



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 09:58 PM UTC

PDB ID : 2KFP / pdb_00002kfp
BMRB ID : 16186
Title : Solution NMR structure of PSPTO_3016 from *Pseudomonas syringae*. Northeast Structural Genomics Consortium target PsR293.
Authors : Feldmann, E.A.; Ramelot, T.A.; Zhao, L.; Hamilton, K.; Ciccocanti, C.; Xiao, R.; Nair, R.; Everett, J.K.; Swapna, G.; Acton, T.B.; Rost, B.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2009-02-24

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

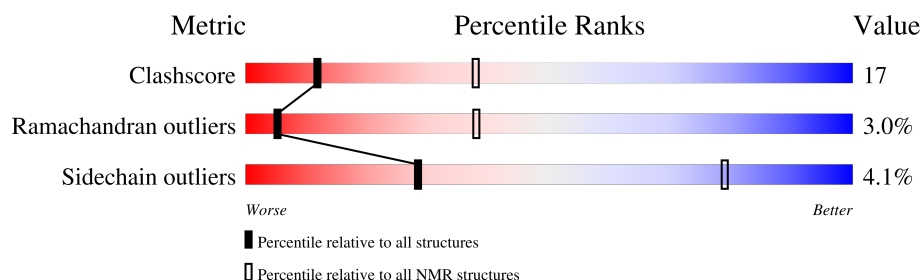
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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	125	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:117 (117)	1.01	1

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2071 atoms, of which 1022 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PSPTO_3016 protein.

Mol	Chain	Residues	Atoms						Trace
1	A	125	Total	C	H	N	O	S	0
			2071	674	1022	187	185	3	

There are 8 discrepancies between the modelled and reference sequences:

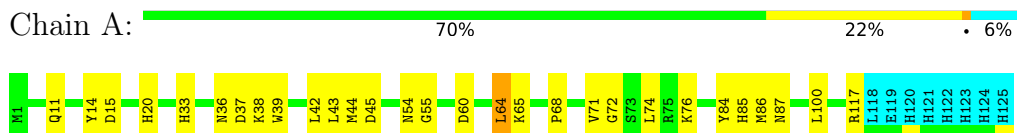
Chain	Residue	Modelled	Actual	Comment	Reference
A	118	LEU	-	expression tag	UNP Q880Y4
A	119	GLU	-	expression tag	UNP Q880Y4
A	120	HIS	-	expression tag	UNP Q880Y4
A	121	HIS	-	expression tag	UNP Q880Y4
A	122	HIS	-	expression tag	UNP Q880Y4
A	123	HIS	-	expression tag	UNP Q880Y4
A	124	HIS	-	expression tag	UNP Q880Y4
A	125	HIS	-	expression tag	UNP Q880Y4

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: PSPTO_3016 protein

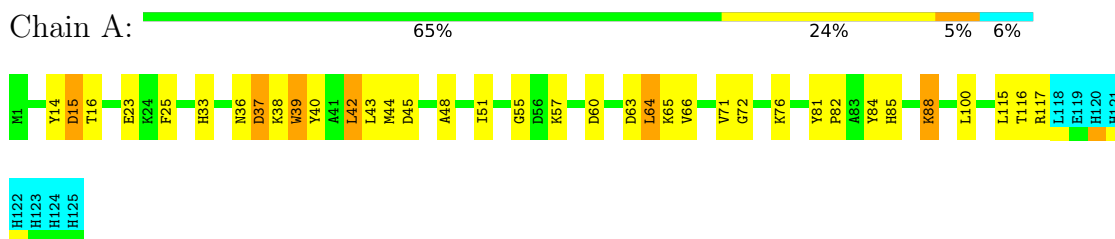


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

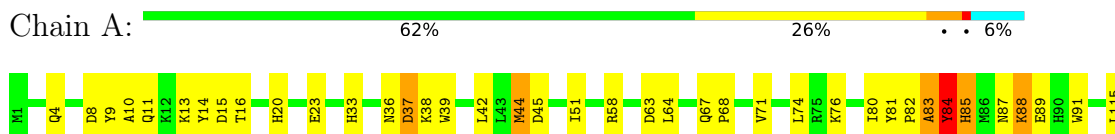
4.2.1 Score per residue for model 1 (medoid)

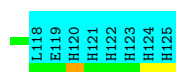
- Molecule 1: PSPTO_3016 protein



4.2.2 Score per residue for model 2

- Molecule 1: PSPTO_3016 protein





4.2.3 Score per residue for model 3

- Molecule 1: PSPTO_3016 protein

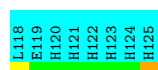
Chain A: 59% 30% 5% 6%



4.2.4 Score per residue for model 4

- Molecule 1: PSPTO_3016 protein

Chain A: 62% 26% 6% 6%



4.2.5 Score per residue for model 5

- Molecule 1: PSPTO_3016 protein

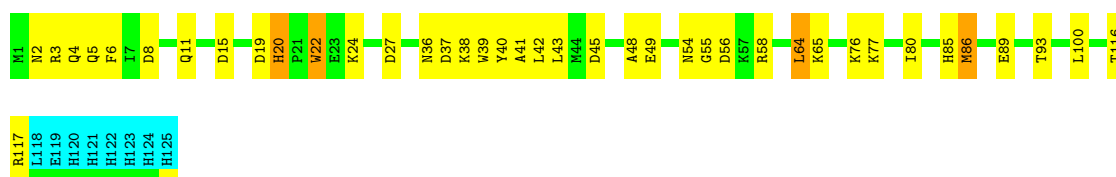
Chain A: 67% 24% 6%



4.2.6 Score per residue for model 6

- Molecule 1: PSPTO_3016 protein

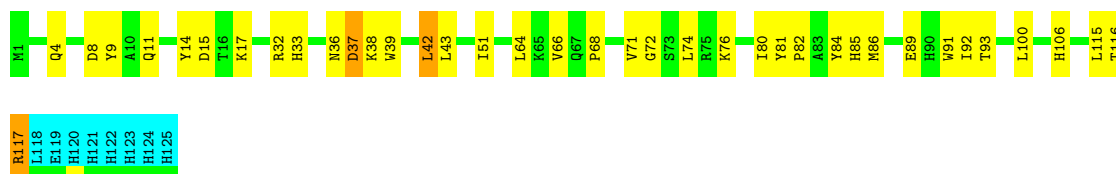
Chain A: 62% 29% 6%



4.2.7 Score per residue for model 7

- Molecule 1: PSPTO_3016 protein

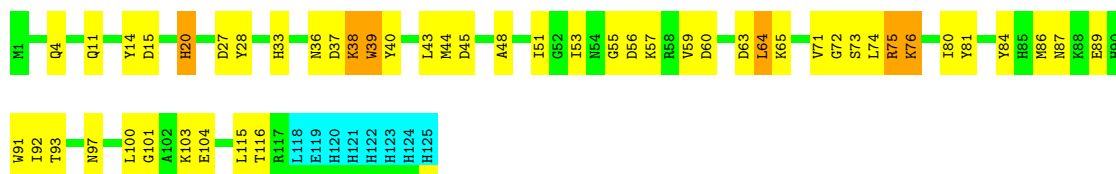
Chain A: 63% 28% 6%



4.2.8 Score per residue for model 8

- Molecule 1: PSPTO_3016 protein

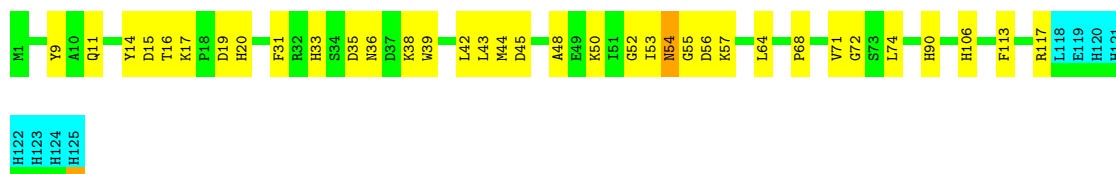
Chain A: 54% 34% 5% 6%



4.2.9 Score per residue for model 9

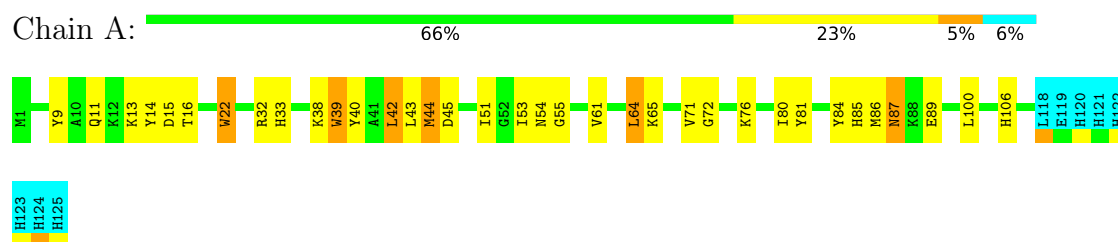
- Molecule 1: PSPTO_3016 protein

Chain A: 66% 27% 6%



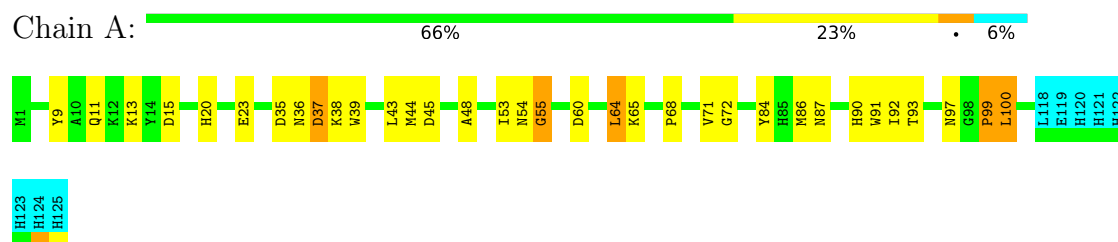
4.2.10 Score per residue for model 10

- Molecule 1: PSPTO_3016 protein



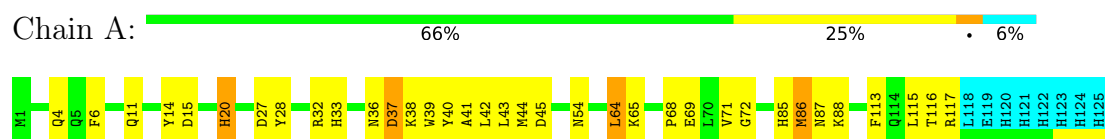
4.2.11 Score per residue for model 11

- Molecule 1: PSPTO_3016 protein



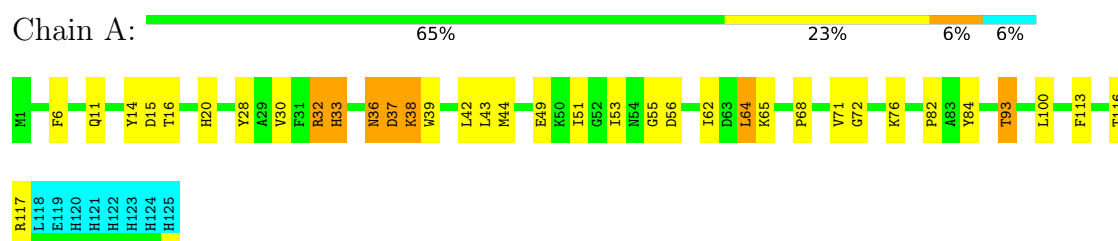
4.2.12 Score per residue for model 12

- Molecule 1: PSPTO_3016 protein



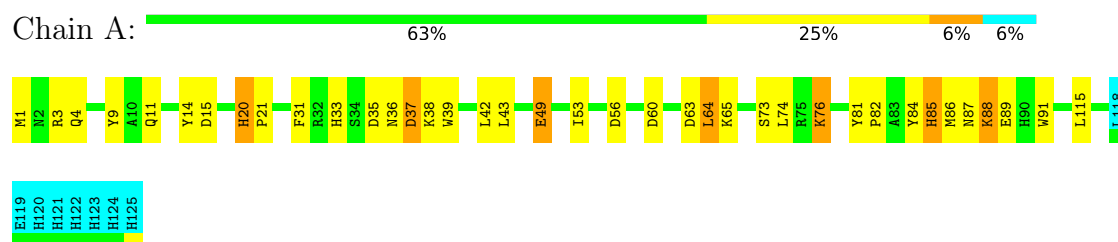
4.2.13 Score per residue for model 13

- Molecule 1: PSPTO_3016 protein



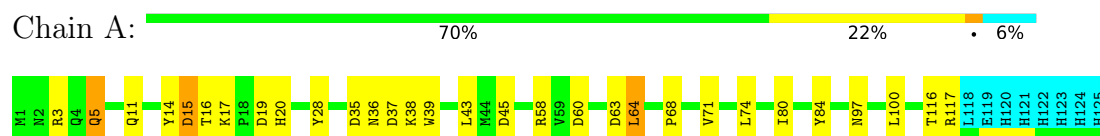
4.2.14 Score per residue for model 14

- Molecule 1: PSPTO_3016 protein



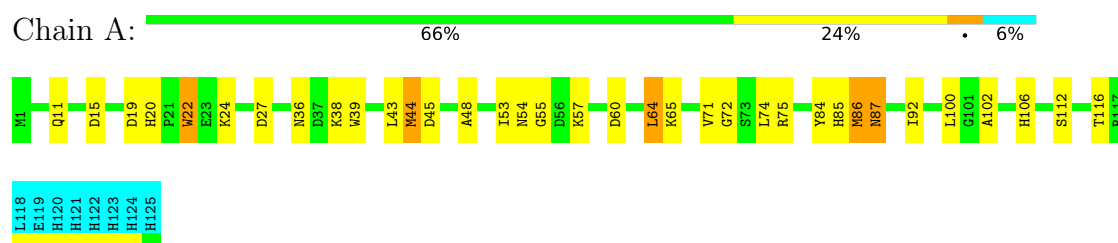
4.2.15 Score per residue for model 15

- Molecule 1: PSPTO_3016 protein



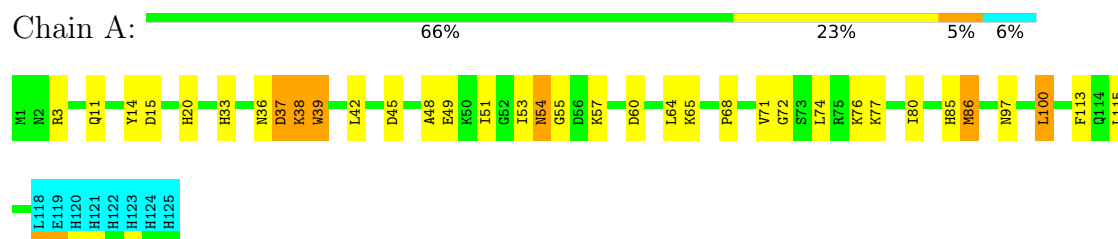
4.2.16 Score per residue for model 16

- Molecule 1: PSPTO_3016 protein



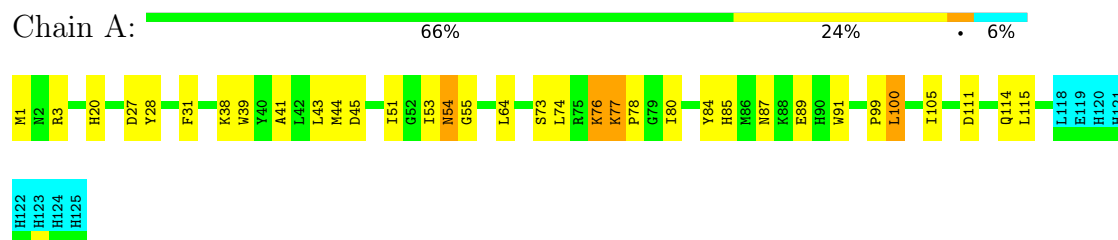
4.2.17 Score per residue for model 17

- Molecule 1: PSPTO_3016 protein



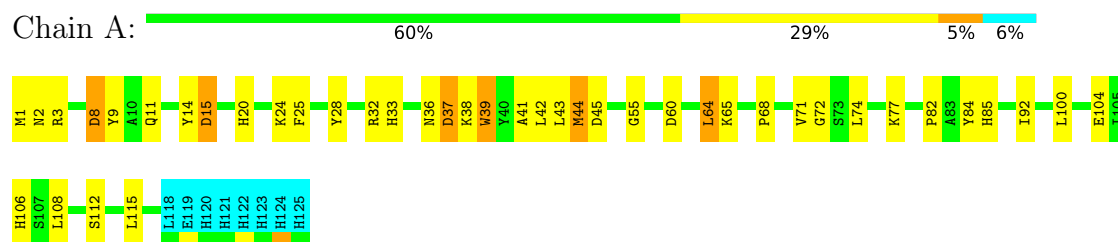
4.2.18 Score per residue for model 18

- Molecule 1: PSPTO_3016 protein



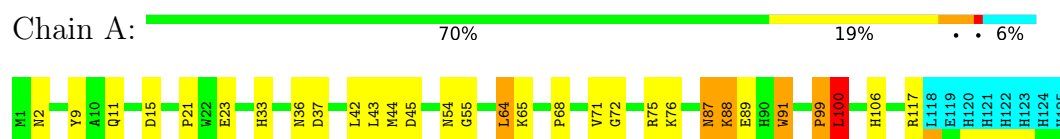
4.2.19 Score per residue for model 19

- Molecule 1: PSPTO_3016 protein



4.2.20 Score per residue for model 20

- Molecule 1: PSPTO_3016 protein



5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.20
PSVS	structure solution	1.3
PSVS	refinement	1.3

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1569
Number of shifts mapped to atoms	1569
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

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	1.43±0.02	0±0/1000 (0.0± 0.0%)	1.23±0.01	0±0/1355 (0.0± 0.0%)
All	All	1.43	2/20000 (0.0%)	1.23	3/27100 (0.0%)

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

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

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	101	GLY	N-CA	5.24	1.50	1.44	8	2

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	25	PHE	CA-CB-CG	-5.19	108.61	113.80	4	1
1	A	38	LYS	N-CA-C	-5.18	108.72	114.62	13	1
1	A	31	PHE	CA-CB-CG	-5.03	108.77	113.80	14	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	58	ARG	Sidechain	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	971	963	963	34±6
All	All	19420	19260	19260	676

