



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 04:59 PM EST

PDB ID : 2LOV
BMRB ID : 18226
Title : AR55 solubilised in LPPG micelles
Authors : Langelaan, D.N.; Rainey, J.K.
Deposited on : 2012-01-27

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 : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

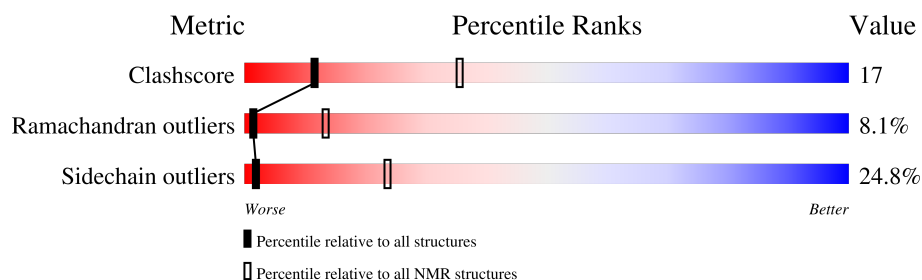
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	64	

2 Ensemble composition and analysis

This entry contains 40 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:27-A:43 (17)	0.94	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 7 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 6, 7, 9, 11, 14, 16, 18, 26, 28, 36, 38
2	3, 10, 15, 19, 20, 22, 27, 32, 33
3	2, 17, 31
4	24, 29, 39
5	13, 34
6	8, 12
7	23, 30
Single-model clusters	21; 25; 35; 37; 40

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 988 atoms, of which 472 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apelin receptor.

Mol	Chain	Residues	Atoms						Trace
1	A	64	Total	C	H	N	O	S	0
			988	329	472	88	96	3	

There are 9 discrepancies between the modelled and reference sequences:

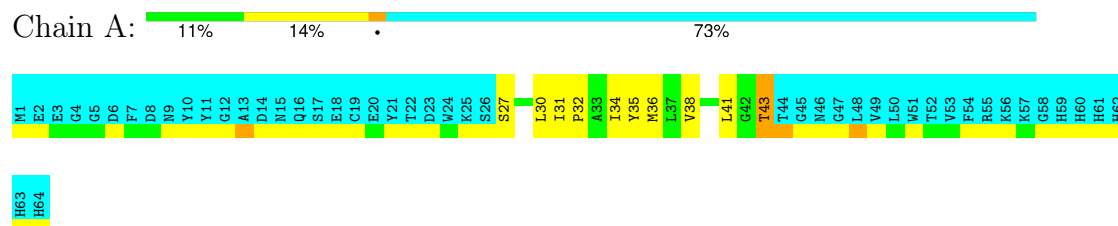
Chain	Residue	Modelled	Actual	Comment	Reference
A	56	LYS	-	expression tag	UNP P35414
A	57	LYS	-	expression tag	UNP P35414
A	58	GLY	-	expression tag	UNP P35414
A	59	HIS	-	expression tag	UNP P35414
A	60	HIS	-	expression tag	UNP P35414
A	61	HIS	-	expression tag	UNP P35414
A	62	HIS	-	expression tag	UNP P35414
A	63	HIS	-	expression tag	UNP P35414
A	64	HIS	-	expression tag	UNP P35414

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Apelin receptor

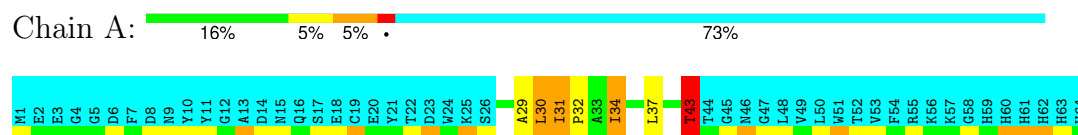


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

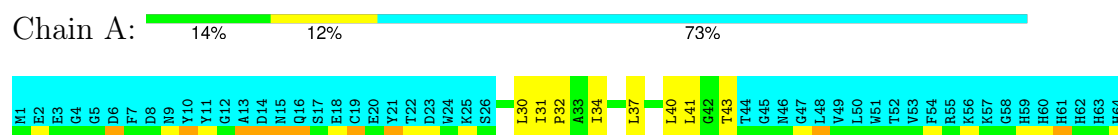
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Apelin receptor



