



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 09:44 PM UTC

PDB ID : 2M7W / pdb_00002m7w
BMRB ID : 19215
Title : Independently verified structure of gp41-M-MAT, a membrane associated MPER trimer from HIV-1 gp41
Authors : Martin, J.W.; Reardon, P.N.; Sage, H.S.; Moses, D.S.; Munir, A.S.; Haynes, B.F.; Spicer, L.D.; Donald, B.R.
Deposited on : 2013-05-01

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

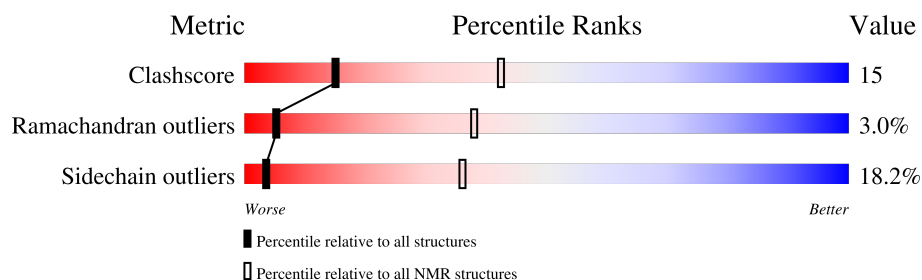
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 19%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	59	 51% 41% 7% .
1	B	59	 49% 42% 7% .
1	C	59	 49% 42% 7% .

2 Ensemble composition and analysis

This entry contains 18 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:1-A:59, B:1-B:59, C:1-C:59 (177)	2.01	5

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2913 atoms, of which 1413 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Envelope glycoprotein.

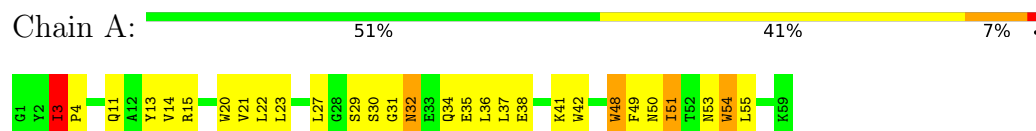
Mol	Chain	Residues	Atoms					Trace
1	A	59	Total	C	H	N	O	0
			971	329	471	80	91	
1	B	59	Total	C	H	N	O	0
			971	329	471	80	91	
1	C	59	Total	C	H	N	O	0
			971	329	471	80	91	

4 Residue-property plots [i](#)

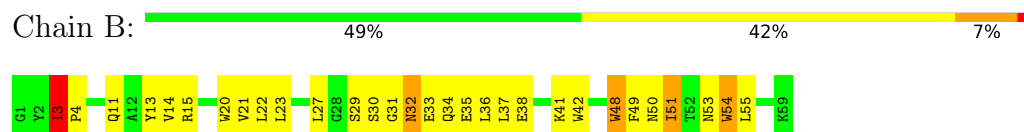
4.1 Average score per residue in the NMR ensemble

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

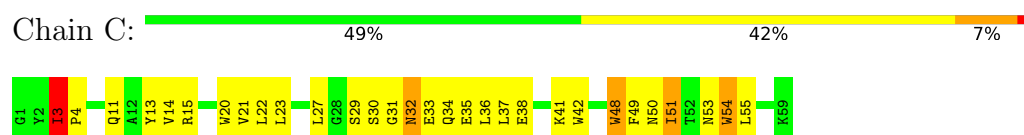
- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

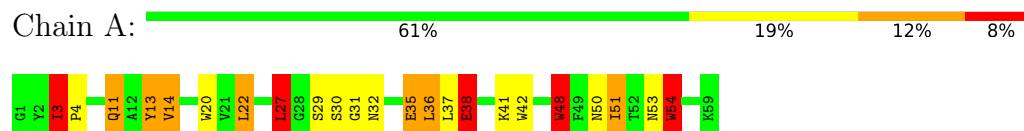


4.2 Scores per residue for each member of the ensemble

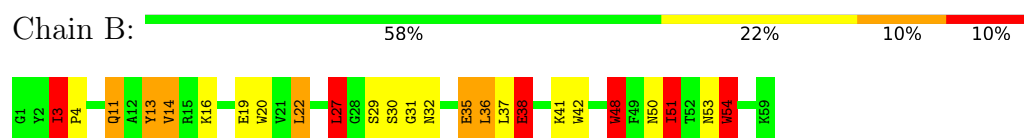
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

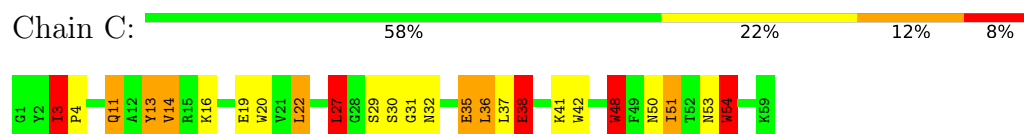
- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

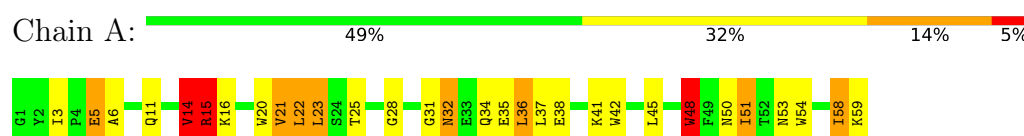


- Molecule 1: Envelope glycoprotein

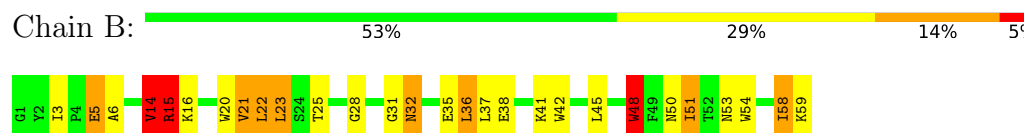


4.2.2 Score per residue for model 2

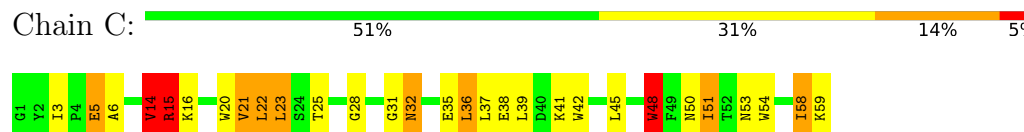
- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

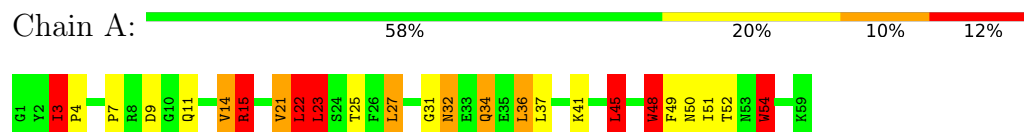


- Molecule 1: Envelope glycoprotein



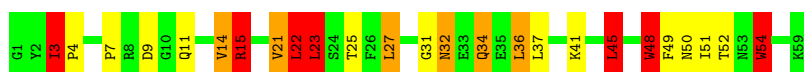
4.2.3 Score per residue for model 3

- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein





- Molecule 1: Envelope glycoprotein

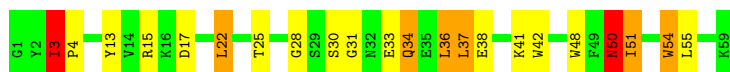


4.2.4 Score per residue for model 4

- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

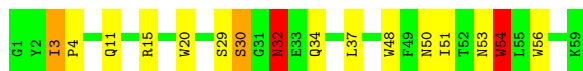


4.2.5 Score per residue for model 5 (medoid)

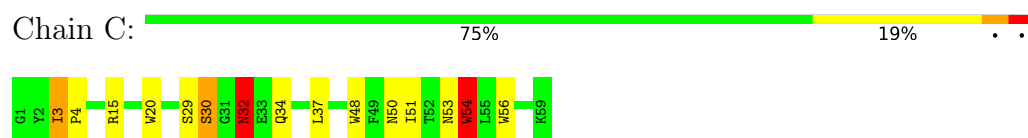
- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

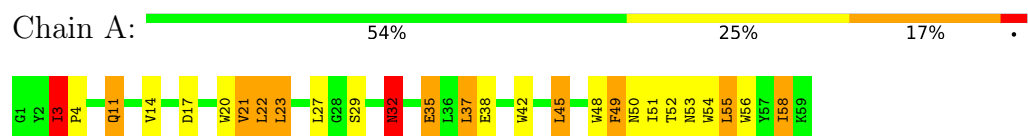


- Molecule 1: Envelope glycoprotein

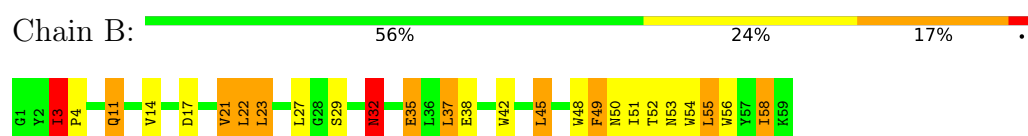


4.2.6 Score per residue for model 6

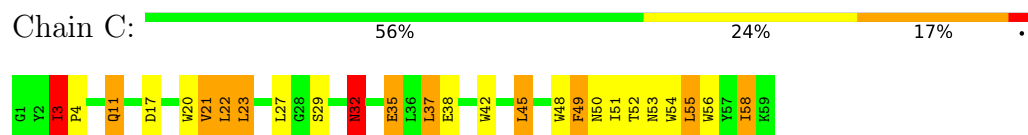
- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

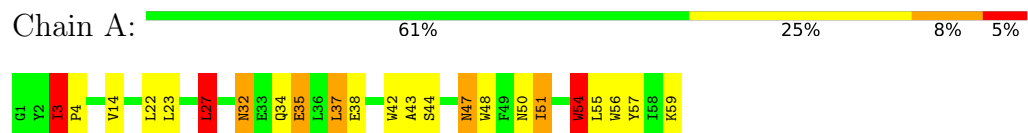


- Molecule 1: Envelope glycoprotein

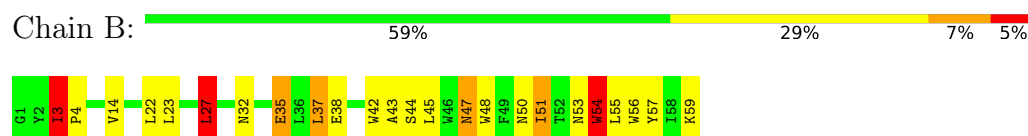


4.2.7 Score per residue for model 7

- Molecule 1: Envelope glycoprotein

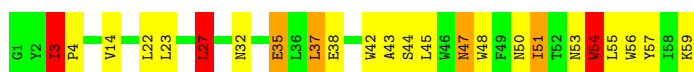


- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein





4.2.8 Score per residue for model 8

- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein



4.2.9 Score per residue for model 9

- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

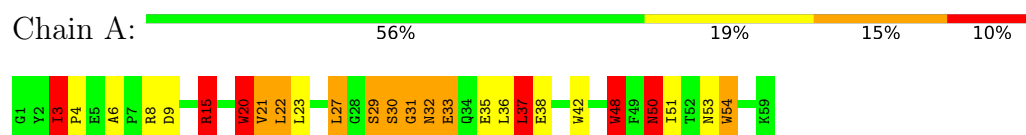


- Molecule 1: Envelope glycoprotein

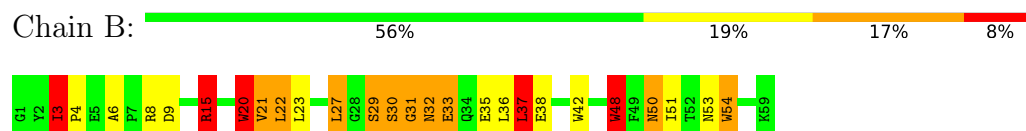


4.2.10 Score per residue for model 10

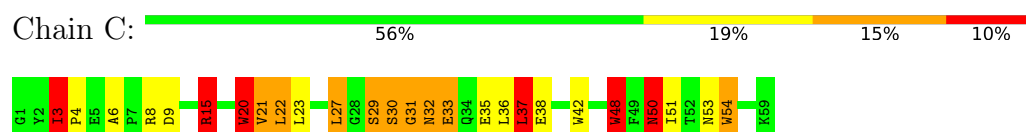
- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

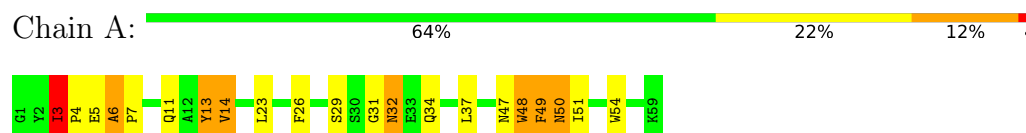


- Molecule 1: Envelope glycoprotein

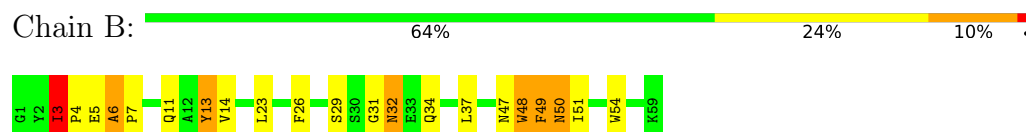


4.2.11 Score per residue for model 11

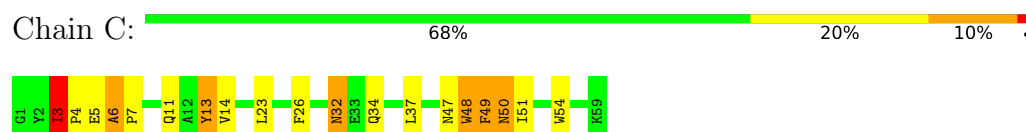
- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein



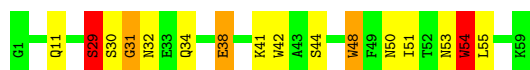
- Molecule 1: Envelope glycoprotein



4.2.12 Score per residue for model 12

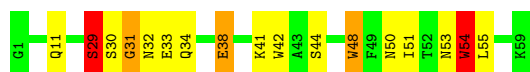
- Molecule 1: Envelope glycoprotein

Chain A:  73% 19% 5%



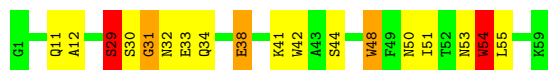
- Molecule 1: Envelope glycoprotein

Chain B:  71% 20% 5%



- Molecule 1: Envelope glycoprotein

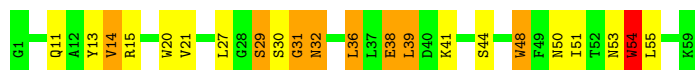
Chain C:  69% 22% 5%



4.2.13 Score per residue for model 13

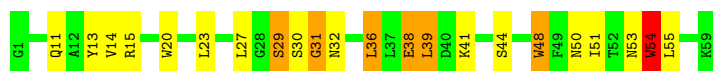
- Molecule 1: Envelope glycoprotein

Chain A:  63% 22% 14%



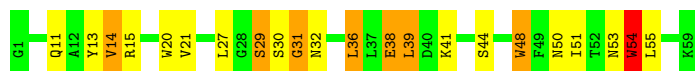
- Molecule 1: Envelope glycoprotein

Chain B:  63% 25% 10%



- Molecule 1: Envelope glycoprotein

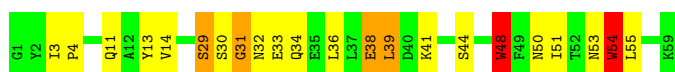
Chain C:  63% 24% 12%



4.2.14 Score per residue for model 14

- Molecule 1: Envelope glycoprotein

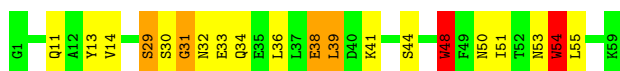
Chain A:  63% 27% 7%



- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein



4.2.15 Score per residue for model 15

- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

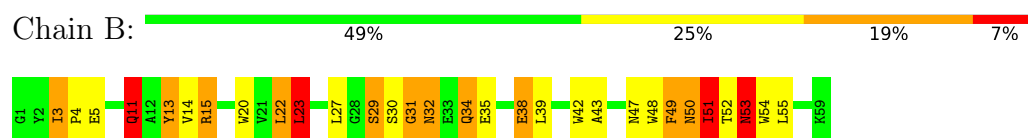


4.2.16 Score per residue for model 16

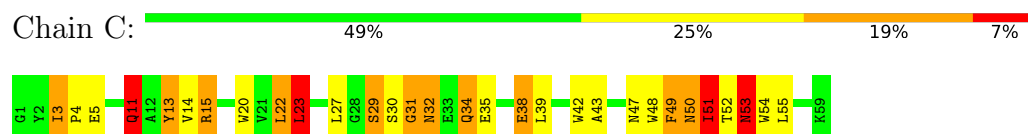
- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

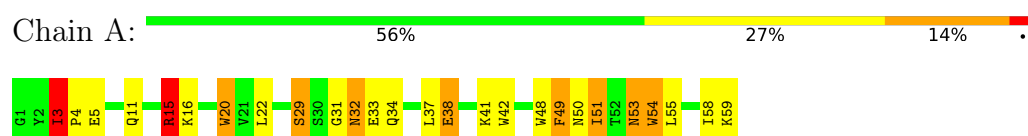


- Molecule 1: Envelope glycoprotein

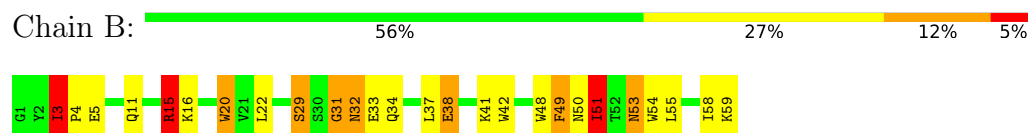


4.2.17 Score per residue for model 17

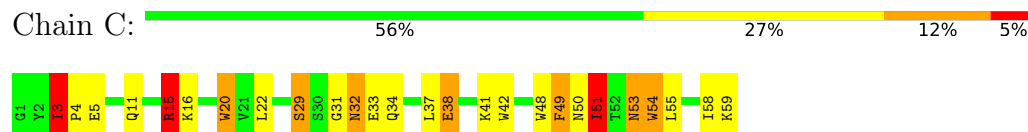
- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein

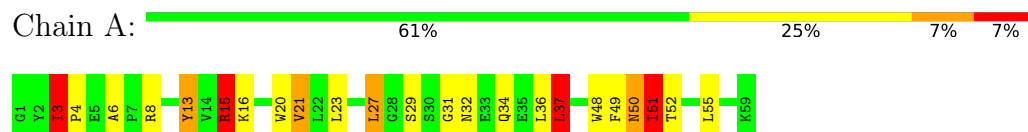


- Molecule 1: Envelope glycoprotein



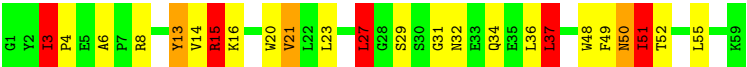
4.2.18 Score per residue for model 18

- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein





● Molecule 1: Envelope glycoprotein



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 18 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
DISCO	structure solution	1
X-PLOR NIH	structure solution	2.33
X-PLOR NIH	refinement	2.33

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	485
Number of shifts mapped to atoms	485
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	19%

6 Model quality i

6.1 Standard geometry i

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	1.71±0.14	8±4/518 (1.6± 0.8%)	1.28±0.05	2±1/706 (0.2± 0.2%)
1	B	1.71±0.14	8±4/518 (1.6± 0.8%)	1.28±0.05	2±2/706 (0.3± 0.2%)
1	C	1.71±0.14	8±4/518 (1.6± 0.8%)	1.28±0.05	2±1/706 (0.2± 0.2%)
All	All	1.72	445/27972 (1.6%)	1.28	89/38124 (0.2%)

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
1	A	51	ILE	CA-CB	10.09	1.66	1.54	2	7
1	B	51	ILE	CA-CB	9.94	1.66	1.54	2	8
1	C	51	ILE	CA-CB	9.89	1.66	1.54	2	7
1	C	58	ILE	CA-CB	8.31	1.65	1.54	6	1
1	A	58	ILE	CA-CB	8.24	1.64	1.54	6	1
1	B	58	ILE	CA-CB	8.23	1.64	1.54	6	1
1	A	15	ARG	CA-CB	8.12	1.64	1.53	10	8
1	C	15	ARG	CA-CB	8.09	1.64	1.53	10	8
1	B	15	ARG	CA-CB	8.08	1.64	1.53	10	8
1	B	3	ILE	CA-CB	8.04	1.64	1.54	7	12
1	C	3	ILE	CA-CB	7.96	1.64	1.54	7	12
1	A	3	ILE	CA-CB	7.91	1.64	1.54	7	12
1	B	21	VAL	CA-CB	7.58	1.63	1.54	6	4
1	C	21	VAL	CA-CB	7.52	1.63	1.54	6	4
1	A	21	VAL	CA-CB	7.42	1.63	1.54	6	4
1	A	20	TRP	CA-CB	7.08	1.61	1.53	2	6
1	B	20	TRP	CA-CB	7.04	1.61	1.53	2	6
1	C	20	TRP	CA-CB	6.98	1.61	1.53	2	6
1	A	54	TRP	CA-CB	6.98	1.64	1.53	9	9
1	C	54	TRP	CA-CB	6.97	1.64	1.53	9	9
1	B	54	TRP	CA-CB	6.96	1.64	1.53	9	9
1	B	22	LEU	CA-CB	6.88	1.64	1.53	3	9
1	C	22	LEU	CA-CB	6.87	1.64	1.53	3	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	22	LEU	CA-CB	6.85	1.64	1.53	3	9
1	C	15	ARG	N-CA	6.85	1.54	1.46	4	4
1	A	36	LEU	CA-CB	6.82	1.64	1.53	3	4
1	C	36	LEU	CA-CB	6.81	1.64	1.53	3	4
1	A	15	ARG	N-CA	6.77	1.54	1.46	4	4
1	B	36	LEU	CA-CB	6.75	1.64	1.53	3	4
1	B	15	ARG	N-CA	6.68	1.54	1.46	4	4
1	C	21	VAL	N-CA	6.67	1.54	1.46	2	3
1	B	21	VAL	N-CA	6.54	1.54	1.46	2	3
1	A	21	VAL	N-CA	6.50	1.54	1.46	2	3
1	B	41	LYS	CA-CB	6.44	1.63	1.53	17	4
1	C	37	LEU	CA-CB	6.44	1.65	1.53	10	4
1	A	37	LEU	CA-CB	6.44	1.65	1.53	10	4
1	A	41	LYS	CA-CB	6.42	1.63	1.53	17	4
1	B	14	VAL	CA-CB	6.40	1.64	1.54	1	3
1	B	37	LEU	CA-CB	6.39	1.65	1.53	10	4
1	A	14	VAL	CA-CB	6.37	1.64	1.54	1	3
1	C	14	VAL	CA-CB	6.35	1.64	1.54	1	3
1	A	38	GLU	CA-CB	6.33	1.63	1.53	1	3
1	B	38	GLU	CA-CB	6.33	1.63	1.53	1	3
1	C	41	LYS	CA-CB	6.29	1.63	1.53	17	4
1	C	38	GLU	CA-CB	6.26	1.63	1.53	1	3
1	B	58	ILE	CB-CG1	6.15	1.65	1.53	2	1
1	C	58	ILE	CB-CG1	6.12	1.65	1.53	2	1
1	A	58	ILE	CB-CG1	6.09	1.65	1.53	2	1
1	B	23	LEU	CA-CB	6.06	1.63	1.53	6	4
1	B	22	LEU	CB-CG	6.05	1.65	1.53	16	2
1	A	22	LEU	CB-CG	6.05	1.65	1.53	16	2
1	C	23	LEU	CA-CB	6.02	1.63	1.53	6	4
1	C	48	TRP	CA-CB	6.00	1.63	1.53	14	8
1	A	23	LEU	CA-CB	5.99	1.63	1.53	6	4
1	C	22	LEU	CB-CG	5.97	1.65	1.53	16	2
1	B	48	TRP	CA-CB	5.93	1.63	1.53	13	8
1	A	48	TRP	CA-CB	5.91	1.63	1.53	14	8
1	B	34	GLN	CA-CB	5.84	1.62	1.53	16	2
1	B	27	LEU	CA-CB	5.83	1.62	1.53	8	1
1	C	27	LEU	CA-CB	5.82	1.62	1.53	8	1
1	A	7	PRO	CA-CB	5.81	1.60	1.53	3	1
1	C	55	LEU	CA-CB	5.80	1.63	1.53	6	2
1	C	34	GLN	CA-CB	5.80	1.62	1.53	16	2
1	A	55	LEU	CA-CB	5.79	1.63	1.53	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	55	LEU	CA-CB	5.79	1.63	1.53	6	2
1	A	27	LEU	CA-CB	5.79	1.62	1.53	8	1
1	A	34	GLN	CA-CB	5.78	1.62	1.53	16	2
1	B	7	PRO	CA-CB	5.78	1.60	1.53	3	1
1	C	27	LEU	CB-CG	5.77	1.65	1.53	10	5
1	C	7	PRO	CA-CB	5.74	1.60	1.53	3	1
1	A	27	LEU	CB-CG	5.74	1.65	1.53	10	5
1	A	33	GLU	N-CA	-5.71	1.39	1.46	15	1
1	B	27	LEU	CB-CG	5.70	1.64	1.53	10	5
1	C	33	GLU	N-CA	-5.70	1.39	1.46	15	1
1	B	33	GLU	N-CA	-5.70	1.39	1.46	15	1
1	A	53	ASN	N-CA	5.68	1.53	1.46	17	1
1	A	5	GLU	CA-CB	5.66	1.62	1.54	2	1
1	B	53	ASN	N-CA	5.66	1.53	1.46	17	1
1	B	5	GLU	CA-CB	5.64	1.62	1.54	2	1
1	C	5	GLU	CA-CB	5.63	1.62	1.54	2	1
1	A	35	GLU	CA-CB	5.57	1.62	1.53	6	1
1	C	53	ASN	N-CA	5.57	1.53	1.46	17	1
1	A	35	GLU	N-CA	5.56	1.53	1.46	1	1
1	A	14	VAL	N-CA	5.56	1.52	1.46	14	6
1	C	35	GLU	N-CA	5.56	1.53	1.46	1	1
1	B	14	VAL	N-CA	5.55	1.52	1.46	3	4
1	C	55	LEU	CB-CG	5.54	1.64	1.53	6	1
1	A	11	GLN	CA-CB	5.53	1.62	1.53	16	4
1	C	45	LEU	CA-CB	5.52	1.61	1.53	3	2
1	B	35	GLU	N-CA	5.51	1.53	1.46	1	1
1	A	51	ILE	CB-CG1	5.51	1.64	1.53	4	2
1	A	49	PHE	CA-CB	5.51	1.62	1.53	6	2
1	B	37	LEU	N-CA	5.51	1.53	1.46	10	1
1	B	47	ASN	CA-CB	5.51	1.61	1.53	11	1
1	A	47	ASN	CA-CB	5.51	1.61	1.53	11	1
1	C	11	GLN	CA-CB	5.50	1.62	1.53	16	3
1	C	47	ASN	CA-CB	5.50	1.61	1.53	11	1
1	C	14	VAL	N-CA	5.49	1.52	1.46	14	3
1	B	49	PHE	CA-CB	5.49	1.63	1.53	11	3
1	B	35	GLU	CA-CB	5.49	1.62	1.53	6	1
1	B	33	GLU	CA-CB	5.48	1.63	1.53	8	1
1	C	35	GLU	CA-CB	5.48	1.62	1.53	6	1
1	A	45	LEU	CA-CB	5.48	1.61	1.53	3	2
1	B	55	LEU	CB-CG	5.48	1.64	1.53	6	1
1	B	32	ASN	CA-CB	5.47	1.62	1.53	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	32	ASN	CA-CB	5.47	1.62	1.53	5	1
1	A	54	TRP	N-CA	5.47	1.53	1.46	3	3
1	B	54	TRP	N-CA	5.47	1.53	1.46	3	3
1	A	37	LEU	N-CA	5.47	1.53	1.46	10	1
1	B	11	GLN	CA-CB	5.46	1.62	1.53	16	3
1	A	33	GLU	CA-CB	5.46	1.63	1.53	8	1
1	B	51	ILE	CB-CG1	5.45	1.64	1.53	4	2
1	B	39	LEU	CB-CG	5.45	1.64	1.53	14	2
1	B	45	LEU	CA-CB	5.44	1.61	1.53	3	2
1	A	55	LEU	CB-CG	5.44	1.64	1.53	6	1
1	C	54	TRP	N-CA	5.43	1.53	1.46	3	4
1	C	37	LEU	N-CA	5.43	1.53	1.46	10	1
1	A	36	LEU	CB-CG	5.42	1.64	1.53	13	2
1	C	49	PHE	CA-CB	5.42	1.62	1.53	6	2
1	B	3	ILE	CB-CG1	5.42	1.64	1.53	15	1
1	C	3	ILE	CB-CG1	5.42	1.64	1.53	15	1
1	C	39	LEU	CB-CG	5.41	1.64	1.53	13	2
1	C	36	LEU	CB-CG	5.40	1.64	1.53	13	2
1	C	33	GLU	CA-CB	5.40	1.62	1.53	8	1
1	C	32	ASN	CA-CB	5.39	1.62	1.53	5	1
1	C	51	ILE	CB-CG1	5.38	1.64	1.53	4	2
1	B	36	LEU	CB-CG	5.37	1.64	1.53	13	2
1	A	39	LEU	CB-CG	5.35	1.64	1.53	14	2
1	B	39	LEU	CA-CB	5.33	1.61	1.53	9	1
1	A	3	ILE	CB-CG1	5.33	1.64	1.53	15	1
1	A	39	LEU	CA-CB	5.32	1.61	1.53	9	1
1	B	50	ASN	N-CA	-5.28	1.39	1.46	18	2
1	B	37	LEU	CB-CG	5.27	1.64	1.53	6	1
1	C	37	LEU	CB-CG	5.24	1.64	1.53	6	1
1	C	50	ASN	N-CA	-5.22	1.39	1.46	16	2
1	A	50	ASN	N-CA	-5.18	1.39	1.46	16	2
1	C	39	LEU	CA-CB	5.17	1.61	1.53	9	1
1	B	33	GLU	CA-C	-5.17	1.45	1.52	10	1
1	A	37	LEU	CB-CG	5.17	1.63	1.53	6	1
1	C	33	GLU	CA-C	-5.16	1.45	1.52	10	1
1	C	53	ASN	CA-CB	5.14	1.61	1.53	16	1
1	B	16	LYS	CA-CB	5.13	1.61	1.53	2	1
1	A	33	GLU	CA-C	-5.12	1.45	1.52	10	1
1	A	16	LYS	CA-CB	5.10	1.61	1.53	2	1
1	A	50	ASN	CA-CB	5.09	1.61	1.53	10	1
1	C	16	LYS	CA-CB	5.09	1.61	1.53	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	20	TRP	C-N	5.07	1.39	1.33	6	1
1	B	53	ASN	CA-CB	5.04	1.61	1.53	16	1
1	A	53	ASN	CA-CB	5.03	1.61	1.53	16	1
1	C	20	TRP	C-N	5.03	1.39	1.33	6	1
1	C	50	ASN	CA-CB	5.00	1.61	1.53	10	1
1	C	12	ALA	C-N	5.00	1.37	1.33	12	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(°)	Ideal(°)	Models	
								Worst	Total
1	A	50	ASN	N-CA-C	-7.42	103.49	112.54	4	3
1	B	50	ASN	N-CA-C	-7.42	103.49	112.54	4	3
1	C	50	ASN	N-CA-C	-7.34	103.59	112.54	4	3
1	C	31	GLY	N-CA-C	-6.98	105.18	115.72	16	7
1	A	31	GLY	N-CA-C	-6.95	105.22	115.72	16	7
1	B	31	GLY	N-CA-C	-6.93	105.26	115.72	16	8
1	C	32	ASN	N-CA-C	-6.33	105.14	112.86	17	3
1	B	32	ASN	N-CA-C	-6.29	105.19	112.86	17	3
1	A	32	ASN	N-CA-C	-6.29	104.16	113.72	10	4
1	C	30	SER	N-CA-C	-6.26	105.69	113.15	13	3
1	A	30	SER	N-CA-C	-6.26	105.70	113.15	13	4
1	B	30	SER	N-CA-C	-6.23	105.74	113.15	13	3
1	B	51	ILE	CA-C-N	6.15	128.81	120.44	4	1
1	B	51	ILE	C-N-CA	6.15	128.81	120.44	4	1
1	B	28	GLY	N-CA-C	-5.96	107.03	115.43	4	2
1	C	28	GLY	N-CA-C	-5.93	107.07	115.43	4	2
1	A	28	GLY	N-CA-C	-5.93	107.08	115.43	4	2
1	B	32	ASN	CA-C-N	5.81	128.06	120.28	16	1
1	B	32	ASN	C-N-CA	5.81	128.06	120.28	16	1
1	B	36	LEU	N-CA-C	5.65	118.64	111.69	9	2
1	C	20	TRP	CB-CG-CD2	5.55	134.57	126.80	10	1
1	A	36	LEU	N-CA-C	5.54	118.51	111.69	9	2
1	C	48	TRP	N-CA-C	-5.52	106.50	113.18	11	1
1	B	20	TRP	CB-CG-CD2	5.51	134.52	126.80	10	1
1	A	20	TRP	CB-CG-CD2	5.47	134.46	126.80	10	1
1	A	48	TRP	N-CA-C	-5.46	106.57	113.18	11	1
1	B	48	TRP	N-CA-C	-5.45	106.58	113.18	11	1
1	C	36	LEU	N-CA-C	5.43	118.37	111.69	9	2
1	C	32	ASN	CA-C-N	5.39	128.04	120.28	16	1
1	C	32	ASN	C-N-CA	5.39	128.04	120.28	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	32	ASN	CA-C-N	5.39	128.04	120.28	16	1
1	A	32	ASN	C-N-CA	5.39	128.04	120.28	16	1
1	B	5	GLU	N-CA-C	-5.30	107.48	114.31	9	3
1	C	5	GLU	N-CA-C	-5.30	107.48	114.31	17	3
1	A	5	GLU	N-CA-C	-5.25	107.54	114.31	17	2
1	B	45	LEU	N-CA-CB	5.23	117.81	110.12	2	1
1	C	45	LEU	N-CA-CB	5.22	117.79	110.12	2	1
1	A	45	LEU	N-CA-CB	5.21	117.78	110.12	2	1
1	B	23	LEU	N-CA-C	-5.07	105.88	111.71	13	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	500	471	471	16±6
1	B	500	471	471	16±6
1	C	500	471	471	16±6
All	All	27000	25434	25434	784