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LEU:H	1:A:74:LEU:HD23	0.80	1.35	8	7
1:A:91:TRP:C	1:A:92:ILE:HD12	0.80	2.02	7	1
1:A:75:ARG:CZ	1:A:92:ILE:HG21	0.73	2.12	8	1
1:A:48:ALA:HB3	1:A:55:GLY:O	0.71	1.84	11	6
1:A:80:ILE:N	1:A:80:ILE:HD12	0.70	2.00	7	6
1:A:91:TRP:O	1:A:92:ILE:HD13	0.70	1.86	11	1
1:A:51:ILE:HD12	1:A:53:ILE:HD12	0.70	1.64	5	5
1:A:77:LYS:HZ3	1:A:108:LEU:HD21	0.68	1.46	19	1
1:A:77:LYS:NZ	1:A:108:LEU:HD21	0.65	2.07	19	1
1:A:43:LEU:C	1:A:43:LEU:HD23	0.64	2.18	10	14
1:A:22:TRP:CD1	1:A:22:TRP:H	0.64	2.09	16	3
1:A:9:TYR:CE1	1:A:106:HIS:CD2	0.63	2.86	10	2
1:A:84:TYR:CZ	1:A:85:HIS:CE1	0.63	2.87	10	2
1:A:33:HIS:ND1	1:A:39:TRP:NE1	0.63	2.47	2	1
1:A:87:ASN:ND2	1:A:91:TRP:CZ3	0.62	2.68	14	5
1:A:9:TYR:CE2	1:A:106:HIS:CD2	0.62	2.88	19	1
1:A:33:HIS:CD2	1:A:39:TRP:NE1	0.62	2.67	3	1
1:A:39:TRP:CD2	1:A:39:TRP:N	0.61	2.68	10	2
1:A:33:HIS:ND1	1:A:39:TRP:CD1	0.61	2.69	2	3
1:A:87:ASN:ND2	1:A:91:TRP:CE3	0.61	2.69	3	2
1:A:14:TYR:CD1	1:A:33:HIS:NE2	0.61	2.69	19	1
1:A:33:HIS:CD2	1:A:39:TRP:HE1	0.61	2.14	3	1
1:A:14:TYR:N	1:A:14:TYR:CD1	0.61	2.68	4	1
1:A:14:TYR:CE1	1:A:33:HIS:NE2	0.61	2.69	14	1
1:A:33:HIS:N	1:A:39:TRP:HE1	0.60	1.94	13	2
1:A:20:HIS:N	1:A:20:HIS:ND1	0.60	2.48	9	3
1:A:75:ARG:NH1	1:A:88:LYS:NZ	0.60	2.49	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:LEU:HD13	1:A:65:LYS:N	0.60	2.11	12	14
1:A:36:ASN:O	1:A:38:LYS:N	0.59	2.35	13	10
1:A:28:TYR:CE2	1:A:44:MET:SD	0.59	2.96	5	6
1:A:14:TYR:CG	1:A:33:HIS:NE2	0.59	2.70	7	1
1:A:23:GLU:H	1:A:23:GLU:CD	0.59	2.06	11	2
1:A:53:ILE:HD11	1:A:81:TYR:CZ	0.59	2.32	14	2
1:A:85:HIS:CG	1:A:86:MET:N	0.58	2.72	7	2
1:A:87:ASN:C	1:A:89:GLU:H	0.58	2.07	3	2
1:A:39:TRP:N	1:A:39:TRP:CE3	0.58	2.71	10	1
1:A:11:GLN:O	1:A:15:ASP:N	0.58	2.37	2	16
1:A:14:TYR:CE1	1:A:33:HIS:CD2	0.58	2.92	14	1
1:A:83:ALA:O	1:A:85:HIS:N	0.57	2.37	2	1
1:A:68:PRO:O	1:A:71:VAL:HG12	0.57	2.00	11	11
1:A:53:ILE:O	1:A:55:GLY:N	0.57	2.38	17	5
1:A:39:TRP:CZ3	1:A:41:ALA:HB2	0.56	2.35	3	1
1:A:84:TYR:CE1	1:A:85:HIS:CE1	0.56	2.93	10	2
1:A:99:PRO:O	1:A:100:LEU:C	0.56	2.47	20	2
1:A:20:HIS:H	1:A:20:HIS:CD2	0.56	2.18	12	1
1:A:39:TRP:O	1:A:39:TRP:CD1	0.56	2.59	7	3
1:A:60:ASP:H	1:A:97:ASN:ND2	0.56	1.99	15	4
1:A:87:ASN:O	1:A:89:GLU:N	0.56	2.39	20	4
1:A:14:TYR:CD1	1:A:33:HIS:CE1	0.55	2.95	19	2
1:A:27:ASP:OD1	1:A:27:ASP:N	0.55	2.39	16	3
1:A:89:GLU:OE1	1:A:89:GLU:N	0.55	2.39	10	1
1:A:69:GLU:OE1	1:A:69:GLU:N	0.55	2.39	12	1
1:A:38:LYS:C	1:A:39:TRP:CG	0.55	2.84	10	2
1:A:14:TYR:CZ	1:A:33:HIS:NE2	0.55	2.75	14	1
1:A:39:TRP:H	1:A:39:TRP:CD1	0.55	2.19	3	1
1:A:63:ASP:OD1	1:A:63:ASP:N	0.55	2.40	2	1
1:A:86:MET:O	1:A:88:LYS:N	0.55	2.40	12	1
1:A:85:HIS:CG	1:A:86:MET:H	0.55	2.20	7	2
1:A:91:TRP:C	1:A:92:ILE:HD13	0.55	2.26	11	1
1:A:14:TYR:CZ	1:A:39:TRP:CE2	0.54	2.94	15	1
1:A:87:ASN:ND2	1:A:91:TRP:CH2	0.54	2.76	4	2
1:A:36:ASN:N	1:A:36:ASN:OD1	0.54	2.41	5	3
1:A:14:TYR:CE1	1:A:33:HIS:CE1	0.54	2.96	8	1
1:A:40:TYR:CE2	1:A:63:ASP:OD2	0.54	2.61	8	1
1:A:11:GLN:NE2	1:A:16:THR:O	0.54	2.41	4	2
1:A:80:ILE:N	1:A:80:ILE:CD1	0.54	2.71	3	5
1:A:100:LEU:HD22	1:A:100:LEU:N	0.54	2.18	6	2
1:A:55:GLY:O	1:A:57:LYS:N	0.54	2.41	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ASN:ND2	1:A:116:THR:O	0.53	2.41	1	5
1:A:74:LEU:CD2	1:A:74:LEU:N	0.53	2.71	17	1
1:A:33:HIS:O	1:A:39:TRP:NE1	0.53	2.41	1	2
1:A:43:LEU:HD21	1:A:60:ASP:OD1	0.53	2.03	1	2
1:A:71:VAL:O	1:A:75:ARG:NH1	0.53	2.41	8	1
1:A:9:TYR:CE2	1:A:13:LYS:NZ	0.53	2.71	11	1
1:A:75:ARG:NE	1:A:92:ILE:HG21	0.53	2.18	8	1
1:A:20:HIS:N	1:A:20:HIS:CD2	0.53	2.76	15	2
1:A:3:ARG:NH2	1:A:45:ASP:OD2	0.53	2.42	19	2
1:A:37:ASP:OD1	1:A:38:LYS:N	0.53	2.41	1	1
1:A:63:ASP:OD1	1:A:64:LEU:N	0.53	2.41	3	4
1:A:100:LEU:HD12	1:A:100:LEU:C	0.53	2.28	8	1
1:A:14:TYR:CB	1:A:33:HIS:HE2	0.53	2.17	7	1
1:A:9:TYR:CD1	1:A:106:HIS:NE2	0.53	2.76	10	2
1:A:5:GLN:N	1:A:5:GLN:OE1	0.53	2.41	15	1
1:A:39:TRP:O	1:A:40:TYR:CD2	0.53	2.62	6	2
1:A:14:TYR:CE1	1:A:113:PHE:CD1	0.53	2.97	9	1
1:A:33:HIS:O	1:A:37:ASP:N	0.52	2.42	20	2
1:A:56:ASP:N	1:A:56:ASP:OD1	0.52	2.42	5	2
1:A:3:ARG:NH2	1:A:45:ASP:CG	0.52	2.67	19	2
1:A:45:ASP:OD2	1:A:58:ARG:NH2	0.52	2.41	6	1
1:A:100:LEU:N	1:A:100:LEU:CD2	0.52	2.72	6	6
1:A:113:PHE:O	1:A:117:ARG:N	0.52	2.43	13	4
1:A:14:TYR:OH	1:A:113:PHE:CD1	0.52	2.62	17	1
1:A:19:ASP:OD1	1:A:20:HIS:N	0.52	2.42	9	3
1:A:8:ASP:OD1	1:A:9:TYR:N	0.52	2.43	19	1
1:A:115:LEU:N	1:A:115:LEU:HD12	0.52	2.20	1	6
1:A:27:ASP:N	1:A:27:ASP:OD1	0.52	2.42	8	1
1:A:53:ILE:C	1:A:55:GLY:H	0.52	2.12	9	3
1:A:9:TYR:CE1	1:A:106:HIS:CG	0.52	2.97	10	1
1:A:32:ARG:CD	1:A:32:ARG:N	0.52	2.72	13	1
1:A:74:LEU:HD23	1:A:74:LEU:N	0.52	2.20	2	6
1:A:39:TRP:CD1	1:A:39:TRP:C	0.52	2.87	6	6
1:A:33:HIS:H	1:A:39:TRP:NE1	0.52	2.03	10	1
1:A:24:LYS:C	1:A:25:PHE:CD1	0.52	2.88	5	2
1:A:39:TRP:CH2	1:A:41:ALA:HB2	0.51	2.40	3	1
1:A:87:ASN:CG	1:A:90:HIS:ND1	0.51	2.69	11	1
1:A:3:ARG:NH2	1:A:45:ASP:OD1	0.51	2.43	17	3
1:A:20:HIS:O	1:A:20:HIS:ND1	0.51	2.43	19	1
1:A:39:TRP:O	1:A:40:TYR:CG	0.51	2.62	1	3
1:A:16:THR:OG1	1:A:33:HIS:NE2	0.51	2.42	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:MET:O	1:A:2:ASN:ND2	0.51	2.43	19	1
1:A:45:ASP:OD2	1:A:58:ARG:NH1	0.51	2.44	2	1
1:A:75:ARG:HH21	1:A:80:ILE:CG2	0.51	2.18	8	1
1:A:49:GLU:N	1:A:55:GLY:O	0.51	2.44	17	1
1:A:85:HIS:O	1:A:85:HIS:CG	0.51	2.63	14	2
1:A:77:LYS:CB	1:A:77:LYS:NZ	0.51	2.72	18	1
1:A:84:TYR:O	1:A:84:TYR:CG	0.51	2.64	13	2
1:A:36:ASN:C	1:A:38:LYS:N	0.51	2.68	4	5
1:A:24:LYS:C	1:A:25:PHE:CG	0.50	2.90	19	2
1:A:37:ASP:O	1:A:38:LYS:C	0.50	2.53	8	1
1:A:84:TYR:CZ	1:A:85:HIS:NE2	0.50	2.79	10	1
1:A:82:PRO:O	1:A:84:TYR:N	0.50	2.43	2	1
1:A:71:VAL:HG13	1:A:72:GLY:N	0.50	2.21	12	12
1:A:37:ASP:O	1:A:38:LYS:CB	0.50	2.60	1	1
1:A:74:LEU:H	1:A:74:LEU:CD2	0.50	2.18	2	6
1:A:55:GLY:C	1:A:57:LYS:N	0.50	2.68	3	2
1:A:103:LYS:NZ	1:A:104:GLU:OE2	0.50	2.45	8	1
1:A:24:LYS:O	1:A:25:PHE:CD1	0.50	2.65	19	1
1:A:14:TYR:O	1:A:15:ASP:C	0.50	2.54	1	6
1:A:14:TYR:CG	1:A:33:HIS:CE1	0.50	3.00	3	1
1:A:32:ARG:CB	1:A:39:TRP:CD1	0.50	2.94	12	2
1:A:37:ASP:O	1:A:39:TRP:CE3	0.50	2.65	12	2
1:A:8:ASP:OD2	1:A:12:LYS:NZ	0.49	2.45	3	1
1:A:51:ILE:O	1:A:81:TYR:CD1	0.49	2.65	1	4
1:A:3:ARG:NH1	1:A:45:ASP:OD2	0.49	2.46	15	1
1:A:75:ARG:NH1	1:A:88:LYS:HZ1	0.49	2.04	20	1
1:A:1:MET:O	1:A:3:ARG:NH2	0.49	2.45	14	1
1:A:14:TYR:CZ	1:A:39:TRP:CZ2	0.49	2.99	15	1
1:A:90:HIS:CD2	1:A:90:HIS:N	0.49	2.80	11	2
1:A:20:HIS:O	1:A:20:HIS:CG	0.49	2.65	18	5
1:A:83:ALA:C	1:A:84:TYR:CG	0.49	2.90	2	1
1:A:36:ASN:C	1:A:38:LYS:H	0.49	2.15	16	4
1:A:24:LYS:O	1:A:25:PHE:CG	0.48	2.66	19	2
1:A:36:ASN:O	1:A:37:ASP:CG	0.48	2.55	20	1
1:A:84:TYR:CD1	1:A:84:TYR:O	0.48	2.66	18	1
1:A:64:LEU:HD21	1:A:112:SER:OG	0.48	2.08	19	1
1:A:73:SER:O	1:A:76:LYS:NZ	0.48	2.45	8	1
1:A:41:ALA:C	1:A:42:LEU:HD22	0.48	2.34	6	4
1:A:20:HIS:ND1	1:A:20:HIS:N	0.48	2.61	6	1
1:A:84:TYR:CZ	1:A:93:THR:HG21	0.48	2.42	11	1
1:A:4:GLN:HE22	1:A:8:ASP:CG	0.48	2.17	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LYS:NZ	1:A:14:TYR:CZ	0.48	2.77	10	1
1:A:33:HIS:CG	1:A:39:TRP:NE1	0.48	2.81	2	1
1:A:115:LEU:HD22	1:A:115:LEU:N	0.48	2.23	19	1
1:A:51:ILE:O	1:A:81:TYR:CD2	0.48	2.67	8	1
1:A:11:GLN:HE22	1:A:16:THR:C	0.48	2.17	10	1
1:A:22:TRP:CD1	1:A:22:TRP:N	0.48	2.80	6	3
1:A:74:LEU:N	1:A:74:LEU:HD22	0.48	2.24	17	1
1:A:36:ASN:ND2	1:A:117:ARG:O	0.47	2.47	4	2
1:A:115:LEU:N	1:A:115:LEU:CD1	0.47	2.76	8	2
1:A:87:ASN:C	1:A:89:GLU:N	0.47	2.72	3	2
1:A:20:HIS:ND1	1:A:28:TYR:O	0.47	2.47	15	1
1:A:19:ASP:C	1:A:20:HIS:CD2	0.47	2.91	15	2
1:A:115:LEU:N	1:A:115:LEU:CD2	0.47	2.76	19	1
1:A:48:ALA:HB2	1:A:57:LYS:O	0.47	2.10	1	4
1:A:9:TYR:OH	1:A:13:LYS:NZ	0.47	2.48	3	2
1:A:33:HIS:CG	1:A:39:TRP:HE1	0.47	2.27	2	1
1:A:3:ARG:NH2	1:A:27:ASP:O	0.47	2.48	6	1
1:A:85:HIS:O	1:A:85:HIS:CD2	0.47	2.68	14	1
1:A:64:LEU:HD12	1:A:66:VAL:HG13	0.47	1.85	1	1
1:A:14:TYR:O	1:A:15:ASP:CG	0.47	2.58	12	2
1:A:44:MET:SD	1:A:44:MET:O	0.47	2.73	2	2
1:A:54:ASN:O	1:A:55:GLY:C	0.47	2.56	11	3
1:A:84:TYR:C	1:A:86:MET:H	0.47	2.18	8	1
1:A:75:ARG:HH21	1:A:92:ILE:CD1	0.47	2.22	16	1
1:A:14:TYR:CE2	1:A:39:TRP:CZ2	0.47	3.03	15	1
1:A:8:ASP:CG	1:A:9:TYR:N	0.47	2.73	19	1
1:A:44:MET:SD	1:A:61:VAL:CG2	0.47	3.03	10	1
1:A:43:LEU:C	1:A:43:LEU:CD2	0.46	2.88	10	6
1:A:20:HIS:CD2	1:A:20:HIS:N	0.46	2.82	12	1
1:A:74:LEU:CD1	1:A:75:ARG:HH22	0.46	2.23	8	1
1:A:102:ALA:O	1:A:106:HIS:ND1	0.46	2.49	16	1
1:A:53:ILE:O	1:A:54:ASN:C	0.46	2.58	18	2
1:A:66:VAL:HG11	1:A:74:LEU:HD13	0.46	1.86	7	2
1:A:85:HIS:CD2	1:A:86:MET:N	0.46	2.83	12	1
1:A:114:GLN:CG	1:A:115:LEU:N	0.46	2.78	18	1
1:A:36:ASN:O	1:A:37:ASP:O	0.46	2.34	1	1
1:A:100:LEU:HD12	1:A:100:LEU:O	0.46	2.10	17	2
1:A:16:THR:HG22	1:A:17:LYS:N	0.46	2.25	9	1
1:A:72:GLY:O	1:A:76:LYS:CG	0.46	2.63	17	4
1:A:35:ASP:N	1:A:35:ASP:OD1	0.46	2.48	14	1
1:A:31:PHE:HB2	1:A:41:ALA:HB3	0.46	1.87	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:PRO:O	1:A:100:LEU:O	0.46	2.33	18	1
1:A:85:HIS:O	1:A:86:MET:O	0.46	2.34	17	4
1:A:14:TYR:O	1:A:16:THR:N	0.46	2.49	15	3
1:A:28:TYR:CZ	1:A:44:MET:SD	0.46	3.08	5	1
1:A:3:ARG:NH2	1:A:60:ASP:OD1	0.46	2.48	4	1
1:A:86:MET:O	1:A:87:ASN:O	0.46	2.34	10	2
1:A:36:ASN:O	1:A:37:ASP:C	0.46	2.59	14	3
1:A:74:LEU:CD2	1:A:92:ILE:HG21	0.46	2.41	19	2
1:A:8:ASP:CG	1:A:12:LYS:NZ	0.46	2.74	3	1
1:A:86:MET:O	1:A:87:ASN:CG	0.46	2.58	10	1
1:A:56:ASP:OD1	1:A:56:ASP:N	0.46	2.49	8	3
1:A:36:ASN:OD1	1:A:37:ASP:N	0.46	2.49	15	1
1:A:14:TYR:C	1:A:15:ASP:CG	0.45	2.84	19	4
1:A:44:MET:SD	1:A:44:MET:C	0.45	2.99	2	4
1:A:31:PHE:O	1:A:41:ALA:HB3	0.45	2.11	3	2
1:A:116:THR:O	1:A:117:ARG:O	0.45	2.34	4	2
1:A:85:HIS:O	1:A:86:MET:C	0.45	2.60	6	1
1:A:115:LEU:CD1	1:A:115:LEU:N	0.45	2.79	7	1
1:A:60:ASP:H	1:A:97:ASN:HD22	0.45	1.54	8	1
1:A:73:SER:O	1:A:76:LYS:CD	0.45	2.64	14	2
1:A:44:MET:CE	1:A:84:TYR:OH	0.45	2.64	19	1
1:A:14:TYR:O	1:A:15:ASP:OD1	0.45	2.35	5	4
1:A:31:PHE:CD1	1:A:31:PHE:N	0.45	2.84	9	1
1:A:43:LEU:HD23	1:A:44:MET:N	0.45	2.26	16	4
1:A:84:TYR:O	1:A:85:HIS:C	0.45	2.60	14	2
1:A:32:ARG:NH2	1:A:37:ASP:O	0.45	2.49	19	2
1:A:38:LYS:O	1:A:39:TRP:O	0.45	2.35	4	2
1:A:45:ASP:OD1	1:A:45:ASP:N	0.45	2.50	9	4
1:A:30:VAL:CG1	1:A:32:ARG:HE	0.45	2.25	13	1
1:A:8:ASP:OD1	1:A:8:ASP:C	0.45	2.60	19	1
1:A:104:GLU:OE1	1:A:104:GLU:N	0.45	2.46	5	1
1:A:9:TYR:CD2	1:A:106:HIS:NE2	0.45	2.85	20	1
1:A:14:TYR:C	1:A:15:ASP:OD1	0.45	2.60	13	2
1:A:37:ASP:O	1:A:38:LYS:O	0.45	2.35	3	2
1:A:45:ASP:O	1:A:45:ASP:OD1	0.45	2.35	11	4
1:A:45:ASP:OD1	1:A:45:ASP:O	0.45	2.35	9	2
1:A:9:TYR:C	1:A:9:TYR:CD1	0.45	2.95	14	1
1:A:111:ASP:O	1:A:114:GLN:NE2	0.45	2.50	18	1
1:A:100:LEU:N	1:A:100:LEU:HD22	0.45	2.27	16	4
1:A:23:GLU:C	1:A:23:GLU:OE1	0.45	2.60	20	2
1:A:55:GLY:O	1:A:56:ASP:CG	0.45	2.60	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:TRP:O	1:A:39:TRP:CG	0.44	2.69	2	1
1:A:75:ARG:NH2	1:A:80:ILE:HG21	0.44	2.27	8	1
1:A:85:HIS:CD2	1:A:86:MET:H	0.44	2.30	12	1
1:A:116:THR:O	1:A:117:ARG:C	0.44	2.59	7	6
1:A:15:ASP:OD1	1:A:15:ASP:O	0.44	2.35	5	1
1:A:42:LEU:HD13	1:A:43:LEU:N	0.44	2.26	7	1
1:A:92:ILE:HD12	1:A:92:ILE:N	0.44	2.28	7	1
1:A:81:TYR:O	1:A:93:THR:O	0.44	2.35	8	1
1:A:48:ALA:HB1	1:A:53:ILE:HB	0.44	1.89	11	1
1:A:77:LYS:HB2	1:A:80:ILE:HD12	0.44	1.89	6	1
1:A:84:TYR:CD1	1:A:84:TYR:N	0.44	2.84	16	1
1:A:71:VAL:CG1	1:A:72:GLY:N	0.44	2.81	13	6
1:A:91:TRP:CD1	1:A:91:TRP:N	0.44	2.84	8	1
1:A:87:ASN:CG	1:A:91:TRP:CD1	0.44	2.96	20	1
1:A:2:ASN:OD1	1:A:5:GLN:OE1	0.44	2.36	6	1
1:A:45:ASP:OD1	1:A:60:ASP:OD1	0.44	2.36	17	7
1:A:51:ILE:O	1:A:81:TYR:CE1	0.44	2.71	3	1
1:A:53:ILE:C	1:A:55:GLY:N	0.44	2.76	9	3
1:A:73:SER:OG	1:A:74:LEU:N	0.44	2.51	14	1
1:A:33:HIS:CE1	1:A:39:TRP:NE1	0.44	2.86	17	2
1:A:49:GLU:OE2	1:A:56:ASP:OD1	0.44	2.35	5	2
1:A:17:LYS:CD	1:A:17:LYS:N	0.43	2.81	7	1
1:A:42:LEU:HD12	1:A:44:MET:HE2	0.43	1.90	1	1
1:A:87:ASN:O	1:A:88:LYS:O	0.43	2.35	2	1
1:A:22:TRP:C	1:A:24:LYS:N	0.43	2.75	16	2
1:A:36:ASN:C	1:A:36:ASN:OD1	0.43	2.60	9	1
1:A:63:ASP:OD1	1:A:63:ASP:C	0.43	2.60	14	3
1:A:45:ASP:OD1	1:A:59:VAL:O	0.43	2.36	8	1
1:A:75:ARG:NH2	1:A:92:ILE:HG21	0.43	2.27	8	1
1:A:54:ASN:OD1	1:A:54:ASN:C	0.43	2.59	17	2
1:A:40:TYR:CE2	1:A:42:LEU:CD2	0.43	3.00	10	1
1:A:3:ARG:O	1:A:4:GLN:C	0.43	2.60	14	1
1:A:39:TRP:O	1:A:39:TRP:CE3	0.43	2.72	14	1
1:A:38:LYS:O	1:A:39:TRP:C	0.43	2.59	17	1
1:A:73:SER:O	1:A:76:LYS:CE	0.43	2.66	8	1
1:A:87:ASN:O	1:A:91:TRP:O	0.43	2.36	8	1
1:A:49:GLU:OE1	1:A:49:GLU:C	0.43	2.60	14	1
1:A:14:TYR:CE1	1:A:113:PHE:CE1	0.43	3.06	9	1
1:A:5:GLN:OE1	1:A:5:GLN:CA	0.43	2.66	15	1
1:A:78:PRO:C	1:A:80:ILE:H	0.43	2.22	18	1
1:A:5:GLN:CD	1:A:5:GLN:N	0.43	2.77	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ASN:ND2	1:A:116:THR:C	0.43	2.76	1	1
1:A:84:TYR:N	1:A:84:TYR:CD1	0.43	2.86	2	1
1:A:42:LEU:HD13	1:A:42:LEU:C	0.43	2.39	7	1
1:A:42:LEU:C	1:A:42:LEU:CD1	0.43	2.91	7	1
1:A:86:MET:O	1:A:87:ASN:OD1	0.43	2.36	10	1
1:A:82:PRO:O	1:A:83:ALA:O	0.43	2.37	4	1
1:A:87:ASN:OD1	1:A:89:GLU:N	0.43	2.52	8	1
1:A:33:HIS:H	1:A:39:TRP:CD1	0.43	2.32	10	1
1:A:49:GLU:OE2	1:A:54:ASN:O	0.42	2.36	6	1
1:A:82:PRO:CB	1:A:88:LYS:NZ	0.42	2.82	1	2
1:A:20:HIS:CD2	1:A:20:HIS:O	0.42	2.72	2	1
1:A:55:GLY:C	1:A:56:ASP:OD1	0.42	2.61	3	1
1:A:56:ASP:O	1:A:56:ASP:OD1	0.42	2.37	4	1
1:A:15:ASP:C	1:A:15:ASP:OD1	0.42	2.62	5	1
1:A:64:LEU:HD13	1:A:64:LEU:C	0.42	2.39	1	1
1:A:82:PRO:O	1:A:93:THR:OG1	0.42	2.37	13	2
1:A:11:GLN:O	1:A:15:ASP:OD1	0.42	2.38	20	3
1:A:77:LYS:NZ	1:A:104:GLU:OE2	0.42	2.50	19	1
1:A:39:TRP:C	1:A:40:TYR:CG	0.42	2.98	12	1
1:A:67:GLN:CD	1:A:115:LEU:HD22	0.42	2.39	2	1
1:A:35:ASP:OD1	1:A:35:ASP:C	0.42	2.62	11	2
1:A:14:TYR:C	1:A:16:THR:N	0.42	2.76	13	2
1:A:84:TYR:CD2	1:A:85:HIS:ND1	0.42	2.87	16	1
1:A:36:ASN:O	1:A:37:ASP:OD2	0.42	2.37	20	1
1:A:19:ASP:OD1	1:A:19:ASP:C	0.42	2.62	6	1
1:A:23:GLU:CD	1:A:23:GLU:N	0.42	2.77	11	1
1:A:88:LYS:O	1:A:89:GLU:CB	0.42	2.67	2	1
1:A:37:ASP:OD1	1:A:37:ASP:C	0.42	2.61	1	1
1:A:6:PHE:CD1	1:A:6:PHE:C	0.42	2.98	6	1
1:A:55:GLY:O	1:A:56:ASP:C	0.42	2.60	3	1
1:A:9:TYR:CE1	1:A:106:HIS:CE1	0.42	3.08	9	1
1:A:3:ARG:HE	1:A:43:LEU:HD21	0.42	1.75	6	1
1:A:4:GLN:CD	1:A:4:GLN:C	0.42	2.88	6	3
1:A:33:HIS:O	1:A:37:ASP:OD1	0.42	2.37	13	1
1:A:112:SER:O	1:A:116:THR:HG23	0.41	2.14	16	1
1:A:87:ASN:CG	1:A:91:TRP:CE3	0.41	2.99	2	1
1:A:84:TYR:O	1:A:86:MET:N	0.41	2.51	8	1
1:A:86:MET:O	1:A:87:ASN:C	0.41	2.61	8	2
1:A:37:ASP:O	1:A:37:ASP:OD1	0.41	2.39	2	1
1:A:37:ASP:O	1:A:39:TRP:CD1	0.41	2.73	14	1
1:A:110:GLU:CD	1:A:110:GLU:C	0.41	2.88	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:ARG:CA	1:A:3:ARG:NE	0.41	2.84	14	1
1:A:10:ALA:O	1:A:14:TYR:N	0.41	2.54	2	1
1:A:51:ILE:O	1:A:81:TYR:CE2	0.41	2.73	8	1
1:A:51:ILE:CD1	1:A:53:ILE:HD12	0.41	2.45	10	1
1:A:2:ASN:CG	1:A:5:GLN:OE1	0.41	2.64	6	1
1:A:50:LYS:C	1:A:52:GLY:H	0.41	2.23	9	1
1:A:11:GLN:C	1:A:15:ASP:H	0.41	2.24	11	1
1:A:1:MET:N	1:A:105:ILE:CD1	0.41	2.83	18	1
1:A:9:TYR:CE2	1:A:106:HIS:NE2	0.41	2.89	19	1
1:A:39:TRP:C	1:A:40:TYR:CD2	0.41	2.99	1	2
1:A:6:PHE:CD2	1:A:43:LEU:CD1	0.41	3.03	12	1
1:A:36:ASN:O	1:A:36:ASN:OD1	0.41	2.39	19	1
1:A:23:GLU:CG	1:A:24:LYS:N	0.41	2.84	4	1
1:A:35:ASP:C	1:A:35:ASP:OD1	0.41	2.62	9	1
1:A:6:PHE:CE1	1:A:62:ILE:CD1	0.41	3.03	13	1
1:A:81:TYR:O	1:A:93:THR:OG1	0.40	2.38	4	1
1:A:9:TYR:CD1	1:A:106:HIS:CD2	0.40	3.09	10	1
1:A:36:ASN:OD1	1:A:36:ASN:C	0.40	2.63	15	1
1:A:2:ASN:OD1	1:A:2:ASN:C	0.40	2.63	20	1
1:A:64:LEU:C	1:A:64:LEU:CD1	0.40	2.94	5	3
1:A:84:TYR:CD1	1:A:84:TYR:C	0.40	2.99	15	1
1:A:23:GLU:C	1:A:25:PHE:N	0.40	2.80	1	1
1:A:64:LEU:CD1	1:A:64:LEU:C	0.40	2.94	11	1
1:A:43:LEU:HD21	1:A:60:ASP:OD2	0.40	2.17	14	1
1:A:9:TYR:CD2	1:A:106:HIS:CE1	0.40	3.09	20	1
1:A:4:GLN:OE1	1:A:8:ASP:OD2	0.40	2.38	2	1
1:A:88:LYS:O	1:A:92:ILE:HD13	0.40	2.17	4	1
1:A:35:ASP:C	1:A:36:ASN:OD1	0.40	2.65	5	1
1:A:75:ARG:NH2	1:A:80:ILE:CG2	0.40	2.85	8	1
1:A:32:ARG:NE	1:A:39:TRP:CH2	0.40	2.88	10	1
1:A:86:MET:C	1:A:87:ASN:CG	0.40	2.88	10	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	116/125 (93%)	108±2 (93±2%)	5±2 (4±1%)	3±1 (3±1%)	5	38
All	All	2320/2500 (93%)	2156 (93%)	95 (4%)	69 (3%)	5	38

