Full wwPDB NMR Structure Validation Report (i)

Nov 7, 2023 – 03:41 PM EST

PDB ID	:	2K03
BMRB ID	:	15635
Title	:	Structure of SDF1 in complex with the CXCR4 N-terminus containing a sulfotyrosine at postition 21
Authors	:	Volkman, B.F.; Veldkamp, C.T.; Peterson, F.C.
Deposited on	:	2008-01-24

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

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

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

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

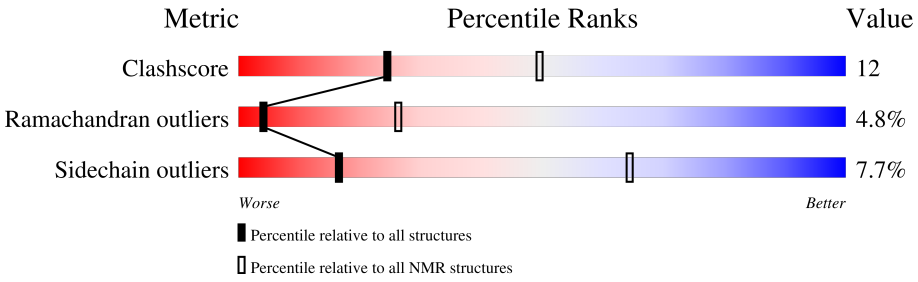
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 88%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	70	56% 24% • 16% •
1	C	70	53% 29% 16% •
2	B	40	22% 10% 62% 5%
2	D	40	25% 12% 58% 5%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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:8-A:43, A:47-A:67, B:114-B:120, B:122-B:127, C:208-C:243, C:247-C:267, D:312-D:320, D:322-D:327 (142)	1.02	11

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3417 atoms, of which 1686 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Stromal cell-derived factor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			1136	353	579	106	92	6	
1	C	68	Total	C	H	N	O	S	0
			1136	353	579	106	92	6	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P48061
A	0	MET	-	expression tag	UNP P48061
A	36	CYS	LEU	engineered mutation	UNP P48061
A	65	CYS	ALA	engineered mutation	UNP P48061
C	199	GLY	-	expression tag	UNP P48061
C	200	MET	-	expression tag	UNP P48061
C	236	CYS	LEU	engineered mutation	UNP P48061
C	265	CYS	ALA	engineered mutation	UNP P48061

- Molecule 2 is a protein called C-X-C chemokine receptor type 4.

Mol	Chain	Residues	Atoms						Trace
2	B	38	Total	C	H	N	O	S	0
			572	185	264	47	72	4	
2	D	38	Total	C	H	N	O	S	0
			573	185	264	47	73	4	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	99	GLY	-	expression tag	UNP P61073
B	100	SER	-	expression tag	UNP P61073
B	128	ALA	CYS	engineered mutation	UNP P61073
D	299	GLY	-	expression tag	UNP P61073
D	300	SER	-	expression tag	UNP P61073
D	328	ALA	CYS	engineered mutation	UNP P61073

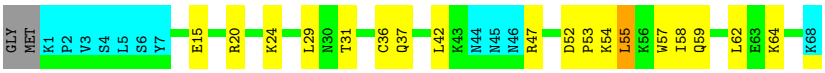
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

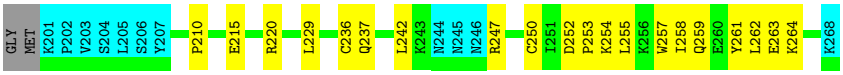
• Molecule 1: Stromal cell-derived factor 1

Chain A:



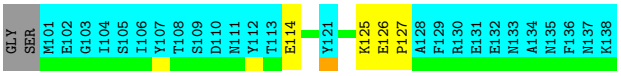
• Molecule 1: Stromal cell-derived factor 1

Chain C:



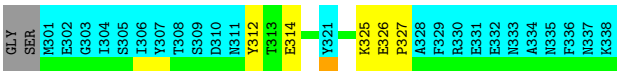
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

Chain D:



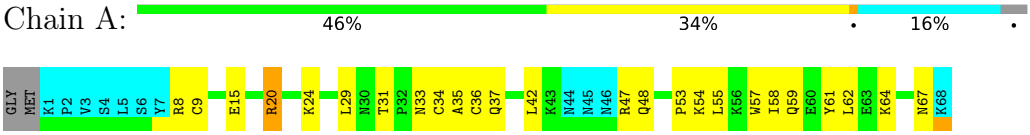
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

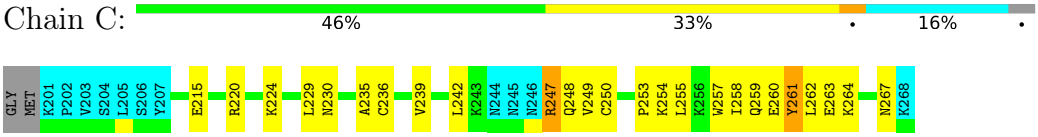
• Molecule 1: Stromal cell-derived factor 1

Chain A:



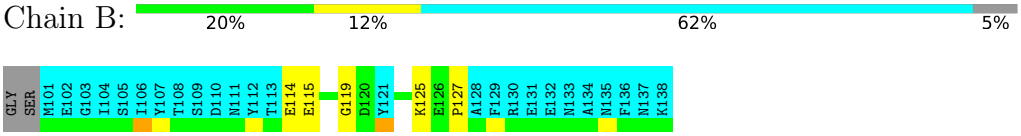
• Molecule 1: Stromal cell-derived factor 1

Chain C:



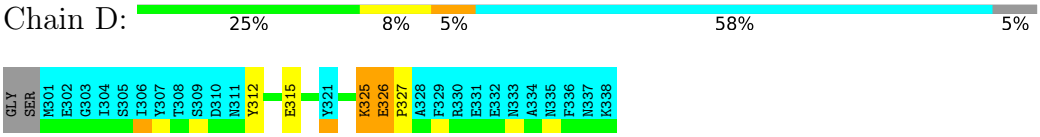
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

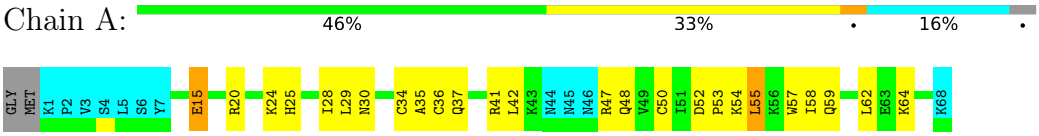
Chain D:



4.2.2 Score per residue for model 2

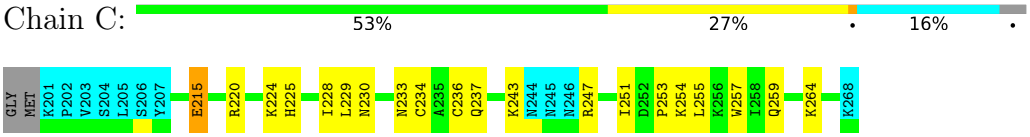
• Molecule 1: Stromal cell-derived factor 1

Chain A:



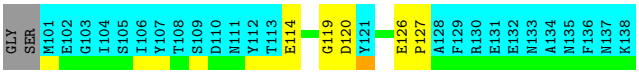
• Molecule 1: Stromal cell-derived factor 1

Chain C:



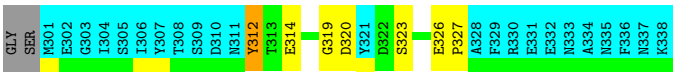
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

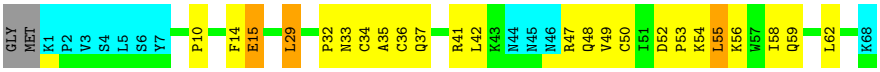
Chain D:



4.2.3 Score per residue for model 3

• Molecule 1: Stromal cell-derived factor 1

Chain A:

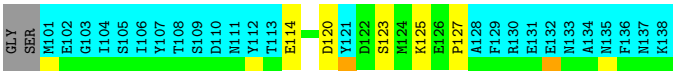


• Molecule 1: Stromal cell-derived factor 1

Chain C:

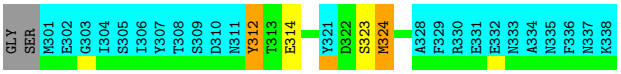
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

Chain D:



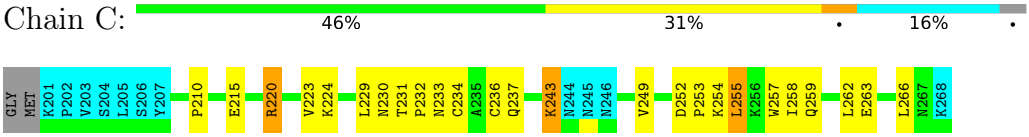
4.2.4 Score per residue for model 4

• Molecule 1: Stromal cell-derived factor 1

Chain A:

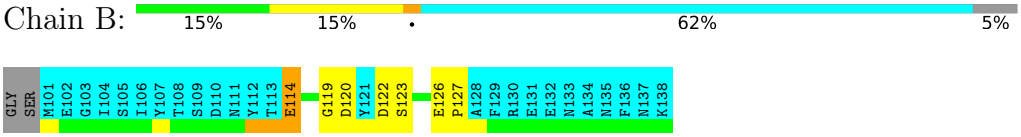
• Molecule 1: Stromal cell-derived factor 1

Chain C:



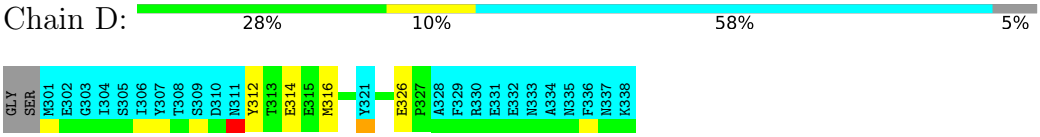
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

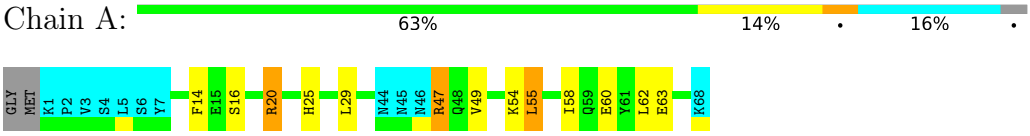
Chain D:



4.2.5 Score per residue for model 5

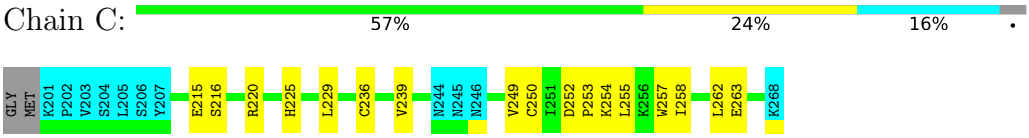
• Molecule 1: Stromal cell-derived factor 1

Chain A:



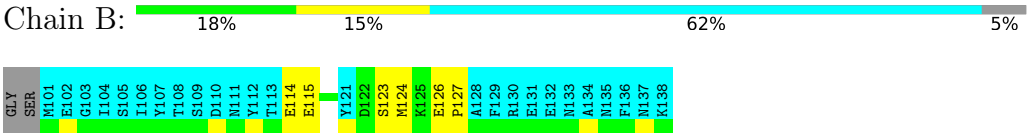
• Molecule 1: Stromal cell-derived factor 1

Chain C:



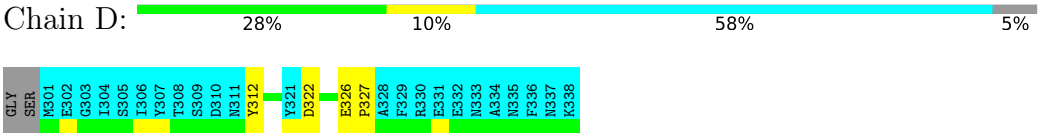
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

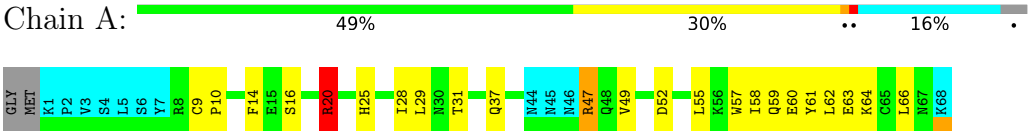
Chain D:



4.2.6 Score per residue for model 6

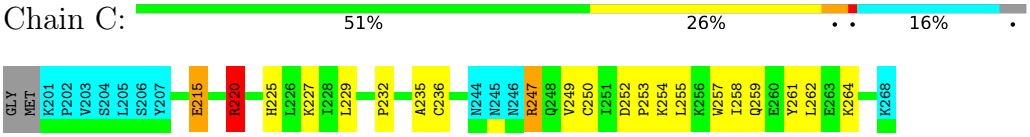
• Molecule 1: Stromal cell-derived factor 1

Chain A:



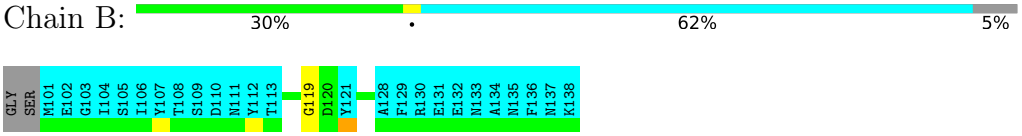
• Molecule 1: Stromal cell-derived factor 1

Chain C:



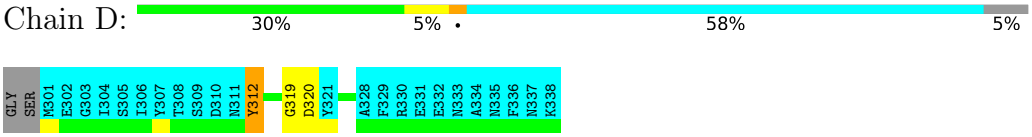
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

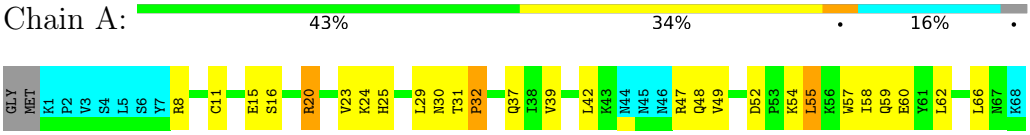
Chain D:



4.2.7 Score per residue for model 7

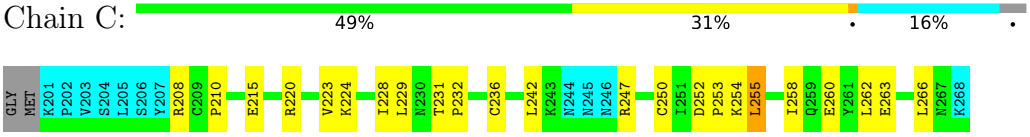
• Molecule 1: Stromal cell-derived factor 1

Chain A:



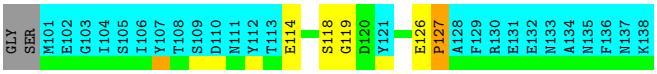
• Molecule 1: Stromal cell-derived factor 1

Chain C:



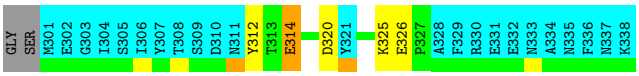
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

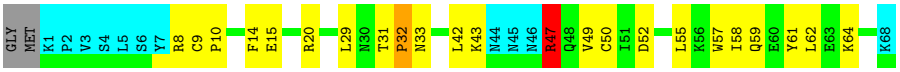
Chain D:



4.2.8 Score per residue for model 8

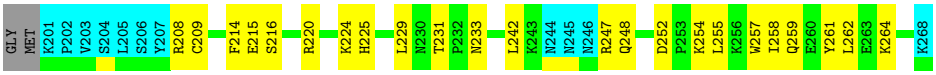
• Molecule 1: Stromal cell-derived factor 1

Chain A:



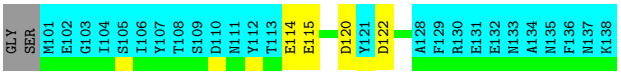
• Molecule 1: Stromal cell-derived factor 1

Chain C:



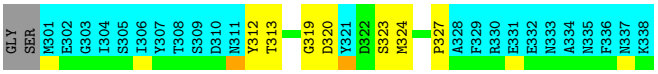
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

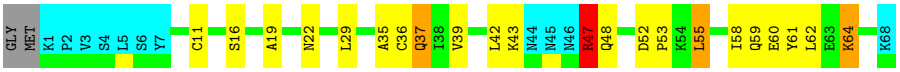
Chain D:



4.2.9 Score per residue for model 9

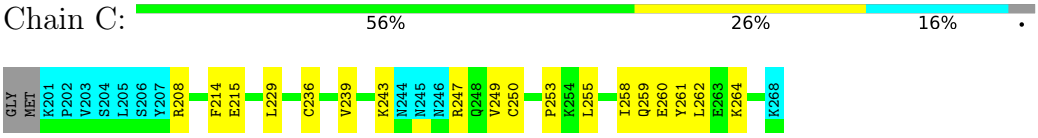
• Molecule 1: Stromal cell-derived factor 1

Chain A:



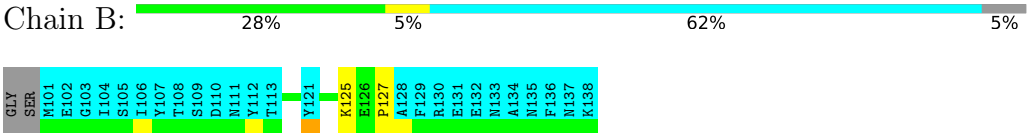
• Molecule 1: Stromal cell-derived factor 1

Chain C:



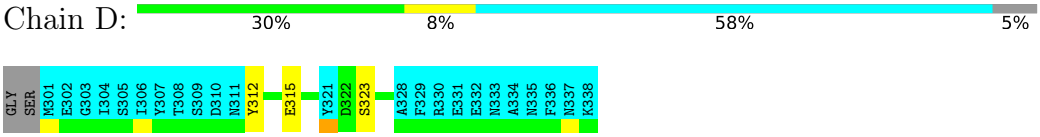
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

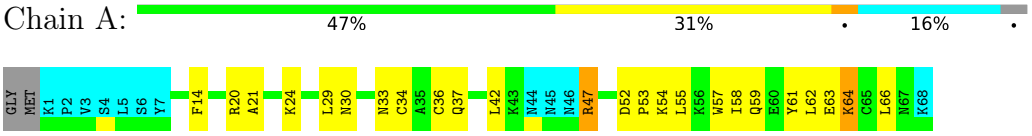
Chain D:



4.2.10 Score per residue for model 10

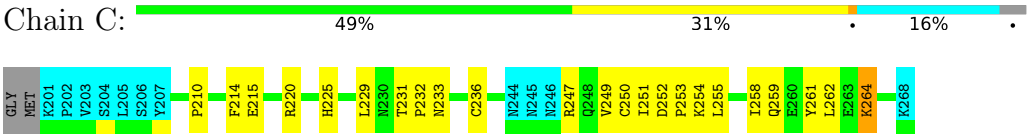
• Molecule 1: Stromal cell-derived factor 1

Chain A:



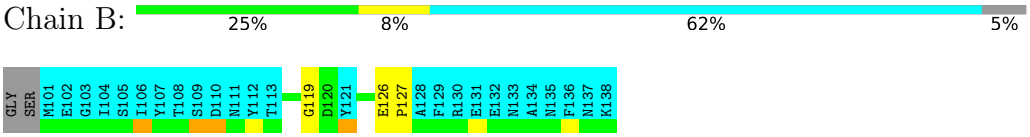
• Molecule 1: Stromal cell-derived factor 1

Chain C:



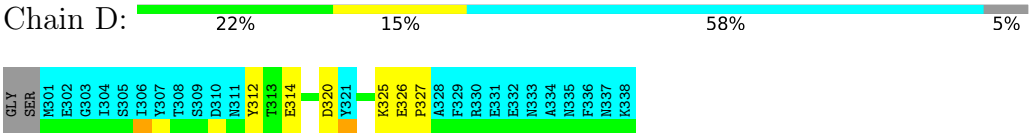
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

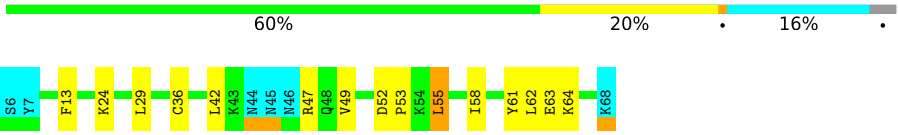
Chain D:



4.2.11 Score per residue for model 11 (medoid)

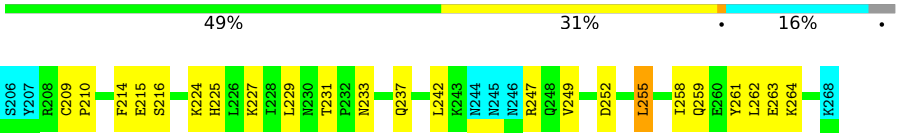
• Molecule 1: Stromal cell-derived factor 1

Chain A:



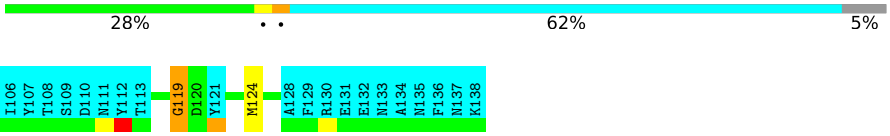
• Molecule 1: Stromal cell-derived factor 1

Chain C:



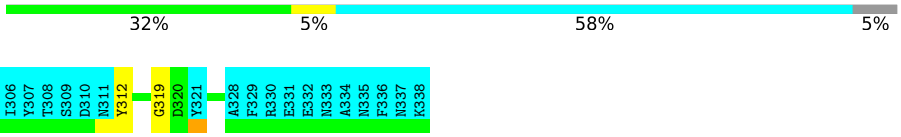
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

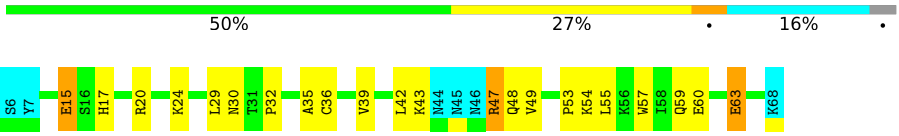
Chain D:



4.2.12 Score per residue for model 12

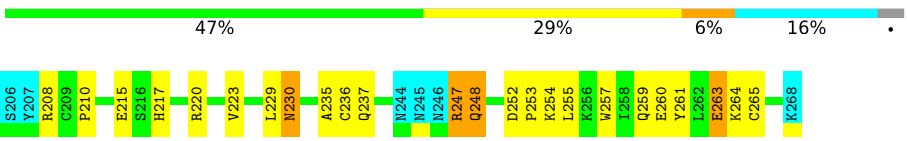
• Molecule 1: Stromal cell-derived factor 1

Chain A:



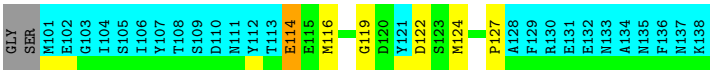
• Molecule 1: Stromal cell-derived factor 1

Chain C:



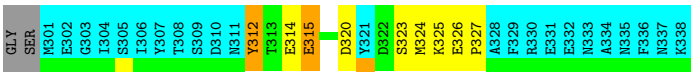
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

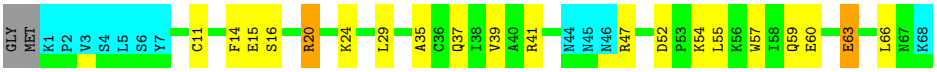
Chain D:



4.2.13 Score per residue for model 13

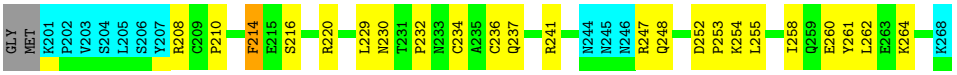
• Molecule 1: Stromal cell-derived factor 1

Chain A:



• Molecule 1: Stromal cell-derived factor 1

Chain C:

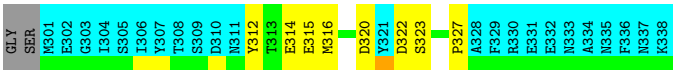


• Molecule 2: C-X-C chemokine receptor type 4

Chain B:

• Molecule 2: C-X-C chemokine receptor type 4

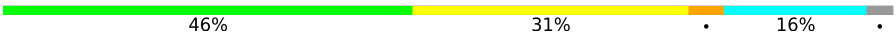
Chain D:

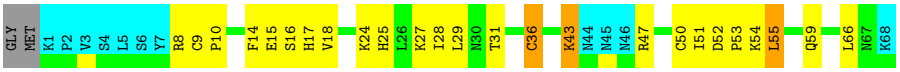


4.2.14 Score per residue for model 14

• Molecule 1: Stromal cell-derived factor 1

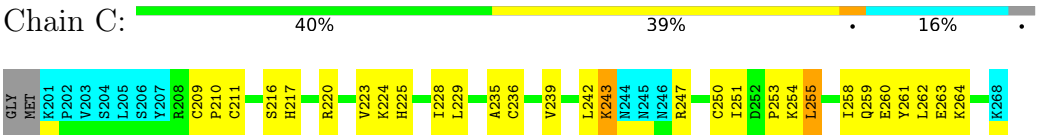
Chain A:





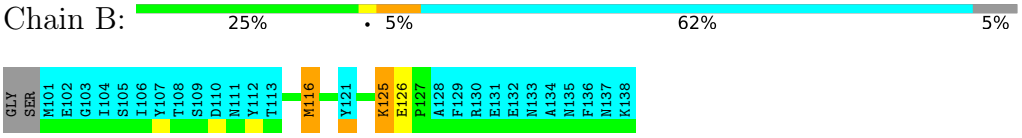
• Molecule 1: Stromal cell-derived factor 1

Chain C:



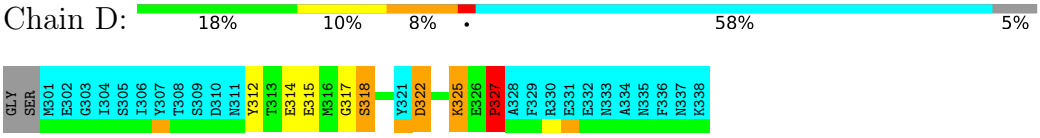
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

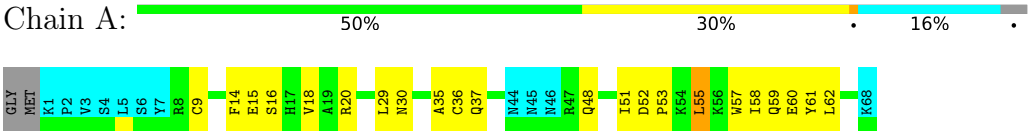
Chain D:



4.2.15 Score per residue for model 15

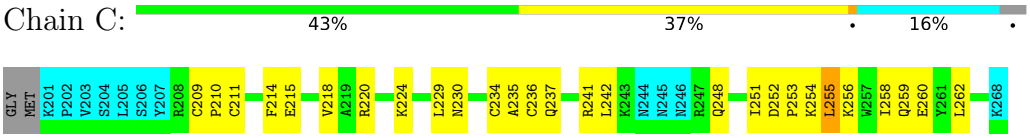
• Molecule 1: Stromal cell-derived factor 1

Chain A:



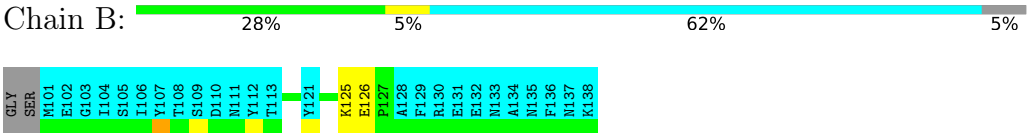
• Molecule 1: Stromal cell-derived factor 1

Chain C:



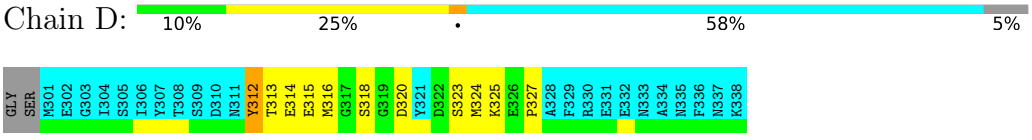
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

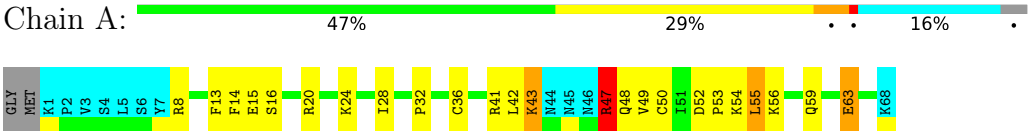
Chain D:



4.2.16 Score per residue for model 16

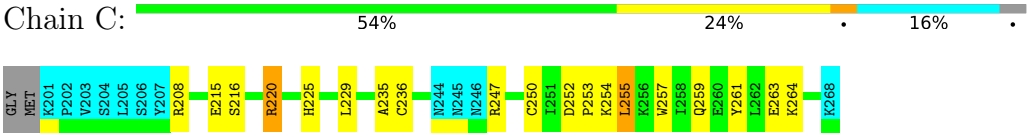
• Molecule 1: Stromal cell-derived factor 1

Chain A:



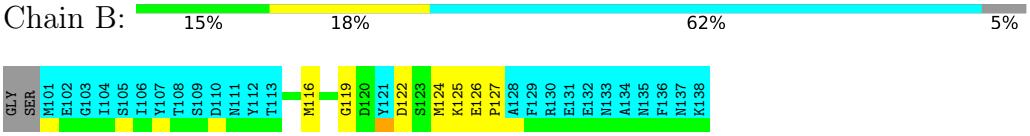
• Molecule 1: Stromal cell-derived factor 1

Chain C:



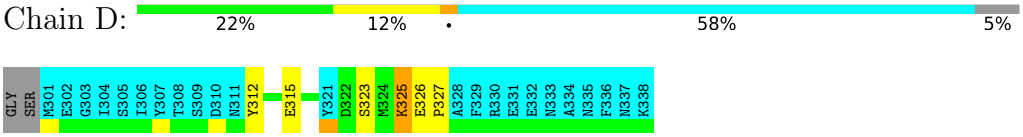
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

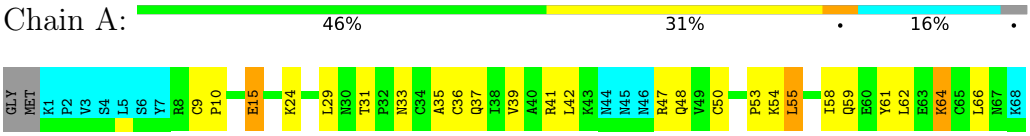
Chain D:



4.2.17 Score per residue for model 17

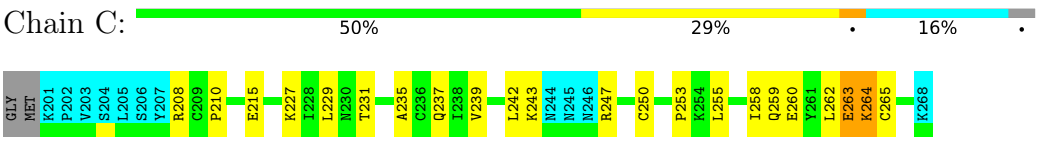
• Molecule 1: Stromal cell-derived factor 1

Chain A:



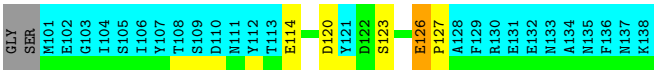
• Molecule 1: Stromal cell-derived factor 1

Chain C:



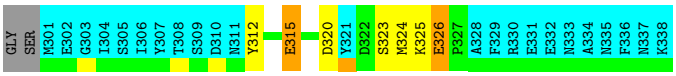
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

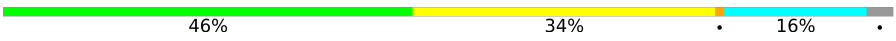
Chain D:

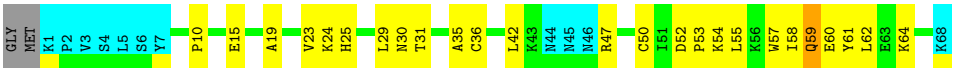


4.2.18 Score per residue for model 18

• Molecule 1: Stromal cell-derived factor 1

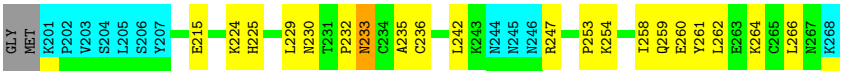
Chain A:





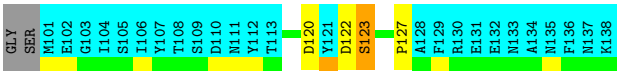
• Molecule 1: Stromal cell-derived factor 1

Chain C:



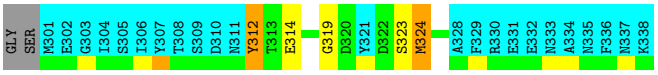
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

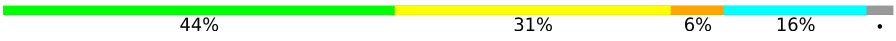
Chain D:



4.2.19 Score per residue for model 19

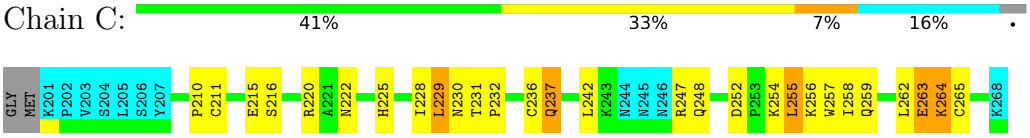
• Molecule 1: Stromal cell-derived factor 1

Chain A:



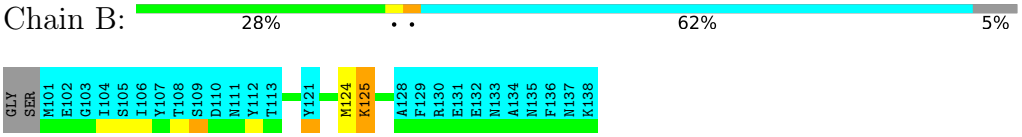
• Molecule 1: Stromal cell-derived factor 1

Chain C:



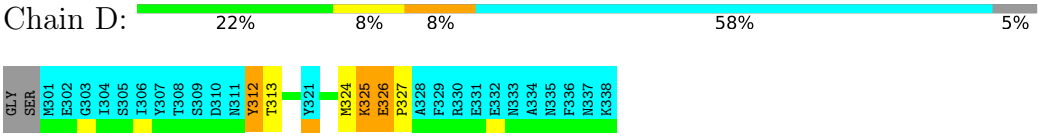
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

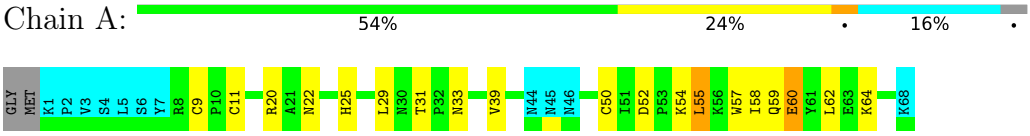
Chain D:



4.2.20 Score per residue for model 20

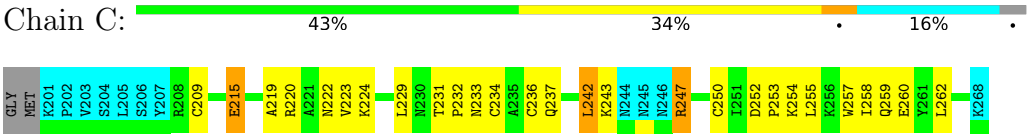
• Molecule 1: Stromal cell-derived factor 1

Chain A:



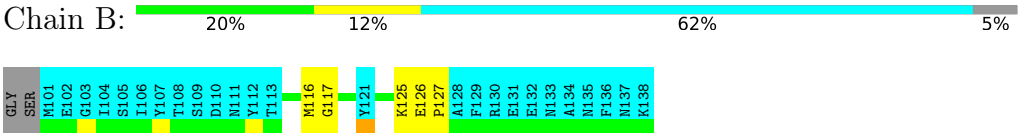
• Molecule 1: Stromal cell-derived factor 1

Chain C:



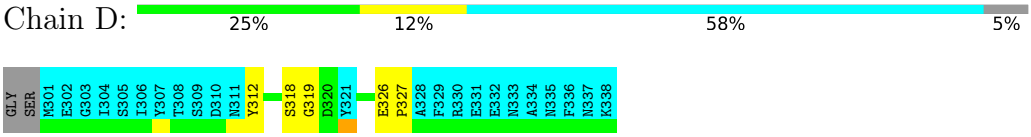
• Molecule 2: C-X-C chemokine receptor type 4

Chain B:



• Molecule 2: C-X-C chemokine receptor type 4

Chain D:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT.*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Xplor-NIH	refinement	2.9.3

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	2478
Number of shifts mapped to atoms	2478
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality

6.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.85±0.03	0±0/479 (0.0± 0.0%)	0.75±0.03	0±0/646 (0.0± 0.0%)
1	C	0.86±0.03	0±0/479 (0.0± 0.0%)	0.74±0.03	0±0/646 (0.0± 0.0%)
2	B	0.89±0.10	0±0/95 (0.0± 0.0%)	0.88±0.07	0±0/124 (0.0± 0.0%)
2	D	0.93±0.07	0±0/115 (0.0± 0.0%)	0.92±0.10	0±0/152 (0.0± 0.1%)
All	All	0.86	0/23360 (0.0%)	0.77	1/31360 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.4
1	C	0.0±0.0	0.1±0.2
All	All	0	4

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	D	312	TYR	CB-CG-CD1	-5.57	117.66	121.00	2	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	47	ARG	Sidechain	2
1	A	20	ARG	Sidechain	1

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Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	C	220	ARG	Sidechain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	469	489	487	12±3
1	C	469	489	487	14±3
2	B	95	80	80	2±1
2	D	114	96	96	4±2
All	All	22940	23080	23000	543