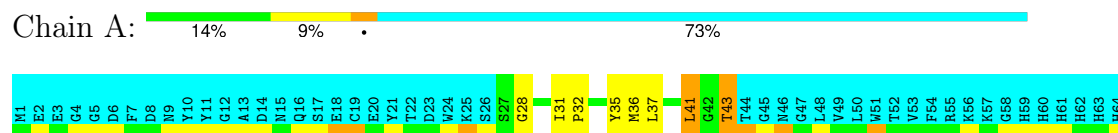
4.2.2 Score per residue for model 2

- Molecule 1: Apelin receptor



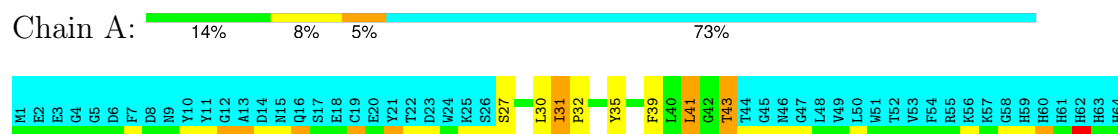
4.2.3 Score per residue for model 3

- Molecule 1: Apelin receptor



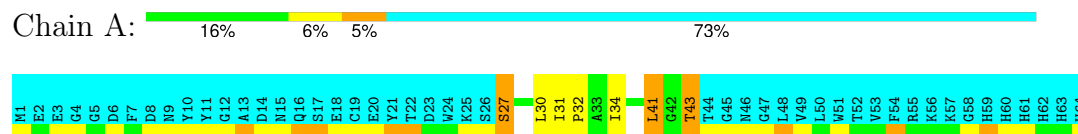
4.2.4 Score per residue for model 4

- Molecule 1: Apelin receptor



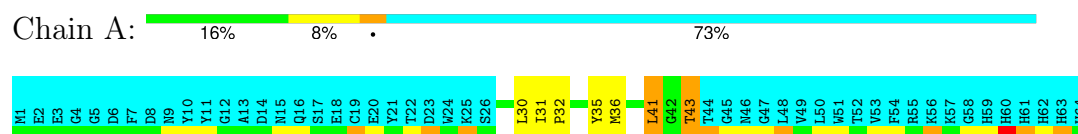
4.2.5 Score per residue for model 5

- Molecule 1: Apelin receptor



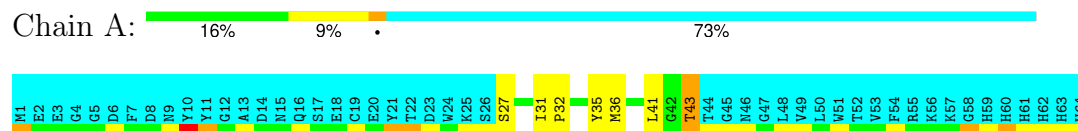
4.2.6 Score per residue for model 6

- Molecule 1: Apelin receptor



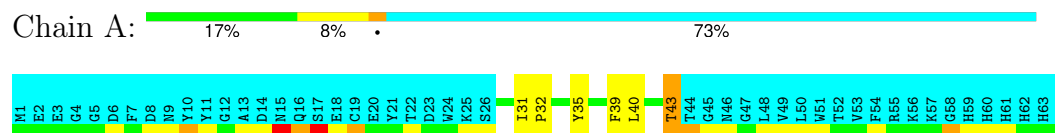
4.2.7 Score per residue for model 7

- Molecule 1: Apelin receptor



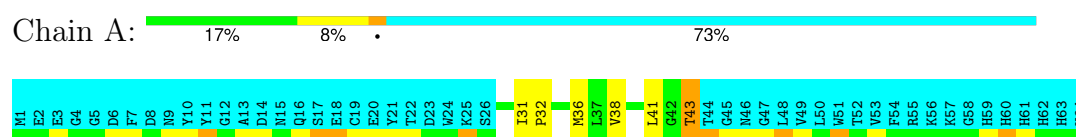
4.2.8 Score per residue for model 8

- Molecule 1: Apelin receptor