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:6:ALA:HB1	1:B:8:ARG:HH12	0.83	1.33	10	2
1:A:6:ALA:HB1	1:A:8:ARG:HH12	0.83	1.33	10	2
1:A:51:ILE:HD13	1:A:52:THR:N	0.82	1.90	18	2
1:C:6:ALA:HB1	1:C:8:ARG:HH12	0.81	1.33	10	2
1:B:51:ILE:HD13	1:B:52:THR:N	0.81	1.90	18	2
1:C:51:ILE:HD13	1:C:52:THR:N	0.80	1.90	18	2
1:B:36:LEU:HD13	1:C:32:ASN:ND2	0.75	1.97	14	1
1:A:36:LEU:HD13	1:B:32:ASN:ND2	0.74	1.97	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ASN:ND2	1:C:36:LEU:HD13	0.73	1.97	14	1
1:A:48:TRP:O	1:A:51:ILE:HG23	0.70	1.87	5	8
1:C:48:TRP:O	1:C:51:ILE:HG23	0.70	1.87	5	9
1:B:48:TRP:O	1:B:51:ILE:HG23	0.70	1.87	5	9
1:A:54:TRP:H	1:A:54:TRP:CD1	0.62	2.12	1	7
1:B:54:TRP:CD1	1:B:54:TRP:H	0.62	2.12	1	8
1:C:54:TRP:H	1:C:54:TRP:CD1	0.61	2.12	1	7
1:B:36:LEU:HD23	1:C:32:ASN:HD21	0.61	1.55	18	1
1:B:33:GLU:O	1:B:37:LEU:HD22	0.59	1.98	10	1
1:A:32:ASN:OD1	1:A:36:LEU:HD23	0.59	1.98	10	1
1:A:33:GLU:O	1:A:37:LEU:HD22	0.59	1.98	10	1
1:B:32:ASN:OD1	1:B:36:LEU:HD23	0.59	1.98	10	1
1:A:23:LEU:HD11	1:C:23:LEU:HD11	0.59	1.75	10	1
1:C:27:LEU:HD12	1:C:32:ASN:HD21	0.58	1.57	1	1
1:C:32:ASN:OD1	1:C:36:LEU:HD23	0.58	1.98	10	1
1:C:33:GLU:O	1:C:37:LEU:HD22	0.58	1.98	10	1
1:A:27:LEU:HD12	1:A:32:ASN:HD21	0.58	1.57	1	1
1:C:6:ALA:HB1	1:C:8:ARG:NH1	0.58	2.10	10	2
1:C:27:LEU:HD12	1:C:32:ASN:ND2	0.58	2.14	1	1
1:A:32:ASN:HD21	1:C:36:LEU:HD23	0.58	1.59	18	1
1:B:27:LEU:HD12	1:B:32:ASN:ND2	0.58	2.14	1	1
1:A:23:LEU:HD11	1:B:23:LEU:HD11	0.58	1.76	10	1
1:B:27:LEU:HD12	1:B:32:ASN:HD21	0.57	1.57	1	1
1:B:3:ILE:H	1:B:4:PRO:CD	0.57	2.13	5	12
1:A:27:LEU:HD12	1:A:32:ASN:ND2	0.57	2.13	1	1
1:B:23:LEU:HD11	1:C:23:LEU:HD11	0.57	1.77	10	1
1:C:37:LEU:HD13	1:C:37:LEU:O	0.57	2.00	2	1
1:C:3:ILE:H	1:C:4:PRO:CD	0.57	2.13	5	12
1:B:37:LEU:O	1:B:37:LEU:HD13	0.56	2.00	2	1
1:A:3:ILE:H	1:A:4:PRO:CD	0.56	2.13	3	12
1:A:26:PHE:CE2	1:C:27:LEU:HD22	0.56	2.35	8	1
1:A:39:LEU:H	1:A:39:LEU:HD23	0.56	1.59	9	1
1:A:36:LEU:HD23	1:B:32:ASN:HD21	0.56	1.59	18	1
1:B:39:LEU:H	1:B:39:LEU:HD23	0.56	1.59	9	1
1:A:6:ALA:HB1	1:A:8:ARG:NH1	0.56	2.10	10	2
1:A:37:LEU:HD13	1:A:37:LEU:O	0.56	2.00	2	1
1:B:6:ALA:HB1	1:B:8:ARG:NH1	0.56	2.10	10	2
1:C:39:LEU:HD23	1:C:39:LEU:H	0.56	1.59	9	1
1:A:27:LEU:HD22	1:B:26:PHE:CE2	0.55	2.35	8	1
1:B:27:LEU:HD22	1:C:26:PHE:CE2	0.55	2.36	8	1
1:A:51:ILE:HD13	1:A:52:THR:H	0.55	1.62	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:51:ILE:HD13	1:C:52:THR:H	0.55	1.62	16	1
1:B:51:ILE:HD13	1:B:52:THR:H	0.55	1.62	16	2
1:A:14:VAL:HG22	1:A:15:ARG:N	0.54	2.17	3	2
1:A:20:TRP:CE3	1:B:15:ARG:NH2	0.54	2.75	17	2
1:A:15:ARG:NH2	1:C:20:TRP:CE3	0.54	2.76	17	2
1:B:20:TRP:CE3	1:C:15:ARG:NH2	0.54	2.76	17	1
1:C:14:VAL:HG22	1:C:15:ARG:N	0.54	2.18	3	2
1:A:54:TRP:N	1:A:54:TRP:CD1	0.54	2.75	7	2
1:B:22:LEU:O	1:B:25:THR:HG22	0.54	2.03	3	1
1:A:15:ARG:NH1	1:C:20:TRP:CE3	0.54	2.76	18	2
1:B:54:TRP:CD1	1:B:54:TRP:N	0.54	2.75	7	9
1:C:13:TYR:CD1	1:C:13:TYR:N	0.54	2.76	18	1
1:B:14:VAL:HG22	1:B:15:ARG:N	0.54	2.17	3	2
1:A:20:TRP:CE3	1:B:15:ARG:NH1	0.54	2.76	18	2
1:A:42:TRP:H	1:A:42:TRP:CD1	0.53	2.20	16	3
1:C:22:LEU:O	1:C:25:THR:HG22	0.53	2.03	3	1
1:B:11:GLN:NE2	1:B:22:LEU:HD21	0.53	2.18	17	1
1:B:20:TRP:CE3	1:C:15:ARG:NH1	0.53	2.77	18	2
1:B:23:LEU:HD13	1:C:14:VAL:HG21	0.53	1.79	7	2
1:B:27:LEU:HD21	1:C:27:LEU:HD12	0.53	1.80	8	1
1:C:54:TRP:CD1	1:C:54:TRP:N	0.53	2.75	7	9
1:A:11:GLN:NE2	1:A:22:LEU:HD21	0.53	2.18	17	1
1:B:13:TYR:N	1:B:13:TYR:CD1	0.53	2.76	18	1
1:A:23:LEU:HD11	1:B:23:LEU:HD21	0.53	1.81	16	1
1:C:11:GLN:NE2	1:C:22:LEU:HD21	0.53	2.19	17	1
1:C:42:TRP:H	1:C:42:TRP:CD1	0.53	2.20	16	3
1:A:11:GLN:NE2	1:A:13:TYR:CD2	0.53	2.77	16	1
1:B:11:GLN:NE2	1:B:13:TYR:CD2	0.53	2.77	16	1
1:A:23:LEU:CD1	1:B:23:LEU:HD21	0.52	2.34	16	1
1:A:27:LEU:HD21	1:B:27:LEU:HD12	0.52	1.81	8	1
1:C:11:GLN:NE2	1:C:13:TYR:CD2	0.52	2.77	16	1
1:B:42:TRP:H	1:B:42:TRP:CD1	0.52	2.21	16	3
1:B:29:SER:C	1:B:31:GLY:H	0.52	2.13	13	7
1:C:29:SER:C	1:C:31:GLY:H	0.52	2.13	14	6
1:A:29:SER:C	1:A:31:GLY:H	0.52	2.13	14	7
1:A:23:LEU:HD21	1:C:23:LEU:CD1	0.52	2.35	16	1
1:A:13:TYR:CD1	1:A:13:TYR:N	0.52	2.76	18	1
1:A:22:LEU:O	1:A:25:THR:HG22	0.52	2.03	3	1
1:A:50:ASN:ND2	1:A:53:ASN:HD22	0.51	2.03	10	1
1:B:23:LEU:CD1	1:C:23:LEU:HD21	0.51	2.35	16	1
1:B:37:LEU:C	1:B:37:LEU:HD12	0.51	2.31	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:HG21	1:C:23:LEU:HD13	0.51	1.80	7	2
1:B:56:TRP:CD1	1:B:57:TYR:N	0.51	2.79	7	1
1:B:58:ILE:C	1:B:58:ILE:HD12	0.51	2.30	17	1
1:C:37:LEU:C	1:C:37:LEU:HD12	0.51	2.31	5	1
1:A:56:TRP:CD1	1:A:57:TYR:N	0.51	2.79	7	1
1:C:56:TRP:CD1	1:C:57:TYR:N	0.51	2.79	7	1
1:C:58:ILE:C	1:C:58:ILE:HD12	0.51	2.30	17	1
1:A:23:LEU:HD13	1:B:14:VAL:HG21	0.51	1.80	7	2
1:C:45:LEU:H	1:C:45:LEU:HD23	0.51	1.65	3	1
1:B:50:ASN:ND2	1:B:53:ASN:HD22	0.51	2.03	10	1
1:A:45:LEU:H	1:A:45:LEU:HD23	0.51	1.65	3	1
1:C:50:ASN:ND2	1:C:53:ASN:HD22	0.51	2.03	10	1
1:A:23:LEU:HD21	1:C:23:LEU:HD11	0.51	1.81	16	1
1:B:45:LEU:HD23	1:B:45:LEU:H	0.51	1.65	3	1
1:A:37:LEU:HD12	1:A:37:LEU:C	0.51	2.31	5	1
1:A:27:LEU:HD12	1:C:27:LEU:HD21	0.51	1.81	8	1
1:A:58:ILE:HD12	1:A:58:ILE:C	0.50	2.30	17	1
1:A:36:LEU:C	1:A:36:LEU:HD12	0.50	2.31	18	1
1:C:36:LEU:C	1:C:36:LEU:HD12	0.50	2.31	18	1
1:A:37:LEU:HD23	1:A:37:LEU:O	0.50	2.06	9	3
1:C:37:LEU:O	1:C:37:LEU:HD23	0.50	2.06	9	2
1:B:36:LEU:HD12	1:B:36:LEU:C	0.50	2.31	18	1
1:B:23:LEU:HD11	1:C:23:LEU:HD21	0.50	1.82	16	1
1:C:51:ILE:C	1:C:51:ILE:HD12	0.50	2.32	15	2
1:B:37:LEU:HD23	1:B:37:LEU:O	0.49	2.06	9	3
1:A:15:ARG:HH21	1:C:15:ARG:CA	0.49	2.20	2	1
1:A:51:ILE:HD12	1:A:51:ILE:C	0.49	2.33	15	2
1:A:23:LEU:HD21	1:C:23:LEU:HD13	0.49	1.83	3	1
1:B:51:ILE:HD12	1:B:51:ILE:C	0.49	2.33	15	2
1:B:23:LEU:HD13	1:C:23:LEU:HD21	0.49	1.83	3	1
1:C:50:ASN:ND2	1:C:54:TRP:HE1	0.49	2.06	3	1
1:A:54:TRP:CD1	1:A:54:TRP:H	0.49	2.24	7	1
1:B:53:ASN:O	1:B:56:TRP:CD1	0.49	2.66	6	2
1:C:55:LEU:C	1:C:55:LEU:HD23	0.49	2.33	18	1
1:B:50:ASN:ND2	1:B:54:TRP:HE1	0.48	2.06	3	1
1:A:55:LEU:HD23	1:A:55:LEU:C	0.48	2.33	18	1
1:B:27:LEU:HD12	1:B:27:LEU:N	0.48	2.23	3	1
1:A:23:LEU:HD13	1:B:23:LEU:HD21	0.48	1.83	3	1
1:C:54:TRP:CD1	1:C:54:TRP:H	0.48	2.25	7	1
1:A:27:LEU:N	1:A:27:LEU:HD12	0.48	2.24	3	1
1:C:53:ASN:O	1:C:56:TRP:CD1	0.48	2.66	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ASN:ND2	1:A:54:TRP:HE1	0.48	2.06	3	1
1:B:55:LEU:C	1:B:55:LEU:HD23	0.48	2.33	18	1
1:C:38:GLU:O	1:C:42:TRP:CD1	0.47	2.67	6	8
1:A:50:ASN:O	1:A:54:TRP:CD1	0.47	2.68	17	14
1:A:53:ASN:O	1:A:56:TRP:CD1	0.47	2.66	6	1
1:B:47:ASN:OD1	1:B:48:TRP:N	0.47	2.48	15	2
1:C:37:LEU:C	1:C:37:LEU:HD23	0.47	2.35	1	1
1:C:50:ASN:O	1:C:54:TRP:CD1	0.47	2.68	9	14
1:C:27:LEU:HD12	1:C:27:LEU:N	0.47	2.23	3	1
1:A:37:LEU:C	1:A:37:LEU:HD23	0.47	2.35	1	1
1:B:31:GLY:C	1:B:33:GLU:N	0.47	2.73	15	5
1:B:37:LEU:C	1:B:37:LEU:HD23	0.47	2.35	1	1
1:B:38:GLU:O	1:B:42:TRP:CD1	0.47	2.67	6	8
1:B:50:ASN:O	1:B:54:TRP:CD1	0.47	2.68	11	14
1:A:38:GLU:O	1:A:42:TRP:NE1	0.47	2.48	9	1
1:A:31:GLY:C	1:A:33:GLU:N	0.47	2.73	15	4
1:B:6:ALA:N	1:B:7:PRO:CD	0.47	2.78	11	1
1:A:47:ASN:OD1	1:A:48:TRP:N	0.47	2.48	15	2
1:A:35:GLU:OE1	1:A:35:GLU:N	0.47	2.48	7	2
1:B:15:ARG:CA	1:C:15:ARG:HH21	0.47	2.22	2	1
1:C:38:GLU:O	1:C:42:TRP:NE1	0.47	2.48	9	1
1:C:48:TRP:C	1:C:50:ASN:H	0.47	2.18	18	3
1:A:38:GLU:O	1:A:42:TRP:CD1	0.47	2.67	6	8
1:C:35:GLU:N	1:C:35:GLU:OE1	0.47	2.48	7	1
1:B:38:GLU:O	1:B:42:TRP:NE1	0.47	2.48	9	1
1:A:48:TRP:C	1:A:50:ASN:H	0.47	2.18	18	3
1:C:45:LEU:O	1:C:45:LEU:HD23	0.46	2.10	8	2
1:C:29:SER:C	1:C:31:GLY:N	0.46	2.73	10	4
1:B:11:GLN:NE2	1:B:13:TYR:CE2	0.46	2.84	16	1
1:C:48:TRP:O	1:C:50:ASN:N	0.46	2.48	16	3
1:B:27:LEU:HD21	1:C:27:LEU:CD1	0.46	2.40	8	1
1:B:36:LEU:HD12	1:B:37:LEU:N	0.46	2.26	18	1
1:B:29:SER:C	1:B:31:GLY:N	0.46	2.73	10	5
1:A:6:ALA:N	1:A:7:PRO:CD	0.46	2.78	11	1
1:A:36:LEU:HD12	1:A:37:LEU:N	0.46	2.26	18	1
1:B:36:LEU:CD2	1:C:32:ASN:HD21	0.46	2.24	18	1
1:A:47:ASN:ND2	1:A:48:TRP:H	0.46	2.09	7	2
1:A:27:LEU:HD21	1:B:27:LEU:CD1	0.46	2.41	8	1
1:A:45:LEU:O	1:A:45:LEU:HD23	0.46	2.10	8	1
1:C:6:ALA:N	1:C:7:PRO:CD	0.46	2.78	11	1
1:B:48:TRP:O	1:B:50:ASN:N	0.46	2.49	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:50:ASN:O	1:B:54:TRP:NE1	0.46	2.49	8	9
1:C:50:ASN:O	1:C:54:TRP:NE1	0.46	2.48	3	9
1:C:44:SER:O	1:C:47:ASN:ND2	0.46	2.49	7	2
1:A:27:LEU:CD1	1:C:27:LEU:HD21	0.46	2.40	8	1
1:C:47:ASN:OD1	1:C:48:TRP:N	0.46	2.48	15	2
1:A:48:TRP:O	1:A:50:ASN:N	0.46	2.48	16	3
1:A:15:ARG:CZ	1:C:20:TRP:CE3	0.46	2.99	17	1
1:C:32:ASN:C	1:C:34:GLN:N	0.46	2.74	11	4
1:B:35:GLU:N	1:B:35:GLU:OE1	0.46	2.48	7	1
1:B:11:GLN:N	1:B:11:GLN:OE1	0.46	2.49	12	3
1:C:11:GLN:NE2	1:C:13:TYR:CE2	0.46	2.84	16	1
1:C:27:LEU:HD12	1:C:27:LEU:H	0.46	1.71	3	1
1:A:38:GLU:N	1:A:38:GLU:OE1	0.46	2.49	14	4
1:A:11:GLN:NE2	1:A:13:TYR:CE2	0.46	2.84	16	1
1:A:29:SER:OG	1:A:30:SER:N	0.46	2.49	5	1
1:B:44:SER:O	1:B:47:ASN:ND2	0.46	2.49	7	2
1:B:48:TRP:C	1:B:50:ASN:H	0.46	2.19	18	3
1:C:36:LEU:HD12	1:C:37:LEU:N	0.46	2.26	18	1
1:A:50:ASN:O	1:A:54:TRP:NE1	0.46	2.49	8	9
1:B:48:TRP:CD1	1:B:48:TRP:C	0.46	2.94	9	8
1:B:29:SER:OG	1:B:30:SER:N	0.46	2.49	5	1
1:B:32:ASN:C	1:B:34:GLN:N	0.46	2.74	11	3
1:C:11:GLN:N	1:C:11:GLN:OE1	0.46	2.49	12	3
1:C:38:GLU:N	1:C:38:GLU:OE1	0.46	2.49	14	4
1:B:20:TRP:CE3	1:C:15:ARG:CZ	0.46	2.99	17	1
1:C:29:SER:OG	1:C:30:SER:N	0.45	2.49	5	1
1:A:44:SER:O	1:A:47:ASN:ND2	0.45	2.49	7	2
1:B:45:LEU:HD23	1:B:45:LEU:O	0.45	2.10	8	2
1:A:29:SER:O	1:A:32:ASN:N	0.45	2.50	1	4
1:A:54:TRP:CD1	1:A:54:TRP:N	0.45	2.84	1	5
1:C:34:GLN:C	1:C:34:GLN:HE21	0.45	2.19	4	1
1:C:50:ASN:OD1	1:C:54:TRP:NE1	0.45	2.49	11	1
1:B:38:GLU:OE1	1:B:38:GLU:N	0.45	2.49	14	4
1:A:20:TRP:CE3	1:B:15:ARG:CZ	0.45	2.99	17	1
1:A:15:ARG:HH21	1:C:15:ARG:N	0.45	2.09	2	1
1:A:27:LEU:HD12	1:A:27:LEU:H	0.45	1.71	3	1
1:B:47:ASN:ND2	1:B:48:TRP:H	0.45	2.09	7	2
1:A:15:ARG:CA	1:B:15:ARG:HH21	0.45	2.24	2	1
1:A:34:GLN:HE21	1:A:34:GLN:C	0.45	2.20	4	1
1:A:53:ASN:OD1	1:A:54:TRP:N	0.45	2.49	17	1
1:B:53:ASN:O	1:B:56:TRP:NE1	0.45	2.50	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:53:ASN:OD1	1:B:54:TRP:N	0.45	2.49	17	1
1:A:15:ARG:HH21	1:C:14:VAL:C	0.45	2.19	2	2
1:B:31:GLY:O	1:B:32:ASN:ND2	0.45	2.50	2	2
1:A:50:ASN:OD1	1:A:54:TRP:NE1	0.45	2.49	11	1
1:A:48:TRP:C	1:A:48:TRP:CD1	0.45	2.95	10	4
1:B:53:ASN:OD1	1:B:54:TRP:CE2	0.45	2.70	2	1
1:C:31:GLY:O	1:C:32:ASN:ND2	0.45	2.50	2	2
1:C:53:ASN:O	1:C:56:TRP:NE1	0.45	2.50	5	1
1:C:55:LEU:O	1:C:59:LYS:N	0.45	2.50	17	2
1:C:42:TRP:CD1	1:C:42:TRP:N	0.45	2.83	9	2
1:B:11:GLN:NE2	1:B:11:GLN:C	0.45	2.75	11	2
1:C:11:GLN:NE2	1:C:11:GLN:C	0.45	2.75	11	2
1:A:11:GLN:N	1:A:11:GLN:OE1	0.45	2.49	12	3
1:C:20:TRP:CD1	1:C:20:TRP:N	0.45	2.85	18	1
1:C:48:TRP:C	1:C:48:TRP:CD1	0.45	2.94	9	3
1:C:9:ASP:N	1:C:9:ASP:OD1	0.45	2.50	10	2
1:B:55:LEU:O	1:B:59:LYS:N	0.45	2.50	17	2
1:C:47:ASN:ND2	1:C:48:TRP:H	0.45	2.09	7	2
1:B:42:TRP:N	1:B:42:TRP:CD1	0.45	2.84	9	1
1:A:50:ASN:O	1:A:53:ASN:N	0.45	2.50	14	5
1:B:50:ASN:O	1:B:53:ASN:N	0.45	2.50	9	5
1:A:32:ASN:C	1:A:34:GLN:N	0.45	2.75	5	6
1:A:48:TRP:CD1	1:A:48:TRP:C	0.45	2.95	2	5
1:A:53:ASN:OD1	1:A:54:TRP:CE2	0.45	2.70	2	1
1:C:53:ASN:OD1	1:C:54:TRP:CE2	0.45	2.70	2	1
1:C:56:TRP:H	1:C:56:TRP:CD1	0.45	2.29	8	1
1:B:53:ASN:OD1	1:B:54:TRP:CD2	0.44	2.70	2	1
1:C:35:GLU:OE1	1:C:35:GLU:N	0.44	2.50	2	1
1:C:31:GLY:C	1:C:33:GLU:N	0.44	2.73	15	5
1:A:20:TRP:CD1	1:A:20:TRP:N	0.44	2.85	18	1
1:C:3:ILE:N	1:C:4:PRO:CD	0.44	2.81	1	9
1:C:11:GLN:OE1	1:C:13:TYR:CG	0.44	2.71	1	1
1:A:31:GLY:O	1:A:32:ASN:ND2	0.44	2.51	3	2
1:C:53:ASN:OD1	1:C:54:TRP:CD2	0.44	2.70	2	1
1:A:27:LEU:HD11	1:B:27:LEU:HA	0.44	1.89	7	1
1:A:55:LEU:O	1:A:59:LYS:N	0.44	2.50	17	2
1:C:53:ASN:OD1	1:C:54:TRP:N	0.44	2.49	17	1
1:C:50:ASN:O	1:C:53:ASN:N	0.44	2.50	9	5
1:B:35:GLU:OE1	1:B:35:GLU:N	0.44	2.50	2	1
1:A:9:ASP:N	1:A:9:ASP:OD1	0.44	2.50	3	2
1:A:52:THR:O	1:A:56:TRP:CD1	0.44	2.70	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:ALA:O	1:B:47:ASN:N	0.44	2.50	16	1
1:B:34:GLN:HE21	1:B:34:GLN:C	0.44	2.19	4	1
1:B:43:ALA:O	1:B:47:ASN:ND2	0.44	2.51	7	1
1:A:56:TRP:CD1	1:A:56:TRP:H	0.44	2.29	8	1
1:A:3:ILE:N	1:A:4:PRO:CD	0.44	2.81	1	8
1:B:3:ILE:N	1:B:4:PRO:CD	0.44	2.81	1	9
1:C:48:TRP:CD1	1:C:48:TRP:C	0.44	2.95	1	5
1:A:53:ASN:O	1:A:56:TRP:NE1	0.44	2.50	5	1
1:C:52:THR:O	1:C:56:TRP:CD1	0.44	2.70	9	1
1:B:50:ASN:OD1	1:B:54:TRP:NE1	0.44	2.49	11	1
1:C:48:TRP:C	1:C:50:ASN:N	0.44	2.75	18	3
1:B:32:ASN:ND2	1:B:35:GLU:CD	0.44	2.76	10	2
1:C:32:ASN:ND2	1:C:35:GLU:OE1	0.44	2.50	1	1
1:A:29:SER:C	1:A:31:GLY:N	0.44	2.73	10	3
1:B:15:ARG:CG	1:C:15:ARG:HH21	0.44	2.25	10	1
1:B:20:TRP:CD1	1:B:20:TRP:N	0.44	2.85	18	1
1:C:29:SER:O	1:C:32:ASN:N	0.44	2.49	15	4
1:C:32:ASN:ND2	1:C:35:GLU:CD	0.44	2.76	10	2
1:A:53:ASN:OD1	1:A:54:TRP:CD2	0.44	2.70	2	1
1:A:43:ALA:O	1:A:47:ASN:ND2	0.44	2.51	7	1
1:C:30:SER:C	1:C:32:ASN:N	0.44	2.76	10	1
1:A:11:GLN:OE1	1:A:13:TYR:CG	0.44	2.71	1	1
1:B:27:LEU:HD11	1:C:27:LEU:HA	0.44	1.89	7	1
1:C:43:ALA:O	1:C:47:ASN:ND2	0.44	2.51	7	1
1:A:11:GLN:C	1:A:11:GLN:NE2	0.44	2.75	11	1
1:A:20:TRP:CD1	1:A:20:TRP:H	0.44	2.31	15	1
1:B:11:GLN:OE1	1:B:13:TYR:CG	0.44	2.71	1	1
1:B:29:SER:O	1:B:32:ASN:N	0.44	2.49	1	4
1:A:15:ARG:CG	1:B:15:ARG:HH21	0.44	2.26	10	1
1:A:32:ASN:ND2	1:A:35:GLU:CD	0.43	2.76	10	2
1:A:27:LEU:HA	1:C:27:LEU:HD11	0.43	1.90	7	1
1:B:48:TRP:C	1:B:50:ASN:N	0.43	2.76	18	3
1:B:9:ASP:N	1:B:9:ASP:OD1	0.43	2.50	3	1
1:B:20:TRP:CZ3	1:C:15:ARG:NH1	0.43	2.86	5	1
1:A:15:ARG:NH1	1:C:20:TRP:CZ3	0.43	2.85	5	1
1:A:30:SER:C	1:A:32:ASN:N	0.43	2.76	10	1
1:B:9:ASP:OD1	1:B:9:ASP:N	0.43	2.50	10	1
1:C:30:SER:C	1:C:32:ASN:H	0.43	2.22	1	2
1:A:15:ARG:HH21	1:C:15:ARG:CG	0.43	2.27	10	1
1:A:43:ALA:O	1:A:47:ASN:N	0.43	2.50	16	1
1:B:52:THR:O	1:B:56:TRP:CD1	0.43	2.70	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:TRP:C	1:A:50:ASN:N	0.43	2.76	18	3
1:C:48:TRP:CD1	1:C:49:PHE:N	0.43	2.87	17	2
1:B:27:LEU:HD12	1:B:27:LEU:H	0.43	1.71	3	1
1:B:56:TRP:H	1:B:56:TRP:CD1	0.43	2.29	8	1
1:B:30:SER:C	1:B:32:ASN:N	0.43	2.76	10	1
1:A:48:TRP:CD1	1:A:49:PHE:N	0.43	2.87	17	2
1:B:11:GLN:OE1	1:B:11:GLN:N	0.43	2.50	5	1
1:A:23:LEU:O	1:A:26:PHE:N	0.43	2.51	11	1
1:A:35:GLU:HG3	1:C:39:LEU:HD22	0.43	1.90	2	1
1:A:20:TRP:CZ3	1:B:15:ARG:NH1	0.43	2.86	5	1
1:B:53:ASN:O	1:B:56:TRP:CE2	0.43	2.72	8	1
1:B:48:TRP:CD1	1:B:49:PHE:N	0.43	2.87	17	2
1:C:37:LEU:HD23	1:C:37:LEU:O	0.43	2.14	1	1
1:A:5:GLU:O	1:A:6:ALA:HB3	0.43	2.14	11	2
1:A:53:ASN:O	1:A:56:TRP:CE2	0.43	2.72	8	1
1:C:53:ASN:O	1:C:56:TRP:CE2	0.43	2.72	8	1
1:A:42:TRP:CD1	1:A:42:TRP:N	0.43	2.87	16	2
1:B:42:TRP:CD1	1:B:42:TRP:N	0.43	2.87	16	1
1:B:5:GLU:O	1:B:6:ALA:HB3	0.42	2.14	11	2
1:A:32:ASN:HD21	1:C:36:LEU:CD2	0.42	2.27	18	1
1:B:14:VAL:CG2	1:B:15:ARG:N	0.42	2.82	3	1
1:C:20:TRP:H	1:C:20:TRP:CD1	0.42	2.31	15	1
1:A:15:ARG:CZ	1:C:20:TRP:CZ3	0.42	3.03	13	1
1:B:13:TYR:OH	1:C:15:ARG:NE	0.42	2.52	4	1
1:C:30:SER:OG	1:C:32:ASN:N	0.42	2.53	16	1
1:A:15:ARG:NH2	1:C:20:TRP:CZ3	0.42	2.87	10	1
1:C:43:ALA:O	1:C:47:ASN:N	0.42	2.50	16	1
1:C:14:VAL:CG2	1:C:15:ARG:N	0.42	2.82	3	1
1:B:31:GLY:C	1:B:33:GLU:H	0.42	2.22	4	2
1:C:23:LEU:O	1:C:26:PHE:N	0.42	2.51	11	1
1:B:32:ASN:HD21	1:B:35:GLU:CD	0.42	2.23	1	1
1:B:14:VAL:C	1:C:15:ARG:HH21	0.42	2.23	2	2
1:B:23:LEU:O	1:B:26:PHE:N	0.42	2.51	11	1
1:A:20:TRP:CZ3	1:B:15:ARG:CZ	0.42	3.03	13	1
1:B:20:TRP:CD1	1:B:20:TRP:H	0.42	2.31	15	1
1:A:30:SER:OG	1:A:32:ASN:N	0.42	2.53	16	1
1:B:16:LYS:O	1:B:19:GLU:N	0.42	2.53	1	1
1:A:14:VAL:C	1:B:15:ARG:HH21	0.42	2.23	3	2
1:C:5:GLU:O	1:C:6:ALA:HB3	0.42	2.14	11	2
1:C:47:ASN:ND2	1:C:48:TRP:N	0.42	2.68	7	1
1:A:12:ALA:O	1:A:22:LEU:HD23	0.42	2.14	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:12:ALA:O	1:B:22:LEU:HD23	0.42	2.14	8	1
1:B:20:TRP:CZ3	1:C:15:ARG:CZ	0.42	3.03	13	1
1:B:39:LEU:H	1:B:39:LEU:CD2	0.42	2.28	9	1
1:B:47:ASN:ND2	1:B:48:TRP:N	0.41	2.68	7	1
1:A:20:TRP:CZ3	1:B:15:ARG:NH2	0.41	2.88	10	1
1:B:30:SER:OG	1:B:32:ASN:N	0.41	2.53	16	1
1:A:47:ASN:ND2	1:A:48:TRP:N	0.41	2.68	7	1
1:C:16:LYS:O	1:C:19:GLU:N	0.41	2.53	1	1
1:A:31:GLY:C	1:A:33:GLU:H	0.41	2.23	10	2
1:C:31:GLY:C	1:C:33:GLU:H	0.41	2.23	4	1
1:B:13:TYR:O	1:C:14:VAL:CG2	0.41	2.69	11	1
1:B:50:ASN:CG	1:B:54:TRP:HE1	0.41	2.23	11	1
1:A:11:GLN:NE2	1:A:11:GLN:C	0.41	2.79	16	1
1:B:15:ARG:N	1:C:15:ARG:HH21	0.41	2.13	2	1
1:C:32:ASN:C	1:C:32:ASN:ND2	0.41	2.78	6	1
1:B:30:SER:C	1:B:32:ASN:H	0.41	2.22	1	1
1:A:14:VAL:CG2	1:A:15:ARG:N	0.41	2.82	3	1
1:A:23:LEU:HD12	1:B:14:VAL:HG21	0.41	1.91	18	1
1:A:39:LEU:H	1:A:39:LEU:CD2	0.41	2.28	9	1
1:B:20:TRP:CZ3	1:C:15:ARG:NH2	0.41	2.89	10	1
1:B:32:ASN:ND2	1:B:35:GLU:OE1	0.41	2.50	1	1
1:B:32:ASN:C	1:B:32:ASN:ND2	0.41	2.78	6	1
1:C:12:ALA:O	1:C:22:LEU:HD23	0.41	2.15	8	1
1:A:14:VAL:N	1:A:21:VAL:O	0.41	2.54	13	1
1:C:14:VAL:N	1:C:21:VAL:O	0.41	2.54	13	1
1:B:53:ASN:OD1	1:B:54:TRP:NE1	0.41	2.54	16	1
1:A:30:SER:C	1:A:32:ASN:H	0.41	2.22	1	1
1:A:37:LEU:HD23	1:A:37:LEU:C	0.41	2.41	9	1
1:B:15:ARG:CB	1:C:15:ARG:HH21	0.41	2.29	10	1
1:C:50:ASN:CG	1:C:54:TRP:HE1	0.41	2.23	11	1
1:C:53:ASN:OD1	1:C:54:TRP:NE1	0.41	2.54	16	1
1:B:36:LEU:CD2	1:C:27:LEU:O	0.41	2.69	18	1
1:B:26:PHE:O	1:B:26:PHE:CD1	0.40	2.75	8	1
1:C:37:LEU:HD23	1:C:37:LEU:C	0.40	2.41	9	1
1:A:14:VAL:CG2	1:C:13:TYR:O	0.40	2.69	11	1
1:A:13:TYR:N	1:A:13:TYR:CD1	0.40	2.89	16	1
1:C:13:TYR:N	1:C:13:TYR:CD1	0.40	2.89	16	1
1:B:23:LEU:HD12	1:C:14:VAL:HG21	0.40	1.91	18	1
1:B:37:LEU:HD23	1:B:37:LEU:C	0.40	2.42	9	1
1:A:32:ASN:C	1:A:32:ASN:ND2	0.40	2.78	6	1
1:A:13:TYR:O	1:B:14:VAL:CG2	0.40	2.69	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:38:GLU:OE1	1:C:42:TRP:NE1	0.40	2.55	15	1
1:B:13:TYR:CD1	1:B:13:TYR:N	0.40	2.89	16	1
1:A:32:ASN:ND2	1:A:35:GLU:OE1	0.40	2.50	1	1
1:A:15:ARG:NE	1:C:13:TYR:OH	0.40	2.55	4	1
1:A:50:ASN:CG	1:A:54:TRP:HE1	0.40	2.24	11	1
1:B:38:GLU:OE1	1:B:42:TRP:NE1	0.40	2.55	15	1
1:A:36:LEU:CD2	1:B:27:LEU:O	0.40	2.70	18	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	57/59 (97%)	48±2 (84±3%)	7±2 (13±3%)	2±1 (3±1%)	5	38
1	B	57/59 (97%)	48±2 (84±4%)	7±2 (13±3%)	2±1 (3±1%)	5	38
1	C	57/59 (97%)	48±2 (84±3%)	7±2 (13±3%)	2±1 (3±2%)	5	39
All	All	3078/3186 (97%)	2594 (84%)	392 (13%)	92 (3%)	5	38