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:254:LYS:O	2:D:327:PRO:HA	0.75	1.81	14	9
1:C:229:LEU:HG	2:D:312:TYR:CE2	0.72	2.19	16	7
1:C:220:ARG:HG2	1:C:257:TRP:CE3	0.65	2.25	6	3
1:C:215:GLU:HG2	1:C:250:CYS:O	0.65	1.91	3	4
1:A:10:PRO:HA	2:B:114:GLU:O	0.64	1.92	8	1
1:A:9:CYS:HA	1:A:31:THR:HG21	0.64	1.70	6	1
1:A:20:ARG:HG2	1:A:57:TRP:CE3	0.64	2.28	6	4
1:C:220:ARG:HB3	1:C:257:TRP:CE3	0.64	2.28	5	5
1:A:54:LYS:O	2:B:127:PRO:HA	0.62	1.94	20	9
1:C:236:CYS:O	1:C:253:PRO:HG3	0.62	1.94	4	16
1:C:234:CYS:HB3	1:C:237:GLN:OE1	0.61	1.94	20	6
2:D:325:LYS:H	2:D:325:LYS:HE2	0.61	1.56	14	1
1:A:36:CYS:O	1:A:53:PRO:HG3	0.61	1.94	4	13
1:C:215:GLU:HB3	2:D:320:ASP:O	0.61	1.96	7	3
1:C:229:LEU:HD13	2:D:312:TYR:CD1	0.60	2.32	3	2
1:C:224:LYS:HE3	1:C:242:LEU:O	0.60	1.97	18	4
1:C:259:GLN:O	1:C:263:GLU:HB2	0.58	1.97	12	4
1:C:210:PRO:HD2	1:C:237:GLN:OE1	0.58	1.98	17	1
1:C:209:CYS:O	2:D:315:GLU:HA	0.57	1.99	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:229:LEU:HD22	2:D:312:TYR:CD2	0.57	2.34	5	11
1:A:9:CYS:HA	1:A:31:THR:OG1	0.57	1.98	14	4
2:B:125:LYS:N	2:B:125:LYS:HE2	0.57	2.15	14	1
1:C:252:ASP:O	1:C:255:LEU:HB2	0.56	2.00	3	10
1:C:254:LYS:HA	1:C:259:GLN:NE2	0.56	2.15	2	5
1:A:59:GLN:O	1:A:63:GLU:HB2	0.56	2.01	12	3
1:A:24:LYS:HE2	1:A:42:LEU:O	0.56	2.00	18	4
1:C:261:TYR:O	1:C:264:LYS:HG2	0.56	2.01	11	10
1:A:15:GLU:HB3	2:B:120:ASP:O	0.56	2.01	2	2
1:A:42:LEU:HD23	1:A:43:LYS:N	0.56	2.15	9	2
1:A:15:GLU:HG2	1:A:50:CYS:O	0.55	1.99	17	6
1:A:54:LYS:HA	1:A:59:GLN:NE2	0.55	2.17	12	6
1:C:255:LEU:O	1:C:259:GLN:HG2	0.55	2.00	1	15
1:A:52:ASP:O	1:A:55:LEU:HB2	0.55	2.02	16	13
1:C:220:ARG:HB3	1:C:257:TRP:CZ3	0.55	2.37	12	2
1:A:28:ILE:O	1:C:225:HIS:HB2	0.54	2.01	14	4
1:A:20:ARG:HB3	1:A:57:TRP:CE3	0.54	2.37	15	4
1:A:55:LEU:O	1:A:59:GLN:HG2	0.54	2.02	20	16
1:C:224:LYS:CG	1:C:243:LYS:HA	0.54	2.32	20	3
2:D:323:SER:O	2:D:324:MET:HG3	0.54	2.02	3	2
2:D:320:ASP:O	2:D:323:SER:HB2	0.54	2.03	15	5
1:A:54:LYS:HB3	2:B:127:PRO:HD3	0.54	1.80	17	1
1:A:47:ARG:NH1	1:A:49:VAL:HG12	0.53	2.18	4	4
1:A:20:ARG:HB3	1:A:57:TRP:CZ3	0.53	2.38	8	1
1:C:229:LEU:HG	2:D:312:TYR:CD2	0.53	2.38	15	5
2:D:326:GLU:OE2	2:D:327:PRO:HD2	0.53	2.04	1	1
1:A:11:CYS:HB3	1:A:37:GLN:OE1	0.53	2.04	7	1
1:C:208:ARG:O	1:C:231:THR:HB	0.53	2.03	17	1
2:B:125:LYS:HE2	2:B:125:LYS:H	0.52	1.62	14	1
1:C:215:GLU:HG2	2:D:320:ASP:N	0.52	2.19	10	1
1:A:34:CYS:HB3	1:A:37:GLN:OE1	0.52	2.05	10	4
1:C:216:SER:O	1:C:255:LEU:HD11	0.52	2.04	3	3
2:B:114:GLU:H	2:B:114:GLU:CD	0.52	2.08	12	2
1:A:20:ARG:HG2	1:A:57:TRP:CD2	0.52	2.40	6	1
1:A:20:ARG:HG3	1:A:57:TRP:CE3	0.52	2.40	2	1
1:A:15:GLU:OE1	1:A:49:VAL:HB	0.52	2.05	7	2
1:A:61:TYR:O	1:A:64:LYS:HG2	0.51	2.05	18	6
1:C:258:ILE:O	1:C:262:LEU:HG	0.51	2.05	20	17
1:C:252:ASP:OD1	1:C:254:LYS:HB2	0.51	2.05	19	6
1:A:25:HIS:HB2	1:C:228:ILE:O	0.51	2.06	19	4
1:A:47:ARG:HG2	1:A:48:GLN:H	0.51	1.66	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:237:GLN:HE21	1:C:237:GLN:N	0.51	2.02	19	1
1:A:59:GLN:O	1:A:63:GLU:HG3	0.51	2.04	6	1
1:A:58:ILE:O	1:A:62:LEU:HG	0.51	2.05	5	16
1:C:259:GLN:O	1:C:263:GLU:HG3	0.51	2.04	1	1
1:A:59:GLN:HA	1:A:59:GLN:HE21	0.51	1.66	18	1
1:A:60:GLU:O	1:A:64:LYS:HG2	0.51	2.05	20	1
2:B:125:LYS:HA	2:B:125:LYS:HE2	0.51	1.83	19	2
1:A:9:CYS:O	2:B:115:GLU:HA	0.50	2.06	8	1
1:A:15:GLU:HG3	2:B:120:ASP:O	0.50	2.06	8	1
1:C:214:PHE:O	2:D:323:SER:HA	0.50	2.06	9	1
1:A:25:HIS:CB	1:C:229:LEU:HG	0.50	2.36	2	5
1:A:16:SER:O	1:A:55:LEU:HD11	0.50	2.05	13	3
2:D:325:LYS:HG2	2:D:326:GLU:H	0.50	1.67	17	1
1:C:220:ARG:HG3	1:C:257:TRP:CE3	0.50	2.41	2	1
1:C:209:CYS:HA	1:C:231:THR:OG1	0.50	2.06	11	3
1:A:24:LYS:HE3	1:A:42:LEU:O	0.49	2.07	10	4
1:C:229:LEU:HD22	2:D:312:TYR:CG	0.49	2.41	13	4
2:B:126:GLU:HB2	2:B:127:PRO:CD	0.49	2.37	17	1
1:C:247:ARG:NH1	1:C:249:VAL:HA	0.49	2.22	6	1
1:C:210:PRO:HA	2:D:314:GLU:C	0.49	2.28	14	1
1:A:13:PHE:HB2	2:B:119:GLY:HA3	0.49	1.83	16	2
1:C:216:SER:CB	2:D:325:LYS:HB2	0.49	2.37	19	1
1:C:230:ASN:OD1	1:C:236:CYS:HA	0.49	2.08	13	1
1:C:264:LYS:HD3	1:C:265:CYS:N	0.49	2.23	17	2
1:A:11:CYS:HA	2:B:117:GLY:H	0.49	1.66	20	1
1:C:215:GLU:OE2	1:C:249:VAL:HB	0.49	2.07	1	2
1:A:47:ARG:NH1	1:A:49:VAL:HA	0.49	2.22	6	1
2:D:325:LYS:HE2	2:D:325:LYS:N	0.49	2.23	14	1
1:A:52:ASP:OD1	1:A:54:LYS:HB2	0.49	2.07	13	3
1:A:9:CYS:HA	1:A:31:THR:CG2	0.48	2.37	6	1
1:C:210:PRO:HA	2:D:314:GLU:HB2	0.48	1.85	3	1
1:C:220:ARG:O	1:C:223:VAL:HG22	0.48	2.09	14	3
1:A:67:ASN:OD1	2:D:327:PRO:HG3	0.48	2.09	19	1
2:D:312:TYR:CE2	2:D:314:GLU:HB2	0.48	2.43	18	1
1:A:57:TRP:O	1:A:61:TYR:HB2	0.48	2.09	1	4
1:C:251:ILE:CG2	1:C:255:LEU:HD12	0.48	2.38	14	2
1:A:24:LYS:HE2	1:A:43:LYS:HA	0.48	1.84	16	1
1:A:15:GLU:HG2	2:B:120:ASP:H	0.48	1.69	4	1
1:A:61:TYR:O	1:A:64:LYS:HG3	0.48	2.09	17	2
1:C:247:ARG:HG2	1:C:248:GLN:N	0.48	2.24	12	1
1:A:24:LYS:CE	1:A:43:LYS:HA	0.48	2.39	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:216:SER:HB3	2:D:325:LYS:HB2	0.48	1.84	19	1
1:C:222:ASN:HD21	1:C:242:LEU:HD13	0.48	1.69	19	1
1:C:219:ALA:O	1:C:222:ASN:HB3	0.48	2.09	20	1
1:C:210:PRO:HA	2:D:314:GLU:CB	0.48	2.38	3	1
1:A:10:PRO:HD3	1:A:31:THR:OG1	0.47	2.09	18	4
1:C:242:LEU:HB2	1:C:247:ARG:O	0.47	2.09	14	2
1:C:210:PRO:HD3	1:C:231:THR:OG1	0.47	2.09	10	1
1:C:252:ASP:HB3	1:C:255:LEU:HG	0.47	1.85	10	1
1:A:54:LYS:HB3	2:B:127:PRO:N	0.47	2.24	3	2
1:C:247:ARG:CZ	1:C:249:VAL:HG12	0.47	2.39	6	2
1:A:16:SER:HB3	2:B:125:LYS:CG	0.47	2.39	9	1
1:A:54:LYS:HA	1:A:59:GLN:OE1	0.47	2.09	4	1
2:B:120:ASP:O	2:B:123:SER:HB2	0.47	2.09	17	4
1:C:208:ARG:HA	1:C:208:ARG:NE	0.47	2.25	7	2
1:A:27:LYS:HG2	1:A:29:LEU:CD2	0.47	2.38	14	1
1:C:239:VAL:HG22	1:C:250:CYS:SG	0.47	2.50	1	5
1:C:220:ARG:HB3	1:C:257:TRP:CD2	0.47	2.44	4	1
1:A:8:ARG:O	1:A:31:THR:HG22	0.47	2.09	7	1
1:C:224:LYS:HE2	1:C:242:LEU:O	0.47	2.09	15	2
1:A:11:CYS:SG	2:B:117:GLY:HA3	0.47	2.49	13	1
1:A:10:PRO:HD2	1:A:37:GLN:OE1	0.47	2.08	17	1
1:C:216:SER:HA	1:C:255:LEU:HD11	0.47	1.87	5	4
1:A:36:CYS:O	1:A:53:PRO:HB3	0.47	2.08	17	1
1:A:52:ASP:CG	2:B:125:LYS:HB3	0.46	2.29	3	1
1:A:18:VAL:HG21	1:A:51:ILE:HD12	0.46	1.87	15	1
1:C:216:SER:HA	1:C:255:LEU:HG	0.46	1.86	16	1
1:C:229:LEU:HD13	2:D:312:TYR:CE1	0.46	2.45	18	2
1:A:18:VAL:HG11	1:A:51:ILE:HD12	0.46	1.86	14	2
1:A:31:THR:CG2	1:A:32:PRO:HD2	0.46	2.41	4	1
1:C:247:ARG:NH1	1:C:249:VAL:HG12	0.46	2.25	10	1
1:C:254:LYS:HB3	2:D:327:PRO:HD3	0.46	1.87	13	1
1:A:29:LEU:HG	1:C:225:HIS:CB	0.46	2.40	2	3
1:A:47:ARG:NH2	1:A:49:VAL:HA	0.46	2.26	5	1
1:A:31:THR:HG22	1:A:32:PRO:HD2	0.46	1.88	4	1
2:D:314:GLU:H	2:D:314:GLU:CD	0.46	2.14	10	1
1:C:252:ASP:OD2	1:C:254:LYS:HB2	0.46	2.11	7	3
1:C:250:CYS:SG	2:D:318:SER:HB2	0.45	2.51	20	1
2:D:325:LYS:HG2	2:D:326:GLU:N	0.45	2.26	17	1
1:C:208:ARG:HD2	2:D:315:GLU:OE2	0.45	2.11	13	1
1:A:11:CYS:HA	2:B:117:GLY:N	0.45	2.25	20	1
1:C:210:PRO:O	2:D:316:MET:HB3	0.45	2.11	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:325:LYS:HG3	2:D:326:GLU:OE2	0.45	2.12	19	1
1:C:214:PHE:CD1	1:C:252:ASP:HA	0.45	2.46	8	2
1:A:15:GLU:OE2	1:A:49:VAL:HB	0.44	2.13	12	1
1:A:39:VAL:HG22	1:A:50:CYS:SG	0.44	2.52	17	2
1:C:242:LEU:HD23	1:C:243:LYS:N	0.44	2.27	17	1
1:C:241:ARG:HG2	1:C:248:GLN:HB3	0.44	1.88	13	1
1:C:217:HIS:HB2	2:D:322:ASP:HB3	0.44	1.88	14	1
1:A:9:CYS:H	2:B:115:GLU:HA	0.44	1.73	1	1
1:C:215:GLU:OE1	1:C:249:VAL:HB	0.44	2.12	9	3
1:C:218:VAL:HG21	1:C:251:ILE:HD12	0.44	1.90	15	1
1:C:224:LYS:HE2	1:C:243:LYS:HA	0.44	1.88	4	1
1:C:215:GLU:HA	2:D:320:ASP:O	0.44	2.13	6	1
1:A:24:LYS:HG2	1:A:41:ARG:O	0.44	2.13	16	2
1:A:17:HIS:CD2	2:B:122:ASP:HB3	0.44	2.48	12	2
1:A:15:GLU:OE1	2:B:118:SER:HB2	0.44	2.13	7	1
1:A:42:LEU:HB2	1:A:47:ARG:O	0.44	2.12	8	2
1:A:41:ARG:HG2	1:A:48:GLN:HG2	0.43	1.89	3	2
1:C:227:LYS:O	1:C:238:ILE:HA	0.43	2.12	3	1
1:C:210:PRO:HG2	1:C:237:GLN:HG2	0.43	1.89	12	2
1:C:227:LYS:HG2	1:C:229:LEU:CD2	0.43	2.43	11	3
1:C:220:ARG:O	1:C:220:ARG:HD2	0.43	2.13	14	1
1:C:208:ARG:NH1	2:D:315:GLU:HB3	0.43	2.27	17	1
1:C:230:ASN:ND2	1:C:236:CYS:HA	0.43	2.28	19	1
1:C:210:PRO:HD3	1:C:231:THR:CB	0.43	2.44	7	2
1:A:9:CYS:SG	1:A:33:ASN:HB3	0.43	2.53	19	1
1:A:19:ALA:O	1:A:22:ASN:HB3	0.43	2.12	9	1
1:C:215:GLU:HA	2:D:323:SER:HA	0.43	1.91	3	1
1:A:29:LEU:HD13	1:C:225:HIS:HB3	0.43	1.90	6	1
1:A:15:GLU:HB3	1:A:50:CYS:O	0.43	2.14	8	1
1:A:20:ARG:HB3	1:A:57:TRP:CD2	0.43	2.49	7	2
1:C:210:PRO:HB3	2:D:312:TYR:HE2	0.43	1.74	13	1
2:B:125:LYS:HG2	2:B:126:GLU:H	0.43	1.73	15	1
1:A:29:LEU:HD21	1:C:225:HIS:HB3	0.43	1.90	18	1
1:C:210:PRO:HD3	1:C:231:THR:CG2	0.42	2.44	19	2
1:C:232:PRO:O	1:C:233:ASN:HB2	0.42	2.14	18	1
1:A:25:HIS:HB2	1:C:229:LEU:HG	0.42	1.90	20	1
1:C:251:ILE:HG23	1:C:255:LEU:HD12	0.42	1.90	2	1
1:A:11:CYS:SG	1:A:39:VAL:HG22	0.42	2.54	9	1
1:A:24:LYS:HG3	1:A:41:ARG:O	0.42	2.14	13	2
1:A:8:ARG:O	1:A:31:THR:HB	0.42	2.14	1	2
1:A:52:ASP:OD2	1:A:54:LYS:HB2	0.42	2.13	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:CYS:HB3	1:A:37:GLN:OE1	0.42	2.13	15	1
1:C:224:LYS:CE	1:C:241:ARG:HD2	0.42	2.43	15	1
1:A:64:LYS:HB2	1:A:64:LYS:NZ	0.42	2.28	17	1
1:A:54:LYS:HA	1:A:59:GLN:CD	0.42	2.35	4	1
2:D:314:GLU:O	2:D:315:GLU:HB2	0.42	2.13	12	1
1:A:37:GLN:HE21	1:A:37:GLN:N	0.42	2.13	9	1
1:A:47:ARG:CG	1:A:48:GLN:H	0.42	2.28	9	1
1:A:24:LYS:HE2	1:A:43:LYS:O	0.42	2.15	14	1
1:C:211:CYS:SG	2:D:318:SER:HB2	0.42	2.54	14	2
1:A:10:PRO:O	2:B:116:MET:HB3	0.42	2.15	14	1
1:A:16:SER:O	1:A:55:LEU:HD21	0.42	2.15	15	2
1:C:222:ASN:ND2	1:C:242:LEU:HD13	0.42	2.30	19	1
1:A:18:VAL:HG21	1:A:49:VAL:HG21	0.42	1.90	4	1
1:A:59:GLN:O	1:A:63:GLU:HG2	0.42	2.15	10	1
2:B:125:LYS:HA	2:B:125:LYS:CE	0.42	2.44	19	1
1:C:261:TYR:O	1:C:264:LYS:HG3	0.41	2.15	10	1
1:A:53:PRO:HA	1:A:58:ILE:HG21	0.41	1.92	2	1
1:C:215:GLU:HB2	1:C:250:CYS:O	0.41	2.14	20	3
1:A:47:ARG:HG2	1:A:48:GLN:O	0.41	2.15	16	1
1:C:254:LYS:HD2	2:D:327:PRO:HD3	0.41	1.90	8	1
1:A:15:GLU:HG2	2:B:120:ASP:N	0.41	2.30	13	1
2:D:325:LYS:HD2	2:D:325:LYS:N	0.41	2.31	16	2
1:A:54:LYS:HD2	2:B:127:PRO:HD3	0.41	1.92	2	1
1:A:16:SER:HA	1:A:55:LEU:CD1	0.41	2.46	5	1
1:C:220:ARG:HG2	1:C:220:ARG:O	0.41	2.15	7	1
1:A:29:LEU:HG	1:C:225:HIS:HB3	0.41	1.92	8	1
1:C:215:GLU:HG3	2:D:320:ASP:C	0.41	2.35	2	1
1:A:10:PRO:CG	1:A:37:GLN:HG2	0.41	2.46	6	1
1:A:25:HIS:HB3	1:C:229:LEU:HD13	0.41	1.91	6	1
1:A:29:LEU:HG	1:C:225:HIS:HB2	0.41	1.92	11	1
1:A:15:GLU:HG3	1:A:49:VAL:HB	0.41	1.91	16	1
1:C:231:THR:CG2	2:D:314:GLU:HB2	0.41	2.46	7	1
2:D:325:LYS:HG3	2:D:326:GLU:H	0.41	1.76	12	1
1:C:208:ARG:HB3	2:D:315:GLU:HA	0.40	1.92	9	1
1:A:29:LEU:CD2	1:C:225:HIS:HB3	0.40	2.45	18	1
1:C:261:TYR:HA	1:C:264:LYS:CD	0.40	2.45	18	1
1:C:220:ARG:HG3	1:C:257:TRP:CZ3	0.40	2.52	3	1
1:A:47:ARG:CZ	1:A:49:VAL:HG12	0.40	2.46	4	1
1:A:20:ARG:O	1:A:23:VAL:HG22	0.40	2.16	7	1
1:A:54:LYS:CB	2:B:127:PRO:HD3	0.40	2.45	17	1
1:A:14:PHE:O	2:B:123:SER:HA	0.40	2.16	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:209:CYS:SG	1:C:210:PRO:HD2	0.40	2.56	11	1
1:A:16:SER:HB2	2:B:124:MET:O	0.40	2.17	16	1
1:A:10:PRO:HA	2:B:114:GLU:CB	0.40	2.47	3	1
1:A:15:GLU:HA	2:B:123:SER:HA	0.40	1.92	3	1
1:A:16:SER:HA	1:A:55:LEU:HD11	0.40	1.93	5	1
1:C:239:VAL:HG21	2:D:312:TYR:OH	0.40	2.16	14	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	57/70 (81%)	51±1 (90±2%)	4±1 (7±2%)	1±1 (2±2%)	9	45
1	C	57/70 (81%)	52±2 (90±3%)	4±2 (7±3%)	1±1 (2±1%)	9	45
2	B	13/40 (32%)	7±2 (55±15%)	4±2 (31±12%)	2±1 (14±7%)	1	5
2	D	15/40 (38%)	8±2 (55±10%)	5±1 (31±8%)	2±1 (15±7%)	0	4
All	All	2840/4400 (65%)	2367 (83%)	337 (12%)	136 (5%)	4	26

All 36 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	35	ALA	8
2	B	119	GLY	8
1	C	235	ALA	8
2	B	126	GLU	8
2	D	326	GLU	7
1	C	232	PRO	7
1	C	233	ASN	7
2	D	324	MET	7
2	D	319	GLY	6
1	A	32	PRO	6
1	A	33	ASN	6
2	D	314	GLU	5

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Mol	Chain	Res	Type	Models (Total)
2	D	312	TYR	5
2	B	116	MET	5
2	B	114	GLU	4
2	D	315	GLU	4
2	B	124	MET	4
1	A	43	LYS	4
1	C	243	LYS	3
2	B	127	PRO	3
1	A	67	ASN	2
2	D	322	ASP	2
2	D	327	PRO	2
2	B	123	SER	2
2	D	313	THR	2
1	C	267	ASN	1
2	B	115	GLU	1
2	B	122	ASP	1
2	D	323	SER	1
1	A	47	ARG	1
2	D	316	MET	1
1	A	36	CYS	1
2	D	317	GLY	1
2	D	318	SER	1
1	C	211	CYS	1
1	C	225	HIS	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	53/65 (82%)	48±1 (91±3%)	5±1 (9±3%)	13	60
1	C	53/65 (82%)	49±2 (92±3%)	4±2 (8±3%)	16	64
2	B	11/33 (33%)	10±1 (95±5%)	0±1 (5±5%)	31	80
2	D	13/33 (39%)	12±1 (95±5%)	1±1 (5±5%)	28	77
All	All	2600/3920 (66%)	2401 (92%)	199 (8%)	16	64

All 49 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	47	ARG	16
1	C	247	ARG	14
1	A	55	LEU	11
1	C	260	GLU	10
1	A	14	PHE	9
1	C	255	LEU	9
1	A	60	GLU	9
1	C	263	GLU	8
2	D	325	LYS	7
1	C	215	GLU	7
1	A	20	ARG	6
1	A	48	GLN	6
2	B	125	LYS	6
1	A	15	GLU	6
1	C	220	ARG	6
1	A	66	LEU	6
1	C	248	GLN	5
1	A	63	GLU	5
1	C	230	ASN	4
1	A	64	LYS	4
1	A	30	ASN	4
1	C	214	PHE	4
1	A	37	GLN	3
1	C	266	LEU	3
2	D	326	GLU	3
1	C	264	LYS	3
2	B	114	GLU	2
1	C	208	ARG	2
1	C	261	TYR	1
1	C	233	ASN	1
1	A	29	LEU	1
1	C	231	THR	1
2	D	312	TYR	1
2	D	316	MET	1
2	B	126	GLU	1
1	A	32	PRO	1
1	A	8	ARG	1
2	B	124	MET	1
2	D	327	PRO	1
1	C	253	PRO	1
1	A	59	GLN	1
1	A	31	THR	1
1	A	42	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	56	LYS	1
1	C	229	LEU	1
1	C	237	GLN	1
1	C	256	LYS	1
1	A	22	ASN	1
1	C	242	LEU	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	TYS	B	121	2	15,16,17	2.69±0.21	2±0 (10±3%)
2	TYS	D	321	2	15,16,17	2.69±0.19	2±1 (11±3%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	TYS	B	121	2	18,22,24	1.04±0.03	2±1 (9±3%)
2	TYS	D	321	2	18,22,24	1.03±0.04	1±1 (7±3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYS	B	121	2	-	0±0,10,11,13	0±0,1,1,1
2	TYS	D	321	2	-	0±0,10,11,13	0±0,1,1,1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	D	321	TYS	OH-S	11.03	1.41	1.58	4	20
2	B	121	TYS	OH-S	10.93	1.41	1.58	8	20
2	D	321	TYS	OH-CZ	2.81	1.38	1.42	4	12
2	B	121	TYS	OH-CZ	2.74	1.38	1.42	20	11
2	D	321	TYS	CB-CG	2.00	1.46	1.51	1	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	D	321	TYS	OH-S-O2	3.08	116.68	107.71	14	19
2	B	121	TYS	OH-S-O2	2.87	116.07	107.71	4	20
2	B	121	TYS	O3-S-O2	2.21	100.82	108.49	4	11
2	D	321	TYS	O3-S-O2	2.12	101.12	108.49	10	8
2	D	321	TYS	OH-S-O1	2.06	113.72	107.71	6	1
2	B	121	TYS	OH-S-O1	2.06	113.70	107.71	20	2

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 84% 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	2478
Number of shifts mapped to atoms	2478
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	200	-0.48 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	192	-0.42 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	186	-0.27 ± 0.07	None needed (< 0.5 ppm)
^{15}N	192	-0.49 ± 0.43	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 88%, i.e. 1759 atoms were assigned a chemical shift out of a possible 2002. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	676/698 (97%)	276/280 (99%)	266/284 (94%)	134/134 (100%)
Sidechain	1001/1181 (85%)	684/760 (90%)	303/363 (83%)	14/58 (24%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	82/123 (67%)	48/60 (80%)	32/53 (60%)	2/10 (20%)
Overall	1759/2002 (88%)	1008/1100 (92%)	601/700 (86%)	150/202 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 2450 atoms were assigned a chemical shift out of a possible 2908. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	976/1036 (94%)	398/416 (96%)	386/420 (92%)	192/200 (96%)
Sidechain	1338/1664 (80%)	918/1066 (86%)	404/514 (79%)	16/84 (19%)
Aromatic	136/208 (65%)	84/100 (84%)	50/98 (51%)	2/10 (20%)
Overall	2450/2908 (84%)	1400/1582 (88%)	840/1032 (81%)	210/294 (71%)

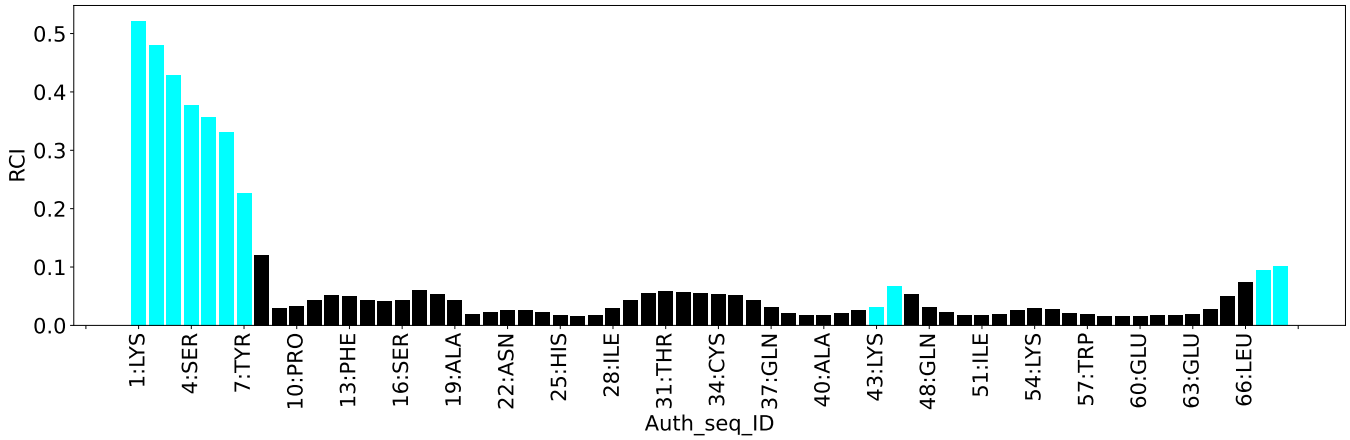
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

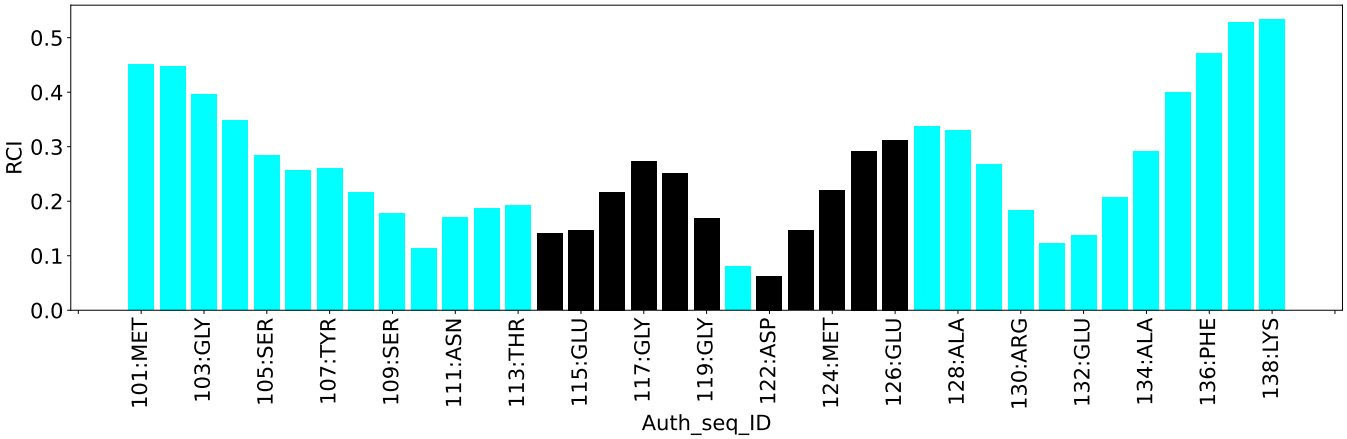
7.1.5 Random Coil Index (RCI) plots (i)

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

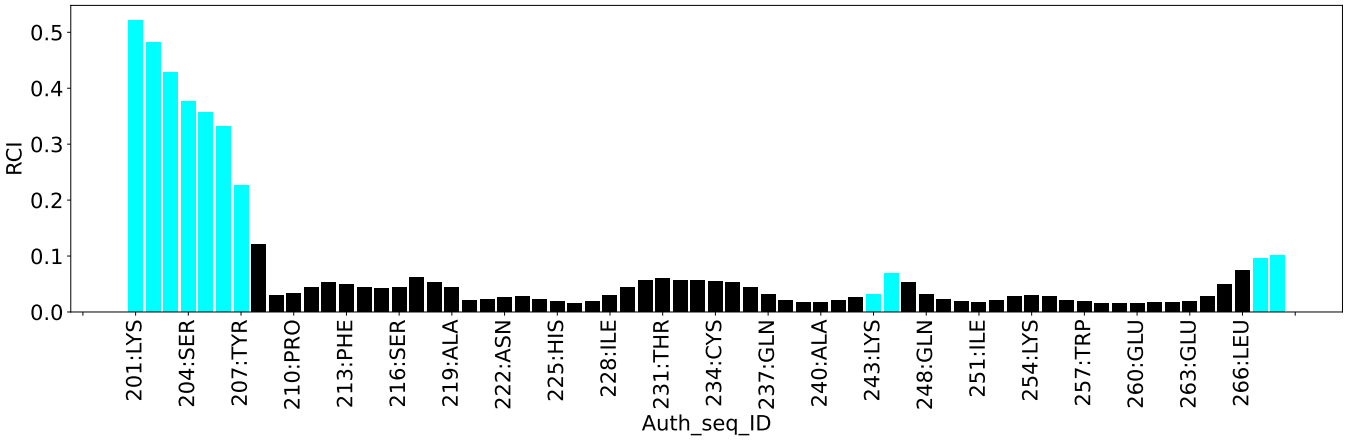
Random coil index (RCI) for chain A:



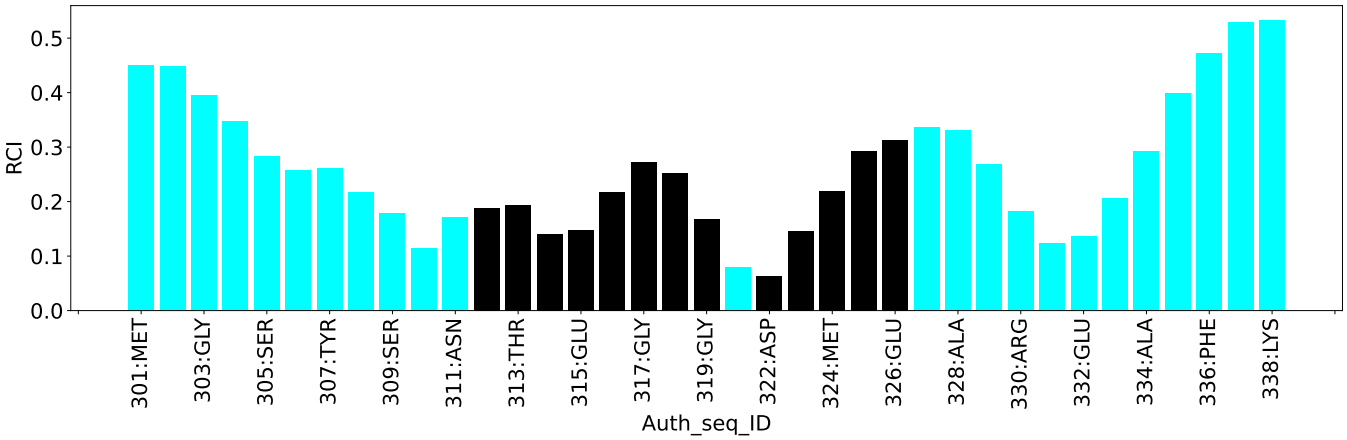
Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:



Random coil index (RCI) for chain D:



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	1694
Intra-residue (|i-j|=0)	528
Sequential (|i-j|=1)	408
Medium range (|i-j|>1 and |i-j|<5)	197
Long range (|i-j|≥5)	376
Inter-chain	185
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	128
Number of unmapped restraints	0
Number of restraints per residue	8.3
Number of long range restraints per residue[1]	1.7

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	42.4	0.2
0.2-0.5 (Medium)	25.8	0.5
>0.5 (Large)	0.2	0.7

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)	20.2	5.04
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

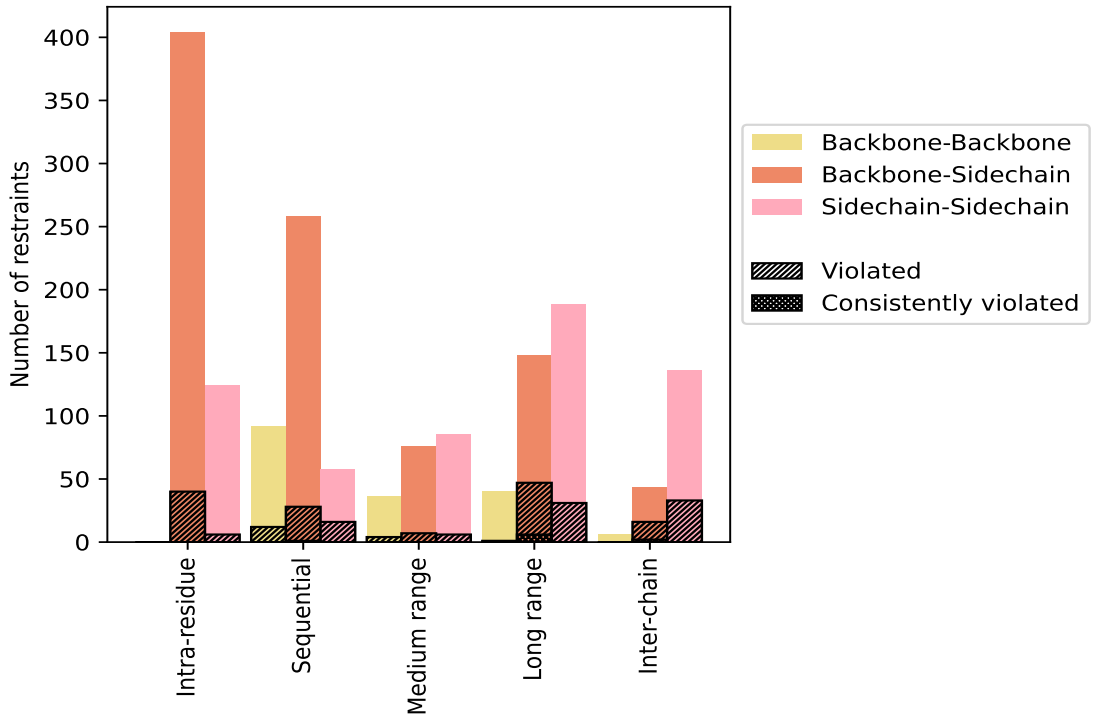
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	528	31.2	46	8.7	2.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	404	23.8	40	9.9	2.4	0	0.0	0.0
Sidechain-Sidechain	124	7.3	6	4.8	0.4	0	0.0	0.0
Sequential (|i-j|=1)	408	24.1	56	13.7	3.3	1	0.2	0.1
Backbone-Backbone	92	5.4	12	13.0	0.7	0	0.0	0.0
Backbone-Sidechain	258	15.2	28	10.9	1.7	1	0.4	0.1
Sidechain-Sidechain	58	3.4	16	27.6	0.9	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	197	11.6	17	8.6	1.0	0	0.0	0.0
Backbone-Backbone	36	2.1	4	11.1	0.2	0	0.0	0.0
Backbone-Sidechain	76	4.5	7	9.2	0.4	0	0.0	0.0
Sidechain-Sidechain	85	5.0	6	7.1	0.4	0	0.0	0.0
Long range (|i-j|≥5)	376	22.2	79	21.0	4.7	6	1.6	0.4
Backbone-Backbone	40	2.4	1	2.5	0.1	0	0.0	0.0
Backbone-Sidechain	148	8.7	47	31.8	2.8	6	4.1	0.4
Sidechain-Sidechain	188	11.1	31	16.5	1.8	0	0.0	0.0
Inter-chain	185	10.9	49	26.5	2.9	2	1.1	0.1
Backbone-Backbone	6	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	43	2.5	16	37.2	0.9	2	4.7	0.1
Sidechain-Sidechain	136	8.0	33	24.3	1.9	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1694	100.0	247	14.6	14.6	9	0.5	0.5
Backbone-Backbone	174	10.3	17	9.8	1.0	0	0.0	0.0
Backbone-Sidechain	929	54.8	138	14.9	8.1	9	1.0	0.5
Sidechain-Sidechain	591	34.9	92	15.6	5.4	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	9	10	1	35	13	68	0.21	0.42	0.1	0.19
2	9	12	2	35	17	75	0.19	0.42	0.09	0.15
3	14	11	6	31	20	82	0.18	0.59	0.08	0.16
4	13	12	2	26	16	69	0.19	0.7	0.1	0.16
5	16	18	1	29	14	78	0.2	0.43	0.1	0.16
6	12	11	6	32	15	76	0.21	0.44	0.1	0.16
7	10	16	4	28	16	74	0.19	0.42	0.08	0.16
8	10	14	4	31	15	74	0.21	0.44	0.09	0.16
9	12	15	1	34	11	73	0.2	0.45	0.09	0.17
10	13	14	1	28	15	71	0.2	0.41	0.08	0.17
11	7	15	3	25	12	62	0.2	0.44	0.09	0.18