All 19 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	37	ASP	11
1	A	86	MET	8
1	A	54	ASN	7
1	A	55	GLY	5
1	A	39	TRP	5
1	A	88	LYS	4
1	A	38	LYS	4
1	A	87	ASN	4
1	A	85	HIS	3
1	A	100	LEU	3
1	A	15	ASP	2
1	A	83	ALA	2
1	A	117	ARG	2
1	A	89	GLU	2
1	A	99	PRO	2
1	A	21	PRO	2
1	A	84	TYR	1
1	A	56	ASP	1
1	A	82	PRO	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	105/113 (93%)	101±1 (96±1%)	4±1 (4±1%)	28	79
All	All	2100/2260 (93%)	2013 (96%)	87 (4%)	28	79

All 28 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	64	LEU	20
1	A	42	LEU	11
1	A	76	LYS	9
1	A	44	MET	6
1	A	100	LEU	6
1	A	20	HIS	4
1	A	39	TRP	3
1	A	22	TRP	3
1	A	17	LYS	2
1	A	36	ASN	2
1	A	93	THR	2
1	A	33	HIS	2
1	A	77	LYS	2
1	A	84	TYR	1
1	A	23	GLU	1
1	A	14	TYR	1
1	A	74	LEU	1
1	A	56	ASP	1
1	A	75	ARG	1
1	A	57	LYS	1
1	A	32	ARG	1
1	A	49	GLU	1
1	A	115	LEU	1
1	A	5	GLN	1
1	A	65	LYS	1
1	A	8	ASP	1
1	A	15	ASP	1
1	A	91	TRP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 87% 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	1569
Number of shifts mapped to atoms	1569
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	120	0.00 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	114	0.21 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	110	0.07 ± 0.13	None needed (< 0.5 ppm)
^{15}N	106	0.68 ± 0.24	Should be applied

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 89%, i.e. 1498 atoms were assigned a chemical shift out of a possible 1674. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	535/575 (93%)	219/232 (94%)	217/234 (93%)	99/109 (91%)
Sidechain	855/934 (92%)	570/603 (95%)	270/294 (92%)	15/37 (41%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	108/165 (65%)	55/82 (67%)	50/75 (67%)	3/8 (38%)
Overall	1498/1674 (89%)	844/917 (92%)	537/603 (89%)	117/154 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1566 atoms were assigned a chemical shift out of a possible 1794. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	569/615 (93%)	233/248 (94%)	230/250 (92%)	106/117 (91%)
Sidechain	889/972 (91%)	593/628 (94%)	281/307 (92%)	15/37 (41%)
Aromatic	108/207 (52%)	55/106 (52%)	50/87 (57%)	3/14 (21%)
Overall	1566/1794 (87%)	881/982 (90%)	561/644 (87%)	124/168 (74%)

7.1.4 Statistically unusual chemical shifts ⓘ

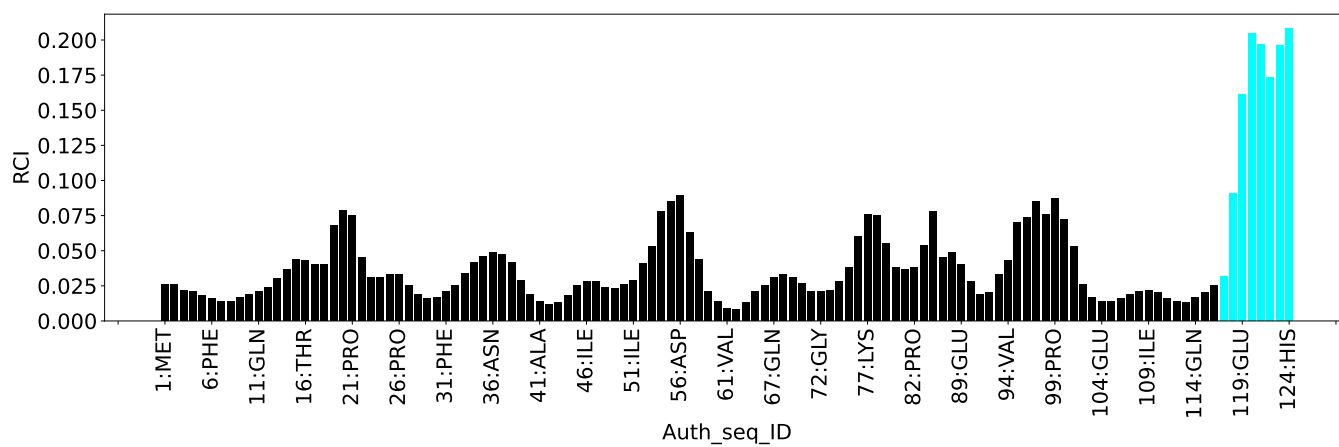
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	16	THR	HG1	6.25	0.08 – 2.19	24.2
1	A	116	THR	HG1	5.35	0.08 – 2.19	20.0
1	A	93	THR	HG1	4.80	0.08 – 2.19	17.4
1	A	13	LYS	HG3	-0.31	0.04 – 2.67	-6.3
1	A	13	LYS	HB2	0.43	0.58 – 2.97	-5.6
1	A	13	LYS	HB3	0.32	0.46 – 3.04	-5.5
1	A	21	PRO	HG2	0.30	0.41 – 3.45	-5.4
1	A	13	LYS	HG2	0.09	0.13 – 2.61	-5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis [i](#)

8.1 Conformationally restricting restraints [i](#)

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

Description	Value
Total distance restraints	1908
Intra-residue ($ i-j =0$)	419
Sequential ($ i-j =1$)	486
Medium range ($ i-j >1$ and $ i-j <5$)	370
Long range ($ i-j \geq 5$)	553
Inter-chain	0
Hydrogen bond restraints	80
Disulfide bond restraints	0
Total dihedral-angle restraints	172
Number of unmapped restraints	0
Number of restraints per residue	16.6
Number of long range restraints per residue ¹	4.7

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

8.2 Residual restraint violations [i](#)

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

8.2.1 Average number of distance violations per model [i](#)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	13.0	0.2
0.2-0.5 (Medium)	3.8	0.42
>0.5 (Large)	0.1	0.82

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)	6.3	7.62
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis [i](#)

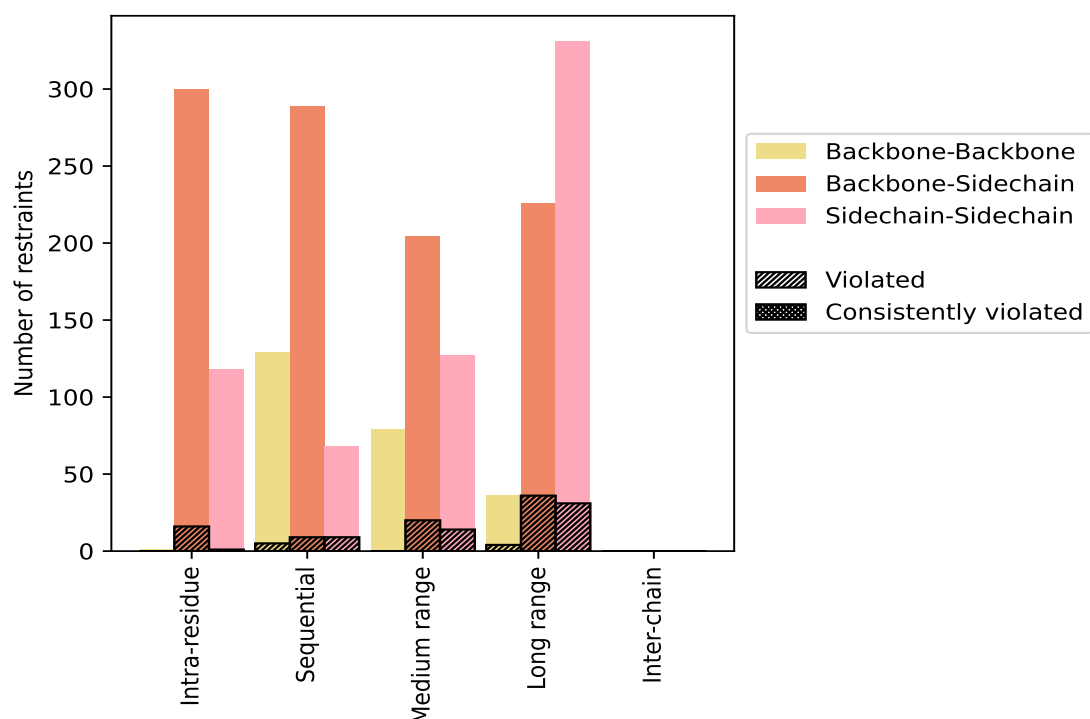
9.1 Summary of distance violations [i](#)

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	419	22.0	17	4.1	0.9	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	300	15.7	16	5.3	0.8	0	0.0	0.0
Sidechain-Sidechain	118	6.2	1	0.8	0.1	0	0.0	0.0
Sequential (i-j =1)	486	25.5	23	4.7	1.2	0	0.0	0.0
Backbone-Backbone	129	6.8	5	3.9	0.3	0	0.0	0.0
Backbone-Sidechain	289	15.1	9	3.1	0.5	0	0.0	0.0
Sidechain-Sidechain	68	3.6	9	13.2	0.5	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	370	19.4	30	8.1	1.6	0	0.0	0.0
Backbone-Backbone	79	4.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	164	8.6	16	9.8	0.8	0	0.0	0.0
Sidechain-Sidechain	127	6.7	14	11.0	0.7	0	0.0	0.0
Long range (i-j ≥5)	553	29.0	57	10.3	3.0	0	0.0	0.0
Backbone-Backbone	36	1.9	4	11.1	0.2	0	0.0	0.0
Backbone-Sidechain	186	9.7	22	11.8	1.2	0	0.0	0.0
Sidechain-Sidechain	331	17.3	31	9.4	1.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	80	4.2	18	22.5	0.9	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1908	100.0	145	7.6	7.6	0	0.0	0.0
Backbone-Backbone	245	12.8	9	3.7	0.5	0	0.0	0.0
Backbone-Sidechain	1019	53.4	81	7.9	4.2	0	0.0	0.0
Sidechain-Sidechain	644	33.8	55	8.5	2.9	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	1	2	1	5	0	9	0.22	0.64	0.17	0.15
2	5	0	2	10	0	17	0.18	0.36	0.07	0.17
3	1	4	3	6	0	14	0.17	0.35	0.06	0.16
4	4	3	3	8	0	18	0.19	0.82	0.16	0.14
5	3	2	5	11	0	21	0.18	0.36	0.07	0.15
6	2	3	2	18	0	25	0.18	0.37	0.08	0.15
7	2	2	3	13	0	20	0.17	0.29	0.07	0.13
8	4	5	2	13	0	24	0.16	0.38	0.06	0.15
9	1	0	1	13	0	15	0.17	0.26	0.06	0.15
10	1	2	3	8	0	14	0.16	0.23	0.04	0.16

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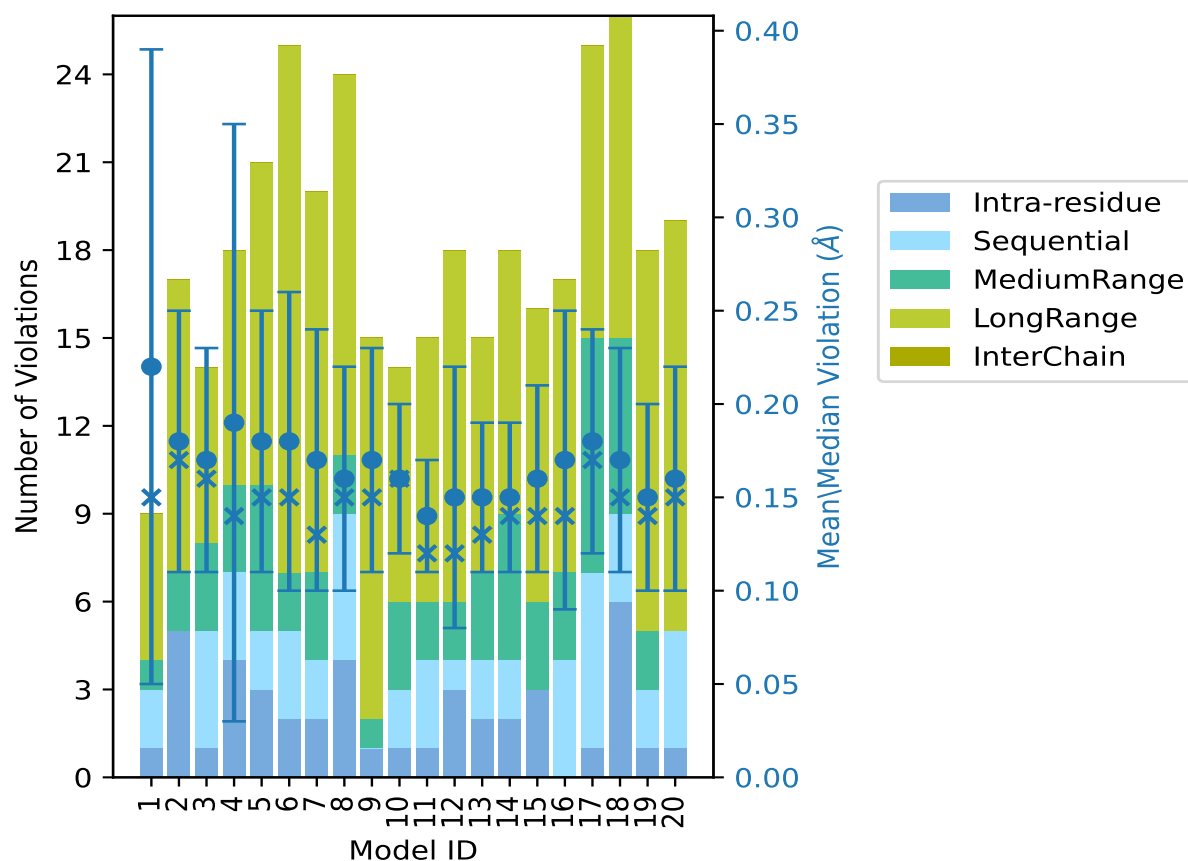
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	3	2	9	0	15	0.14	0.21	0.03	0.12
12	3	1	2	12	0	18	0.15	0.32	0.07	0.12
13	2	2	3	8	0	15	0.15	0.24	0.04	0.13
14	2	2	5	9	0	18	0.15	0.24	0.04	0.14
15	3	0	3	10	0	16	0.16	0.29	0.05	0.14
16	0	4	3	10	0	17	0.17	0.42	0.08	0.14
17	1	6	8	10	0	25	0.18	0.31	0.06	0.17
18	6	3	6	11	0	26	0.17	0.31	0.06	0.15
19	1	2	2	13	0	18	0.15	0.26	0.05	0.14
20	1	4	0	14	0	19	0.16	0.32	0.06	0.15

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

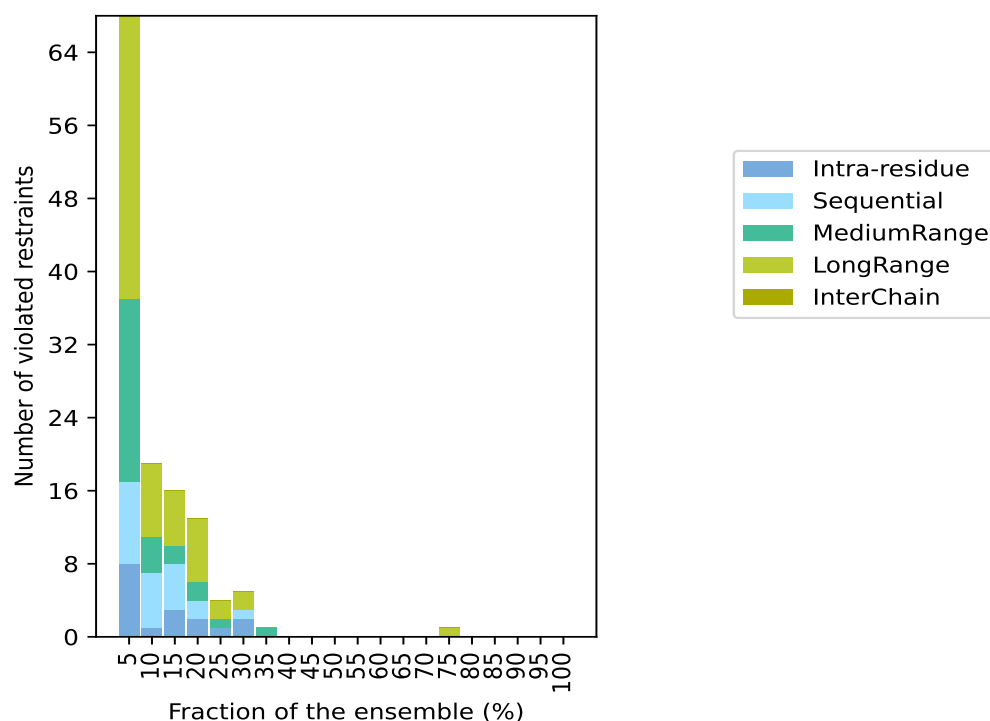
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1701(IR:402, SQ:463, MR:340, LR:496, IC:0) restraints are 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	%
8	9	20	31	0	68	1	5.0
1	6	4	8	0	19	2	10.0
3	5	2	6	0	16	3	15.0
2	2	2	7	0	13	4	20.0
1	0	1	2	0	4	5	25.0
2	1	0	2	0	5	6	30.0
0	0	1	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	1	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