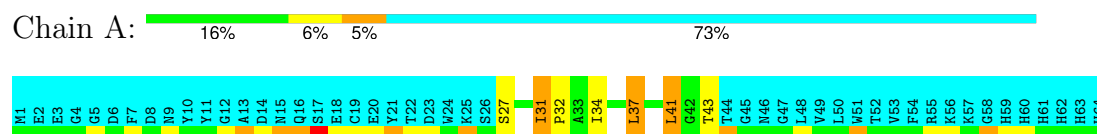
4.2.9 Score per residue for model 9

- Molecule 1: Apelin receptor



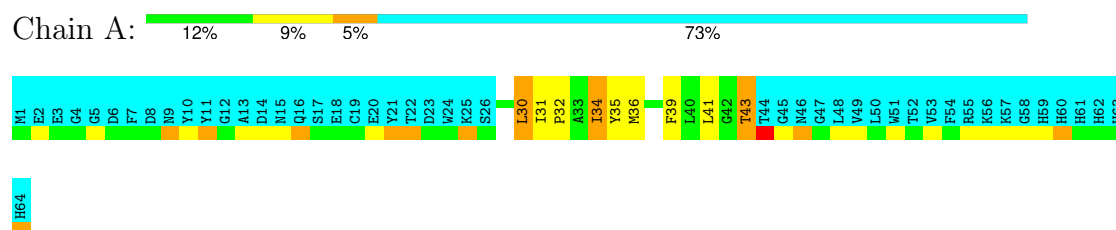
4.2.10 Score per residue for model 10

- Molecule 1: Apelin receptor



4.2.11 Score per residue for model 11

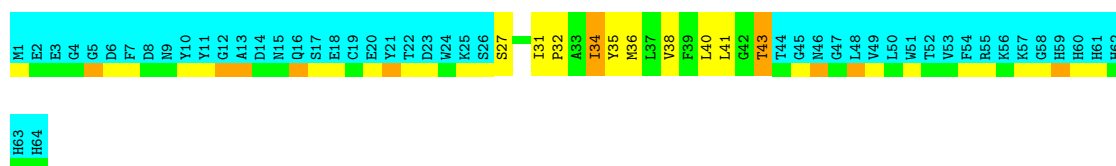
- Molecule 1: Apelin receptor



4.2.12 Score per residue for model 12

- Molecule 1: Apelin receptor

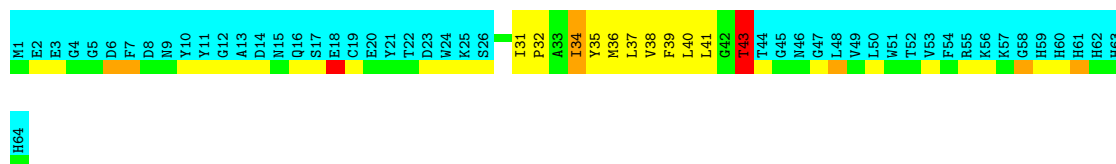




4.2.13 Score per residue for model 13

- Molecule 1: Apelin receptor

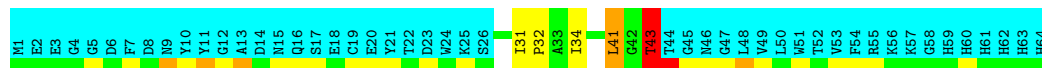
Chain A: 9% 14% . . 73%



4.2.14 Score per residue for model 14

- Molecule 1: Apelin receptor

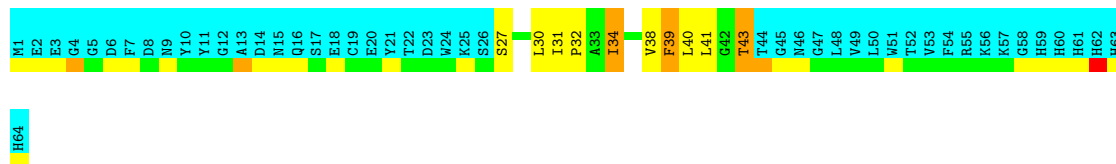
Chain A: 19% 5% . . 73%



4.2.15 Score per residue for model 15