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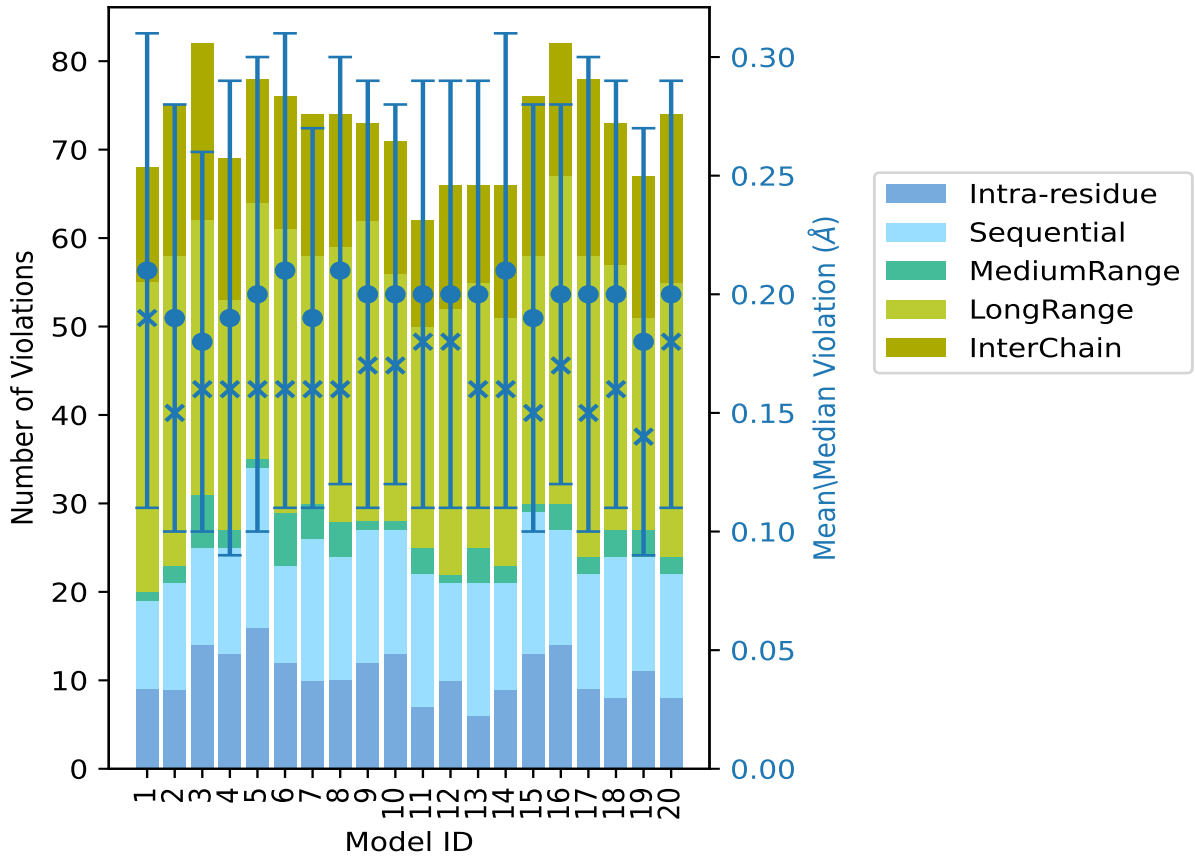
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	10	11	1	30	14	66	0.2	0.55	0.09	0.18
13	6	15	4	30	11	66	0.2	0.41	0.09	0.16
14	9	12	2	28	15	66	0.21	0.5	0.1	0.16
15	13	16	1	28	18	76	0.19	0.45	0.09	0.15
16	14	13	3	37	15	82	0.2	0.5	0.08	0.17
17	9	13	2	34	20	78	0.2	0.44	0.1	0.15
18	8	16	3	30	16	73	0.2	0.54	0.09	0.16
19	11	13	3	24	16	67	0.18	0.64	0.09	0.14
20	8	14	2	31	19	74	0.2	0.44	0.09	0.18

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

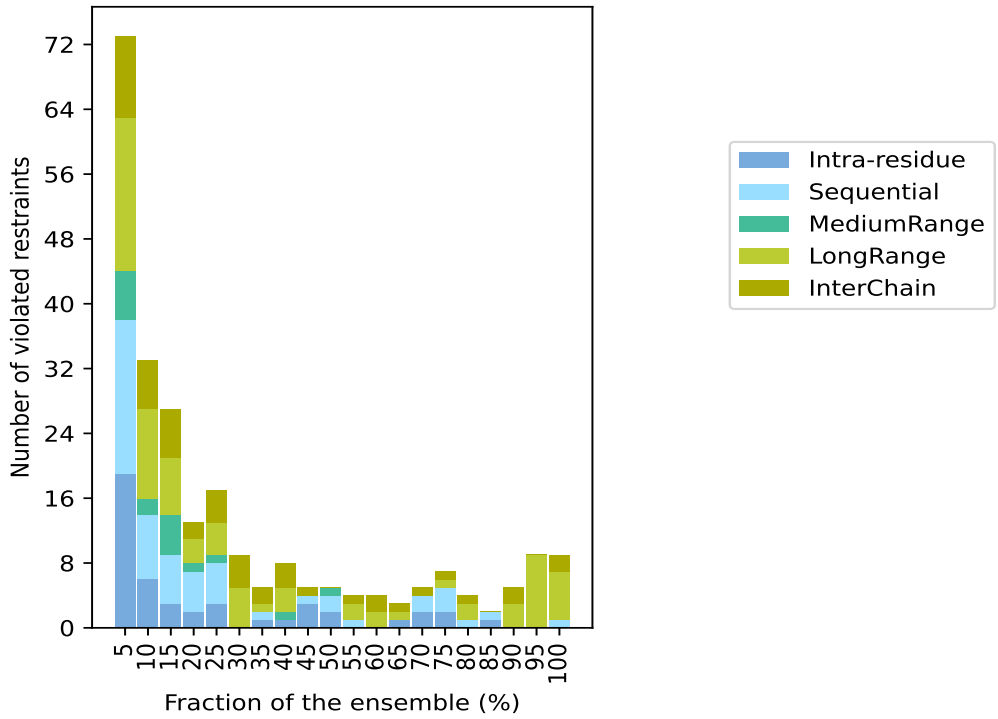
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1447(IR:482, SQ:352, MR:180, LR:297, IC:136) 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]	%
19	19	6	19	10	73	1	5.0
6	8	2	11	6	33	2	10.0
3	6	5	7	6	27	3	15.0
2	5	1	3	2	13	4	20.0
3	5	1	4	4	17	5	25.0
0	0	0	5	4	9	6	30.0
1	1	0	1	2	5	7	35.0
1	0	1	3	3	8	8	40.0
3	1	0	0	1	5	9	45.0
2	2	1	0	0	5	10	50.0
0	1	0	2	1	4	11	55.0
0	0	0	2	2	4	12	60.0
1	0	0	1	1	3	13	65.0
2	2	0	0	1	5	14	70.0
2	3	0	1	1	7	15	75.0
0	1	0	2	1	4	16	80.0
1	1	0	0	0	2	17	85.0
0	0	0	3	2	5	18	90.0
0	0	0	9	0	9	19	95.0
0	1	0	6	2	9	20	100.0

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

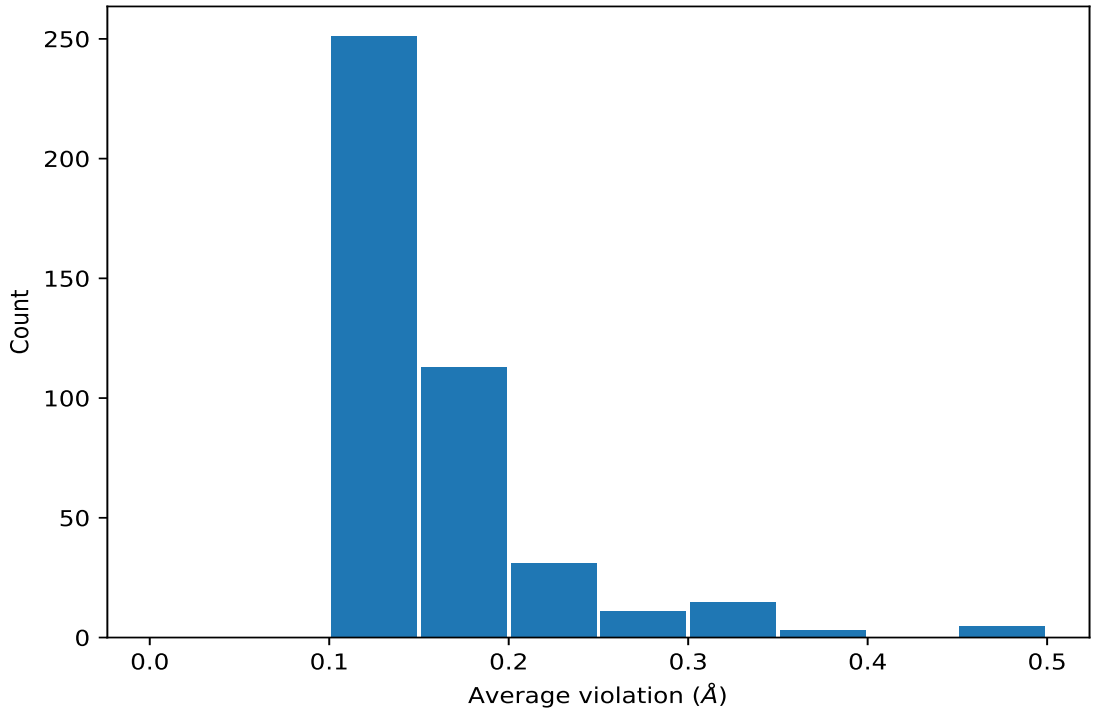
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (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)
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	20	0.36	0.03	0.36
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	20	0.35	0.05	0.36
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	20	0.31	0.07	0.32
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	20	0.3	0.05	0.31
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	20	0.3	0.06	0.32
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	20	0.29	0.04	0.3
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	20	0.28	0.06	0.32
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	20	0.28	0.06	0.29
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	20	0.12	0.01	0.12
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	19	0.35	0.09	0.36
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	19	0.34	0.05	0.37
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	19	0.33	0.06	0.32
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	19	0.32	0.05	0.33
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	19	0.29	0.07	0.28
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	19	0.28	0.07	0.28
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	19	0.25	0.05	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	19	0.22	0.06	0.23
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	19	0.2	0.05	0.19
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	18	0.33	0.1	0.34
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	18	0.23	0.07	0.24
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	18	0.23	0.04	0.23
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	18	0.21	0.06	0.2
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	18	0.2	0.05	0.2
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	17	0.21	0.06	0.22
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	17	0.21	0.06	0.22
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	17	0.21	0.06	0.22
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	17	0.21	0.06	0.22
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	17	0.15	0.03	0.15
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	17	0.15	0.03	0.15
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	16	0.26	0.07	0.26
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	16	0.19	0.05	0.18
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	16	0.19	0.05	0.18
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	16	0.19	0.05	0.18
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	16	0.19	0.05	0.18
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	16	0.18	0.05	0.16
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	16	0.15	0.04	0.14
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	16	0.15	0.04	0.14
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	16	0.15	0.04	0.14
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	16	0.15	0.04	0.14
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	16	0.15	0.04	0.14
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	16	0.15	0.04	0.14
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	15	0.28	0.11	0.28
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	15	0.2	0.05	0.19
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	15	0.16	0.04	0.16
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	15	0.16	0.04	0.16
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	15	0.16	0.05	0.15
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	15	0.16	0.05	0.15
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	15	0.16	0.02	0.15
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	15	0.16	0.02	0.15
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	15	0.16	0.02	0.15
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	15	0.16	0.02	0.15
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	15	0.14	0.03	0.13
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	15	0.14	0.03	0.13
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	15	0.12	0.01	0.12
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	14	0.18	0.06	0.16
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	14	0.18	0.06	0.16
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	14	0.18	0.06	0.16
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	14	0.17	0.04	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	14	0.17	0.02	0.16
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	14	0.17	0.02	0.16
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	14	0.17	0.02	0.16
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	14	0.17	0.02	0.16
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	14	0.13	0.02	0.12
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	14	0.12	0.01	0.12
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	13	0.23	0.08	0.2
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	13	0.19	0.04	0.18
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	13	0.19	0.04	0.18
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	13	0.19	0.04	0.18
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	13	0.13	0.02	0.14
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	12	0.19	0.06	0.2
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	12	0.16	0.04	0.17
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	12	0.16	0.04	0.17
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	12	0.16	0.04	0.17
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	12	0.16	0.04	0.17
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	12	0.16	0.04	0.17
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	12	0.16	0.04	0.17
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	12	0.16	0.04	0.17
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	12	0.16	0.04	0.17
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	12	0.16	0.04	0.17
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	12	0.16	0.04	0.17
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	12	0.16	0.04	0.17
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	12	0.16	0.04	0.17
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	12	0.15	0.04	0.14
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	12	0.15	0.04	0.14
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	12	0.15	0.04	0.14
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	12	0.15	0.04	0.14
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	12	0.15	0.04	0.15
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	11	0.26	0.09	0.27
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	11	0.17	0.04	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	11	0.17	0.04	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	11	0.17	0.04	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	11	0.17	0.04	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	11	0.17	0.04	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	11	0.17	0.04	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	11	0.17	0.04	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	11	0.17	0.04	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	11	0.17	0.04	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	11	0.17	0.04	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	11	0.17	0.04	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	11	0.17	0.04	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	11	0.15	0.02	0.15
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	11	0.15	0.02	0.15
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	11	0.15	0.02	0.15
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	11	0.15	0.02	0.15
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	11	0.15	0.02	0.15
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	11	0.15	0.02	0.15
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	11	0.14	0.03	0.13
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD1	10	0.36	0.06	0.38
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD2	10	0.36	0.06	0.38
(1,991)	1:220:C:ARG:HD2	1:223:C:VAL:H	10	0.31	0.11	0.34
(1,991)	1:220:C:ARG:HD3	1:223:C:VAL:H	10	0.31	0.11	0.34
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE1	10	0.14	0.02	0.15
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE2	10	0.14	0.02	0.15
(1,411)	1:43:A:LYS:H	1:43:A:LYS:HD3	10	0.14	0.03	0.14
(1,1453)	1:264:C:LYS:HB3	1:265:C:CYS:H	10	0.13	0.03	0.12
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD1	9	0.35	0.05	0.33
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD2	9	0.35	0.05	0.33
(1,1328)	1:255:C:LEU:H	1:255:C:LEU:HG	9	0.18	0.04	0.18
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD1	9	0.16	0.03	0.16
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD2	9	0.16	0.03	0.16
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD1	9	0.16	0.03	0.16
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD2	9	0.16	0.03	0.16
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD1	9	0.16	0.03	0.16
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD2	9	0.16	0.03	0.16
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE1	9	0.13	0.02	0.13
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE2	9	0.13	0.02	0.13
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE1	9	0.12	0.01	0.12
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE2	9	0.12	0.01	0.12
(1,86)	1:18:A:VAL:HG23	2:121:B:TYS:HD2	8	0.45	0.18	0.46
(1,86)	1:18:A:VAL:HG23	2:121:B:TYS:HE1	8	0.45	0.18	0.46
(1,86)	1:18:A:VAL:HG11	2:121:B:TYS:HD2	8	0.45	0.18	0.46
(1,86)	1:18:A:VAL:HG23	2:121:B:TYS:HD1	8	0.45	0.18	0.46
(1,86)	1:18:A:VAL:HG23	2:121:B:TYS:HE2	8	0.45	0.18	0.46
(1,115)	1:20:A:ARG:HD2	1:23:A:VAL:H	8	0.22	0.1	0.24
(1,115)	1:20:A:ARG:HD3	1:23:A:VAL:H	8	0.22	0.1	0.24
(1,1040)	1:224:C:LYS:HE2	1:241:C:ARG:H	8	0.19	0.04	0.17
(1,1040)	1:224:C:LYS:HE3	1:241:C:ARG:H	8	0.19	0.04	0.17
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD1	8	0.16	0.05	0.15
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD2	8	0.16	0.05	0.15
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD1	8	0.16	0.05	0.15
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD2	8	0.16	0.05	0.15
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE2	8	0.15	0.04	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE3	8	0.15	0.04	0.15
(1,1152)	1:237:C:GLN:HE21	1:253:C:PRO:HG3	8	0.15	0.03	0.16
(1,1152)	1:237:C:GLN:HE22	1:253:C:PRO:HG3	8	0.15	0.03	0.16
(1,167)	1:24:A:LYS:HE2	1:41:A:ARG:H	8	0.14	0.03	0.12
(1,167)	1:24:A:LYS:HE3	1:41:A:ARG:H	8	0.14	0.03	0.12
(1,1372)	1:257:C:TRP:H	1:257:C:TRP:HE1	8	0.12	0.01	0.12
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD2	7	0.17	0.04	0.14
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD3	7	0.17	0.04	0.14
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD2	7	0.17	0.04	0.14
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD3	7	0.17	0.04	0.14
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE1	7	0.16	0.04	0.17
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE2	7	0.16	0.04	0.17
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE1	7	0.16	0.04	0.17
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE2	7	0.16	0.04	0.17
(1,399)	1:42:A:LEU:HB3	1:47:A:ARG:H	7	0.13	0.02	0.14
(1,252)	1:27:A:LYS:HE2	1:225:C:HIS:HE1	7	0.13	0.02	0.12
(1,252)	1:27:A:LYS:HE3	1:225:C:HIS:HE1	7	0.13	0.02	0.12
(1,656)	1:64:A:LYS:HB2	1:65:A:CYS:H	7	0.12	0.02	0.12
(3,29)	1:227:C:LYS:H	1:239:C:VAL:O	6	0.19	0.05	0.18
(1,1132)	1:231:C:THR:HG21	2:314:D:GLU:HB2	6	0.18	0.06	0.18
(1,1132)	1:231:C:THR:HG22	2:314:D:GLU:HB2	6	0.18	0.06	0.18
(1,1132)	1:231:C:THR:HG23	2:314:D:GLU:HB2	6	0.18	0.06	0.18
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE1	6	0.17	0.04	0.16
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE2	6	0.17	0.04	0.16
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE1	6	0.17	0.04	0.16
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE2	6	0.17	0.04	0.16
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE1	6	0.17	0.04	0.16
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE2	6	0.17	0.04	0.16
(3,22)	1:40:A:ALA:O	1:49:A:VAL:H	6	0.16	0.03	0.16
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG21	6	0.15	0.05	0.13
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG22	6	0.15	0.05	0.13
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG23	6	0.15	0.05	0.13
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD1	6	0.15	0.03	0.14
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD2	6	0.15	0.03	0.14
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD1	6	0.15	0.03	0.14
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD2	6	0.15	0.03	0.14
(1,1219)	1:242:C:LEU:HB3	1:247:C:ARG:H	6	0.13	0.02	0.12
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD1	6	0.13	0.01	0.12
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD2	6	0.13	0.01	0.12
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD1	6	0.13	0.01	0.12
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD2	6	0.13	0.01	0.12
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD1	6	0.13	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD2	6	0.13	0.01	0.12
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG21	6	0.12	0.02	0.12
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG22	6	0.12	0.02	0.12
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG23	6	0.12	0.02	0.12
(1,971)	1:218:C:VAL:HG21	2:321:D:TYS:HD1	5	0.31	0.16	0.29
(1,971)	1:218:C:VAL:HG21	2:321:D:TYS:HD2	5	0.31	0.16	0.29
(1,971)	1:218:C:VAL:HG21	2:321:D:TYS:HE1	5	0.31	0.16	0.29
(1,971)	1:218:C:VAL:HG21	2:321:D:TYS:HE2	5	0.31	0.16	0.29
(1,62)	1:15:A:GLU:HG2	2:123:B:SER:HA	5	0.17	0.06	0.16
(1,62)	1:15:A:GLU:HG3	2:123:B:SER:HA	5	0.17	0.06	0.16
(1,332)	1:37:A:GLN:HE21	1:53:A:PRO:HG3	5	0.16	0.03	0.14
(1,332)	1:37:A:GLN:HE22	1:53:A:PRO:HG3	5	0.16	0.03	0.14
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE1	5	0.14	0.03	0.14
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE2	5	0.14	0.03	0.14
(1,839)	2:128:B:ALA:HA	2:129:B:PHE:H	5	0.14	0.02	0.13
(1,386)	1:41:A:ARG:HD2	1:42:A:LEU:H	5	0.14	0.02	0.15
(1,386)	1:41:A:ARG:HD3	1:42:A:LEU:H	5	0.14	0.02	0.15
(1,1367)	1:256:C:LYS:HD2	1:257:C:TRP:H	5	0.14	0.02	0.14
(1,1367)	1:256:C:LYS:HD3	1:257:C:TRP:H	5	0.14	0.02	0.14
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE1	5	0.13	0.04	0.11
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE2	5	0.13	0.04	0.11
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE1	5	0.13	0.04	0.11
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE2	5	0.13	0.04	0.11
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD1	5	0.13	0.03	0.11
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD2	5	0.13	0.03	0.11
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD1	5	0.13	0.03	0.11
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD2	5	0.13	0.03	0.11
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD1	5	0.13	0.03	0.11
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD2	5	0.13	0.03	0.11
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD1	5	0.13	0.03	0.11
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD2	5	0.13	0.03	0.11
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD1	5	0.13	0.03	0.11
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD2	5	0.13	0.03	0.11
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD1	5	0.13	0.03	0.11
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD2	5	0.13	0.03	0.11
(1,1015)	1:223:C:VAL:HB	1:242:C:LEU:H	5	0.13	0.02	0.11
(1,1206)	1:241:C:ARG:HD2	1:242:C:LEU:H	5	0.12	0.02	0.11
(1,1206)	1:241:C:ARG:HD3	1:242:C:LEU:H	5	0.12	0.02	0.11
(1,1451)	1:264:C:LYS:HB2	1:265:C:CYS:H	5	0.12	0.02	0.13
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE1	5	0.12	0.01	0.12
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE2	5	0.12	0.01	0.12
(1,397)	1:42:A:LEU:HB2	1:47:A:ARG:H	5	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG11	5	0.12	0.01	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG12	5	0.12	0.01	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG13	5	0.12	0.01	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG21	5	0.12	0.01	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG22	5	0.12	0.01	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG23	5	0.12	0.01	0.12
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE2	5	0.11	0.01	0.11
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE3	5	0.11	0.01	0.11
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE2	5	0.11	0.01	0.11
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE3	5	0.11	0.01	0.11
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG2	5	0.11	0.01	0.11
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG3	5	0.11	0.01	0.11
(1,1066)	1:226:C:LEU:HD11	1:227:C:LYS:H	4	0.24	0.06	0.26
(1,1066)	1:226:C:LEU:HD12	1:227:C:LYS:H	4	0.24	0.06	0.26
(1,1066)	1:226:C:LEU:HD13	1:227:C:LYS:H	4	0.24	0.06	0.26
(1,1066)	1:226:C:LEU:HD21	1:227:C:LYS:H	4	0.24	0.06	0.26
(1,1066)	1:226:C:LEU:HD22	1:227:C:LYS:H	4	0.24	0.06	0.26
(1,1066)	1:226:C:LEU:HD23	1:227:C:LYS:H	4	0.24	0.06	0.26
(1,215)	1:26:A:LEU:HD11	1:27:A:LYS:H	4	0.22	0.04	0.22
(1,215)	1:26:A:LEU:HD12	1:27:A:LYS:H	4	0.22	0.04	0.22
(1,215)	1:26:A:LEU:HD13	1:27:A:LYS:H	4	0.22	0.04	0.22
(1,215)	1:26:A:LEU:HD21	1:27:A:LYS:H	4	0.22	0.04	0.22
(1,215)	1:26:A:LEU:HD22	1:27:A:LYS:H	4	0.22	0.04	0.22
(1,215)	1:26:A:LEU:HD23	1:27:A:LYS:H	4	0.22	0.04	0.22
(1,309)	1:31:A:THR:HG21	2:114:B:GLU:HB2	4	0.18	0.05	0.16
(1,309)	1:31:A:THR:HG22	2:114:B:GLU:HB2	4	0.18	0.05	0.16
(1,309)	1:31:A:THR:HG23	2:114:B:GLU:HB2	4	0.18	0.05	0.16
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD11	4	0.15	0.03	0.15
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD12	4	0.15	0.03	0.15
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD13	4	0.15	0.03	0.15
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD21	4	0.15	0.03	0.15
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD22	4	0.15	0.03	0.15
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD23	4	0.15	0.03	0.15
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD11	4	0.15	0.03	0.15
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD12	4	0.15	0.03	0.15
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD13	4	0.15	0.03	0.15
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD21	4	0.15	0.03	0.15
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD22	4	0.15	0.03	0.15
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD23	4	0.15	0.03	0.15
(1,1602)	2:328:D:ALA:HA	2:329:D:PHE:H	4	0.15	0.03	0.15
(1,824)	2:125:B:LYS:HB2	2:125:B:LYS:HD2	4	0.15	0.02	0.15
(1,824)	2:125:B:LYS:HB2	2:125:B:LYS:HD3	4	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,824)	2:125:B:LYS:HB3	2:125:B:LYS:HD2	4	0.15	0.02	0.15
(1,824)	2:125:B:LYS:HB3	2:125:B:LYS:HD3	4	0.15	0.02	0.15
(1,746)	2:106:B:ILE:HA	2:107:B:TYR:H	4	0.13	0.02	0.14
(2,6)	1:11:A:CYS:SG	1:50:A:CYS:CB	4	0.12	0.02	0.12
(1,1515)	2:306:D:ILE:HA	2:307:D:TYR:H	4	0.12	0.01	0.12
(1,328)	1:37:A:GLN:H	1:53:A:PRO:HG3	4	0.12	0.01	0.12
(2,5)	1:11:A:CYS:CB	1:50:A:CYS:SG	4	0.12	0.02	0.11
(1,471)	1:52:A:ASP:H	1:55:A:LEU:H	4	0.11	0.01	0.11
(1,1554)	2:315:D:GLU:HA	2:315:D:GLU:HG2	4	0.11	0.01	0.11
(1,1554)	2:315:D:GLU:HA	2:315:D:GLU:HG3	4	0.11	0.01	0.11
(1,814)	2:125:B:LYS:H	2:125:B:LYS:HD2	3	0.2	0.04	0.21
(1,814)	2:125:B:LYS:H	2:125:B:LYS:HD3	3	0.2	0.04	0.21
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG21	3	0.17	0.05	0.16
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG22	3	0.17	0.05	0.16
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG23	3	0.17	0.05	0.16
(1,882)	1:210:C:PRO:HA	2:312:D:TYR:HE1	3	0.17	0.03	0.17
(1,882)	1:210:C:PRO:HA	2:312:D:TYR:HE2	3	0.17	0.03	0.17
(1,938)	1:215:C:GLU:HG2	2:323:D:SER:HA	3	0.17	0.04	0.18
(1,938)	1:215:C:GLU:HG3	2:323:D:SER:HA	3	0.17	0.04	0.18
(1,552)	1:57:A:TRP:H	1:57:A:TRP:HE1	3	0.16	0.04	0.15
(1,752)	2:106:B:ILE:HD11	2:107:B:TYR:HE1	3	0.16	0.03	0.17
(1,752)	2:106:B:ILE:HD11	2:107:B:TYR:HE2	3	0.16	0.03	0.17
(1,752)	2:106:B:ILE:HD12	2:107:B:TYR:HE1	3	0.16	0.03	0.17
(1,752)	2:106:B:ILE:HD12	2:107:B:TYR:HE2	3	0.16	0.03	0.17
(1,752)	2:106:B:ILE:HD13	2:107:B:TYR:HE1	3	0.16	0.03	0.17
(1,752)	2:106:B:ILE:HD13	2:107:B:TYR:HE2	3	0.16	0.03	0.17
(1,783)	2:114:B:GLU:HA	2:114:B:GLU:HG2	3	0.15	0.01	0.15
(1,783)	2:114:B:GLU:HA	2:114:B:GLU:HG3	3	0.15	0.01	0.15
(1,242)	1:27:A:LYS:HG2	2:112:B:TYR:HE1	3	0.15	0.0	0.15
(1,242)	1:27:A:LYS:HG2	2:112:B:TYR:HE2	3	0.15	0.0	0.15
(1,189)	1:25:A:HIS:HE1	1:41:A:ARG:HD2	3	0.14	0.02	0.13
(1,189)	1:25:A:HIS:HE1	1:41:A:ARG:HD3	3	0.14	0.02	0.13
(1,1050)	1:225:C:HIS:HE1	1:227:C:LYS:HE2	3	0.14	0.03	0.12
(1,1050)	1:225:C:HIS:HE1	1:227:C:LYS:HE3	3	0.14	0.03	0.12
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG11	3	0.13	0.03	0.12
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG12	3	0.13	0.03	0.12
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG13	3	0.13	0.03	0.12
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG21	3	0.13	0.03	0.12
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG22	3	0.13	0.03	0.12
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG23	3	0.13	0.03	0.12
(1,14)	1:10:A:PRO:HB3	1:11:A:CYS:H	3	0.13	0.02	0.12
(1,1012)	1:222:C:ASN:HD21	1:242:C:LEU:HB2	3	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1012)	1:222:C:ASN:HD22	1:242:C:LEU:HB2	3	0.13	0.01	0.13
(1,1162)	1:238:C:ILE:HB	1:239:C:VAL:H	3	0.12	0.01	0.12
(1,239)	1:27:A:LYS:HD3	2:112:B:TYR:HD1	3	0.12	0.02	0.11
(1,239)	1:27:A:LYS:HD3	2:112:B:TYR:HD2	3	0.12	0.02	0.11
(2,17)	1:211:C:CYS:CB	1:250:C:CYS:SG	3	0.12	0.01	0.12
(1,1148)	1:237:C:GLN:H	1:253:C:PRO:HG3	3	0.12	0.02	0.11
(1,749)	2:106:B:ILE:HB	2:107:B:TYR:HD1	3	0.12	0.0	0.12
(1,749)	2:106:B:ILE:HB	2:107:B:TYR:HD2	3	0.12	0.0	0.12
(1,831)	2:127:B:PRO:HA	2:128:B:ALA:H	3	0.12	0.01	0.11
(1,7)	1:10:A:PRO:HB2	2:112:B:TYR:HD1	3	0.11	0.02	0.1
(1,7)	1:10:A:PRO:HB2	2:112:B:TYR:HD2	3	0.11	0.02	0.1
(1,1431)	1:262:C:LEU:HA	1:265:C:CYS:H	3	0.11	0.01	0.11
(1,489)	1:53:A:PRO:HB3	1:54:A:LYS:H	3	0.11	0.01	0.11
(1,1052)	1:225:C:HIS:HE1	1:241:C:ARG:HD2	3	0.11	0.01	0.11
(1,1052)	1:225:C:HIS:HE1	1:241:C:ARG:HD3	3	0.11	0.01	0.11
(1,687)	1:66:A:LEU:HD11	1:263:C:GLU:H	3	0.11	0.01	0.11
(1,687)	1:66:A:LEU:HD12	1:263:C:GLU:H	3	0.11	0.01	0.11
(1,687)	1:66:A:LEU:HD13	1:263:C:GLU:H	3	0.11	0.01	0.11
(1,1368)	1:256:C:LYS:HD2	1:260:C:GLU:HG2	3	0.11	0.01	0.1
(1,1368)	1:256:C:LYS:HD3	1:260:C:GLU:HG2	3	0.11	0.01	0.1
(2,14)	1:209:C:CYS:CB	1:234:C:CYS:SG	3	0.11	0.0	0.11
(1,187)	1:25:A:HIS:HE1	1:27:A:LYS:HE2	3	0.1	0.0	0.1
(1,187)	1:25:A:HIS:HE1	1:27:A:LYS:HE3	3	0.1	0.0	0.1
(1,1519)	2:306:D:ILE:HD11	2:307:D:TYR:H	2	0.2	0.0	0.2
(1,1519)	2:306:D:ILE:HD12	2:307:D:TYR:H	2	0.2	0.0	0.2
(1,1519)	2:306:D:ILE:HD13	2:307:D:TYR:H	2	0.2	0.0	0.2
(1,750)	2:106:B:ILE:HD11	2:107:B:TYR:H	2	0.18	0.05	0.18
(1,750)	2:106:B:ILE:HD12	2:107:B:TYR:H	2	0.18	0.05	0.18
(1,750)	2:106:B:ILE:HD13	2:107:B:TYR:H	2	0.18	0.05	0.18
(1,114)	1:20:A:ARG:HB2	1:57:A:TRP:HH2	2	0.17	0.03	0.17
(1,114)	1:20:A:ARG:HB3	1:57:A:TRP:HH2	2	0.17	0.03	0.17
(1,966)	1:218:C:VAL:HG11	1:252:C:ASP:H	2	0.16	0.01	0.16
(1,966)	1:218:C:VAL:HG12	1:252:C:ASP:H	2	0.16	0.01	0.16
(1,966)	1:218:C:VAL:HG13	1:252:C:ASP:H	2	0.16	0.01	0.16
(1,966)	1:218:C:VAL:HG21	1:252:C:ASP:H	2	0.16	0.01	0.16
(1,966)	1:218:C:VAL:HG22	1:252:C:ASP:H	2	0.16	0.01	0.16
(1,966)	1:218:C:VAL:HG23	1:252:C:ASP:H	2	0.16	0.01	0.16
(1,1553)	2:315:D:GLU:H	2:315:D:GLU:HG2	2	0.15	0.02	0.15
(1,1553)	2:315:D:GLU:H	2:315:D:GLU:HG3	2	0.15	0.02	0.15
(3,9)	1:27:A:LYS:H	1:39:A:VAL:O	2	0.15	0.04	0.15
(1,139)	1:23:A:VAL:HB	1:42:A:LEU:H	2	0.14	0.01	0.14
(2,18)	1:211:C:CYS:SG	1:250:C:CYS:CB	2	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,293)	1:29:A:LEU:HD11	1:225:C:HIS:HE1	2	0.13	0.02	0.13
(1,293)	1:29:A:LEU:HD12	1:225:C:HIS:HE1	2	0.13	0.02	0.13
(1,293)	1:29:A:LEU:HD13	1:225:C:HIS:HE1	2	0.13	0.02	0.13
(1,241)	1:27:A:LYS:HD3	1:225:C:HIS:HE1	2	0.12	0.02	0.12
(1,313)	1:31:A:THR:HG21	1:37:A:GLN:HE21	2	0.12	0.01	0.12
(1,313)	1:31:A:THR:HG21	1:37:A:GLN:HE22	2	0.12	0.01	0.12
(1,313)	1:31:A:THR:HG22	1:37:A:GLN:HE21	2	0.12	0.01	0.12
(1,313)	1:31:A:THR:HG22	1:37:A:GLN:HE22	2	0.12	0.01	0.12
(1,313)	1:31:A:THR:HG23	1:37:A:GLN:HE21	2	0.12	0.01	0.12
(1,313)	1:31:A:THR:HG23	1:37:A:GLN:HE22	2	0.12	0.01	0.12
(1,1022)	1:224:C:LYS:H	1:224:C:LYS:HD2	2	0.12	0.01	0.12
(1,1022)	1:224:C:LYS:H	1:224:C:LYS:HD3	2	0.12	0.01	0.12
(1,1036)	1:224:C:LYS:HB2	1:225:C:HIS:HE1	2	0.12	0.02	0.12
(1,1036)	1:224:C:LYS:HB3	1:225:C:HIS:HE1	2	0.12	0.02	0.12
(1,92)	1:18:A:VAL:HG11	1:52:A:ASP:H	2	0.12	0.01	0.12
(1,92)	1:18:A:VAL:HG12	1:52:A:ASP:H	2	0.12	0.01	0.12
(1,92)	1:18:A:VAL:HG13	1:52:A:ASP:H	2	0.12	0.01	0.12
(1,92)	1:18:A:VAL:HG21	1:52:A:ASP:H	2	0.12	0.01	0.12
(1,92)	1:18:A:VAL:HG22	1:52:A:ASP:H	2	0.12	0.01	0.12
(1,92)	1:18:A:VAL:HG23	1:52:A:ASP:H	2	0.12	0.01	0.12
(1,777)	2:113:B:THR:HA	2:113:B:THR:HG21	2	0.12	0.0	0.12
(1,777)	2:113:B:THR:HA	2:113:B:THR:HG22	2	0.12	0.0	0.12
(1,777)	2:113:B:THR:HA	2:113:B:THR:HG23	2	0.12	0.0	0.12
(1,825)	2:125:B:LYS:HB2	2:125:B:LYS:HE2	2	0.12	0.01	0.12
(1,825)	2:125:B:LYS:HB2	2:125:B:LYS:HE3	2	0.12	0.01	0.12
(1,825)	2:125:B:LYS:HB3	2:125:B:LYS:HE2	2	0.12	0.01	0.12
(1,825)	2:125:B:LYS:HB3	2:125:B:LYS:HE3	2	0.12	0.01	0.12
(1,886)	1:210:C:PRO:HB2	2:312:D:TYR:HD1	2	0.12	0.02	0.12
(1,886)	1:210:C:PRO:HB2	2:312:D:TYR:HD2	2	0.12	0.02	0.12
(1,1291)	1:252:C:ASP:H	1:255:C:LEU:H	2	0.12	0.02	0.12
(1,70)	1:16:A:SER:HB2	1:52:A:ASP:H	2	0.12	0.0	0.12
(1,70)	1:16:A:SER:HB3	1:52:A:ASP:H	2	0.12	0.0	0.12
(1,627)	1:62:A:LEU:HA	1:65:A:CYS:H	2	0.12	0.0	0.12
(1,744)	2:106:B:ILE:HA	2:106:B:ILE:HD11	2	0.12	0.0	0.12
(1,744)	2:106:B:ILE:HA	2:106:B:ILE:HD12	2	0.12	0.0	0.12
(1,744)	2:106:B:ILE:HA	2:106:B:ILE:HD13	2	0.12	0.0	0.12
(1,816)	2:125:B:LYS:HA	2:125:B:LYS:HD2	2	0.12	0.0	0.12
(1,816)	2:125:B:LYS:HA	2:125:B:LYS:HD3	2	0.12	0.0	0.12
(1,946)	1:216:C:SER:HB2	1:252:C:ASP:H	2	0.12	0.0	0.12
(1,946)	1:216:C:SER:HB3	1:252:C:ASP:H	2	0.12	0.0	0.12
(1,1265)	1:249:C:VAL:HG21	2:321:D:TYS:HE1	2	0.12	0.0	0.12
(1,1265)	1:249:C:VAL:HG21	2:321:D:TYS:HE2	2	0.12	0.0	0.12