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

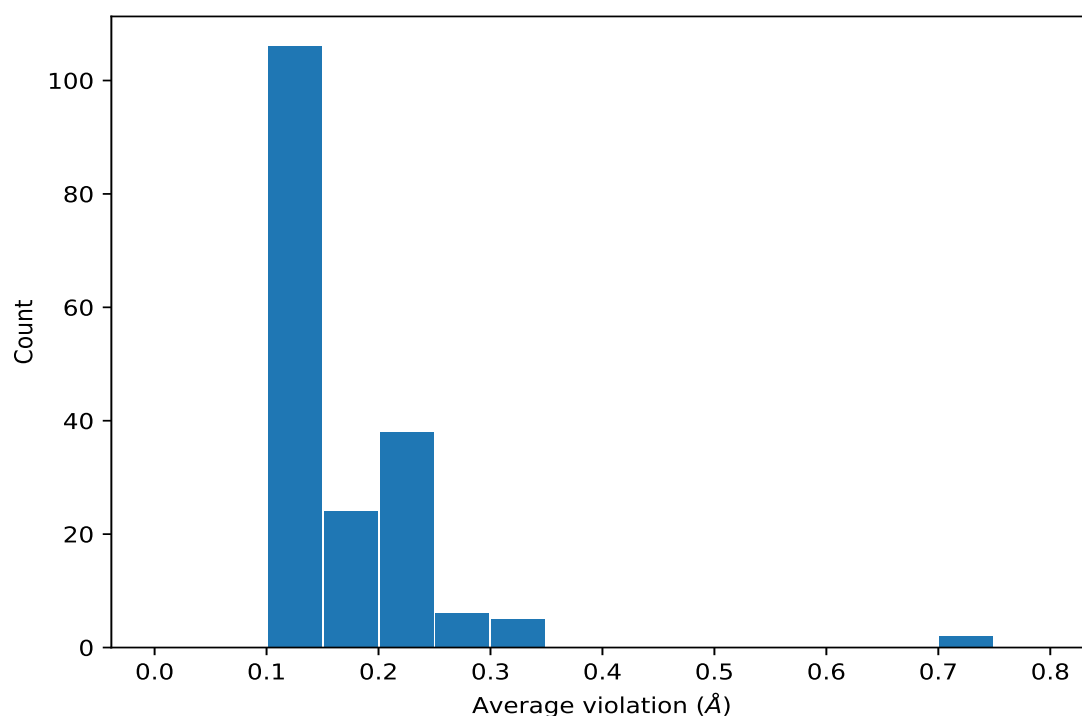
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	19	0.18	0.05	0.18
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	15	0.17	0.05	0.16
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	12	0.15	0.03	0.15
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	12	0.14	0.02	0.15
(1,849)	1:53:A:ILE:HD11	1:55:A:GLY:H	7	0.15	0.03	0.13
(1,849)	1:53:A:ILE:HD12	1:55:A:GLY:H	7	0.15	0.03	0.13
(1,849)	1:53:A:ILE:HD13	1:55:A:GLY:H	7	0.15	0.03	0.13
(2,57)	1:95:A:LEU:H	1:79:A:GLY:O	7	0.13	0.02	0.12
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG2	6	0.31	0.08	0.32
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG3	6	0.31	0.08	0.32
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD21	6	0.26	0.02	0.26
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD22	6	0.26	0.02	0.26
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD23	6	0.26	0.02	0.26
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD11	6	0.24	0.04	0.25
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD12	6	0.24	0.04	0.25
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD13	6	0.24	0.04	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD21	6	0.14	0.03	0.12
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD22	6	0.14	0.03	0.12
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD23	6	0.14	0.03	0.12
(1,762)	1:49:A:GLU:HA	1:56:A:ASP:HA	6	0.13	0.02	0.13
(1,1325)	1:76:A:LYS:H	1:76:A:LYS:HD3	5	0.34	0.04	0.35
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG2	5	0.15	0.03	0.14
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG3	5	0.15	0.03	0.14
(2,25)	1:31:A:PHE:H	1:41:A:ALA:O	5	0.15	0.03	0.14
(1,1007)	1:64:A:LEU:HD11	1:109:A:ILE:HA	5	0.14	0.02	0.15
(1,1007)	1:64:A:LEU:HD12	1:109:A:ILE:HA	5	0.14	0.02	0.15
(1,1007)	1:64:A:LEU:HD13	1:109:A:ILE:HA	5	0.14	0.02	0.15
(2,31)	1:46:A:ILE:H	1:59:A:VAL:O	5	0.12	0.01	0.12
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG21	5	0.12	0.01	0.12
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG22	5	0.12	0.01	0.12
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG23	5	0.12	0.01	0.12
(1,1598)	1:104:A:GLU:H	1:104:A:GLU:HG2	4	0.2	0.01	0.2
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG21	4	0.19	0.1	0.16
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG22	4	0.19	0.1	0.16
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG23	4	0.19	0.1	0.16
(1,1824)	1:121:A:HIS:HA	1:122:A:HIS:H	4	0.19	0.04	0.2
(1,577)	1:38:A:LYS:H	1:38:A:LYS:HD2	4	0.17	0.05	0.17
(1,577)	1:38:A:LYS:H	1:38:A:LYS:HD3	4	0.17	0.05	0.17
(1,530)	1:32:A:ARG:HB2	1:39:A:TRP:HD1	4	0.17	0.05	0.16
(1,530)	1:32:A:ARG:HB3	1:39:A:TRP:HD1	4	0.17	0.05	0.16
(1,1815)	1:119:A:GLU:HG2	1:120:A:HIS:HA	4	0.16	0.04	0.16
(1,1815)	1:119:A:GLU:HG3	1:120:A:HIS:HA	4	0.16	0.04	0.16
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG21	4	0.14	0.03	0.13
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG22	4	0.14	0.03	0.13
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG23	4	0.14	0.03	0.13
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD21	4	0.14	0.02	0.14
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD22	4	0.14	0.02	0.14
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD23	4	0.14	0.02	0.14
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD11	4	0.14	0.02	0.14
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD12	4	0.14	0.02	0.14
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD13	4	0.14	0.02	0.14
(2,45)	1:64:A:LEU:H	1:92:A:ILE:O	4	0.14	0.02	0.13
(1,1235)	1:74:A:LEU:HA	1:76:A:LYS:HE2	4	0.14	0.01	0.14
(1,1235)	1:74:A:LEU:HA	1:76:A:LYS:HE3	4	0.14	0.01	0.14
(1,1016)	1:64:A:LEU:HD21	1:112:A:SER:HA	4	0.13	0.03	0.12
(1,1016)	1:64:A:LEU:HD22	1:112:A:SER:HA	4	0.13	0.03	0.12
(1,1016)	1:64:A:LEU:HD23	1:112:A:SER:HA	4	0.13	0.03	0.12
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD21	4	0.13	0.03	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD22	4	0.13	0.03	0.12
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD23	4	0.13	0.03	0.12
(1,526)	1:32:A:ARG:HA	1:40:A:TYR:H	4	0.11	0.01	0.12
(2,17)	1:19:A:ASP:H	1:30:A:VAL:O	4	0.11	0.01	0.11
(1,1434)	1:89:A:GLU:H	1:89:A:GLU:HG2	3	0.31	0.04	0.29
(1,1434)	1:89:A:GLU:H	1:89:A:GLU:HG3	3	0.31	0.04	0.29
(1,1520)	1:100:A:LEU:HA	1:101:A:GLY:H	3	0.25	0.04	0.24
(1,1808)	1:118:A:LEU:H	1:118:A:LEU:HG	3	0.25	0.02	0.26
(1,1770)	1:115:A:LEU:H	1:115:A:LEU:HG	3	0.24	0.01	0.24
(1,240)	1:10:A:ALA:HB1	1:11:A:GLN:HG2	3	0.23	0.02	0.24
(1,240)	1:10:A:ALA:HB1	1:11:A:GLN:HG3	3	0.23	0.02	0.24
(1,240)	1:10:A:ALA:HB2	1:11:A:GLN:HG2	3	0.23	0.02	0.24
(1,240)	1:10:A:ALA:HB2	1:11:A:GLN:HG3	3	0.23	0.02	0.24
(1,240)	1:10:A:ALA:HB3	1:11:A:GLN:HG2	3	0.23	0.02	0.24
(1,240)	1:10:A:ALA:HB3	1:11:A:GLN:HG3	3	0.23	0.02	0.24
(1,1803)	1:118:A:LEU:HD21	1:119:A:GLU:HG2	3	0.23	0.07	0.21
(1,1803)	1:118:A:LEU:HD21	1:119:A:GLU:HG3	3	0.23	0.07	0.21
(1,1803)	1:118:A:LEU:HD22	1:119:A:GLU:HG2	3	0.23	0.07	0.21
(1,1803)	1:118:A:LEU:HD22	1:119:A:GLU:HG3	3	0.23	0.07	0.21
(1,1803)	1:118:A:LEU:HD23	1:119:A:GLU:HG2	3	0.23	0.07	0.21
(1,1803)	1:118:A:LEU:HD23	1:119:A:GLU:HG3	3	0.23	0.07	0.21
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG11	3	0.21	0.02	0.21
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG12	3	0.21	0.02	0.21
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG13	3	0.21	0.02	0.21
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG11	3	0.21	0.02	0.21
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG12	3	0.21	0.02	0.21
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG13	3	0.21	0.02	0.21
(1,1812)	1:119:A:GLU:HA	1:120:A:HIS:H	3	0.21	0.08	0.16
(1,1278)	1:75:A:ARG:HD2	1:88:A:LYS:HD2	3	0.2	0.07	0.18
(1,1278)	1:75:A:ARG:HD2	1:88:A:LYS:HD3	3	0.2	0.07	0.18
(1,1278)	1:75:A:ARG:HD3	1:88:A:LYS:HD2	3	0.2	0.07	0.18
(1,1278)	1:75:A:ARG:HD3	1:88:A:LYS:HD3	3	0.2	0.07	0.18
(1,1292)	1:75:A:ARG:HG3	1:82:A:PRO:HD2	3	0.14	0.04	0.11
(1,1292)	1:75:A:ARG:HG3	1:82:A:PRO:HD3	3	0.14	0.04	0.11
(1,1198)	1:71:A:VAL:HG21	1:75:A:ARG:HB2	3	0.13	0.03	0.12
(1,1198)	1:71:A:VAL:HG21	1:75:A:ARG:HB3	3	0.13	0.03	0.12
(1,1198)	1:71:A:VAL:HG22	1:75:A:ARG:HB2	3	0.13	0.03	0.12
(1,1198)	1:71:A:VAL:HG22	1:75:A:ARG:HB3	3	0.13	0.03	0.12
(1,1198)	1:71:A:VAL:HG23	1:75:A:ARG:HB2	3	0.13	0.03	0.12
(1,1198)	1:71:A:VAL:HG23	1:75:A:ARG:HB3	3	0.13	0.03	0.12
(1,1431)	1:89:A:GLU:HG2	1:90:A:HIS:HD1	3	0.13	0.02	0.13
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG21	3	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG22	3	0.13	0.02	0.13
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG23	3	0.13	0.02	0.13
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG21	3	0.13	0.02	0.13
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG22	3	0.13	0.02	0.13
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG23	3	0.13	0.02	0.13
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG21	3	0.13	0.02	0.13
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG22	3	0.13	0.02	0.13
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG23	3	0.13	0.02	0.13
(1,1083)	1:66:A:VAL:HG21	1:88:A:LYS:HG2	3	0.13	0.0	0.13
(1,1083)	1:66:A:VAL:HG21	1:88:A:LYS:HG3	3	0.13	0.0	0.13
(1,1083)	1:66:A:VAL:HG22	1:88:A:LYS:HG2	3	0.13	0.0	0.13
(1,1083)	1:66:A:VAL:HG22	1:88:A:LYS:HG3	3	0.13	0.0	0.13
(1,1083)	1:66:A:VAL:HG23	1:88:A:LYS:HG2	3	0.13	0.0	0.13
(1,1083)	1:66:A:VAL:HG23	1:88:A:LYS:HG3	3	0.13	0.0	0.13
(2,37)	1:59:A:VAL:H	1:46:A:ILE:O	3	0.11	0.01	0.11
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD21	3	0.11	0.0	0.11
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD22	3	0.11	0.0	0.11
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD23	3	0.11	0.0	0.11
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD11	3	0.11	0.01	0.11
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD12	3	0.11	0.01	0.11
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD13	3	0.11	0.01	0.11
(1,1426)	1:89:A:GLU:HB3	1:90:A:HIS:HD2	2	0.73	0.09	0.73
(1,1426)	1:89:A:GLU:HB2	1:90:A:HIS:HD2	2	0.73	0.09	0.73
(1,1347)	1:78:A:PRO:HA	1:99:A:PRO:HG3	2	0.26	0.11	0.26
(1,760)	1:49:A:GLU:HA	1:53:A:ILE:HG21	2	0.22	0.04	0.22
(1,760)	1:49:A:GLU:HA	1:53:A:ILE:HG22	2	0.22	0.04	0.22
(1,760)	1:49:A:GLU:HA	1:53:A:ILE:HG23	2	0.22	0.04	0.22
(1,1797)	1:118:A:LEU:HA	1:119:A:GLU:H	2	0.2	0.02	0.2
(1,1445)	1:91:A:TRP:H	1:92:A:ILE:HD11	2	0.2	0.03	0.2
(1,1445)	1:91:A:TRP:H	1:92:A:ILE:HD12	2	0.2	0.03	0.2
(1,1445)	1:91:A:TRP:H	1:92:A:ILE:HD13	2	0.2	0.03	0.2
(1,80)	1:3:A:ARG:HG2	1:43:A:LEU:HD11	2	0.2	0.05	0.2
(1,80)	1:3:A:ARG:HG2	1:43:A:LEU:HD12	2	0.2	0.05	0.2
(1,80)	1:3:A:ARG:HG2	1:43:A:LEU:HD13	2	0.2	0.05	0.2
(1,1765)	1:115:A:LEU:HB2	1:116:A:THR:HA	2	0.19	0.01	0.19
(1,1429)	1:89:A:GLU:HG3	1:90:A:HIS:HD1	2	0.18	0.01	0.18
(1,1256)	1:74:A:LEU:HD21	1:76:A:LYS:H	2	0.18	0.06	0.18
(1,1256)	1:74:A:LEU:HD22	1:76:A:LYS:H	2	0.18	0.06	0.18
(1,1256)	1:74:A:LEU:HD23	1:76:A:LYS:H	2	0.18	0.06	0.18
(1,699)	1:47:A:PRO:HA	1:58:A:ARG:HG2	2	0.16	0.02	0.16
(1,699)	1:47:A:PRO:HA	1:58:A:ARG:HG3	2	0.16	0.02	0.16
(2,43)	1:63:A:ASP:H	1:42:A:LEU:O	2	0.16	0.06	0.16

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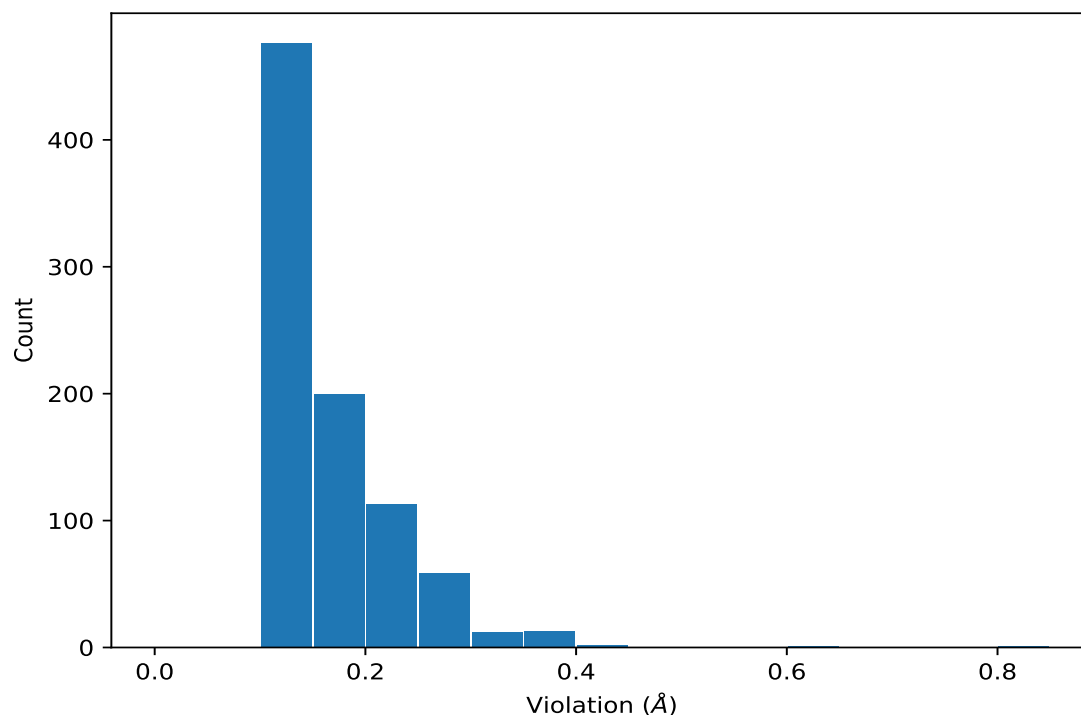
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1643)	1:106:A:HIS:H	1:106:A:HIS:HD2	2	0.16	0.02	0.16
(1,1343)	1:77:A:LYS:H	1:80:A:ILE:HD11	2	0.16	0.02	0.16
(1,1343)	1:77:A:LYS:H	1:80:A:ILE:HD12	2	0.16	0.02	0.16
(1,1343)	1:77:A:LYS:H	1:80:A:ILE:HD13	2	0.16	0.02	0.16
(1,1032)	1:65:A:LYS:HD2	1:66:A:VAL:H	2	0.15	0.04	0.15
(1,1032)	1:65:A:LYS:HD3	1:66:A:VAL:H	2	0.15	0.04	0.15
(2,49)	1:81:A:TYR:H	1:93:A:THR:O	2	0.14	0.02	0.14
(1,539)	1:33:A:HIS:HB2	1:38:A:LYS:H	2	0.12	0.02	0.12
(1,539)	1:33:A:HIS:HB3	1:38:A:LYS:H	2	0.12	0.02	0.12
(1,559)	1:36:A:ASN:HB2	1:118:A:LEU:HG	2	0.12	0.02	0.12
(1,559)	1:36:A:ASN:HB3	1:118:A:LEU:HG	2	0.12	0.02	0.12
(1,1059)	1:66:A:VAL:HA	1:115:A:LEU:HD21	2	0.12	0.02	0.12
(1,1059)	1:66:A:VAL:HA	1:115:A:LEU:HD22	2	0.12	0.02	0.12
(1,1059)	1:66:A:VAL:HA	1:115:A:LEU:HD23	2	0.12	0.02	0.12
(1,1086)	1:66:A:VAL:HG21	1:92:A:ILE:HD11	2	0.12	0.02	0.12
(1,1086)	1:66:A:VAL:HG21	1:92:A:ILE:HD12	2	0.12	0.02	0.12
(1,1086)	1:66:A:VAL:HG21	1:92:A:ILE:HD13	2	0.12	0.02	0.12
(1,1086)	1:66:A:VAL:HG22	1:92:A:ILE:HD11	2	0.12	0.02	0.12
(1,1086)	1:66:A:VAL:HG22	1:92:A:ILE:HD12	2	0.12	0.02	0.12
(1,1086)	1:66:A:VAL:HG22	1:92:A:ILE:HD13	2	0.12	0.02	0.12
(1,1086)	1:66:A:VAL:HG23	1:92:A:ILE:HD11	2	0.12	0.02	0.12
(1,1086)	1:66:A:VAL:HG23	1:92:A:ILE:HD12	2	0.12	0.02	0.12
(1,1086)	1:66:A:VAL:HG23	1:92:A:ILE:HD13	2	0.12	0.02	0.12
(2,47)	1:66:A:VAL:H	1:90:A:HIS:O	2	0.12	0.01	0.12
(2,61)	1:105:A:ILE:H	1:101:A:GLY:O	2	0.12	0.01	0.12
(1,160)	1:6:A:PHE:HZ	1:64:A:LEU:HD21	2	0.11	0.0	0.11
(1,160)	1:6:A:PHE:HZ	1:64:A:LEU:HD22	2	0.11	0.0	0.11
(1,160)	1:6:A:PHE:HZ	1:64:A:LEU:HD23	2	0.11	0.0	0.11
(1,597)	1:42:A:LEU:HD11	1:44:A:MET:HE1	2	0.11	0.0	0.11
(1,597)	1:42:A:LEU:HD11	1:44:A:MET:HE2	2	0.11	0.0	0.11
(1,597)	1:42:A:LEU:HD11	1:44:A:MET:HE3	2	0.11	0.0	0.11
(1,597)	1:42:A:LEU:HD12	1:44:A:MET:HE1	2	0.11	0.0	0.11
(1,597)	1:42:A:LEU:HD12	1:44:A:MET:HE2	2	0.11	0.0	0.11
(1,597)	1:42:A:LEU:HD12	1:44:A:MET:HE3	2	0.11	0.0	0.11
(1,597)	1:42:A:LEU:HD13	1:44:A:MET:HE1	2	0.11	0.0	0.11
(1,597)	1:42:A:LEU:HD13	1:44:A:MET:HE2	2	0.11	0.0	0.11
(1,597)	1:42:A:LEU:HD13	1:44:A:MET:HE3	2	0.11	0.0	0.11
(2,30)	1:44:A:MET:N	1:61:A:VAL:O	2	0.11	0.0	0.11
(2,39)	1:61:A:VAL:H	1:44:A:MET:O	2	0.1	0.0	0.1