- Molecule 1: Apelin receptor

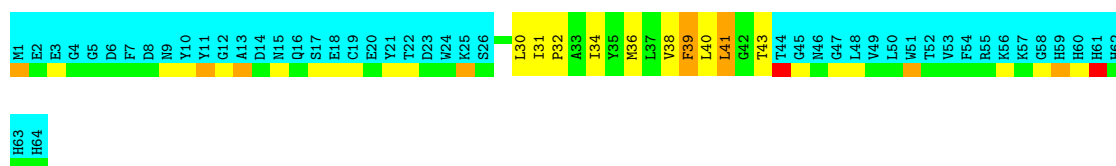
Chain A: 11% 11% 5% 73%



4.2.16 Score per residue for model 16

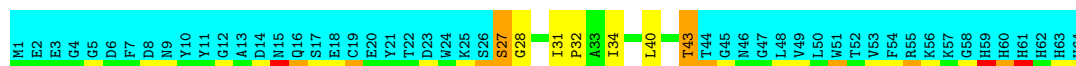
- Molecule 1: Apelin receptor

Chain A: 11% 12% . 73%



4.2.17 Score per residue for model 17

- Molecule 1: Apelin receptor



4.2.18 Score per residue for model 18

- Molecule 1: Apelin receptor



4.2.19 Score per residue for model 19

- Molecule 1: Apelin receptor



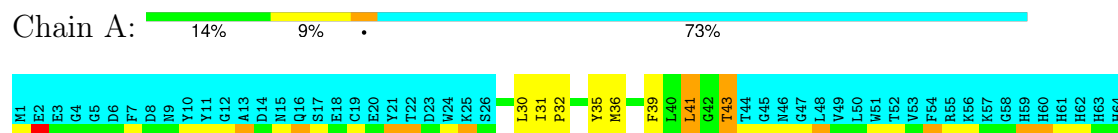
4.2.20 Score per residue for model 20

- Molecule 1: Apelin receptor



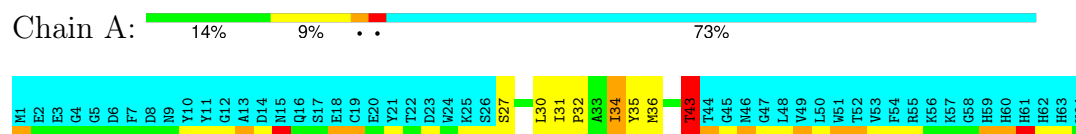
4.2.21 Score per residue for model 21

- Molecule 1: Apelin receptor



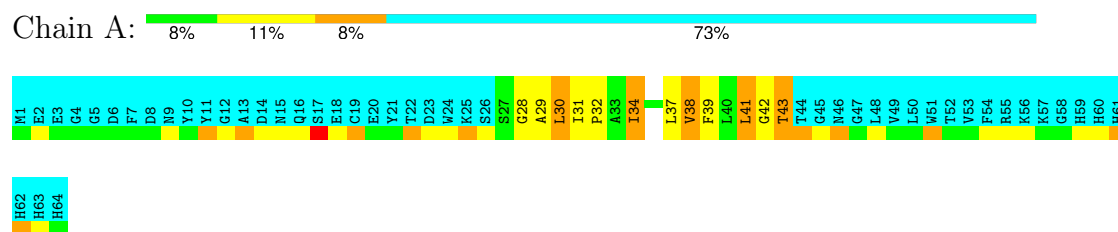
4.2.22 Score per residue for model 22

- Molecule 1: Apelin receptor