All 21 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	3	ILE	13
1	B	3	ILE	13
1	C	3	ILE	13
1	A	29	SER	6
1	B	29	SER	6
1	C	29	SER	6
1	A	32	ASN	5
1	B	32	ASN	5
1	C	32	ASN	5
1	A	49	PHE	4
1	B	49	PHE	4
1	C	49	PHE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	30	SER	1
1	B	30	SER	1
1	C	30	SER	1
1	A	17	ASP	1
1	B	17	ASP	1
1	C	17	ASP	1
1	A	6	ALA	1
1	B	6	ALA	1
1	C	6	ALA	1

6.3.2 Protein sidechains ⓘ

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	51/51 (100%)	42±4 (82±7%)	9±4 (18±7%)	3	36
1	B	51/51 (100%)	42±4 (82±7%)	9±4 (18±7%)	3	36
1	C	51/51 (100%)	42±4 (82±7%)	9±4 (18±7%)	3	36
All	All	2754/2754 (100%)	2253 (82%)	501 (18%)	3	36

All 111 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	3	ILE	11
1	A	51	ILE	11
1	B	3	ILE	11
1	B	51	ILE	11
1	C	3	ILE	11
1	C	51	ILE	11
1	A	22	LEU	10
1	A	54	TRP	10
1	B	22	LEU	10
1	B	54	TRP	10
1	C	22	LEU	10
1	C	54	TRP	10
1	A	27	LEU	9
1	B	27	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	C	27	LEU	9
1	A	48	TRP	8
1	B	48	TRP	8
1	C	48	TRP	8
1	A	15	ARG	7
1	B	15	ARG	7
1	C	15	ARG	7
1	A	37	LEU	7
1	B	37	LEU	7
1	C	37	LEU	7
1	A	13	TYR	6
1	A	38	GLU	6
1	B	13	TYR	6
1	B	38	GLU	6
1	C	13	TYR	6
1	C	38	GLU	6
1	A	55	LEU	6
1	B	55	LEU	6
1	C	55	LEU	6
1	A	11	GLN	5
1	A	36	LEU	5
1	B	11	GLN	5
1	B	36	LEU	5
1	C	11	GLN	5
1	C	36	LEU	5
1	A	21	VAL	5
1	A	23	LEU	5
1	B	21	VAL	5
1	B	23	LEU	5
1	C	21	VAL	5
1	C	23	LEU	5
1	A	34	GLN	5
1	A	41	LYS	5
1	B	34	GLN	5
1	B	41	LYS	5
1	C	34	GLN	5
1	C	41	LYS	5
1	A	32	ASN	4
1	B	32	ASN	4
1	C	32	ASN	4
1	A	29	SER	4
1	A	35	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	B	29	SER	4
1	B	35	GLU	4
1	C	29	SER	4
1	C	35	GLU	4
1	A	39	LEU	4
1	B	39	LEU	4
1	C	39	LEU	4
1	A	49	PHE	3
1	B	49	PHE	3
1	C	49	PHE	3
1	A	44	SER	3
1	B	44	SER	3
1	C	44	SER	3
1	A	14	VAL	2
1	B	14	VAL	2
1	C	14	VAL	2
1	A	25	THR	2
1	A	58	ILE	2
1	A	59	LYS	2
1	B	25	THR	2
1	B	58	ILE	2
1	B	59	LYS	2
1	C	25	THR	2
1	C	58	ILE	2
1	C	59	LYS	2
1	A	45	LEU	2
1	A	52	THR	2
1	B	45	LEU	2
1	B	52	THR	2
1	C	45	LEU	2
1	C	52	THR	2
1	A	50	ASN	2
1	B	50	ASN	2
1	C	50	ASN	2
1	A	30	SER	2
1	B	30	SER	2
1	C	30	SER	2
1	A	47	ASN	2
1	B	47	ASN	2
1	C	47	ASN	2
1	A	16	LYS	2
1	B	16	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	C	16	LYS	2
1	A	17	ASP	1
1	B	17	ASP	1
1	C	17	ASP	1
1	A	33	GLU	1
1	B	33	GLU	1
1	C	33	GLU	1
1	A	20	TRP	1
1	B	20	TRP	1
1	C	20	TRP	1
1	A	53	ASN	1
1	B	53	ASN	1
1	C	53	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 19% for the well-defined parts and 19% 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	485
Number of shifts mapped to atoms	485
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	55	0.13 ± 0.37	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	49	0.63 ± 0.16	Should be applied
$^{13}\text{C}'$	42	-0.44 ± 0.25	None needed (< 0.5 ppm)
^{15}N	55	-0.28 ± 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 19%, i.e. 485 atoms were assigned a chemical shift out of a possible 2505. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	252/888 (28%)	100/363 (28%)	97/354 (27%)	55/171 (32%)
Sidechain	221/1260 (18%)	163/816 (20%)	55/399 (14%)	3/45 (7%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	12/357 (3%)	6/174 (3%)	0/165 (0%)	6/18 (33%)
Overall	485/2505 (19%)	269/1353 (20%)	152/918 (17%)	64/234 (27%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 19%, i.e. 485 atoms were assigned a chemical shift out of a possible 2505. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	252/888 (28%)	100/363 (28%)	97/354 (27%)	55/171 (32%)
Sidechain	221/1260 (18%)	163/816 (20%)	55/399 (14%)	3/45 (7%)
Aromatic	12/357 (3%)	6/174 (3%)	0/165 (0%)	6/18 (33%)
Overall	485/2505 (19%)	269/1353 (20%)	152/918 (17%)	64/234 (27%)

7.1.4 Statistically unusual chemical shifts [i](#)

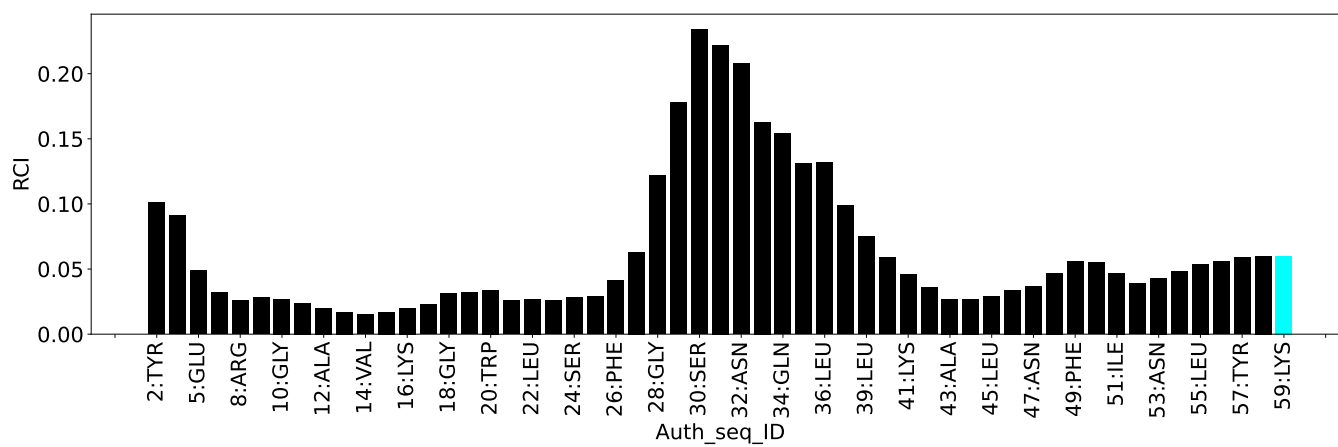
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	6	ALA	HB1	-0.42	0.14 – 2.58	-7.3
1	A	6	ALA	HB2	-0.42	0.14 – 2.58	-7.3
1	A	6	ALA	HB3	-0.42	0.14 – 2.58	-7.3

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	949
Intra-residue ($ i-j =0$)	48
Sequential ($ i-j =1$)	333
Medium range ($ i-j >1$ and $ i-j <5$)	456
Long range ($ i-j \geq 5$)	70
Inter-chain	42
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	255
Number of unmapped restraints	0
Number of restraints per residue	6.8
Number of long range restraints per residue ¹	0.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	59.7	0.2
0.2-0.5 (Medium)	46.4	0.5
>0.5 (Large)	2.0	0.79

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)	7.7	4.76
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

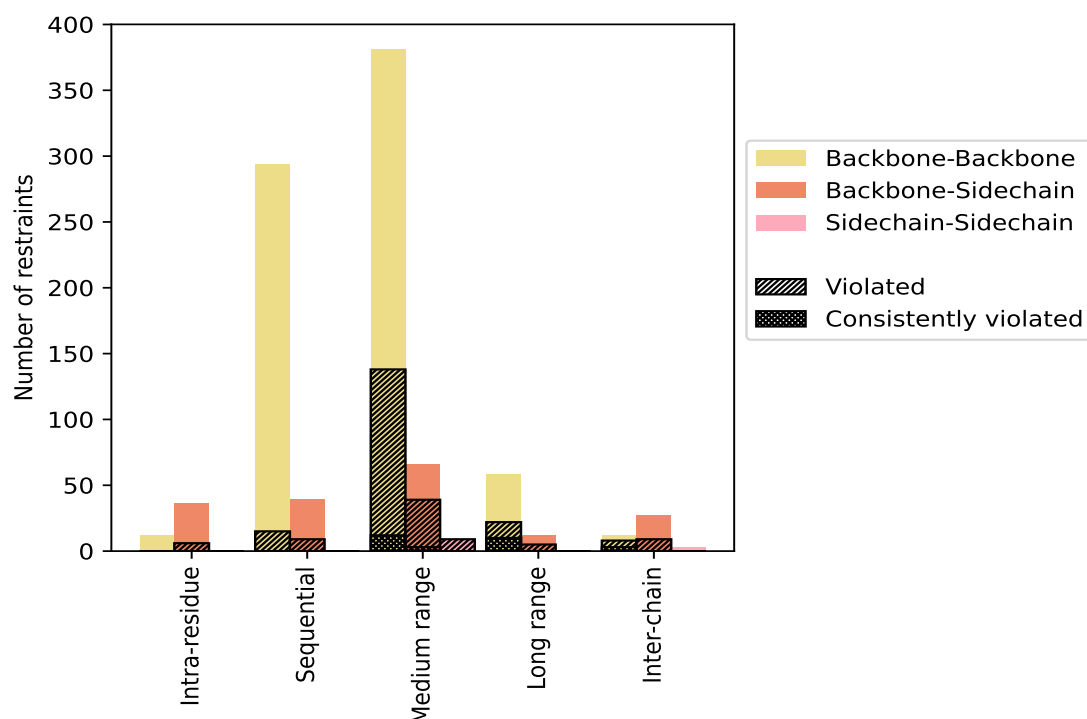
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	48	5.1	6	12.5	0.6	0	0.0	0.0
Backbone-Backbone	12	1.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	36	3.8	6	16.7	0.6	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	333	35.1	24	7.2	2.5	0	0.0	0.0
Backbone-Backbone	294	31.0	15	5.1	1.6	0	0.0	0.0
Backbone-Sidechain	39	4.1	9	23.1	0.9	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	456	48.1	186	40.8	19.6	15	3.3	1.6
Backbone-Backbone	381	40.1	138	36.2	14.5	12	3.1	1.3
Backbone-Sidechain	66	7.0	39	59.1	4.1	3	4.5	0.3
Sidechain-Sidechain	9	0.9	9	100.0	0.9	0	0.0	0.0
Long range (i-j ≥5)	70	7.4	27	38.6	2.8	10	14.3	1.1
Backbone-Backbone	58	6.1	22	37.9	2.3	10	17.2	1.1
Backbone-Sidechain	12	1.3	5	41.7	0.5	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	42	4.4	17	40.5	1.8	3	7.1	0.3
Backbone-Backbone	12	1.3	8	66.7	0.8	3	25.0	0.3
Backbone-Sidechain	27	2.8	9	33.3	0.9	0	0.0	0.0
Sidechain-Sidechain	3	0.3	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	949	100.0	260	27.4	27.4	28	3.0	3.0
Backbone-Backbone	757	79.8	183	24.2	19.3	25	3.3	2.6
Backbone-Sidechain	180	19.0	68	37.8	7.2	3	1.7	0.3
Sidechain-Sidechain	12	1.3	9	75.0	0.9	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 [i](#)



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	6	9	93	16	6	130	0.21	0.57	0.09	0.17
2	6	12	78	13	7	116	0.22	0.46	0.1	0.18
3	0	12	90	16	9	127	0.21	0.46	0.09	0.19
4	0	16	88	13	3	120	0.24	0.51	0.11	0.2
5	0	6	65	16	3	90	0.23	0.45	0.1	0.23
6	0	6	96	19	3	124	0.22	0.52	0.1	0.19
7	0	6	57	16	3	82	0.21	0.38	0.07	0.21
8	0	6	75	13	4	98	0.23	0.41	0.08	0.2
9	0	3	99	19	3	124	0.21	0.66	0.12	0.17
10	6	9	87	16	3	121	0.23	0.5	0.11	0.18

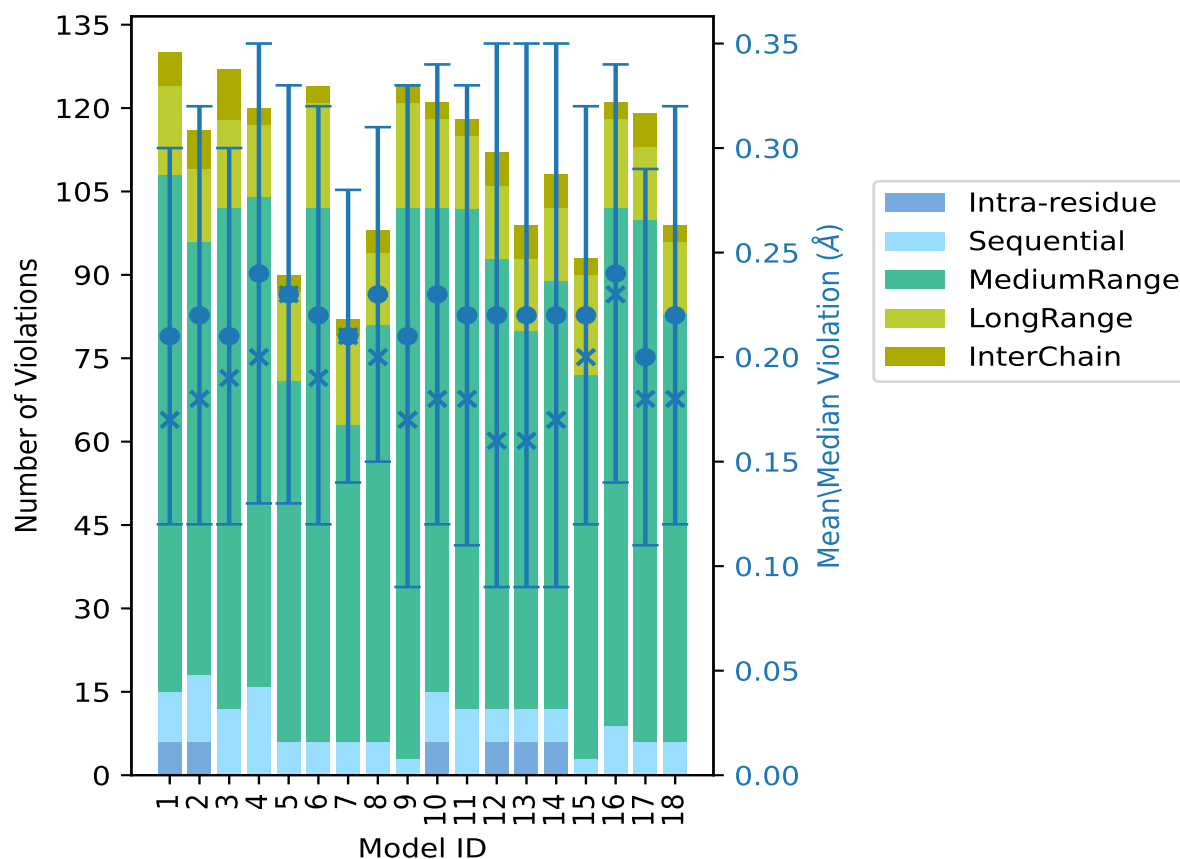
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	12	90	13	3	118	0.22	0.65	0.11	0.18
12	6	6	81	13	6	112	0.22	0.79	0.13	0.16
13	6	6	68	13	6	99	0.22	0.7	0.13	0.16
14	6	6	77	13	6	108	0.22	0.74	0.13	0.17
15	0	3	69	18	3	93	0.22	0.64	0.1	0.2
16	0	9	93	16	3	121	0.24	0.52	0.1	0.23
17	0	6	94	13	6	119	0.2	0.52	0.09	0.18
18	0	6	77	13	3	99	0.22	0.5	0.1	0.18

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

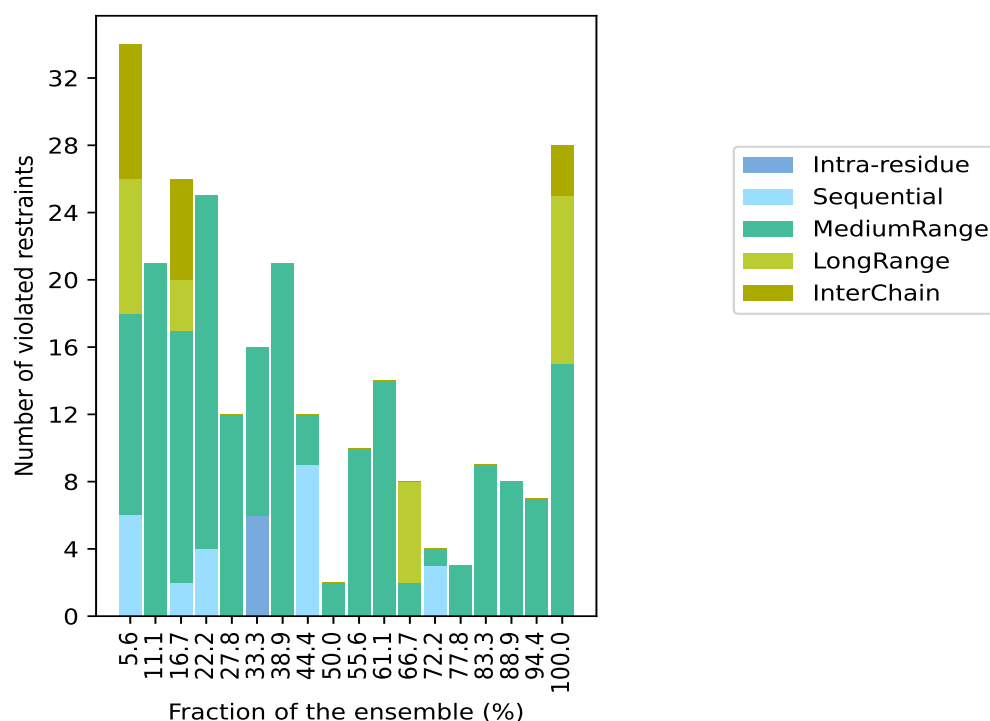
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 689(IR:42, SQ:309, MR:270, LR:43, IC:25) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	6	12	8	8	34	1	5.6
0	0	21	0	0	21	2	11.1
0	2	15	3	6	26	3	16.7
0	4	21	0	0	25	4	22.2
0	0	12	0	0	12	5	27.8
6	0	10	0	0	16	6	33.3
0	0	21	0	0	21	7	38.9
0	9	3	0	0	12	8	44.4
0	0	2	0	0	2	9	50.0
0	0	10	0	0	10	10	55.6
0	0	14	0	0	14	11	61.1
0	0	2	6	0	8	12	66.7
0	3	1	0	0	4	13	72.2
0	0	3	0	0	3	14	77.8
0	0	9	0	0	9	15	83.3
0	0	8	0	0	8	16	88.9
0	0	7	0	0	7	17	94.4
0	0	15	10	3	28	18	100.0