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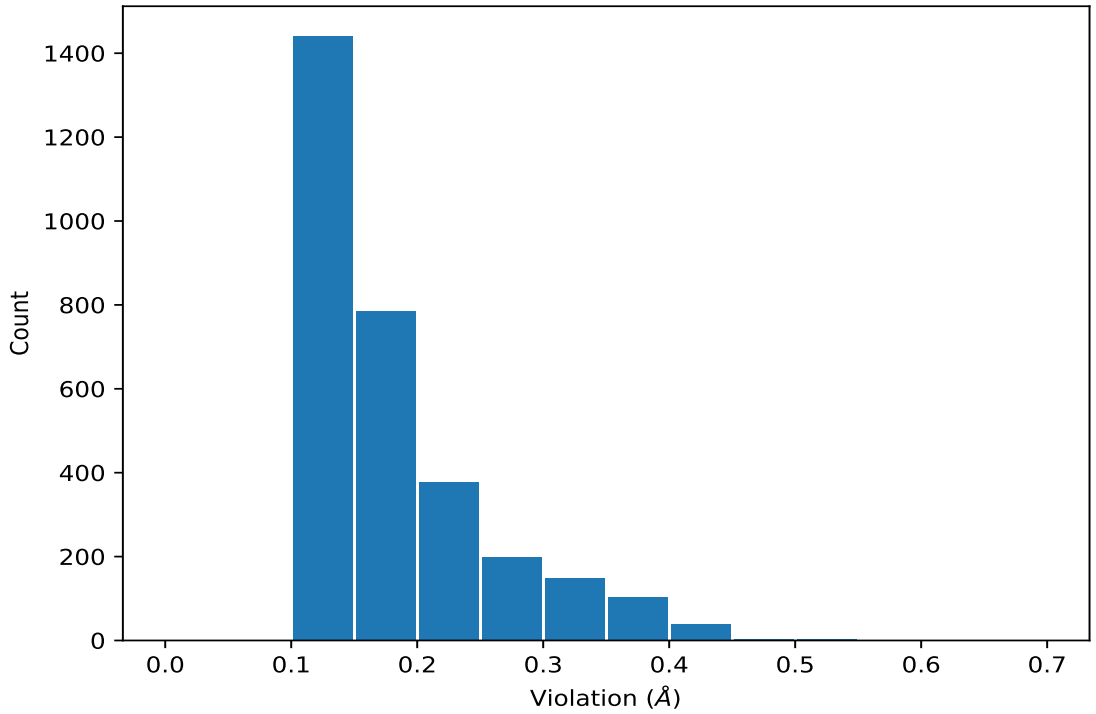
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1265)	1:249:C:VAL:HG22	2:321:D:TYS:HE1	2	0.12	0.0	0.12
(1,1265)	1:249:C:VAL:HG22	2:321:D:TYS:HE2	2	0.12	0.0	0.12
(1,1265)	1:249:C:VAL:HG23	2:321:D:TYS:HE1	2	0.12	0.0	0.12
(1,1265)	1:249:C:VAL:HG23	2:321:D:TYS:HE2	2	0.12	0.0	0.12
(1,547)	1:56:A:LYS:HD2	1:57:A:TRP:H	2	0.11	0.01	0.11
(1,547)	1:56:A:LYS:HD3	1:57:A:TRP:H	2	0.11	0.01	0.11
(1,699)	1:66:A:LEU:HD11	2:327:D:PRO:HB2	2	0.11	0.0	0.11
(1,699)	1:66:A:LEU:HD11	2:327:D:PRO:HB3	2	0.11	0.0	0.11
(1,699)	1:66:A:LEU:HD12	2:327:D:PRO:HB2	2	0.11	0.0	0.11
(1,699)	1:66:A:LEU:HD12	2:327:D:PRO:HB3	2	0.11	0.0	0.11
(1,699)	1:66:A:LEU:HD13	2:327:D:PRO:HB2	2	0.11	0.0	0.11
(1,699)	1:66:A:LEU:HD13	2:327:D:PRO:HB3	2	0.11	0.0	0.11
(1,699)	1:66:A:LEU:HD21	2:327:D:PRO:HB2	2	0.11	0.0	0.11
(1,699)	1:66:A:LEU:HD21	2:327:D:PRO:HB3	2	0.11	0.0	0.11
(1,699)	1:66:A:LEU:HD22	2:327:D:PRO:HB2	2	0.11	0.0	0.11
(1,699)	1:66:A:LEU:HD22	2:327:D:PRO:HB3	2	0.11	0.0	0.11
(1,699)	1:66:A:LEU:HD23	2:327:D:PRO:HB2	2	0.11	0.0	0.11
(1,699)	1:66:A:LEU:HD23	2:327:D:PRO:HB3	2	0.11	0.0	0.11
(1,798)	2:120:B:ASP:HB3	2:121:B:TYS:HE1	2	0.11	0.01	0.11
(1,798)	2:120:B:ASP:HB3	2:121:B:TYS:HE2	2	0.11	0.01	0.11
(1,888)	1:210:C:PRO:HB3	1:211:C:CYS:H	2	0.11	0.0	0.11
(1,957)	1:218:C:VAL:HB	1:251:C:ILE:HG21	2	0.11	0.0	0.11
(1,957)	1:218:C:VAL:HB	1:251:C:ILE:HG22	2	0.11	0.0	0.11
(1,957)	1:218:C:VAL:HB	1:251:C:ILE:HG23	2	0.11	0.0	0.11
(1,188)	1:25:A:HIS:HE1	1:41:A:ARG:HB2	2	0.11	0.0	0.11
(1,188)	1:25:A:HIS:HE1	1:41:A:ARG:HB3	2	0.11	0.0	0.11
(1,1564)	2:320:D:ASP:HB3	2:321:D:TYS:HE1	2	0.11	0.0	0.11
(1,1564)	2:320:D:ASP:HB3	2:321:D:TYS:HE2	2	0.11	0.0	0.11
(2,11)	1:65:A:CYS:CB	1:236:C:CYS:SG	2	0.11	0.0	0.11
(1,758)	2:106:B:ILE:HG21	2:107:B:TYR:HE1	2	0.1	0.0	0.1
(1,758)	2:106:B:ILE:HG21	2:107:B:TYR:HE2	2	0.1	0.0	0.1
(1,758)	2:106:B:ILE:HG22	2:107:B:TYR:HE1	2	0.1	0.0	0.1
(1,758)	2:106:B:ILE:HG22	2:107:B:TYR:HE2	2	0.1	0.0	0.1
(1,758)	2:106:B:ILE:HG23	2:107:B:TYR:HE1	2	0.1	0.0	0.1
(1,758)	2:106:B:ILE:HG23	2:107:B:TYR:HE2	2	0.1	0.0	0.1