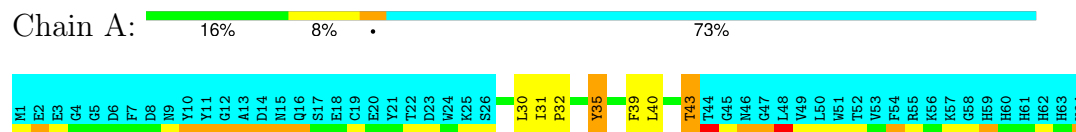
4.2.23 Score per residue for model 23

- Molecule 1: Apelin receptor



4.2.24 Score per residue for model 24

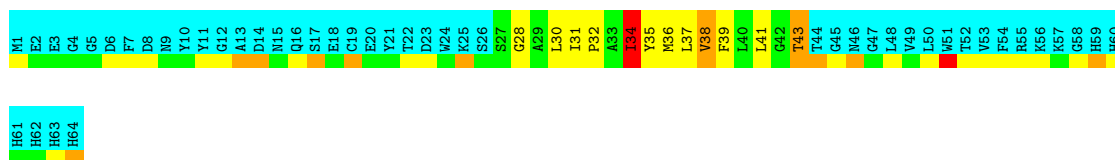
- Molecule 1: Apelin receptor



4.2.25 Score per residue for model 25

- Molecule 1: Apelin receptor

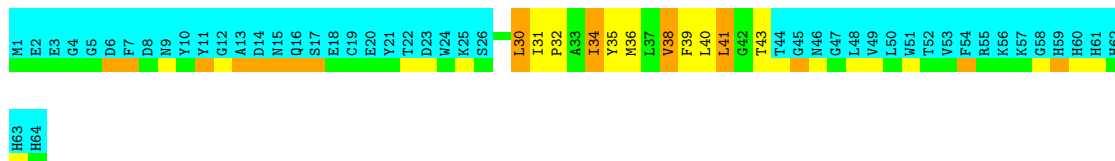




4.2.26 Score per residue for model 26

- Molecule 1: Apelin receptor

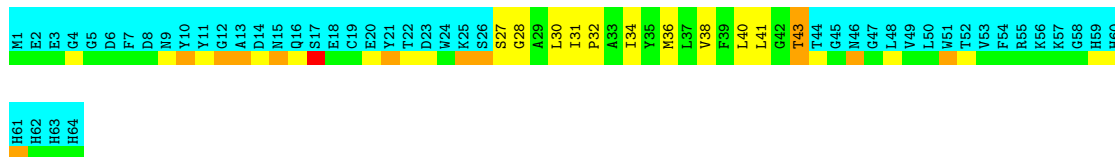
Chain A: 9% 11% 6% 73%



4.2.27 Score per residue for model 27

- Molecule 1: Apelin receptor

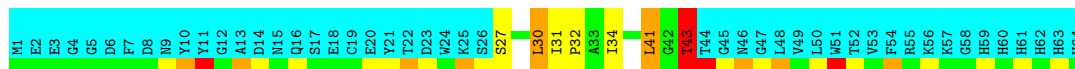
Chain A: 9% 16% . 73%



4.2.28 Score per residue for model 28

- Molecule 1: Apelin receptor

Chain A: 16% 6% . . 73%



4.2.29 Score per residue for model 29