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

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

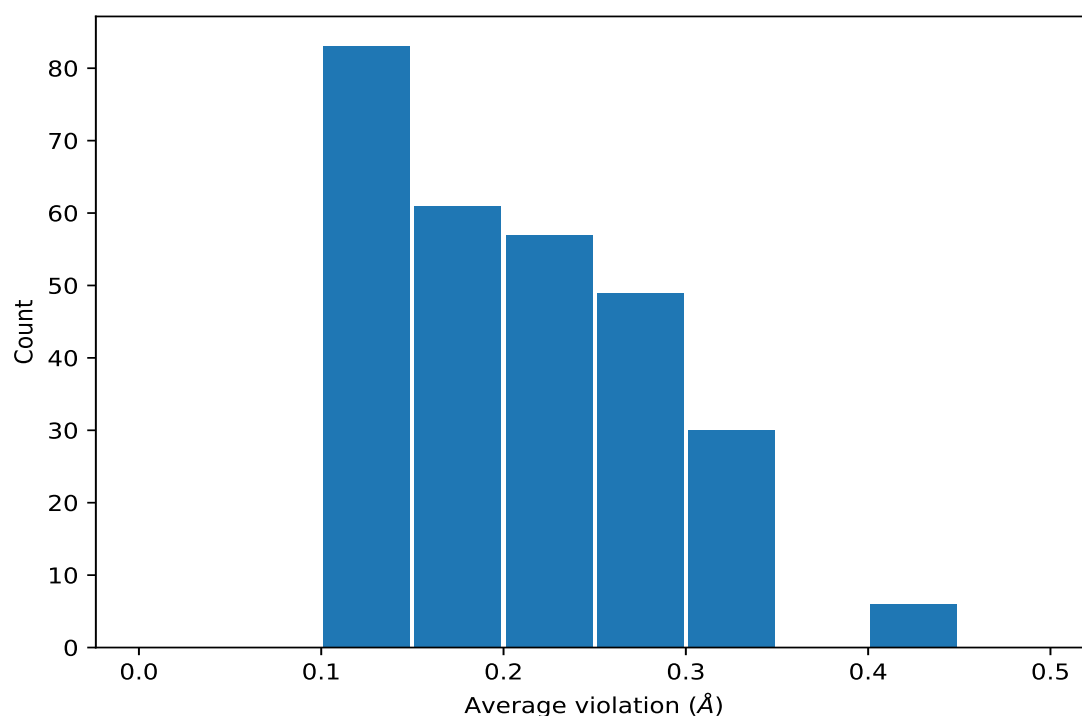
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	18	0.33	0.04	0.31
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	18	0.33	0.04	0.31
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	18	0.33	0.04	0.31
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	18	0.33	0.04	0.31
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	18	0.33	0.04	0.31
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	18	0.33	0.04	0.31
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	18	0.29	0.05	0.28
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	18	0.29	0.05	0.28
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	18	0.28	0.05	0.28
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	18	0.28	0.05	0.28
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	18	0.28	0.05	0.28
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	18	0.28	0.05	0.28
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	18	0.28	0.04	0.29
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	18	0.28	0.04	0.29
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	18	0.28	0.04	0.29
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	18	0.28	0.04	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	18	0.27	0.11	0.25
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	18	0.26	0.11	0.25
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	18	0.26	0.11	0.24
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	18	0.24	0.09	0.2
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	18	0.24	0.09	0.2
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	18	0.24	0.09	0.2
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	18	0.22	0.06	0.21
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	18	0.22	0.06	0.21
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	18	0.22	0.06	0.21
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	18	0.21	0.07	0.21
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	18	0.21	0.07	0.21
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	18	0.21	0.07	0.21
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	18	0.21	0.07	0.21
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	18	0.21	0.07	0.21
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	18	0.21	0.07	0.21
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	17	0.32	0.09	0.35
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	17	0.32	0.09	0.35
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	17	0.32	0.09	0.35
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	17	0.16	0.03	0.16
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	17	0.16	0.03	0.16
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	17	0.16	0.03	0.16
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	17	0.16	0.03	0.16
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	16	0.23	0.09	0.2
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	16	0.23	0.09	0.2
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	16	0.23	0.09	0.2
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	16	0.23	0.11	0.22
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	16	0.23	0.11	0.22
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	16	0.23	0.11	0.22
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	16	0.23	0.11	0.22
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	16	0.23	0.11	0.22
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	16	0.23	0.11	0.22
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	16	0.15	0.03	0.14
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	16	0.15	0.03	0.14
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	15	0.44	0.23	0.5
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	15	0.44	0.23	0.5
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	15	0.44	0.23	0.5
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	15	0.44	0.23	0.5
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	15	0.44	0.23	0.5
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	15	0.44	0.23	0.5
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	15	0.17	0.05	0.15
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	15	0.17	0.05	0.15
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	15	0.17	0.05	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	15	0.17	0.05	0.15
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	15	0.17	0.05	0.15
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	15	0.17	0.05	0.15
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	14	0.34	0.12	0.34
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	14	0.34	0.12	0.34
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	14	0.34	0.12	0.34
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	14	0.34	0.12	0.34
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	14	0.34	0.12	0.34
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	14	0.34	0.12	0.34
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	14	0.34	0.12	0.34
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	14	0.34	0.12	0.34
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	14	0.34	0.12	0.34
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	13	0.35	0.09	0.38
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	13	0.35	0.09	0.38
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	13	0.35	0.09	0.37
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	13	0.14	0.04	0.14
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	12	0.23	0.08	0.21
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	12	0.23	0.08	0.2
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	12	0.23	0.08	0.2
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	12	0.17	0.06	0.16
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	12	0.17	0.06	0.16
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	12	0.17	0.06	0.16
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	12	0.15	0.04	0.15
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	12	0.15	0.04	0.14
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	11	0.24	0.1	0.2
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	11	0.24	0.1	0.2
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	11	0.24	0.1	0.2
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	11	0.24	0.1	0.2
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	11	0.24	0.1	0.2
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	11	0.24	0.1	0.2
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	11	0.15	0.02	0.15
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	11	0.15	0.02	0.15
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	11	0.15	0.02	0.15
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	11	0.15	0.02	0.15
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	11	0.15	0.02	0.15
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	11	0.15	0.02	0.15
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	11	0.15	0.03	0.15
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	11	0.15	0.03	0.15
(2,73)	1:50:A:ASN:H	1:47:A:ASN:H	10	0.19	0.05	0.18
(2,74)	1:50:B:ASN:H	1:47:B:ASN:H	10	0.19	0.05	0.18
(2,75)	1:50:C:ASN:H	1:47:C:ASN:H	10	0.19	0.05	0.18
(2,341)	1:47:A:ASN:H	1:50:A:ASN:H	10	0.19	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,577)	1:47:B:ASN:H	1:50:B:ASN:H	10	0.19	0.05	0.18
(2,813)	1:47:C:ASN:H	1:50:C:ASN:H	10	0.19	0.05	0.18
(2,545)	1:14:B:VAL:H	1:16:B:LYS:H	10	0.15	0.03	0.16
(2,561)	1:14:B:VAL:H	1:16:B:LYS:H	10	0.15	0.03	0.16
(2,781)	1:14:C:VAL:H	1:16:C:LYS:H	10	0.15	0.03	0.16
(2,797)	1:14:C:VAL:H	1:16:C:LYS:H	10	0.15	0.03	0.16
(2,317)	1:21:A:VAL:H	1:23:A:LEU:H	9	0.16	0.04	0.13
(2,323)	1:21:A:VAL:H	1:23:A:LEU:H	9	0.16	0.04	0.13
(2,389)	1:32:B:ASN:HB2	1:33:B:GLU:H	8	0.34	0.08	0.36
(2,389)	1:32:B:ASN:HB3	1:33:B:GLU:H	8	0.34	0.08	0.36
(2,625)	1:32:C:ASN:HB2	1:33:C:GLU:H	8	0.34	0.08	0.36
(2,625)	1:32:C:ASN:HB3	1:33:C:GLU:H	8	0.34	0.08	0.36
(2,155)	1:32:A:ASN:HB2	1:33:A:GLU:H	8	0.34	0.08	0.36
(2,155)	1:32:A:ASN:HB3	1:33:A:GLU:H	8	0.34	0.08	0.36
(2,292)	1:32:A:ASN:HB2	1:34:A:GLN:H	8	0.3	0.19	0.23
(2,292)	1:32:A:ASN:HB3	1:34:A:GLN:H	8	0.3	0.19	0.23
(2,526)	1:32:B:ASN:HB2	1:34:B:GLN:H	8	0.3	0.19	0.22
(2,526)	1:32:B:ASN:HB3	1:34:B:GLN:H	8	0.3	0.19	0.22
(2,762)	1:32:C:ASN:HB2	1:34:C:GLN:H	8	0.3	0.19	0.22
(2,762)	1:32:C:ASN:HB3	1:34:C:GLN:H	8	0.3	0.19	0.22
(1,57)	1:42:B:TRP:HE1	1:43:B:ALA:H	8	0.18	0.03	0.17
(1,63)	1:42:B:TRP:HE1	1:43:B:ALA:H	8	0.18	0.03	0.17
(1,85)	1:42:C:TRP:HE1	1:43:C:ALA:H	8	0.18	0.03	0.17
(1,91)	1:42:C:TRP:HE1	1:43:C:ALA:H	8	0.18	0.03	0.17
(1,29)	1:42:A:TRP:HE1	1:43:A:ALA:H	8	0.17	0.03	0.17
(1,35)	1:42:A:TRP:HE1	1:43:A:ALA:H	8	0.17	0.03	0.17
(2,108)	1:34:C:GLN:H	1:30:C:SER:H	7	0.34	0.11	0.36
(2,106)	1:34:A:GLN:H	1:30:A:SER:H	7	0.34	0.11	0.36
(2,107)	1:34:B:GLN:H	1:30:B:SER:H	7	0.34	0.11	0.36
(2,293)	1:32:A:ASN:HB2	1:35:A:GLU:H	7	0.29	0.09	0.27
(2,293)	1:32:A:ASN:HB3	1:35:A:GLU:H	7	0.29	0.09	0.27
(2,527)	1:32:B:ASN:HB2	1:35:B:GLU:H	7	0.29	0.09	0.27
(2,527)	1:32:B:ASN:HB3	1:35:B:GLU:H	7	0.29	0.09	0.27
(2,763)	1:32:C:ASN:HB2	1:35:C:GLU:H	7	0.29	0.09	0.27
(2,763)	1:32:C:ASN:HB3	1:35:C:GLU:H	7	0.29	0.09	0.27
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD11	7	0.26	0.08	0.26
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD12	7	0.26	0.08	0.26
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD13	7	0.26	0.08	0.26
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD11	7	0.26	0.08	0.26
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD12	7	0.26	0.08	0.26
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD13	7	0.26	0.08	0.26
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD11	7	0.26	0.08	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD12	7	0.26	0.08	0.26
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD13	7	0.26	0.08	0.26
(2,257)	1:29:A:SER:HA	1:32:A:ASN:H	7	0.23	0.11	0.19
(2,302)	1:29:A:SER:HA	1:32:A:ASN:H	7	0.23	0.11	0.19
(2,491)	1:29:B:SER:HA	1:32:B:ASN:H	7	0.23	0.11	0.19
(2,536)	1:29:B:SER:HA	1:32:B:ASN:H	7	0.23	0.11	0.19
(2,727)	1:29:C:SER:HA	1:32:C:ASN:H	7	0.23	0.11	0.19
(2,772)	1:29:C:SER:HA	1:32:C:ASN:H	7	0.23	0.11	0.19
(2,787)	1:21:C:VAL:H	1:23:C:LEU:H	7	0.16	0.04	0.15
(2,794)	1:21:C:VAL:H	1:23:C:LEU:H	7	0.16	0.04	0.15
(2,551)	1:21:B:VAL:H	1:23:B:LEU:H	7	0.16	0.04	0.15
(2,558)	1:21:B:VAL:H	1:23:B:LEU:H	7	0.16	0.04	0.15
(2,255)	1:30:A:SER:HA	1:33:A:GLU:H	7	0.14	0.03	0.13
(2,303)	1:30:A:SER:HA	1:33:A:GLU:H	7	0.14	0.03	0.13
(2,471)	1:52:B:THR:H	1:54:B:TRP:H	6	0.17	0.04	0.18
(2,518)	1:52:B:THR:H	1:54:B:TRP:H	6	0.17	0.04	0.18
(2,237)	1:52:A:THR:H	1:54:A:TRP:H	6	0.17	0.04	0.18
(2,284)	1:52:A:THR:H	1:54:A:TRP:H	6	0.17	0.04	0.18
(2,707)	1:52:C:THR:H	1:54:C:TRP:H	6	0.17	0.04	0.18
(2,754)	1:52:C:THR:H	1:54:C:TRP:H	6	0.17	0.04	0.18
(2,489)	1:30:B:SER:HA	1:33:B:GLU:H	6	0.15	0.02	0.15
(2,537)	1:30:B:SER:HA	1:33:B:GLU:H	6	0.15	0.02	0.15
(2,725)	1:30:C:SER:HA	1:33:C:GLU:H	6	0.15	0.03	0.15
(2,773)	1:30:C:SER:HA	1:33:C:GLU:H	6	0.15	0.03	0.15
(2,540)	1:48:B:TRP:H	1:48:B:TRP:HE1	6	0.12	0.02	0.12
(2,555)	1:48:B:TRP:H	1:48:B:TRP:HE1	6	0.12	0.02	0.12
(2,307)	1:48:A:TRP:H	1:48:A:TRP:HE1	6	0.12	0.02	0.12
(2,320)	1:48:A:TRP:H	1:48:A:TRP:HE1	6	0.12	0.02	0.12
(2,776)	1:48:C:TRP:H	1:48:C:TRP:HE1	6	0.12	0.02	0.11
(2,791)	1:48:C:TRP:H	1:48:C:TRP:HE1	6	0.12	0.02	0.11
(2,256)	1:33:A:GLU:H	1:36:A:LEU:HG	5	0.25	0.08	0.31
(2,490)	1:33:B:GLU:H	1:36:B:LEU:HG	5	0.25	0.08	0.31
(2,726)	1:33:C:GLU:H	1:36:C:LEU:HG	5	0.25	0.08	0.31
(2,94)	1:44:A:SER:H	1:47:A:ASN:H	5	0.15	0.02	0.16
(2,95)	1:44:B:SER:H	1:47:B:ASN:H	5	0.15	0.02	0.16
(2,96)	1:44:C:SER:H	1:47:C:ASN:H	5	0.15	0.02	0.16
(2,544)	1:8:B:ARG:H	1:10:B:GLY:H	5	0.12	0.01	0.11
(2,560)	1:8:B:ARG:H	1:10:B:GLY:H	5	0.12	0.01	0.11
(2,310)	1:8:A:ARG:H	1:10:A:GLY:H	5	0.11	0.01	0.11
(2,325)	1:8:A:ARG:H	1:10:A:GLY:H	5	0.11	0.01	0.11
(2,780)	1:8:C:ARG:H	1:10:C:GLY:H	5	0.11	0.01	0.11
(2,796)	1:8:C:ARG:H	1:10:C:GLY:H	5	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,22)	1:51:A:ILE:HG12	1:48:A:TRP:HE1	4	0.24	0.13	0.22
(1,22)	1:51:A:ILE:HG13	1:48:A:TRP:HE1	4	0.24	0.13	0.22
(1,23)	1:51:B:ILE:HG12	1:48:B:TRP:HE1	4	0.24	0.13	0.22
(1,23)	1:51:B:ILE:HG13	1:48:B:TRP:HE1	4	0.24	0.13	0.22
(1,24)	1:51:C:ILE:HG12	1:48:C:TRP:HE1	4	0.24	0.13	0.22
(1,24)	1:51:C:ILE:HG13	1:48:C:TRP:HE1	4	0.24	0.13	0.22
(2,290)	1:27:A:LEU:HB2	1:29:A:SER:H	4	0.2	0.05	0.2
(2,290)	1:27:A:LEU:HB3	1:29:A:SER:H	4	0.2	0.05	0.2
(2,524)	1:27:B:LEU:HB2	1:29:B:SER:H	4	0.2	0.05	0.2
(2,524)	1:27:B:LEU:HB3	1:29:B:SER:H	4	0.2	0.05	0.2
(2,760)	1:27:C:LEU:HB2	1:29:C:SER:H	4	0.2	0.05	0.2
(2,760)	1:27:C:LEU:HB3	1:29:C:SER:H	4	0.2	0.05	0.2
(2,180)	1:33:A:GLU:H	1:35:A:GLU:H	4	0.19	0.05	0.18
(2,202)	1:33:A:GLU:H	1:35:A:GLU:H	4	0.19	0.05	0.18
(2,335)	1:32:A:ASN:H	1:35:A:GLU:H	4	0.19	0.05	0.2
(2,571)	1:32:B:ASN:H	1:35:B:GLU:H	4	0.19	0.05	0.2
(2,650)	1:33:C:GLU:H	1:35:C:GLU:H	4	0.19	0.05	0.18
(2,672)	1:33:C:GLU:H	1:35:C:GLU:H	4	0.19	0.05	0.18
(2,414)	1:33:B:GLU:H	1:35:B:GLU:H	4	0.19	0.05	0.18
(2,436)	1:33:B:GLU:H	1:35:B:GLU:H	4	0.19	0.05	0.18
(2,807)	1:32:C:ASN:H	1:35:C:GLU:H	4	0.19	0.05	0.2
(2,418)	1:43:B:ALA:H	1:45:B:LEU:H	4	0.15	0.04	0.14
(2,452)	1:43:B:ALA:H	1:45:B:LEU:H	4	0.15	0.04	0.14
(2,184)	1:43:A:ALA:H	1:45:A:LEU:H	4	0.14	0.04	0.13
(2,218)	1:43:A:ALA:H	1:45:A:LEU:H	4	0.14	0.04	0.13
(2,654)	1:43:C:ALA:H	1:45:C:LEU:H	4	0.14	0.04	0.13
(2,688)	1:43:C:ALA:H	1:45:C:LEU:H	4	0.14	0.04	0.13
(2,164)	1:14:A:VAL:H	1:15:A:ARG:H	4	0.11	0.01	0.11
(2,194)	1:14:A:VAL:H	1:15:A:ARG:H	4	0.11	0.01	0.11
(2,634)	1:14:C:VAL:H	1:15:C:ARG:H	4	0.11	0.01	0.11
(2,664)	1:14:C:VAL:H	1:15:C:ARG:H	4	0.11	0.01	0.11
(2,41)	1:34:B:GLN:H	1:36:B:LEU:HG	3	0.21	0.07	0.23
(2,492)	1:34:B:GLN:H	1:36:B:LEU:HG	3	0.21	0.07	0.23
(2,40)	1:34:A:GLN:H	1:36:A:LEU:HG	3	0.2	0.07	0.22
(2,42)	1:34:C:GLN:H	1:36:C:LEU:HG	3	0.2	0.07	0.22
(2,258)	1:34:A:GLN:H	1:36:A:LEU:HG	3	0.2	0.07	0.22
(2,728)	1:34:C:GLN:H	1:36:C:LEU:HG	3	0.2	0.07	0.22
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD21	3	0.19	0.09	0.14
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD22	3	0.19	0.09	0.14
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD23	3	0.19	0.09	0.14
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD21	3	0.19	0.09	0.14
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD22	3	0.19	0.09	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD23	3	0.19	0.09	0.14
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD21	3	0.19	0.09	0.14
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD22	3	0.19	0.09	0.14
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD23	3	0.19	0.09	0.14
(2,79)	1:34:A:GLN:H	1:31:A:GLY:H	3	0.18	0.06	0.16
(2,80)	1:34:B:GLN:H	1:31:B:GLY:H	3	0.18	0.06	0.16
(2,81)	1:34:C:GLN:H	1:31:C:GLY:H	3	0.18	0.06	0.16
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG21	3	0.14	0.0	0.14
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG22	3	0.14	0.0	0.14
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG23	3	0.14	0.0	0.14
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG21	3	0.13	0.03	0.12
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG22	3	0.13	0.03	0.12
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG23	3	0.13	0.03	0.12
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG21	3	0.13	0.0	0.13
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG22	3	0.13	0.0	0.13
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG23	3	0.13	0.0	0.13
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG21	3	0.13	0.0	0.13
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG22	3	0.13	0.0	0.13
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG23	3	0.13	0.0	0.13
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG21	3	0.13	0.03	0.12
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG22	3	0.13	0.03	0.12
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG23	3	0.13	0.03	0.12
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG21	3	0.12	0.01	0.12
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG22	3	0.12	0.01	0.12
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG23	3	0.12	0.01	0.12
(1,10)	1:26:A:PHE:H	1:29:A:SER:H	3	0.12	0.02	0.12
(1,11)	1:26:B:PHE:H	1:29:B:SER:H	3	0.12	0.02	0.12
(1,12)	1:26:C:PHE:H	1:29:C:SER:H	3	0.12	0.02	0.11
(2,208)	1:40:A:ASP:H	1:42:A:TRP:H	3	0.11	0.0	0.11
(2,442)	1:40:B:ASP:H	1:42:B:TRP:H	3	0.11	0.0	0.11
(2,678)	1:40:C:ASP:H	1:42:C:TRP:H	3	0.11	0.0	0.11
(2,398)	1:14:B:VAL:H	1:15:B:ARG:H	3	0.11	0.01	0.11
(2,428)	1:14:B:VAL:H	1:15:B:ARG:H	3	0.11	0.01	0.11
(2,52)	1:33:A:GLU:HG2	1:31:A:GLY:H	2	0.26	0.02	0.26
(2,52)	1:33:A:GLU:HG3	1:31:A:GLY:H	2	0.26	0.02	0.26
(2,53)	1:33:B:GLU:HG2	1:31:B:GLY:H	2	0.26	0.02	0.26
(2,53)	1:33:B:GLU:HG3	1:31:B:GLY:H	2	0.26	0.02	0.26
(2,54)	1:33:C:GLU:HG2	1:31:C:GLY:H	2	0.26	0.02	0.26
(2,54)	1:33:C:GLU:HG3	1:31:C:GLY:H	2	0.26	0.02	0.26
(2,121)	1:31:A:GLY:H	1:33:A:GLU:HG2	2	0.26	0.02	0.26
(2,121)	1:31:A:GLY:H	1:33:A:GLU:HG3	2	0.26	0.02	0.26
(2,122)	1:31:B:GLY:H	1:33:B:GLU:HG2	2	0.26	0.02	0.26

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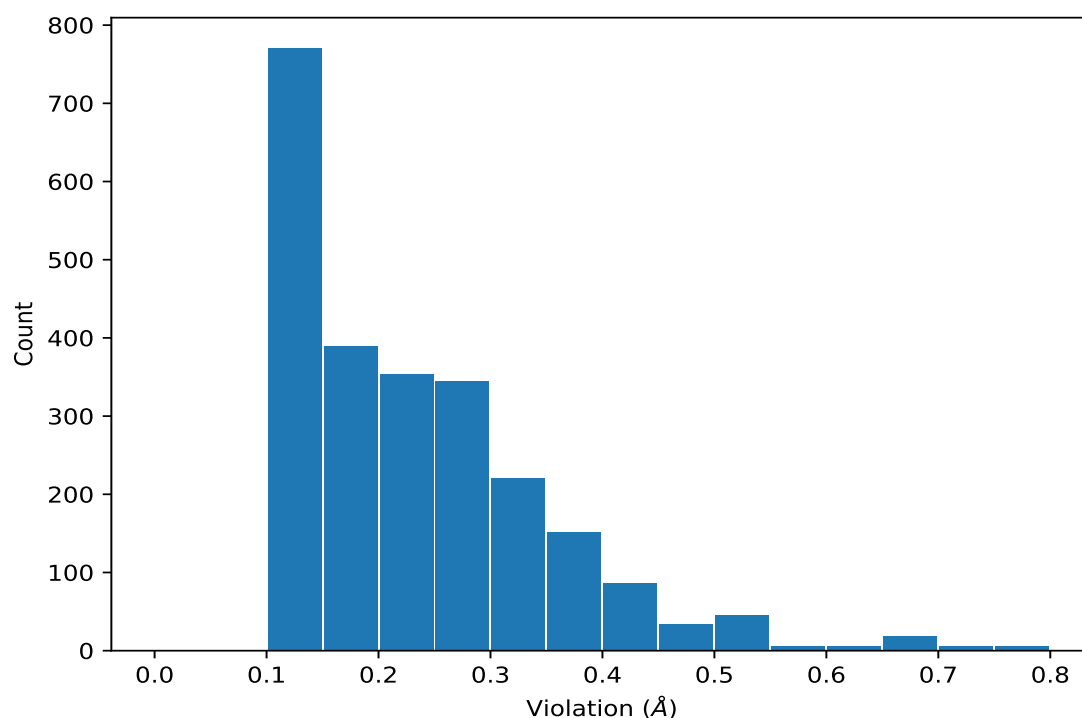
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,122)	1:31:B:GLY:H	1:33:B:GLU:HG3	2	0.26	0.02	0.26
(2,123)	1:31:C:GLY:H	1:33:C:GLU:HG2	2	0.26	0.02	0.26
(2,123)	1:31:C:GLY:H	1:33:C:GLU:HG3	2	0.26	0.02	0.26
(1,43)	1:23:A:LEU:H	1:27:A:LEU:H	2	0.2	0.02	0.2
(1,71)	1:23:B:LEU:H	1:27:B:LEU:H	2	0.2	0.02	0.2
(1,99)	1:23:C:LEU:H	1:27:C:LEU:H	2	0.2	0.02	0.2
(2,248)	1:56:A:TRP:H	1:58:A:ILE:H	2	0.18	0.01	0.18
(2,718)	1:56:C:TRP:H	1:58:C:ILE:H	2	0.18	0.01	0.18
(2,482)	1:56:B:TRP:H	1:58:B:ILE:H	2	0.18	0.02	0.18
(2,300)	1:34:A:GLN:H	1:36:A:LEU:H	2	0.14	0.02	0.14
(2,534)	1:34:B:GLN:H	1:36:B:LEU:H	2	0.14	0.02	0.14
(2,770)	1:34:C:GLN:H	1:36:C:LEU:H	2	0.14	0.02	0.14
(2,177)	1:23:A:LEU:H	1:25:A:THR:H	2	0.13	0.02	0.13
(2,207)	1:23:A:LEU:H	1:25:A:THR:H	2	0.13	0.02	0.13
(2,411)	1:23:B:LEU:H	1:25:B:THR:H	2	0.13	0.02	0.13
(2,441)	1:23:B:LEU:H	1:25:B:THR:H	2	0.13	0.02	0.13
(2,647)	1:23:C:LEU:H	1:25:C:THR:H	2	0.13	0.02	0.13
(2,677)	1:23:C:LEU:H	1:25:C:THR:H	2	0.13	0.02	0.13