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:18:A:VAL:HG11	2:121:B:TYS:HD2	4	0.7
(1,86)	1:18:A:VAL:HG23	2:121:B:TYS:HE2	19	0.64
(1,86)	1:18:A:VAL:HG23	2:121:B:TYS:HE1	3	0.59
(1,971)	1:218:C:VAL:HG21	2:321:D:TYS:HE1	12	0.55
(1,86)	1:18:A:VAL:HG23	2:121:B:TYS:HE1	18	0.54
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	16	0.5
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	14	0.5
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	14	0.46
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	9	0.45
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	15	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	11	0.44
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	17	0.44
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	20	0.44
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	20	0.44
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD1	6	0.44
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD2	6	0.44
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD1	8	0.44
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD2	8	0.44
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD1	6	0.44
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD2	6	0.44
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	5	0.43
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	4	0.43
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	15	0.43
(1,991)	1:220:C:ARG:HD2	1:223:C:VAL:H	8	0.43
(1,991)	1:220:C:ARG:HD3	1:223:C:VAL:H	8	0.43
(1,971)	1:218:C:VAL:HG21	2:321:D:TYS:HD2	17	0.43
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	1	0.42
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	1	0.42
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	14	0.42
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	2	0.42
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	20	0.42
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	6	0.42
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	7	0.42
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	18	0.41
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	5	0.41
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	18	0.41
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	13	0.41
(1,991)	1:220:C:ARG:HD2	1:223:C:VAL:H	20	0.41
(1,991)	1:220:C:ARG:HD3	1:223:C:VAL:H	20	0.41
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD1	10	0.41
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD2	10	0.41
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	6	0.4
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	15	0.4
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	16	0.4
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	4	0.4
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	2	0.4
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	6	0.4
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	17	0.4
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD1	5	0.4
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD2	5	0.4
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	2	0.39
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	6	0.39
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	15	0.39
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	1	0.39
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	5	0.39
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	1	0.39
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	6	0.39
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	1	0.39
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	17	0.39
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	20	0.39
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	7	0.39
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	16	0.39
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	10	0.39
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	11	0.39
(1,991)	1:220:C:ARG:HD2	1:223:C:VAL:H	19	0.39
(1,991)	1:220:C:ARG:HD3	1:223:C:VAL:H	19	0.39
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD1	18	0.39
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD2	18	0.39
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	5	0.38
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	1	0.38
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	2	0.38
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	17	0.38
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	12	0.38
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	19	0.38
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	14	0.38
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	2	0.38
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	17	0.38
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	20	0.38
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	14	0.38
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	1	0.38
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD1	13	0.38
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD2	13	0.38
(1,991)	1:220:C:ARG:HD2	1:223:C:VAL:H	9	0.38
(1,991)	1:220:C:ARG:HD3	1:223:C:VAL:H	9	0.38
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD1	8	0.38
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD2	8	0.38
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	14	0.37
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	15	0.37
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	18	0.37
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	9	0.37
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	6	0.37
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	14	0.37
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	13	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	3	0.37
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	5	0.37
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	8	0.37
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	1	0.37
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	20	0.37
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	6	0.37
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	5	0.37
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	9	0.37
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	13	0.37
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	14	0.37
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	15	0.37
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	6	0.37
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	14	0.37
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	9	0.37
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD1	5	0.37
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD2	5	0.37
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD1	13	0.37
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD2	13	0.37
(1,115)	1:20:A:ARG:HD2	1:23:A:VAL:H	11	0.37
(1,115)	1:20:A:ARG:HD3	1:23:A:VAL:H	11	0.37
(1,86)	1:18:A:VAL:HG23	2:121:B:TYS:HD2	1	0.37
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	11	0.36
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	17	0.36
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	2	0.36
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	15	0.36
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	17	0.36
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	10	0.36
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	19	0.36
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	10	0.36
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	13	0.36
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	18	0.36
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	18	0.36
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	1	0.36
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	2	0.36
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	6	0.36
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	17	0.36
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	6	0.36
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	9	0.36
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	8	0.36
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	8	0.35
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	17	0.35
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	13	0.35
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	6	0.35
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	7	0.35
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	12	0.35
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	13	0.35
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	12	0.35
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	15	0.35
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	17	0.35
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	14	0.35
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	4	0.35
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	9	0.35
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	13	0.35
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	4	0.35
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	8	0.35
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	12	0.35
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	7	0.35
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	18	0.35
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	10	0.34
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	12	0.34
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	6	0.34
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	13	0.34
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	16	0.34
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	14	0.34
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	20	0.34
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	10	0.34
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	9	0.34
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	15	0.34
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	13	0.34
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	2	0.34
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	7	0.34
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	17	0.34
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	10	0.34
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	20	0.34
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	8	0.34
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	10	0.34
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	5	0.34
(1,991)	1:220:C:ARG:HD2	1:223:C:VAL:H	3	0.34
(1,991)	1:220:C:ARG:HD3	1:223:C:VAL:H	3	0.34
(1,991)	1:220:C:ARG:HD2	1:223:C:VAL:H	11	0.34
(1,991)	1:220:C:ARG:HD3	1:223:C:VAL:H	11	0.34
(1,86)	1:18:A:VAL:HG23	2:121:B:TYS:HE1	8	0.34
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	5	0.33
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	9	0.33
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	3	0.33
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	9	0.33
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	6	0.33
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	16	0.33
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	11	0.33
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	6	0.33
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	17	0.33
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	12	0.33
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	5	0.33
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	14	0.33
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	18	0.33
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	5	0.33
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	15	0.33
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	11	0.33
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	18	0.33
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	1	0.33
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	17	0.33
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	20	0.33
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD1	14	0.33
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD2	14	0.33
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD1	15	0.33
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD2	15	0.33
(1,115)	1:20:A:ARG:HD2	1:23:A:VAL:H	3	0.33
(1,115)	1:20:A:ARG:HD3	1:23:A:VAL:H	3	0.33
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	1	0.32
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	3	0.32
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	7	0.32
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	8	0.32
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	14	0.32
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	11	0.32
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	13	0.32
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	5	0.32
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	16	0.32
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	4	0.32
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	8	0.32
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	10	0.32
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	17	0.32
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	4	0.32
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	6	0.32
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	11	0.32
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	6	0.32
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	3	0.32
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	5	0.32
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	8	0.32
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	12	0.32
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	15	0.32
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	17	0.32
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	10	0.32
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	11	0.32
(1,1462)	1:265:C:CYS:H	1:268:C:LYS:HD2	16	0.32
(1,1462)	1:265:C:CYS:H	1:268:C:LYS:HD3	16	0.32
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	12	0.32
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	12	0.32
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	12	0.32
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	19	0.31
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	11	0.31
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	12	0.31
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	18	0.31
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	9	0.31
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	2	0.31
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	1	0.31
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	6	0.31
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	16	0.31
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	19	0.31
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	9	0.31
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	19	0.31
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	8	0.31
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	12	0.31
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	9	0.31
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	15	0.31
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	13	0.31
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	7	0.31
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	17	0.31
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	8	0.31
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	13	0.31
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	8	0.31
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD1	1	0.31
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD2	1	0.31
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD1	16	0.31
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD2	16	0.31
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	20	0.3
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	3	0.3
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	9	0.3
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	20	0.3
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	3	0.3
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	15	0.3
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	1	0.3
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	2	0.3
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	5	0.3
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	8	0.3
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	12	0.3
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	7	0.3
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	10	0.3
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	16	0.3
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	10	0.3
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	5	0.3
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	12	0.3
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD1	15	0.3
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD2	15	0.3
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD1	20	0.3
(1,1530)	2:307:D:TYR:HA	2:307:D:TYR:HD2	20	0.3
(1,1132)	1:231:C:THR:HG21	2:314:D:GLU:HB2	19	0.3
(1,1132)	1:231:C:THR:HG22	2:314:D:GLU:HB2	19	0.3
(1,1132)	1:231:C:THR:HG23	2:314:D:GLU:HB2	19	0.3
(1,1066)	1:226:C:LEU:HD11	1:227:C:LYS:H	18	0.3
(1,1066)	1:226:C:LEU:HD12	1:227:C:LYS:H	18	0.3
(1,1066)	1:226:C:LEU:HD13	1:227:C:LYS:H	18	0.3
(1,1066)	1:226:C:LEU:HD21	1:227:C:LYS:H	18	0.3
(1,1066)	1:226:C:LEU:HD22	1:227:C:LYS:H	18	0.3
(1,1066)	1:226:C:LEU:HD23	1:227:C:LYS:H	18	0.3
(1,991)	1:220:C:ARG:HD2	1:223:C:VAL:H	2	0.3
(1,991)	1:220:C:ARG:HD3	1:223:C:VAL:H	2	0.3
(1,991)	1:220:C:ARG:HD2	1:223:C:VAL:H	7	0.3
(1,991)	1:220:C:ARG:HD3	1:223:C:VAL:H	7	0.3
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	3	0.3
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	3	0.3
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	3	0.3
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	3	0.3
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD1	16	0.3
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD2	16	0.3
(1,86)	1:18:A:VAL:HG23	2:121:B:TYS:HE2	14	0.3
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	7	0.29
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	16	0.29
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	12	0.29
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	3	0.29
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	1	0.29
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	8	0.29
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	18	0.29
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	6	0.29
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	16	0.29
(3,19)	1:38:A:ILE:O	1:51:A:ILE:N	7	0.29
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	12	0.29
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	3	0.29
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	13	0.29
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	20	0.29
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	4	0.29
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	8	0.29
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	17	0.29
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	10	0.29
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	2	0.29
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	11	0.29
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	17	0.29
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	18	0.29
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	5	0.29
(1,1066)	1:226:C:LEU:HD11	1:227:C:LYS:H	20	0.29
(1,1066)	1:226:C:LEU:HD12	1:227:C:LYS:H	20	0.29
(1,1066)	1:226:C:LEU:HD13	1:227:C:LYS:H	20	0.29
(1,1066)	1:226:C:LEU:HD21	1:227:C:LYS:H	20	0.29
(1,1066)	1:226:C:LEU:HD22	1:227:C:LYS:H	20	0.29
(1,1066)	1:226:C:LEU:HD23	1:227:C:LYS:H	20	0.29
(1,971)	1:218:C:VAL:HG21	2:321:D:TYS:HE2	18	0.29
(1,215)	1:26:A:LEU:HD11	1:27:A:LYS:H	18	0.29
(1,215)	1:26:A:LEU:HD12	1:27:A:LYS:H	18	0.29
(1,215)	1:26:A:LEU:HD13	1:27:A:LYS:H	18	0.29
(1,215)	1:26:A:LEU:HD21	1:27:A:LYS:H	18	0.29
(1,215)	1:26:A:LEU:HD22	1:27:A:LYS:H	18	0.29
(1,215)	1:26:A:LEU:HD23	1:27:A:LYS:H	18	0.29
(1,115)	1:20:A:ARG:HD2	1:23:A:VAL:H	20	0.29
(1,115)	1:20:A:ARG:HD3	1:23:A:VAL:H	20	0.29
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	6	0.28
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	20	0.28
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	10	0.28
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	18	0.28
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	20	0.28
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	11	0.28
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	17	0.28
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	2	0.28
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	9	0.28
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	7	0.28
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	14	0.28
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	18	0.28
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	10	0.28
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	12	0.28
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	1	0.28
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	5	0.28
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	19	0.28
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	8	0.28
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	12	0.28
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	5	0.28
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	14	0.28
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	16	0.28
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	7	0.28
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	7	0.28
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	7	0.28
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	16	0.28
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	16	0.28
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	16	0.28
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	16	0.28
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD1	7	0.28
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD2	7	0.28
(1,115)	1:20:A:ARG:HD2	1:23:A:VAL:H	2	0.28
(1,115)	1:20:A:ARG:HD3	1:23:A:VAL:H	2	0.28
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	4	0.27
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	10	0.27
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	7	0.27
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	10	0.27
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	11	0.27
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	13	0.27
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	15	0.27
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	7	0.27
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	3	0.27
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	5	0.27
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	19	0.27
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	11	0.27
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	7	0.27
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	16	0.27
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	6	0.27
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	2	0.27
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	4	0.27
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	4	0.27
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	3	0.27
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	16	0.27
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	4	0.27
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	18	0.27
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	16	0.27
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	9	0.27
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	10	0.27
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	17	0.27
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	17	0.27
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	17	0.27
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	14	0.27
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	14	0.27
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	14	0.27
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	14	0.27
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	1	0.27
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	1	0.27
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	1	0.27
(1,309)	1:31:A:THR:HG21	2:114:B:GLU:HB2	8	0.27
(1,309)	1:31:A:THR:HG22	2:114:B:GLU:HB2	8	0.27
(1,309)	1:31:A:THR:HG23	2:114:B:GLU:HB2	8	0.27
(1,62)	1:15:A:GLU:HG2	2:123:B:SER:HA	17	0.27
(1,62)	1:15:A:GLU:HG3	2:123:B:SER:HA	17	0.27
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	10	0.26
(3,34)	1:238:C:ILE:O	1:251:C:ILE:N	9	0.26
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	7	0.26
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	12	0.26
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	19	0.26
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	1	0.26
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	14	0.26
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	16	0.26
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	8	0.26
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	1	0.26
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	3	0.26
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	10	0.26
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	5	0.26
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	7	0.26
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	17	0.26
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	13	0.26
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	3	0.26
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	11	0.26
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	13	0.26
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	10	0.26
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	12	0.26
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	15	0.26
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	4	0.26
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	2	0.26
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	1	0.26
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	1	0.26
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	1	0.26
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	1	0.26
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	10	0.26
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	10	0.26
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	10	0.26
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	10	0.26
(1,1040)	1:224:C:LYS:HE2	1:241:C:ARG:H	17	0.26
(1,1040)	1:224:C:LYS:HE3	1:241:C:ARG:H	17	0.26
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	11	0.26
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	11	0.26
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	11	0.26
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	11	0.26
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD1	14	0.26
(1,761)	2:107:B:TYR:HA	2:107:B:TYR:HD2	14	0.26
(1,429)	1:47:A:ARG:HA	1:48:A:GLN:H	9	0.26
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	5	0.25
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	16	0.25
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	10	0.25
(3,29)	1:227:C:LYS:H	1:239:C:VAL:O	14	0.25
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	4	0.25
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	16	0.25
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	1	0.25
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	2	0.25
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	1	0.25
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	3	0.25
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	18	0.25
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	19	0.25
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	19	0.25
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	18	0.25
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	8	0.25
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	8	0.25
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	8	0.25
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	8	0.25
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	13	0.25
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	13	0.25
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	13	0.25
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	13	0.25
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG21	8	0.25
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG22	8	0.25
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG23	8	0.25
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	17	0.25
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	17	0.25
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	17	0.25
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	17	0.25
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	18	0.25
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	18	0.25
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	18	0.25
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	18	0.25
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	9	0.25
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	7	0.25
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	7	0.25
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	7	0.25
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	6	0.25
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	6	0.25
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	6	0.25
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	6	0.25
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	3	0.24
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	6	0.24
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	3	0.24
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	4	0.24
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	5	0.24
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	18	0.24
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	11	0.24
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	13	0.24
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	16	0.24
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	11	0.24
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	9	0.24
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	1	0.24
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	13	0.24
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	1	0.24
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	11	0.24
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	11	0.24
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	11	0.24
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	11	0.24
(1,1328)	1:255:C:LEU:H	1:255:C:LEU:HG	7	0.24
(1,1066)	1:226:C:LEU:HD11	1:227:C:LYS:H	16	0.24
(1,1066)	1:226:C:LEU:HD12	1:227:C:LYS:H	16	0.24
(1,1066)	1:226:C:LEU:HD13	1:227:C:LYS:H	16	0.24
(1,1066)	1:226:C:LEU:HD21	1:227:C:LYS:H	16	0.24
(1,1066)	1:226:C:LEU:HD22	1:227:C:LYS:H	16	0.24
(1,1066)	1:226:C:LEU:HD23	1:227:C:LYS:H	16	0.24
(1,814)	2:125:B:LYS:H	2:125:B:LYS:HD2	9	0.24
(1,814)	2:125:B:LYS:H	2:125:B:LYS:HD3	9	0.24
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	19	0.24
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	19	0.24
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	19	0.24
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD1	4	0.24
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD2	4	0.24
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD1	4	0.24
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD2	4	0.24
(3,37)	1:240:C:ALA:O	1:249:C:VAL:H	10	0.23
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	20	0.23
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	3	0.23
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	5	0.23
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	12	0.23
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	19	0.23
(3,29)	1:227:C:LYS:H	1:239:C:VAL:O	5	0.23
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	1	0.23
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	11	0.23
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	14	0.23
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	7	0.23
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	5	0.23
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	9	0.23
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	16	0.23
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	11	0.23
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	15	0.23
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	10	0.23
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	16	0.23
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	2	0.23
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	11	0.23
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	20	0.23
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	20	0.23
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD2	15	0.23
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD3	15	0.23
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD2	15	0.23
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD3	15	0.23
(1,1328)	1:255:C:LEU:H	1:255:C:LEU:HG	16	0.23
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE1	14	0.23
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE2	14	0.23
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE1	14	0.23
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE2	14	0.23
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE1	14	0.23
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE2	14	0.23
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE1	3	0.23
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE2	3	0.23
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE1	3	0.23
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE2	3	0.23
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	5	0.23
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	5	0.23
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	9	0.23
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	9	0.23
(1,1040)	1:224:C:LYS:HE2	1:241:C:ARG:H	1	0.23
(1,1040)	1:224:C:LYS:HE3	1:241:C:ARG:H	1	0.23
(1,1040)	1:224:C:LYS:HE2	1:241:C:ARG:H	16	0.23
(1,1040)	1:224:C:LYS:HE3	1:241:C:ARG:H	16	0.23
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	7	0.23
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	7	0.23
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	7	0.23
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	7	0.23
(1,750)	2:106:B:ILE:HD11	2:107:B:TYR:H	15	0.23
(1,750)	2:106:B:ILE:HD12	2:107:B:TYR:H	15	0.23
(1,750)	2:106:B:ILE:HD13	2:107:B:TYR:H	15	0.23
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	4	0.23
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	4	0.23
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	4	0.23
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	4	0.23
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	4	0.23
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	4	0.23
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	4	0.23
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	4	0.23
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	4	0.23
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	4	0.23
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	4	0.23
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD1	8	0.23
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD2	8	0.23
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD1	8	0.23
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD2	8	0.23
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	8	0.23
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	8	0.23
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	8	0.23
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	8	0.23
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	8	0.23
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	8	0.23
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	6	0.23
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	6	0.23
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG21	2	0.23
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG22	2	0.23
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG23	2	0.23
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	2	0.22
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	10	0.22
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	19	0.22
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	17	0.22
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	1	0.22
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	5	0.22
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	9	0.22
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	20	0.22
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	4	0.22
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	7	0.22
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	3	0.22
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	4	0.22
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	12	0.22
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	6	0.22
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	2	0.22
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	9	0.22
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD2	3	0.22
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD3	3	0.22
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD2	3	0.22
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD3	3	0.22
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	19	0.22
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	19	0.22
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	19	0.22
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	19	0.22
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	19	0.22
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	19	0.22
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	19	0.22
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	19	0.22
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	19	0.22
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	19	0.22
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	19	0.22
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	1	0.22
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	1	0.22
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	1	0.22
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	1	0.22
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	13	0.22
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	13	0.22
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	13	0.22
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	13	0.22
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	15	0.22
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	15	0.22
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	15	0.22
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	15	0.22
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	12	0.22
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	12	0.22
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	12	0.22
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	12	0.22
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	12	0.22
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	12	0.22
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	12	0.22
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	12	0.22
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	12	0.22
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	12	0.22
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	12	0.22
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	12	0.22
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	15	0.22
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	15	0.22
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	15	0.22
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	9	0.22
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	9	0.22
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	9	0.22
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	9	0.22
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	9	0.22
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	9	0.22
(1,215)	1:26:A:LEU:HD11	1:27:A:LYS:H	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:26:A:LEU:HD12	1:27:A:LYS:H	16	0.22
(1,215)	1:26:A:LEU:HD13	1:27:A:LYS:H	16	0.22
(1,215)	1:26:A:LEU:HD21	1:27:A:LYS:H	16	0.22
(1,215)	1:26:A:LEU:HD22	1:27:A:LYS:H	16	0.22
(1,215)	1:26:A:LEU:HD23	1:27:A:LYS:H	16	0.22
(1,215)	1:26:A:LEU:HD11	1:27:A:LYS:H	20	0.22
(1,215)	1:26:A:LEU:HD12	1:27:A:LYS:H	20	0.22
(1,215)	1:26:A:LEU:HD13	1:27:A:LYS:H	20	0.22
(1,215)	1:26:A:LEU:HD21	1:27:A:LYS:H	20	0.22
(1,215)	1:26:A:LEU:HD22	1:27:A:LYS:H	20	0.22
(1,215)	1:26:A:LEU:HD23	1:27:A:LYS:H	20	0.22
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	4	0.22
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	4	0.22
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	8	0.21
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	9	0.21
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	13	0.21
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	18	0.21
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	19	0.21
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	4	0.21
(3,18)	1:38:A:ILE:O	1:51:A:ILE:H	7	0.21
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	10	0.21
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	11	0.21
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	12	0.21
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	8	0.21
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	18	0.21
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	9	0.21
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	18	0.21
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	12	0.21
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	12	0.21
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	12	0.21
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	12	0.21
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	15	0.21
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	15	0.21
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	15	0.21
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	15	0.21
(1,1519)	2:306:D:ILE:HD11	2:307:D:TYR:H	10	0.21
(1,1519)	2:306:D:ILE:HD12	2:307:D:TYR:H	10	0.21
(1,1519)	2:306:D:ILE:HD13	2:307:D:TYR:H	10	0.21
(1,1453)	1:264:C:LYS:HB3	1:265:C:CYS:H	20	0.21
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD1	4	0.21
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD2	4	0.21
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD1	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD2	4	0.21
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD1	4	0.21
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD2	4	0.21
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE1	15	0.21
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE2	15	0.21
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE1	15	0.21
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE2	15	0.21
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE1	15	0.21
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE2	15	0.21
(1,938)	1:215:C:GLU:HG2	2:323:D:SER:HA	8	0.21
(1,938)	1:215:C:GLU:HG3	2:323:D:SER:HA	8	0.21
(1,814)	2:125:B:LYS:H	2:125:B:LYS:HD2	17	0.21
(1,814)	2:125:B:LYS:H	2:125:B:LYS:HD3	17	0.21
(1,713)	1:67:A:ASN:HB2	1:68:A:LYS:H	19	0.21
(1,713)	1:67:A:ASN:HB3	1:68:A:LYS:H	19	0.21
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	13	0.21
(1,552)	1:57:A:TRP:H	1:57:A:TRP:HE1	10	0.21
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	5	0.21
(1,332)	1:37:A:GLN:HE21	1:53:A:PRO:HG3	14	0.21
(1,332)	1:37:A:GLN:HE22	1:53:A:PRO:HG3	14	0.21
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	3	0.21
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	3	0.21
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	3	0.21
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	3	0.21
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE2	18	0.21
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE3	18	0.21
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	5	0.21
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	5	0.21
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	9	0.21
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	9	0.21
(1,167)	1:24:A:LYS:HE2	1:41:A:ARG:H	16	0.21
(1,167)	1:24:A:LYS:HE3	1:41:A:ARG:H	16	0.21
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE1	7	0.21
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE2	7	0.21
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE1	7	0.21
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE2	7	0.21
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	19	0.2
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	20	0.2
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	20	0.2
(3,32)	1:227:C:LYS:O	1:239:C:VAL:N	19	0.2
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	18	0.2
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,22)	1:40:A:ALA:O	1:49:A:VAL:H	7	0.2
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	12	0.2
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	13	0.2
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	20	0.2
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	5	0.2
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	19	0.2
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	18	0.2
(3,12)	1:27:A:LYS:O	1:39:A:VAL:N	3	0.2
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	2	0.2
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	16	0.2
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	20	0.2
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	7	0.2
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	20	0.2
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	12	0.2
(1,1602)	2:328:D:ALA:HA	2:329:D:PHE:H	4	0.2
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD2	12	0.2
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD3	12	0.2
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD2	12	0.2
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD3	12	0.2
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	9	0.2
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	9	0.2
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	9	0.2
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	9	0.2
(1,1519)	2:306:D:ILE:HD11	2:307:D:TYR:H	11	0.2
(1,1519)	2:306:D:ILE:HD12	2:307:D:TYR:H	11	0.2
(1,1519)	2:306:D:ILE:HD13	2:307:D:TYR:H	11	0.2
(1,1328)	1:255:C:LEU:H	1:255:C:LEU:HG	4	0.2
(1,1132)	1:231:C:THR:HG21	2:314:D:GLU:HB2	8	0.2
(1,1132)	1:231:C:THR:HG22	2:314:D:GLU:HB2	8	0.2
(1,1132)	1:231:C:THR:HG23	2:314:D:GLU:HB2	8	0.2
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	6	0.2
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	6	0.2
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	20	0.2
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	20	0.2
(1,882)	1:210:C:PRO:HA	2:312:D:TYR:HE1	20	0.2
(1,882)	1:210:C:PRO:HA	2:312:D:TYR:HE2	20	0.2
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	17	0.2
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	17	0.2
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	17	0.2
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	17	0.2
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	7	0.2
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	20	0.2
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	20	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	3	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	3	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	3	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	3	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	3	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	3	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	3	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	3	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	3	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	3	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	3	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	3	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	4	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	4	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	4	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	4	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	4	0.2
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	4	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	4	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	4	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	4	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	4	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	4	0.2
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	4	0.2
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	6	0.2
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	6	0.2
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	6	0.2
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	6	0.2
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	6	0.2
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	6	0.2
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	6	0.2
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	6	0.2
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	6	0.2
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	6	0.2
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	6	0.2
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	6	0.2
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	17	0.2
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	17	0.2
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	17	0.2
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	17	0.2
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	17	0.2
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	17	0.2
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	17	0.2
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	17	0.2
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	17	0.2
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	17	0.2
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	17	0.2
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	14	0.2
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	15	0.2
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	14	0.2
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	14	0.2
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	14	0.2
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	17	0.2
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	17	0.2
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	17	0.2
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE2	7	0.2
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE3	7	0.2
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	8	0.2
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	8	0.2
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	12	0.2
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	12	0.2
(1,136)	1:22:A:ASN:HD21	1:42:A:LEU:HB2	20	0.2
(1,136)	1:22:A:ASN:HD22	1:42:A:LEU:HB2	20	0.2
(1,115)	1:20:A:ARG:HD2	1:23:A:VAL:H	17	0.2
(1,115)	1:20:A:ARG:HD3	1:23:A:VAL:H	17	0.2
(1,114)	1:20:A:ARG:HB2	1:57:A:TRP:HH2	6	0.2
(1,114)	1:20:A:ARG:HB3	1:57:A:TRP:HH2	6	0.2
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	15	0.19
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	10	0.19
(3,33)	1:238:C:ILE:O	1:251:C:ILE:H	4	0.19
(3,29)	1:227:C:LYS:H	1:239:C:VAL:O	9	0.19
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	4	0.19
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	16	0.19
(3,22)	1:40:A:ALA:O	1:49:A:VAL:H	16	0.19
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	18	0.19
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	5	0.19
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	7	0.19
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	10	0.19
(3,9)	1:27:A:LYS:H	1:39:A:VAL:O	6	0.19
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	1	0.19
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	16	0.19
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	18	0.19
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	16	0.19
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	7	0.19
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	7	0.19
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	7	0.19
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	7	0.19
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	10	0.19
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	10	0.19
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	10	0.19
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	10	0.19
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	11	0.19
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	11	0.19
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	11	0.19
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	11	0.19
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	16	0.19
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	16	0.19
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	16	0.19
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	16	0.19
(1,1527)	2:306:D:ILE:HG21	2:307:D:TYR:HE1	11	0.19
(1,1527)	2:306:D:ILE:HG21	2:307:D:TYR:HE2	11	0.19
(1,1527)	2:306:D:ILE:HG22	2:307:D:TYR:HE1	11	0.19
(1,1527)	2:306:D:ILE:HG22	2:307:D:TYR:HE2	11	0.19
(1,1527)	2:306:D:ILE:HG23	2:307:D:TYR:HE1	11	0.19
(1,1527)	2:306:D:ILE:HG23	2:307:D:TYR:HE2	11	0.19
(1,1328)	1:255:C:LEU:H	1:255:C:LEU:HG	14	0.19
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	1	0.19
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	1	0.19
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	1	0.19
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	10	0.19
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	10	0.19
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	10	0.19
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	11	0.19
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	11	0.19
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	11	0.19
(1,1132)	1:231:C:THR:HG21	2:314:D:GLU:HB2	3	0.19
(1,1132)	1:231:C:THR:HG22	2:314:D:GLU:HB2	3	0.19
(1,1132)	1:231:C:THR:HG23	2:314:D:GLU:HB2	3	0.19
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD1	2	0.19
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD2	2	0.19
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD1	2	0.19
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD2	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	1	0.19
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	1	0.19
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	1	0.19
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	1	0.19
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	1	0.19
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	1	0.19
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	11	0.19
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	11	0.19
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	11	0.19
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	11	0.19
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	12	0.19
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	12	0.19
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	12	0.19
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	12	0.19
(1,867)	2:132:B:GLU:H	2:132:B:GLU:HG2	3	0.19
(1,867)	2:132:B:GLU:H	2:132:B:GLU:HG3	3	0.19
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD11	2	0.19
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD12	2	0.19
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD13	2	0.19
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD21	2	0.19
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD22	2	0.19
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD23	2	0.19
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD11	2	0.19
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD12	2	0.19
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD13	2	0.19
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD21	2	0.19
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD22	2	0.19
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD23	2	0.19
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	7	0.19
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	7	0.19
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	7	0.19
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	7	0.19
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	7	0.19
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	7	0.19
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	7	0.19
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	7	0.19
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	7	0.19
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	7	0.19
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	7	0.19
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	7	0.19
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE1	16	0.19
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE2	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	2:106:B:ILE:HD11	2:107:B:TYR:HE1	11	0.19
(1,752)	2:106:B:ILE:HD11	2:107:B:TYR:HE2	11	0.19
(1,752)	2:106:B:ILE:HD12	2:107:B:TYR:HE1	11	0.19
(1,752)	2:106:B:ILE:HD12	2:107:B:TYR:HE2	11	0.19
(1,752)	2:106:B:ILE:HD13	2:107:B:TYR:HE1	11	0.19
(1,752)	2:106:B:ILE:HD13	2:107:B:TYR:HE2	11	0.19
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD1	20	0.19
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD2	20	0.19
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD1	20	0.19
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD2	20	0.19
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD1	20	0.19
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD2	20	0.19
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD1	20	0.19
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD2	20	0.19
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD1	20	0.19
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD2	20	0.19
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD1	20	0.19
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD2	20	0.19
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	19	0.19
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	19	0.19
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	19	0.19
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	19	0.19
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	19	0.19
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	19	0.19
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	19	0.19
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	19	0.19
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	19	0.19
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	19	0.19
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	19	0.19
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	19	0.19
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	7	0.19
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	3	0.19
(1,62)	1:15:A:GLU:HG2	2:123:B:SER:HA	18	0.19
(1,62)	1:15:A:GLU:HG3	2:123:B:SER:HA	18	0.19
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE1	6	0.19
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE2	6	0.19
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	20	0.18
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	14	0.18
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	20	0.18
(3,29)	1:227:C:LYS:H	1:239:C:VAL:O	13	0.18
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	12	0.18
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	14	0.18
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	12	0.18
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	13	0.18
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	20	0.18
(3,16)	1:28:A:ILE:O	1:226:C:LEU:N	3	0.18
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	14	0.18
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	20	0.18
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	2	0.18
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	6	0.18
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	2	0.18
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	7	0.18
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	12	0.18
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	6	0.18
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	6	0.18
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	6	0.18
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	6	0.18
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	16	0.18
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	16	0.18
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	16	0.18
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	16	0.18
(1,1629)	2:332:D:GLU:H	2:332:D:GLU:HG2	3	0.18
(1,1629)	2:332:D:GLU:H	2:332:D:GLU:HG3	3	0.18
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE1	8	0.18
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE2	8	0.18
(1,1328)	1:255:C:LEU:H	1:255:C:LEU:HG	3	0.18
(1,1152)	1:237:C:GLN:HE21	1:253:C:PRO:HG3	9	0.18
(1,1152)	1:237:C:GLN:HE22	1:253:C:PRO:HG3	9	0.18
(1,1152)	1:237:C:GLN:HE21	1:253:C:PRO:HG3	14	0.18
(1,1152)	1:237:C:GLN:HE22	1:253:C:PRO:HG3	14	0.18
(1,1138)	1:235:C:ALA:HB1	1:254:C:LYS:HD2	11	0.18
(1,1138)	1:235:C:ALA:HB1	1:254:C:LYS:HD3	11	0.18
(1,1138)	1:235:C:ALA:HB2	1:254:C:LYS:HD2	11	0.18
(1,1138)	1:235:C:ALA:HB2	1:254:C:LYS:HD3	11	0.18
(1,1138)	1:235:C:ALA:HB3	1:254:C:LYS:HD2	11	0.18
(1,1138)	1:235:C:ALA:HB3	1:254:C:LYS:HD3	11	0.18
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD1	15	0.18
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD2	15	0.18
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD1	15	0.18
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD2	15	0.18
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD1	15	0.18
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD2	15	0.18
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE1	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE2	17	0.18
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE1	17	0.18
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE2	17	0.18
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE1	19	0.18
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE2	19	0.18
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE1	19	0.18
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE2	19	0.18
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD1	10	0.18
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD2	10	0.18
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD1	10	0.18
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD2	10	0.18
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	5	0.18
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	5	0.18
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	5	0.18
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	5	0.18
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	5	0.18
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	5	0.18
(1,1051)	1:225:C:HIS:HE1	1:241:C:ARG:HB2	3	0.18
(1,1051)	1:225:C:HIS:HE1	1:241:C:ARG:HB3	3	0.18
(1,1050)	1:225:C:HIS:HE1	1:227:C:LYS:HE2	18	0.18
(1,1050)	1:225:C:HIS:HE1	1:227:C:LYS:HE3	18	0.18
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	8	0.18
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	8	0.18
(1,938)	1:215:C:GLU:HG2	2:323:D:SER:HA	17	0.18
(1,938)	1:215:C:GLU:HG3	2:323:D:SER:HA	17	0.18
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	6	0.18
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	6	0.18
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	6	0.18
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	6	0.18
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	7	0.18
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	7	0.18
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	7	0.18
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	7	0.18
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	16	0.18
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	16	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	5	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	5	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	5	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	5	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	5	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	5	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	5	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	5	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	5	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	5	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	5	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	12	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	12	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	12	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	12	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	12	0.18
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	12	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	12	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	12	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	12	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	12	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	12	0.18
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	12	0.18
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	6	0.18
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	6	0.18
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	6	0.18
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	6	0.18
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	9	0.18
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	9	0.18
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	9	0.18
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	9	0.18
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	16	0.18
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	16	0.18
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	16	0.18
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	16	0.18
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	16	0.18
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	16	0.18
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	16	0.18
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	16	0.18
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	16	0.18
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	16	0.18
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	16	0.18
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	16	0.18
(1,411)	1:43:A:LYS:H	1:43:A:LYS:HD3	6	0.18
(1,332)	1:37:A:GLN:HE21	1:53:A:PRO:HG3	1	0.18
(1,332)	1:37:A:GLN:HE22	1:53:A:PRO:HG3	1	0.18
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	18	0.18
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	18	0.18
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	14	0.18
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	14	0.18
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	14	0.18
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	14	0.18
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	14	0.18
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	14	0.18
(1,167)	1:24:A:LYS:HE2	1:41:A:ARG:H	17	0.18
(1,167)	1:24:A:LYS:HE3	1:41:A:ARG:H	17	0.18
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG11	8	0.18
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG12	8	0.18
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG13	8	0.18
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG21	8	0.18
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG22	8	0.18
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG23	8	0.18
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	5	0.17
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	9	0.17
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	16	0.17
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	4	0.17
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	2	0.17
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	16	0.17
(3,22)	1:40:A:ALA:O	1:49:A:VAL:H	9	0.17
(3,11)	1:27:A:LYS:O	1:39:A:VAL:H	3	0.17
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	20	0.17
(2,18)	1:211:C:CYS:SG	1:250:C:CYS:CB	3	0.17
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	9	0.17
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	13	0.17
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	15	0.17
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	1	0.17
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	1	0.17
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	1	0.17
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	1	0.17
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	12	0.17
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	12	0.17
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	5	0.17
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	5	0.17
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	5	0.17
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	5	0.17
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE1	10	0.17
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE2	10	0.17
(1,1553)	2:315:D:GLU:H	2:315:D:GLU:HG2	12	0.17
(1,1553)	2:315:D:GLU:H	2:315:D:GLU:HG3	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1367)	1:256:C:LYS:HD2	1:257:C:TRP:H	2	0.17
(1,1367)	1:256:C:LYS:HD3	1:257:C:TRP:H	2	0.17
(1,1328)	1:255:C:LEU:H	1:255:C:LEU:HG	11	0.17
(1,1328)	1:255:C:LEU:H	1:255:C:LEU:HG	17	0.17
(1,1219)	1:242:C:LEU:HB3	1:247:C:ARG:H	13	0.17
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD1	5	0.17
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD2	5	0.17
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD1	5	0.17
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD2	5	0.17
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD1	5	0.17
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD2	5	0.17
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD1	9	0.17
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD2	9	0.17
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD1	9	0.17
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD2	9	0.17
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD1	9	0.17
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD2	9	0.17
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE1	16	0.17
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE2	16	0.17
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE1	16	0.17
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE2	16	0.17
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE1	16	0.17
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE2	16	0.17
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE1	4	0.17
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE2	4	0.17
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE1	4	0.17
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE2	4	0.17
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	13	0.17
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	13	0.17
(1,1040)	1:224:C:LYS:HE2	1:241:C:ARG:H	4	0.17
(1,1040)	1:224:C:LYS:HE3	1:241:C:ARG:H	4	0.17
(1,1040)	1:224:C:LYS:HE2	1:241:C:ARG:H	15	0.17
(1,1040)	1:224:C:LYS:HE3	1:241:C:ARG:H	15	0.17
(1,1015)	1:223:C:VAL:HB	1:242:C:LEU:H	11	0.17
(1,1010)	1:222:C:ASN:HB3	1:223:C:VAL:H	8	0.17
(1,966)	1:218:C:VAL:HG11	1:252:C:ASP:H	20	0.17
(1,966)	1:218:C:VAL:HG12	1:252:C:ASP:H	20	0.17
(1,966)	1:218:C:VAL:HG13	1:252:C:ASP:H	20	0.17
(1,966)	1:218:C:VAL:HG21	1:252:C:ASP:H	20	0.17
(1,966)	1:218:C:VAL:HG22	1:252:C:ASP:H	20	0.17
(1,966)	1:218:C:VAL:HG23	1:252:C:ASP:H	20	0.17
(1,882)	1:210:C:PRO:HA	2:312:D:TYR:HE1	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,882)	1:210:C:PRO:HA	2:312:D:TYR:HE2	19	0.17
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	3	0.17
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	3	0.17
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	16	0.17
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	16	0.17
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	16	0.17
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	16	0.17
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	16	0.17
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	16	0.17
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	16	0.17
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	16	0.17
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	16	0.17
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	16	0.17
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	16	0.17
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	16	0.17
(1,783)	2:114:B:GLU:HA	2:114:B:GLU:HG2	12	0.17
(1,783)	2:114:B:GLU:HA	2:114:B:GLU:HG3	12	0.17
(1,752)	2:106:B:ILE:HD11	2:107:B:TYR:HE1	9	0.17
(1,752)	2:106:B:ILE:HD11	2:107:B:TYR:HE2	9	0.17
(1,752)	2:106:B:ILE:HD12	2:107:B:TYR:HE1	9	0.17
(1,752)	2:106:B:ILE:HD12	2:107:B:TYR:HE2	9	0.17
(1,752)	2:106:B:ILE:HD13	2:107:B:TYR:HE1	9	0.17
(1,752)	2:106:B:ILE:HD13	2:107:B:TYR:HE2	9	0.17
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	16	0.17
(1,411)	1:43:A:LYS:H	1:43:A:LYS:HD3	15	0.17
(1,399)	1:42:A:LEU:HB3	1:47:A:ARG:H	6	0.17
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	10	0.17
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	10	0.17
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	10	0.17
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	12	0.17
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	12	0.17
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	12	0.17
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD1	10	0.17
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD2	10	0.17
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD1	10	0.17
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD2	10	0.17
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	16	0.17
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	16	0.17
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	16	0.17
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	16	0.17
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	16	0.17
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	18	0.17
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	18	0.17
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	18	0.17
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	18	0.17
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	18	0.17
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	18	0.17
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	20	0.17
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	20	0.17
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	20	0.17
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	20	0.17
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	20	0.17
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	20	0.17
(1,215)	1:26:A:LEU:HD11	1:27:A:LYS:H	15	0.17
(1,215)	1:26:A:LEU:HD12	1:27:A:LYS:H	15	0.17
(1,215)	1:26:A:LEU:HD13	1:27:A:LYS:H	15	0.17
(1,215)	1:26:A:LEU:HD21	1:27:A:LYS:H	15	0.17
(1,215)	1:26:A:LEU:HD22	1:27:A:LYS:H	15	0.17
(1,215)	1:26:A:LEU:HD23	1:27:A:LYS:H	15	0.17
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	18	0.17
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	18	0.17
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	9	0.16
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	12	0.16
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	17	0.16
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	18	0.16
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	9	0.16
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	15	0.16
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	4	0.16
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	8	0.16
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	8	0.16
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	8	0.16
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	13	0.16
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	11	0.16
(2,6)	1:11:A:CYS:SG	1:50:A:CYS:CB	3	0.16
(2,4)	1:11:A:CYS:CB	1:50:A:CYS:CB	1	0.16
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	6	0.16
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	6	0.16
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	19	0.16
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	19	0.16
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	6	0.16
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	6	0.16
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	6	0.16
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE1	13	0.16
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE2	13	0.16
(1,1549)	2:314:D:GLU:HA	2:314:D:GLU:HG2	10	0.16
(1,1549)	2:314:D:GLU:HA	2:314:D:GLU:HG3	10	0.16
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	5	0.16
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	7	0.16
(1,1152)	1:237:C:GLN:HE21	1:253:C:PRO:HG3	1	0.16
(1,1152)	1:237:C:GLN:HE22	1:253:C:PRO:HG3	1	0.16
(1,1152)	1:237:C:GLN:HE21	1:253:C:PRO:HG3	2	0.16
(1,1152)	1:237:C:GLN:HE22	1:253:C:PRO:HG3	2	0.16
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	14	0.16
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	14	0.16
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	14	0.16
(1,1132)	1:231:C:THR:HG21	2:314:D:GLU:HB2	18	0.16
(1,1132)	1:231:C:THR:HG22	2:314:D:GLU:HB2	18	0.16
(1,1132)	1:231:C:THR:HG23	2:314:D:GLU:HB2	18	0.16
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD1	7	0.16
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD2	7	0.16
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD1	7	0.16
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD2	7	0.16
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD1	7	0.16
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD2	7	0.16
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE1	10	0.16
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE2	10	0.16
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE1	10	0.16
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE2	10	0.16
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE1	10	0.16
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE2	10	0.16
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD1	16	0.16
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD2	16	0.16
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD1	16	0.16
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD2	16	0.16
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	12	0.16
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	12	0.16
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	12	0.16
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	12	0.16
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	12	0.16
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	12	0.16
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	17	0.16
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	17	0.16
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	17	0.16
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	17	0.16
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	17	0.16
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	2	0.16
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	2	0.16
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	15	0.16
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	15	0.16
(1,990)	1:220:C:ARG:HB2	1:257:C:TRP:HH2	6	0.16
(1,990)	1:220:C:ARG:HB3	1:257:C:TRP:HH2	6	0.16
(1,966)	1:218:C:VAL:HG11	1:252:C:ASP:H	2	0.16
(1,966)	1:218:C:VAL:HG12	1:252:C:ASP:H	2	0.16
(1,966)	1:218:C:VAL:HG13	1:252:C:ASP:H	2	0.16
(1,966)	1:218:C:VAL:HG21	1:252:C:ASP:H	2	0.16
(1,966)	1:218:C:VAL:HG22	1:252:C:ASP:H	2	0.16
(1,966)	1:218:C:VAL:HG23	1:252:C:ASP:H	2	0.16
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	10	0.16
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	10	0.16
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	10	0.16
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	10	0.16
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	16	0.16
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	16	0.16
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	16	0.16
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	16	0.16
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD11	14	0.16
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD12	14	0.16
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD13	14	0.16
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD21	14	0.16
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD22	14	0.16
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD23	14	0.16
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD11	14	0.16
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD12	14	0.16
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD13	14	0.16
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD21	14	0.16
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD22	14	0.16
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD23	14	0.16
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	18	0.16
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	18	0.16
(1,839)	2:128:B:ALA:HA	2:129:B:PHE:H	4	0.16
(1,839)	2:128:B:ALA:HA	2:129:B:PHE:H	5	0.16
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	15	0.16
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	15	0.16
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	15	0.16
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	15	0.16
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	15	0.16
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	15	0.16
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	15	0.16
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	15	0.16
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	15	0.16
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	15	0.16
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	15	0.16
(1,824)	2:125:B:LYS:HB2	2:125:B:LYS:HD2	3	0.16
(1,824)	2:125:B:LYS:HB2	2:125:B:LYS:HD3	3	0.16
(1,824)	2:125:B:LYS:HB3	2:125:B:LYS:HD2	3	0.16
(1,824)	2:125:B:LYS:HB3	2:125:B:LYS:HD3	3	0.16
(1,824)	2:125:B:LYS:HB2	2:125:B:LYS:HD2	20	0.16
(1,824)	2:125:B:LYS:HB2	2:125:B:LYS:HD3	20	0.16
(1,824)	2:125:B:LYS:HB3	2:125:B:LYS:HD2	20	0.16
(1,824)	2:125:B:LYS:HB3	2:125:B:LYS:HD3	20	0.16
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	2	0.16
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	2	0.16
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	2	0.16
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	2	0.16
(1,746)	2:106:B:ILE:HA	2:107:B:TYR:H	10	0.16
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	17	0.16
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	14	0.16
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	14	0.16
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	14	0.16
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	14	0.16
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	14	0.16
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	14	0.16
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	14	0.16
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	14	0.16
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	14	0.16
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	14	0.16
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	14	0.16
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	14	0.16
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	3	0.16
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	4	0.16
(1,411)	1:43:A:LYS:H	1:43:A:LYS:HD3	8	0.16
(1,386)	1:41:A:ARG:HD2	1:42:A:LEU:H	11	0.16
(1,386)	1:41:A:ARG:HD3	1:42:A:LEU:H	11	0.16
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	6	0.16
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	6	0.16
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:31:A:THR:HG21	2:114:B:GLU:HB2	6	0.16
(1,309)	1:31:A:THR:HG22	2:114:B:GLU:HB2	6	0.16
(1,309)	1:31:A:THR:HG23	2:114:B:GLU:HB2	6	0.16
(1,309)	1:31:A:THR:HG21	2:114:B:GLU:HB2	18	0.16
(1,309)	1:31:A:THR:HG22	2:114:B:GLU:HB2	18	0.16
(1,309)	1:31:A:THR:HG23	2:114:B:GLU:HB2	18	0.16
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	19	0.16
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	19	0.16
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	19	0.16
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	19	0.16
(1,189)	1:25:A:HIS:HE1	1:41:A:ARG:HD2	8	0.16
(1,189)	1:25:A:HIS:HE1	1:41:A:ARG:HD3	8	0.16
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE2	8	0.16
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE3	8	0.16
(1,62)	1:15:A:GLU:HG2	2:123:B:SER:HA	16	0.16
(1,62)	1:15:A:GLU:HG3	2:123:B:SER:HA	16	0.16
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG21	3	0.16
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG22	3	0.16
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG23	3	0.16
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	2	0.15
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	18	0.15
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	2	0.15
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	16	0.15
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	6	0.15
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	11	0.15
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	4	0.15
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	12	0.15
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	17	0.15
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	7	0.15
(2,16)	1:211:C:CYS:CB	1:250:C:CYS:CB	3	0.15
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	13	0.15
(2,5)	1:11:A:CYS:CB	1:50:A:CYS:SG	19	0.15
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	18	0.15
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	2	0.15
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	2	0.15
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	2	0.15
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	2	0.15
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	14	0.15
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	14	0.15
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	14	0.15
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	14	0.15
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	18	0.15
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	18	0.15
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	18	0.15
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	20	0.15
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	20	0.15
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	20	0.15
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	20	0.15
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	3	0.15
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	3	0.15
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	15	0.15
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	15	0.15
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	16	0.15
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	16	0.15
(1,1602)	2:328:D:ALA:HA	2:329:D:PHE:H	19	0.15
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	3	0.15
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	3	0.15
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	3	0.15
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	3	0.15
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	12	0.15
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	12	0.15
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	12	0.15
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	12	0.15
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE1	3	0.15
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE2	3	0.15