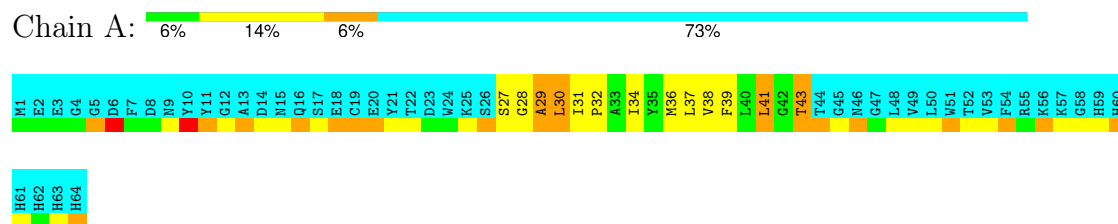
- Molecule 1: Apelin receptor

Chain A: 14% 11% . 73%



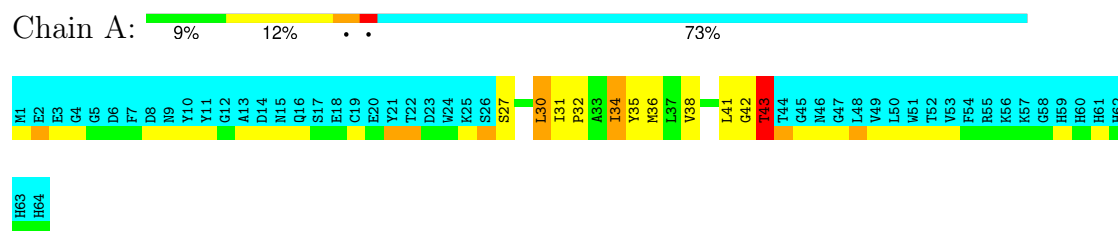
4.2.30 Score per residue for model 30

- Molecule 1: Apelin receptor



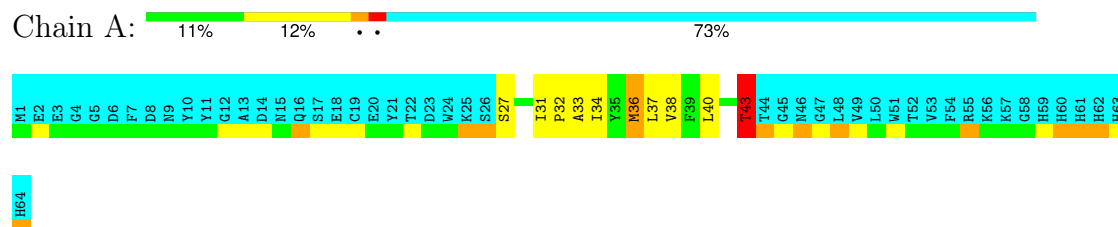
4.2.31 Score per residue for model 31

- Molecule 1: Apelin receptor



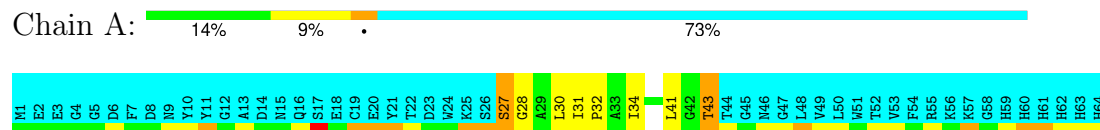
4.2.32 Score per residue for model 32

- Molecule 1: Apelin receptor



4.2.33 Score per residue for model 33

- Molecule 1: Apelin receptor



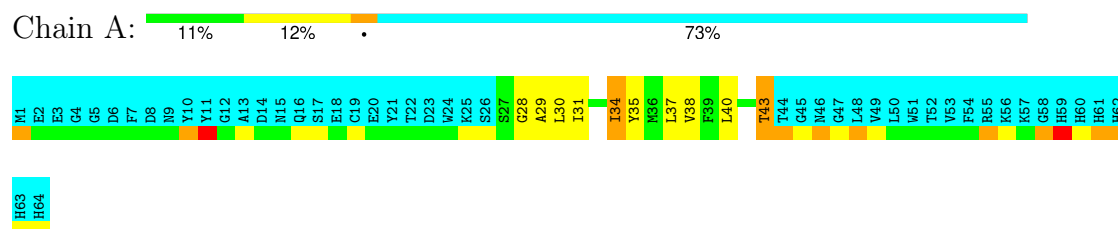
4.2.34 Score per residue for model 34

- Molecule 1: Apelin receptor



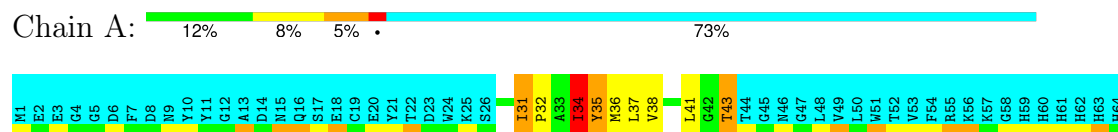
4.2.35 Score per residue for model 35

- Molecule 1: Apelin receptor



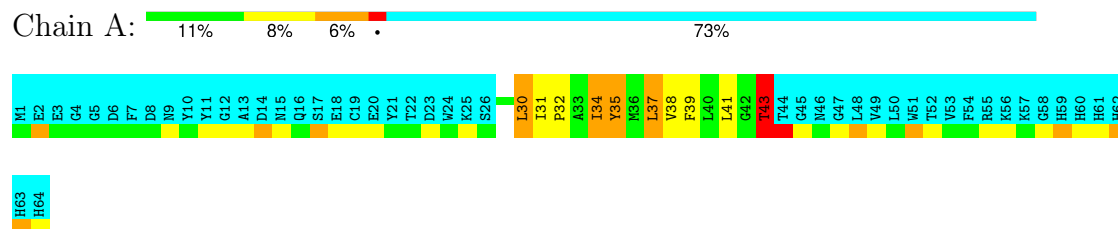