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	12	0.79
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	12	0.79
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	12	0.78
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	12	0.78
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	12	0.78
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	12	0.78
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	14	0.74
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	14	0.74
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	14	0.74
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	14	0.74
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	14	0.74
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	14	0.74
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	13	0.7
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	13	0.7
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	13	0.7
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	13	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	13	0.7
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	13	0.7
(2,762)	1:32:C:ASN:HB2	1:34:C:GLN:H	9	0.66
(2,762)	1:32:C:ASN:HB3	1:34:C:GLN:H	9	0.66
(2,526)	1:32:B:ASN:HB2	1:34:B:GLN:H	9	0.66
(2,526)	1:32:B:ASN:HB3	1:34:B:GLN:H	9	0.66
(2,292)	1:32:A:ASN:HB2	1:34:A:GLN:H	9	0.66
(2,292)	1:32:A:ASN:HB3	1:34:A:GLN:H	9	0.66
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	11	0.65
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	11	0.65
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	11	0.65
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	11	0.65
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	11	0.65
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	11	0.65
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	15	0.64
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	15	0.64
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	15	0.64
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	15	0.64
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	15	0.64
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	15	0.64
(2,762)	1:32:C:ASN:HB2	1:34:C:GLN:H	1	0.57
(2,762)	1:32:C:ASN:HB3	1:34:C:GLN:H	1	0.57
(2,526)	1:32:B:ASN:HB2	1:34:B:GLN:H	1	0.57
(2,526)	1:32:B:ASN:HB3	1:34:B:GLN:H	1	0.57
(2,292)	1:32:A:ASN:HB2	1:34:A:GLN:H	1	0.57
(2,292)	1:32:A:ASN:HB3	1:34:A:GLN:H	1	0.57
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	6	0.52
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	6	0.52
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	6	0.52
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	6	0.52
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	6	0.52
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	6	0.52
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	16	0.52
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	16	0.52
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	17	0.52
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	17	0.52
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	16	0.52
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	16	0.52
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	17	0.52
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	17	0.52
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	16	0.52
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	16	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	17	0.52
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	17	0.52
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	4	0.51
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	4	0.51
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	4	0.51
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	9	0.51
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	9	0.51
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	9	0.51
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	4	0.51
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	4	0.51
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	4	0.51
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	9	0.51
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	9	0.51
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	9	0.51
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	4	0.51
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	4	0.51
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	4	0.51
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	9	0.51
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	9	0.51
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	9	0.51
(2,108)	1:34:C:GLN:H	1:30:C:SER:H	10	0.5
(2,107)	1:34:B:GLN:H	1:30:B:SER:H	10	0.5
(2,106)	1:34:A:GLN:H	1:30:A:SER:H	10	0.5
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	18	0.5
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	18	0.5
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	18	0.5
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	18	0.5
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	18	0.5
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	18	0.5
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	4	0.49
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	4	0.49
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	12	0.48
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	12	0.48
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	12	0.48
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	4	0.48
(2,763)	1:32:C:ASN:HB2	1:35:C:GLU:H	10	0.47
(2,763)	1:32:C:ASN:HB3	1:35:C:GLU:H	10	0.47
(2,527)	1:32:B:ASN:HB2	1:35:B:GLU:H	10	0.47
(2,527)	1:32:B:ASN:HB3	1:35:B:GLU:H	10	0.47
(2,293)	1:32:A:ASN:HB2	1:35:A:GLU:H	10	0.47
(2,293)	1:32:A:ASN:HB3	1:35:A:GLU:H	10	0.47
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	14	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	14	0.47
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	14	0.47
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	3	0.46
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	3	0.46
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	3	0.46
(2,108)	1:34:C:GLN:H	1:30:C:SER:H	9	0.46
(2,107)	1:34:B:GLN:H	1:30:B:SER:H	9	0.46
(2,106)	1:34:A:GLN:H	1:30:A:SER:H	9	0.46
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	10	0.46
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	10	0.46
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	10	0.46
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	2	0.46
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	5	0.45
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	5	0.45
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	5	0.45
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	10	0.45
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	10	0.45
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	10	0.45
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	10	0.45
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	10	0.45
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	10	0.45
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	2	0.44
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	2	0.44
(2,625)	1:32:C:ASN:HB2	1:33:C:GLU:H	13	0.43
(2,625)	1:32:C:ASN:HB3	1:33:C:GLU:H	13	0.43
(2,389)	1:32:B:ASN:HB2	1:33:B:GLU:H	13	0.43
(2,389)	1:32:B:ASN:HB3	1:33:B:GLU:H	13	0.43
(2,155)	1:32:A:ASN:HB2	1:33:A:GLU:H	13	0.43
(2,155)	1:32:A:ASN:HB3	1:33:A:GLU:H	13	0.43
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	4	0.43
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	3	0.43
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	2	0.42
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	2	0.42
(2,625)	1:32:C:ASN:HB2	1:33:C:GLU:H	11	0.42
(2,625)	1:32:C:ASN:HB3	1:33:C:GLU:H	11	0.42
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	2	0.42
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	2	0.42
(2,389)	1:32:B:ASN:HB2	1:33:B:GLU:H	11	0.42
(2,389)	1:32:B:ASN:HB3	1:33:B:GLU:H	11	0.42
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	2	0.42
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	2	0.42
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:32:A:ASN:HB2	1:33:A:GLU:H	11	0.42
(2,155)	1:32:A:ASN:HB3	1:33:A:GLU:H	11	0.42
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	4	0.42
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	4	0.42
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	15	0.42
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	3	0.42
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	3	0.42
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	6	0.41
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	6	0.41
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	2	0.41
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	6	0.41
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	6	0.41
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	2	0.41
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	6	0.41
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	6	0.41
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	5	0.41
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	5	0.41
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	5	0.41
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	6	0.41
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	6	0.41
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	6	0.41
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	11	0.41
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	11	0.41
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	11	0.41
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	5	0.41
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	5	0.41
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	5	0.41
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	6	0.41
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	6	0.41
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	6	0.41
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	11	0.41
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	11	0.41
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	11	0.41
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	5	0.41
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	5	0.41
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	5	0.41
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	6	0.41
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	6	0.41
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	6	0.41
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	11	0.41
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	11	0.41
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	5	0.41
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	13	0.41
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	15	0.41
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	5	0.41
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	13	0.41
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	15	0.41
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	5	0.41
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	13	0.41
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	8	0.41
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	8	0.41
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	8	0.41
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	16	0.4
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	16	0.4
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	16	0.4
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	16	0.4
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	16	0.4
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	16	0.4
(1,24)	1:51:C:ILE:HG12	1:48:C:TRP:HE1	18	0.4
(1,24)	1:51:C:ILE:HG13	1:48:C:TRP:HE1	18	0.4
(1,23)	1:51:B:ILE:HG12	1:48:B:TRP:HE1	18	0.4
(1,23)	1:51:B:ILE:HG13	1:48:B:TRP:HE1	18	0.4
(1,22)	1:51:A:ILE:HG12	1:48:A:TRP:HE1	18	0.4
(1,22)	1:51:A:ILE:HG13	1:48:A:TRP:HE1	18	0.4
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	11	0.39
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	11	0.39
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	4	0.39
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	10	0.39
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	10	0.39
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	13	0.39
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	11	0.39
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	11	0.39
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	4	0.39
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	10	0.39
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	10	0.39
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	11	0.39
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	11	0.39
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	4	0.39
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	10	0.39
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	10	0.39
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	13	0.39
(2,108)	1:34:C:GLN:H	1:30:C:SER:H	1	0.39
(2,107)	1:34:B:GLN:H	1:30:B:SER:H	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:34:A:GLN:H	1:30:A:SER:H	1	0.39
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	4	0.39
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	4	0.39
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	4	0.39
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	1	0.39
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	1	0.39
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	1	0.39
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	1	0.39
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	1	0.39
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	1	0.39
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	7	0.38
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	7	0.38
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	8	0.38
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	11	0.38
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	14	0.38
(2,625)	1:32:C:ASN:HB2	1:33:C:GLU:H	14	0.38
(2,625)	1:32:C:ASN:HB3	1:33:C:GLU:H	14	0.38
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	7	0.38
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	7	0.38
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	1	0.38
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	1	0.38
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	8	0.38
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	13	0.38
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	14	0.38
(2,389)	1:32:B:ASN:HB2	1:33:B:GLU:H	14	0.38
(2,389)	1:32:B:ASN:HB3	1:33:B:GLU:H	14	0.38
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	8	0.38
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	11	0.38
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	14	0.38
(2,155)	1:32:A:ASN:HB2	1:33:A:GLU:H	14	0.38
(2,155)	1:32:A:ASN:HB3	1:33:A:GLU:H	14	0.38
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	10	0.38
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	10	0.38
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	10	0.38
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	3	0.38
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	3	0.38
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	3	0.38
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	18	0.38
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	4	0.38
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	18	0.38
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	4	0.38
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	1	0.37
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	1	0.37
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	4	0.37
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	4	0.37
(2,625)	1:32:C:ASN:HB2	1:33:C:GLU:H	17	0.37
(2,625)	1:32:C:ASN:HB3	1:33:C:GLU:H	17	0.37
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	11	0.37
(2,389)	1:32:B:ASN:HB2	1:33:B:GLU:H	17	0.37
(2,389)	1:32:B:ASN:HB3	1:33:B:GLU:H	17	0.37
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	1	0.37
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	1	0.37
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	2	0.37
(2,155)	1:32:A:ASN:HB2	1:33:A:GLU:H	17	0.37
(2,155)	1:32:A:ASN:HB3	1:33:A:GLU:H	17	0.37
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD11	10	0.37
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD12	10	0.37
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD13	10	0.37
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD11	10	0.37
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD12	10	0.37
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD13	10	0.37
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD11	10	0.37
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD12	10	0.37
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD13	10	0.37
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	9	0.37
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	9	0.37
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	9	0.37
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	9	0.37
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	9	0.37
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	9	0.37
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	4	0.37
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	17	0.37
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	17	0.37
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	16	0.37
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	16	0.37
(2,772)	1:29:C:SER:HA	1:32:C:ASN:H	12	0.36
(2,772)	1:29:C:SER:HA	1:32:C:ASN:H	13	0.36
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	3	0.36
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	3	0.36
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	5	0.36
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	5	0.36
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	8	0.36
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,727)	1:29:C:SER:HA	1:32:C:ASN:H	12	0.36
(2,727)	1:29:C:SER:HA	1:32:C:ASN:H	13	0.36
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	2	0.36
(2,625)	1:32:C:ASN:HB2	1:33:C:GLU:H	12	0.36
(2,625)	1:32:C:ASN:HB3	1:33:C:GLU:H	12	0.36
(2,536)	1:29:B:SER:HA	1:32:B:ASN:H	12	0.36
(2,536)	1:29:B:SER:HA	1:32:B:ASN:H	13	0.36
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	3	0.36
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	3	0.36
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	4	0.36
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	4	0.36
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	5	0.36
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	5	0.36
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	8	0.36
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	8	0.36
(2,491)	1:29:B:SER:HA	1:32:B:ASN:H	12	0.36
(2,491)	1:29:B:SER:HA	1:32:B:ASN:H	13	0.36
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	2	0.36
(2,389)	1:32:B:ASN:HB2	1:33:B:GLU:H	12	0.36
(2,389)	1:32:B:ASN:HB3	1:33:B:GLU:H	12	0.36
(2,302)	1:29:A:SER:HA	1:32:A:ASN:H	12	0.36
(2,302)	1:29:A:SER:HA	1:32:A:ASN:H	13	0.36
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	3	0.36
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	3	0.36
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	4	0.36
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	4	0.36
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	5	0.36
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	5	0.36
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	8	0.36
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	8	0.36
(2,257)	1:29:A:SER:HA	1:32:A:ASN:H	12	0.36
(2,257)	1:29:A:SER:HA	1:32:A:ASN:H	13	0.36
(2,108)	1:34:C:GLN:H	1:30:C:SER:H	16	0.36
(2,107)	1:34:B:GLN:H	1:30:B:SER:H	16	0.36
(2,106)	1:34:A:GLN:H	1:30:A:SER:H	16	0.36
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	7	0.36
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	7	0.36
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	7	0.36
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	7	0.36
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	7	0.36
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	7	0.36
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	7	0.36
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	7	0.36
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	17	0.36
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	8	0.36
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	8	0.36
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	16	0.36
(2,763)	1:32:C:ASN:HB2	1:35:C:GLU:H	9	0.35
(2,763)	1:32:C:ASN:HB3	1:35:C:GLU:H	9	0.35
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	6	0.35
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	4	0.35
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	6	0.35
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	4	0.35
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	6	0.35
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	3	0.35
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	7	0.35
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	10	0.35
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	12	0.35
(2,625)	1:32:C:ASN:HB2	1:33:C:GLU:H	4	0.35
(2,625)	1:32:C:ASN:HB3	1:33:C:GLU:H	4	0.35
(2,527)	1:32:B:ASN:HB2	1:35:B:GLU:H	9	0.35
(2,527)	1:32:B:ASN:HB3	1:35:B:GLU:H	9	0.35
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	6	0.35
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	4	0.35
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	6	0.35
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	4	0.35
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	6	0.35
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	3	0.35
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	7	0.35
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	10	0.35
(2,389)	1:32:B:ASN:HB2	1:33:B:GLU:H	4	0.35
(2,389)	1:32:B:ASN:HB3	1:33:B:GLU:H	4	0.35
(2,293)	1:32:A:ASN:HB2	1:35:A:GLU:H	9	0.35
(2,293)	1:32:A:ASN:HB3	1:35:A:GLU:H	9	0.35
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	6	0.35
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	4	0.35
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	6	0.35
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	4	0.35
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	6	0.35
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	3	0.35
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	7	0.35
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	10	0.35
(2,155)	1:32:A:ASN:HB2	1:33:A:GLU:H	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:32:A:ASN:HB3	1:33:A:GLU:H	4	0.35
(2,155)	1:32:A:ASN:HB2	1:33:A:GLU:H	12	0.35
(2,155)	1:32:A:ASN:HB3	1:33:A:GLU:H	12	0.35
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	5	0.35
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	5	0.35
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	5	0.35
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	5	0.35
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	5	0.35
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	5	0.35
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	16	0.35
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	16	0.35
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	16	0.35
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	8	0.35
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	8	0.34
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	8	0.34
(2,772)	1:29:C:SER:HA	1:32:C:ASN:H	14	0.34
(2,727)	1:29:C:SER:HA	1:32:C:ASN:H	14	0.34
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	18	0.34
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	8	0.34
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	8	0.34
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	18	0.34
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	8	0.34
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	8	0.34
(2,536)	1:29:B:SER:HA	1:32:B:ASN:H	14	0.34
(2,491)	1:29:B:SER:HA	1:32:B:ASN:H	14	0.34
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	18	0.34
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	8	0.34
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	8	0.34
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	18	0.34
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	12	0.34
(2,302)	1:29:A:SER:HA	1:32:A:ASN:H	14	0.34
(2,257)	1:29:A:SER:HA	1:32:A:ASN:H	14	0.34
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	18	0.34
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	8	0.34
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	8	0.34
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	18	0.34
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	12	0.34
(1,24)	1:51:C:ILE:HG12	1:48:C:TRP:HE1	16	0.34
(1,24)	1:51:C:ILE:HG13	1:48:C:TRP:HE1	16	0.34
(1,23)	1:51:B:ILE:HG12	1:48:B:TRP:HE1	16	0.34
(1,23)	1:51:B:ILE:HG13	1:48:B:TRP:HE1	16	0.34
(1,22)	1:51:A:ILE:HG12	1:48:A:TRP:HE1	16	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:51:A:ILE:HG13	1:48:A:TRP:HE1	16	0.34
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	4	0.33
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	15	0.33
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	15	0.33
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	4	0.33
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	16	0.33
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	16	0.33
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	16	0.33
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	16	0.33
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	16	0.33
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	16	0.33
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD11	18	0.33
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD12	18	0.33
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD13	18	0.33
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD11	18	0.33
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD12	18	0.33
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD13	18	0.33
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD11	18	0.33
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD12	18	0.33
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD13	18	0.33
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	2	0.33
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	16	0.33
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	2	0.33
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	16	0.33
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	2	0.33
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	16	0.33
(2,813)	1:47:C:ASN:H	1:50:C:ASN:H	2	0.32
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	18	0.32
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	18	0.32
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	15	0.32
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	15	0.32
(2,726)	1:33:C:GLU:H	1:36:C:LEU:HG	2	0.32
(2,726)	1:33:C:GLU:H	1:36:C:LEU:HG	3	0.32
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	2	0.32
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	16	0.32
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	2	0.32
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	16	0.32
(2,577)	1:47:B:ASN:H	1:50:B:ASN:H	2	0.32
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	18	0.32
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	18	0.32
(2,490)	1:33:B:GLU:H	1:36:B:LEU:HG	2	0.32
(2,490)	1:33:B:GLU:H	1:36:B:LEU:HG	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	2	0.32
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	16	0.32
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	2	0.32
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	16	0.32
(2,341)	1:47:A:ASN:H	1:50:A:ASN:H	2	0.32
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	15	0.32
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	15	0.32
(2,256)	1:33:A:GLU:H	1:36:A:LEU:HG	2	0.32
(2,256)	1:33:A:GLU:H	1:36:A:LEU:HG	3	0.32
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	2	0.32
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	16	0.32
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	2	0.32
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	16	0.32
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	4	0.32
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD11	11	0.32
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD12	11	0.32
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD13	11	0.32
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD11	11	0.32
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD12	11	0.32
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD13	11	0.32
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD11	11	0.32
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD12	11	0.32
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD13	11	0.32
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD21	10	0.32
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD22	10	0.32
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD23	10	0.32
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD21	10	0.32
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD22	10	0.32
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD23	10	0.32
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD21	10	0.32
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD22	10	0.32
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD23	10	0.32
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	6	0.32
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	6	0.32
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	6	0.32
(2,75)	1:50:C:ASN:H	1:47:C:ASN:H	2	0.32
(2,74)	1:50:B:ASN:H	1:47:B:ASN:H	2	0.32
(2,73)	1:50:A:ASN:H	1:47:A:ASN:H	2	0.32
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	1	0.32
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	1	0.32
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	1	0.32
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	1	0.32
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	1	0.32
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	1	0.32
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	1	0.32
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	1	0.32
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	15	0.32
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	15	0.32
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	15	0.32
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	9	0.31
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	9	0.31
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	6	0.31
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	6	0.31
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	13	0.31
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	13	0.31
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	17	0.31
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	17	0.31
(2,763)	1:32:C:ASN:HB2	1:35:C:GLU:H	1	0.31
(2,763)	1:32:C:ASN:HB3	1:35:C:GLU:H	1	0.31
(2,726)	1:33:C:GLU:H	1:36:C:LEU:HG	5	0.31
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	3	0.31
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	3	0.31
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	6	0.31
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	6	0.31
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	6	0.31
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	12	0.31
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	12	0.31
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	13	0.31
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	13	0.31
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	17	0.31
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	17	0.31
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	18	0.31
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	18	0.31
(2,527)	1:32:B:ASN:HB2	1:35:B:GLU:H	1	0.31
(2,527)	1:32:B:ASN:HB3	1:35:B:GLU:H	1	0.31
(2,490)	1:33:B:GLU:H	1:36:B:LEU:HG	5	0.31
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	3	0.31
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	3	0.31
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	6	0.31
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	6	0.31
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	6	0.31
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	12	0.31
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	12	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	13	0.31
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	13	0.31
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	17	0.31
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	17	0.31
(2,293)	1:32:A:ASN:HB2	1:35:A:GLU:H	1	0.31
(2,293)	1:32:A:ASN:HB3	1:35:A:GLU:H	1	0.31
(2,256)	1:33:A:GLU:H	1:36:A:LEU:HG	5	0.31
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	3	0.31
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	3	0.31
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	6	0.31
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	14	0.31
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	14	0.31
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	14	0.31
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	14	0.31
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	5	0.31
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	5	0.31
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	5	0.31
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	1	0.3
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	3	0.3
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	6	0.3
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	1	0.3
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	3	0.3
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	6	0.3
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	12	0.3
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	12	0.3
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	16	0.3
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	16	0.3
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	18	0.3
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	18	0.3
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	2	0.3
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	17	0.3
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	1	0.3
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	3	0.3
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	6	0.3
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	9	0.3
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	1	0.3
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	3	0.3
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	6	0.3
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	9	0.3
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	16	0.3
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	16	0.3
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	17	0.3
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	16	0.3
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	16	0.3
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	18	0.3
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	18	0.3
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	2	0.3
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	17	0.3
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	14	0.3
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	14	0.3
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	6	0.3
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	6	0.3
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	6	0.3
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	2	0.3
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	2	0.3
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	2	0.3
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	11	0.3
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	15	0.3
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	15	0.3
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	15	0.3
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	10	0.29
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	15	0.29
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	16	0.29
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	10	0.29
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	15	0.29
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	16	0.29
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	7	0.29
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	7	0.29
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	9	0.29
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	9	0.29
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	14	0.29
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	14	0.29
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	8	0.29
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	8	0.29
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	4	0.29
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	12	0.29
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	12	0.29
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	4	0.29
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	9	0.29
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	10	0.29
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	15	0.29
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	16	0.29
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	15	0.29
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	16	0.29
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	7	0.29
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	7	0.29
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	9	0.29
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	9	0.29
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	14	0.29
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	14	0.29
(2,526)	1:32:B:ASN:HB2	1:34:B:GLN:H	10	0.29
(2,526)	1:32:B:ASN:HB3	1:34:B:GLN:H	10	0.29
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	8	0.29
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	8	0.29
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	12	0.29
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	12	0.29
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	7	0.29
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	7	0.29
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	9	0.29
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	9	0.29
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	14	0.29
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	14	0.29
(2,292)	1:32:A:ASN:HB2	1:34:A:GLN:H	10	0.29
(2,292)	1:32:A:ASN:HB3	1:34:A:GLN:H	10	0.29
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	8	0.29
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	8	0.29
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	12	0.29
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	12	0.29
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	9	0.29
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	11	0.29
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	11	0.29
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	6	0.29
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	10	0.29
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	10	0.29
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	10	0.29
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	5	0.29
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	5	0.29
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	5	0.29
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	17	0.28
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	17	0.28
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB2	10	0.28
(2,764)	1:38:C:GLU:H	1:40:C:ASP:HB3	10	0.28
(2,762)	1:32:C:ASN:HB2	1:34:C:GLN:H	10	0.28
(2,762)	1:32:C:ASN:HB3	1:34:C:GLN:H	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,760)	1:27:C:LEU:HB2	1:29:C:SER:H	17	0.28
(2,760)	1:27:C:LEU:HB3	1:29:C:SER:H	17	0.28
(2,728)	1:34:C:GLN:H	1:36:C:LEU:HG	1	0.28
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	5	0.28
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	18	0.28
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	5	0.28
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	18	0.28
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	17	0.28
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	17	0.28
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB2	10	0.28
(2,528)	1:38:B:GLU:H	1:40:B:ASP:HB3	10	0.28
(2,524)	1:27:B:LEU:HB2	1:29:B:SER:H	17	0.28
(2,524)	1:27:B:LEU:HB3	1:29:B:SER:H	17	0.28
(2,492)	1:34:B:GLN:H	1:36:B:LEU:HG	1	0.28
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	4	0.28
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	5	0.28
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	18	0.28
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	5	0.28
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	18	0.28
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	4	0.28
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	9	0.28
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB2	10	0.28
(2,294)	1:38:A:GLU:H	1:40:A:ASP:HB3	10	0.28
(2,290)	1:27:A:LEU:HB2	1:29:A:SER:H	17	0.28
(2,290)	1:27:A:LEU:HB3	1:29:A:SER:H	17	0.28
(2,258)	1:34:A:GLN:H	1:36:A:LEU:HG	1	0.28
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	4	0.28
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	5	0.28
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	18	0.28
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	5	0.28
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	18	0.28
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	4	0.28
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	18	0.28
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	18	0.28
(2,123)	1:31:C:GLY:H	1:33:C:GLU:HG2	16	0.28
(2,123)	1:31:C:GLY:H	1:33:C:GLU:HG3	16	0.28
(2,122)	1:31:B:GLY:H	1:33:B:GLU:HG2	16	0.28
(2,122)	1:31:B:GLY:H	1:33:B:GLU:HG3	16	0.28
(2,121)	1:31:A:GLY:H	1:33:A:GLU:HG2	16	0.28
(2,121)	1:31:A:GLY:H	1:33:A:GLU:HG3	16	0.28
(2,108)	1:34:C:GLN:H	1:30:C:SER:H	5	0.28
(2,107)	1:34:B:GLN:H	1:30:B:SER:H	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:34:A:GLN:H	1:30:A:SER:H	5	0.28
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	8	0.28
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	11	0.28
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	8	0.28
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	11	0.28
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	8	0.28
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	11	0.28
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	10	0.28
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	10	0.28
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	10	0.28
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	16	0.28
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	16	0.28
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	16	0.28
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	16	0.28
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	16	0.28
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	16	0.28
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	16	0.28
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	16	0.28
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	16	0.28
(2,54)	1:33:C:GLU:HG2	1:31:C:GLY:H	16	0.28
(2,54)	1:33:C:GLU:HG3	1:31:C:GLY:H	16	0.28
(2,53)	1:33:B:GLU:HG2	1:31:B:GLY:H	16	0.28
(2,53)	1:33:B:GLU:HG3	1:31:B:GLY:H	16	0.28
(2,52)	1:33:A:GLU:HG2	1:31:A:GLY:H	16	0.28
(2,52)	1:33:A:GLU:HG3	1:31:A:GLY:H	16	0.28
(2,42)	1:34:C:GLN:H	1:36:C:LEU:HG	1	0.28
(2,41)	1:34:B:GLN:H	1:36:B:LEU:HG	1	0.28
(2,40)	1:34:A:GLN:H	1:36:A:LEU:HG	1	0.28
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	11	0.28
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	11	0.28
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	11	0.28
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	6	0.28
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	6	0.28
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	1	0.27
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	16	0.27
(2,763)	1:32:C:ASN:HB2	1:35:C:GLU:H	8	0.27
(2,763)	1:32:C:ASN:HB3	1:35:C:GLU:H	8	0.27
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	8	0.27
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	11	0.27
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	11	0.27
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	15	0.27
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	16	0.27
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	11	0.27
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	11	0.27
(2,527)	1:32:B:ASN:HB2	1:35:B:GLU:H	8	0.27
(2,527)	1:32:B:ASN:HB3	1:35:B:GLU:H	8	0.27
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	8	0.27
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	11	0.27
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	11	0.27
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	15	0.27
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	1	0.27
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	16	0.27
(2,293)	1:32:A:ASN:HB2	1:35:A:GLU:H	8	0.27
(2,293)	1:32:A:ASN:HB3	1:35:A:GLU:H	8	0.27
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	8	0.27
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	17	0.27
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	11	0.27
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	13	0.27
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	11	0.27
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	13	0.27
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	17	0.27
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	15	0.27
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	18	0.27
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	18	0.27
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	18	0.27
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	18	0.27
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	17	0.27
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	17	0.27
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	17	0.27
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	8	0.27
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	8	0.27
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	8	0.27
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	10	0.27
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	10	0.27
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	10	0.27
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	7	0.27
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	7	0.27
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	4	0.26
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	11	0.26
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	11	0.26
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	11	0.26
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	4	0.26
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	3	0.26
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	12	0.26
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	14	0.26
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	17	0.26
(2,672)	1:33:C:GLU:H	1:35:C:GLU:H	18	0.26
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	13	0.26
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	14	0.26
(2,650)	1:33:C:GLU:H	1:35:C:GLU:H	18	0.26
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	13	0.26
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	14	0.26
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	17	0.26
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	4	0.26
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	11	0.26
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	4	0.26
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	11	0.26
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	3	0.26
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	12	0.26
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	14	0.26
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	17	0.26
(2,436)	1:33:B:GLU:H	1:35:B:GLU:H	18	0.26
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	13	0.26
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	14	0.26
(2,414)	1:33:B:GLU:H	1:35:B:GLU:H	18	0.26
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	13	0.26
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	14	0.26
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	17	0.26
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	3	0.26
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	12	0.26
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	14	0.26
(2,202)	1:33:A:GLU:H	1:35:A:GLU:H	18	0.26
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	14	0.26
(2,180)	1:33:A:GLU:H	1:35:A:GLU:H	18	0.26
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	14	0.26
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	9	0.26
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	9	0.26
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	12	0.26
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	12	0.26
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	9	0.26
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	9	0.26
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	12	0.26
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	12	0.26
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	9	0.26
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	12	0.26
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	12	0.26
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD11	16	0.26
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD12	16	0.26
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD13	16	0.26
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD11	16	0.26
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD12	16	0.26
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD13	16	0.26
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD11	16	0.26
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD12	16	0.26
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD13	16	0.26
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	3	0.26
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	3	0.26
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	3	0.26
(2,81)	1:34:C:GLN:H	1:31:C:GLY:H	11	0.26
(2,80)	1:34:B:GLN:H	1:31:B:GLY:H	11	0.26
(2,79)	1:34:A:GLN:H	1:31:A:GLY:H	11	0.26
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	3	0.26
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	3	0.26
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	3	0.26
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	8	0.26
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	8	0.26
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	8	0.26
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	3	0.26
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	3	0.26
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	3	0.26
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	8	0.26
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	8	0.26
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	8	0.26
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	8	0.26
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	8	0.26
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	8	0.26
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	7	0.26
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	4	0.26
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	4	0.26
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	4	0.26
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	7	0.25
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	7	0.25
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	7	0.25
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	7	0.25
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	11	0.25
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	7	0.25
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	7	0.25
(2,108)	1:34:C:GLN:H	1:30:C:SER:H	15	0.25
(2,107)	1:34:B:GLN:H	1:30:B:SER:H	15	0.25
(2,106)	1:34:A:GLN:H	1:30:A:SER:H	15	0.25
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	9	0.25
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	2	0.25
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	2	0.25
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	2	0.25
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	2	0.25
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	2	0.25
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	2	0.25
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	2	0.25
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	2	0.25
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	2	0.25
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	3	0.25
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	3	0.25
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	3	0.25
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	10	0.25
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	10	0.25
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	10	0.25
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	10	0.25
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	17	0.25
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	17	0.25
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	17	0.25
(2,807)	1:32:C:ASN:H	1:35:C:GLU:H	14	0.24
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	2	0.24
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	13	0.24
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	14	0.24
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	2	0.24
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	13	0.24
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	14	0.24
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	7	0.24
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	6	0.24
(2,571)	1:32:B:ASN:H	1:35:B:GLU:H	14	0.24
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	2	0.24
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	13	0.24
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	14	0.24
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	2	0.24
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	13	0.24
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	7	0.24
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	13	0.24
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	6	0.24
(2,335)	1:32:A:ASN:H	1:35:A:GLU:H	14	0.24
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	7	0.24
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	6	0.24
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	13	0.24
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	13	0.24
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	13	0.24
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	13	0.24
(2,123)	1:31:C:GLY:H	1:33:C:GLU:HG2	15	0.24
(2,123)	1:31:C:GLY:H	1:33:C:GLU:HG3	15	0.24
(2,122)	1:31:B:GLY:H	1:33:B:GLU:HG2	15	0.24
(2,122)	1:31:B:GLY:H	1:33:B:GLU:HG3	15	0.24
(2,121)	1:31:A:GLY:H	1:33:A:GLU:HG2	15	0.24
(2,121)	1:31:A:GLY:H	1:33:A:GLU:HG3	15	0.24
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	9	0.24
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	9	0.24
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	7	0.24
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	7	0.24
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	7	0.24
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	10	0.24
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	10	0.24
(2,54)	1:33:C:GLU:HG2	1:31:C:GLY:H	15	0.24
(2,54)	1:33:C:GLU:HG3	1:31:C:GLY:H	15	0.24
(2,53)	1:33:B:GLU:HG2	1:31:B:GLY:H	15	0.24
(2,53)	1:33:B:GLU:HG3	1:31:B:GLY:H	15	0.24
(2,52)	1:33:A:GLU:HG2	1:31:A:GLY:H	15	0.24
(2,52)	1:33:A:GLU:HG3	1:31:A:GLY:H	15	0.24
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	7	0.23
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	5	0.23
(2,799)	1:13:C:TYR:H	1:21:C:VAL:H	12	0.23
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	5	0.23
(2,777)	1:13:C:TYR:H	1:21:C:VAL:H	12	0.23
(2,754)	1:52:C:THR:H	1:54:C:TRP:H	3	0.23
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	5	0.23
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	16	0.23
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	13	0.23
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	5	0.23
(2,707)	1:52:C:THR:H	1:54:C:TRP:H	3	0.23
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	7	0.23
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	7	0.23
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	17	0.23
(2,625)	1:32:C:ASN:HB2	1:33:C:GLU:H	5	0.23
(2,625)	1:32:C:ASN:HB3	1:33:C:GLU:H	5	0.23
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	7	0.23
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	5	0.23
(2,563)	1:13:B:TYR:H	1:21:B:VAL:H	12	0.23
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	5	0.23
(2,541)	1:13:B:TYR:H	1:21:B:VAL:H	12	0.23
(2,526)	1:32:B:ASN:HB2	1:34:B:GLN:H	16	0.23
(2,526)	1:32:B:ASN:HB3	1:34:B:GLN:H	16	0.23
(2,518)	1:52:B:THR:H	1:54:B:TRP:H	3	0.23
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	5	0.23
(2,492)	1:34:B:GLN:H	1:36:B:LEU:HG	9	0.23
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	16	0.23
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	5	0.23
(2,471)	1:52:B:THR:H	1:54:B:TRP:H	3	0.23
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	7	0.23
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	17	0.23
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	7	0.23
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	17	0.23
(2,389)	1:32:B:ASN:HB2	1:33:B:GLU:H	5	0.23
(2,389)	1:32:B:ASN:HB3	1:33:B:GLU:H	5	0.23
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	7	0.23
(2,292)	1:32:A:ASN:HB2	1:34:A:GLN:H	5	0.23
(2,292)	1:32:A:ASN:HB3	1:34:A:GLN:H	5	0.23
(2,292)	1:32:A:ASN:HB2	1:34:A:GLN:H	16	0.23
(2,292)	1:32:A:ASN:HB3	1:34:A:GLN:H	16	0.23
(2,284)	1:52:A:THR:H	1:54:A:TRP:H	3	0.23
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	5	0.23
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	16	0.23
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	13	0.23
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	5	0.23
(2,237)	1:52:A:THR:H	1:54:A:TRP:H	3	0.23
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	7	0.23
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	17	0.23
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	7	0.23
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	17	0.23
(2,155)	1:32:A:ASN:HB2	1:33:A:GLU:H	5	0.23
(2,155)	1:32:A:ASN:HB3	1:33:A:GLU:H	5	0.23
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	13	0.23
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD11	15	0.23
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD12	15	0.23
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD13	15	0.23
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD11	15	0.23
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD12	15	0.23
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD13	15	0.23
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	18	0.23
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	18	0.23
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	18	0.23
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	16	0.23
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	16	0.23
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	16	0.23
(2,41)	1:34:B:GLN:H	1:36:B:LEU:HG	9	0.23
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	11	0.23
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	18	0.23
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	11	0.23
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	18	0.23
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	11	0.23
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	18	0.23
(1,91)	1:42:C:TRP:HE1	1:43:C:ALA:H	2	0.23
(1,85)	1:42:C:TRP:HE1	1:43:C:ALA:H	2	0.23
(1,63)	1:42:B:TRP:HE1	1:43:B:ALA:H	2	0.23
(1,57)	1:42:B:TRP:HE1	1:43:B:ALA:H	2	0.23
(1,35)	1:42:A:TRP:HE1	1:43:A:ALA:H	2	0.23
(1,29)	1:42:A:TRP:HE1	1:43:A:ALA:H	2	0.23
(2,807)	1:32:C:ASN:H	1:35:C:GLU:H	12	0.22
(2,763)	1:32:C:ASN:HB2	1:35:C:GLU:H	7	0.22
(2,763)	1:32:C:ASN:HB3	1:35:C:GLU:H	7	0.22
(2,762)	1:32:C:ASN:HB2	1:34:C:GLN:H	5	0.22
(2,762)	1:32:C:ASN:HB3	1:34:C:GLN:H	5	0.22
(2,762)	1:32:C:ASN:HB2	1:34:C:GLN:H	16	0.22
(2,762)	1:32:C:ASN:HB3	1:34:C:GLN:H	16	0.22
(2,728)	1:34:C:GLN:H	1:36:C:LEU:HG	9	0.22
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	6	0.22
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	12	0.22
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	14	0.22
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	15	0.22
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	15	0.22
(2,571)	1:32:B:ASN:H	1:35:B:GLU:H	12	0.22
(2,527)	1:32:B:ASN:HB2	1:35:B:GLU:H	7	0.22
(2,527)	1:32:B:ASN:HB3	1:35:B:GLU:H	7	0.22
(2,526)	1:32:B:ASN:HB2	1:34:B:GLN:H	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,526)	1:32:B:ASN:HB3	1:34:B:GLN:H	5	0.22
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	6	0.22
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	12	0.22
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	14	0.22
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	15	0.22
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	15	0.22
(2,341)	1:47:A:ASN:H	1:50:A:ASN:H	8	0.22
(2,335)	1:32:A:ASN:H	1:35:A:GLU:H	12	0.22
(2,323)	1:21:A:VAL:H	1:23:A:LEU:H	6	0.22
(2,323)	1:21:A:VAL:H	1:23:A:LEU:H	11	0.22
(2,317)	1:21:A:VAL:H	1:23:A:LEU:H	6	0.22
(2,317)	1:21:A:VAL:H	1:23:A:LEU:H	11	0.22
(2,293)	1:32:A:ASN:HB2	1:35:A:GLU:H	7	0.22
(2,293)	1:32:A:ASN:HB3	1:35:A:GLU:H	7	0.22
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	4	0.22
(2,258)	1:34:A:GLN:H	1:36:A:LEU:HG	9	0.22
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	6	0.22
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	12	0.22
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	14	0.22
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	4	0.22
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	9	0.22
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	15	0.22
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	9	0.22
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	15	0.22
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD11	15	0.22
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD12	15	0.22
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD13	15	0.22
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	14	0.22
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	14	0.22
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	14	0.22
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	6	0.22
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	12	0.22
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	14	0.22
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	6	0.22
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	12	0.22
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	14	0.22
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	6	0.22
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	12	0.22
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	14	0.22
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	15	0.22
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	15	0.22
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,73)	1:50:A:ASN:H	1:47:A:ASN:H	8	0.22
(2,42)	1:34:C:GLN:H	1:36:C:LEU:HG	9	0.22
(2,40)	1:34:A:GLN:H	1:36:A:LEU:HG	9	0.22
(2,813)	1:47:C:ASN:H	1:50:C:ASN:H	8	0.21
(2,794)	1:21:C:VAL:H	1:23:C:LEU:H	11	0.21
(2,787)	1:21:C:VAL:H	1:23:C:LEU:H	11	0.21
(2,762)	1:32:C:ASN:HB2	1:34:C:GLN:H	17	0.21
(2,762)	1:32:C:ASN:HB3	1:34:C:GLN:H	17	0.21
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	4	0.21
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	4	0.21
(2,688)	1:43:C:ALA:H	1:45:C:LEU:H	1	0.21
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	1	0.21
(2,671)	1:14:C:VAL:H	1:22:C:LEU:H	9	0.21
(2,654)	1:43:C:ALA:H	1:45:C:LEU:H	1	0.21
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	1	0.21
(2,642)	1:14:C:VAL:H	1:22:C:LEU:H	9	0.21
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	1	0.21
(2,577)	1:47:B:ASN:H	1:50:B:ASN:H	8	0.21
(2,526)	1:32:B:ASN:HB2	1:34:B:GLN:H	17	0.21
(2,526)	1:32:B:ASN:HB3	1:34:B:GLN:H	17	0.21
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	4	0.21
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	4	0.21
(2,452)	1:43:B:ALA:H	1:45:B:LEU:H	1	0.21
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	1	0.21
(2,435)	1:14:B:VAL:H	1:22:B:LEU:H	9	0.21
(2,418)	1:43:B:ALA:H	1:45:B:LEU:H	1	0.21
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	1	0.21
(2,406)	1:14:B:VAL:H	1:22:B:LEU:H	9	0.21
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	1	0.21
(2,323)	1:21:A:VAL:H	1:23:A:LEU:H	3	0.21
(2,317)	1:21:A:VAL:H	1:23:A:LEU:H	3	0.21
(2,292)	1:32:A:ASN:HB2	1:34:A:GLN:H	17	0.21
(2,292)	1:32:A:ASN:HB3	1:34:A:GLN:H	17	0.21
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	18	0.21
(2,218)	1:43:A:ALA:H	1:45:A:LEU:H	1	0.21
(2,201)	1:14:A:VAL:H	1:22:A:LEU:H	1	0.21
(2,184)	1:43:A:ALA:H	1:45:A:LEU:H	1	0.21
(2,172)	1:14:A:VAL:H	1:22:A:LEU:H	1	0.21
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	1	0.21
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	5	0.21
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	7	0.21
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	1	0.21
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	5	0.21
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	7	0.21
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	12	0.21
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	5	0.21
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	7	0.21
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	12	0.21
(2,75)	1:50:C:ASN:H	1:47:C:ASN:H	8	0.21
(2,74)	1:50:B:ASN:H	1:47:B:ASN:H	8	0.21
(1,99)	1:23:C:LEU:H	1:27:C:LEU:H	12	0.21
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	16	0.21
(1,71)	1:23:B:LEU:H	1:27:B:LEU:H	12	0.21
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	16	0.21