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE1	18	0.15
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE2	18	0.15
(1,1453)	1:264:C:LYS:HB3	1:265:C:CYS:H	5	0.15
(1,1453)	1:264:C:LYS:HB3	1:265:C:CYS:H	7	0.15
(1,1451)	1:264:C:LYS:HB2	1:265:C:CYS:H	16	0.15
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	15	0.15
(1,1367)	1:256:C:LYS:HD2	1:257:C:TRP:H	7	0.15
(1,1367)	1:256:C:LYS:HD3	1:257:C:TRP:H	7	0.15
(1,1328)	1:255:C:LEU:H	1:255:C:LEU:HG	15	0.15
(1,1295)	1:252:C:ASP:HB2	1:255:C:LEU:H	10	0.15
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	8	0.15
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	9	0.15
(1,1206)	1:241:C:ARG:HD2	1:242:C:LEU:H	11	0.15
(1,1206)	1:241:C:ARG:HD3	1:242:C:LEU:H	11	0.15
(1,1152)	1:237:C:GLN:HE21	1:253:C:PRO:HG3	15	0.15
(1,1152)	1:237:C:GLN:HE22	1:253:C:PRO:HG3	15	0.15
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	13	0.15
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	13	0.15
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	20	0.15
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	20	0.15
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	20	0.15
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD1	2	0.15
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD2	2	0.15
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD1	2	0.15
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD2	2	0.15
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD1	2	0.15
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD2	2	0.15
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	6	0.15
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	6	0.15
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	6	0.15
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	6	0.15
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	6	0.15
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	6	0.15
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	16	0.15
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	16	0.15
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	16	0.15
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	16	0.15
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	16	0.15
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	16	0.15
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	20	0.15
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	20	0.15
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	20	0.15
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	20	0.15
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	20	0.15
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	20	0.15
(1,1066)	1:226:C:LEU:HD11	1:227:C:LYS:H	15	0.15
(1,1066)	1:226:C:LEU:HD12	1:227:C:LYS:H	15	0.15
(1,1066)	1:226:C:LEU:HD13	1:227:C:LYS:H	15	0.15
(1,1066)	1:226:C:LEU:HD21	1:227:C:LYS:H	15	0.15
(1,1066)	1:226:C:LEU:HD22	1:227:C:LYS:H	15	0.15
(1,1066)	1:226:C:LEU:HD23	1:227:C:LYS:H	15	0.15
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	18	0.15
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	18	0.15
(1,1040)	1:224:C:LYS:HE2	1:241:C:ARG:H	7	0.15
(1,1040)	1:224:C:LYS:HE3	1:241:C:ARG:H	7	0.15
(1,1040)	1:224:C:LYS:HE2	1:241:C:ARG:H	18	0.15
(1,1040)	1:224:C:LYS:HE3	1:241:C:ARG:H	18	0.15
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	4	0.15
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	4	0.15
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	4	0.15
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	9	0.15
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	9	0.15
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	9	0.15
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	9	0.15
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	14	0.15
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	14	0.15
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	14	0.15
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	14	0.15
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	8	0.15
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	8	0.15
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	11	0.15
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	11	0.15
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	12	0.15
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	12	0.15
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	15	0.15
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	15	0.15
(1,783)	2:114:B:GLU:HA	2:114:B:GLU:HG2	4	0.15
(1,783)	2:114:B:GLU:HA	2:114:B:GLU:HG3	4	0.15
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	20	0.15
(1,552)	1:57:A:TRP:H	1:57:A:TRP:HE1	6	0.15
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	7	0.15
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	11	0.15
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	16	0.15
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	17	0.15
(1,426)	1:47:A:ARG:H	1:47:A:ARG:HG2	9	0.15
(1,426)	1:47:A:ARG:H	1:47:A:ARG:HG3	9	0.15
(1,414)	1:43:A:LYS:H	1:43:A:LYS:HE2	20	0.15
(1,414)	1:43:A:LYS:H	1:43:A:LYS:HE3	20	0.15
(1,411)	1:43:A:LYS:H	1:43:A:LYS:HD3	2	0.15
(1,411)	1:43:A:LYS:H	1:43:A:LYS:HD3	10	0.15
(1,386)	1:41:A:ARG:HD2	1:42:A:LEU:H	12	0.15
(1,386)	1:41:A:ARG:HD3	1:42:A:LEU:H	12	0.15
(1,386)	1:41:A:ARG:HD2	1:42:A:LEU:H	17	0.15
(1,386)	1:41:A:ARG:HD3	1:42:A:LEU:H	17	0.15
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	5	0.15
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	5	0.15
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	5	0.15
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	20	0.15
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	20	0.15
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD1	9	0.15
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD2	9	0.15
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD1	9	0.15
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD2	9	0.15
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD1	9	0.15
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD2	9	0.15
(1,293)	1:29:A:LEU:HD11	1:225:C:HIS:HE1	3	0.15
(1,293)	1:29:A:LEU:HD12	1:225:C:HIS:HE1	3	0.15
(1,293)	1:29:A:LEU:HD13	1:225:C:HIS:HE1	3	0.15
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	7	0.15
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	7	0.15
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	7	0.15
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	7	0.15
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	15	0.15
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	15	0.15
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	15	0.15
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	15	0.15
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD1	9	0.15
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD2	9	0.15
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD1	9	0.15
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD2	9	0.15
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD1	18	0.15
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD2	18	0.15
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD1	18	0.15
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD2	18	0.15
(1,252)	1:27:A:LYS:HE2	1:225:C:HIS:HE1	6	0.15
(1,252)	1:27:A:LYS:HE3	1:225:C:HIS:HE1	6	0.15
(1,252)	1:27:A:LYS:HE2	1:225:C:HIS:HE1	17	0.15
(1,252)	1:27:A:LYS:HE3	1:225:C:HIS:HE1	17	0.15
(1,242)	1:27:A:LYS:HG2	2:112:B:TYR:HE1	3	0.15
(1,242)	1:27:A:LYS:HG2	2:112:B:TYR:HE2	3	0.15
(1,242)	1:27:A:LYS:HG2	2:112:B:TYR:HE1	19	0.15
(1,242)	1:27:A:LYS:HG2	2:112:B:TYR:HE2	19	0.15
(1,239)	1:27:A:LYS:HD3	2:112:B:TYR:HD1	6	0.15
(1,239)	1:27:A:LYS:HD3	2:112:B:TYR:HD2	6	0.15
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	5	0.15
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	5	0.15
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	5	0.15
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	5	0.15
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	5	0.15
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	5	0.15
(1,190)	1:25:A:HIS:HE1	1:41:A:ARG:HG2	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:25:A:HIS:HE1	1:41:A:ARG:HG3	19	0.15
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE2	2	0.15
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE3	2	0.15
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	10	0.15
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	10	0.15
(1,167)	1:24:A:LYS:HE2	1:41:A:ARG:H	1	0.15
(1,167)	1:24:A:LYS:HE3	1:41:A:ARG:H	1	0.15
(1,139)	1:23:A:VAL:HB	1:42:A:LEU:H	11	0.15
(1,86)	1:18:A:VAL:HG23	2:121:B:TYS:HD1	12	0.15
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG21	7	0.15
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG22	7	0.15
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG23	7	0.15
(1,14)	1:10:A:PRO:HB3	1:11:A:CYS:H	1	0.15
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE1	15	0.15
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE2	15	0.15
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	12	0.14
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	12	0.14
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	17	0.14
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	18	0.14
(3,31)	1:227:C:LYS:O	1:239:C:VAL:H	19	0.14
(3,29)	1:227:C:LYS:H	1:239:C:VAL:O	1	0.14
(3,22)	1:40:A:ALA:O	1:49:A:VAL:H	13	0.14
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	7	0.14
(3,14)	1:28:A:ILE:N	1:226:C:LEU:O	15	0.14
(3,13)	1:28:A:ILE:H	1:226:C:LEU:O	19	0.14
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	9	0.14
(3,8)	1:26:A:LEU:O	1:228:C:ILE:N	16	0.14
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	8	0.14
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	4	0.14
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	15	0.14
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	9	0.14
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	9	0.14
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	9	0.14
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	9	0.14
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	15	0.14
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	15	0.14
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	15	0.14
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	15	0.14
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE1	10	0.14
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE2	10	0.14
(1,1602)	2:328:D:ALA:HA	2:329:D:PHE:H	18	0.14
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD3	1	0.14
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD2	1	0.14
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD3	1	0.14
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD2	10	0.14
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD3	10	0.14
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD2	10	0.14
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD3	10	0.14
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD2	16	0.14
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD3	16	0.14
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD2	16	0.14
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD3	16	0.14
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	7	0.14
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	7	0.14
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	7	0.14
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	7	0.14
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	19	0.14
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	19	0.14
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	19	0.14
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	19	0.14
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	20	0.14
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	20	0.14
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	20	0.14
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	20	0.14
(1,1570)	2:321:D:TYS:H	2:321:D:TYS:HE1	12	0.14
(1,1570)	2:321:D:TYS:H	2:321:D:TYS:HE2	12	0.14
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE1	4	0.14
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE2	4	0.14
(1,1515)	2:306:D:ILE:HA	2:307:D:TYR:H	9	0.14
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	4	0.14
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	10	0.14
(1,1453)	1:264:C:LYS:HB3	1:265:C:CYS:H	15	0.14
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	20	0.14
(1,1372)	1:257:C:TRP:H	1:257:C:TRP:HE1	3	0.14
(1,1372)	1:257:C:TRP:H	1:257:C:TRP:HE1	4	0.14
(1,1372)	1:257:C:TRP:H	1:257:C:TRP:HE1	7	0.14
(1,1367)	1:256:C:LYS:HD2	1:257:C:TRP:H	14	0.14
(1,1367)	1:256:C:LYS:HD3	1:257:C:TRP:H	14	0.14
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	10	0.14
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	16	0.14
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	18	0.14
(1,1219)	1:242:C:LEU:HB3	1:247:C:ARG:H	9	0.14
(1,1162)	1:238:C:ILE:HB	1:239:C:VAL:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:237:C:GLN:H	1:253:C:PRO:HG3	9	0.14
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	2	0.14
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	2	0.14
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	2	0.14
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	8	0.14
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	8	0.14
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	8	0.14
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	15	0.14
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	15	0.14
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	15	0.14
(1,1132)	1:231:C:THR:HG21	2:314:D:GLU:HB2	11	0.14
(1,1132)	1:231:C:THR:HG22	2:314:D:GLU:HB2	11	0.14
(1,1132)	1:231:C:THR:HG23	2:314:D:GLU:HB2	11	0.14
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE1	17	0.14
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE2	17	0.14
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE1	17	0.14
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE2	17	0.14
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE1	17	0.14
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE2	17	0.14
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE1	1	0.14
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE2	1	0.14
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE1	1	0.14
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE2	1	0.14
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	9	0.14
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	9	0.14
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	9	0.14
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	9	0.14
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	9	0.14
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	9	0.14
(1,1040)	1:224:C:LYS:HE2	1:241:C:ARG:H	11	0.14
(1,1040)	1:224:C:LYS:HE3	1:241:C:ARG:H	11	0.14
(1,1036)	1:224:C:LYS:HB2	1:225:C:HIS:HE1	9	0.14
(1,1036)	1:224:C:LYS:HB3	1:225:C:HIS:HE1	9	0.14
(1,1015)	1:223:C:VAL:HB	1:242:C:LEU:H	17	0.14
(1,1012)	1:222:C:ASN:HD21	1:242:C:LEU:HB2	19	0.14
(1,1012)	1:222:C:ASN:HD22	1:242:C:LEU:HB2	19	0.14
(1,971)	1:218:C:VAL:HG21	2:321:D:TYS:HD1	3	0.14
(1,964)	1:218:C:VAL:HG11	1:222:C:ASN:HD21	13	0.14
(1,964)	1:218:C:VAL:HG11	1:222:C:ASN:HD22	13	0.14
(1,964)	1:218:C:VAL:HG12	1:222:C:ASN:HD21	13	0.14
(1,964)	1:218:C:VAL:HG12	1:222:C:ASN:HD22	13	0.14
(1,964)	1:218:C:VAL:HG13	1:222:C:ASN:HD21	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,964)	1:218:C:VAL:HG13	1:222:C:ASN:HD22	13	0.14
(1,964)	1:218:C:VAL:HG21	1:222:C:ASN:HD21	13	0.14
(1,964)	1:218:C:VAL:HG21	1:222:C:ASN:HD22	13	0.14
(1,964)	1:218:C:VAL:HG22	1:222:C:ASN:HD21	13	0.14
(1,964)	1:218:C:VAL:HG22	1:222:C:ASN:HD22	13	0.14
(1,964)	1:218:C:VAL:HG23	1:222:C:ASN:HD21	13	0.14
(1,964)	1:218:C:VAL:HG23	1:222:C:ASN:HD22	13	0.14
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG21	10	0.14
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG22	10	0.14
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG23	10	0.14
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG21	14	0.14
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG22	14	0.14
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG23	14	0.14
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG11	13	0.14
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG12	13	0.14
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG13	13	0.14
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG21	13	0.14
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG22	13	0.14
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG23	13	0.14
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	2	0.14
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	2	0.14
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	2	0.14
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	2	0.14
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	5	0.14
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	5	0.14
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	5	0.14
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	5	0.14
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	15	0.14
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	15	0.14
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	15	0.14
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	15	0.14
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD11	7	0.14
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD12	7	0.14
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD13	7	0.14
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD21	7	0.14
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD22	7	0.14
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD23	7	0.14
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD11	7	0.14
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD12	7	0.14
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD13	7	0.14
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD21	7	0.14
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD22	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD23	7	0.14
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	2	0.14
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	2	0.14
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	13	0.14
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	13	0.14
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	20	0.14
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	20	0.14
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	20	0.14
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	20	0.14
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	20	0.14
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	20	0.14
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	20	0.14
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	20	0.14
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	20	0.14
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	20	0.14
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	20	0.14
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	20	0.14
(1,814)	2:125:B:LYS:H	2:125:B:LYS:HD2	19	0.14
(1,814)	2:125:B:LYS:H	2:125:B:LYS:HD3	19	0.14
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	10	0.14
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	10	0.14
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	10	0.14
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	10	0.14
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	12	0.14
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	12	0.14
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	12	0.14
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	12	0.14
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE1	1	0.14
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE2	1	0.14
(1,783)	2:114:B:GLU:HA	2:114:B:GLU:HG2	15	0.14
(1,783)	2:114:B:GLU:HA	2:114:B:GLU:HG3	15	0.14
(1,746)	2:106:B:ILE:HA	2:107:B:TYR:H	13	0.14
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	4	0.14
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	9	0.14
(1,656)	1:64:A:LYS:HB2	1:65:A:CYS:H	6	0.14
(1,656)	1:64:A:LYS:HB2	1:65:A:CYS:H	14	0.14
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	3	0.14
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	12	0.14
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	20	0.14
(1,399)	1:42:A:LEU:HB3	1:47:A:ARG:H	3	0.14
(1,399)	1:42:A:LEU:HB3	1:47:A:ARG:H	5	0.14
(1,399)	1:42:A:LEU:HB3	1:47:A:ARG:H	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:42:A:LEU:HB2	1:47:A:ARG:H	16	0.14
(1,332)	1:37:A:GLN:HE21	1:53:A:PRO:HG3	2	0.14
(1,332)	1:37:A:GLN:HE22	1:53:A:PRO:HG3	2	0.14
(1,332)	1:37:A:GLN:HE21	1:53:A:PRO:HG3	18	0.14
(1,332)	1:37:A:GLN:HE22	1:53:A:PRO:HG3	18	0.14
(1,318)	1:35:A:ALA:HB1	1:54:A:LYS:HD2	16	0.14
(1,318)	1:35:A:ALA:HB1	1:54:A:LYS:HD3	16	0.14
(1,318)	1:35:A:ALA:HB2	1:54:A:LYS:HD2	16	0.14
(1,318)	1:35:A:ALA:HB2	1:54:A:LYS:HD3	16	0.14
(1,318)	1:35:A:ALA:HB3	1:54:A:LYS:HD2	16	0.14
(1,318)	1:35:A:ALA:HB3	1:54:A:LYS:HD3	16	0.14
(1,309)	1:31:A:THR:HG21	2:114:B:GLU:HB2	19	0.14
(1,309)	1:31:A:THR:HG22	2:114:B:GLU:HB2	19	0.14
(1,309)	1:31:A:THR:HG23	2:114:B:GLU:HB2	19	0.14
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	13	0.14
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	13	0.14
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	13	0.14
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	13	0.14
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	16	0.14
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	16	0.14
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	16	0.14
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	16	0.14
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	20	0.14
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	20	0.14
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	20	0.14
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	20	0.14
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD1	5	0.14
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD2	5	0.14
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD1	5	0.14
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD2	5	0.14
(1,252)	1:27:A:LYS:HE2	1:225:C:HIS:HE1	5	0.14
(1,252)	1:27:A:LYS:HE3	1:225:C:HIS:HE1	5	0.14
(1,242)	1:27:A:LYS:HG2	2:112:B:TYR:HE1	18	0.14
(1,242)	1:27:A:LYS:HG2	2:112:B:TYR:HE2	18	0.14
(1,241)	1:27:A:LYS:HD3	1:225:C:HIS:HE1	16	0.14
(1,238)	1:27:A:LYS:HD2	1:225:C:HIS:HE1	18	0.14
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	1	0.14
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	1	0.14
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	1	0.14
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	1	0.14
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	1	0.14
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	6	0.14
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	6	0.14
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	6	0.14
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	6	0.14
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	6	0.14
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	6	0.14
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE2	20	0.14
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE3	20	0.14
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	13	0.14
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	13	0.14
(1,114)	1:20:A:ARG:HB2	1:57:A:TRP:HH2	13	0.14
(1,114)	1:20:A:ARG:HB3	1:57:A:TRP:HH2	13	0.14
(1,91)	1:18:A:VAL:HG11	1:23:A:VAL:H	15	0.14
(1,91)	1:18:A:VAL:HG12	1:23:A:VAL:H	15	0.14
(1,91)	1:18:A:VAL:HG13	1:23:A:VAL:H	15	0.14
(1,91)	1:18:A:VAL:HG21	1:23:A:VAL:H	15	0.14
(1,91)	1:18:A:VAL:HG22	1:23:A:VAL:H	15	0.14
(1,91)	1:18:A:VAL:HG23	1:23:A:VAL:H	15	0.14
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG21	4	0.14
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG22	4	0.14
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG23	4	0.14
(1,7)	1:10:A:PRO:HB2	2:112:B:TYR:HD1	8	0.14
(1,7)	1:10:A:PRO:HB2	2:112:B:TYR:HD2	8	0.14
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE1	4	0.14
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE2	4	0.14
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	6	0.13
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	16	0.13
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	8	0.13
(3,35)	1:240:C:ALA:H	1:249:C:VAL:O	14	0.13
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	17	0.13
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	2	0.13
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	7	0.13
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	8	0.13
(3,20)	1:40:A:ALA:H	1:49:A:VAL:O	14	0.13
(3,15)	1:28:A:ILE:O	1:226:C:LEU:H	3	0.13
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	14	0.13
(3,6)	1:26:A:LEU:N	1:228:C:ILE:O	3	0.13
(3,3)	1:24:A:LYS:H	1:41:A:ARG:O	20	0.13
(2,17)	1:211:C:CYS:CB	1:250:C:CYS:SG	3	0.13
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	2	0.13
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	8	0.13
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:36:A:CYS:CB	1:265:C:CYS:CB	13	0.13
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE2	5	0.13
(1,1637)	2:338:D:LYS:HB2	2:338:D:LYS:HE3	5	0.13
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE2	5	0.13
(1,1637)	2:338:D:LYS:HB3	2:338:D:LYS:HE3	5	0.13
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	5	0.13
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	5	0.13
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	11	0.13
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	11	0.13
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	13	0.13
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	13	0.13
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	17	0.13
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	17	0.13
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	18	0.13
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	18	0.13
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE2	11	0.13
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE3	11	0.13
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE2	11	0.13
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE3	11	0.13
(1,1582)	2:325:D:LYS:HA	2:325:D:LYS:HD2	2	0.13
(1,1582)	2:325:D:LYS:HA	2:325:D:LYS:HD3	2	0.13
(1,1553)	2:315:D:GLU:H	2:315:D:GLU:HG2	16	0.13
(1,1553)	2:315:D:GLU:H	2:315:D:GLU:HG3	16	0.13
(1,1482)	1:267:C:ASN:HB2	1:268:C:LYS:H	6	0.13
(1,1482)	1:267:C:ASN:HB3	1:268:C:LYS:H	6	0.13
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	18	0.13
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	20	0.13
(1,1453)	1:264:C:LYS:HB3	1:265:C:CYS:H	17	0.13
(1,1451)	1:264:C:LYS:HB2	1:265:C:CYS:H	1	0.13
(1,1451)	1:264:C:LYS:HB2	1:265:C:CYS:H	4	0.13
(1,1448)	1:264:C:LYS:HA	1:264:C:LYS:HE2	4	0.13
(1,1448)	1:264:C:LYS:HA	1:264:C:LYS:HE3	4	0.13
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	1	0.13
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	8	0.13
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	10	0.13
(1,1431)	1:262:C:LEU:HA	1:265:C:CYS:H	16	0.13
(1,1291)	1:252:C:ASP:H	1:255:C:LEU:H	6	0.13
(1,1246)	1:247:C:ARG:H	1:247:C:ARG:HG2	12	0.13
(1,1246)	1:247:C:ARG:H	1:247:C:ARG:HG3	12	0.13
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	14	0.13
(1,1219)	1:242:C:LEU:HB3	1:247:C:ARG:H	4	0.13
(1,1206)	1:241:C:ARG:HD2	1:242:C:LEU:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:241:C:ARG:HD3	1:242:C:LEU:H	13	0.13
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD1	16	0.13
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD2	16	0.13
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD1	16	0.13
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD2	16	0.13
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD1	16	0.13
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD2	16	0.13
(1,1112)	1:229:C:LEU:HA	1:237:C:GLN:HB2	8	0.13
(1,1112)	1:229:C:LEU:HA	1:237:C:GLN:HB3	8	0.13
(1,1093)	1:227:C:LYS:HB2	1:239:C:VAL:H	19	0.13
(1,1093)	1:227:C:LYS:HB3	1:239:C:VAL:H	19	0.13
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	2	0.13
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	2	0.13
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	2	0.13
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	2	0.13
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	2	0.13
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	2	0.13
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	8	0.13
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	8	0.13
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	8	0.13
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	8	0.13
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	8	0.13
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	8	0.13
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	1	0.13
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	1	0.13
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	10	0.13
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	10	0.13
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	16	0.13
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	16	0.13
(1,1022)	1:224:C:LYS:H	1:224:C:LYS:HD2	14	0.13
(1,1022)	1:224:C:LYS:H	1:224:C:LYS:HD3	14	0.13
(1,1012)	1:222:C:ASN:HD21	1:242:C:LEU:HB2	20	0.13
(1,1012)	1:222:C:ASN:HD22	1:242:C:LEU:HB2	20	0.13
(1,971)	1:218:C:VAL:HG21	2:321:D:TYS:HD2	7	0.13
(1,886)	1:210:C:PRO:HB2	2:312:D:TYR:HD1	15	0.13
(1,886)	1:210:C:PRO:HB2	2:312:D:TYR:HD2	15	0.13
(1,882)	1:210:C:PRO:HA	2:312:D:TYR:HE1	13	0.13
(1,882)	1:210:C:PRO:HA	2:312:D:TYR:HE2	13	0.13
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	18	0.13
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	18	0.13
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	18	0.13
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE2	20	0.13
(1,875)	2:138:B:LYS:HB2	2:138:B:LYS:HE3	20	0.13
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE2	20	0.13
(1,875)	2:138:B:LYS:HB3	2:138:B:LYS:HE3	20	0.13
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE1	1	0.13
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE2	1	0.13
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE1	15	0.13
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE2	15	0.13
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	5	0.13
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	5	0.13
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	6	0.13
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	6	0.13
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	19	0.13
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	19	0.13
(1,839)	2:128:B:ALA:HA	2:129:B:PHE:H	8	0.13
(1,839)	2:128:B:ALA:HA	2:129:B:PHE:H	13	0.13
(1,831)	2:127:B:PRO:HA	2:128:B:ALA:H	10	0.13
(1,825)	2:125:B:LYS:HB2	2:125:B:LYS:HE2	5	0.13
(1,825)	2:125:B:LYS:HB2	2:125:B:LYS:HE3	5	0.13
(1,825)	2:125:B:LYS:HB3	2:125:B:LYS:HE2	5	0.13
(1,825)	2:125:B:LYS:HB3	2:125:B:LYS:HE3	5	0.13
(1,824)	2:125:B:LYS:HB2	2:125:B:LYS:HD2	1	0.13
(1,824)	2:125:B:LYS:HB2	2:125:B:LYS:HD3	1	0.13
(1,824)	2:125:B:LYS:HB3	2:125:B:LYS:HD2	1	0.13
(1,824)	2:125:B:LYS:HB3	2:125:B:LYS:HD3	1	0.13
(1,824)	2:125:B:LYS:HB2	2:125:B:LYS:HD2	16	0.13
(1,824)	2:125:B:LYS:HB2	2:125:B:LYS:HD3	16	0.13
(1,824)	2:125:B:LYS:HB3	2:125:B:LYS:HD2	16	0.13
(1,824)	2:125:B:LYS:HB3	2:125:B:LYS:HD3	16	0.13
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	5	0.13
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	5	0.13
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	5	0.13
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	5	0.13
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE1	2	0.13
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE2	2	0.13
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE1	6	0.13
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE2	6	0.13
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE1	14	0.13
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE2	14	0.13
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE1	18	0.13
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE2	18	0.13
(1,750)	2:106:B:ILE:HD11	2:107:B:TYR:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	2:106:B:ILE:HD12	2:107:B:TYR:H	7	0.13
(1,750)	2:106:B:ILE:HD13	2:107:B:TYR:H	7	0.13
(1,746)	2:106:B:ILE:HA	2:107:B:TYR:H	5	0.13
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	5	0.13
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	6	0.13
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	20	0.13
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD1	14	0.13
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD2	14	0.13
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD1	14	0.13
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD2	14	0.13
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD1	14	0.13
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD2	14	0.13
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD1	14	0.13
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD2	14	0.13
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD1	14	0.13
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD2	14	0.13
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD1	14	0.13
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD2	14	0.13
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	2	0.13
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	2	0.13
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	2	0.13
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	2	0.13
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	2	0.13
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	2	0.13
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	2	0.13
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	2	0.13
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	2	0.13
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	2	0.13
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	2	0.13
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	2	0.13
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	20	0.13
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	20	0.13
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	20	0.13
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	20	0.13
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	20	0.13
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	20	0.13
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	20	0.13
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	20	0.13
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	20	0.13
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	20	0.13
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	20	0.13
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	2	0.13
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	4	0.13
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	5	0.13
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	15	0.13
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	8	0.13
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	11	0.13
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	18	0.13
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	20	0.13
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	2	0.13
(1,411)	1:43:A:LYS:H	1:43:A:LYS:HD3	1	0.13
(1,399)	1:42:A:LEU:HB3	1:47:A:ARG:H	2	0.13
(1,328)	1:37:A:GLN:H	1:53:A:PRO:HG3	11	0.13
(1,313)	1:31:A:THR:HG21	1:37:A:GLN:HE21	6	0.13
(1,313)	1:31:A:THR:HG21	1:37:A:GLN:HE22	6	0.13
(1,313)	1:31:A:THR:HG22	1:37:A:GLN:HE21	6	0.13
(1,313)	1:31:A:THR:HG22	1:37:A:GLN:HE22	6	0.13
(1,313)	1:31:A:THR:HG23	1:37:A:GLN:HE21	6	0.13
(1,313)	1:31:A:THR:HG23	1:37:A:GLN:HE22	6	0.13
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD1	10	0.13
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD2	10	0.13
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD1	10	0.13
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD2	10	0.13
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD1	10	0.13
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD2	10	0.13
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD1	16	0.13
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD2	16	0.13
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD1	16	0.13
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD2	16	0.13
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD1	16	0.13
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD2	16	0.13
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	11	0.13
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	11	0.13
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	11	0.13
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	11	0.13
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	4	0.13
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	4	0.13
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	4	0.13
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	4	0.13
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	4	0.13
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	4	0.13
(1,189)	1:25:A:HIS:HE1	1:41:A:ARG:HD2	16	0.13
(1,189)	1:25:A:HIS:HE1	1:41:A:ARG:HD3	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:24:A:LYS:HG2	1:43:A:LYS:H	16	0.13
(1,171)	1:24:A:LYS:HG3	1:43:A:LYS:H	16	0.13
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	20	0.13
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	20	0.13
(1,167)	1:24:A:LYS:HE2	1:41:A:ARG:H	13	0.13
(1,167)	1:24:A:LYS:HE3	1:41:A:ARG:H	13	0.13
(1,139)	1:23:A:VAL:HB	1:42:A:LEU:H	2	0.13
(1,93)	1:18:A:VAL:HG11	1:57:A:TRP:HE1	10	0.13
(1,93)	1:18:A:VAL:HG12	1:57:A:TRP:HE1	10	0.13
(1,93)	1:18:A:VAL:HG13	1:57:A:TRP:HE1	10	0.13
(1,93)	1:18:A:VAL:HG21	1:57:A:TRP:HE1	10	0.13
(1,93)	1:18:A:VAL:HG22	1:57:A:TRP:HE1	10	0.13
(1,93)	1:18:A:VAL:HG23	1:57:A:TRP:HE1	10	0.13
(1,92)	1:18:A:VAL:HG11	1:52:A:ASP:H	20	0.13
(1,92)	1:18:A:VAL:HG12	1:52:A:ASP:H	20	0.13
(1,92)	1:18:A:VAL:HG13	1:52:A:ASP:H	20	0.13
(1,92)	1:18:A:VAL:HG21	1:52:A:ASP:H	20	0.13
(1,92)	1:18:A:VAL:HG22	1:52:A:ASP:H	20	0.13
(1,92)	1:18:A:VAL:HG23	1:52:A:ASP:H	20	0.13
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG21	8	0.13
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG22	8	0.13
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG23	8	0.13
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE1	14	0.13
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE2	14	0.13
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	4	0.12
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	11	0.12
(3,36)	1:240:C:ALA:N	1:249:C:VAL:O	13	0.12
(3,30)	1:227:C:LYS:N	1:239:C:VAL:O	17	0.12
(3,29)	1:227:C:LYS:H	1:239:C:VAL:O	10	0.12
(3,28)	1:224:C:LYS:N	1:241:C:ARG:O	15	0.12
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	6	0.12
(3,22)	1:40:A:ALA:O	1:49:A:VAL:H	1	0.12
(3,22)	1:40:A:ALA:O	1:49:A:VAL:H	3	0.12
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	10	0.12
(3,21)	1:40:A:ALA:N	1:49:A:VAL:O	15	0.12
(2,17)	1:211:C:CYS:CB	1:250:C:CYS:SG	19	0.12
(2,13)	1:209:C:CYS:CB	1:234:C:CYS:CB	15	0.12
(2,10)	1:65:A:CYS:CB	1:236:C:CYS:CB	11	0.12
(2,6)	1:11:A:CYS:SG	1:50:A:CYS:CB	19	0.12
(2,1)	1:9:A:CYS:CB	1:34:A:CYS:CB	5	0.12
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE1	1	0.12
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE1	3	0.12
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE2	3	0.12
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE1	4	0.12
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE2	4	0.12
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE1	17	0.12
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE2	17	0.12
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	8	0.12
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	8	0.12
(1,1602)	2:328:D:ALA:HA	2:329:D:PHE:H	8	0.12
(1,1597)	2:327:D:PRO:HA	2:328:D:ALA:H	10	0.12
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE2	13	0.12
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE3	13	0.12
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE2	13	0.12
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE3	13	0.12
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE1	1	0.12
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE2	1	0.12
(1,1554)	2:315:D:GLU:HA	2:315:D:GLU:HG2	3	0.12
(1,1554)	2:315:D:GLU:HA	2:315:D:GLU:HG3	3	0.12
(1,1543)	2:313:D:THR:HA	2:313:D:THR:HG21	19	0.12
(1,1543)	2:313:D:THR:HA	2:313:D:THR:HG22	19	0.12
(1,1543)	2:313:D:THR:HA	2:313:D:THR:HG23	19	0.12
(1,1521)	2:306:D:ILE:HD11	2:307:D:TYR:HE1	18	0.12
(1,1521)	2:306:D:ILE:HD11	2:307:D:TYR:HE2	18	0.12
(1,1521)	2:306:D:ILE:HD12	2:307:D:TYR:HE1	18	0.12
(1,1521)	2:306:D:ILE:HD12	2:307:D:TYR:HE2	18	0.12
(1,1521)	2:306:D:ILE:HD13	2:307:D:TYR:HE1	18	0.12
(1,1521)	2:306:D:ILE:HD13	2:307:D:TYR:HE2	18	0.12
(1,1518)	2:306:D:ILE:HB	2:307:D:TYR:HD1	17	0.12
(1,1518)	2:306:D:ILE:HB	2:307:D:TYR:HD2	17	0.12
(1,1515)	2:306:D:ILE:HA	2:307:D:TYR:H	5	0.12
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	1	0.12
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	9	0.12
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	14	0.12
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	17	0.12
(1,1453)	1:264:C:LYS:HB3	1:265:C:CYS:H	6	0.12
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	2	0.12
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	3	0.12
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	6	0.12
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	9	0.12
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	11	0.12
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	13	0.12
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:257:C:TRP:H	1:257:C:TRP:HE1	6	0.12
(1,1372)	1:257:C:TRP:H	1:257:C:TRP:HE1	8	0.12
(1,1368)	1:256:C:LYS:HD2	1:260:C:GLU:HG2	3	0.12
(1,1368)	1:256:C:LYS:HD3	1:260:C:GLU:HG2	3	0.12
(1,1309)	1:253:C:PRO:HB3	1:254:C:LYS:H	11	0.12
(1,1265)	1:249:C:VAL:HG21	2:321:D:TYS:HE1	10	0.12
(1,1265)	1:249:C:VAL:HG21	2:321:D:TYS:HE2	10	0.12
(1,1265)	1:249:C:VAL:HG22	2:321:D:TYS:HE1	10	0.12
(1,1265)	1:249:C:VAL:HG22	2:321:D:TYS:HE2	10	0.12
(1,1265)	1:249:C:VAL:HG23	2:321:D:TYS:HE1	10	0.12
(1,1265)	1:249:C:VAL:HG23	2:321:D:TYS:HE2	10	0.12
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	4	0.12
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	6	0.12
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	15	0.12
(1,1219)	1:242:C:LEU:HB3	1:247:C:ARG:H	5	0.12
(1,1219)	1:242:C:LEU:HB3	1:247:C:ARG:H	10	0.12
(1,1162)	1:238:C:ILE:HB	1:239:C:VAL:H	12	0.12
(1,1152)	1:237:C:GLN:HE21	1:253:C:PRO:HG3	6	0.12
(1,1152)	1:237:C:GLN:HE22	1:253:C:PRO:HG3	6	0.12
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	16	0.12
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	16	0.12
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	16	0.12
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD1	13	0.12
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD2	13	0.12
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD1	13	0.12
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD2	13	0.12
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD1	13	0.12
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD2	13	0.12
(1,1130)	1:231:C:THR:HG21	1:237:C:GLN:HE21	17	0.12
(1,1130)	1:231:C:THR:HG21	1:237:C:GLN:HE22	17	0.12
(1,1130)	1:231:C:THR:HG22	1:237:C:GLN:HE21	17	0.12
(1,1130)	1:231:C:THR:HG22	1:237:C:GLN:HE22	17	0.12
(1,1130)	1:231:C:THR:HG23	1:237:C:GLN:HE21	17	0.12
(1,1130)	1:231:C:THR:HG23	1:237:C:GLN:HE22	17	0.12
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD1	7	0.12
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD2	7	0.12
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD1	7	0.12
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD2	7	0.12
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD1	15	0.12
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD2	15	0.12
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD1	15	0.12
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD2	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1052)	1:225:C:HIS:HE1	1:241:C:ARG:HD2	15	0.12
(1,1052)	1:225:C:HIS:HE1	1:241:C:ARG:HD3	15	0.12
(1,1050)	1:225:C:HIS:HE1	1:227:C:LYS:HE2	7	0.12
(1,1050)	1:225:C:HIS:HE1	1:227:C:LYS:HE3	7	0.12
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	3	0.12
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	3	0.12
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	12	0.12
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	12	0.12
(1,1022)	1:224:C:LYS:H	1:224:C:LYS:HD2	9	0.12
(1,1022)	1:224:C:LYS:H	1:224:C:LYS:HD3	9	0.12
(1,991)	1:220:C:ARG:HD2	1:223:C:VAL:H	6	0.12
(1,991)	1:220:C:ARG:HD3	1:223:C:VAL:H	6	0.12
(1,946)	1:216:C:SER:HB2	1:252:C:ASP:H	17	0.12
(1,946)	1:216:C:SER:HB3	1:252:C:ASP:H	17	0.12
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG21	3	0.12
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG22	3	0.12
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG23	3	0.12
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG21	16	0.12
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG22	16	0.12
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG23	16	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG11	8	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG12	8	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG13	8	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG21	8	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG22	8	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG23	8	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG11	15	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG12	15	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG13	15	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG21	15	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG22	15	0.12
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG23	15	0.12
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE1	9	0.12
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE2	9	0.12
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD11	20	0.12
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD12	20	0.12
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD13	20	0.12
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD21	20	0.12
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD22	20	0.12
(1,846)	2:129:B:PHE:HD1	1:266:C:LEU:HD23	20	0.12
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD11	20	0.12
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD12	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD13	20	0.12
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD21	20	0.12
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD22	20	0.12
(1,846)	2:129:B:PHE:HD2	1:266:C:LEU:HD23	20	0.12
(1,839)	2:128:B:ALA:HA	2:129:B:PHE:H	15	0.12
(1,816)	2:125:B:LYS:HA	2:125:B:LYS:HD2	2	0.12
(1,816)	2:125:B:LYS:HA	2:125:B:LYS:HD3	2	0.12
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB2	19	0.12
(1,808)	2:121:B:TYS:HD1	2:122:B:ASP:HB3	19	0.12
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB2	19	0.12
(1,808)	2:121:B:TYS:HD2	2:122:B:ASP:HB3	19	0.12
(1,798)	2:120:B:ASP:HB3	2:121:B:TYS:HE1	8	0.12
(1,798)	2:120:B:ASP:HB3	2:121:B:TYS:HE2	8	0.12
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE1	15	0.12
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE2	15	0.12
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG2	1	0.12
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG3	1	0.12
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG2	5	0.12
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG3	5	0.12
(1,777)	2:113:B:THR:HA	2:113:B:THR:HG21	9	0.12
(1,777)	2:113:B:THR:HA	2:113:B:THR:HG22	9	0.12
(1,777)	2:113:B:THR:HA	2:113:B:THR:HG23	9	0.12
(1,777)	2:113:B:THR:HA	2:113:B:THR:HG21	19	0.12
(1,777)	2:113:B:THR:HA	2:113:B:THR:HG22	19	0.12
(1,777)	2:113:B:THR:HA	2:113:B:THR:HG23	19	0.12
(1,749)	2:106:B:ILE:HB	2:107:B:TYR:HD1	12	0.12
(1,749)	2:106:B:ILE:HB	2:107:B:TYR:HD2	12	0.12
(1,749)	2:106:B:ILE:HB	2:107:B:TYR:HD1	17	0.12
(1,749)	2:106:B:ILE:HB	2:107:B:TYR:HD2	17	0.12
(1,744)	2:106:B:ILE:HA	2:106:B:ILE:HD11	5	0.12
(1,744)	2:106:B:ILE:HA	2:106:B:ILE:HD12	5	0.12
(1,744)	2:106:B:ILE:HA	2:106:B:ILE:HD13	5	0.12
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	11	0.12
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	13	0.12
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	14	0.12
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	18	0.12
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	3	0.12
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	3	0.12
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	3	0.12
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	3	0.12
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	3	0.12
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	3	0.12
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	3	0.12
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	3	0.12
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	3	0.12
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	3	0.12
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	3	0.12
(1,687)	1:66:A:LEU:HD11	1:263:C:GLU:H	2	0.12
(1,687)	1:66:A:LEU:HD12	1:263:C:GLU:H	2	0.12
(1,687)	1:66:A:LEU:HD13	1:263:C:GLU:H	2	0.12
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	14	0.12
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	19	0.12
(1,656)	1:64:A:LYS:HB2	1:65:A:CYS:H	8	0.12
(1,656)	1:64:A:LYS:HB2	1:65:A:CYS:H	17	0.12
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	2	0.12
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	6	0.12
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	7	0.12
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	9	0.12
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	10	0.12
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	13	0.12
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	15	0.12
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	16	0.12
(1,627)	1:62:A:LEU:HA	1:65:A:CYS:H	14	0.12
(1,552)	1:57:A:TRP:H	1:57:A:TRP:HE1	3	0.12
(1,547)	1:56:A:LYS:HD2	1:57:A:TRP:H	2	0.12
(1,547)	1:56:A:LYS:HD3	1:57:A:TRP:H	2	0.12
(1,508)	1:55:A:LEU:H	1:55:A:LEU:HG	8	0.12
(1,489)	1:53:A:PRO:HB3	1:54:A:LYS:H	11	0.12
(1,471)	1:52:A:ASP:H	1:55:A:LEU:H	6	0.12
(1,445)	1:49:A:VAL:HG21	1:50:A:CYS:H	16	0.12
(1,445)	1:49:A:VAL:HG22	1:50:A:CYS:H	16	0.12
(1,445)	1:49:A:VAL:HG23	1:50:A:CYS:H	16	0.12
(1,411)	1:43:A:LYS:H	1:43:A:LYS:HD3	5	0.12
(1,397)	1:42:A:LEU:HB2	1:47:A:ARG:H	20	0.12
(1,386)	1:41:A:ARG:HD2	1:42:A:LEU:H	15	0.12
(1,386)	1:41:A:ARG:HD3	1:42:A:LEU:H	15	0.12
(1,385)	1:41:A:ARG:HB2	1:48:A:GLN:HG2	8	0.12
(1,385)	1:41:A:ARG:HB2	1:48:A:GLN:HG3	8	0.12
(1,385)	1:41:A:ARG:HB3	1:48:A:GLN:HG2	8	0.12
(1,385)	1:41:A:ARG:HB3	1:48:A:GLN:HG3	8	0.12
(1,342)	1:38:A:ILE:HB	1:39:A:VAL:H	13	0.12
(1,332)	1:37:A:GLN:HE21	1:53:A:PRO:HG3	3	0.12
(1,332)	1:37:A:GLN:HE22	1:53:A:PRO:HG3	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:37:A:GLN:H	1:53:A:PRO:HG3	7	0.12
(1,313)	1:31:A:THR:HG21	1:37:A:GLN:HE21	7	0.12
(1,313)	1:31:A:THR:HG21	1:37:A:GLN:HE22	7	0.12
(1,313)	1:31:A:THR:HG22	1:37:A:GLN:HE21	7	0.12
(1,313)	1:31:A:THR:HG22	1:37:A:GLN:HE22	7	0.12
(1,313)	1:31:A:THR:HG23	1:37:A:GLN:HE21	7	0.12
(1,313)	1:31:A:THR:HG23	1:37:A:GLN:HE22	7	0.12
(1,310)	1:31:A:THR:HG21	2:115:B:GLU:HA	11	0.12
(1,310)	1:31:A:THR:HG22	2:115:B:GLU:HA	11	0.12
(1,310)	1:31:A:THR:HG23	2:115:B:GLU:HA	11	0.12
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD1	15	0.12
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD2	15	0.12
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD1	15	0.12
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD2	15	0.12
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD1	15	0.12
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD2	15	0.12
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD1	17	0.12
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD2	17	0.12
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD1	17	0.12
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD2	17	0.12
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD1	17	0.12
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD2	17	0.12
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	1	0.12
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	1	0.12
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	1	0.12
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	1	0.12
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	12	0.12
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	12	0.12
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	12	0.12
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	12	0.12
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD1	14	0.12
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD2	14	0.12
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD1	14	0.12
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD2	14	0.12
(1,252)	1:27:A:LYS:HE2	1:225:C:HIS:HE1	11	0.12
(1,252)	1:27:A:LYS:HE3	1:225:C:HIS:HE1	11	0.12
(1,252)	1:27:A:LYS:HE2	1:225:C:HIS:HE1	14	0.12
(1,252)	1:27:A:LYS:HE3	1:225:C:HIS:HE1	14	0.12
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	7	0.12
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	7	0.12
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	7	0.12
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	7	0.12
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	7	0.12
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	15	0.12
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	15	0.12
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	15	0.12
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	15	0.12
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	15	0.12
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	15	0.12
(1,207)	1:26:A:LEU:HD21	1:228:C:ILE:H	3	0.12
(1,207)	1:26:A:LEU:HD22	1:228:C:ILE:H	3	0.12
(1,207)	1:26:A:LEU:HD23	1:228:C:ILE:H	3	0.12
(1,189)	1:25:A:HIS:HE1	1:41:A:ARG:HD2	13	0.12
(1,189)	1:25:A:HIS:HE1	1:41:A:ARG:HD3	13	0.12
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	7	0.12
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	7	0.12
(1,167)	1:24:A:LYS:HE2	1:41:A:ARG:H	2	0.12
(1,167)	1:24:A:LYS:HE3	1:41:A:ARG:H	2	0.12
(1,167)	1:24:A:LYS:HE2	1:41:A:ARG:H	10	0.12
(1,167)	1:24:A:LYS:HE3	1:41:A:ARG:H	10	0.12
(1,167)	1:24:A:LYS:HE2	1:41:A:ARG:H	14	0.12
(1,167)	1:24:A:LYS:HE3	1:41:A:ARG:H	14	0.12
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE1	17	0.12
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE2	17	0.12
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE1	17	0.12
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE2	17	0.12
(1,115)	1:20:A:ARG:HD2	1:23:A:VAL:H	6	0.12
(1,115)	1:20:A:ARG:HD3	1:23:A:VAL:H	6	0.12
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG21	9	0.12
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG22	9	0.12
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG23	9	0.12
(1,70)	1:16:A:SER:HB2	1:52:A:ASP:H	17	0.12
(1,70)	1:16:A:SER:HB3	1:52:A:ASP:H	17	0.12
(1,62)	1:15:A:GLU:HG2	2:123:B:SER:HA	2	0.12
(1,62)	1:15:A:GLU:HG3	2:123:B:SER:HA	2	0.12
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG21	14	0.12
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG22	14	0.12
(1,60)	1:15:A:GLU:HB3	1:51:A:ILE:HG23	14	0.12
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG11	13	0.12
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG12	13	0.12
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG13	13	0.12
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG21	13	0.12
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG22	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG23	13	0.12
(1,14)	1:10:A:PRO:HB3	1:11:A:CYS:H	12	0.12
(1,2)	1:6:A:SER:HB2	1:7:A:TYR:HD1	7	0.12
(1,2)	1:6:A:SER:HB2	1:7:A:TYR:HD2	7	0.12
(1,2)	1:6:A:SER:HB3	1:7:A:TYR:HD1	7	0.12
(1,2)	1:6:A:SER:HB3	1:7:A:TYR:HD2	7	0.12
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	1	0.11
(3,38)	1:240:C:ALA:O	1:249:C:VAL:N	17	0.11
(3,27)	1:224:C:LYS:H	1:241:C:ARG:O	4	0.11
(3,10)	1:27:A:LYS:N	1:39:A:VAL:O	8	0.11
(3,9)	1:27:A:LYS:H	1:39:A:VAL:O	1	0.11
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	18	0.11
(3,7)	1:26:A:LEU:O	1:228:C:ILE:H	20	0.11
(3,4)	1:24:A:LYS:N	1:41:A:ARG:O	14	0.11
(2,18)	1:211:C:CYS:SG	1:250:C:CYS:CB	19	0.11
(2,17)	1:211:C:CYS:CB	1:250:C:CYS:SG	16	0.11
(2,14)	1:209:C:CYS:CB	1:234:C:CYS:SG	11	0.11
(2,14)	1:209:C:CYS:CB	1:234:C:CYS:SG	14	0.11
(2,11)	1:65:A:CYS:CB	1:236:C:CYS:SG	9	0.11
(2,6)	1:11:A:CYS:SG	1:50:A:CYS:CB	12	0.11
(2,5)	1:11:A:CYS:CB	1:50:A:CYS:SG	12	0.11
(2,5)	1:11:A:CYS:CB	1:50:A:CYS:SG	16	0.11
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE1	5	0.11
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE2	5	0.11
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE1	14	0.11
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE2	14	0.11
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE1	16	0.11
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE2	16	0.11
(1,1613)	2:330:D:ARG:HA	2:331:D:GLU:H	17	0.11
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE2	5	0.11
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE3	5	0.11
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE2	5	0.11
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE3	5	0.11
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE2	9	0.11
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE3	9	0.11
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE2	9	0.11
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE3	9	0.11
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD2	7	0.11
(1,1590)	2:325:D:LYS:HB2	2:325:D:LYS:HD3	7	0.11
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD2	7	0.11
(1,1590)	2:325:D:LYS:HB3	2:325:D:LYS:HD3	7	0.11
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB2	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1574)	2:321:D:TYS:HD1	2:322:D:ASP:HB3	17	0.11
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB2	17	0.11
(1,1574)	2:321:D:TYS:HD2	2:322:D:ASP:HB3	17	0.11
(1,1564)	2:320:D:ASP:HB3	2:321:D:TYS:HE1	17	0.11
(1,1564)	2:320:D:ASP:HB3	2:321:D:TYS:HE2	17	0.11
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE1	16	0.11
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE2	16	0.11
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE1	19	0.11
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE2	19	0.11
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE1	20	0.11
(1,1561)	2:320:D:ASP:HB2	2:321:D:TYS:HE2	20	0.11
(1,1554)	2:315:D:GLU:HA	2:315:D:GLU:HG2	1	0.11
(1,1554)	2:315:D:GLU:HA	2:315:D:GLU:HG3	1	0.11
(1,1515)	2:306:D:ILE:HA	2:307:D:TYR:H	8	0.11
(1,1515)	2:306:D:ILE:HA	2:307:D:TYR:H	19	0.11
(1,1513)	2:306:D:ILE:HA	2:306:D:ILE:HD11	5	0.11
(1,1513)	2:306:D:ILE:HA	2:306:D:ILE:HD12	5	0.11
(1,1513)	2:306:D:ILE:HA	2:306:D:ILE:HD13	5	0.11
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	2	0.11
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	15	0.11
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	16	0.11
(1,1453)	1:264:C:LYS:HB3	1:265:C:CYS:H	3	0.11
(1,1453)	1:264:C:LYS:HB3	1:265:C:CYS:H	9	0.11
(1,1453)	1:264:C:LYS:HB3	1:265:C:CYS:H	11	0.11
(1,1453)	1:264:C:LYS:HB3	1:265:C:CYS:H	19	0.11
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	5	0.11
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	16	0.11
(1,1434)	1:262:C:LEU:HG	1:263:C:GLU:H	18	0.11
(1,1431)	1:262:C:LEU:HA	1:265:C:CYS:H	1	0.11
(1,1372)	1:257:C:TRP:H	1:257:C:TRP:HE1	2	0.11
(1,1372)	1:257:C:TRP:H	1:257:C:TRP:HE1	10	0.11
(1,1367)	1:256:C:LYS:HD2	1:257:C:TRP:H	5	0.11
(1,1367)	1:256:C:LYS:HD3	1:257:C:TRP:H	5	0.11
(1,1367)	1:256:C:LYS:HD2	1:257:C:TRP:H	12	0.11
(1,1367)	1:256:C:LYS:HD3	1:257:C:TRP:H	12	0.11
(1,1328)	1:255:C:LEU:H	1:255:C:LEU:HG	19	0.11
(1,1265)	1:249:C:VAL:HG21	2:321:D:TYS:HE1	3	0.11
(1,1265)	1:249:C:VAL:HG21	2:321:D:TYS:HE2	3	0.11
(1,1265)	1:249:C:VAL:HG22	2:321:D:TYS:HE1	3	0.11
(1,1265)	1:249:C:VAL:HG22	2:321:D:TYS:HE2	3	0.11
(1,1265)	1:249:C:VAL:HG23	2:321:D:TYS:HE1	3	0.11
(1,1265)	1:249:C:VAL:HG23	2:321:D:TYS:HE2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	17	0.11
(1,1231)	1:243:C:LYS:H	1:243:C:LYS:HD3	19	0.11
(1,1219)	1:242:C:LEU:HB3	1:247:C:ARG:H	2	0.11
(1,1206)	1:241:C:ARG:HD2	1:242:C:LEU:H	12	0.11
(1,1206)	1:241:C:ARG:HD3	1:242:C:LEU:H	12	0.11
(1,1206)	1:241:C:ARG:HD2	1:242:C:LEU:H	18	0.11
(1,1206)	1:241:C:ARG:HD3	1:242:C:LEU:H	18	0.11
(1,1206)	1:241:C:ARG:HD2	1:242:C:LEU:H	20	0.11
(1,1206)	1:241:C:ARG:HD3	1:242:C:LEU:H	20	0.11
(1,1162)	1:238:C:ILE:HB	1:239:C:VAL:H	13	0.11
(1,1152)	1:237:C:GLN:HE21	1:253:C:PRO:HG3	3	0.11
(1,1152)	1:237:C:GLN:HE22	1:253:C:PRO:HG3	3	0.11
(1,1148)	1:237:C:GLN:H	1:253:C:PRO:HG3	17	0.11
(1,1133)	1:231:C:THR:HG21	2:315:D:GLU:HA	5	0.11
(1,1133)	1:231:C:THR:HG22	2:315:D:GLU:HA	5	0.11
(1,1133)	1:231:C:THR:HG23	2:315:D:GLU:HA	5	0.11
(1,1132)	1:231:C:THR:HG21	2:314:D:GLU:HB2	20	0.11
(1,1132)	1:231:C:THR:HG22	2:314:D:GLU:HB2	20	0.11
(1,1132)	1:231:C:THR:HG23	2:314:D:GLU:HB2	20	0.11
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD1	10	0.11
(1,1131)	1:231:C:THR:HG21	2:312:D:TYR:HD2	10	0.11
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD1	10	0.11
(1,1131)	1:231:C:THR:HG22	2:312:D:TYR:HD2	10	0.11
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD1	10	0.11
(1,1131)	1:231:C:THR:HG23	2:312:D:TYR:HD2	10	0.11
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE1	6	0.11
(1,1117)	1:229:C:LEU:HD11	2:312:D:TYR:HE2	6	0.11
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE1	6	0.11
(1,1117)	1:229:C:LEU:HD12	2:312:D:TYR:HE2	6	0.11
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE1	6	0.11
(1,1117)	1:229:C:LEU:HD13	2:312:D:TYR:HE2	6	0.11
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE1	11	0.11
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE2	11	0.11
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE1	11	0.11
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE2	11	0.11
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE1	20	0.11
(1,1114)	1:229:C:LEU:HB2	2:312:D:TYR:HE2	20	0.11
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE1	20	0.11
(1,1114)	1:229:C:LEU:HB3	2:312:D:TYR:HE2	20	0.11
(1,1101)	1:228:C:ILE:HB	1:229:C:LEU:H	7	0.11
(1,1052)	1:225:C:HIS:HE1	1:241:C:ARG:HD2	17	0.11
(1,1052)	1:225:C:HIS:HE1	1:241:C:ARG:HD3	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1050)	1:225:C:HIS:HE1	1:227:C:LYS:HE2	3	0.11
(1,1050)	1:225:C:HIS:HE1	1:227:C:LYS:HE3	3	0.11
(1,1043)	1:224:C:LYS:HG2	1:225:C:HIS:H	14	0.11
(1,1043)	1:224:C:LYS:HG3	1:225:C:HIS:H	14	0.11
(1,1015)	1:223:C:VAL:HB	1:242:C:LEU:H	3	0.11
(1,1015)	1:223:C:VAL:HB	1:242:C:LEU:H	18	0.11
(1,1015)	1:223:C:VAL:HB	1:242:C:LEU:H	20	0.11
(1,1012)	1:222:C:ASN:HD21	1:242:C:LEU:HB2	12	0.11
(1,1012)	1:222:C:ASN:HD22	1:242:C:LEU:HB2	12	0.11
(1,965)	1:218:C:VAL:HG11	1:223:C:VAL:H	15	0.11
(1,965)	1:218:C:VAL:HG12	1:223:C:VAL:H	15	0.11
(1,965)	1:218:C:VAL:HG13	1:223:C:VAL:H	15	0.11
(1,965)	1:218:C:VAL:HG21	1:223:C:VAL:H	15	0.11
(1,965)	1:218:C:VAL:HG22	1:223:C:VAL:H	15	0.11
(1,965)	1:218:C:VAL:HG23	1:223:C:VAL:H	15	0.11
(1,957)	1:218:C:VAL:HB	1:251:C:ILE:HG21	9	0.11
(1,957)	1:218:C:VAL:HB	1:251:C:ILE:HG22	9	0.11
(1,957)	1:218:C:VAL:HB	1:251:C:ILE:HG23	9	0.11
(1,957)	1:218:C:VAL:HB	1:251:C:ILE:HG21	15	0.11
(1,957)	1:218:C:VAL:HB	1:251:C:ILE:HG22	15	0.11
(1,957)	1:218:C:VAL:HB	1:251:C:ILE:HG23	15	0.11
(1,946)	1:216:C:SER:HB2	1:252:C:ASP:H	3	0.11
(1,946)	1:216:C:SER:HB3	1:252:C:ASP:H	3	0.11
(1,938)	1:215:C:GLU:HG2	2:323:D:SER:HA	3	0.11
(1,938)	1:215:C:GLU:HG3	2:323:D:SER:HA	3	0.11
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG21	17	0.11
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG22	17	0.11
(1,936)	1:215:C:GLU:HB3	1:251:C:ILE:HG23	17	0.11
(1,888)	1:210:C:PRO:HB3	1:211:C:CYS:H	2	0.11
(1,888)	1:210:C:PRO:HB3	1:211:C:CYS:H	7	0.11
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE1	3	0.11
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE2	3	0.11
(1,851)	2:130:B:ARG:HA	2:131:B:GLU:H	11	0.11
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	4	0.11
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	4	0.11
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	10	0.11
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	10	0.11
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE1	17	0.11
(1,844)	2:129:B:PHE:HA	2:129:B:PHE:HE2	17	0.11
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	1	0.11
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	1	0.11
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	1	0.11
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	1	0.11
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	1	0.11
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	1	0.11
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	1	0.11
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	1	0.11
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	1	0.11
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	1	0.11
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	1	0.11
(1,831)	2:127:B:PRO:HA	2:128:B:ALA:H	4	0.11
(1,831)	2:127:B:PRO:HA	2:128:B:ALA:H	14	0.11
(1,825)	2:125:B:LYS:HB2	2:125:B:LYS:HE2	18	0.11
(1,825)	2:125:B:LYS:HB2	2:125:B:LYS:HE3	18	0.11
(1,825)	2:125:B:LYS:HB3	2:125:B:LYS:HE2	18	0.11
(1,825)	2:125:B:LYS:HB3	2:125:B:LYS:HE3	18	0.11
(1,816)	2:125:B:LYS:HA	2:125:B:LYS:HD2	10	0.11
(1,816)	2:125:B:LYS:HA	2:125:B:LYS:HD3	10	0.11
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE1	19	0.11
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE2	19	0.11
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG2	3	0.11
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG3	3	0.11
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG2	8	0.11
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG3	8	0.11
(1,787)	2:115:B:GLU:H	2:115:B:GLU:HG2	10	0.11
(1,787)	2:115:B:GLU:H	2:115:B:GLU:HG3	10	0.11
(1,776)	2:113:B:THR:HA	2:113:B:THR:HB	4	0.11
(1,764)	2:107:B:TYR:HE1	1:223:C:VAL:HG11	17	0.11
(1,764)	2:107:B:TYR:HE1	1:223:C:VAL:HG12	17	0.11
(1,764)	2:107:B:TYR:HE1	1:223:C:VAL:HG13	17	0.11
(1,764)	2:107:B:TYR:HE1	1:223:C:VAL:HG21	17	0.11
(1,764)	2:107:B:TYR:HE1	1:223:C:VAL:HG22	17	0.11
(1,764)	2:107:B:TYR:HE1	1:223:C:VAL:HG23	17	0.11
(1,764)	2:107:B:TYR:HE2	1:223:C:VAL:HG11	17	0.11
(1,764)	2:107:B:TYR:HE2	1:223:C:VAL:HG12	17	0.11
(1,764)	2:107:B:TYR:HE2	1:223:C:VAL:HG13	17	0.11
(1,764)	2:107:B:TYR:HE2	1:223:C:VAL:HG21	17	0.11
(1,764)	2:107:B:TYR:HE2	1:223:C:VAL:HG22	17	0.11
(1,764)	2:107:B:TYR:HE2	1:223:C:VAL:HG23	17	0.11
(1,757)	2:106:B:ILE:HG21	2:107:B:TYR:HD1	9	0.11
(1,757)	2:106:B:ILE:HG21	2:107:B:TYR:HD2	9	0.11
(1,757)	2:106:B:ILE:HG22	2:107:B:TYR:HD1	9	0.11
(1,757)	2:106:B:ILE:HG22	2:107:B:TYR:HD2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,757)	2:106:B:ILE:HG23	2:107:B:TYR:HD1	9	0.11
(1,757)	2:106:B:ILE:HG23	2:107:B:TYR:HD2	9	0.11
(1,752)	2:106:B:ILE:HD11	2:107:B:TYR:HE1	7	0.11
(1,752)	2:106:B:ILE:HD11	2:107:B:TYR:HE2	7	0.11
(1,752)	2:106:B:ILE:HD12	2:107:B:TYR:HE1	7	0.11
(1,752)	2:106:B:ILE:HD12	2:107:B:TYR:HE2	7	0.11
(1,752)	2:106:B:ILE:HD13	2:107:B:TYR:HE1	7	0.11
(1,752)	2:106:B:ILE:HD13	2:107:B:TYR:HE2	7	0.11
(1,749)	2:106:B:ILE:HB	2:107:B:TYR:HD1	20	0.11
(1,749)	2:106:B:ILE:HB	2:107:B:TYR:HD2	20	0.11
(1,744)	2:106:B:ILE:HA	2:106:B:ILE:HD11	8	0.11
(1,744)	2:106:B:ILE:HA	2:106:B:ILE:HD12	8	0.11
(1,744)	2:106:B:ILE:HA	2:106:B:ILE:HD13	8	0.11
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	7	0.11
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	10	0.11
(1,707)	1:67:A:ASN:HA	1:68:A:LYS:H	15	0.11
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD1	4	0.11
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD2	4	0.11
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD1	4	0.11
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD2	4	0.11
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD1	4	0.11
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD2	4	0.11
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD1	4	0.11
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD2	4	0.11
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD1	4	0.11
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD2	4	0.11
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD1	4	0.11
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD2	4	0.11
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD1	7	0.11
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD2	7	0.11
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD1	7	0.11
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD2	7	0.11
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD1	7	0.11
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD2	7	0.11
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD1	7	0.11
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD2	7	0.11
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD1	7	0.11
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD2	7	0.11
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD1	7	0.11
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD2	7	0.11
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	15	0.11
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	15	0.11
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	15	0.11
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	15	0.11
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	15	0.11
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	15	0.11
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	15	0.11
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	15	0.11
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	15	0.11
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	15	0.11
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	15	0.11
(1,699)	1:66:A:LEU:HD11	2:327:D:PRO:HB2	1	0.11
(1,699)	1:66:A:LEU:HD11	2:327:D:PRO:HB3	1	0.11
(1,699)	1:66:A:LEU:HD12	2:327:D:PRO:HB2	1	0.11
(1,699)	1:66:A:LEU:HD12	2:327:D:PRO:HB3	1	0.11
(1,699)	1:66:A:LEU:HD13	2:327:D:PRO:HB2	1	0.11
(1,699)	1:66:A:LEU:HD13	2:327:D:PRO:HB3	1	0.11
(1,699)	1:66:A:LEU:HD21	2:327:D:PRO:HB2	1	0.11
(1,699)	1:66:A:LEU:HD21	2:327:D:PRO:HB3	1	0.11
(1,699)	1:66:A:LEU:HD22	2:327:D:PRO:HB2	1	0.11
(1,699)	1:66:A:LEU:HD22	2:327:D:PRO:HB3	1	0.11
(1,699)	1:66:A:LEU:HD23	2:327:D:PRO:HB2	1	0.11
(1,699)	1:66:A:LEU:HD23	2:327:D:PRO:HB3	1	0.11
(1,699)	1:66:A:LEU:HD11	2:327:D:PRO:HB2	2	0.11
(1,699)	1:66:A:LEU:HD11	2:327:D:PRO:HB3	2	0.11
(1,699)	1:66:A:LEU:HD12	2:327:D:PRO:HB2	2	0.11
(1,699)	1:66:A:LEU:HD12	2:327:D:PRO:HB3	2	0.11
(1,699)	1:66:A:LEU:HD13	2:327:D:PRO:HB2	2	0.11
(1,699)	1:66:A:LEU:HD13	2:327:D:PRO:HB3	2	0.11
(1,699)	1:66:A:LEU:HD21	2:327:D:PRO:HB2	2	0.11
(1,699)	1:66:A:LEU:HD21	2:327:D:PRO:HB3	2	0.11
(1,699)	1:66:A:LEU:HD22	2:327:D:PRO:HB2	2	0.11
(1,699)	1:66:A:LEU:HD22	2:327:D:PRO:HB3	2	0.11
(1,699)	1:66:A:LEU:HD23	2:327:D:PRO:HB2	2	0.11
(1,699)	1:66:A:LEU:HD23	2:327:D:PRO:HB3	2	0.11
(1,694)	1:66:A:LEU:HD11	1:262:C:LEU:H	4	0.11
(1,694)	1:66:A:LEU:HD12	1:262:C:LEU:H	4	0.11
(1,694)	1:66:A:LEU:HD13	1:262:C:LEU:H	4	0.11
(1,694)	1:66:A:LEU:HD21	1:262:C:LEU:H	4	0.11
(1,694)	1:66:A:LEU:HD22	1:262:C:LEU:H	4	0.11
(1,694)	1:66:A:LEU:HD23	1:262:C:LEU:H	4	0.11
(1,687)	1:66:A:LEU:HD11	1:263:C:GLU:H	15	0.11
(1,687)	1:66:A:LEU:HD12	1:263:C:GLU:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,687)	1:66:A:LEU:HD13	1:263:C:GLU:H	15	0.11
(1,658)	1:64:A:LYS:HB3	1:65:A:CYS:H	18	0.11
(1,653)	1:64:A:LYS:HA	1:64:A:LYS:HE2	4	0.11
(1,653)	1:64:A:LYS:HA	1:64:A:LYS:HE3	4	0.11
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	1	0.11
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	5	0.11
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	12	0.11
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	14	0.11
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	17	0.11
(1,627)	1:62:A:LEU:HA	1:65:A:CYS:H	16	0.11
(1,618)	1:61:A:TYR:HE1	1:65:A:CYS:HB2	7	0.11
(1,618)	1:61:A:TYR:HE2	1:65:A:CYS:HB2	7	0.11
(1,548)	1:56:A:LYS:HD2	1:60:A:GLU:HG2	3	0.11
(1,548)	1:56:A:LYS:HD3	1:60:A:GLU:HG2	3	0.11
(1,489)	1:53:A:PRO:HB3	1:54:A:LYS:H	7	0.11
(1,471)	1:52:A:ASP:H	1:55:A:LEU:H	13	0.11
(1,471)	1:52:A:ASP:H	1:55:A:LEU:H	18	0.11
(1,450)	1:51:A:ILE:H	1:51:A:ILE:HD11	5	0.11
(1,450)	1:51:A:ILE:H	1:51:A:ILE:HD12	5	0.11
(1,450)	1:51:A:ILE:H	1:51:A:ILE:HD13	5	0.11
(1,411)	1:43:A:LYS:H	1:43:A:LYS:HD3	4	0.11
(1,411)	1:43:A:LYS:H	1:43:A:LYS:HD3	18	0.11
(1,399)	1:42:A:LEU:HB3	1:47:A:ARG:H	10	0.11
(1,399)	1:42:A:LEU:HB3	1:47:A:ARG:H	15	0.11
(1,397)	1:42:A:LEU:HB2	1:47:A:ARG:H	6	0.11
(1,397)	1:42:A:LEU:HB2	1:47:A:ARG:H	9	0.11
(1,372)	1:40:A:ALA:HB1	1:51:A:ILE:H	7	0.11
(1,372)	1:40:A:ALA:HB2	1:51:A:ILE:H	7	0.11
(1,372)	1:40:A:ALA:HB3	1:51:A:ILE:H	7	0.11
(1,328)	1:37:A:GLN:H	1:53:A:PRO:HG3	8	0.11
(1,328)	1:37:A:GLN:H	1:53:A:PRO:HG3	12	0.11
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD1	2	0.11
(1,308)	1:31:A:THR:HG21	2:112:B:TYR:HD2	2	0.11
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD1	2	0.11
(1,308)	1:31:A:THR:HG22	2:112:B:TYR:HD2	2	0.11
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD1	2	0.11
(1,308)	1:31:A:THR:HG23	2:112:B:TYR:HD2	2	0.11
(1,297)	1:29:A:LEU:HD21	1:225:C:HIS:HE1	19	0.11
(1,297)	1:29:A:LEU:HD22	1:225:C:HIS:HE1	19	0.11
(1,297)	1:29:A:LEU:HD23	1:225:C:HIS:HE1	19	0.11
(1,293)	1:29:A:LEU:HD11	1:225:C:HIS:HE1	19	0.11
(1,293)	1:29:A:LEU:HD12	1:225:C:HIS:HE1	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,293)	1:29:A:LEU:HD13	1:225:C:HIS:HE1	19	0.11
(1,292)	1:29:A:LEU:HD11	2:112:B:TYR:HE1	12	0.11
(1,292)	1:29:A:LEU:HD11	2:112:B:TYR:HE2	12	0.11
(1,292)	1:29:A:LEU:HD12	2:112:B:TYR:HE1	12	0.11
(1,292)	1:29:A:LEU:HD12	2:112:B:TYR:HE2	12	0.11
(1,292)	1:29:A:LEU:HD13	2:112:B:TYR:HE1	12	0.11
(1,292)	1:29:A:LEU:HD13	2:112:B:TYR:HE2	12	0.11
(1,252)	1:27:A:LYS:HE2	1:225:C:HIS:HE1	9	0.11
(1,252)	1:27:A:LYS:HE3	1:225:C:HIS:HE1	9	0.11
(1,241)	1:27:A:LYS:HD3	1:225:C:HIS:HE1	7	0.11
(1,239)	1:27:A:LYS:HD3	2:112:B:TYR:HD1	20	0.11
(1,239)	1:27:A:LYS:HD3	2:112:B:TYR:HD2	20	0.11
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	2	0.11
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	2	0.11
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	2	0.11
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	2	0.11
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	2	0.11
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	2	0.11
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	12	0.11
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	12	0.11
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	12	0.11
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	12	0.11
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	12	0.11
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	12	0.11
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	17	0.11
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	17	0.11
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	17	0.11
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	17	0.11
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	17	0.11
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	17	0.11
(1,188)	1:25:A:HIS:HE1	1:41:A:ARG:HB2	19	0.11
(1,188)	1:25:A:HIS:HE1	1:41:A:ARG:HB3	19	0.11
(1,187)	1:25:A:HIS:HE1	1:27:A:LYS:HE2	6	0.11
(1,187)	1:25:A:HIS:HE1	1:27:A:LYS:HE3	6	0.11
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE2	6	0.11
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE3	6	0.11
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	3	0.11
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	3	0.11
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	15	0.11
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	15	0.11
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	19	0.11
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	1:24:A:LYS:HE2	1:41:A:ARG:H	11	0.11
(1,167)	1:24:A:LYS:HE3	1:41:A:ARG:H	11	0.11
(1,163)	1:24:A:LYS:HB2	1:25:A:HIS:HE1	4	0.11
(1,163)	1:24:A:LYS:HB3	1:25:A:HIS:HE1	4	0.11
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE1	5	0.11
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE2	5	0.11
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE1	5	0.11
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE2	5	0.11
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE1	9	0.11
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE2	9	0.11
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE1	9	0.11
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE2	9	0.11
(1,115)	1:20:A:ARG:HD2	1:23:A:VAL:H	19	0.11
(1,115)	1:20:A:ARG:HD3	1:23:A:VAL:H	19	0.11
(1,101)	1:19:A:ALA:HA	1:57:A:TRP:HE1	6	0.11
(1,92)	1:18:A:VAL:HG11	1:52:A:ASP:H	2	0.11
(1,92)	1:18:A:VAL:HG12	1:52:A:ASP:H	2	0.11
(1,92)	1:18:A:VAL:HG13	1:52:A:ASP:H	2	0.11
(1,92)	1:18:A:VAL:HG21	1:52:A:ASP:H	2	0.11
(1,92)	1:18:A:VAL:HG22	1:52:A:ASP:H	2	0.11
(1,92)	1:18:A:VAL:HG23	1:52:A:ASP:H	2	0.11
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG21	1	0.11
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG22	1	0.11
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG23	1	0.11
(1,70)	1:16:A:SER:HB2	1:52:A:ASP:H	9	0.11
(1,70)	1:16:A:SER:HB3	1:52:A:ASP:H	9	0.11
(1,62)	1:15:A:GLU:HG2	2:123:B:SER:HA	3	0.11
(1,62)	1:15:A:GLU:HG3	2:123:B:SER:HA	3	0.11
(1,14)	1:10:A:PRO:HB3	1:11:A:CYS:H	2	0.11
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE1	17	0.11
(1,6)	1:10:A:PRO:HA	2:112:B:TYR:HE2	17	0.11
(3,23)	1:40:A:ALA:O	1:49:A:VAL:N	18	0.1
(2,14)	1:209:C:CYS:CB	1:234:C:CYS:SG	3	0.1
(2,11)	1:65:A:CYS:CB	1:236:C:CYS:SG	19	0.1
(2,9)	1:36:A:CYS:SG	1:265:C:CYS:CB	15	0.1
(2,6)	1:11:A:CYS:SG	1:50:A:CYS:CB	1	0.1
(2,5)	1:11:A:CYS:CB	1:50:A:CYS:SG	1	0.1
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE1	9	0.1
(1,1633)	2:336:D:PHE:HA	2:336:D:PHE:HE2	9	0.1
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	2	0.1
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	2	0.1
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE1	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1607)	2:329:D:PHE:HA	2:329:D:PHE:HE2	7	0.1
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE2	6	0.1
(1,1591)	2:325:D:LYS:HB2	2:325:D:LYS:HE3	6	0.1
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE2	6	0.1
(1,1591)	2:325:D:LYS:HB3	2:325:D:LYS:HE3	6	0.1
(1,1580)	2:325:D:LYS:H	2:325:D:LYS:HD2	19	0.1
(1,1580)	2:325:D:LYS:H	2:325:D:LYS:HD3	19	0.1
(1,1564)	2:320:D:ASP:HB3	2:321:D:TYS:HE1	5	0.1
(1,1564)	2:320:D:ASP:HB3	2:321:D:TYS:HE2	5	0.1
(1,1554)	2:315:D:GLU:HA	2:315:D:GLU:HG2	13	0.1
(1,1554)	2:315:D:GLU:HA	2:315:D:GLU:HG3	13	0.1
(1,1554)	2:315:D:GLU:HA	2:315:D:GLU:HG2	19	0.1
(1,1554)	2:315:D:GLU:HA	2:315:D:GLU:HG3	19	0.1
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	5	0.1
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	8	0.1
(1,1476)	1:267:C:ASN:HA	1:268:C:LYS:H	13	0.1
(1,1451)	1:264:C:LYS:HB2	1:265:C:CYS:H	17	0.1
(1,1451)	1:264:C:LYS:HB2	1:265:C:CYS:H	18	0.1
(1,1431)	1:262:C:LEU:HA	1:265:C:CYS:H	17	0.1
(1,1372)	1:257:C:TRP:H	1:257:C:TRP:HE1	9	0.1
(1,1368)	1:256:C:LYS:HD2	1:260:C:GLU:HG2	11	0.1
(1,1368)	1:256:C:LYS:HD3	1:260:C:GLU:HG2	11	0.1
(1,1368)	1:256:C:LYS:HD2	1:260:C:GLU:HG2	14	0.1
(1,1368)	1:256:C:LYS:HD3	1:260:C:GLU:HG2	14	0.1
(1,1291)	1:252:C:ASP:H	1:255:C:LEU:H	5	0.1
(1,1270)	1:251:C:ILE:H	1:251:C:ILE:HD11	6	0.1
(1,1270)	1:251:C:ILE:H	1:251:C:ILE:HD12	6	0.1
(1,1270)	1:251:C:ILE:H	1:251:C:ILE:HD13	6	0.1
(1,1152)	1:237:C:GLN:HE21	1:253:C:PRO:HG3	13	0.1
(1,1152)	1:237:C:GLN:HE22	1:253:C:PRO:HG3	13	0.1
(1,1148)	1:237:C:GLN:H	1:253:C:PRO:HG3	4	0.1
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD1	5	0.1
(1,1113)	1:229:C:LEU:HB2	2:312:D:TYR:HD2	5	0.1
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD1	5	0.1
(1,1113)	1:229:C:LEU:HB3	2:312:D:TYR:HD2	5	0.1
(1,1110)	1:229:C:LEU:H	1:237:C:GLN:H	14	0.1
(1,1076)	1:226:C:LEU:HD11	1:262:C:LEU:H	18	0.1
(1,1076)	1:226:C:LEU:HD12	1:262:C:LEU:H	18	0.1
(1,1076)	1:226:C:LEU:HD13	1:262:C:LEU:H	18	0.1
(1,1076)	1:226:C:LEU:HD21	1:262:C:LEU:H	18	0.1
(1,1076)	1:226:C:LEU:HD22	1:262:C:LEU:H	18	0.1
(1,1076)	1:226:C:LEU:HD23	1:262:C:LEU:H	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1052)	1:225:C:HIS:HE1	1:241:C:ARG:HD2	16	0.1
(1,1052)	1:225:C:HIS:HE1	1:241:C:ARG:HD3	16	0.1
(1,1044)	1:224:C:LYS:HG2	1:243:C:LYS:H	17	0.1
(1,1044)	1:224:C:LYS:HG3	1:243:C:LYS:H	17	0.1
(1,1036)	1:224:C:LYS:HB2	1:225:C:HIS:HE1	14	0.1
(1,1036)	1:224:C:LYS:HB3	1:225:C:HIS:HE1	14	0.1
(1,991)	1:220:C:ARG:HD2	1:223:C:VAL:H	4	0.1
(1,991)	1:220:C:ARG:HD3	1:223:C:VAL:H	4	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG11	4	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG12	4	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG13	4	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG21	4	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG22	4	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG23	4	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG11	18	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG12	18	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG13	18	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG21	18	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG22	18	0.1
(1,931)	1:215:C:GLU:H	1:218:C:VAL:HG23	18	0.1
(1,886)	1:210:C:PRO:HB2	2:312:D:TYR:HD1	20	0.1
(1,886)	1:210:C:PRO:HB2	2:312:D:TYR:HD2	20	0.1
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE1	16	0.1
(1,871)	2:136:B:PHE:HA	2:136:B:PHE:HE2	16	0.1
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD11	2	0.1
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD12	2	0.1
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD13	2	0.1
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD21	2	0.1
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD22	2	0.1
(1,835)	2:127:B:PRO:HD2	1:266:C:LEU:HD23	2	0.1
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD11	2	0.1
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD12	2	0.1
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD13	2	0.1
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD21	2	0.1
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD22	2	0.1
(1,835)	2:127:B:PRO:HD3	1:266:C:LEU:HD23	2	0.1
(1,798)	2:120:B:ASP:HB3	2:121:B:TYS:HE1	5	0.1
(1,798)	2:120:B:ASP:HB3	2:121:B:TYS:HE2	5	0.1
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE1	3	0.1
(1,795)	2:120:B:ASP:HB2	2:121:B:TYS:HE2	3	0.1
(1,789)	2:115:B:GLU:HA	2:116:B:MET:H	7	0.1
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG2	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,788)	2:115:B:GLU:HA	2:115:B:GLU:HG3	19	0.1
(1,758)	2:106:B:ILE:HG21	2:107:B:TYR:HE1	3	0.1
(1,758)	2:106:B:ILE:HG21	2:107:B:TYR:HE2	3	0.1
(1,758)	2:106:B:ILE:HG22	2:107:B:TYR:HE1	3	0.1
(1,758)	2:106:B:ILE:HG22	2:107:B:TYR:HE2	3	0.1
(1,758)	2:106:B:ILE:HG23	2:107:B:TYR:HE1	3	0.1
(1,758)	2:106:B:ILE:HG23	2:107:B:TYR:HE2	3	0.1
(1,758)	2:106:B:ILE:HG21	2:107:B:TYR:HE1	8	0.1
(1,758)	2:106:B:ILE:HG21	2:107:B:TYR:HE2	8	0.1
(1,758)	2:106:B:ILE:HG22	2:107:B:TYR:HE1	8	0.1
(1,758)	2:106:B:ILE:HG22	2:107:B:TYR:HE2	8	0.1
(1,758)	2:106:B:ILE:HG23	2:107:B:TYR:HE1	8	0.1
(1,758)	2:106:B:ILE:HG23	2:107:B:TYR:HE2	8	0.1
(1,746)	2:106:B:ILE:HA	2:107:B:TYR:H	19	0.1
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD1	10	0.1
(1,702)	1:66:A:LEU:HD11	2:329:D:PHE:HD2	10	0.1
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD1	10	0.1
(1,702)	1:66:A:LEU:HD12	2:329:D:PHE:HD2	10	0.1
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD1	10	0.1
(1,702)	1:66:A:LEU:HD13	2:329:D:PHE:HD2	10	0.1
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD1	10	0.1
(1,702)	1:66:A:LEU:HD21	2:329:D:PHE:HD2	10	0.1
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD1	10	0.1
(1,702)	1:66:A:LEU:HD22	2:329:D:PHE:HD2	10	0.1
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD1	10	0.1
(1,702)	1:66:A:LEU:HD23	2:329:D:PHE:HD2	10	0.1
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD2	5	0.1
(1,700)	1:66:A:LEU:HD11	2:327:D:PRO:HD3	5	0.1
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD2	5	0.1
(1,700)	1:66:A:LEU:HD12	2:327:D:PRO:HD3	5	0.1
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD2	5	0.1
(1,700)	1:66:A:LEU:HD13	2:327:D:PRO:HD3	5	0.1
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD2	5	0.1
(1,700)	1:66:A:LEU:HD21	2:327:D:PRO:HD3	5	0.1
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD2	5	0.1
(1,700)	1:66:A:LEU:HD22	2:327:D:PRO:HD3	5	0.1
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD2	5	0.1
(1,700)	1:66:A:LEU:HD23	2:327:D:PRO:HD3	5	0.1
(1,687)	1:66:A:LEU:HD11	1:263:C:GLU:H	20	0.1
(1,687)	1:66:A:LEU:HD12	1:263:C:GLU:H	20	0.1
(1,687)	1:66:A:LEU:HD13	1:263:C:GLU:H	20	0.1
(1,668)	1:65:A:CYS:H	1:68:A:LYS:HG2	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:65:A:CYS:H	1:68:A:LYS:HG3	6	0.1
(1,656)	1:64:A:LYS:HB2	1:65:A:CYS:H	4	0.1
(1,656)	1:64:A:LYS:HB2	1:65:A:CYS:H	9	0.1
(1,656)	1:64:A:LYS:HB2	1:65:A:CYS:H	11	0.1
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	4	0.1
(1,631)	1:62:A:LEU:HG	1:63:A:GLU:H	19	0.1
(1,547)	1:56:A:LYS:HD2	1:57:A:TRP:H	5	0.1
(1,547)	1:56:A:LYS:HD3	1:57:A:TRP:H	5	0.1
(1,489)	1:53:A:PRO:HB3	1:54:A:LYS:H	5	0.1
(1,471)	1:52:A:ASP:H	1:55:A:LEU:H	7	0.1
(1,411)	1:43:A:LYS:H	1:43:A:LYS:HD3	17	0.1
(1,397)	1:42:A:LEU:HB2	1:47:A:ARG:H	19	0.1
(1,386)	1:41:A:ARG:HD2	1:42:A:LEU:H	10	0.1
(1,386)	1:41:A:ARG:HD3	1:42:A:LEU:H	10	0.1
(1,334)	1:38:A:ILE:H	1:38:A:ILE:HD11	19	0.1
(1,334)	1:38:A:ILE:H	1:38:A:ILE:HD12	19	0.1
(1,334)	1:38:A:ILE:H	1:38:A:ILE:HD13	19	0.1
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE1	17	0.1
(1,290)	1:29:A:LEU:HB2	2:112:B:TYR:HE2	17	0.1
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE1	17	0.1
(1,290)	1:29:A:LEU:HB3	2:112:B:TYR:HE2	17	0.1
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD1	2	0.1
(1,289)	1:29:A:LEU:HB2	2:112:B:TYR:HD2	2	0.1
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD1	2	0.1
(1,289)	1:29:A:LEU:HB3	2:112:B:TYR:HD2	2	0.1
(1,267)	1:28:A:ILE:HB	1:29:A:LEU:H	7	0.1
(1,252)	1:27:A:LYS:HE2	1:225:C:HIS:HE1	8	0.1
(1,252)	1:27:A:LYS:HE3	1:225:C:HIS:HE1	8	0.1
(1,239)	1:27:A:LYS:HD3	2:112:B:TYR:HD1	12	0.1
(1,239)	1:27:A:LYS:HD3	2:112:B:TYR:HD2	12	0.1
(1,225)	1:26:A:LEU:HD11	1:62:A:LEU:H	13	0.1
(1,225)	1:26:A:LEU:HD12	1:62:A:LEU:H	13	0.1
(1,225)	1:26:A:LEU:HD13	1:62:A:LEU:H	13	0.1
(1,225)	1:26:A:LEU:HD21	1:62:A:LEU:H	13	0.1
(1,225)	1:26:A:LEU:HD22	1:62:A:LEU:H	13	0.1
(1,225)	1:26:A:LEU:HD23	1:62:A:LEU:H	13	0.1
(1,188)	1:25:A:HIS:HE1	1:41:A:ARG:HB2	2	0.1
(1,188)	1:25:A:HIS:HE1	1:41:A:ARG:HB3	2	0.1
(1,187)	1:25:A:HIS:HE1	1:27:A:LYS:HE2	3	0.1
(1,187)	1:25:A:HIS:HE1	1:27:A:LYS:HE3	3	0.1
(1,187)	1:25:A:HIS:HE1	1:27:A:LYS:HE2	12	0.1
(1,187)	1:25:A:HIS:HE1	1:27:A:LYS:HE3	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE2	4	0.1
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE3	4	0.1
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE2	17	0.1
(1,185)	1:25:A:HIS:HE1	1:227:C:LYS:HE3	17	0.1
(1,170)	1:24:A:LYS:HG2	1:25:A:HIS:H	2	0.1
(1,170)	1:24:A:LYS:HG3	1:25:A:HIS:H	2	0.1
(1,149)	1:24:A:LYS:H	1:24:A:LYS:HD2	4	0.1
(1,149)	1:24:A:LYS:H	1:24:A:LYS:HD3	4	0.1
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE1	18	0.1
(1,117)	1:20:A:ARG:HD2	1:61:A:TYR:HE2	18	0.1
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE1	18	0.1
(1,117)	1:20:A:ARG:HD3	1:61:A:TYR:HE2	18	0.1
(1,115)	1:20:A:ARG:HD2	1:23:A:VAL:H	8	0.1
(1,115)	1:20:A:ARG:HD3	1:23:A:VAL:H	8	0.1
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG21	15	0.1
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG22	15	0.1
(1,82)	1:18:A:VAL:HB	1:51:A:ILE:HG23	15	0.1
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG11	19	0.1
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG12	19	0.1
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG13	19	0.1
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG21	19	0.1
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG22	19	0.1
(1,55)	1:15:A:GLU:H	1:18:A:VAL:HG23	19	0.1
(1,7)	1:10:A:PRO:HB2	2:112:B:TYR:HD1	6	0.1
(1,7)	1:10:A:PRO:HB2	2:112:B:TYR:HD2	6	0.1
(1,7)	1:10:A:PRO:HB2	2:112:B:TYR:HD1	13	0.1
(1,7)	1:10:A:PRO:HB2	2:112:B:TYR:HD2	13	0.1