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)
(1,1426)	1:89:A:GLU:HB2	1:90:A:HIS:HD2	4	0.82
(1,1426)	1:89:A:GLU:HB3	1:90:A:HIS:HD2	1	0.64
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG2	16	0.42
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG3	16	0.42
(1,1325)	1:76:A:LYS:H	1:76:A:LYS:HD3	1	0.39
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG2	8	0.38
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG3	8	0.38
(1,1347)	1:78:A:PRO:HA	1:99:A:PRO:HG3	6	0.37
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG2	6	0.37
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG3	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1434)	1:89:A:GLU:H	1:89:A:GLU:HG2	2	0.36
(1,1434)	1:89:A:GLU:H	1:89:A:GLU:HG3	2	0.36
(1,1325)	1:76:A:LYS:H	1:76:A:LYS:HD3	5	0.36
(1,1325)	1:76:A:LYS:H	1:76:A:LYS:HD3	3	0.35
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG21	6	0.35
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG22	6	0.35
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG23	6	0.35
(1,1812)	1:119:A:GLU:HA	1:120:A:HIS:H	20	0.32
(1,1803)	1:118:A:LEU:HD21	1:119:A:GLU:HG2	12	0.32
(1,1803)	1:118:A:LEU:HD21	1:119:A:GLU:HG3	12	0.32
(1,1803)	1:118:A:LEU:HD22	1:119:A:GLU:HG2	12	0.32
(1,1803)	1:118:A:LEU:HD22	1:119:A:GLU:HG3	12	0.32
(1,1803)	1:118:A:LEU:HD23	1:119:A:GLU:HG2	12	0.32
(1,1803)	1:118:A:LEU:HD23	1:119:A:GLU:HG3	12	0.32
(1,1325)	1:76:A:LYS:H	1:76:A:LYS:HD3	12	0.32
(1,1520)	1:100:A:LEU:HA	1:101:A:GLY:H	18	0.31
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD11	17	0.31
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD12	17	0.31
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD13	17	0.31
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	7	0.29
(1,1434)	1:89:A:GLU:H	1:89:A:GLU:HG2	18	0.29
(1,1434)	1:89:A:GLU:H	1:89:A:GLU:HG3	18	0.29
(1,1414)	1:87:A:ASN:HB2	1:89:A:GLU:H	2	0.29
(1,1414)	1:87:A:ASN:HB3	1:89:A:GLU:H	2	0.29
(1,1278)	1:75:A:ARG:HD2	1:88:A:LYS:HD2	16	0.29
(1,1278)	1:75:A:ARG:HD2	1:88:A:LYS:HD3	16	0.29
(1,1278)	1:75:A:ARG:HD3	1:88:A:LYS:HD2	16	0.29
(1,1278)	1:75:A:ARG:HD3	1:88:A:LYS:HD3	16	0.29
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD21	15	0.29
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD22	15	0.29
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD23	15	0.29
(1,1434)	1:89:A:GLU:H	1:89:A:GLU:HG2	6	0.28
(1,1434)	1:89:A:GLU:H	1:89:A:GLU:HG3	6	0.28
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD11	7	0.28
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD12	7	0.28
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD13	7	0.28
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	17	0.27
(1,1808)	1:118:A:LEU:H	1:118:A:LEU:HG	2	0.27
(1,1325)	1:76:A:LYS:H	1:76:A:LYS:HD3	7	0.27
(1,1808)	1:118:A:LEU:H	1:118:A:LEU:HG	5	0.26
(1,1227)	1:73:A:SER:HA	1:76:A:LYS:HG2	5	0.26
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD11	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD12	9	0.26
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD13	9	0.26
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD21	7	0.26
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD22	7	0.26
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD23	7	0.26
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD21	9	0.26
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD22	9	0.26
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD23	9	0.26
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD21	18	0.26
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD22	18	0.26
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD23	18	0.26
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	9	0.26
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	17	0.26
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG2	5	0.26
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG3	5	0.26
(1,760)	1:49:A:GLU:HA	1:53:A:ILE:HG21	5	0.26
(1,760)	1:49:A:GLU:HA	1:53:A:ILE:HG22	5	0.26
(1,760)	1:49:A:GLU:HA	1:53:A:ILE:HG23	5	0.26
(1,240)	1:10:A:ALA:HB1	1:11:A:GLN:HG2	19	0.26
(1,240)	1:10:A:ALA:HB1	1:11:A:GLN:HG3	19	0.26
(1,240)	1:10:A:ALA:HB2	1:11:A:GLN:HG2	19	0.26
(1,240)	1:10:A:ALA:HB2	1:11:A:GLN:HG3	19	0.26
(1,240)	1:10:A:ALA:HB3	1:11:A:GLN:HG2	19	0.26
(1,240)	1:10:A:ALA:HB3	1:11:A:GLN:HG3	19	0.26
(1,1770)	1:115:A:LEU:H	1:115:A:LEU:HG	4	0.25
(1,1288)	1:75:A:ARG:HG2	1:93:A:THR:H	8	0.25
(1,1288)	1:75:A:ARG:HG3	1:93:A:THR:H	8	0.25
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD21	17	0.25
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD22	17	0.25
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD23	17	0.25
(1,866)	1:53:A:ILE:HG21	1:56:A:ASP:H	17	0.25
(1,866)	1:53:A:ILE:HG22	1:56:A:ASP:H	17	0.25
(1,866)	1:53:A:ILE:HG23	1:56:A:ASP:H	17	0.25
(1,80)	1:3:A:ARG:HG2	1:43:A:LEU:HD11	6	0.25
(1,80)	1:3:A:ARG:HG2	1:43:A:LEU:HD12	6	0.25
(1,80)	1:3:A:ARG:HG2	1:43:A:LEU:HD13	6	0.25
(1,1824)	1:121:A:HIS:HA	1:122:A:HIS:H	8	0.24
(1,1770)	1:115:A:LEU:H	1:115:A:LEU:HG	14	0.24
(1,1520)	1:100:A:LEU:HA	1:101:A:GLY:H	20	0.24
(1,1055)	1:66:A:VAL:HA	1:67:A:GLN:HG2	17	0.24
(1,1055)	1:66:A:VAL:HA	1:67:A:GLN:HG3	17	0.24
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD11	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD12	18	0.24
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD13	18	0.24
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD21	2	0.24
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD22	2	0.24
(1,994)	1:64:A:LEU:HA	1:64:A:LEU:HD23	2	0.24
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG11	19	0.24
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG12	19	0.24
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG13	19	0.24
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG11	19	0.24
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG12	19	0.24
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG13	19	0.24
(1,577)	1:38:A:LYS:H	1:38:A:LYS:HD2	13	0.24
(1,577)	1:38:A:LYS:H	1:38:A:LYS:HD3	13	0.24
(1,240)	1:10:A:ALA:HB1	1:11:A:GLN:HG2	7	0.24
(1,240)	1:10:A:ALA:HB1	1:11:A:GLN:HG3	7	0.24
(1,240)	1:10:A:ALA:HB2	1:11:A:GLN:HG2	7	0.24
(1,240)	1:10:A:ALA:HB2	1:11:A:GLN:HG3	7	0.24
(1,240)	1:10:A:ALA:HB3	1:11:A:GLN:HG2	7	0.24
(1,240)	1:10:A:ALA:HB3	1:11:A:GLN:HG3	7	0.24
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	8	0.23
(1,1819)	1:119:A:GLU:H	1:119:A:GLU:HG3	12	0.23
(1,1770)	1:115:A:LEU:H	1:115:A:LEU:HG	6	0.23
(1,1445)	1:91:A:TRP:H	1:92:A:ILE:HD11	3	0.23
(1,1445)	1:91:A:TRP:H	1:92:A:ILE:HD12	3	0.23
(1,1445)	1:91:A:TRP:H	1:92:A:ILE:HD13	3	0.23
(1,1256)	1:74:A:LEU:HD21	1:76:A:LYS:H	17	0.23
(1,1256)	1:74:A:LEU:HD22	1:76:A:LYS:H	17	0.23
(1,1256)	1:74:A:LEU:HD23	1:76:A:LYS:H	17	0.23
(1,530)	1:32:A:ARG:HB2	1:39:A:TRP:HD1	10	0.23
(1,530)	1:32:A:ARG:HB3	1:39:A:TRP:HD1	10	0.23
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	15	0.22
(2,43)	1:63:A:ASP:H	1:42:A:LEU:O	10	0.22
(1,1808)	1:118:A:LEU:H	1:118:A:LEU:HG	13	0.22
(1,1797)	1:118:A:LEU:HA	1:119:A:GLU:H	3	0.22
(1,1598)	1:104:A:GLU:H	1:104:A:GLU:HG2	20	0.22
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG21	19	0.22
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG22	19	0.22
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG23	19	0.22
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG2	17	0.22
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG3	17	0.22
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG2	18	0.22
(1,883)	1:56:A:ASP:HA	1:57:A:LYS:HG3	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	6	0.21
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	9	0.21
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	14	0.21
(1,1824)	1:121:A:HIS:HA	1:122:A:HIS:H	11	0.21
(1,1806)	1:118:A:LEU:H	1:118:A:LEU:HD11	4	0.21
(1,1806)	1:118:A:LEU:H	1:118:A:LEU:HD12	4	0.21
(1,1806)	1:118:A:LEU:H	1:118:A:LEU:HD13	4	0.21
(1,1803)	1:118:A:LEU:HD21	1:119:A:GLU:HG2	18	0.21
(1,1803)	1:118:A:LEU:HD21	1:119:A:GLU:HG3	18	0.21
(1,1803)	1:118:A:LEU:HD22	1:119:A:GLU:HG2	18	0.21
(1,1803)	1:118:A:LEU:HD22	1:119:A:GLU:HG3	18	0.21
(1,1803)	1:118:A:LEU:HD23	1:119:A:GLU:HG2	18	0.21
(1,1803)	1:118:A:LEU:HD23	1:119:A:GLU:HG3	18	0.21
(1,1532)	1:100:A:LEU:HD11	1:104:A:GLU:HA	17	0.21
(1,1532)	1:100:A:LEU:HD12	1:104:A:GLU:HA	17	0.21
(1,1532)	1:100:A:LEU:HD13	1:104:A:GLU:HA	17	0.21
(1,1520)	1:100:A:LEU:HA	1:101:A:GLY:H	11	0.21
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	2	0.21
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	14	0.21
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	20	0.21
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG11	9	0.21
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG12	9	0.21
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG13	9	0.21
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG11	9	0.21
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG12	9	0.21
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG13	9	0.21
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	2	0.2
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	13	0.2
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	19	0.2
(1,1815)	1:119:A:GLU:HG2	1:120:A:HIS:HA	14	0.2
(1,1815)	1:119:A:GLU:HG3	1:120:A:HIS:HA	14	0.2
(1,1765)	1:115:A:LEU:HB2	1:116:A:THR:HA	4	0.2
(1,1598)	1:104:A:GLU:H	1:104:A:GLU:HG2	15	0.2
(1,1598)	1:104:A:GLU:H	1:104:A:GLU:HG2	18	0.2
(1,1598)	1:104:A:GLU:H	1:104:A:GLU:HG2	19	0.2
(1,1292)	1:75:A:ARG:HG3	1:82:A:PRO:HD2	16	0.2
(1,1292)	1:75:A:ARG:HG3	1:82:A:PRO:HD3	16	0.2
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD11	2	0.2
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD12	2	0.2
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD13	2	0.2
(1,849)	1:53:A:ILE:HD11	1:55:A:GLY:H	5	0.2
(1,849)	1:53:A:ILE:HD12	1:55:A:GLY:H	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:53:A:ILE:HD13	1:55:A:GLY:H	5	0.2
(1,692)	1:46:A:ILE:H	1:58:A:ARG:HG2	15	0.2
(1,692)	1:46:A:ILE:H	1:58:A:ARG:HG3	15	0.2
(1,577)	1:38:A:LYS:H	1:38:A:LYS:HD2	4	0.2
(1,577)	1:38:A:LYS:H	1:38:A:LYS:HD3	4	0.2
(1,573)	1:37:A:ASP:H	1:38:A:LYS:H	5	0.2
(1,530)	1:32:A:ARG:HB2	1:39:A:TRP:HD1	1	0.2
(1,530)	1:32:A:ARG:HB3	1:39:A:TRP:HD1	1	0.2
(1,253)	1:10:A:ALA:HB1	1:41:A:ALA:HB1	10	0.2
(1,253)	1:10:A:ALA:HB1	1:41:A:ALA:HB2	10	0.2
(1,253)	1:10:A:ALA:HB1	1:41:A:ALA:HB3	10	0.2
(1,253)	1:10:A:ALA:HB2	1:41:A:ALA:HB1	10	0.2
(1,253)	1:10:A:ALA:HB2	1:41:A:ALA:HB2	10	0.2
(1,253)	1:10:A:ALA:HB2	1:41:A:ALA:HB3	10	0.2
(1,253)	1:10:A:ALA:HB3	1:41:A:ALA:HB1	10	0.2
(1,253)	1:10:A:ALA:HB3	1:41:A:ALA:HB2	10	0.2
(1,253)	1:10:A:ALA:HB3	1:41:A:ALA:HB3	10	0.2
(1,240)	1:10:A:ALA:HB1	1:11:A:GLN:HG2	10	0.2
(1,240)	1:10:A:ALA:HB1	1:11:A:GLN:HG3	10	0.2
(1,240)	1:10:A:ALA:HB2	1:11:A:GLN:HG2	10	0.2
(1,240)	1:10:A:ALA:HB2	1:11:A:GLN:HG3	10	0.2
(1,240)	1:10:A:ALA:HB3	1:11:A:GLN:HG2	10	0.2
(1,240)	1:10:A:ALA:HB3	1:11:A:GLN:HG3	10	0.2
(2,25)	1:31:A:PHE:H	1:41:A:ALA:O	7	0.19
(1,1815)	1:119:A:GLU:HG2	1:120:A:HIS:HA	4	0.19
(1,1815)	1:119:A:GLU:HG3	1:120:A:HIS:HA	4	0.19
(1,1797)	1:118:A:LEU:HA	1:119:A:GLU:H	17	0.19
(1,1515)	1:99:A:PRO:HD2	1:100:A:LEU:HG	6	0.19
(1,1515)	1:99:A:PRO:HD3	1:100:A:LEU:HG	6	0.19
(1,1429)	1:89:A:GLU:HG3	1:90:A:HIS:HD1	10	0.19
(1,1416)	1:87:A:ASN:HB2	1:91:A:TRP:HE1	7	0.19
(1,1416)	1:87:A:ASN:HB3	1:91:A:TRP:HE1	7	0.19
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD21	8	0.19
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD22	8	0.19
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD23	8	0.19
(1,1032)	1:65:A:LYS:HD2	1:66:A:VAL:H	8	0.19
(1,1032)	1:65:A:LYS:HD3	1:66:A:VAL:H	8	0.19
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	7	0.19
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG21	20	0.19
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG22	20	0.19
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG23	20	0.19
(1,699)	1:47:A:PRO:HA	1:58:A:ARG:HG2	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,699)	1:47:A:PRO:HA	1:58:A:ARG:HG3	20	0.19
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG2	3	0.19
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG3	3	0.19
(2,57)	1:95:A:LEU:H	1:79:A:GLY:O	12	0.18
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	18	0.18
(2,45)	1:64:A:LEU:H	1:92:A:ILE:O	9	0.18
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	10	0.18
(1,1824)	1:121:A:HIS:HA	1:122:A:HIS:H	3	0.18
(1,1821)	1:119:A:GLU:H	1:120:A:HIS:HB2	20	0.18
(1,1821)	1:119:A:GLU:H	1:120:A:HIS:HB3	20	0.18
(1,1765)	1:115:A:LEU:HB2	1:116:A:THR:HA	6	0.18
(1,1429)	1:89:A:GLU:HG3	1:90:A:HIS:HD1	17	0.18
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD21	16	0.18
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD22	16	0.18
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD23	16	0.18
(1,1343)	1:77:A:LYS:H	1:80:A:ILE:HD11	14	0.18
(1,1343)	1:77:A:LYS:H	1:80:A:ILE:HD12	14	0.18
(1,1343)	1:77:A:LYS:H	1:80:A:ILE:HD13	14	0.18
(1,1278)	1:75:A:ARG:HD2	1:88:A:LYS:HD2	5	0.18
(1,1278)	1:75:A:ARG:HD2	1:88:A:LYS:HD3	5	0.18
(1,1278)	1:75:A:ARG:HD3	1:88:A:LYS:HD2	5	0.18
(1,1278)	1:75:A:ARG:HD3	1:88:A:LYS:HD3	5	0.18
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD21	8	0.18
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD22	8	0.18
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD23	8	0.18
(1,1202)	1:71:A:VAL:HG21	1:75:A:ARG:HG3	8	0.18
(1,1202)	1:71:A:VAL:HG22	1:75:A:ARG:HG3	8	0.18
(1,1202)	1:71:A:VAL:HG23	1:75:A:ARG:HG3	8	0.18
(1,1016)	1:64:A:LEU:HD21	1:112:A:SER:HA	18	0.18
(1,1016)	1:64:A:LEU:HD22	1:112:A:SER:HA	18	0.18
(1,1016)	1:64:A:LEU:HD23	1:112:A:SER:HA	18	0.18
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD11	15	0.18
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD12	15	0.18
(1,995)	1:64:A:LEU:HA	1:74:A:LEU:HD13	15	0.18
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	18	0.18
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG11	15	0.18
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG12	15	0.18
(1,895)	1:57:A:LYS:HG2	1:59:A:VAL:HG13	15	0.18
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG11	15	0.18
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG12	15	0.18
(1,895)	1:57:A:LYS:HG3	1:59:A:VAL:HG13	15	0.18
(1,849)	1:53:A:ILE:HD11	1:55:A:GLY:H	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:53:A:ILE:HD12	1:55:A:GLY:H	17	0.18
(1,849)	1:53:A:ILE:HD13	1:55:A:GLY:H	17	0.18
(1,849)	1:53:A:ILE:HD11	1:55:A:GLY:H	18	0.18
(1,849)	1:53:A:ILE:HD12	1:55:A:GLY:H	18	0.18
(1,849)	1:53:A:ILE:HD13	1:55:A:GLY:H	18	0.18
(1,581)	1:40:A:TYR:HB2	1:91:A:TRP:HD1	16	0.18
(1,581)	1:40:A:TYR:HB3	1:91:A:TRP:HD1	16	0.18
(1,73)	1:3:A:ARG:HE	1:43:A:LEU:HD11	2	0.18
(1,73)	1:3:A:ARG:HE	1:43:A:LEU:HD12	2	0.18
(1,73)	1:3:A:ARG:HE	1:43:A:LEU:HD13	2	0.18
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	10	0.17
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	4	0.17
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	20	0.17
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	3	0.17
(1,1643)	1:106:A:HIS:H	1:106:A:HIS:HD2	8	0.17
(1,1445)	1:91:A:TRP:H	1:92:A:ILE:HD11	8	0.17
(1,1445)	1:91:A:TRP:H	1:92:A:ILE:HD12	8	0.17
(1,1445)	1:91:A:TRP:H	1:92:A:ILE:HD13	8	0.17
(1,1374)	1:80:A:ILE:HG12	1:100:A:LEU:HD11	17	0.17
(1,1374)	1:80:A:ILE:HG12	1:100:A:LEU:HD12	17	0.17
(1,1374)	1:80:A:ILE:HG12	1:100:A:LEU:HD13	17	0.17
(1,1374)	1:80:A:ILE:HG13	1:100:A:LEU:HD11	17	0.17
(1,1374)	1:80:A:ILE:HG13	1:100:A:LEU:HD12	17	0.17
(1,1374)	1:80:A:ILE:HG13	1:100:A:LEU:HD13	17	0.17
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD21	2	0.17
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD22	2	0.17
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD23	2	0.17
(1,1198)	1:71:A:VAL:HG21	1:75:A:ARG:HB2	11	0.17
(1,1198)	1:71:A:VAL:HG21	1:75:A:ARG:HB3	11	0.17
(1,1198)	1:71:A:VAL:HG22	1:75:A:ARG:HB2	11	0.17
(1,1198)	1:71:A:VAL:HG22	1:75:A:ARG:HB3	11	0.17
(1,1198)	1:71:A:VAL:HG23	1:75:A:ARG:HB2	11	0.17
(1,1198)	1:71:A:VAL:HG23	1:75:A:ARG:HB3	11	0.17
(1,760)	1:49:A:GLU:HA	1:53:A:ILE:HG21	18	0.17
(1,760)	1:49:A:GLU:HA	1:53:A:ILE:HG22	18	0.17
(1,760)	1:49:A:GLU:HA	1:53:A:ILE:HG23	18	0.17
(2,57)	1:95:A:LEU:H	1:79:A:GLY:O	20	0.16
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	5	0.16
(2,49)	1:81:A:TYR:H	1:93:A:THR:O	6	0.16
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	10	0.16
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	16	0.16
(1,1812)	1:119:A:GLU:HA	1:120:A:HIS:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1803)	1:118:A:LEU:HD21	1:119:A:GLU:HG2	13	0.16
(1,1803)	1:118:A:LEU:HD21	1:119:A:GLU:HG3	13	0.16
(1,1803)	1:118:A:LEU:HD22	1:119:A:GLU:HG2	13	0.16
(1,1803)	1:118:A:LEU:HD22	1:119:A:GLU:HG3	13	0.16
(1,1803)	1:118:A:LEU:HD23	1:119:A:GLU:HG2	13	0.16
(1,1803)	1:118:A:LEU:HD23	1:119:A:GLU:HG3	13	0.16
(1,1431)	1:89:A:GLU:HG2	1:90:A:HIS:HD1	17	0.16
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD11	6	0.16
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD12	6	0.16
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD13	6	0.16
(1,1082)	1:66:A:VAL:HG21	1:74:A:LEU:HD21	16	0.16
(1,1082)	1:66:A:VAL:HG21	1:74:A:LEU:HD22	16	0.16
(1,1082)	1:66:A:VAL:HG21	1:74:A:LEU:HD23	16	0.16
(1,1082)	1:66:A:VAL:HG22	1:74:A:LEU:HD21	16	0.16
(1,1082)	1:66:A:VAL:HG22	1:74:A:LEU:HD22	16	0.16
(1,1082)	1:66:A:VAL:HG22	1:74:A:LEU:HD23	16	0.16
(1,1082)	1:66:A:VAL:HG23	1:74:A:LEU:HD21	16	0.16
(1,1082)	1:66:A:VAL:HG23	1:74:A:LEU:HD22	16	0.16
(1,1082)	1:66:A:VAL:HG23	1:74:A:LEU:HD23	16	0.16
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	3	0.16
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	6	0.16
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	19	0.16
(1,762)	1:49:A:GLU:HA	1:56:A:ASP:HA	5	0.16
(1,567)	1:36:A:ASN:HD21	1:119:A:GLU:H	2	0.16
(1,567)	1:36:A:ASN:HD22	1:119:A:GLU:H	2	0.16
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG2	8	0.16
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG3	8	0.16
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	11	0.15
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	16	0.15
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	6	0.15
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	13	0.15
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	5	0.15
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	12	0.15
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	19	0.15
(2,25)	1:31:A:PHE:H	1:41:A:ALA:O	12	0.15
(1,1812)	1:119:A:GLU:HA	1:120:A:HIS:H	13	0.15
(1,1743)	1:114:A:GLN:HA	1:117:A:ARG:HB2	11	0.15
(1,1743)	1:114:A:GLN:HA	1:117:A:ARG:HB3	11	0.15
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD21	20	0.15
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD22	20	0.15
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD23	20	0.15
(1,1347)	1:78:A:PRO:HA	1:99:A:PRO:HG3	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:74:A:LEU:HA	1:76:A:LYS:HE2	1	0.15
(1,1235)	1:74:A:LEU:HA	1:76:A:LYS:HE3	1	0.15
(1,1235)	1:74:A:LEU:HA	1:76:A:LYS:HE2	3	0.15
(1,1235)	1:74:A:LEU:HA	1:76:A:LYS:HE3	3	0.15
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD11	17	0.15
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD12	17	0.15
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD13	17	0.15
(1,1086)	1:66:A:VAL:HG21	1:92:A:ILE:HD11	15	0.15
(1,1086)	1:66:A:VAL:HG21	1:92:A:ILE:HD12	15	0.15
(1,1086)	1:66:A:VAL:HG21	1:92:A:ILE:HD13	15	0.15
(1,1086)	1:66:A:VAL:HG22	1:92:A:ILE:HD11	15	0.15
(1,1086)	1:66:A:VAL:HG22	1:92:A:ILE:HD12	15	0.15
(1,1086)	1:66:A:VAL:HG22	1:92:A:ILE:HD13	15	0.15
(1,1086)	1:66:A:VAL:HG23	1:92:A:ILE:HD11	15	0.15
(1,1086)	1:66:A:VAL:HG23	1:92:A:ILE:HD12	15	0.15
(1,1086)	1:66:A:VAL:HG23	1:92:A:ILE:HD13	15	0.15
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG21	19	0.15
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG22	19	0.15
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG23	19	0.15
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG21	19	0.15
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG22	19	0.15
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG23	19	0.15
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG21	19	0.15
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG22	19	0.15
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG23	19	0.15
(1,1058)	1:66:A:VAL:HA	1:115:A:LEU:HD11	4	0.15
(1,1058)	1:66:A:VAL:HA	1:115:A:LEU:HD12	4	0.15
(1,1058)	1:66:A:VAL:HA	1:115:A:LEU:HD13	4	0.15
(1,1007)	1:64:A:LEU:HD11	1:109:A:ILE:HA	2	0.15
(1,1007)	1:64:A:LEU:HD12	1:109:A:ILE:HA	2	0.15
(1,1007)	1:64:A:LEU:HD13	1:109:A:ILE:HA	2	0.15
(1,1007)	1:64:A:LEU:HD11	1:109:A:ILE:HA	7	0.15
(1,1007)	1:64:A:LEU:HD12	1:109:A:ILE:HA	7	0.15
(1,1007)	1:64:A:LEU:HD13	1:109:A:ILE:HA	7	0.15
(1,1007)	1:64:A:LEU:HD11	1:109:A:ILE:HA	9	0.15
(1,1007)	1:64:A:LEU:HD12	1:109:A:ILE:HA	9	0.15
(1,1007)	1:64:A:LEU:HD13	1:109:A:ILE:HA	9	0.15
(1,1007)	1:64:A:LEU:HD11	1:109:A:ILE:HA	18	0.15
(1,1007)	1:64:A:LEU:HD12	1:109:A:ILE:HA	18	0.15
(1,1007)	1:64:A:LEU:HD13	1:109:A:ILE:HA	18	0.15
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	8	0.15
(1,539)	1:33:A:HIS:HB2	1:38:A:LYS:H	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:33:A:HIS:HB3	1:38:A:LYS:H	1	0.15
(1,176)	1:7:A:ILE:HD11	1:31:A:PHE:HD1	4	0.15
(1,176)	1:7:A:ILE:HD11	1:31:A:PHE:HD2	4	0.15
(1,176)	1:7:A:ILE:HD12	1:31:A:PHE:HD1	4	0.15
(1,176)	1:7:A:ILE:HD12	1:31:A:PHE:HD2	4	0.15
(1,176)	1:7:A:ILE:HD13	1:31:A:PHE:HD1	4	0.15
(1,176)	1:7:A:ILE:HD13	1:31:A:PHE:HD2	4	0.15
(1,66)	1:3:A:ARG:HB2	1:96:A:LEU:HD11	14	0.15
(1,66)	1:3:A:ARG:HB2	1:96:A:LEU:HD12	14	0.15
(1,66)	1:3:A:ARG:HB2	1:96:A:LEU:HD13	14	0.15
(1,66)	1:3:A:ARG:HB3	1:96:A:LEU:HD11	14	0.15
(1,66)	1:3:A:ARG:HB3	1:96:A:LEU:HD12	14	0.15
(1,66)	1:3:A:ARG:HB3	1:96:A:LEU:HD13	14	0.15
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	1	0.14
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	16	0.14
(2,31)	1:46:A:ILE:H	1:59:A:VAL:O	6	0.14
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	11	0.14
(2,25)	1:31:A:PHE:H	1:41:A:ALA:O	3	0.14
(2,25)	1:31:A:PHE:H	1:41:A:ALA:O	6	0.14
(1,1825)	1:121:A:HIS:HB2	1:122:A:HIS:H	16	0.14
(1,1825)	1:121:A:HIS:HB3	1:122:A:HIS:H	16	0.14
(1,1728)	1:112:A:SER:HB3	1:116:A:THR:HG21	18	0.14
(1,1728)	1:112:A:SER:HB3	1:116:A:THR:HG22	18	0.14
(1,1728)	1:112:A:SER:HB3	1:116:A:THR:HG23	18	0.14
(1,1643)	1:106:A:HIS:H	1:106:A:HIS:HD2	12	0.14
(1,1286)	1:75:A:ARG:HG2	1:82:A:PRO:HB2	19	0.14
(1,1286)	1:75:A:ARG:HG2	1:82:A:PRO:HB3	19	0.14
(1,1286)	1:75:A:ARG:HG3	1:82:A:PRO:HB2	19	0.14
(1,1286)	1:75:A:ARG:HG3	1:82:A:PRO:HB3	19	0.14
(1,1231)	1:73:A:SER:HB2	1:76:A:LYS:HE2	14	0.14
(1,1231)	1:73:A:SER:HB2	1:76:A:LYS:HE3	14	0.14
(1,1231)	1:73:A:SER:HB3	1:76:A:LYS:HE2	14	0.14
(1,1231)	1:73:A:SER:HB3	1:76:A:LYS:HE3	14	0.14
(1,1059)	1:66:A:VAL:HA	1:115:A:LEU:HD21	15	0.14
(1,1059)	1:66:A:VAL:HA	1:115:A:LEU:HD22	15	0.14
(1,1059)	1:66:A:VAL:HA	1:115:A:LEU:HD23	15	0.14
(1,1016)	1:64:A:LEU:HD21	1:112:A:SER:HA	17	0.14
(1,1016)	1:64:A:LEU:HD22	1:112:A:SER:HA	17	0.14
(1,1016)	1:64:A:LEU:HD23	1:112:A:SER:HA	17	0.14
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	5	0.14