(1,43)	1:23:A:LEU:H	1:27:A:LEU:H	12	0.21
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	9	0.21
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	16	0.21
(2,813)	1:47:C:ASN:H	1:50:C:ASN:H	3	0.2
(2,813)	1:47:C:ASN:H	1:50:C:ASN:H	16	0.2
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	6	0.2
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	4	0.2
(2,797)	1:14:C:VAL:H	1:16:C:LYS:H	4	0.2
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	3	0.2
(2,794)	1:21:C:VAL:H	1:23:C:LEU:H	3	0.2
(2,794)	1:21:C:VAL:H	1:23:C:LEU:H	6	0.2
(2,787)	1:21:C:VAL:H	1:23:C:LEU:H	3	0.2
(2,787)	1:21:C:VAL:H	1:23:C:LEU:H	6	0.2
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	4	0.2
(2,781)	1:14:C:VAL:H	1:16:C:LYS:H	4	0.2
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	3	0.2
(2,763)	1:32:C:ASN:HB2	1:35:C:GLU:H	6	0.2
(2,763)	1:32:C:ASN:HB3	1:35:C:GLU:H	6	0.2
(2,760)	1:27:C:LEU:HB2	1:29:C:SER:H	5	0.2
(2,760)	1:27:C:LEU:HB3	1:29:C:SER:H	5	0.2
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	1	0.2
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	13	0.2
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	9	0.2
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	18	0.2
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	15	0.2
(2,672)	1:33:C:GLU:H	1:35:C:GLU:H	10	0.2
(2,650)	1:33:C:GLU:H	1:35:C:GLU:H	10	0.2
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	15	0.2
(2,577)	1:47:B:ASN:H	1:50:B:ASN:H	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,577)	1:47:B:ASN:H	1:50:B:ASN:H	16	0.2
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	6	0.2
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	4	0.2
(2,561)	1:14:B:VAL:H	1:16:B:LYS:H	4	0.2
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	3	0.2
(2,558)	1:21:B:VAL:H	1:23:B:LEU:H	3	0.2
(2,558)	1:21:B:VAL:H	1:23:B:LEU:H	6	0.2
(2,558)	1:21:B:VAL:H	1:23:B:LEU:H	11	0.2
(2,551)	1:21:B:VAL:H	1:23:B:LEU:H	3	0.2
(2,551)	1:21:B:VAL:H	1:23:B:LEU:H	6	0.2
(2,551)	1:21:B:VAL:H	1:23:B:LEU:H	11	0.2
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	4	0.2
(2,545)	1:14:B:VAL:H	1:16:B:LYS:H	4	0.2
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	3	0.2
(2,527)	1:32:B:ASN:HB2	1:35:B:GLU:H	6	0.2
(2,527)	1:32:B:ASN:HB3	1:35:B:GLU:H	6	0.2
(2,524)	1:27:B:LEU:HB2	1:29:B:SER:H	5	0.2
(2,524)	1:27:B:LEU:HB3	1:29:B:SER:H	5	0.2
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	1	0.2
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	13	0.2
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	9	0.2
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	18	0.2
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	15	0.2
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	15	0.2
(2,341)	1:47:A:ASN:H	1:50:A:ASN:H	3	0.2
(2,341)	1:47:A:ASN:H	1:50:A:ASN:H	16	0.2
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	6	0.2
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	4	0.2
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	4	0.2
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	4	0.2
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	4	0.2
(2,293)	1:32:A:ASN:HB2	1:35:A:GLU:H	6	0.2
(2,293)	1:32:A:ASN:HB3	1:35:A:GLU:H	6	0.2
(2,290)	1:27:A:LEU:HB2	1:29:A:SER:H	5	0.2
(2,290)	1:27:A:LEU:HB3	1:29:A:SER:H	5	0.2
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	1	0.2
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	13	0.2
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	9	0.2
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	15	0.2
(2,202)	1:33:A:GLU:H	1:35:A:GLU:H	10	0.2
(2,180)	1:33:A:GLU:H	1:35:A:GLU:H	10	0.2
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	2	0.2
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	2	0.2
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	15	0.2
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	15	0.2
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	2	0.2
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	2	0.2
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	15	0.2
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	15	0.2
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	2	0.2
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	2	0.2
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	15	0.2
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	15	0.2
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	1	0.2
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	1	0.2
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	1	0.2
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	13	0.2
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	1	0.2
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	13	0.2
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	1	0.2
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	13	0.2
(2,75)	1:50:C:ASN:H	1:47:C:ASN:H	3	0.2
(2,75)	1:50:C:ASN:H	1:47:C:ASN:H	16	0.2
(2,74)	1:50:B:ASN:H	1:47:B:ASN:H	3	0.2
(2,74)	1:50:B:ASN:H	1:47:B:ASN:H	16	0.2
(2,73)	1:50:A:ASN:H	1:47:A:ASN:H	3	0.2
(2,73)	1:50:A:ASN:H	1:47:A:ASN:H	16	0.2
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	14	0.2
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	14	0.2
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	14	0.2
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	14	0.2
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	14	0.2
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	14	0.2
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	14	0.2
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	14	0.2
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	14	0.2
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	9	0.2
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	9	0.2
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	9	0.2
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	1	0.2
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	5	0.2
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	5	0.2
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	9	0.2
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	9	0.2
(2,815)	1:54:C:TRP:H	1:57:C:TYR:H	6	0.19
(2,772)	1:29:C:SER:HA	1:32:C:ASN:H	16	0.19
(2,763)	1:32:C:ASN:HB2	1:35:C:GLU:H	15	0.19
(2,763)	1:32:C:ASN:HB3	1:35:C:GLU:H	15	0.19
(2,760)	1:27:C:LEU:HB2	1:29:C:SER:H	13	0.19
(2,760)	1:27:C:LEU:HB3	1:29:C:SER:H	13	0.19
(2,754)	1:52:C:THR:H	1:54:C:TRP:H	8	0.19
(2,754)	1:52:C:THR:H	1:54:C:TRP:H	17	0.19
(2,727)	1:29:C:SER:HA	1:32:C:ASN:H	16	0.19
(2,718)	1:56:C:TRP:H	1:58:C:ILE:H	8	0.19
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	11	0.19
(2,707)	1:52:C:THR:H	1:54:C:TRP:H	8	0.19
(2,707)	1:52:C:THR:H	1:54:C:TRP:H	17	0.19
(2,579)	1:54:B:TRP:H	1:57:B:TYR:H	6	0.19
(2,577)	1:47:B:ASN:H	1:50:B:ASN:H	6	0.19
(2,536)	1:29:B:SER:HA	1:32:B:ASN:H	16	0.19
(2,527)	1:32:B:ASN:HB2	1:35:B:GLU:H	15	0.19
(2,527)	1:32:B:ASN:HB3	1:35:B:GLU:H	15	0.19
(2,524)	1:27:B:LEU:HB2	1:29:B:SER:H	13	0.19
(2,524)	1:27:B:LEU:HB3	1:29:B:SER:H	13	0.19
(2,518)	1:52:B:THR:H	1:54:B:TRP:H	8	0.19
(2,518)	1:52:B:THR:H	1:54:B:TRP:H	17	0.19
(2,491)	1:29:B:SER:HA	1:32:B:ASN:H	16	0.19
(2,482)	1:56:B:TRP:H	1:58:B:ILE:H	8	0.19
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	11	0.19
(2,471)	1:52:B:THR:H	1:54:B:TRP:H	8	0.19
(2,471)	1:52:B:THR:H	1:54:B:TRP:H	17	0.19
(2,436)	1:33:B:GLU:H	1:35:B:GLU:H	10	0.19
(2,414)	1:33:B:GLU:H	1:35:B:GLU:H	10	0.19
(2,343)	1:54:A:TRP:H	1:57:A:TYR:H	6	0.19
(2,341)	1:47:A:ASN:H	1:50:A:ASN:H	6	0.19
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	2	0.19
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	2	0.19
(2,302)	1:29:A:SER:HA	1:32:A:ASN:H	16	0.19
(2,293)	1:32:A:ASN:HB2	1:35:A:GLU:H	15	0.19
(2,293)	1:32:A:ASN:HB3	1:35:A:GLU:H	15	0.19
(2,290)	1:27:A:LEU:HB2	1:29:A:SER:H	13	0.19
(2,290)	1:27:A:LEU:HB3	1:29:A:SER:H	13	0.19
(2,284)	1:52:A:THR:H	1:54:A:TRP:H	8	0.19
(2,284)	1:52:A:THR:H	1:54:A:TRP:H	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,257)	1:29:A:SER:HA	1:32:A:ASN:H	16	0.19
(2,248)	1:56:A:TRP:H	1:58:A:ILE:H	8	0.19
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	11	0.19
(2,237)	1:52:A:THR:H	1:54:A:TRP:H	8	0.19
(2,237)	1:52:A:THR:H	1:54:A:TRP:H	17	0.19
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD11	17	0.19
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD12	17	0.19
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD13	17	0.19
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD11	17	0.19
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD12	17	0.19
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD13	17	0.19
(2,74)	1:50:B:ASN:H	1:47:B:ASN:H	6	0.19
(2,73)	1:50:A:ASN:H	1:47:A:ASN:H	6	0.19
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	2	0.19
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	2	0.19
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	2	0.19
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	2	0.19
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	2	0.19
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	2	0.19
(2,36)	1:32:C:ASN:H	1:33:C:GLU:HA	1	0.19
(2,35)	1:32:B:ASN:H	1:33:B:GLU:HA	1	0.19
(2,34)	1:32:A:ASN:H	1:33:A:GLU:HA	1	0.19
(1,91)	1:42:C:TRP:HE1	1:43:C:ALA:H	3	0.19
(1,91)	1:42:C:TRP:HE1	1:43:C:ALA:H	4	0.19
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	7	0.19
(1,85)	1:42:C:TRP:HE1	1:43:C:ALA:H	3	0.19
(1,85)	1:42:C:TRP:HE1	1:43:C:ALA:H	4	0.19
(1,63)	1:42:B:TRP:HE1	1:43:B:ALA:H	3	0.19
(1,63)	1:42:B:TRP:HE1	1:43:B:ALA:H	4	0.19
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	7	0.19
(1,57)	1:42:B:TRP:HE1	1:43:B:ALA:H	3	0.19
(1,57)	1:42:B:TRP:HE1	1:43:B:ALA:H	4	0.19
(1,35)	1:42:A:TRP:HE1	1:43:A:ALA:H	3	0.19
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	7	0.19
(1,29)	1:42:A:TRP:HE1	1:43:A:ALA:H	3	0.19
(2,813)	1:47:C:ASN:H	1:50:C:ASN:H	4	0.18
(2,813)	1:47:C:ASN:H	1:50:C:ASN:H	6	0.18
(2,813)	1:47:C:ASN:H	1:50:C:ASN:H	10	0.18
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	2	0.18
(2,797)	1:14:C:VAL:H	1:16:C:LYS:H	15	0.18
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	4	0.18
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,781)	1:14:C:VAL:H	1:16:C:LYS:H	15	0.18
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	4	0.18
(2,773)	1:30:C:SER:HA	1:33:C:GLU:H	11	0.18
(2,725)	1:30:C:SER:HA	1:33:C:GLU:H	11	0.18
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	10	0.18
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	17	0.18
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	11	0.18
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	11	0.18
(2,625)	1:32:C:ASN:HB2	1:33:C:GLU:H	18	0.18
(2,625)	1:32:C:ASN:HB3	1:33:C:GLU:H	18	0.18
(2,577)	1:47:B:ASN:H	1:50:B:ASN:H	10	0.18
(2,571)	1:32:B:ASN:H	1:35:B:GLU:H	17	0.18
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	2	0.18
(2,561)	1:14:B:VAL:H	1:16:B:LYS:H	15	0.18
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	2	0.18
(2,545)	1:14:B:VAL:H	1:16:B:LYS:H	15	0.18
(2,537)	1:30:B:SER:HA	1:33:B:GLU:H	11	0.18
(2,489)	1:30:B:SER:HA	1:33:B:GLU:H	11	0.18
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	10	0.18
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	17	0.18
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	11	0.18
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	11	0.18
(2,389)	1:32:B:ASN:HB2	1:33:B:GLU:H	18	0.18
(2,389)	1:32:B:ASN:HB3	1:33:B:GLU:H	18	0.18
(2,341)	1:47:A:ASN:H	1:50:A:ASN:H	10	0.18
(2,335)	1:32:A:ASN:H	1:35:A:GLU:H	17	0.18
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	8	0.18
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	15	0.18
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	3	0.18
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	8	0.18
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	15	0.18
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	3	0.18
(2,303)	1:30:A:SER:HA	1:33:A:GLU:H	11	0.18
(2,255)	1:30:A:SER:HA	1:33:A:GLU:H	11	0.18
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	10	0.18
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	17	0.18
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	11	0.18
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	11	0.18
(2,155)	1:32:A:ASN:HB2	1:33:A:GLU:H	18	0.18
(2,155)	1:32:A:ASN:HB3	1:33:A:GLU:H	18	0.18
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD11	17	0.18
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD12	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD13	17	0.18
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	3	0.18
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	13	0.18
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	15	0.18
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	3	0.18
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	13	0.18
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	15	0.18
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	3	0.18
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	13	0.18
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	15	0.18
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	10	0.18
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	17	0.18
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	10	0.18
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	17	0.18
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	10	0.18
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	17	0.18
(2,96)	1:44:C:SER:H	1:47:C:ASN:H	2	0.18
(2,95)	1:44:B:SER:H	1:47:B:ASN:H	2	0.18
(2,94)	1:44:A:SER:H	1:47:A:ASN:H	2	0.18
(2,75)	1:50:C:ASN:H	1:47:C:ASN:H	4	0.18
(2,75)	1:50:C:ASN:H	1:47:C:ASN:H	6	0.18
(2,75)	1:50:C:ASN:H	1:47:C:ASN:H	10	0.18
(2,74)	1:50:B:ASN:H	1:47:B:ASN:H	10	0.18
(2,73)	1:50:A:ASN:H	1:47:A:ASN:H	10	0.18
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	1	0.18
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	1	0.18
(2,12)	1:13:A:TYR:H	1:15:B:ARG:H	17	0.18
(2,9)	1:15:A:ARG:H	1:13:C:TYR:H	17	0.18
(2,8)	1:13:B:TYR:H	1:15:C:ARG:H	17	0.18
(1,99)	1:23:C:LEU:H	1:27:C:LEU:H	6	0.18
(1,91)	1:42:C:TRP:HE1	1:43:C:ALA:H	11	0.18
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	1	0.18
(1,85)	1:42:C:TRP:HE1	1:43:C:ALA:H	11	0.18
(1,71)	1:23:B:LEU:H	1:27:B:LEU:H	6	0.18
(1,63)	1:42:B:TRP:HE1	1:43:B:ALA:H	11	0.18
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	1	0.18
(1,57)	1:42:B:TRP:HE1	1:43:B:ALA:H	11	0.18
(1,43)	1:23:A:LEU:H	1:27:A:LEU:H	6	0.18
(1,35)	1:42:A:TRP:HE1	1:43:A:ALA:H	4	0.18
(1,35)	1:42:A:TRP:HE1	1:43:A:ALA:H	11	0.18
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	1	0.18
(1,29)	1:42:A:TRP:HE1	1:43:A:ALA:H	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:42:A:TRP:HE1	1:43:A:ALA:H	11	0.18
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	3	0.17
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	10	0.17
(2,807)	1:32:C:ASN:H	1:35:C:GLU:H	17	0.17
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	17	0.17
(2,797)	1:14:C:VAL:H	1:16:C:LYS:H	8	0.17
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	1	0.17
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	7	0.17
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	17	0.17
(2,781)	1:14:C:VAL:H	1:16:C:LYS:H	8	0.17
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	1	0.17
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	7	0.17
(2,773)	1:30:C:SER:HA	1:33:C:GLU:H	18	0.17
(2,754)	1:52:C:THR:H	1:54:C:TRP:H	4	0.17
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	9	0.17
(2,725)	1:30:C:SER:HA	1:33:C:GLU:H	18	0.17
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	9	0.17
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	4	0.17
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	7	0.17
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	11	0.17
(2,718)	1:56:C:TRP:H	1:58:C:ILE:H	6	0.17
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	9	0.17
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	10	0.17
(2,707)	1:52:C:THR:H	1:54:C:TRP:H	4	0.17
(2,672)	1:33:C:GLU:H	1:35:C:GLU:H	3	0.17
(2,650)	1:33:C:GLU:H	1:35:C:GLU:H	3	0.17
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	10	0.17
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	17	0.17
(2,577)	1:47:B:ASN:H	1:50:B:ASN:H	4	0.17
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	3	0.17
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	10	0.17
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	17	0.17
(2,561)	1:14:B:VAL:H	1:16:B:LYS:H	8	0.17
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	1	0.17
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	4	0.17
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	7	0.17
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	17	0.17
(2,545)	1:14:B:VAL:H	1:16:B:LYS:H	8	0.17
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	1	0.17
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	4	0.17
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	7	0.17
(2,537)	1:30:B:SER:HA	1:33:B:GLU:H	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,518)	1:52:B:THR:H	1:54:B:TRP:H	4	0.17
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	9	0.17
(2,489)	1:30:B:SER:HA	1:33:B:GLU:H	18	0.17
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	9	0.17
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	4	0.17
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	7	0.17
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	11	0.17
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	9	0.17
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	10	0.17
(2,471)	1:52:B:THR:H	1:54:B:TRP:H	4	0.17
(2,436)	1:33:B:GLU:H	1:35:B:GLU:H	3	0.17
(2,414)	1:33:B:GLU:H	1:35:B:GLU:H	3	0.17
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	10	0.17
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	17	0.17
(2,341)	1:47:A:ASN:H	1:50:A:ASN:H	4	0.17
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	3	0.17
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	10	0.17
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	17	0.17
(2,323)	1:21:A:VAL:H	1:23:A:LEU:H	2	0.17
(2,317)	1:21:A:VAL:H	1:23:A:LEU:H	2	0.17
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	17	0.17
(2,303)	1:30:A:SER:HA	1:33:A:GLU:H	18	0.17
(2,284)	1:52:A:THR:H	1:54:A:TRP:H	4	0.17
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	9	0.17
(2,255)	1:30:A:SER:HA	1:33:A:GLU:H	18	0.17
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	9	0.17
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	4	0.17
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	7	0.17
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	11	0.17
(2,248)	1:56:A:TRP:H	1:58:A:ILE:H	6	0.17
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	9	0.17
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	10	0.17
(2,237)	1:52:A:THR:H	1:54:A:TRP:H	4	0.17
(2,202)	1:33:A:GLU:H	1:35:A:GLU:H	3	0.17
(2,180)	1:33:A:GLU:H	1:35:A:GLU:H	3	0.17
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	10	0.17
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	17	0.17
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	4	0.17
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	4	0.17
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	4	0.17
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	9	0.17
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	9	0.17
(2,96)	1:44:C:SER:H	1:47:C:ASN:H	8	0.17
(2,95)	1:44:B:SER:H	1:47:B:ASN:H	8	0.17
(2,94)	1:44:A:SER:H	1:47:A:ASN:H	8	0.17
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	1	0.17
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	8	0.17
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	14	0.17
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	1	0.17
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	8	0.17
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	14	0.17
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	1	0.17
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	8	0.17
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	14	0.17
(2,74)	1:50:B:ASN:H	1:47:B:ASN:H	4	0.17
(2,73)	1:50:A:ASN:H	1:47:A:ASN:H	4	0.17
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG21	2	0.17
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG22	2	0.17
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG23	2	0.17
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG21	2	0.17
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG22	2	0.17
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG23	2	0.17
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	17	0.17
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	17	0.17
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	17	0.17
(2,813)	1:47:C:ASN:H	1:50:C:ASN:H	7	0.16
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	6	0.16
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	15	0.16
(2,797)	1:14:C:VAL:H	1:16:C:LYS:H	16	0.16
(2,797)	1:14:C:VAL:H	1:16:C:LYS:H	17	0.16
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	2	0.16
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	6	0.16
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	8	0.16
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	10	0.16
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	16	0.16
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	6	0.16
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	15	0.16
(2,781)	1:14:C:VAL:H	1:16:C:LYS:H	16	0.16
(2,781)	1:14:C:VAL:H	1:16:C:LYS:H	17	0.16
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	2	0.16
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	6	0.16
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	8	0.16
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	16	0.16
(2,773)	1:30:C:SER:HA	1:33:C:GLU:H	9	0.16
(2,772)	1:29:C:SER:HA	1:32:C:ASN:H	18	0.16
(2,770)	1:34:C:GLN:H	1:36:C:LEU:H	1	0.16
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	3	0.16
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	16	0.16
(2,727)	1:29:C:SER:HA	1:32:C:ASN:H	18	0.16
(2,726)	1:33:C:GLU:H	1:36:C:LEU:HG	4	0.16
(2,726)	1:33:C:GLU:H	1:36:C:LEU:HG	13	0.16
(2,725)	1:30:C:SER:HA	1:33:C:GLU:H	9	0.16
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	5	0.16
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	3	0.16
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	16	0.16
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	12	0.16
(2,577)	1:47:B:ASN:H	1:50:B:ASN:H	7	0.16
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	6	0.16
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	15	0.16
(2,561)	1:14:B:VAL:H	1:16:B:LYS:H	16	0.16
(2,561)	1:14:B:VAL:H	1:16:B:LYS:H	17	0.16
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	2	0.16
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	8	0.16
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	10	0.16
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	16	0.16
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	6	0.16
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	15	0.16
(2,545)	1:14:B:VAL:H	1:16:B:LYS:H	16	0.16
(2,545)	1:14:B:VAL:H	1:16:B:LYS:H	17	0.16
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	2	0.16
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	8	0.16
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	10	0.16
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	16	0.16
(2,537)	1:30:B:SER:HA	1:33:B:GLU:H	9	0.16
(2,536)	1:29:B:SER:HA	1:32:B:ASN:H	18	0.16
(2,534)	1:34:B:GLN:H	1:36:B:LEU:H	1	0.16
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	3	0.16
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	16	0.16
(2,491)	1:29:B:SER:HA	1:32:B:ASN:H	18	0.16
(2,490)	1:33:B:GLU:H	1:36:B:LEU:HG	4	0.16
(2,490)	1:33:B:GLU:H	1:36:B:LEU:HG	13	0.16
(2,489)	1:30:B:SER:HA	1:33:B:GLU:H	9	0.16
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	5	0.16
(2,482)	1:56:B:TRP:H	1:58:B:ILE:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	3	0.16
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	16	0.16
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	12	0.16
(2,341)	1:47:A:ASN:H	1:50:A:ASN:H	7	0.16
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	6	0.16
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	15	0.16
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	16	0.16
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	17	0.16
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	4	0.16
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	6	0.16
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	15	0.16
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	16	0.16
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	17	0.16
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	4	0.16
(2,303)	1:30:A:SER:HA	1:33:A:GLU:H	9	0.16
(2,302)	1:29:A:SER:HA	1:32:A:ASN:H	18	0.16
(2,300)	1:34:A:GLN:H	1:36:A:LEU:H	1	0.16
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	3	0.16
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	16	0.16
(2,257)	1:29:A:SER:HA	1:32:A:ASN:H	18	0.16
(2,256)	1:33:A:GLU:H	1:36:A:LEU:HG	4	0.16
(2,256)	1:33:A:GLU:H	1:36:A:LEU:HG	13	0.16
(2,255)	1:30:A:SER:HA	1:33:A:GLU:H	9	0.16
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	5	0.16
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	3	0.16
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	16	0.16
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	3	0.16
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	12	0.16
(2,108)	1:34:C:GLN:H	1:30:C:SER:H	6	0.16
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	5	0.16
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	5	0.16
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	5	0.16
(2,96)	1:44:C:SER:H	1:47:C:ASN:H	7	0.16
(2,95)	1:44:B:SER:H	1:47:B:ASN:H	7	0.16
(2,94)	1:44:A:SER:H	1:47:A:ASN:H	7	0.16
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	9	0.16
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	12	0.16
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	9	0.16
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	12	0.16
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	9	0.16
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	12	0.16
(2,81)	1:34:C:GLN:H	1:31:C:GLY:H	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,80)	1:34:B:GLN:H	1:31:B:GLY:H	17	0.16
(2,79)	1:34:A:GLN:H	1:31:A:GLY:H	17	0.16
(2,75)	1:50:C:ASN:H	1:47:C:ASN:H	7	0.16
(2,74)	1:50:B:ASN:H	1:47:B:ASN:H	7	0.16
(2,73)	1:50:A:ASN:H	1:47:A:ASN:H	7	0.16
(1,91)	1:42:C:TRP:HE1	1:43:C:ALA:H	7	0.16
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	3	0.16
(1,85)	1:42:C:TRP:HE1	1:43:C:ALA:H	7	0.16
(1,63)	1:42:B:TRP:HE1	1:43:B:ALA:H	7	0.16
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	3	0.16
(1,57)	1:42:B:TRP:HE1	1:43:B:ALA:H	7	0.16
(1,35)	1:42:A:TRP:HE1	1:43:A:ALA:H	7	0.16
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	3	0.16
(1,29)	1:42:A:TRP:HE1	1:43:A:ALA:H	7	0.16
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	3	0.15
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	11	0.15
(2,797)	1:14:C:VAL:H	1:16:C:LYS:H	1	0.15
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	13	0.15
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	14	0.15
(2,794)	1:21:C:VAL:H	1:23:C:LEU:H	2	0.15
(2,791)	1:48:C:TRP:H	1:48:C:TRP:HE1	1	0.15
(2,787)	1:21:C:VAL:H	1:23:C:LEU:H	2	0.15
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	3	0.15
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	11	0.15
(2,781)	1:14:C:VAL:H	1:16:C:LYS:H	1	0.15
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	13	0.15
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	14	0.15
(2,776)	1:48:C:TRP:H	1:48:C:TRP:HE1	1	0.15
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	12	0.15
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	13	0.15
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	14	0.15
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	5	0.15
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	15	0.15
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	16	0.15
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	12	0.15
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	13	0.15
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	14	0.15
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	3	0.15
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	14	0.15
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	5	0.15
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	8	0.15
(2,677)	1:23:C:LEU:H	1:25:C:THR:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,674)	1:14:C:VAL:H	1:23:C:LEU:H	6	0.15
(2,647)	1:23:C:LEU:H	1:25:C:THR:H	16	0.15
(2,635)	1:14:C:VAL:H	1:23:C:LEU:H	6	0.15
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	5	0.15
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	8	0.15
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	3	0.15
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	11	0.15
(2,561)	1:14:B:VAL:H	1:16:B:LYS:H	1	0.15
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	6	0.15
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	13	0.15
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	14	0.15
(2,558)	1:21:B:VAL:H	1:23:B:LEU:H	2	0.15
(2,555)	1:48:B:TRP:H	1:48:B:TRP:HE1	1	0.15
(2,551)	1:21:B:VAL:H	1:23:B:LEU:H	2	0.15
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	3	0.15
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	11	0.15
(2,545)	1:14:B:VAL:H	1:16:B:LYS:H	1	0.15
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	6	0.15
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	13	0.15
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	14	0.15
(2,540)	1:48:B:TRP:H	1:48:B:TRP:HE1	1	0.15
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	12	0.15
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	13	0.15
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	14	0.15
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	5	0.15
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	15	0.15
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	16	0.15
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	12	0.15
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	13	0.15
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	14	0.15
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	3	0.15
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	10	0.15
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	14	0.15
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	5	0.15
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	8	0.15
(2,452)	1:43:B:ALA:H	1:45:B:LEU:H	2	0.15
(2,441)	1:23:B:LEU:H	1:25:B:THR:H	16	0.15
(2,438)	1:14:B:VAL:H	1:23:B:LEU:H	6	0.15
(2,418)	1:43:B:ALA:H	1:45:B:LEU:H	2	0.15
(2,411)	1:23:B:LEU:H	1:25:B:THR:H	16	0.15
(2,399)	1:14:B:VAL:H	1:23:B:LEU:H	6	0.15
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	8	0.15
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	3	0.15
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	11	0.15
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	1	0.15
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	1	0.15
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	2	0.15
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	7	0.15
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	10	0.15
(2,320)	1:48:A:TRP:H	1:48:A:TRP:HE1	1	0.15
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	3	0.15
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	11	0.15
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	1	0.15
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	1	0.15
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	2	0.15
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	7	0.15
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	10	0.15
(2,307)	1:48:A:TRP:H	1:48:A:TRP:HE1	1	0.15
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	12	0.15
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	13	0.15
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	14	0.15
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	5	0.15
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	15	0.15
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	16	0.15
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	12	0.15
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	13	0.15
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	14	0.15
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	10	0.15
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	14	0.15
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	5	0.15
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	8	0.15
(2,207)	1:23:A:LEU:H	1:25:A:THR:H	16	0.15
(2,204)	1:14:A:VAL:H	1:23:A:LEU:H	6	0.15
(2,177)	1:23:A:LEU:H	1:25:A:THR:H	16	0.15
(2,165)	1:14:A:VAL:H	1:23:A:LEU:H	6	0.15
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	5	0.15
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	8	0.15
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	1	0.15
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	1	0.15
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	1	0.15
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	1	0.15
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	1	0.15
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:28:C:GLY:H	1:25:C:THR:HA	4	0.15
(2,113)	1:28:B:GLY:H	1:25:B:THR:HA	4	0.15
(2,112)	1:28:A:GLY:H	1:25:A:THR:HA	4	0.15
(2,107)	1:34:B:GLN:H	1:30:B:SER:H	6	0.15
(2,106)	1:34:A:GLN:H	1:30:A:SER:H	6	0.15
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	2	0.15
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	2	0.15
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	2	0.15
(2,94)	1:44:A:SER:H	1:47:A:ASN:H	3	0.15
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	13	0.15
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	17	0.15
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	13	0.15
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	17	0.15
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	13	0.15
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	17	0.15
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	12	0.15
(2,6)	1:26:B:PHE:H	1:27:A:LEU:HD21	3	0.15
(2,6)	1:26:B:PHE:H	1:27:A:LEU:HD22	3	0.15
(2,6)	1:26:B:PHE:H	1:27:A:LEU:HD23	3	0.15
(2,4)	1:26:A:PHE:H	1:27:C:LEU:HD21	3	0.15
(2,4)	1:26:A:PHE:H	1:27:C:LEU:HD22	3	0.15
(2,4)	1:26:A:PHE:H	1:27:C:LEU:HD23	3	0.15
(1,91)	1:42:C:TRP:HE1	1:43:C:ALA:H	1	0.15
(1,91)	1:42:C:TRP:HE1	1:43:C:ALA:H	6	0.15
(1,91)	1:42:C:TRP:HE1	1:43:C:ALA:H	8	0.15
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	18	0.15
(1,85)	1:42:C:TRP:HE1	1:43:C:ALA:H	1	0.15
(1,85)	1:42:C:TRP:HE1	1:43:C:ALA:H	6	0.15
(1,85)	1:42:C:TRP:HE1	1:43:C:ALA:H	8	0.15
(1,63)	1:42:B:TRP:HE1	1:43:B:ALA:H	1	0.15
(1,63)	1:42:B:TRP:HE1	1:43:B:ALA:H	6	0.15
(1,63)	1:42:B:TRP:HE1	1:43:B:ALA:H	8	0.15
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	18	0.15
(1,57)	1:42:B:TRP:HE1	1:43:B:ALA:H	1	0.15
(1,57)	1:42:B:TRP:HE1	1:43:B:ALA:H	6	0.15
(1,57)	1:42:B:TRP:HE1	1:43:B:ALA:H	8	0.15
(1,35)	1:42:A:TRP:HE1	1:43:A:ALA:H	1	0.15
(1,35)	1:42:A:TRP:HE1	1:43:A:ALA:H	6	0.15
(1,35)	1:42:A:TRP:HE1	1:43:A:ALA:H	8	0.15
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	18	0.15
(1,29)	1:42:A:TRP:HE1	1:43:A:ALA:H	1	0.15
(1,29)	1:42:A:TRP:HE1	1:43:A:ALA:H	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:42:A:TRP:HE1	1:43:A:ALA:H	8	0.15
(2,813)	1:47:C:ASN:H	1:50:C:ASN:H	1	0.14
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	11	0.14
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	9	0.14
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	18	0.14
(2,796)	1:8:C:ARG:H	1:10:C:GLY:H	1	0.14
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	5	0.14
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	9	0.14
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	12	0.14
(2,791)	1:48:C:TRP:H	1:48:C:TRP:HE1	2	0.14
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	9	0.14
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	18	0.14
(2,780)	1:8:C:ARG:H	1:10:C:GLY:H	1	0.14
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	5	0.14
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	9	0.14
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	12	0.14
(2,776)	1:48:C:TRP:H	1:48:C:TRP:HE1	2	0.14
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	1	0.14
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	1	0.14
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	8	0.14
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	9	0.14
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	10	0.14
(2,688)	1:43:C:ALA:H	1:45:C:LEU:H	2	0.14
(2,654)	1:43:C:ALA:H	1:45:C:LEU:H	2	0.14
(2,577)	1:47:B:ASN:H	1:50:B:ASN:H	1	0.14
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	11	0.14
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	9	0.14
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	18	0.14
(2,560)	1:8:B:ARG:H	1:10:B:GLY:H	1	0.14
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	5	0.14
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	9	0.14
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	12	0.14
(2,555)	1:48:B:TRP:H	1:48:B:TRP:HE1	2	0.14
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	9	0.14
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	18	0.14
(2,544)	1:8:B:ARG:H	1:10:B:GLY:H	1	0.14
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	5	0.14
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	9	0.14
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	12	0.14
(2,540)	1:48:B:TRP:H	1:48:B:TRP:HE1	2	0.14
(2,518)	1:52:B:THR:H	1:54:B:TRP:H	14	0.14
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	18	0.14
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	1	0.14
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	9	0.14
(2,471)	1:52:B:THR:H	1:54:B:TRP:H	14	0.14
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	11	0.14
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	9	0.14
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	18	0.14
(2,325)	1:8:A:ARG:H	1:10:A:GLY:H	1	0.14
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	6	0.14
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	8	0.14
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	13	0.14
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	14	0.14
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	16	0.14
(2,320)	1:48:A:TRP:H	1:48:A:TRP:HE1	2	0.14
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	9	0.14
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	18	0.14
(2,310)	1:8:A:ARG:H	1:10:A:GLY:H	1	0.14
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	6	0.14
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	8	0.14
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	13	0.14
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	14	0.14
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	16	0.14
(2,307)	1:48:A:TRP:H	1:48:A:TRP:HE1	2	0.14
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	1	0.14
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	1	0.14
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	9	0.14
(2,218)	1:43:A:ALA:H	1:45:A:LEU:H	2	0.14
(2,184)	1:43:A:ALA:H	1:45:A:LEU:H	2	0.14
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	8	0.14
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	8	0.14
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	8	0.14
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	8	0.14
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	8	0.14
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	8	0.14
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD21	15	0.14
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD22	15	0.14
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD23	15	0.14
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD21	15	0.14
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD22	15	0.14
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD23	15	0.14
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD21	15	0.14
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD22	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD23	15	0.14
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	18	0.14
(2,96)	1:44:C:SER:H	1:47:C:ASN:H	3	0.14
(2,95)	1:44:B:SER:H	1:47:B:ASN:H	3	0.14
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	18	0.14
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	18	0.14
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	18	0.14
(2,75)	1:50:C:ASN:H	1:47:C:ASN:H	1	0.14
(2,74)	1:50:B:ASN:H	1:47:B:ASN:H	1	0.14
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	7	0.14
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	7	0.14
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	7	0.14
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	7	0.14
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	7	0.14
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	7	0.14
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG21	12	0.14
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG22	12	0.14
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG23	12	0.14
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG21	12	0.14
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG22	12	0.14
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG23	12	0.14
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG21	12	0.14
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG22	12	0.14
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG23	12	0.14
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG21	13	0.14
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG22	13	0.14
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG23	13	0.14
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG21	14	0.14
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG22	14	0.14
(2,28)	1:14:A:VAL:H	1:14:B:VAL:HG23	14	0.14
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG21	2	0.14
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG22	2	0.14
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG23	2	0.14
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	9	0.14
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	13	0.14
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	12	0.14
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	12	0.14
(2,5)	1:26:C:PHE:H	1:27:B:LEU:HD21	3	0.14
(2,5)	1:26:C:PHE:H	1:27:B:LEU:HD22	3	0.14
(2,5)	1:26:C:PHE:H	1:27:B:LEU:HD23	3	0.14
(1,12)	1:26:C:PHE:H	1:29:C:SER:H	12	0.14
(1,11)	1:26:B:PHE:H	1:29:B:SER:H	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:26:A:PHE:H	1:29:A:SER:H	12	0.14
(2,813)	1:47:C:ASN:H	1:50:C:ASN:H	9	0.13
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	13	0.13
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	14	0.13
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	12	0.13
(2,794)	1:21:C:VAL:H	1:23:C:LEU:H	4	0.13
(2,787)	1:21:C:VAL:H	1:23:C:LEU:H	4	0.13
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	12	0.13
(2,773)	1:30:C:SER:HA	1:33:C:GLU:H	12	0.13
(2,762)	1:32:C:ASN:HB2	1:34:C:GLN:H	15	0.13
(2,762)	1:32:C:ASN:HB3	1:34:C:GLN:H	15	0.13
(2,760)	1:27:C:LEU:HB2	1:29:C:SER:H	12	0.13
(2,760)	1:27:C:LEU:HB3	1:29:C:SER:H	12	0.13
(2,754)	1:52:C:THR:H	1:54:C:TRP:H	14	0.13
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	11	0.13
(2,725)	1:30:C:SER:HA	1:33:C:GLU:H	12	0.13
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	18	0.13
(2,721)	1:24:C:SER:H	1:27:C:LEU:H	1	0.13
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	11	0.13
(2,707)	1:52:C:THR:H	1:54:C:TRP:H	14	0.13
(2,672)	1:33:C:GLU:H	1:35:C:GLU:H	11	0.13
(2,650)	1:33:C:GLU:H	1:35:C:GLU:H	11	0.13
(2,577)	1:47:B:ASN:H	1:50:B:ASN:H	9	0.13
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	14	0.13
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	12	0.13
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	12	0.13
(2,537)	1:30:B:SER:HA	1:33:B:GLU:H	12	0.13
(2,526)	1:32:B:ASN:HB2	1:34:B:GLN:H	15	0.13
(2,526)	1:32:B:ASN:HB3	1:34:B:GLN:H	15	0.13
(2,524)	1:27:B:LEU:HB2	1:29:B:SER:H	12	0.13
(2,524)	1:27:B:LEU:HB3	1:29:B:SER:H	12	0.13
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	11	0.13
(2,489)	1:30:B:SER:HA	1:33:B:GLU:H	12	0.13
(2,485)	1:24:B:SER:H	1:27:B:LEU:H	1	0.13
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	11	0.13
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	8	0.13
(2,436)	1:33:B:GLU:H	1:35:B:GLU:H	11	0.13
(2,414)	1:33:B:GLU:H	1:35:B:GLU:H	11	0.13
(2,341)	1:47:A:ASN:H	1:50:A:ASN:H	1	0.13
(2,341)	1:47:A:ASN:H	1:50:A:ASN:H	9	0.13
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	13	0.13
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,331)	1:16:A:LYS:H	1:20:A:TRP:H	14	0.13
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	12	0.13
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	5	0.13
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	9	0.13
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	12	0.13
(2,323)	1:21:A:VAL:H	1:23:A:LEU:H	4	0.13
(2,323)	1:21:A:VAL:H	1:23:A:LEU:H	9	0.13
(2,323)	1:21:A:VAL:H	1:23:A:LEU:H	14	0.13
(2,317)	1:21:A:VAL:H	1:23:A:LEU:H	4	0.13
(2,317)	1:21:A:VAL:H	1:23:A:LEU:H	9	0.13
(2,317)	1:21:A:VAL:H	1:23:A:LEU:H	14	0.13
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	12	0.13
(2,314)	1:16:A:LYS:H	1:20:A:TRP:H	14	0.13
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	5	0.13
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	9	0.13
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	12	0.13
(2,303)	1:30:A:SER:HA	1:33:A:GLU:H	12	0.13
(2,290)	1:27:A:LEU:HB2	1:29:A:SER:H	12	0.13
(2,290)	1:27:A:LEU:HB3	1:29:A:SER:H	12	0.13
(2,284)	1:52:A:THR:H	1:54:A:TRP:H	14	0.13
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	11	0.13
(2,255)	1:30:A:SER:HA	1:33:A:GLU:H	12	0.13
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	18	0.13
(2,251)	1:24:A:SER:H	1:27:A:LEU:H	1	0.13
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	11	0.13
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	8	0.13
(2,237)	1:52:A:THR:H	1:54:A:TRP:H	14	0.13
(2,202)	1:33:A:GLU:H	1:35:A:GLU:H	11	0.13
(2,180)	1:33:A:GLU:H	1:35:A:GLU:H	11	0.13
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	4	0.13
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	4	0.13
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	4	0.13
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	4	0.13
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	4	0.13
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	4	0.13
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	18	0.13
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	18	0.13
(2,75)	1:50:C:ASN:H	1:47:C:ASN:H	9	0.13
(2,74)	1:50:B:ASN:H	1:47:B:ASN:H	9	0.13
(2,73)	1:50:A:ASN:H	1:47:A:ASN:H	1	0.13
(2,73)	1:50:A:ASN:H	1:47:A:ASN:H	9	0.13
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG21	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG22	13	0.13
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG23	13	0.13
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG21	14	0.13
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG22	14	0.13
(2,30)	1:14:C:VAL:H	1:14:A:VAL:HG23	14	0.13
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG21	13	0.13
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG22	13	0.13
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG23	13	0.13
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG21	14	0.13
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG22	14	0.13
(2,29)	1:14:B:VAL:H	1:14:C:VAL:HG23	14	0.13
(2,24)	1:15:B:ARG:H	1:14:A:VAL:H	14	0.13
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	13	0.13
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	9	0.13
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	13	0.13
(2,22)	1:15:A:ARG:H	1:14:C:VAL:H	14	0.13
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	9	0.12
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	12	0.12
(2,807)	1:32:C:ASN:H	1:35:C:GLU:H	13	0.12
(2,803)	1:16:C:LYS:H	1:20:C:TRP:H	14	0.12
(2,797)	1:14:C:VAL:H	1:16:C:LYS:H	2	0.12
(2,797)	1:14:C:VAL:H	1:16:C:LYS:H	7	0.12
(2,797)	1:14:C:VAL:H	1:16:C:LYS:H	18	0.12
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	18	0.12
(2,784)	1:16:C:LYS:H	1:20:C:TRP:H	14	0.12
(2,781)	1:14:C:VAL:H	1:16:C:LYS:H	2	0.12
(2,781)	1:14:C:VAL:H	1:16:C:LYS:H	7	0.12
(2,781)	1:14:C:VAL:H	1:16:C:LYS:H	18	0.12
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	18	0.12
(2,773)	1:30:C:SER:HA	1:33:C:GLU:H	1	0.12
(2,772)	1:29:C:SER:HA	1:32:C:ASN:H	17	0.12
(2,762)	1:32:C:ASN:HB2	1:34:C:GLN:H	6	0.12
(2,762)	1:32:C:ASN:HB3	1:34:C:GLN:H	6	0.12
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	10	0.12
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	17	0.12
(2,727)	1:29:C:SER:HA	1:32:C:ASN:H	17	0.12
(2,725)	1:30:C:SER:HA	1:33:C:GLU:H	1	0.12
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	10	0.12
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	17	0.12
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	15	0.12
(2,713)	1:50:C:ASN:H	1:54:C:TRP:HE1	2	0.12
(2,688)	1:43:C:ALA:H	1:45:C:LEU:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,678)	1:40:C:ASP:H	1:42:C:TRP:H	10	0.12
(2,664)	1:14:C:VAL:H	1:15:C:ARG:H	2	0.12
(2,654)	1:43:C:ALA:H	1:45:C:LEU:H	3	0.12
(2,634)	1:14:C:VAL:H	1:15:C:ARG:H	2	0.12
(2,628)	1:50:C:ASN:H	1:54:C:TRP:HE1	2	0.12
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	9	0.12
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	12	0.12
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	13	0.12
(2,571)	1:32:B:ASN:H	1:35:B:GLU:H	13	0.12
(2,567)	1:16:B:LYS:H	1:20:B:TRP:H	14	0.12
(2,561)	1:14:B:VAL:H	1:16:B:LYS:H	2	0.12
(2,561)	1:14:B:VAL:H	1:16:B:LYS:H	7	0.12
(2,561)	1:14:B:VAL:H	1:16:B:LYS:H	18	0.12
(2,560)	1:8:B:ARG:H	1:10:B:GLY:H	4	0.12
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	17	0.12
(2,559)	1:19:B:GLU:H	1:21:B:VAL:H	18	0.12
(2,558)	1:21:B:VAL:H	1:23:B:LEU:H	4	0.12
(2,555)	1:48:B:TRP:H	1:48:B:TRP:HE1	10	0.12
(2,555)	1:48:B:TRP:H	1:48:B:TRP:HE1	14	0.12
(2,551)	1:21:B:VAL:H	1:23:B:LEU:H	4	0.12
(2,548)	1:16:B:LYS:H	1:20:B:TRP:H	14	0.12
(2,545)	1:14:B:VAL:H	1:16:B:LYS:H	2	0.12
(2,545)	1:14:B:VAL:H	1:16:B:LYS:H	7	0.12
(2,545)	1:14:B:VAL:H	1:16:B:LYS:H	18	0.12
(2,544)	1:8:B:ARG:H	1:10:B:GLY:H	4	0.12
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	17	0.12
(2,543)	1:19:B:GLU:H	1:21:B:VAL:H	18	0.12
(2,540)	1:48:B:TRP:H	1:48:B:TRP:HE1	10	0.12
(2,540)	1:48:B:TRP:H	1:48:B:TRP:HE1	14	0.12
(2,537)	1:30:B:SER:HA	1:33:B:GLU:H	1	0.12
(2,537)	1:30:B:SER:HA	1:33:B:GLU:H	17	0.12
(2,536)	1:29:B:SER:HA	1:32:B:ASN:H	17	0.12
(2,526)	1:32:B:ASN:HB2	1:34:B:GLN:H	6	0.12
(2,526)	1:32:B:ASN:HB3	1:34:B:GLN:H	6	0.12
(2,518)	1:52:B:THR:H	1:54:B:TRP:H	13	0.12
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	10	0.12
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	17	0.12
(2,491)	1:29:B:SER:HA	1:32:B:ASN:H	17	0.12
(2,489)	1:30:B:SER:HA	1:33:B:GLU:H	1	0.12
(2,489)	1:30:B:SER:HA	1:33:B:GLU:H	17	0.12
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	10	0.12
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	15	0.12
(2,477)	1:50:B:ASN:H	1:54:B:TRP:HE1	2	0.12
(2,471)	1:52:B:THR:H	1:54:B:TRP:H	13	0.12
(2,452)	1:43:B:ALA:H	1:45:B:LEU:H	3	0.12
(2,442)	1:40:B:ASP:H	1:42:B:TRP:H	10	0.12
(2,428)	1:14:B:VAL:H	1:15:B:ARG:H	2	0.12
(2,418)	1:43:B:ALA:H	1:45:B:LEU:H	3	0.12
(2,398)	1:14:B:VAL:H	1:15:B:ARG:H	2	0.12
(2,392)	1:50:B:ASN:H	1:54:B:TRP:HE1	2	0.12
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	9	0.12
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	12	0.12
(2,335)	1:32:A:ASN:H	1:35:A:GLU:H	13	0.12
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	2	0.12
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	7	0.12
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	18	0.12
(2,325)	1:8:A:ARG:H	1:10:A:GLY:H	4	0.12
(2,320)	1:48:A:TRP:H	1:48:A:TRP:HE1	10	0.12
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	2	0.12
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	7	0.12
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	18	0.12
(2,310)	1:8:A:ARG:H	1:10:A:GLY:H	4	0.12
(2,307)	1:48:A:TRP:H	1:48:A:TRP:HE1	10	0.12
(2,303)	1:30:A:SER:HA	1:33:A:GLU:H	1	0.12
(2,303)	1:30:A:SER:HA	1:33:A:GLU:H	17	0.12
(2,302)	1:29:A:SER:HA	1:32:A:ASN:H	17	0.12
(2,292)	1:32:A:ASN:HB2	1:34:A:GLN:H	6	0.12
(2,292)	1:32:A:ASN:HB3	1:34:A:GLN:H	6	0.12
(2,292)	1:32:A:ASN:HB2	1:34:A:GLN:H	15	0.12
(2,292)	1:32:A:ASN:HB3	1:34:A:GLN:H	15	0.12
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	10	0.12
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	17	0.12
(2,257)	1:29:A:SER:HA	1:32:A:ASN:H	17	0.12
(2,255)	1:30:A:SER:HA	1:33:A:GLU:H	1	0.12
(2,255)	1:30:A:SER:HA	1:33:A:GLU:H	17	0.12
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	10	0.12
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	17	0.12
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	15	0.12
(2,243)	1:50:A:ASN:H	1:54:A:TRP:HE1	2	0.12
(2,218)	1:43:A:ALA:H	1:45:A:LEU:H	3	0.12
(2,208)	1:40:A:ASP:H	1:42:A:TRP:H	10	0.12
(2,194)	1:14:A:VAL:H	1:15:A:ARG:H	2	0.12
(2,184)	1:43:A:ALA:H	1:45:A:LEU:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,164)	1:14:A:VAL:H	1:15:A:ARG:H	2	0.12
(2,158)	1:50:A:ASN:H	1:54:A:TRP:HE1	2	0.12
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	3	0.12
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	3	0.12
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	3	0.12
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	3	0.12
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	3	0.12
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	3	0.12
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD11	9	0.12
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD12	9	0.12
(2,129)	1:33:C:GLU:H	1:36:C:LEU:HD13	9	0.12
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD11	9	0.12
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD12	9	0.12
(2,128)	1:33:B:GLU:H	1:36:B:LEU:HD13	9	0.12
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD11	9	0.12
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD12	9	0.12
(2,127)	1:33:A:GLU:H	1:36:A:LEU:HD13	9	0.12
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD21	9	0.12
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD22	9	0.12
(2,117)	1:12:C:ALA:H	1:22:C:LEU:HD23	9	0.12
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD21	9	0.12
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD22	9	0.12
(2,116)	1:12:B:ALA:H	1:22:B:LEU:HD23	9	0.12
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD21	9	0.12
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD22	9	0.12
(2,115)	1:12:A:ALA:H	1:22:A:LEU:HD23	9	0.12
(2,84)	1:43:C:ALA:H	1:47:C:ASN:H	7	0.12
(2,83)	1:43:B:ALA:H	1:47:B:ASN:H	7	0.12
(2,82)	1:43:A:ALA:H	1:47:A:ASN:H	7	0.12
(2,81)	1:34:C:GLN:H	1:31:C:GLY:H	12	0.12
(2,80)	1:34:B:GLN:H	1:31:B:GLY:H	12	0.12
(2,79)	1:34:A:GLN:H	1:31:A:GLY:H	12	0.12
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	8	0.12
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	8	0.12
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	8	0.12
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	8	0.12
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	8	0.12
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	8	0.12
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG21	3	0.12
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG22	3	0.12
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG23	3	0.12
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG21	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG22	3	0.12
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG23	3	0.12
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG21	3	0.12
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG22	3	0.12
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG23	3	0.12
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	9	0.12
(2,23)	1:15:C:ARG:H	1:14:B:VAL:H	14	0.12
(1,89)	1:14:C:VAL:H	1:20:C:TRP:H	2	0.12
(1,61)	1:14:B:VAL:H	1:20:B:TRP:H	2	0.12
(1,33)	1:14:A:VAL:H	1:20:A:TRP:H	2	0.12
(1,11)	1:26:B:PHE:H	1:29:B:SER:H	15	0.12
(1,10)	1:26:A:PHE:H	1:29:A:SER:H	15	0.12
(2,801)	1:22:C:LEU:H	1:24:C:SER:H	5	0.11
(2,797)	1:14:C:VAL:H	1:16:C:LYS:H	3	0.11
(2,796)	1:8:C:ARG:H	1:10:C:GLY:H	4	0.11
(2,796)	1:8:C:ARG:H	1:10:C:GLY:H	9	0.11
(2,796)	1:8:C:ARG:H	1:10:C:GLY:H	10	0.11
(2,795)	1:19:C:GLU:H	1:21:C:VAL:H	17	0.11
(2,794)	1:21:C:VAL:H	1:23:C:LEU:H	9	0.11
(2,794)	1:21:C:VAL:H	1:23:C:LEU:H	14	0.11
(2,791)	1:48:C:TRP:H	1:48:C:TRP:HE1	10	0.11
(2,791)	1:48:C:TRP:H	1:48:C:TRP:HE1	12	0.11
(2,791)	1:48:C:TRP:H	1:48:C:TRP:HE1	13	0.11
(2,791)	1:48:C:TRP:H	1:48:C:TRP:HE1	14	0.11
(2,787)	1:21:C:VAL:H	1:23:C:LEU:H	9	0.11
(2,787)	1:21:C:VAL:H	1:23:C:LEU:H	14	0.11
(2,785)	1:22:C:LEU:H	1:24:C:SER:H	5	0.11
(2,781)	1:14:C:VAL:H	1:16:C:LYS:H	3	0.11
(2,780)	1:8:C:ARG:H	1:10:C:GLY:H	4	0.11
(2,780)	1:8:C:ARG:H	1:10:C:GLY:H	9	0.11
(2,780)	1:8:C:ARG:H	1:10:C:GLY:H	10	0.11
(2,779)	1:19:C:GLU:H	1:21:C:VAL:H	17	0.11
(2,776)	1:48:C:TRP:H	1:48:C:TRP:HE1	10	0.11
(2,776)	1:48:C:TRP:H	1:48:C:TRP:HE1	12	0.11
(2,776)	1:48:C:TRP:H	1:48:C:TRP:HE1	13	0.11
(2,776)	1:48:C:TRP:H	1:48:C:TRP:HE1	14	0.11
(2,773)	1:30:C:SER:HA	1:33:C:GLU:H	17	0.11
(2,772)	1:29:C:SER:HA	1:32:C:ASN:H	11	0.11
(2,770)	1:34:C:GLN:H	1:36:C:LEU:H	17	0.11
(2,754)	1:52:C:THR:H	1:54:C:TRP:H	13	0.11
(2,728)	1:34:C:GLN:H	1:36:C:LEU:HG	10	0.11
(2,727)	1:29:C:SER:HA	1:32:C:ASN:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,725)	1:30:C:SER:HA	1:33:C:GLU:H	17	0.11
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	11	0.11
(2,724)	1:50:C:ASN:H	1:53:C:ASN:H	15	0.11
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	1	0.11
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	18	0.11
(2,707)	1:52:C:THR:H	1:54:C:TRP:H	13	0.11
(2,688)	1:43:C:ALA:H	1:45:C:LEU:H	9	0.11
(2,678)	1:40:C:ASP:H	1:42:C:TRP:H	12	0.11
(2,678)	1:40:C:ASP:H	1:42:C:TRP:H	16	0.11
(2,677)	1:23:C:LEU:H	1:25:C:THR:H	6	0.11
(2,664)	1:14:C:VAL:H	1:15:C:ARG:H	16	0.11
(2,654)	1:43:C:ALA:H	1:45:C:LEU:H	9	0.11
(2,647)	1:23:C:LEU:H	1:25:C:THR:H	6	0.11
(2,634)	1:14:C:VAL:H	1:15:C:ARG:H	16	0.11
(2,627)	1:38:C:GLU:H	1:42:C:TRP:HE1	16	0.11
(2,565)	1:22:B:LEU:H	1:24:B:SER:H	5	0.11
(2,561)	1:14:B:VAL:H	1:16:B:LYS:H	3	0.11
(2,560)	1:8:B:ARG:H	1:10:B:GLY:H	9	0.11
(2,560)	1:8:B:ARG:H	1:10:B:GLY:H	10	0.11
(2,558)	1:21:B:VAL:H	1:23:B:LEU:H	9	0.11
(2,558)	1:21:B:VAL:H	1:23:B:LEU:H	14	0.11
(2,555)	1:48:B:TRP:H	1:48:B:TRP:HE1	12	0.11
(2,555)	1:48:B:TRP:H	1:48:B:TRP:HE1	13	0.11
(2,551)	1:21:B:VAL:H	1:23:B:LEU:H	9	0.11
(2,551)	1:21:B:VAL:H	1:23:B:LEU:H	14	0.11
(2,549)	1:22:B:LEU:H	1:24:B:SER:H	5	0.11
(2,545)	1:14:B:VAL:H	1:16:B:LYS:H	3	0.11
(2,544)	1:8:B:ARG:H	1:10:B:GLY:H	9	0.11
(2,544)	1:8:B:ARG:H	1:10:B:GLY:H	10	0.11
(2,540)	1:48:B:TRP:H	1:48:B:TRP:HE1	12	0.11
(2,540)	1:48:B:TRP:H	1:48:B:TRP:HE1	13	0.11
(2,536)	1:29:B:SER:HA	1:32:B:ASN:H	11	0.11
(2,534)	1:34:B:GLN:H	1:36:B:LEU:H	17	0.11
(2,492)	1:34:B:GLN:H	1:36:B:LEU:HG	10	0.11
(2,491)	1:29:B:SER:HA	1:32:B:ASN:H	11	0.11
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	11	0.11
(2,488)	1:50:B:ASN:H	1:53:B:ASN:H	15	0.11
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	1	0.11
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	18	0.11
(2,452)	1:43:B:ALA:H	1:45:B:LEU:H	9	0.11
(2,442)	1:40:B:ASP:H	1:42:B:TRP:H	12	0.11
(2,442)	1:40:B:ASP:H	1:42:B:TRP:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,441)	1:23:B:LEU:H	1:25:B:THR:H	6	0.11
(2,428)	1:14:B:VAL:H	1:15:B:ARG:H	16	0.11
(2,418)	1:43:B:ALA:H	1:45:B:LEU:H	9	0.11
(2,411)	1:23:B:LEU:H	1:25:B:THR:H	6	0.11
(2,398)	1:14:B:VAL:H	1:15:B:ARG:H	16	0.11
(2,391)	1:38:B:GLU:H	1:42:B:TRP:HE1	16	0.11
(2,329)	1:22:A:LEU:H	1:24:A:SER:H	5	0.11
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	3	0.11
(2,325)	1:8:A:ARG:H	1:10:A:GLY:H	9	0.11
(2,323)	1:21:A:VAL:H	1:23:A:LEU:H	13	0.11
(2,323)	1:21:A:VAL:H	1:23:A:LEU:H	18	0.11
(2,320)	1:48:A:TRP:H	1:48:A:TRP:HE1	12	0.11
(2,320)	1:48:A:TRP:H	1:48:A:TRP:HE1	13	0.11
(2,320)	1:48:A:TRP:H	1:48:A:TRP:HE1	14	0.11
(2,317)	1:21:A:VAL:H	1:23:A:LEU:H	13	0.11
(2,317)	1:21:A:VAL:H	1:23:A:LEU:H	18	0.11
(2,315)	1:22:A:LEU:H	1:24:A:SER:H	5	0.11
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	3	0.11
(2,310)	1:8:A:ARG:H	1:10:A:GLY:H	9	0.11
(2,307)	1:48:A:TRP:H	1:48:A:TRP:HE1	12	0.11
(2,307)	1:48:A:TRP:H	1:48:A:TRP:HE1	13	0.11
(2,307)	1:48:A:TRP:H	1:48:A:TRP:HE1	14	0.11
(2,302)	1:29:A:SER:HA	1:32:A:ASN:H	11	0.11
(2,300)	1:34:A:GLN:H	1:36:A:LEU:H	17	0.11
(2,284)	1:52:A:THR:H	1:54:A:TRP:H	13	0.11
(2,276)	1:54:A:TRP:H	1:56:A:TRP:H	6	0.11
(2,258)	1:34:A:GLN:H	1:36:A:LEU:HG	10	0.11
(2,257)	1:29:A:SER:HA	1:32:A:ASN:H	11	0.11
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	11	0.11
(2,254)	1:50:A:ASN:H	1:53:A:ASN:H	15	0.11
(2,246)	1:54:A:TRP:H	1:56:A:TRP:H	6	0.11
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	1	0.11
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	18	0.11
(2,237)	1:52:A:THR:H	1:54:A:TRP:H	13	0.11
(2,218)	1:43:A:ALA:H	1:45:A:LEU:H	9	0.11
(2,208)	1:40:A:ASP:H	1:42:A:TRP:H	12	0.11
(2,208)	1:40:A:ASP:H	1:42:A:TRP:H	16	0.11
(2,207)	1:23:A:LEU:H	1:25:A:THR:H	6	0.11
(2,194)	1:14:A:VAL:H	1:15:A:ARG:H	16	0.11
(2,184)	1:43:A:ALA:H	1:45:A:LEU:H	9	0.11
(2,177)	1:23:A:LEU:H	1:25:A:THR:H	6	0.11
(2,164)	1:14:A:VAL:H	1:15:A:ARG:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,157)	1:38:A:GLU:H	1:42:A:TRP:HE1	16	0.11
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	10	0.11
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	10	0.11
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	10	0.11
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	10	0.11
(2,105)	1:35:C:GLU:H	1:38:C:GLU:H	16	0.11
(2,104)	1:35:B:GLU:H	1:38:B:GLU:H	16	0.11
(2,103)	1:35:A:GLU:H	1:38:A:GLU:H	16	0.11
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	11	0.11
(2,99)	1:50:C:ASN:H	1:53:C:ASN:H	15	0.11
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	11	0.11
(2,98)	1:50:B:ASN:H	1:53:B:ASN:H	15	0.11
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	11	0.11
(2,97)	1:50:A:ASN:H	1:53:A:ASN:H	15	0.11
(2,96)	1:44:C:SER:H	1:47:C:ASN:H	17	0.11
(2,95)	1:44:B:SER:H	1:47:B:ASN:H	17	0.11
(2,94)	1:44:A:SER:H	1:47:A:ASN:H	17	0.11
(2,60)	1:31:C:GLY:HA2	1:34:C:GLN:H	6	0.11
(2,60)	1:31:C:GLY:HA3	1:34:C:GLN:H	6	0.11
(2,59)	1:31:B:GLY:HA2	1:34:B:GLN:H	6	0.11
(2,59)	1:31:B:GLY:HA3	1:34:B:GLN:H	6	0.11
(2,58)	1:31:A:GLY:HA2	1:34:A:GLN:H	6	0.11
(2,58)	1:31:A:GLY:HA3	1:34:A:GLN:H	6	0.11
(2,42)	1:34:C:GLN:H	1:36:C:LEU:HG	10	0.11
(2,41)	1:34:B:GLN:H	1:36:B:LEU:HG	10	0.11
(2,40)	1:34:A:GLN:H	1:36:A:LEU:HG	10	0.11
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG21	1	0.11
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG22	1	0.11
(2,27)	1:23:C:LEU:H	1:14:A:VAL:HG23	1	0.11
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG21	1	0.11
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG22	1	0.11
(2,26)	1:23:B:LEU:H	1:14:C:VAL:HG23	1	0.11
(2,11)	1:9:A:ASP:H	1:17:B:ASP:H	2	0.11
(2,7)	1:9:B:ASP:H	1:17:C:ASP:H	8	0.11
(1,24)	1:51:C:ILE:HG12	1:48:C:TRP:HE1	13	0.11
(1,24)	1:51:C:ILE:HG13	1:48:C:TRP:HE1	13	0.11
(1,24)	1:51:C:ILE:HG12	1:48:C:TRP:HE1	14	0.11
(1,24)	1:51:C:ILE:HG13	1:48:C:TRP:HE1	14	0.11
(1,23)	1:51:B:ILE:HG12	1:48:B:TRP:HE1	13	0.11
(1,23)	1:51:B:ILE:HG13	1:48:B:TRP:HE1	13	0.11
(1,23)	1:51:B:ILE:HG12	1:48:B:TRP:HE1	14	0.11
(1,23)	1:51:B:ILE:HG13	1:48:B:TRP:HE1	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:51:A:ILE:HG12	1:48:A:TRP:HE1	13	0.11
(1,22)	1:51:A:ILE:HG13	1:48:A:TRP:HE1	13	0.11
(1,22)	1:51:A:ILE:HG12	1:48:A:TRP:HE1	14	0.11
(1,22)	1:51:A:ILE:HG13	1:48:A:TRP:HE1	14	0.11
(1,12)	1:26:C:PHE:H	1:29:C:SER:H	15	0.11
(2,811)	1:12:C:ALA:H	1:24:C:SER:H	5	0.1
(2,796)	1:8:C:ARG:H	1:10:C:GLY:H	11	0.1
(2,780)	1:8:C:ARG:H	1:10:C:GLY:H	11	0.1
(2,746)	1:54:C:TRP:H	1:56:C:TRP:H	6	0.1
(2,716)	1:54:C:TRP:H	1:56:C:TRP:H	6	0.1
(2,715)	1:56:C:TRP:H	1:59:C:LYS:H	13	0.1
(2,685)	1:29:C:SER:H	1:30:C:SER:H	10	0.1
(2,664)	1:14:C:VAL:H	1:15:C:ARG:H	3	0.1
(2,664)	1:14:C:VAL:H	1:15:C:ARG:H	4	0.1
(2,652)	1:29:C:SER:H	1:30:C:SER:H	10	0.1
(2,634)	1:14:C:VAL:H	1:15:C:ARG:H	3	0.1
(2,634)	1:14:C:VAL:H	1:15:C:ARG:H	4	0.1
(2,575)	1:12:B:ALA:H	1:24:B:SER:H	5	0.1
(2,560)	1:8:B:ARG:H	1:10:B:GLY:H	11	0.1
(2,544)	1:8:B:ARG:H	1:10:B:GLY:H	11	0.1
(2,510)	1:54:B:TRP:H	1:56:B:TRP:H	6	0.1
(2,480)	1:54:B:TRP:H	1:56:B:TRP:H	6	0.1
(2,479)	1:56:B:TRP:H	1:59:B:LYS:H	13	0.1
(2,449)	1:29:B:SER:H	1:30:B:SER:H	10	0.1
(2,428)	1:14:B:VAL:H	1:15:B:ARG:H	3	0.1
(2,416)	1:29:B:SER:H	1:30:B:SER:H	10	0.1
(2,398)	1:14:B:VAL:H	1:15:B:ARG:H	3	0.1
(2,339)	1:12:A:ALA:H	1:24:A:SER:H	5	0.1
(2,326)	1:14:A:VAL:H	1:16:A:LYS:H	5	0.1
(2,325)	1:8:A:ARG:H	1:10:A:GLY:H	10	0.1
(2,325)	1:8:A:ARG:H	1:10:A:GLY:H	11	0.1
(2,324)	1:19:A:GLU:H	1:21:A:VAL:H	18	0.1
(2,311)	1:14:A:VAL:H	1:16:A:LYS:H	5	0.1
(2,310)	1:8:A:ARG:H	1:10:A:GLY:H	10	0.1
(2,310)	1:8:A:ARG:H	1:10:A:GLY:H	11	0.1
(2,309)	1:19:A:GLU:H	1:21:A:VAL:H	18	0.1
(2,303)	1:30:A:SER:HA	1:33:A:GLU:H	14	0.1
(2,255)	1:30:A:SER:HA	1:33:A:GLU:H	14	0.1
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	4	0.1
(2,245)	1:56:A:TRP:H	1:59:A:LYS:H	13	0.1
(2,215)	1:29:A:SER:H	1:30:A:SER:H	10	0.1
(2,194)	1:14:A:VAL:H	1:15:A:ARG:H	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,194)	1:14:A:VAL:H	1:15:A:ARG:H	4	0.1
(2,182)	1:29:A:SER:H	1:30:A:SER:H	10	0.1
(2,164)	1:14:A:VAL:H	1:15:A:ARG:H	3	0.1
(2,164)	1:14:A:VAL:H	1:15:A:ARG:H	4	0.1
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB2	17	0.1
(2,132)	1:48:C:TRP:HE1	1:45:C:LEU:HB3	17	0.1
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	10	0.1
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	10	0.1
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB2	17	0.1
(2,131)	1:48:B:TRP:HE1	1:45:B:LEU:HB3	17	0.1
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB2	17	0.1
(2,130)	1:48:A:TRP:HE1	1:45:A:LEU:HB3	17	0.1
(2,110)	1:20:B:TRP:HE1	1:5:B:GLU:H	15	0.1
(2,109)	1:20:A:TRP:HE1	1:5:A:GLU:H	15	0.1
(2,69)	1:51:C:ILE:HG21	1:48:C:TRP:HE1	12	0.1
(2,69)	1:51:C:ILE:HG22	1:48:C:TRP:HE1	12	0.1
(2,69)	1:51:C:ILE:HG23	1:48:C:TRP:HE1	12	0.1
(2,68)	1:51:B:ILE:HG21	1:48:B:TRP:HE1	12	0.1
(2,68)	1:51:B:ILE:HG22	1:48:B:TRP:HE1	12	0.1
(2,68)	1:51:B:ILE:HG23	1:48:B:TRP:HE1	12	0.1
(2,67)	1:51:A:ILE:HG21	1:48:A:TRP:HE1	12	0.1
(2,67)	1:51:A:ILE:HG22	1:48:A:TRP:HE1	12	0.1
(2,67)	1:51:A:ILE:HG23	1:48:A:TRP:HE1	12	0.1
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG21	1	0.1
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG22	1	0.1
(2,25)	1:23:A:LEU:H	1:14:B:VAL:HG23	1	0.1
(1,12)	1:26:C:PHE:H	1:29:C:SER:H	6	0.1
(1,11)	1:26:B:PHE:H	1:29:B:SER:H	6	0.1
(1,10)	1:26:A:PHE:H	1:29:A:SER:H	6	0.1