4.2.36 Score per residue for model 36

- Molecule 1: Apelin receptor



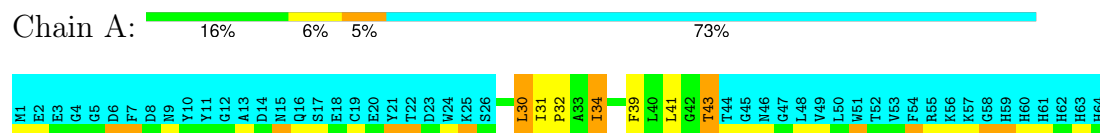
4.2.37 Score per residue for model 37

- Molecule 1: Apelin receptor



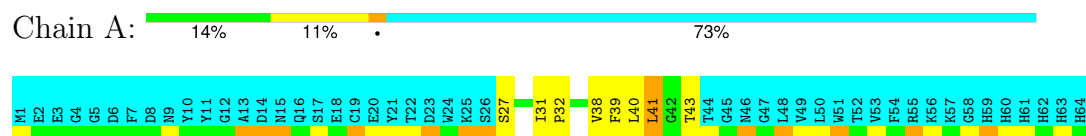
4.2.38 Score per residue for model 38

- Molecule 1: Apelin receptor



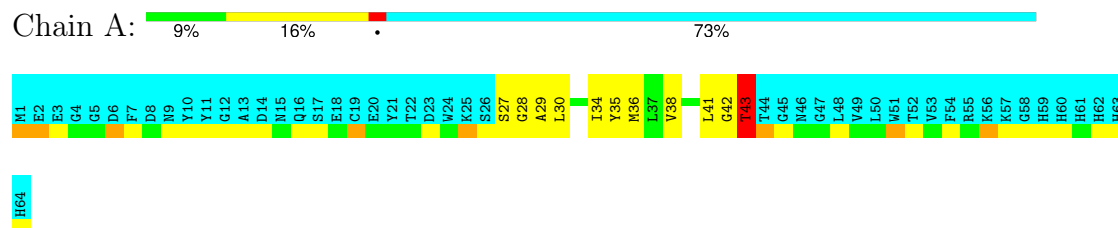
4.2.39 Score per residue for model 39

- Molecule 1: Apelin receptor



4.2.40 Score per residue for model 40

- Molecule 1: Apelin receptor



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 40 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	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	721
Number of shifts mapped to atoms	721
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	124	137	137	5±2
All	All	4960	5480	5480	182