10 Dihedral-angle violation analysis

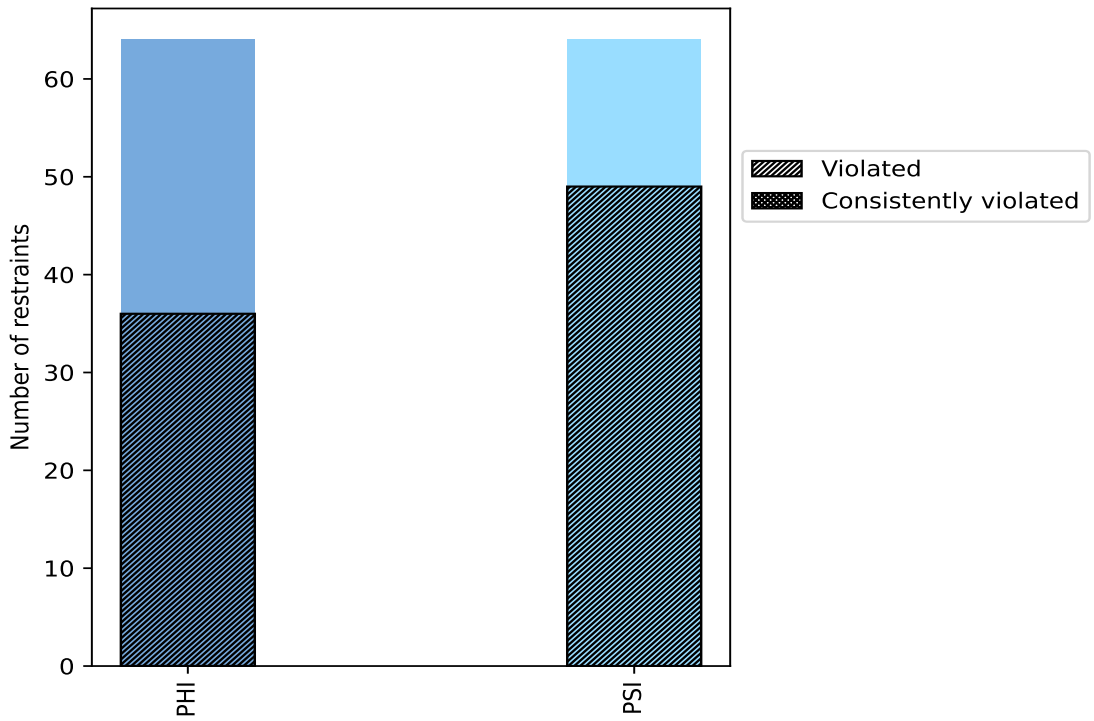
10.1 Summary of dihedral-angle violations

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]
PHI	64	50.0	36	56.2	28.1	0	0.0	0.0
PSI	64	50.0	49	76.6	38.3	0	0.0	0.0
Total	128	100.0	85	66.4	66.4	0	0.0	0.0

[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



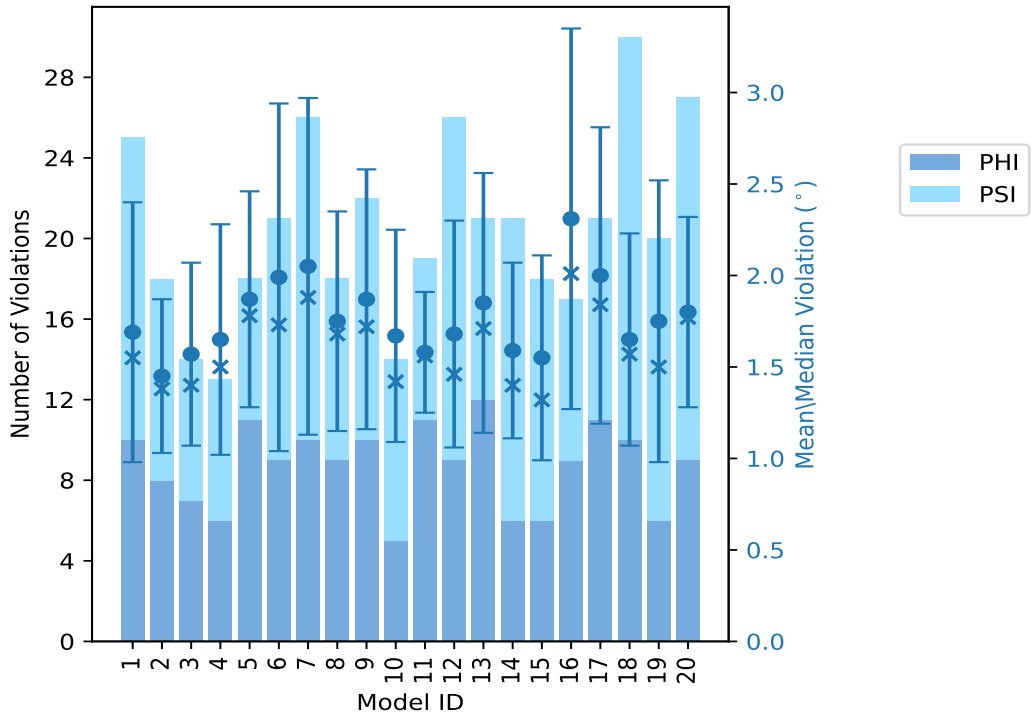
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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 (°)
	PHI	PSI	Total				
1	10	15	25	1.69	4.56	0.71	1.55
2	8	10	18	1.45	2.9	0.42	1.38
3	7	7	14	1.57	2.54	0.5	1.4
4	6	7	13	1.65	3.3	0.63	1.5
5	11	7	18	1.87	3.41	0.59	1.78
6	9	12	21	1.99	5.04	0.95	1.73
7	10	16	26	2.05	4.8	0.92	1.88
8	9	9	18	1.75	3.84	0.6	1.68
9	10	12	22	1.87	3.84	0.71	1.72
10	5	9	14	1.67	2.82	0.58	1.42
11	11	8	19	1.58	2.32	0.33	1.56
12	9	17	26	1.68	3.06	0.62	1.46
13	12	9	21	1.85	3.23	0.71	1.71
14	6	15	21	1.59	2.67	0.48	1.4
15	6	12	18	1.55	2.78	0.56	1.32
16	9	8	17	2.31	4.89	1.04	2.01
17	11	10	21	2.0	4.33	0.81	1.84
18	10	20	30	1.65	3.16	0.58	1.57
19	6	14	20	1.75	4.54	0.77	1.5
20	9	18	27	1.8	3.18	0.52	1.77

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble

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	
PHI	PSI	Total	Count[1]	%
11	9	20	1	5.0
6	9	15	2	10.0
3	7	10	3	15.0
2	4	6	4	20.0
2	5	7	5	25.0
1	0	1	6	30.0
1	3	4	7	35.0
1	2	3	8	40.0
4	1	5	9	45.0
0	3	3	10	50.0
1	2	3	11	55.0

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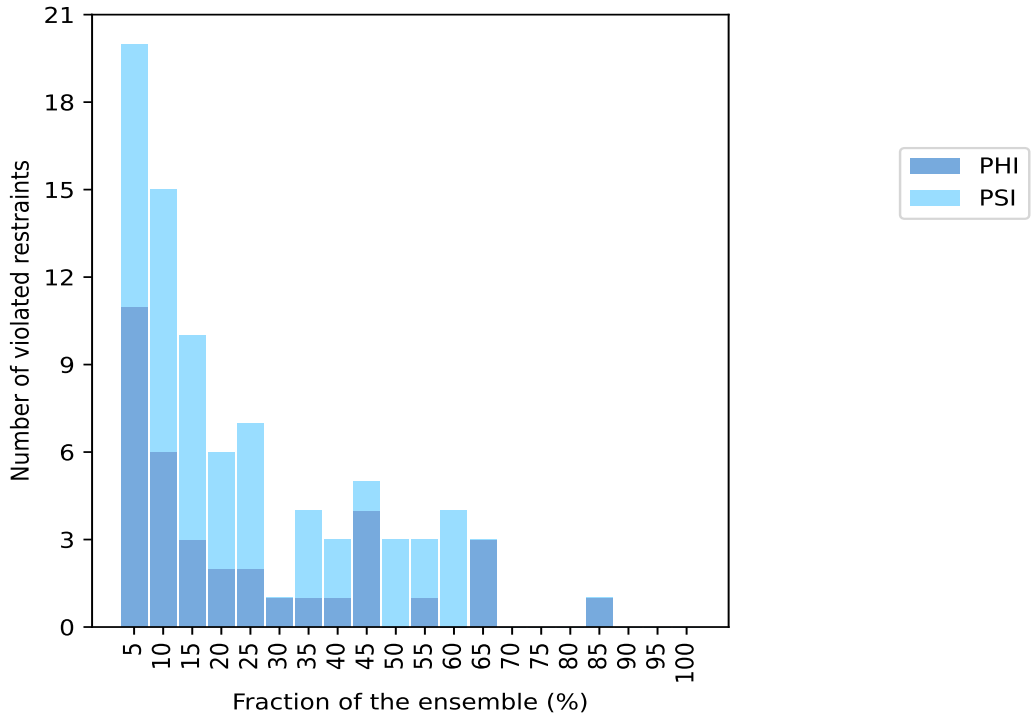
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	4	4	12	60.0
3	0	3	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

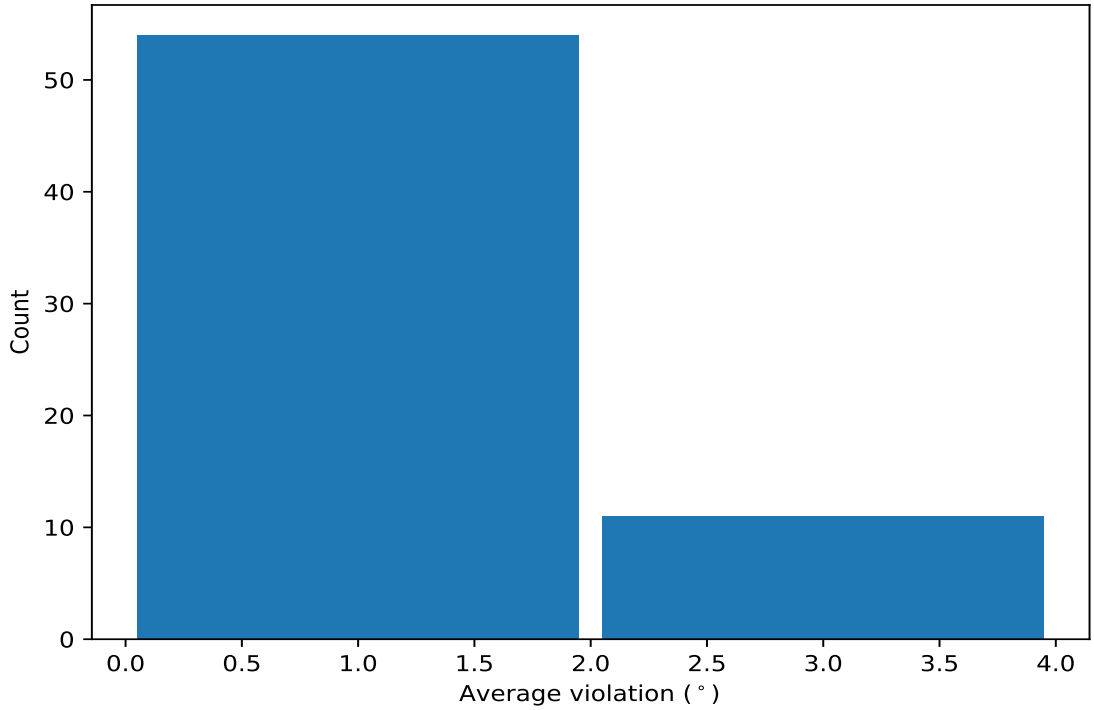


10.4 Most violated dihedral-angle restraints in the ensemble

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

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
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	17	1.86	0.54	1.77
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	13	2.07	0.88	1.83
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	13	2.04	0.76	1.77
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	13	1.91	0.5	1.89
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	12	2.6	0.97	2.74
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	12	1.99	0.48	1.94
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	12	1.84	0.7	1.58
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	12	1.72	0.42	1.73
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	11	2.81	1.19	2.13
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	11	1.86	0.59	1.77
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	11	1.52	0.34	1.41
(1,39)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ARG:N	10	1.57	0.57	1.34
(1,29)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	10	1.54	0.58	1.42
(1,118)	1:259:C:GLN:N	1:259:C:GLN:CA	1:259:C:GLN:C	1:260:C:GLU:N	10	1.53	0.43	1.46
(1,42)	1:47:A:ARG:C	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	9	2.47	0.8	2.32
(1,67)	1:208:C:ARG:C	1:209:C:CYS:N	1:209:C:CYS:CA	1:209:C:CYS:C	9	2.42	1.14	2.1
(1,104)	1:240:C:ALA:C	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	9	2.27	0.91	1.96
(1,3)	1:8:A:ARG:C	1:9:A:CYS:N	1:9:A:CYS:CA	1:9:A:CYS:C	9	2.14	0.94	1.96
(1,41)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:LEU:N	9	1.78	0.72	1.66
(1,106)	1:247:C:ARG:C	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	8	2.27	0.45	2.22