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

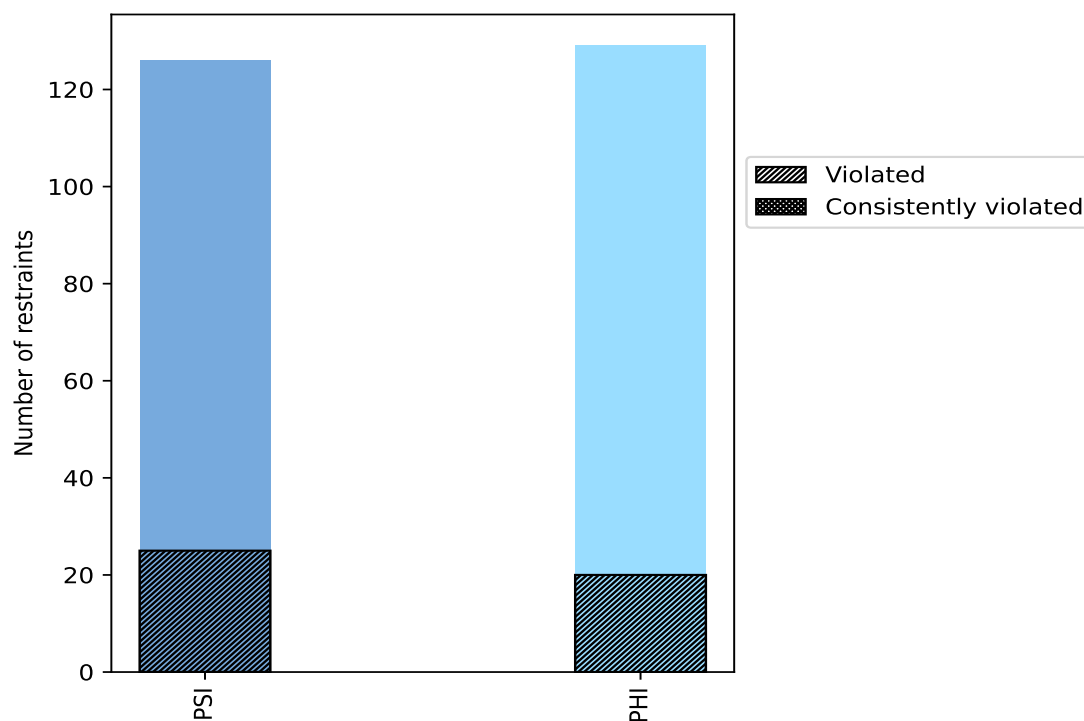
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	126	49.4	25	19.8	9.8	0	0.0	0.0
PHI	129	50.6	20	15.5	7.8	0	0.0	0.0
Total	255	100.0	45	17.6	17.6	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 [i](#)