(1,780)	1:50:A:LYS:H	1:50:A:LYS:HG2	2	0.14
(1,780)	1:50:A:LYS:H	1:50:A:LYS:HG3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,762)	1:49:A:GLU:HA	1:56:A:ASP:HA	8	0.14
(1,699)	1:47:A:PRO:HA	1:58:A:ARG:HG2	14	0.14
(1,699)	1:47:A:PRO:HA	1:58:A:ARG:HG3	14	0.14
(1,577)	1:38:A:LYS:H	1:38:A:LYS:HD2	11	0.14
(1,577)	1:38:A:LYS:H	1:38:A:LYS:HD3	11	0.14
(1,559)	1:36:A:ASN:HB2	1:118:A:LEU:HG	5	0.14
(1,559)	1:36:A:ASN:HB3	1:118:A:LEU:HG	5	0.14
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG2	18	0.14
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG3	18	0.14
(1,189)	1:7:A:ILE:HG21	1:11:A:GLN:HE21	10	0.14
(1,189)	1:7:A:ILE:HG22	1:11:A:GLN:HE21	10	0.14
(1,189)	1:7:A:ILE:HG23	1:11:A:GLN:HE21	10	0.14
(1,137)	1:6:A:PHE:HD1	1:43:A:LEU:HD21	6	0.14
(1,137)	1:6:A:PHE:HD1	1:43:A:LEU:HD22	6	0.14
(1,137)	1:6:A:PHE:HD1	1:43:A:LEU:HD23	6	0.14
(1,137)	1:6:A:PHE:HD2	1:43:A:LEU:HD21	6	0.14
(1,137)	1:6:A:PHE:HD2	1:43:A:LEU:HD22	6	0.14
(1,137)	1:6:A:PHE:HD2	1:43:A:LEU:HD23	6	0.14
(1,80)	1:3:A:ARG:HG2	1:43:A:LEU:HD11	14	0.14
(1,80)	1:3:A:ARG:HG2	1:43:A:LEU:HD12	14	0.14
(1,80)	1:3:A:ARG:HG2	1:43:A:LEU:HD13	14	0.14
(2,61)	1:105:A:ILE:H	1:101:A:GLY:O	15	0.13
(2,57)	1:95:A:LEU:H	1:79:A:GLY:O	19	0.13
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	4	0.13
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	20	0.13
(2,47)	1:66:A:VAL:H	1:90:A:HIS:O	16	0.13
(2,45)	1:64:A:LEU:H	1:92:A:ILE:O	2	0.13
(2,45)	1:64:A:LEU:H	1:92:A:ILE:O	7	0.13
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	5	0.13
(2,37)	1:59:A:VAL:H	1:46:A:ILE:O	19	0.13
(2,31)	1:46:A:ILE:H	1:59:A:VAL:O	18	0.13
(1,1824)	1:121:A:HIS:HA	1:122:A:HIS:H	16	0.13
(1,1431)	1:89:A:GLU:HG2	1:90:A:HIS:HD1	20	0.13
(1,1382)	1:80:A:ILE:H	1:80:A:ILE:HD11	8	0.13
(1,1382)	1:80:A:ILE:H	1:80:A:ILE:HD12	8	0.13
(1,1382)	1:80:A:ILE:H	1:80:A:ILE:HD13	8	0.13
(1,1343)	1:77:A:LYS:H	1:80:A:ILE:HD11	13	0.13
(1,1343)	1:77:A:LYS:H	1:80:A:ILE:HD12	13	0.13
(1,1343)	1:77:A:LYS:H	1:80:A:ILE:HD13	13	0.13
(1,1278)	1:75:A:ARG:HD2	1:88:A:LYS:HD2	6	0.13
(1,1278)	1:75:A:ARG:HD2	1:88:A:LYS:HD3	6	0.13
(1,1278)	1:75:A:ARG:HD3	1:88:A:LYS:HD2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1278)	1:75:A:ARG:HD3	1:88:A:LYS:HD3	6	0.13
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD21	14	0.13
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD22	14	0.13
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD23	14	0.13
(1,1246)	1:74:A:LEU:HB2	1:108:A:LEU:HD21	17	0.13
(1,1246)	1:74:A:LEU:HB2	1:108:A:LEU:HD22	17	0.13
(1,1246)	1:74:A:LEU:HB2	1:108:A:LEU:HD23	17	0.13
(1,1246)	1:74:A:LEU:HB3	1:108:A:LEU:HD21	17	0.13
(1,1246)	1:74:A:LEU:HB3	1:108:A:LEU:HD22	17	0.13
(1,1246)	1:74:A:LEU:HB3	1:108:A:LEU:HD23	17	0.13
(1,1235)	1:74:A:LEU:HA	1:76:A:LYS:HE2	5	0.13
(1,1235)	1:74:A:LEU:HA	1:76:A:LYS:HE3	5	0.13
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG21	12	0.13
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG22	12	0.13
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG23	12	0.13
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD11	3	0.13
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD12	3	0.13
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD13	3	0.13
(1,1093)	1:66:A:VAL:H	1:90:A:HIS:H	20	0.13
(1,1083)	1:66:A:VAL:HG21	1:88:A:LYS:HG2	7	0.13
(1,1083)	1:66:A:VAL:HG21	1:88:A:LYS:HG3	7	0.13
(1,1083)	1:66:A:VAL:HG22	1:88:A:LYS:HG2	7	0.13
(1,1083)	1:66:A:VAL:HG22	1:88:A:LYS:HG3	7	0.13
(1,1083)	1:66:A:VAL:HG23	1:88:A:LYS:HG2	7	0.13
(1,1083)	1:66:A:VAL:HG23	1:88:A:LYS:HG3	7	0.13
(1,1083)	1:66:A:VAL:HG21	1:88:A:LYS:HG2	19	0.13
(1,1083)	1:66:A:VAL:HG21	1:88:A:LYS:HG3	19	0.13
(1,1083)	1:66:A:VAL:HG22	1:88:A:LYS:HG2	19	0.13
(1,1083)	1:66:A:VAL:HG22	1:88:A:LYS:HG3	19	0.13
(1,1083)	1:66:A:VAL:HG23	1:88:A:LYS:HG2	19	0.13
(1,1083)	1:66:A:VAL:HG23	1:88:A:LYS:HG3	19	0.13
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG21	13	0.13
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG22	13	0.13
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG23	13	0.13
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG21	13	0.13
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG22	13	0.13
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG23	13	0.13
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG21	13	0.13
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG22	13	0.13
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG23	13	0.13
(1,877)	1:54:A:ASN:H	1:54:A:ASN:HB2	18	0.13
(1,877)	1:54:A:ASN:H	1:54:A:ASN:HB3	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG21	9	0.13
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG22	9	0.13
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG23	9	0.13
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG21	15	0.13
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG22	15	0.13
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG23	15	0.13
(1,849)	1:53:A:ILE:HD11	1:55:A:GLY:H	4	0.13
(1,849)	1:53:A:ILE:HD12	1:55:A:GLY:H	4	0.13
(1,849)	1:53:A:ILE:HD13	1:55:A:GLY:H	4	0.13
(1,849)	1:53:A:ILE:HD11	1:55:A:GLY:H	14	0.13
(1,849)	1:53:A:ILE:HD12	1:55:A:GLY:H	14	0.13
(1,849)	1:53:A:ILE:HD13	1:55:A:GLY:H	14	0.13
(1,831)	1:51:A:ILE:H	1:51:A:ILE:HG12	10	0.13
(1,762)	1:49:A:GLU:HA	1:56:A:ASP:HA	9	0.13
(1,762)	1:49:A:GLU:HA	1:56:A:ASP:HA	12	0.13
(1,524)	1:31:A:PHE:HZ	1:43:A:LEU:HB2	6	0.13
(1,524)	1:31:A:PHE:HZ	1:43:A:LEU:HB3	6	0.13
(1,272)	1:11:A:GLN:HG2	1:15:A:ASP:HA	13	0.13
(1,272)	1:11:A:GLN:HG3	1:15:A:ASP:HA	13	0.13
(1,248)	1:10:A:ALA:HB1	1:16:A:THR:H	5	0.13
(1,248)	1:10:A:ALA:HB2	1:16:A:THR:H	5	0.13
(1,248)	1:10:A:ALA:HB3	1:16:A:THR:H	5	0.13
(1,239)	1:10:A:ALA:HB1	1:11:A:GLN:HE21	3	0.13
(1,239)	1:10:A:ALA:HB2	1:11:A:GLN:HE21	3	0.13
(1,239)	1:10:A:ALA:HB3	1:11:A:GLN:HE21	3	0.13
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG2	17	0.13
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG3	17	0.13
(1,79)	1:3:A:ARG:HG2	1:7:A:ILE:HD11	14	0.13
(1,79)	1:3:A:ARG:HG2	1:7:A:ILE:HD12	14	0.13
(1,79)	1:3:A:ARG:HG2	1:7:A:ILE:HD13	14	0.13
(2,79)	1:114:A:GLN:H	1:110:A:GLU:O	5	0.12
(2,57)	1:95:A:LEU:H	1:79:A:GLY:O	1	0.12
(2,57)	1:95:A:LEU:H	1:79:A:GLY:O	4	0.12
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	14	0.12
(2,47)	1:66:A:VAL:H	1:90:A:HIS:O	8	0.12
(2,45)	1:64:A:LEU:H	1:92:A:ILE:O	18	0.12
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	19	0.12
(2,31)	1:46:A:ILE:H	1:59:A:VAL:O	7	0.12
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	6	0.12
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	8	0.12
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	20	0.12
(2,17)	1:19:A:ASP:H	1:30:A:VAL:O	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,17)	1:19:A:ASP:H	1:30:A:VAL:O	14	0.12
(1,1815)	1:119:A:GLU:HG2	1:120:A:HIS:HA	11	0.12
(1,1815)	1:119:A:GLU:HG3	1:120:A:HIS:HA	11	0.12
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD21	4	0.12
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD22	4	0.12
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD23	4	0.12
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD21	11	0.12
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD22	11	0.12
(1,1370)	1:80:A:ILE:HA	1:100:A:LEU:HD23	11	0.12
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD21	5	0.12
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD22	5	0.12
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD23	5	0.12
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD21	15	0.12
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD22	15	0.12
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD23	15	0.12
(1,1256)	1:74:A:LEU:HD21	1:76:A:LYS:H	4	0.12
(1,1256)	1:74:A:LEU:HD22	1:76:A:LYS:H	4	0.12
(1,1256)	1:74:A:LEU:HD23	1:76:A:LYS:H	4	0.12
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD21	4	0.12
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD22	4	0.12
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD23	4	0.12
(1,1235)	1:74:A:LEU:HA	1:76:A:LYS:HE2	7	0.12
(1,1235)	1:74:A:LEU:HA	1:76:A:LYS:HE3	7	0.12
(1,1203)	1:71:A:VAL:HG21	1:75:A:ARG:HG2	18	0.12
(1,1203)	1:71:A:VAL:HG22	1:75:A:ARG:HG2	18	0.12
(1,1203)	1:71:A:VAL:HG23	1:75:A:ARG:HG2	18	0.12
(1,1198)	1:71:A:VAL:HG21	1:75:A:ARG:HB2	17	0.12
(1,1198)	1:71:A:VAL:HG21	1:75:A:ARG:HB3	17	0.12
(1,1198)	1:71:A:VAL:HG22	1:75:A:ARG:HB2	17	0.12
(1,1198)	1:71:A:VAL:HG22	1:75:A:ARG:HB3	17	0.12
(1,1198)	1:71:A:VAL:HG23	1:75:A:ARG:HB2	17	0.12
(1,1198)	1:71:A:VAL:HG23	1:75:A:ARG:HB3	17	0.12
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG21	7	0.12
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG22	7	0.12
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG23	7	0.12
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG21	18	0.12
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG22	18	0.12
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG23	18	0.12
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD11	12	0.12
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD12	12	0.12
(1,1184)	1:71:A:VAL:HA	1:74:A:LEU:HD13	12	0.12
(1,1083)	1:66:A:VAL:HG21	1:88:A:LYS:HG2	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1083)	1:66:A:VAL:HG21	1:88:A:LYS:HG3	18	0.12
(1,1083)	1:66:A:VAL:HG22	1:88:A:LYS:HG2	18	0.12
(1,1083)	1:66:A:VAL:HG22	1:88:A:LYS:HG3	18	0.12
(1,1083)	1:66:A:VAL:HG23	1:88:A:LYS:HG2	18	0.12
(1,1083)	1:66:A:VAL:HG23	1:88:A:LYS:HG3	18	0.12
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD11	7	0.12
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD12	7	0.12
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD13	7	0.12
(1,1041)	1:65:A:LYS:HE2	1:115:A:LEU:HB2	14	0.12
(1,1041)	1:65:A:LYS:HE2	1:115:A:LEU:HB3	14	0.12
(1,1034)	1:65:A:LYS:HD2	1:115:A:LEU:HB2	6	0.12
(1,1034)	1:65:A:LYS:HD3	1:115:A:LEU:HB2	6	0.12
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG21	10	0.12
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG22	10	0.12
(1,873)	1:53:A:ILE:H	1:59:A:VAL:HG23	10	0.12
(1,849)	1:53:A:ILE:HD11	1:55:A:GLY:H	13	0.12
(1,849)	1:53:A:ILE:HD12	1:55:A:GLY:H	13	0.12
(1,849)	1:53:A:ILE:HD13	1:55:A:GLY:H	13	0.12
(1,762)	1:49:A:GLU:HA	1:56:A:ASP:HA	20	0.12
(1,533)	1:32:A:ARG:H	1:41:A:ALA:HB1	13	0.12
(1,533)	1:32:A:ARG:H	1:41:A:ALA:HB2	13	0.12
(1,533)	1:32:A:ARG:H	1:41:A:ALA:HB3	13	0.12
(1,530)	1:32:A:ARG:HB2	1:39:A:TRP:HD1	9	0.12
(1,530)	1:32:A:ARG:HB3	1:39:A:TRP:HD1	9	0.12
(1,530)	1:32:A:ARG:HB2	1:39:A:TRP:HD1	14	0.12
(1,530)	1:32:A:ARG:HB3	1:39:A:TRP:HD1	14	0.12
(1,526)	1:32:A:ARG:HA	1:40:A:TYR:H	8	0.12
(1,526)	1:32:A:ARG:HA	1:40:A:TYR:H	13	0.12
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD21	15	0.12
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD22	15	0.12
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD23	15	0.12
(1,235)	1:10:A:ALA:HA	1:14:A:TYR:HD1	4	0.12
(1,235)	1:10:A:ALA:HA	1:14:A:TYR:HD2	4	0.12
(2,61)	1:105:A:ILE:H	1:101:A:GLY:O	7	0.11
(2,57)	1:95:A:LEU:H	1:79:A:GLY:O	6	0.11
(2,57)	1:95:A:LEU:H	1:79:A:GLY:O	11	0.11
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	3	0.11
(2,49)	1:81:A:TYR:H	1:93:A:THR:O	19	0.11
(2,43)	1:63:A:ASP:H	1:42:A:LEU:O	17	0.11
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	11	0.11
(2,41)	1:62:A:ILE:H	1:94:A:VAL:O	12	0.11
(2,37)	1:59:A:VAL:H	1:46:A:ILE:O	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,31)	1:46:A:ILE:H	1:59:A:VAL:O	17	0.11
(2,30)	1:44:A:MET:N	1:61:A:VAL:O	12	0.11
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	1	0.11
(2,29)	1:44:A:MET:H	1:61:A:VAL:O	9	0.11
(2,25)	1:31:A:PHE:H	1:41:A:ALA:O	19	0.11
(1,1815)	1:119:A:GLU:HG2	1:120:A:HIS:HA	1	0.11
(1,1815)	1:119:A:GLU:HG3	1:120:A:HIS:HA	1	0.11
(1,1801)	1:118:A:LEU:HB2	1:119:A:GLU:H	17	0.11
(1,1801)	1:118:A:LEU:HB3	1:119:A:GLU:H	17	0.11
(1,1652)	1:107:A:SER:HB2	1:108:A:LEU:HD21	8	0.11
(1,1652)	1:107:A:SER:HB2	1:108:A:LEU:HD22	8	0.11
(1,1652)	1:107:A:SER:HB2	1:108:A:LEU:HD23	8	0.11
(1,1652)	1:107:A:SER:HB3	1:108:A:LEU:HD21	8	0.11
(1,1652)	1:107:A:SER:HB3	1:108:A:LEU:HD22	8	0.11
(1,1652)	1:107:A:SER:HB3	1:108:A:LEU:HD23	8	0.11
(1,1431)	1:89:A:GLU:HG2	1:90:A:HIS:HD1	16	0.11
(1,1373)	1:80:A:ILE:HD11	1:100:A:LEU:HB2	6	0.11
(1,1373)	1:80:A:ILE:HD11	1:100:A:LEU:HB3	6	0.11
(1,1373)	1:80:A:ILE:HD12	1:100:A:LEU:HB2	6	0.11
(1,1373)	1:80:A:ILE:HD12	1:100:A:LEU:HB3	6	0.11
(1,1373)	1:80:A:ILE:HD13	1:100:A:LEU:HB2	6	0.11
(1,1373)	1:80:A:ILE:HD13	1:100:A:LEU:HB3	6	0.11
(1,1292)	1:75:A:ARG:HG3	1:82:A:PRO:HD2	4	0.11
(1,1292)	1:75:A:ARG:HG3	1:82:A:PRO:HD3	4	0.11
(1,1292)	1:75:A:ARG:HG3	1:82:A:PRO:HD2	11	0.11
(1,1292)	1:75:A:ARG:HG3	1:82:A:PRO:HD3	11	0.11
(1,1283)	1:75:A:ARG:HE	1:82:A:PRO:HG2	8	0.11
(1,1283)	1:75:A:ARG:HE	1:82:A:PRO:HG3	8	0.11
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD21	6	0.11
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD22	6	0.11
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD23	6	0.11
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD21	12	0.11
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD22	12	0.11
(1,1242)	1:74:A:LEU:HA	1:108:A:LEU:HD23	12	0.11
(1,1198)	1:71:A:VAL:HG21	1:75:A:ARG:HB2	16	0.11
(1,1198)	1:71:A:VAL:HG21	1:75:A:ARG:HB3	16	0.11
(1,1198)	1:71:A:VAL:HG22	1:75:A:ARG:HB2	16	0.11
(1,1198)	1:71:A:VAL:HG22	1:75:A:ARG:HB3	16	0.11
(1,1198)	1:71:A:VAL:HG23	1:75:A:ARG:HB2	16	0.11
(1,1198)	1:71:A:VAL:HG23	1:75:A:ARG:HB3	16	0.11
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG21	15	0.11
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG22	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG23	15	0.11
(1,1154)	1:69:A:GLU:HG2	1:70:A:LEU:HD21	7	0.11
(1,1154)	1:69:A:GLU:HG2	1:70:A:LEU:HD22	7	0.11
(1,1154)	1:69:A:GLU:HG2	1:70:A:LEU:HD23	7	0.11
(1,1154)	1:69:A:GLU:HG3	1:70:A:LEU:HD21	7	0.11
(1,1154)	1:69:A:GLU:HG3	1:70:A:LEU:HD22	7	0.11
(1,1154)	1:69:A:GLU:HG3	1:70:A:LEU:HD23	7	0.11
(1,1113)	1:67:A:GLN:HE21	1:69:A:GLU:HG2	2	0.11
(1,1113)	1:67:A:GLN:HE21	1:69:A:GLU:HG3	2	0.11
(1,1113)	1:67:A:GLN:HE22	1:69:A:GLU:HG2	2	0.11
(1,1113)	1:67:A:GLN:HE22	1:69:A:GLU:HG3	2	0.11
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG21	8	0.11
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG22	8	0.11
(1,1070)	1:66:A:VAL:HG11	1:92:A:ILE:HG23	8	0.11
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG21	8	0.11
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG22	8	0.11
(1,1070)	1:66:A:VAL:HG12	1:92:A:ILE:HG23	8	0.11
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG21	8	0.11
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG22	8	0.11
(1,1070)	1:66:A:VAL:HG13	1:92:A:ILE:HG23	8	0.11
(1,1059)	1:66:A:VAL:HA	1:115:A:LEU:HD21	9	0.11
(1,1059)	1:66:A:VAL:HA	1:115:A:LEU:HD22	9	0.11
(1,1059)	1:66:A:VAL:HA	1:115:A:LEU:HD23	9	0.11
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG21	11	0.11
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG22	11	0.11
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG23	11	0.11
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD11	17	0.11
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD12	17	0.11
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD13	17	0.11
(1,1036)	1:65:A:LYS:HE2	1:115:A:LEU:HB2	9	0.11
(1,1036)	1:65:A:LYS:HE2	1:115:A:LEU:HB3	9	0.11
(1,1036)	1:65:A:LYS:HE3	1:115:A:LEU:HB2	9	0.11
(1,1036)	1:65:A:LYS:HE3	1:115:A:LEU:HB3	9	0.11
(1,1032)	1:65:A:LYS:HD2	1:66:A:VAL:H	19	0.11
(1,1032)	1:65:A:LYS:HD3	1:66:A:VAL:H	19	0.11
(1,1016)	1:64:A:LEU:HD21	1:112:A:SER:HA	2	0.11
(1,1016)	1:64:A:LEU:HD22	1:112:A:SER:HA	2	0.11
(1,1016)	1:64:A:LEU:HD23	1:112:A:SER:HA	2	0.11
(1,1007)	1:64:A:LEU:HD11	1:109:A:ILE:HA	15	0.11
(1,1007)	1:64:A:LEU:HD12	1:109:A:ILE:HA	15	0.11
(1,1007)	1:64:A:LEU:HD13	1:109:A:ILE:HA	15	0.11
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	15	0.11
(1,867)	1:53:A:ILE:HG21	1:57:A:LYS:H	10	0.11
(1,867)	1:53:A:ILE:HG22	1:57:A:LYS:H	10	0.11
(1,867)	1:53:A:ILE:HG23	1:57:A:LYS:H	10	0.11
(1,849)	1:53:A:ILE:HD11	1:55:A:GLY:H	19	0.11
(1,849)	1:53:A:ILE:HD12	1:55:A:GLY:H	19	0.11
(1,849)	1:53:A:ILE:HD13	1:55:A:GLY:H	19	0.11
(1,762)	1:49:A:GLU:HA	1:56:A:ASP:HA	3	0.11
(1,691)	1:46:A:ILE:H	1:58:A:ARG:HB2	5	0.11
(1,691)	1:46:A:ILE:H	1:58:A:ARG:HB3	5	0.11
(1,597)	1:42:A:LEU:HD11	1:44:A:MET:HE1	16	0.11
(1,597)	1:42:A:LEU:HD11	1:44:A:MET:HE2	16	0.11
(1,597)	1:42:A:LEU:HD11	1:44:A:MET:HE3	16	0.11
(1,597)	1:42:A:LEU:HD12	1:44:A:MET:HE1	16	0.11
(1,597)	1:42:A:LEU:HD12	1:44:A:MET:HE2	16	0.11
(1,597)	1:42:A:LEU:HD12	1:44:A:MET:HE3	16	0.11
(1,597)	1:42:A:LEU:HD13	1:44:A:MET:HE1	16	0.11
(1,597)	1:42:A:LEU:HD13	1:44:A:MET:HE2	16	0.11
(1,597)	1:42:A:LEU:HD13	1:44:A:MET:HE3	16	0.11
(1,597)	1:42:A:LEU:HD11	1:44:A:MET:HE1	18	0.11
(1,597)	1:42:A:LEU:HD11	1:44:A:MET:HE2	18	0.11
(1,597)	1:42:A:LEU:HD11	1:44:A:MET:HE3	18	0.11
(1,597)	1:42:A:LEU:HD12	1:44:A:MET:HE1	18	0.11
(1,597)	1:42:A:LEU:HD12	1:44:A:MET:HE2	18	0.11
(1,597)	1:42:A:LEU:HD12	1:44:A:MET:HE3	18	0.11
(1,597)	1:42:A:LEU:HD13	1:44:A:MET:HE1	18	0.11
(1,597)	1:42:A:LEU:HD13	1:44:A:MET:HE2	18	0.11
(1,597)	1:42:A:LEU:HD13	1:44:A:MET:HE3	18	0.11
(1,577)	1:38:A:LYS:H	1:38:A:LYS:HD2	8	0.11
(1,577)	1:38:A:LYS:H	1:38:A:LYS:HD3	8	0.11
(1,559)	1:36:A:ASN:HB2	1:118:A:LEU:HG	13	0.11
(1,559)	1:36:A:ASN:HB3	1:118:A:LEU:HG	13	0.11
(1,558)	1:36:A:ASN:HB2	1:118:A:LEU:HD21	5	0.11
(1,558)	1:36:A:ASN:HB2	1:118:A:LEU:HD22	5	0.11
(1,558)	1:36:A:ASN:HB2	1:118:A:LEU:HD23	5	0.11
(1,558)	1:36:A:ASN:HB3	1:118:A:LEU:HD21	5	0.11
(1,558)	1:36:A:ASN:HB3	1:118:A:LEU:HD22	5	0.11
(1,558)	1:36:A:ASN:HB3	1:118:A:LEU:HD23	5	0.11
(1,557)	1:36:A:ASN:HB2	1:118:A:LEU:HD11	7	0.11
(1,557)	1:36:A:ASN:HB2	1:118:A:LEU:HD12	7	0.11
(1,557)	1:36:A:ASN:HB2	1:118:A:LEU:HD13	7	0.11
(1,557)	1:36:A:ASN:HB3	1:118:A:LEU:HD11	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:36:A:ASN:HB3	1:118:A:LEU:HD12	7	0.11
(1,557)	1:36:A:ASN:HB3	1:118:A:LEU:HD13	7	0.11
(1,526)	1:32:A:ARG:HA	1:40:A:TYR:H	2	0.11
(1,497)	1:30:A:VAL:HG11	1:42:A:LEU:HB2	3	0.11
(1,497)	1:30:A:VAL:HG11	1:42:A:LEU:HB3	3	0.11
(1,497)	1:30:A:VAL:HG12	1:42:A:LEU:HB2	3	0.11
(1,497)	1:30:A:VAL:HG12	1:42:A:LEU:HB3	3	0.11
(1,497)	1:30:A:VAL:HG13	1:42:A:LEU:HB2	3	0.11
(1,497)	1:30:A:VAL:HG13	1:42:A:LEU:HB3	3	0.11
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD21	8	0.11
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD22	8	0.11
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD23	8	0.11
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD21	11	0.11
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD22	11	0.11
(1,486)	1:30:A:VAL:HA	1:42:A:LEU:HD23	11	0.11
(1,360)	1:19:A:ASP:HB2	1:30:A:VAL:HG21	6	0.11
(1,360)	1:19:A:ASP:HB2	1:30:A:VAL:HG22	6	0.11
(1,360)	1:19:A:ASP:HB2	1:30:A:VAL:HG23	6	0.11
(1,360)	1:19:A:ASP:HB3	1:30:A:VAL:HG21	6	0.11
(1,360)	1:19:A:ASP:HB3	1:30:A:VAL:HG22	6	0.11
(1,360)	1:19:A:ASP:HB3	1:30:A:VAL:HG23	6	0.11
(1,277)	1:12:A:LYS:HA	1:12:A:LYS:HD2	18	0.11
(1,277)	1:12:A:LYS:HA	1:12:A:LYS:HD3	18	0.11
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG2	10	0.11
(1,204)	1:8:A:ASP:HA	1:11:A:GLN:HG3	10	0.11
(1,160)	1:6:A:PHE:HZ	1:64:A:LEU:HD21	2	0.11
(1,160)	1:6:A:PHE:HZ	1:64:A:LEU:HD22	2	0.11
(1,160)	1:6:A:PHE:HZ	1:64:A:LEU:HD23	2	0.11
(1,160)	1:6:A:PHE:HZ	1:64:A:LEU:HD21	9	0.11
(1,160)	1:6:A:PHE:HZ	1:64:A:LEU:HD22	9	0.11
(1,160)	1:6:A:PHE:HZ	1:64:A:LEU:HD23	9	0.11
(2,73)	1:111:A:ASP:H	1:107:A:SER:O	12	0.1
(2,53)	1:93:A:THR:H	1:81:A:TYR:O	12	0.1
(2,39)	1:61:A:VAL:H	1:44:A:MET:O	18	0.1
(2,39)	1:61:A:VAL:H	1:44:A:MET:O	20	0.1
(2,37)	1:59:A:VAL:H	1:46:A:ILE:O	7	0.1
(2,31)	1:46:A:ILE:H	1:59:A:VAL:O	12	0.1
(2,30)	1:44:A:MET:N	1:61:A:VAL:O	5	0.1
(2,17)	1:19:A:ASP:H	1:30:A:VAL:O	10	0.1
(2,17)	1:19:A:ASP:H	1:30:A:VAL:O	11	0.1
(2,1)	1:6:A:PHE:H	1:2:A:ASN:O	14	0.1
(1,1726)	1:112:A:SER:HA	1:116:A:THR:HG21	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1726)	1:112:A:SER:HA	1:116:A:THR:HG22	17	0.1
(1,1726)	1:112:A:SER:HA	1:116:A:THR:HG23	17	0.1
(1,1422)	1:88:A:LYS:HG2	1:92:A:ILE:HG21	16	0.1
(1,1422)	1:88:A:LYS:HG2	1:92:A:ILE:HG22	16	0.1
(1,1422)	1:88:A:LYS:HG2	1:92:A:ILE:HG23	16	0.1
(1,1422)	1:88:A:LYS:HG3	1:92:A:ILE:HG21	16	0.1
(1,1422)	1:88:A:LYS:HG3	1:92:A:ILE:HG22	16	0.1
(1,1422)	1:88:A:LYS:HG3	1:92:A:ILE:HG23	16	0.1
(1,1369)	1:80:A:ILE:HA	1:100:A:LEU:HD11	8	0.1
(1,1369)	1:80:A:ILE:HA	1:100:A:LEU:HD12	8	0.1
(1,1369)	1:80:A:ILE:HA	1:100:A:LEU:HD13	8	0.1
(1,1340)	1:77:A:LYS:HG2	1:108:A:LEU:HD21	16	0.1
(1,1340)	1:77:A:LYS:HG2	1:108:A:LEU:HD22	16	0.1
(1,1340)	1:77:A:LYS:HG2	1:108:A:LEU:HD23	16	0.1
(1,1340)	1:77:A:LYS:HG3	1:108:A:LEU:HD21	16	0.1
(1,1340)	1:77:A:LYS:HG3	1:108:A:LEU:HD22	16	0.1
(1,1340)	1:77:A:LYS:HG3	1:108:A:LEU:HD23	16	0.1
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD21	18	0.1
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD22	18	0.1
(1,1260)	1:74:A:LEU:H	1:74:A:LEU:HD23	18	0.1
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG21	20	0.1
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG22	20	0.1
(1,1190)	1:71:A:VAL:HB	1:92:A:ILE:HG23	20	0.1
(1,1086)	1:66:A:VAL:HG21	1:92:A:ILE:HD11	20	0.1
(1,1086)	1:66:A:VAL:HG21	1:92:A:ILE:HD12	20	0.1
(1,1086)	1:66:A:VAL:HG21	1:92:A:ILE:HD13	20	0.1
(1,1086)	1:66:A:VAL:HG22	1:92:A:ILE:HD11	20	0.1
(1,1086)	1:66:A:VAL:HG22	1:92:A:ILE:HD12	20	0.1
(1,1086)	1:66:A:VAL:HG22	1:92:A:ILE:HD13	20	0.1
(1,1086)	1:66:A:VAL:HG23	1:92:A:ILE:HD11	20	0.1
(1,1086)	1:66:A:VAL:HG23	1:92:A:ILE:HD12	20	0.1
(1,1086)	1:66:A:VAL:HG23	1:92:A:ILE:HD13	20	0.1
(1,1075)	1:66:A:VAL:HG21	1:70:A:LEU:HD11	6	0.1
(1,1075)	1:66:A:VAL:HG21	1:70:A:LEU:HD12	6	0.1
(1,1075)	1:66:A:VAL:HG21	1:70:A:LEU:HD13	6	0.1
(1,1075)	1:66:A:VAL:HG22	1:70:A:LEU:HD11	6	0.1
(1,1075)	1:66:A:VAL:HG22	1:70:A:LEU:HD12	6	0.1
(1,1075)	1:66:A:VAL:HG22	1:70:A:LEU:HD13	6	0.1
(1,1075)	1:66:A:VAL:HG23	1:70:A:LEU:HD11	6	0.1
(1,1075)	1:66:A:VAL:HG23	1:70:A:LEU:HD12	6	0.1
(1,1075)	1:66:A:VAL:HG23	1:70:A:LEU:HD13	6	0.1
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG21	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG22	8	0.1
(1,1052)	1:65:A:LYS:H	1:116:A:THR:HG23	8	0.1
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD11	18	0.1
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD12	18	0.1
(1,1049)	1:65:A:LYS:H	1:74:A:LEU:HD13	18	0.1
(1,1016)	1:64:A:LEU:HD21	1:112:A:SER:HA	7	0.1
(1,1016)	1:64:A:LEU:HD22	1:112:A:SER:HA	7	0.1
(1,1016)	1:64:A:LEU:HD23	1:112:A:SER:HA	7	0.1
(1,983)	1:62:A:ILE:HG21	1:64:A:LEU:HB2	15	0.1
(1,983)	1:62:A:ILE:HG21	1:64:A:LEU:HB3	15	0.1
(1,983)	1:62:A:ILE:HG22	1:64:A:LEU:HB2	15	0.1
(1,983)	1:62:A:ILE:HG22	1:64:A:LEU:HB3	15	0.1
(1,983)	1:62:A:ILE:HG23	1:64:A:LEU:HB2	15	0.1
(1,983)	1:62:A:ILE:HG23	1:64:A:LEU:HB3	15	0.1
(1,947)	1:60:A:ASP:H	1:97:A:ASN:HA	13	0.1
(1,638)	1:44:A:MET:HE1	1:62:A:ILE:HA	19	0.1
(1,638)	1:44:A:MET:HE2	1:62:A:ILE:HA	19	0.1
(1,638)	1:44:A:MET:HE3	1:62:A:ILE:HA	19	0.1
(1,539)	1:33:A:HIS:HB2	1:38:A:LYS:H	12	0.1
(1,539)	1:33:A:HIS:HB3	1:38:A:LYS:H	12	0.1
(1,526)	1:32:A:ARG:HA	1:40:A:TYR:H	20	0.1
(1,5)	1:1:A:MET:HB2	1:1:A:MET:HE1	4	0.1
(1,5)	1:1:A:MET:HB2	1:1:A:MET:HE2	4	0.1
(1,5)	1:1:A:MET:HB2	1:1:A:MET:HE3	4	0.1
(1,5)	1:1:A:MET:HB3	1:1:A:MET:HE1	4	0.1
(1,5)	1:1:A:MET:HB3	1:1:A:MET:HE2	4	0.1
(1,5)	1:1:A:MET:HB3	1:1:A:MET:HE3	4	0.1