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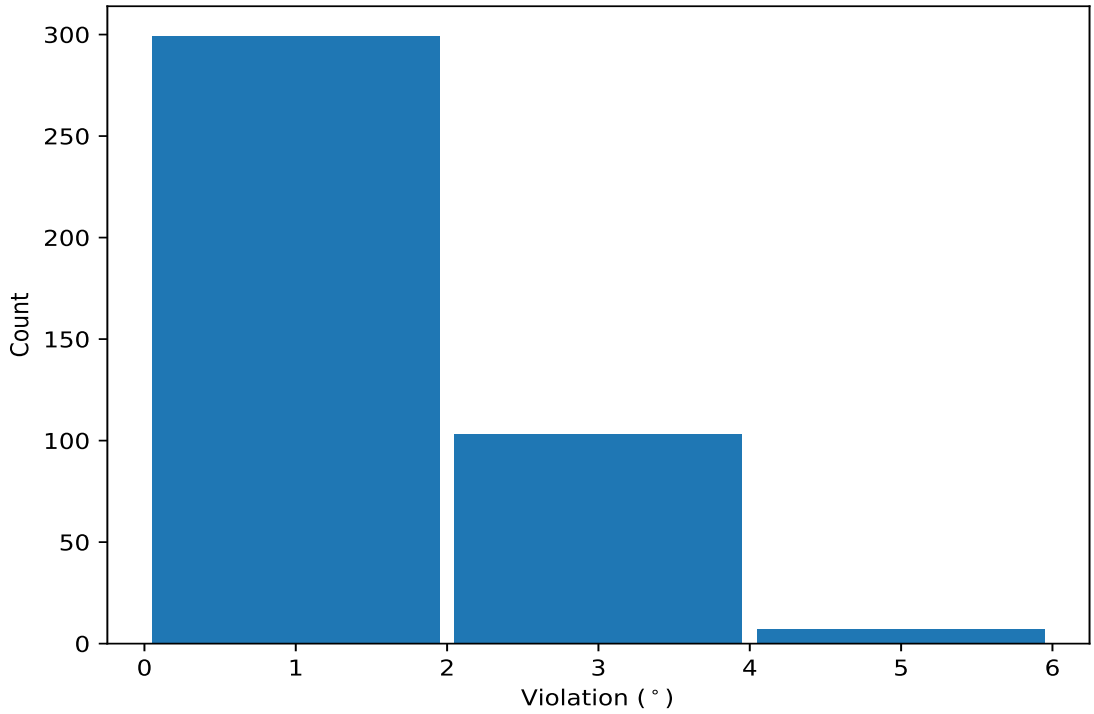
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,33)	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	1:35:A:ALA:N	8	1.51	0.45	1.27
(1,19)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ASN:N	8	1.51	0.36	1.4
(1,83)	1:221:C:ALA:N	1:221:C:ALA:CA	1:221:C:ALA:C	1:222:C:ASN:N	7	1.53	0.45	1.3
(1,125)	1:262:C:LEU:C	1:263:C:GLU:N	1:263:C:GLU:CA	1:263:C:GLU:C	7	1.42	0.23	1.41
(1,56)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:TYR:N	7	1.4	0.34	1.23
(1,85)	1:223:C:VAL:N	1:223:C:VAL:CA	1:223:C:VAL:C	1:224:C:LYS:N	7	1.37	0.22	1.34
(1,32)	1:33:A:ASN:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	6	1.46	0.36	1.38
(1,103)	1:240:C:ALA:N	1:240:C:ALA:CA	1:240:C:ALA:C	1:241:C:ARG:N	5	2.23	0.71	2.45
(1,79)	1:219:C:ALA:N	1:219:C:ALA:CA	1:219:C:ALA:C	1:220:C:ARG:N	5	1.67	0.14	1.71
(1,31)	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	1:32:A:PRO:N	5	1.65	0.36	1.49
(1,35)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	5	1.51	0.21	1.63
(1,12)	1:17:A:HIS:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	5	1.47	0.28	1.55
(1,76)	1:217:C:HIS:C	1:218:C:VAL:N	1:218:C:VAL:CA	1:218:C:VAL:C	5	1.42	0.22	1.32
(1,105)	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	1:242:C:LEU:N	5	1.39	0.32	1.45
(1,96)	1:233:C:ASN:C	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	4	2.16	0.64	2.0
(1,9)	1:14:A:PHE:N	1:14:A:PHE:CA	1:14:A:PHE:C	1:15:A:GLU:N	4	1.85	0.39	1.91
(1,71)	1:213:C:PHE:N	1:213:C:PHE:CA	1:213:C:PHE:C	1:214:C:PHE:N	4	1.45	0.28	1.39
(1,25)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:ILE:N	4	1.32	0.13	1.32
(1,1)	1:7:A:TYR:C	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	4	1.23	0.19	1.22
(1,107)	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	1:249:C:VAL:N	4	1.23	0.13	1.19
(1,89)	1:227:C:LYS:N	1:227:C:LYS:CA	1:227:C:LYS:C	1:228:C:ILE:N	3	1.94	0.38	2.05
(1,21)	1:23:A:VAL:N	1:23:A:VAL:CA	1:23:A:VAL:C	1:24:A:LYS:N	3	1.88	0.58	1.88
(1,93)	1:230:C:ASN:N	1:230:C:ASN:CA	1:230:C:ASN:C	1:231:C:THR:N	3	1.88	0.7	1.65
(1,44)	1:48:A:GLN:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	3	1.81	0.26	1.87
(1,17)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	3	1.72	0.18	1.79
(1,120)	1:260:C:GLU:N	1:260:C:GLU:CA	1:260:C:GLU:C	1:261:C:TYR:N	3	1.51	0.11	1.54
(1,92)	1:229:C:LEU:C	1:230:C:ASN:N	1:230:C:ASN:CA	1:230:C:ASN:C	3	1.48	0.29	1.33
(1,109)	1:249:C:VAL:N	1:249:C:VAL:CA	1:249:C:VAL:C	1:250:C:CYS:N	3	1.48	0.09	1.46
(1,60)	1:62:A:LEU:N	1:62:A:LEU:CA	1:62:A:LEU:C	1:63:A:GLU:N	3	1.36	0.13	1.3
(1,61)	1:62:A:LEU:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	3	1.17	0.15	1.13
(1,5)	1:11:A:CYS:C	1:12:A:ARG:N	1:12:A:ARG:CA	1:12:A:ARG:C	2	1.98	0.9	1.98
(1,7)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:PHE:N	2	1.8	0.38	1.8
(1,110)	1:250:C:CYS:N	1:250:C:CYS:CA	1:250:C:CYS:C	1:251:C:ILE:N	2	1.69	0.23	1.69
(1,11)	1:15:A:GLU:N	1:15:A:GLU:CA	1:15:A:GLU:C	1:16:A:SER:N	2	1.68	0.55	1.68
(1,45)	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	1:50:A:CYS:N	2	1.66	0.56	1.66
(1,69)	1:211:C:CYS:C	1:212:C:ARG:N	1:212:C:ARG:CA	1:212:C:ARG:C	2	1.5	0.37	1.5
(1,119)	1:259:C:GLN:C	1:260:C:GLU:N	1:260:C:GLU:CA	1:260:C:GLU:C	2	1.48	0.24	1.48
(1,77)	1:218:C:VAL:N	1:218:C:VAL:CA	1:218:C:VAL:C	1:219:C:ALA:N	2	1.42	0.34	1.42
(1,13)	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	1:19:A:ALA:N	2	1.29	0.24	1.29
(1,73)	1:214:C:PHE:N	1:214:C:PHE:CA	1:214:C:PHE:C	1:215:C:GLU:N	2	1.29	0.23	1.29
(1,6)	1:12:A:ARG:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	2	1.2	0.17	1.2
(1,80)	1:219:C:ALA:C	1:220:C:ARG:N	1:220:C:ARG:CA	1:220:C:ARG:C	2	1.2	0.11	1.2
(1,58)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:LEU:N	2	1.13	0.12	1.13
(1,16)	1:19:A:ALA:C	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	2	1.11	0.04	1.11
(1,46)	1:50:A:CYS:N	1:50:A:CYS:CA	1:50:A:CYS:C	1:51:A:ILE:N	2	1.02	0.01	1.02

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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

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 (°)
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	6	5.04
(1,67)	1:208:C:ARG:C	1:209:C:CYS:N	1:209:C:CYS:CA	1:209:C:CYS:C	16	4.89
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	7	4.8
(1,3)	1:8:A:ARG:C	1:9:A:CYS:N	1:9:A:CYS:CA	1:9:A:CYS:C	1	4.56
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	19	4.54
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	17	4.33
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	16	4.07
(1,67)	1:208:C:ARG:C	1:209:C:CYS:N	1:209:C:CYS:CA	1:209:C:CYS:C	6	3.97
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	7	3.92
(1,104)	1:240:C:ALA:C	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	9	3.84
(1,42)	1:47:A:ARG:C	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	8	3.84
(1,42)	1:47:A:ARG:C	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	16	3.47
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	5	3.41
(1,104)	1:240:C:ALA:C	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	7	3.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,41)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:LEU:N	17	3.35
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	4	3.3
(1,103)	1:240:C:ALA:N	1:240:C:ALA:CA	1:240:C:ALA:C	1:241:C:ARG:N	7	3.25
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	13	3.23
(1,104)	1:240:C:ALA:C	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	17	3.22
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	13	3.2
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	20	3.18
(1,96)	1:233:C:ASN:C	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	18	3.16
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	16	3.09
(1,29)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	7	3.08
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	12	3.06
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	18	3.03
(1,42)	1:47:A:ARG:C	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	9	2.96
(1,39)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ARG:N	16	2.95
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	2	2.9
(1,5)	1:11:A:CYS:C	1:12:A:ARG:N	1:12:A:ARG:CA	1:12:A:ARG:C	13	2.89
(1,106)	1:247:C:ARG:C	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	12	2.88
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	13	2.88
(1,106)	1:247:C:ARG:C	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	9	2.86
(1,93)	1:230:C:ASN:N	1:230:C:ASN:CA	1:230:C:ASN:C	1:231:C:THR:N	10	2.82
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	6	2.78
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	15	2.78
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	10	2.74
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	5	2.74
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	19	2.73
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	20	2.71
(1,3)	1:8:A:ARG:C	1:9:A:CYS:N	1:9:A:CYS:CA	1:9:A:CYS:C	20	2.7
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	12	2.7
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	5	2.67
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	14	2.67
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	9	2.65
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	17	2.63
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	1	2.61
(1,42)	1:47:A:ARG:C	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	12	2.58
(1,21)	1:23:A:VAL:N	1:23:A:VAL:CA	1:23:A:VAL:C	1:24:A:LYS:N	18	2.58
(1,106)	1:247:C:ARG:C	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	4	2.57
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	6	2.55
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	3	2.54
(1,118)	1:259:C:GLN:N	1:259:C:GLN:CA	1:259:C:GLN:C	1:260:C:GLU:N	15	2.52
(1,41)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:LEU:N	15	2.51
(1,83)	1:221:C:ALA:N	1:221:C:ALA:CA	1:221:C:ALA:C	1:222:C:ASN:N	13	2.48
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	12	2.48
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	3	2.47
(1,103)	1:240:C:ALA:N	1:240:C:ALA:CA	1:240:C:ALA:C	1:241:C:ARG:N	17	2.47
(1,103)	1:240:C:ALA:N	1:240:C:ALA:CA	1:240:C:ALA:C	1:241:C:ARG:N	9	2.45
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	16	2.44
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	13	2.43
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	1	2.42
(1,106)	1:247:C:ARG:C	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	16	2.41
(1,33)	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	1:35:A:ALA:N	18	2.37
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	19	2.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,89)	1:227:C:LYS:N	1:227:C:LYS:CA	1:227:C:LYS:C	1:228:C:ILE:N	14	2.34
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	10	2.33
(1,42)	1:47:A:ARG:C	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	11	2.32
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	20	2.31
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	20	2.3
(1,42)	1:47:A:ARG:C	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	17	2.3
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	9	2.29
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	7	2.26
(1,9)	1:14:A:PHE:N	1:14:A:PHE:CA	1:14:A:PHE:C	1:15:A:GLU:N	20	2.26
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	7	2.25
(1,96)	1:233:C:ASN:C	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	10	2.25
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	7	2.24
(1,11)	1:15:A:GLU:N	1:15:A:GLU:CA	1:15:A:GLU:C	1:16:A:SER:N	14	2.23
(1,45)	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	1:50:A:CYS:N	12	2.22
(1,67)	1:208:C:ARG:C	1:209:C:CYS:N	1:209:C:CYS:CA	1:209:C:CYS:C	3	2.2
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	14	2.2
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	6	2.19
(1,67)	1:208:C:ARG:C	1:209:C:CYS:N	1:209:C:CYS:CA	1:209:C:CYS:C	18	2.19
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	15	2.18
(1,9)	1:14:A:PHE:N	1:14:A:PHE:CA	1:14:A:PHE:C	1:15:A:GLU:N	19	2.18
(1,7)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:PHE:N	12	2.17
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	8	2.16
(1,31)	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	1:32:A:PRO:N	6	2.16
(1,32)	1:33:A:ASN:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	4	2.15
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	14	2.14
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	5	2.13
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	8	2.11
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	6	2.1
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	16	2.1
(1,67)	1:208:C:ARG:C	1:209:C:CYS:N	1:209:C:CYS:CA	1:209:C:CYS:C	8	2.1
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	14	2.1
(1,44)	1:48:A:GLN:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	5	2.1
(1,56)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:TYR:N	9	2.09
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	18	2.07
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	7	2.07
(1,41)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:LEU:N	7	2.06
(1,89)	1:227:C:LYS:N	1:227:C:LYS:CA	1:227:C:LYS:C	1:228:C:ILE:N	1	2.05
(1,39)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ARG:N	12	2.05
(1,106)	1:247:C:ARG:C	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	5	2.04
(1,30)	1:30:A:ASN:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	6	2.04
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	7	2.03
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	5	2.03
(1,104)	1:240:C:ALA:C	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	20	2.02
(1,94)	1:230:C:ASN:C	1:231:C:THR:N	1:231:C:THR:CA	1:231:C:THR:C	16	2.01
(1,3)	1:8:A:ARG:C	1:9:A:CYS:N	1:9:A:CYS:CA	1:9:A:CYS:C	5	2.01
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	1	1.99
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	9	1.99
(1,67)	1:208:C:ARG:C	1:209:C:CYS:N	1:209:C:CYS:CA	1:209:C:CYS:C	17	1.98
(1,19)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ASN:N	18	1.98
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	18	1.97
(1,31)	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	1:32:A:PRO:N	7	1.97

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,3)	1:8:A:ARG:C	1:9:A:CYS:N	1:9:A:CYS:CA	1:9:A:CYS:C	2	1.97
(1,118)	1:259:C:GLN:N	1:259:C:GLN:CA	1:259:C:GLN:C	1:260:C:GLU:N	17	1.96
(1,104)	1:240:C:ALA:C	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	18	1.96
(1,19)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ASN:N	19	1.96
(1,3)	1:8:A:ARG:C	1:9:A:CYS:N	1:9:A:CYS:CA	1:9:A:CYS:C	6	1.96
(1,42)	1:47:A:ARG:C	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	13	1.95
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	18	1.95
(1,106)	1:247:C:ARG:C	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	8	1.94
(1,33)	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	1:35:A:ALA:N	13	1.94
(1,19)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ASN:N	17	1.94
(1,110)	1:250:C:CYS:N	1:250:C:CYS:CA	1:250:C:CYS:C	1:251:C:ILE:N	7	1.92
(1,105)	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	1:242:C:LEU:N	19	1.91
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	9	1.91
(1,81)	1:220:C:ARG:N	1:220:C:ARG:CA	1:220:C:ARG:C	1:221:C:ALA:N	20	1.91
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	13	1.9
(1,17)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	17	1.9
(1,92)	1:229:C:LEU:C	1:230:C:ASN:N	1:230:C:ASN:CA	1:230:C:ASN:C	11	1.89
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	16	1.89
(1,29)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	8	1.88
(1,21)	1:23:A:VAL:N	1:23:A:VAL:CA	1:23:A:VAL:C	1:24:A:LYS:N	11	1.88
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	9	1.87
(1,71)	1:213:C:PHE:N	1:213:C:PHE:CA	1:213:C:PHE:C	1:214:C:PHE:N	20	1.87
(1,69)	1:211:C:CYS:C	1:212:C:ARG:N	1:212:C:ARG:CA	1:212:C:ARG:C	11	1.87
(1,44)	1:48:A:GLN:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	6	1.87
(1,33)	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	1:35:A:ALA:N	20	1.87
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	11	1.86
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	18	1.86
(1,104)	1:240:C:ALA:C	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	13	1.84
(1,79)	1:219:C:ALA:N	1:219:C:ALA:CA	1:219:C:ALA:C	1:220:C:ARG:N	18	1.84
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	17	1.84
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	1	1.84
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	7	1.83
(1,106)	1:247:C:ARG:C	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	11	1.83
(1,103)	1:240:C:ALA:N	1:240:C:ALA:CA	1:240:C:ALA:C	1:241:C:ARG:N	20	1.83
(1,67)	1:208:C:ARG:C	1:209:C:CYS:N	1:209:C:CYS:CA	1:209:C:CYS:C	5	1.83
(1,12)	1:17:A:HIS:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	1	1.83
(1,125)	1:262:C:LEU:C	1:263:C:GLU:N	1:263:C:GLU:CA	1:263:C:GLU:C	20	1.81
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	16	1.81
(1,41)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:LEU:N	12	1.79
(1,39)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ARG:N	1	1.79
(1,39)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ARG:N	19	1.79
(1,17)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	20	1.79
(1,85)	1:223:C:VAL:N	1:223:C:VAL:CA	1:223:C:VAL:C	1:224:C:LYS:N	11	1.78
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	8	1.77
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	14	1.77
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	7	1.77
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	9	1.77
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	1	1.77
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	8	1.77
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	17	1.77
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	20	1.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,77)	1:218:C:VAL:N	1:218:C:VAL:CA	1:218:C:VAL:C	1:219:C:ALA:N	15	1.76
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	1	1.75
(1,96)	1:233:C:ASN:C	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	20	1.75
(1,79)	1:219:C:ALA:N	1:219:C:ALA:CA	1:219:C:ALA:C	1:220:C:ARG:N	20	1.75
(1,35)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	5	1.74
(1,104)	1:240:C:ALA:C	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	3	1.73
(1,83)	1:221:C:ALA:N	1:221:C:ALA:CA	1:221:C:ALA:C	1:222:C:ASN:N	6	1.73
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	4	1.73
(1,66)	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	1:209:C:CYS:N	18	1.73
(1,119)	1:259:C:GLN:C	1:260:C:GLU:N	1:260:C:GLU:CA	1:260:C:GLU:C	11	1.72
(1,43)	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	1:49:A:VAL:N	3	1.72
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	20	1.71
(1,83)	1:221:C:ALA:N	1:221:C:ALA:CA	1:221:C:ALA:C	1:222:C:ASN:N	3	1.71
(1,79)	1:219:C:ALA:N	1:219:C:ALA:CA	1:219:C:ALA:C	1:220:C:ARG:N	12	1.71
(1,56)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:TYR:N	20	1.71
(1,3)	1:8:A:ARG:C	1:9:A:CYS:N	1:9:A:CYS:CA	1:9:A:CYS:C	13	1.71
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	11	1.69
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	2	1.69
(1,76)	1:217:C:HIS:C	1:218:C:VAL:N	1:218:C:VAL:CA	1:218:C:VAL:C	1	1.69
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	8	1.69
(1,3)	1:8:A:ARG:C	1:9:A:CYS:N	1:9:A:CYS:CA	1:9:A:CYS:C	17	1.69
(1,76)	1:217:C:HIS:C	1:218:C:VAL:N	1:218:C:VAL:CA	1:218:C:VAL:C	7	1.68
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	14	1.67
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	8	1.67
(1,41)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:LEU:N	9	1.66
(1,118)	1:259:C:GLN:N	1:259:C:GLN:CA	1:259:C:GLN:C	1:260:C:GLU:N	19	1.65
(1,93)	1:230:C:ASN:N	1:230:C:ASN:CA	1:230:C:ASN:C	1:231:C:THR:N	17	1.65
(1,35)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	20	1.65
(1,29)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	18	1.65
(1,24)	1:26:A:LEU:C	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	15	1.64
(1,9)	1:14:A:PHE:N	1:14:A:PHE:CA	1:14:A:PHE:C	1:15:A:GLU:N	14	1.64
(1,125)	1:262:C:LEU:C	1:263:C:GLU:N	1:263:C:GLU:CA	1:263:C:GLU:C	2	1.63
(1,120)	1:260:C:GLU:N	1:260:C:GLU:CA	1:260:C:GLU:C	1:261:C:TYR:N	7	1.63
(1,35)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	19	1.63
(1,106)	1:247:C:ARG:C	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	10	1.62
(1,42)	1:47:A:ARG:C	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	7	1.62
(1,32)	1:33:A:ASN:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	5	1.62
(1,12)	1:17:A:HIS:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	5	1.62
(1,79)	1:219:C:ALA:N	1:219:C:ALA:CA	1:219:C:ALA:C	1:220:C:ARG:N	8	1.61
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1	1.61
(1,109)	1:249:C:VAL:N	1:249:C:VAL:CA	1:249:C:VAL:C	1:250:C:CYS:N	12	1.6
(1,118)	1:259:C:GLN:N	1:259:C:GLN:CA	1:259:C:GLN:C	1:260:C:GLU:N	18	1.59
(1,85)	1:223:C:VAL:N	1:223:C:VAL:CA	1:223:C:VAL:C	1:224:C:LYS:N	12	1.59
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	6	1.56
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	11	1.56
(1,118)	1:259:C:GLN:N	1:259:C:GLN:CA	1:259:C:GLN:C	1:260:C:GLU:N	1	1.55
(1,71)	1:213:C:PHE:N	1:213:C:PHE:CA	1:213:C:PHE:C	1:214:C:PHE:N	18	1.55
(1,60)	1:62:A:LEU:N	1:62:A:LEU:CA	1:62:A:LEU:C	1:63:A:GLU:N	4	1.55
(1,12)	1:17:A:HIS:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	17	1.55
(1,120)	1:260:C:GLU:N	1:260:C:GLU:CA	1:260:C:GLU:C	1:261:C:TYR:N	9	1.54
(1,13)	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	1:19:A:ALA:N	5	1.53

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,73)	1:214:C:PHE:N	1:214:C:PHE:CA	1:214:C:PHE:C	1:215:C:GLU:N	12	1.52
(1,28)	1:29:A:LEU:C	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	11	1.52
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	4	1.51
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	15	1.51
(1,3)	1:8:A:ARG:C	1:9:A:CYS:N	1:9:A:CYS:CA	1:9:A:CYS:C	15	1.51
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	1	1.51
(1,105)	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	1:242:C:LEU:N	4	1.5
(1,29)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	19	1.5
(1,96)	1:233:C:ASN:C	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	11	1.49
(1,31)	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	1:32:A:PRO:N	19	1.49
(1,1)	1:7:A:TYR:C	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	11	1.49
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	17	1.48
(1,25)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:ILE:N	1	1.48
(1,17)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	19	1.48
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	18	1.47
(1,44)	1:48:A:GLN:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	16	1.47
(1,31)	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	1:32:A:PRO:N	2	1.47
(1,125)	1:262:C:LEU:C	1:263:C:GLU:N	1:263:C:GLU:CA	1:263:C:GLU:C	3	1.46
(1,110)	1:250:C:CYS:N	1:250:C:CYS:CA	1:250:C:CYS:C	1:251:C:ILE:N	16	1.46
(1,109)	1:249:C:VAL:N	1:249:C:VAL:CA	1:249:C:VAL:C	1:250:C:CYS:N	1	1.46
(1,105)	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	1:242:C:LEU:N	10	1.45
(1,32)	1:33:A:ASN:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	8	1.45
(1,29)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	6	1.45
(1,107)	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	1:249:C:VAL:N	10	1.44
(1,89)	1:227:C:LYS:N	1:227:C:LYS:CA	1:227:C:LYS:C	1:228:C:ILE:N	6	1.44
(1,19)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ASN:N	16	1.44
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	13	1.42
(1,79)	1:219:C:ALA:N	1:219:C:ALA:CA	1:219:C:ALA:C	1:220:C:ARG:N	13	1.42
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	20	1.42
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	2	1.42
(1,7)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:PHE:N	2	1.42
(1,125)	1:262:C:LEU:C	1:263:C:GLU:N	1:263:C:GLU:CA	1:263:C:GLU:C	9	1.41
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	19	1.41
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	14	1.41
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	1	1.41
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	10	1.41
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	6	1.41
(1,25)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:ILE:N	6	1.41
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	13	1.4
(1,29)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	14	1.4
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	12	1.39
(1,67)	1:208:C:ARG:C	1:209:C:CYS:N	1:209:C:CYS:CA	1:209:C:CYS:C	20	1.39
(1,118)	1:259:C:GLN:N	1:259:C:GLN:CA	1:259:C:GLN:C	1:260:C:GLU:N	2	1.38
(1,61)	1:62:A:LEU:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	2	1.38
(1,56)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:TYR:N	7	1.38
(1,109)	1:249:C:VAL:N	1:249:C:VAL:CA	1:249:C:VAL:C	1:250:C:CYS:N	15	1.37
(1,39)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ARG:N	9	1.37
(1,6)	1:12:A:ARG:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	2	1.37
(1,125)	1:262:C:LEU:C	1:263:C:GLU:N	1:263:C:GLU:CA	1:263:C:GLU:C	12	1.36
(1,120)	1:260:C:GLU:N	1:260:C:GLU:CA	1:260:C:GLU:C	1:261:C:TYR:N	12	1.36
(1,118)	1:259:C:GLN:N	1:259:C:GLN:CA	1:259:C:GLN:C	1:260:C:GLU:N	8	1.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	14	1.36
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	17	1.35
(1,85)	1:223:C:VAL:N	1:223:C:VAL:CA	1:223:C:VAL:C	1:224:C:LYS:N	7	1.35
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	3	1.35
(1,19)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ASN:N	10	1.35
(1,12)	1:17:A:HIS:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	7	1.35
(1,85)	1:223:C:VAL:N	1:223:C:VAL:CA	1:223:C:VAL:C	1:224:C:LYS:N	1	1.34
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	8	1.34
(1,1)	1:7:A:TYR:C	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	5	1.34
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	8	1.33
(1,92)	1:229:C:LEU:C	1:230:C:ASN:N	1:230:C:ASN:CA	1:230:C:ASN:C	19	1.33
(1,41)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:LEU:N	11	1.33
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	18	1.32
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	10	1.32
(1,76)	1:217:C:HIS:C	1:218:C:VAL:N	1:218:C:VAL:CA	1:218:C:VAL:C	5	1.32
(1,75)	1:215:C:GLU:N	1:215:C:GLU:CA	1:215:C:GLU:C	1:216:C:SER:N	5	1.32
(1,9)	1:14:A:PHE:N	1:14:A:PHE:CA	1:14:A:PHE:C	1:15:A:GLU:N	6	1.32
(1,80)	1:219:C:ALA:C	1:220:C:ARG:N	1:220:C:ARG:CA	1:220:C:ARG:C	9	1.31
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	12	1.31
(1,32)	1:33:A:ASN:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	6	1.31
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	2	1.3
(1,85)	1:223:C:VAL:N	1:223:C:VAL:CA	1:223:C:VAL:C	1:224:C:LYS:N	4	1.3
(1,83)	1:221:C:ALA:N	1:221:C:ALA:CA	1:221:C:ALA:C	1:222:C:ASN:N	17	1.3
(1,60)	1:62:A:LEU:N	1:62:A:LEU:CA	1:62:A:LEU:C	1:63:A:GLU:N	14	1.3
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	12	1.3
(1,39)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ARG:N	13	1.3
(1,35)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	18	1.3
(1,33)	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	1:35:A:ALA:N	9	1.3
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	16	1.3
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	13	1.29
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	3	1.28
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	12	1.28
(1,29)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	15	1.27
(1,83)	1:221:C:ALA:N	1:221:C:ALA:CA	1:221:C:ALA:C	1:222:C:ASN:N	2	1.26
(1,107)	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	1:249:C:VAL:N	11	1.25
(1,58)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:LEU:N	14	1.25
(1,33)	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	1:35:A:ALA:N	19	1.25
(1,19)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ASN:N	9	1.25
(1,2)	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1:9:A:CYS:N	10	1.25
(1,119)	1:259:C:GLN:C	1:260:C:GLU:N	1:260:C:GLU:CA	1:260:C:GLU:C	6	1.24
(1,118)	1:259:C:GLN:N	1:259:C:GLN:CA	1:259:C:GLN:C	1:260:C:GLU:N	9	1.24
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	4	1.24
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	10	1.24
(1,60)	1:62:A:LEU:N	1:62:A:LEU:CA	1:62:A:LEU:C	1:63:A:GLU:N	15	1.24
(1,25)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:ILE:N	7	1.24
(1,71)	1:213:C:PHE:N	1:213:C:PHE:CA	1:213:C:PHE:C	1:214:C:PHE:N	2	1.23
(1,56)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:TYR:N	1	1.23
(1,104)	1:240:C:ALA:C	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	1	1.22
(1,104)	1:240:C:ALA:C	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	16	1.22
(1,92)	1:229:C:LEU:C	1:230:C:ASN:N	1:230:C:ASN:CA	1:230:C:ASN:C	5	1.22
(1,76)	1:217:C:HIS:C	1:218:C:VAL:N	1:218:C:VAL:CA	1:218:C:VAL:C	14	1.22

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:60:A:GLU:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	19	1.22
(1,35)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:VAL:N	8	1.22
(1,67)	1:208:C:ARG:C	1:209:C:CYS:N	1:209:C:CYS:CA	1:209:C:CYS:C	13	1.21
(1,50)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ILE:N	4	1.21
(1,41)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:LEU:N	20	1.21
(1,39)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ARG:N	11	1.21
(1,42)	1:47:A:ARG:C	1:48:A:GLN:N	1:48:A:GLN:CA	1:48:A:GLN:C	20	1.2
(1,56)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:TYR:N	14	1.19
(1,111)	1:250:C:CYS:C	1:251:C:ILE:N	1:251:C:ILE:CA	1:251:C:ILE:C	6	1.18
(1,90)	1:227:C:LYS:C	1:228:C:ILE:N	1:228:C:ILE:CA	1:228:C:ILE:C	19	1.18
(1,83)	1:221:C:ALA:N	1:221:C:ALA:CA	1:221:C:ALA:C	1:222:C:ASN:N	15	1.18
(1,76)	1:217:C:HIS:C	1:218:C:VAL:N	1:218:C:VAL:CA	1:218:C:VAL:C	19	1.18
(1,33)	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	1:35:A:ALA:N	2	1.18
(1,3)	1:8:A:ARG:C	1:9:A:CYS:N	1:9:A:CYS:CA	1:9:A:CYS:C	3	1.18
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	13	1.17
(1,34)	1:37:A:GLN:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	19	1.17
(1,31)	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	1:32:A:PRO:N	14	1.17
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	4	1.17
(1,21)	1:23:A:VAL:N	1:23:A:VAL:CA	1:23:A:VAL:C	1:24:A:LYS:N	16	1.17
(1,15)	1:19:A:ALA:N	1:19:A:ALA:CA	1:19:A:ALA:C	1:20:A:ARG:N	18	1.17
(1,93)	1:230:C:ASN:N	1:230:C:ASN:CA	1:230:C:ASN:C	1:231:C:THR:N	15	1.16
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	11	1.15
(1,71)	1:213:C:PHE:N	1:213:C:PHE:CA	1:213:C:PHE:C	1:214:C:PHE:N	7	1.15
(1,65)	1:207:C:TYR:C	1:208:C:ARG:N	1:208:C:ARG:CA	1:208:C:ARG:C	2	1.15
(1,56)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:TYR:N	18	1.15
(1,33)	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	1:35:A:ALA:N	4	1.15
(1,16)	1:19:A:ALA:C	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	9	1.15
(1,128)	1:264:C:LYS:N	1:264:C:LYS:CA	1:264:C:LYS:C	1:265:C:CYS:N	9	1.14
(1,107)	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	1:249:C:VAL:N	20	1.14
(1,72)	1:213:C:PHE:C	1:214:C:PHE:N	1:214:C:PHE:CA	1:214:C:PHE:C	14	1.14
(1,25)	1:27:A:LYS:N	1:27:A:LYS:CA	1:27:A:LYS:C	1:28:A:ILE:N	14	1.14
(1,19)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ASN:N	2	1.14
(1,125)	1:262:C:LEU:C	1:263:C:GLU:N	1:263:C:GLU:CA	1:263:C:GLU:C	15	1.13
(1,114)	1:257:C:TRP:N	1:257:C:TRP:CA	1:257:C:TRP:C	1:258:C:ILE:N	14	1.13
(1,103)	1:240:C:ALA:N	1:240:C:ALA:CA	1:240:C:ALA:C	1:241:C:ARG:N	4	1.13
(1,85)	1:223:C:VAL:N	1:223:C:VAL:CA	1:223:C:VAL:C	1:224:C:LYS:N	3	1.13
(1,69)	1:211:C:CYS:C	1:212:C:ARG:N	1:212:C:ARG:CA	1:212:C:ARG:C	18	1.13
(1,61)	1:62:A:LEU:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	12	1.13
(1,22)	1:25:A:HIS:C	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	2	1.13
(1,11)	1:15:A:GLU:N	1:15:A:GLU:CA	1:15:A:GLU:C	1:16:A:SER:N	18	1.13
(1,85)	1:223:C:VAL:N	1:223:C:VAL:CA	1:223:C:VAL:C	1:224:C:LYS:N	20	1.12
(1,39)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ARG:N	8	1.12
(1,125)	1:262:C:LEU:C	1:263:C:GLU:N	1:263:C:GLU:CA	1:263:C:GLU:C	13	1.11
(1,105)	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	1:242:C:LEU:N	18	1.11
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	20	1.11
(1,32)	1:33:A:ASN:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	3	1.11
(1,122)	1:261:C:TYR:N	1:261:C:TYR:CA	1:261:C:TYR:C	1:262:C:LEU:N	1	1.1
(1,45)	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	1:50:A:CYS:N	11	1.1
(1,37)	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	1:40:A:ALA:N	12	1.1
(1,32)	1:33:A:ASN:C	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	17	1.1
(1,1)	1:7:A:TYR:C	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	18	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,107)	1:248:C:GLN:N	1:248:C:GLN:CA	1:248:C:GLN:C	1:249:C:VAL:N	1	1.09
(1,86)	1:225:C:HIS:C	1:226:C:LEU:N	1:226:C:LEU:CA	1:226:C:LEU:C	19	1.09
(1,80)	1:219:C:ALA:C	1:220:C:ARG:N	1:220:C:ARG:CA	1:220:C:ARG:C	8	1.09
(1,77)	1:218:C:VAL:N	1:218:C:VAL:CA	1:218:C:VAL:C	1:219:C:ALA:N	18	1.09
(1,55)	1:59:A:GLN:C	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	11	1.09
(1,41)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:LEU:N	10	1.08
(1,29)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	10	1.08
(1,5)	1:11:A:CYS:C	1:12:A:ARG:N	1:12:A:ARG:CA	1:12:A:ARG:C	17	1.08
(1,97)	1:234:C:CYS:N	1:234:C:CYS:CA	1:234:C:CYS:C	1:235:C:ALA:N	7	1.07
(1,56)	1:60:A:GLU:N	1:60:A:GLU:CA	1:60:A:GLU:C	1:61:A:TYR:N	12	1.07
(1,41)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:LEU:N	18	1.07
(1,16)	1:19:A:ALA:C	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	7	1.07
(1,118)	1:259:C:GLN:N	1:259:C:GLN:CA	1:259:C:GLN:C	1:260:C:GLU:N	20	1.06
(1,83)	1:221:C:ALA:N	1:221:C:ALA:CA	1:221:C:ALA:C	1:222:C:ASN:N	18	1.06
(1,73)	1:214:C:PHE:N	1:214:C:PHE:CA	1:214:C:PHE:C	1:215:C:GLU:N	6	1.06
(1,39)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ARG:N	7	1.06
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	15	1.05
(1,39)	1:40:A:ALA:N	1:40:A:ALA:CA	1:40:A:ALA:C	1:41:A:ARG:N	3	1.05
(1,33)	1:34:A:CYS:N	1:34:A:CYS:CA	1:34:A:CYS:C	1:35:A:ALA:N	1	1.05
(1,29)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	17	1.05
(1,13)	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	1:19:A:ALA:N	15	1.05
(1,19)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:ASN:N	15	1.04
(1,54)	1:59:A:GLN:N	1:59:A:GLN:CA	1:59:A:GLN:C	1:60:A:GLU:N	18	1.03
(1,40)	1:40:A:ALA:C	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	12	1.03
(1,29)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:THR:N	12	1.03
(1,6)	1:12:A:ARG:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	12	1.03
(1,99)	1:238:C:ILE:N	1:238:C:ILE:CA	1:238:C:ILE:C	1:239:C:VAL:N	5	1.02
(1,95)	1:231:C:THR:N	1:231:C:THR:CA	1:231:C:THR:C	1:232:C:PRO:N	12	1.02
(1,46)	1:50:A:CYS:N	1:50:A:CYS:CA	1:50:A:CYS:C	1:51:A:ILE:N	1	1.02
(1,118)	1:259:C:GLN:N	1:259:C:GLN:CA	1:259:C:GLN:C	1:260:C:GLU:N	3	1.01
(1,61)	1:62:A:LEU:C	1:63:A:GLU:N	1:63:A:GLU:CA	1:63:A:GLU:C	13	1.01
(1,58)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:LEU:N	13	1.01
(1,47)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	18	1.01
(1,46)	1:50:A:CYS:N	1:50:A:CYS:CA	1:50:A:CYS:C	1:51:A:ILE:N	14	1.01
(1,105)	1:241:C:ARG:N	1:241:C:ARG:CA	1:241:C:ARG:C	1:242:C:LEU:N	9	1.0
(1,98)	1:237:C:GLN:C	1:238:C:ILE:N	1:238:C:ILE:CA	1:238:C:ILE:C	15	1.0
(1,12)	1:17:A:HIS:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	2	1.0
(1,1)	1:7:A:TYR:C	1:8:A:ARG:N	1:8:A:ARG:CA	1:8:A:ARG:C	1	1.0