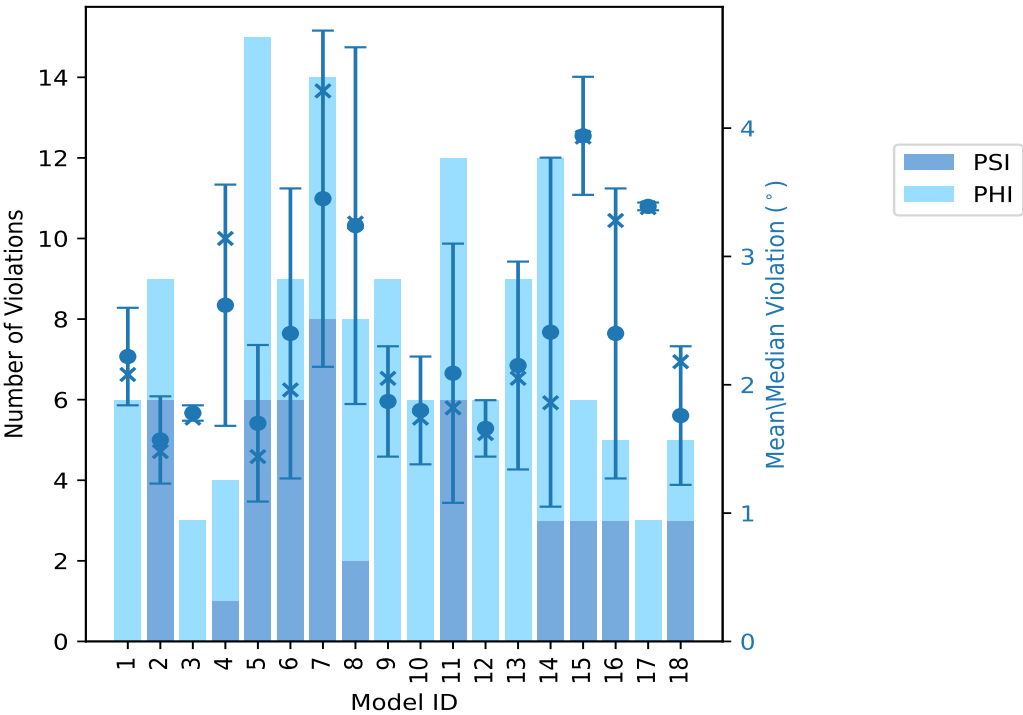
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	0	6	6	2.22	3.06	0.38	2.08
2	6	3	9	1.57	2.1	0.34	1.48
3	0	3	3	1.78	1.86	0.06	1.74
4	1	3	4	2.62	3.22	0.94	3.14
5	6	9	15	1.7	2.76	0.61	1.44
6	6	3	9	2.4	3.95	1.13	1.96
7	8	6	14	3.45	4.63	1.31	4.29
8	2	6	8	3.24	4.76	1.39	3.26
9	0	9	9	1.87	2.32	0.43	2.05
10	0	6	6	1.8	2.69	0.42	1.74
11	6	6	12	2.09	3.85	1.01	1.82
12	0	6	6	1.66	1.93	0.22	1.62
13	0	9	9	2.15	3.27	0.81	2.05
14	3	9	12	2.41	4.74	1.36	1.86
15	3	3	6	3.94	4.54	0.46	3.93
16	3	2	5	2.4	3.36	1.13	3.28
17	0	3	3	3.39	3.43	0.03	3.38
18	3	2	5	1.76	2.21	0.54	2.18

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	
PSI	PHI	Total	Count ¹	%
11	6	17	1	5.6
7	2	9	2	11.1
6	0	6	3	16.7
1	0	1	4	22.2
0	0	0	5	27.8
0	3	3	6	33.3
0	6	6	7	38.9
0	3	3	8	44.4
0	0	0	9	50.0
0	0	0	10	55.6
0	0	0	11	61.1

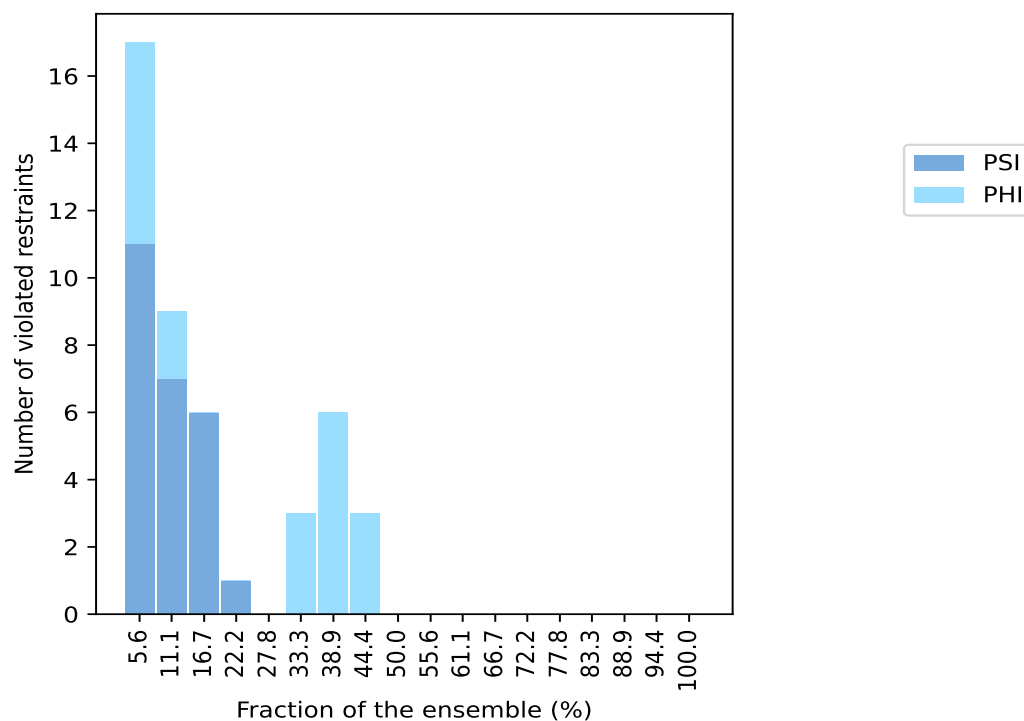
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	66.7
0	0	0	13	72.2
0	0	0	14	77.8
0	0	0	15	83.3
0	0	0	16	88.9
0	0	0	17	94.4
0	0	0	18	100.0

¹ Number of models with violations

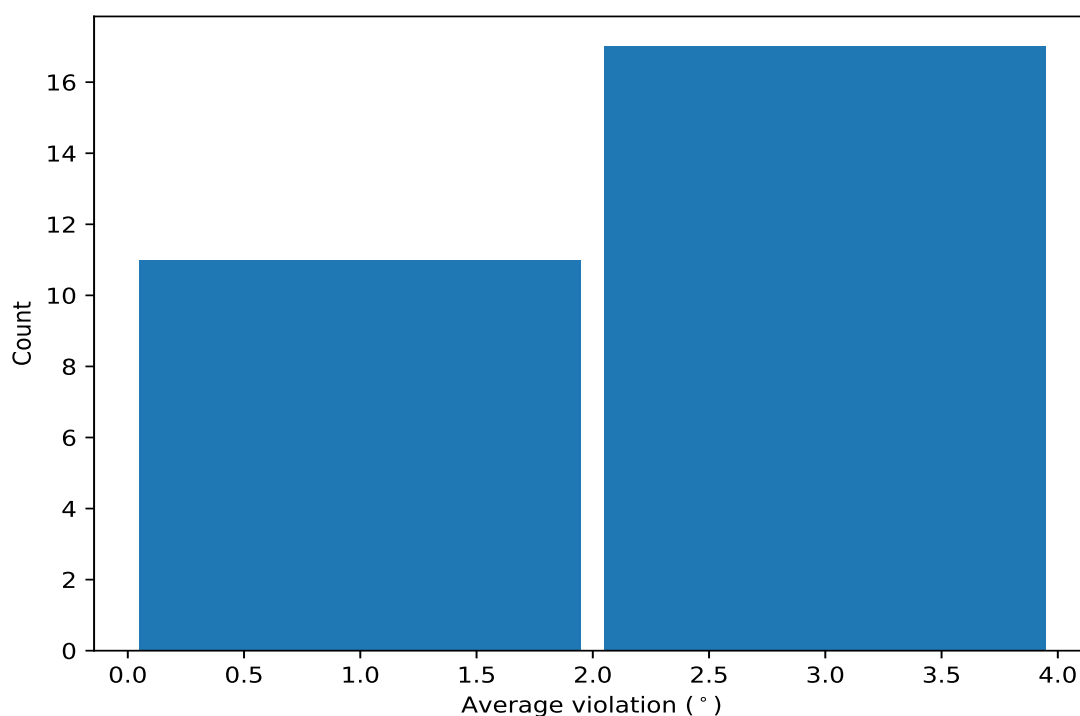
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,34)	1:51:A:ILE:C	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	8	3.15	0.95	3.23
(1,119)	1:51:B:ILE:C	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	8	3.14	1.02	3.22
(1,204)	1:51:C:ILE:C	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	8	3.11	0.95	3.16
(1,16)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	7	2.87	1.46	2.12
(1,101)	1:25:B:THR:C	1:26:B:PHE:N	1:26:B:PHE:CA	1:26:B:PHE:C	7	2.86	1.42	2.1
(1,186)	1:25:C:THR:C	1:26:C:PHE:N	1:26:C:PHE:CA	1:26:C:PHE:C	7	2.82	1.42	2.05
(1,210)	1:57:C:TYR:C	1:58:C:ILE:N	1:58:C:ILE:CA	1:58:C:ILE:C	7	2.49	0.78	2.56
(1,125)	1:57:B:TYR:C	1:58:B:ILE:N	1:58:B:ILE:CA	1:58:B:ILE:C	7	2.32	0.85	1.97
(1,40)	1:57:A:TYR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	7	2.2	0.89	2.05
(1,176)	1:14:C:VAL:C	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	6	1.79	0.47	1.78
(1,6)	1:14:A:VAL:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	6	1.77	0.45	1.74
(1,91)	1:14:B:VAL:C	1:15:B:ARG:N	1:15:B:ARG:CA	1:15:B:ARG:C	6	1.77	0.46	1.74
(1,242)	1:50:C:ASN:N	1:50:C:ASN:CA	1:50:C:ASN:C	1:51:C:ILE:N	4	2.82	1.37	2.74
(1,72)	1:50:A:ASN:N	1:50:A:ASN:CA	1:50:A:ASN:C	1:51:A:ILE:N	3	3.32	1.03	3.55
(1,157)	1:50:B:ASN:N	1:50:B:ASN:CA	1:50:B:ASN:C	1:51:B:ILE:N	3	3.29	0.96	3.32
(1,249)	1:57:C:TYR:N	1:57:C:TYR:CA	1:57:C:TYR:C	1:58:C:ILE:N	3	1.74	0.29	1.73
(1,79)	1:57:A:TYR:N	1:57:A:TYR:CA	1:57:A:TYR:C	1:58:A:ILE:N	3	1.5	0.39	1.54
(1,164)	1:57:B:TYR:N	1:57:B:TYR:CA	1:57:B:TYR:C	1:58:B:ILE:N	3	1.43	0.41	1.2
(1,76)	1:54:A:TRP:N	1:54:A:TRP:CA	1:54:A:TRP:C	1:55:A:LEU:N	3	1.23	0.19	1.2
(1,215)	1:14:C:VAL:N	1:14:C:VAL:CA	1:14:C:VAL:C	1:15:C:ARG:N	2	2.78	0.58	2.78
(1,130)	1:14:B:VAL:N	1:14:B:VAL:CA	1:14:B:VAL:C	1:15:B:ARG:N	2	2.78	0.56	2.78

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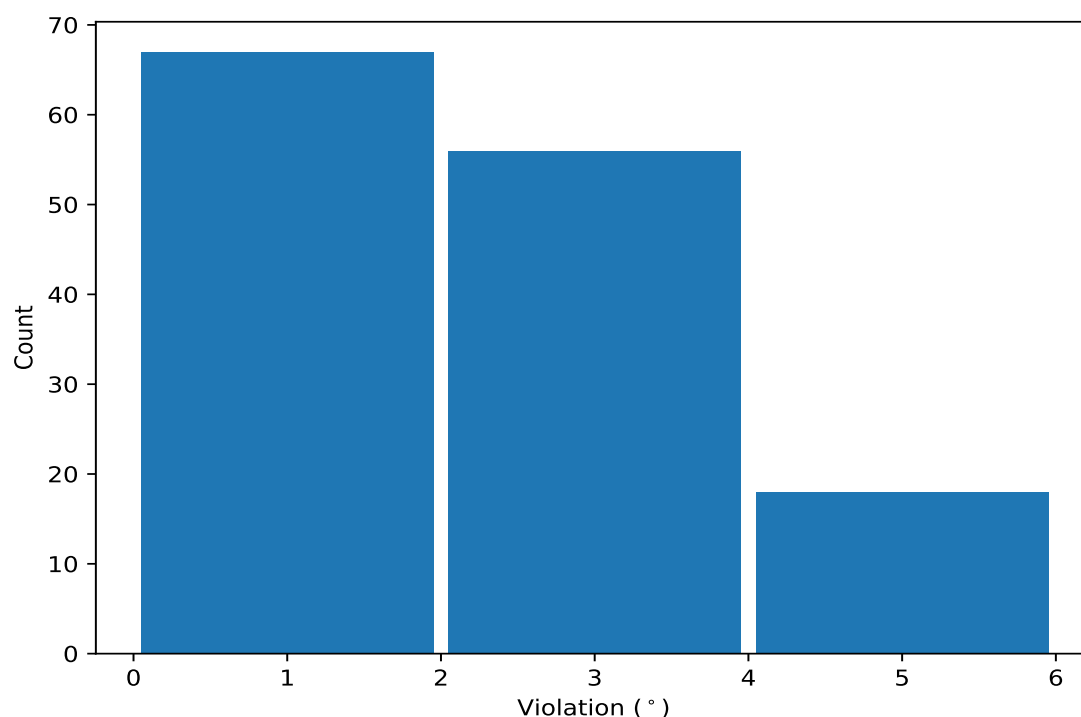
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,45)	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	1:15:A:ARG:N	2	2.73	0.55	2.73
(1,37)	1:54:A:TRP:C	1:55:A:LEU:N	1:55:A:LEU:CA	1:55:A:LEU:C	2	2.48	1.46	2.48
(1,207)	1:54:C:TRP:C	1:55:C:LEU:N	1:55:C:LEU:CA	1:55:C:LEU:C	2	2.48	1.46	2.48
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:ASN:N	2	1.67	0.49	1.67
(1,159)	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	1:53:B:ASN:N	2	1.67	0.64	1.67
(1,244)	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	1:53:C:ASN:N	2	1.56	0.42	1.56
(1,161)	1:54:B:TRP:N	1:54:B:TRP:CA	1:54:B:TRP:C	1:55:B:LEU:N	2	1.31	0.2	1.31

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,16)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	8	4.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,119)	1:51:B:ILE:C	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	14	4.74
(1,204)	1:51:C:ILE:C	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	14	4.67
(1,101)	1:25:B:THR:C	1:26:B:PHE:N	1:26:B:PHE:CA	1:26:B:PHE:C	8	4.65
(1,242)	1:50:C:ASN:N	1:50:C:ASN:CA	1:50:C:ASN:C	1:51:C:ILE:N	7	4.63
(1,186)	1:25:C:THR:C	1:26:C:PHE:N	1:26:C:PHE:CA	1:26:C:PHE:C	8	4.63
(1,34)	1:51:A:ILE:C	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	14	4.55
(1,101)	1:25:B:THR:C	1:26:B:PHE:N	1:26:B:PHE:CA	1:26:B:PHE:C	15	4.54
(1,157)	1:50:B:ASN:N	1:50:B:ASN:CA	1:50:B:ASN:C	1:51:B:ILE:N	7	4.46
(1,119)	1:51:B:ILE:C	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	7	4.45
(1,16)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	7	4.45
(1,72)	1:50:A:ASN:N	1:50:A:ASN:CA	1:50:A:ASN:C	1:51:A:ILE:N	7	4.44
(1,186)	1:25:C:THR:C	1:26:C:PHE:N	1:26:C:PHE:CA	1:26:C:PHE:C	7	4.38
(1,34)	1:51:A:ILE:C	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	7	4.37
(1,16)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	15	4.35
(1,186)	1:25:C:THR:C	1:26:C:PHE:N	1:26:C:PHE:CA	1:26:C:PHE:C	15	4.26
(1,204)	1:51:C:ILE:C	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	7	4.21
(1,101)	1:25:B:THR:C	1:26:B:PHE:N	1:26:B:PHE:CA	1:26:B:PHE:C	7	4.2
(1,122)	1:54:B:TRP:C	1:55:B:LEU:N	1:55:B:LEU:CA	1:55:B:LEU:C	6	3.95
(1,207)	1:54:C:TRP:C	1:55:C:LEU:N	1:55:C:LEU:CA	1:55:C:LEU:C	6	3.94
(1,37)	1:54:A:TRP:C	1:55:A:LEU:N	1:55:A:LEU:CA	1:55:A:LEU:C	6	3.94
(1,210)	1:57:C:TYR:C	1:58:C:ILE:N	1:58:C:ILE:CA	1:58:C:ILE:C	11	3.85
(1,40)	1:57:A:TYR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	11	3.8
(1,242)	1:50:C:ASN:N	1:50:C:ASN:CA	1:50:C:ASN:C	1:51:C:ILE:N	15	3.6
(1,72)	1:50:A:ASN:N	1:50:A:ASN:CA	1:50:A:ASN:C	1:51:A:ILE:N	15	3.55
(1,125)	1:57:B:TYR:C	1:58:B:ILE:N	1:58:B:ILE:CA	1:58:B:ILE:C	11	3.51
(1,34)	1:51:A:ILE:C	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	17	3.43
(1,119)	1:51:B:ILE:C	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	17	3.38
(1,204)	1:51:C:ILE:C	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	17	3.37
(1,215)	1:14:C:VAL:N	1:14:C:VAL:CA	1:14:C:VAL:C	1:15:C:ARG:N	16	3.36
(1,130)	1:14:B:VAL:N	1:14:B:VAL:CA	1:14:B:VAL:C	1:15:B:ARG:N	16	3.34
(1,157)	1:50:B:ASN:N	1:50:B:ASN:CA	1:50:B:ASN:C	1:51:B:ILE:N	15	3.32
(1,34)	1:51:A:ILE:C	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	8	3.31
(1,45)	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	1:15:A:ARG:N	16	3.28
(1,119)	1:51:B:ILE:C	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	13	3.27
(1,40)	1:57:A:TYR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	4	3.22
(1,204)	1:51:C:ILE:C	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	8	3.2
(1,125)	1:57:B:TYR:C	1:58:B:ILE:N	1:58:B:ILE:CA	1:58:B:ILE:C	4	3.2
(1,119)	1:51:B:ILE:C	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	8	3.17
(1,34)	1:51:A:ILE:C	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	13	3.15
(1,204)	1:51:C:ILE:C	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	13	3.12
(1,210)	1:57:C:TYR:C	1:58:C:ILE:N	1:58:C:ILE:CA	1:58:C:ILE:C	4	3.08
(1,125)	1:57:B:TYR:C	1:58:B:ILE:N	1:58:B:ILE:CA	1:58:B:ILE:C	1	3.06
(1,34)	1:51:A:ILE:C	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	5	2.76
(1,210)	1:57:C:TYR:C	1:58:C:ILE:N	1:58:C:ILE:CA	1:58:C:ILE:C	10	2.69
(1,204)	1:51:C:ILE:C	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	5	2.64
(1,210)	1:57:C:TYR:C	1:58:C:ILE:N	1:58:C:ILE:CA	1:58:C:ILE:C	5	2.56
(1,119)	1:51:B:ILE:C	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	5	2.52
(1,91)	1:14:B:VAL:C	1:15:B:ARG:N	1:15:B:ARG:CA	1:15:B:ARG:C	14	2.34
(1,176)	1:14:C:VAL:C	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	9	2.32
(1,176)	1:14:C:VAL:C	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	14	2.31
(1,159)	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	1:53:B:ASN:N	7	2.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,6)	1:14:A:VAL:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	9	2.3
(1,91)	1:14:B:VAL:C	1:15:B:ARG:N	1:15:B:ARG:CA	1:15:B:ARG:C	9	2.27
(1,6)	1:14:A:VAL:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	14	2.27
(1,130)	1:14:B:VAL:N	1:14:B:VAL:CA	1:14:B:VAL:C	1:15:B:ARG:N	18	2.21
(1,215)	1:14:C:VAL:N	1:14:C:VAL:CA	1:14:C:VAL:C	1:15:C:ARG:N	18	2.2
(1,45)	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	1:15:A:ARG:N	18	2.18
(1,70)	1:48:A:TRP:N	1:48:A:TRP:CA	1:48:A:TRP:C	1:49:A:PHE:N	11	2.17
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:ASN:N	7	2.16
(1,240)	1:48:C:TRP:N	1:48:C:TRP:CA	1:48:C:TRP:C	1:49:C:PHE:N	11	2.13
(1,16)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	1	2.12
(1,249)	1:57:C:TYR:N	1:57:C:TYR:CA	1:57:C:TYR:C	1:58:C:ILE:N	2	2.1
(1,157)	1:50:B:ASN:N	1:50:B:ASN:CA	1:50:B:ASN:C	1:51:B:ILE:N	6	2.1
(1,101)	1:25:B:THR:C	1:26:B:PHE:N	1:26:B:PHE:CA	1:26:B:PHE:C	1	2.1
(1,176)	1:14:C:VAL:C	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	13	2.09
(1,155)	1:48:B:TRP:N	1:48:B:TRP:CA	1:48:B:TRP:C	1:49:B:PHE:N	11	2.09
(1,210)	1:57:C:TYR:C	1:58:C:ILE:N	1:58:C:ILE:CA	1:58:C:ILE:C	9	2.05
(1,186)	1:25:C:THR:C	1:26:C:PHE:N	1:26:C:PHE:CA	1:26:C:PHE:C	1	2.05
(1,40)	1:57:A:TYR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1	2.05
(1,40)	1:57:A:TYR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	9	2.05
(1,6)	1:14:A:VAL:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	13	2.05
(1,91)	1:14:B:VAL:C	1:15:B:ARG:N	1:15:B:ARG:CA	1:15:B:ARG:C	13	2.02
(1,164)	1:57:B:TYR:N	1:57:B:TYR:CA	1:57:B:TYR:C	1:58:B:ILE:N	2	2.01
(1,244)	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	1:53:C:ASN:N	7	1.98
(1,125)	1:57:B:TYR:C	1:58:B:ILE:N	1:58:B:ILE:CA	1:58:B:ILE:C	9	1.97
(1,79)	1:57:A:TYR:N	1:57:A:TYR:CA	1:57:A:TYR:C	1:58:A:ILE:N	2	1.96
(1,72)	1:50:A:ASN:N	1:50:A:ASN:CA	1:50:A:ASN:C	1:51:A:ILE:N	6	1.96
(1,210)	1:57:C:TYR:C	1:58:C:ILE:N	1:58:C:ILE:CA	1:58:C:ILE:C	1	1.95
(1,204)	1:51:C:ILE:C	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	12	1.93
(1,34)	1:51:A:ILE:C	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	12	1.92
(1,242)	1:50:C:ASN:N	1:50:C:ASN:CA	1:50:C:ASN:C	1:51:C:ILE:N	6	1.89
(1,119)	1:51:B:ILE:C	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	3	1.86
(1,125)	1:57:B:TYR:C	1:58:B:ILE:N	1:58:B:ILE:CA	1:58:B:ILE:C	5	1.84
(1,16)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	10	1.79
(1,119)	1:51:B:ILE:C	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	12	1.76
(1,186)	1:25:C:THR:C	1:26:C:PHE:N	1:26:C:PHE:CA	1:26:C:PHE:C	10	1.75
(1,204)	1:51:C:ILE:C	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	3	1.74
(1,34)	1:51:A:ILE:C	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	3	1.74
(1,249)	1:57:C:TYR:N	1:57:C:TYR:CA	1:57:C:TYR:C	1:58:C:ILE:N	5	1.73
(1,40)	1:57:A:TYR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	5	1.73
(1,101)	1:25:B:THR:C	1:26:B:PHE:N	1:26:B:PHE:CA	1:26:B:PHE:C	10	1.72
(1,79)	1:57:A:TYR:N	1:57:A:TYR:CA	1:57:A:TYR:C	1:58:A:ILE:N	11	1.54
(1,161)	1:54:B:TRP:N	1:54:B:TRP:CA	1:54:B:TRP:C	1:55:B:LEU:N	2	1.51
(1,76)	1:54:A:TRP:N	1:54:A:TRP:CA	1:54:A:TRP:C	1:55:A:LEU:N	2	1.48
(1,176)	1:14:C:VAL:C	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	12	1.47
(1,246)	1:54:C:TRP:N	1:54:C:TRP:CA	1:54:C:TRP:C	1:55:C:LEU:N	2	1.45
(1,125)	1:57:B:TYR:C	1:58:B:ILE:N	1:58:B:ILE:CA	1:58:B:ILE:C	10	1.45
(1,91)	1:14:B:VAL:C	1:15:B:ARG:N	1:15:B:ARG:CA	1:15:B:ARG:C	12	1.45
(1,186)	1:25:C:THR:C	1:26:C:PHE:N	1:26:C:PHE:CA	1:26:C:PHE:C	14	1.44
(1,6)	1:14:A:VAL:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	5	1.44
(1,6)	1:14:A:VAL:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	12	1.43
(1,101)	1:25:B:THR:C	1:26:B:PHE:N	1:26:B:PHE:CA	1:26:B:PHE:C	9	1.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,91)	1:14:B:VAL:C	1:15:B:ARG:N	1:15:B:ARG:CA	1:15:B:ARG:C	5	1.41
(1,249)	1:57:C:TYR:N	1:57:C:TYR:CA	1:57:C:TYR:C	1:58:C:ILE:N	11	1.4
(1,40)	1:57:A:TYR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	10	1.4
(1,176)	1:14:C:VAL:C	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	5	1.39
(1,60)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:GLU:N	6	1.37
(1,16)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	14	1.37
(1,101)	1:25:B:THR:C	1:26:B:PHE:N	1:26:B:PHE:CA	1:26:B:PHE:C	14	1.36
(1,142)	1:33:B:GLU:N	1:33:B:GLU:CA	1:33:B:GLU:C	1:34:B:GLN:N	14	1.3
(1,57)	1:33:A:GLU:N	1:33:A:GLU:CA	1:33:A:GLU:C	1:34:A:GLN:N	14	1.29
(1,230)	1:37:C:LEU:N	1:37:C:LEU:CA	1:37:C:LEU:C	1:38:C:GLU:N	6	1.27
(1,227)	1:33:C:GLU:N	1:33:C:GLU:CA	1:33:C:GLU:C	1:34:C:GLN:N	14	1.26
(1,210)	1:57:C:TYR:C	1:58:C:ILE:N	1:58:C:ILE:CA	1:58:C:ILE:C	2	1.26
(1,16)	1:25:A:THR:C	1:26:A:PHE:N	1:26:A:PHE:CA	1:26:A:PHE:C	9	1.24
(1,184)	1:23:C:LEU:C	1:24:C:SER:N	1:24:C:SER:CA	1:24:C:SER:C	13	1.22
(1,145)	1:37:B:LEU:N	1:37:B:LEU:CA	1:37:B:LEU:C	1:38:B:GLU:N	6	1.22
(1,99)	1:23:B:LEU:C	1:24:B:SER:N	1:24:B:SER:CA	1:24:B:SER:C	13	1.22
(1,186)	1:25:C:THR:C	1:26:C:PHE:N	1:26:C:PHE:CA	1:26:C:PHE:C	9	1.21
(1,125)	1:57:B:TYR:C	1:58:B:ILE:N	1:58:B:ILE:CA	1:58:B:ILE:C	2	1.21
(1,14)	1:23:A:LEU:C	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	13	1.21
(1,164)	1:57:B:TYR:N	1:57:B:TYR:CA	1:57:B:TYR:C	1:58:B:ILE:N	11	1.2
(1,76)	1:54:A:TRP:N	1:54:A:TRP:CA	1:54:A:TRP:C	1:55:A:LEU:N	7	1.2
(1,74)	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	1:53:A:ASN:N	5	1.18
(1,40)	1:57:A:TYR:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	2	1.17
(1,176)	1:14:C:VAL:C	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	11	1.16
(1,242)	1:50:C:ASN:N	1:50:C:ASN:CA	1:50:C:ASN:C	1:51:C:ILE:N	8	1.15
(1,6)	1:14:A:VAL:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	11	1.15
(1,244)	1:52:C:THR:N	1:52:C:THR:CA	1:52:C:THR:C	1:53:C:ASN:N	5	1.14
(1,91)	1:14:B:VAL:C	1:15:B:ARG:N	1:15:B:ARG:CA	1:15:B:ARG:C	11	1.13
(1,30)	1:47:A:ASN:C	1:48:A:TRP:N	1:48:A:TRP:CA	1:48:A:TRP:C	18	1.11
(1,161)	1:54:B:TRP:N	1:54:B:TRP:CA	1:54:B:TRP:C	1:55:B:LEU:N	7	1.1
(1,164)	1:57:B:TYR:N	1:57:B:TYR:CA	1:57:B:TYR:C	1:58:B:ILE:N	5	1.08
(1,115)	1:47:B:ASN:C	1:48:B:TRP:N	1:48:B:TRP:CA	1:48:B:TRP:C	18	1.08
(1,159)	1:52:B:THR:N	1:52:B:THR:CA	1:52:B:THR:C	1:53:B:ASN:N	5	1.03
(1,76)	1:54:A:TRP:N	1:54:A:TRP:CA	1:54:A:TRP:C	1:55:A:LEU:N	8	1.02
(1,37)	1:54:A:TRP:C	1:55:A:LEU:N	1:55:A:LEU:CA	1:55:A:LEU:C	16	1.02
(1,207)	1:54:C:TRP:C	1:55:C:LEU:N	1:55:C:LEU:CA	1:55:C:LEU:C	16	1.01
(1,80)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:LYS:N	4	1.0
(1,79)	1:57:A:TYR:N	1:57:A:TYR:CA	1:57:A:TYR:C	1:58:A:ILE:N	5	1.0