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

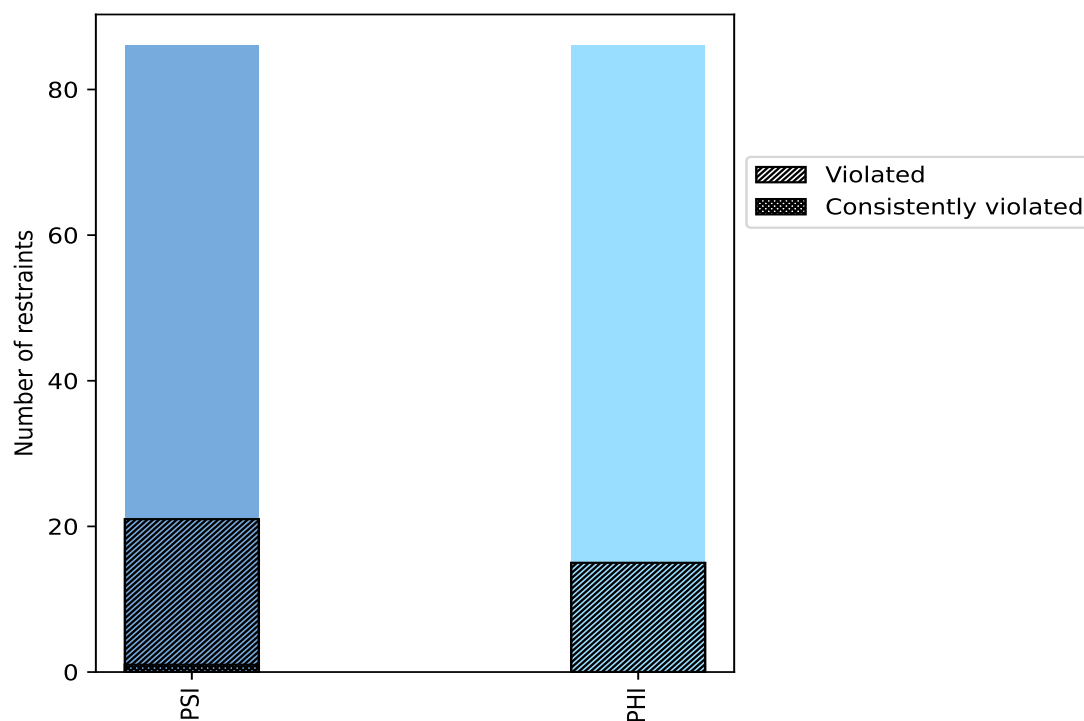
10.1 Summary of dihedral-angle violations [i](#)

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	86	50.0	21	24.4	12.2	1	1.2	0.6
PHI	86	50.0	15	17.4	8.7	0	0.0	0.0
Total	172	100.0	36	20.9	20.9	1	0.6	0.6

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](#)



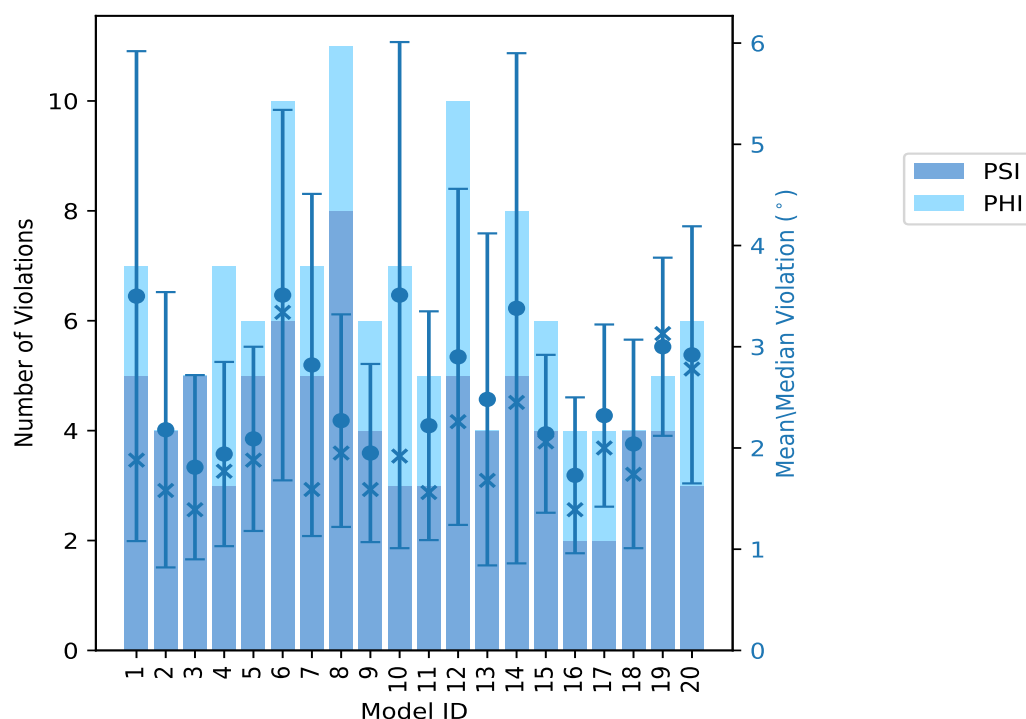
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	5	2	7	3.5	7.28	2.42	1.88
2	4	0	4	2.18	4.49	1.36	1.58
3	5	0	5	1.81	3.57	0.91	1.39
4	3	4	7	1.94	3.83	0.91	1.77
5	5	1	6	2.09	3.98	0.91	1.88
6	6	4	10	3.51	6.54	1.83	3.34
7	5	2	7	2.82	5.04	1.69	1.59
8	8	3	11	2.27	4.5	1.05	1.95
9	4	2	6	1.95	3.76	0.88	1.59
10	3	4	7	3.51	7.49	2.5	1.92
11	3	2	5	2.22	4.0	1.13	1.56
12	5	5	10	2.9	5.65	1.66	2.26
13	4	0	4	2.48	5.3	1.64	1.68
14	5	3	8	3.38	7.62	2.52	2.45
15	4	2	6	2.14	3.6	0.78	2.06
16	2	2	4	1.73	3.02	0.77	1.39
17	2	2	4	2.32	3.76	0.9	2.0
18	4	0	4	2.04	3.58	1.03	1.74
19	4	1	5	3.0	4.26	0.88	3.13
20	3	3	6	2.92	4.99	1.27	2.78

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
10	8	18	1	5.0
3	3	6	2	10.0
3	1	4	3	15.0
0	1	1	4	20.0
1	0	1	5	25.0
0	0	0	6	30.0
0	1	1	7	35.0
0	0	0	8	40.0
1	0	1	9	45.0
1	0	1	10	50.0
0	0	0	11	55.0

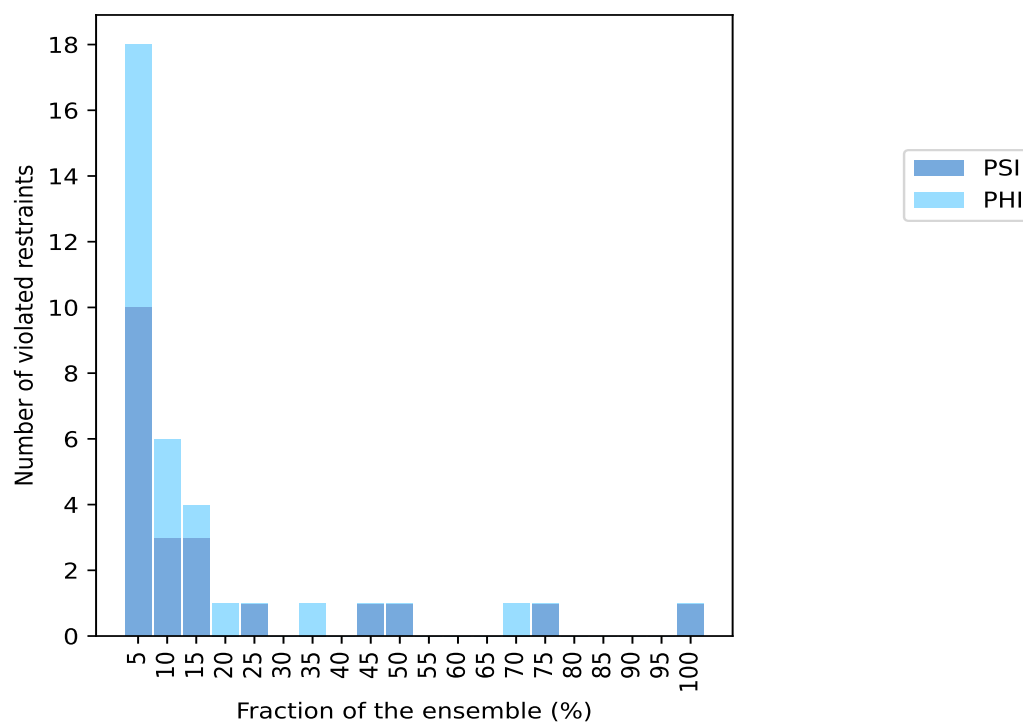
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	1	1	14	70.0
1	0	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
1	0	1	20	100.0

¹ Number of models with violations

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

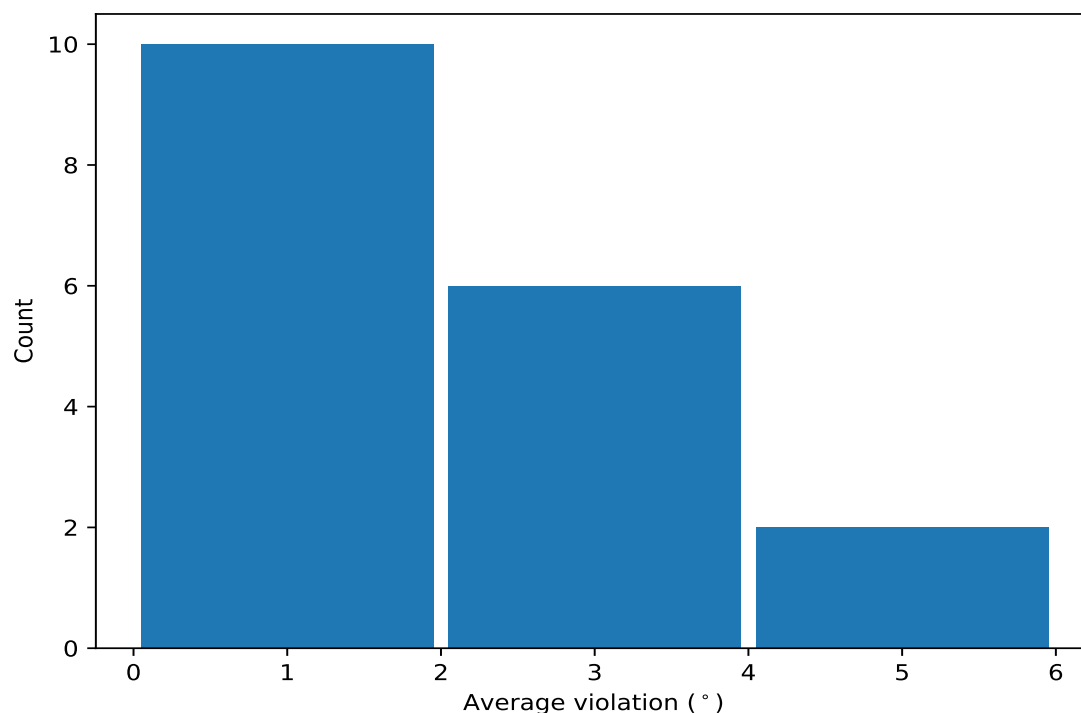


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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.

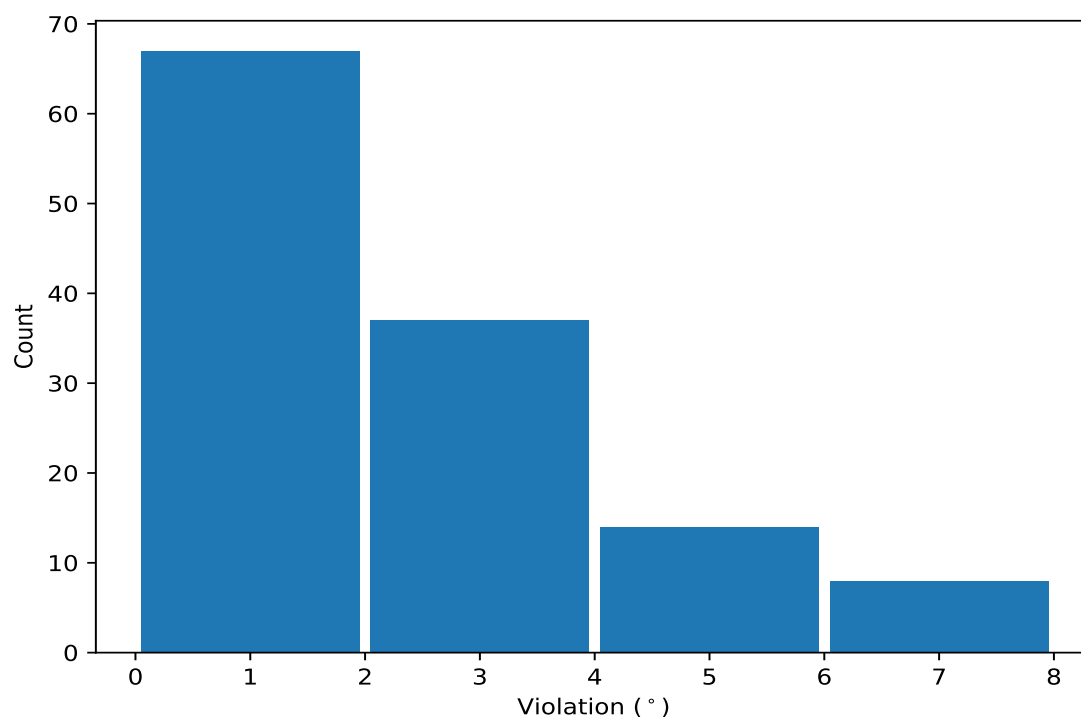
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	20	4.0	0.64	3.9
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	15	1.87	0.45	1.77
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	14	3.99	2.3	3.88
(1,64)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:ALA:N	10	4.95	2.21	5.26
(1,172)	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	1:117:A:ARG:N	9	1.48	0.6	1.27
(1,55)	1:32:A:ARG:C	1:33:A:HIS:N	1:33:A:HIS:CA	1:33:A:HIS:C	7	2.08	1.04	1.51
(1,28)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PRO:N	5	1.85	0.41	1.95
(1,117)	1:73:A:SER:C	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	4	2.23	0.76	1.96
(1,21)	1:12:A:LYS:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	3	2.49	0.63	2.77
(1,60)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:ASN:N	3	1.74	0.44	1.82
(1,122)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:LYS:N	3	1.7	0.24	1.86
(1,114)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:SER:N	3	1.12	0.07	1.08
(1,61)	1:35:A:ASP:C	1:36:A:ASN:N	1:36:A:ASN:CA	1:36:A:ASN:C	2	2.79	0.99	2.79
(1,54)	1:32:A:ARG:N	1:32:A:ARG:CA	1:32:A:ARG:C	1:33:A:HIS:N	2	2.15	0.41	2.15
(1,62)	1:36:A:ASN:N	1:36:A:ASN:CA	1:36:A:ASN:C	1:37:A:ASP:N	2	1.8	0.03	1.8
(1,121)	1:75:A:ARG:C	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	2	1.73	0.18	1.73
(1,63)	1:39:A:TRP:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	2	1.58	0.34	1.58
(1,116)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LEU:N	2	1.44	0.02	1.44

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 (°)
(1,64)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:ALA:N	14	7.62
(1,64)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:ALA:N	10	7.49
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	14	7.29
(1,64)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:ALA:N	1	7.28
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1	7.16
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	10	6.83
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	6	6.54
(1,64)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:ALA:N	6	6.46
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	12	5.65
(1,64)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:ALA:N	12	5.57
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	13	5.3
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	7	5.04
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	20	4.99
(1,64)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:ALA:N	7	4.96

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	6	4.68
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	8	4.5
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	2	4.49
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	19	4.26
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	7	4.25
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	10	4.22
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	12	4.22
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	11	4.0
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	5	3.98
(1,55)	1:32:A:ARG:C	1:33:A:HIS:N	1:33:A:HIS:CA	1:33:A:HIS:C	6	3.92
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	4	3.83
(1,61)	1:35:A:ASP:C	1:36:A:ASN:N	1:36:A:ASN:CA	1:36:A:ASN:C	20	3.78
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	9	3.76
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	17	3.76
(1,64)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:ALA:N	8	3.73
(1,130)	1:81:A:TYR:N	1:81:A:TYR:CA	1:81:A:TYR:C	1:82:A:PRO:N	6	3.6
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	15	3.6
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	18	3.58
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	3	3.57
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	14	3.53
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	19	3.51
(1,55)	1:32:A:ARG:C	1:33:A:HIS:N	1:33:A:HIS:CA	1:33:A:HIS:C	12	3.51
(1,117)	1:73:A:SER:C	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	14	3.47
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	1	3.32
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	20	3.32
(1,64)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:ALA:N	19	3.13
(1,21)	1:12:A:LYS:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	11	3.08
(1,172)	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	1:117:A:ARG:N	6	3.07
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	16	3.02
(1,76)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:PRO:N	8	2.82
(1,21)	1:12:A:LYS:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	12	2.77
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	8	2.63
(1,54)	1:32:A:ARG:N	1:32:A:ARG:CA	1:32:A:ARG:C	1:33:A:HIS:N	6	2.57
(1,118)	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	1:75:A:ARG:N	8	2.49
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	17	2.41
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	18	2.35
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	19	2.33
(1,23)	1:13:A:LYS:C	1:14:A:TYR:N	1:14:A:TYR:CA	1:14:A:TYR:C	4	2.32
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	15	2.3
(1,28)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PRO:N	15	2.29
(1,28)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PRO:N	9	2.27
(1,60)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:ASN:N	20	2.23
(1,117)	1:73:A:SER:C	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	4	2.21
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	5	2.15
(1,64)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:ALA:N	20	2.07
(1,28)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PRO:N	8	1.95
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	13	1.93
(1,63)	1:39:A:TRP:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	10	1.92
(1,121)	1:75:A:ARG:C	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	5	1.91
(1,122)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:LYS:N	1	1.88
(1,122)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:LYS:N	5	1.86

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,62)	1:36:A:ASN:N	1:36:A:ASN:CA	1:36:A:ASN:C	1:37:A:ASP:N	8	1.83
(1,60)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:ASN:N	15	1.82
(1,168)	1:114:A:GLN:N	1:114:A:GLN:CA	1:114:A:GLN:C	1:115:A:LEU:N	6	1.8
(1,61)	1:35:A:ASP:C	1:36:A:ASN:N	1:36:A:ASN:CA	1:36:A:ASN:C	15	1.8
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	4	1.77
(1,62)	1:36:A:ASN:N	1:36:A:ASN:CA	1:36:A:ASN:C	1:37:A:ASP:N	2	1.77
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	3	1.77
(1,172)	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	1:117:A:ARG:N	19	1.76
(1,54)	1:32:A:ARG:N	1:32:A:ARG:CA	1:32:A:ARG:C	1:33:A:HIS:N	12	1.74
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	1	1.73
(1,117)	1:73:A:SER:C	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	9	1.71
(1,55)	1:32:A:ARG:C	1:33:A:HIS:N	1:33:A:HIS:CA	1:33:A:HIS:C	16	1.64
(1,21)	1:12:A:LYS:C	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1	1.61
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	17	1.6
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	7	1.59
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	11	1.56
(1,121)	1:75:A:ARG:C	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	12	1.55
(1,172)	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	1:117:A:ARG:N	1	1.53
(1,117)	1:73:A:SER:C	1:74:A:LEU:N	1:74:A:LEU:CA	1:74:A:LEU:C	8	1.53
(1,55)	1:32:A:ARG:C	1:33:A:HIS:N	1:33:A:HIS:CA	1:33:A:HIS:C	17	1.51
(1,82)	1:49:A:GLU:N	1:49:A:GLU:CA	1:49:A:GLU:C	1:50:A:LYS:N	7	1.48
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	9	1.47
(1,116)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LEU:N	5	1.46
(1,28)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PRO:N	13	1.43
(1,116)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:LEU:N	14	1.42
(1,55)	1:32:A:ARG:C	1:33:A:HIS:N	1:33:A:HIS:CA	1:33:A:HIS:C	7	1.4
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	2	1.4
(1,55)	1:32:A:ARG:C	1:33:A:HIS:N	1:33:A:HIS:CA	1:33:A:HIS:C	10	1.39
(1,24)	1:14:A:TYR:N	1:14:A:TYR:CA	1:14:A:TYR:C	1:15:A:ASP:N	3	1.39
(1,122)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:LYS:N	12	1.36
(1,80)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:GLU:N	10	1.36
(1,171)	1:115:A:LEU:C	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	10	1.35
(1,172)	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	1:117:A:ARG:N	11	1.32
(1,28)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PRO:N	3	1.32
(1,93)	1:59:A:VAL:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	12	1.29
(1,77)	1:46:A:ILE:C	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	14	1.29
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	12	1.29
(1,57)	1:33:A:HIS:C	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	8	1.28
(1,172)	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	1:117:A:ARG:N	13	1.27
(1,133)	1:90:A:HIS:C	1:91:A:TRP:N	1:91:A:TRP:CA	1:91:A:TRP:C	6	1.26
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	9	1.25
(1,63)	1:39:A:TRP:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	6	1.25
(1,172)	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	1:117:A:ARG:N	14	1.23
(1,64)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:ALA:N	9	1.22
(1,55)	1:32:A:ARG:C	1:33:A:HIS:N	1:33:A:HIS:CA	1:33:A:HIS:C	4	1.22
(1,114)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:SER:N	14	1.21
(1,34)	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	1:21:A:PRO:N	4	1.17
(1,60)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:ASN:N	5	1.16
(1,129)	1:80:A:ILE:C	1:81:A:TYR:N	1:81:A:TYR:CA	1:81:A:TYR:C	16	1.14
(1,172)	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	1:117:A:ARG:N	18	1.13
(1,170)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:THR:N	16	1.13

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	11	1.13
(1,58)	1:34:A:SER:N	1:34:A:SER:CA	1:34:A:SER:C	1:35:A:ASP:N	8	1.12
(1,33)	1:19:A:ASP:C	1:20:A:HIS:N	1:20:A:HIS:CA	1:20:A:HIS:C	20	1.1
(1,114)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:SER:N	18	1.08
(1,114)	1:72:A:GLY:N	1:72:A:GLY:CA	1:72:A:GLY:C	1:73:A:SER:N	8	1.06
(1,22)	1:13:A:LYS:N	1:13:A:LYS:CA	1:13:A:LYS:C	1:14:A:TYR:N	2	1.06
(1,66)	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	1:42:A:LEU:N	7	1.04
(1,65)	1:40:A:TYR:C	1:41:A:ALA:N	1:41:A:ALA:CA	1:41:A:ALA:C	15	1.04
(1,172)	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	1:117:A:ARG:N	4	1.03
(1,172)	1:116:A:THR:N	1:116:A:THR:CA	1:116:A:THR:C	1:117:A:ARG:N	3	1.01