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:30:LEU:HD22	1:A:30:LEU:N	0.80	1.92	37	3
1:A:37:LEU:HD12	1:A:37:LEU:O	0.78	1.77	37	1
1:A:34:ILE:HD12	1:A:34:ILE:H	0.71	1.46	37	1
1:A:30:LEU:N	1:A:30:LEU:HD23	0.70	2.02	1	1
1:A:34:ILE:HD12	1:A:34:ILE:N	0.70	2.01	37	1
1:A:30:LEU:H	1:A:30:LEU:HD12	0.69	1.46	30	1
1:A:30:LEU:O	1:A:34:ILE:HD11	0.67	1.90	1	5
1:A:31:ILE:N	1:A:31:ILE:HD13	0.65	2.05	36	1
1:A:31:ILE:HD13	1:A:31:ILE:N	0.64	2.08	4	3
1:A:31:ILE:N	1:A:32:PRO:CD	0.62	2.62	21	38
1:A:36:MET:SD	1:A:36:MET:N	0.62	2.73	32	1
1:A:30:LEU:HD12	1:A:30:LEU:N	0.61	2.09	30	1
1:A:37:LEU:O	1:A:41:LEU:HD12	0.61	1.95	2	3
1:A:28:GLY:O	1:A:29:ALA:HB3	0.61	1.96	23	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:N	1:A:36:MET:SD	0.60	2.75	32	1
1:A:30:LEU:N	1:A:30:LEU:CD2	0.59	2.65	37	4
1:A:36:MET:N	1:A:36:MET:SD	0.58	2.77	26	1
1:A:34:ILE:N	1:A:34:ILE:CD1	0.58	2.67	37	2
1:A:37:LEU:N	1:A:37:LEU:HD12	0.57	2.14	23	2
1:A:27:SER:OG	1:A:28:GLY:N	0.55	2.40	30	1
1:A:35:TYR:O	1:A:35:TYR:CD1	0.54	2.61	36	1
1:A:34:ILE:N	1:A:34:ILE:HD13	0.53	2.18	33	1
1:A:29:ALA:C	1:A:30:LEU:HD23	0.53	2.24	1	1
1:A:34:ILE:O	1:A:37:LEU:N	0.53	2.42	34	3
1:A:37:LEU:HD12	1:A:37:LEU:C	0.53	2.22	37	1
1:A:35:TYR:O	1:A:39:PHE:N	0.52	2.42	34	2
1:A:37:LEU:N	1:A:37:LEU:CD2	0.52	2.73	13	1
1:A:31:ILE:N	1:A:31:ILE:CD1	0.51	2.70	36	4
1:A:35:TYR:CE2	1:A:39:PHE:CD1	0.50	2.98	24	1
1:A:37:LEU:N	1:A:37:LEU:HD22	0.50	2.20	13	1
1:A:38:VAL:O	1:A:42:GLY:N	0.50	2.44	40	3
1:A:37:LEU:N	1:A:37:LEU:CD1	0.49	2.75	23	2
1:A:35:TYR:O	1:A:36:MET:SD	0.49	2.70	22	9
1:A:30:LEU:CD2	1:A:30:LEU:N	0.49	2.74	35	1
1:A:30:LEU:N	1:A:30:LEU:HD22	0.49	2.22	35	1
1:A:36:MET:C	1:A:38:VAL:N	0.48	2.67	32	9
1:A:28:GLY:O	1:A:29:ALA:CB	0.48	2.61	23	3
1:A:36:MET:O	1:A:38:VAL:N	0.48	2.47	32	3
1:A:30:LEU:O	1:A:34:ILE:CG1	0.47	2.62	15	7
1:A:39:PHE:O	1:A:39:PHE:CD2	0.47	2.67	4	2
1:A:38:VAL:C	1:A:40:LEU:N	0.47	2.68	39	6
1:A:38:VAL:O	1:A:40:LEU:N	0.47	2.47	39	6
1:A:30:LEU:N	1:A:30:LEU:CD1	0.46	2.73	30	1
1:A:31:ILE:HD12	1:A:31:ILE:N	0.46	2.25	35	1
1:A:32:PRO:O	1:A:36:MET:CG	0.45	2.64	16	1
1:A:33:ALA:C	1:A:36:MET:SD	0.45	2.95	32	1
1:A:41:LEU:C	1:A:43:THR:N	0.45	2.70	5	8
1:A:34:ILE:C	1:A:36:MET:N	0.45	2.68	12	1
1:A:34:ILE:O	1:A:36:MET:N	0.45	2.49	12	2
1:A:35:TYR:CD1	1:A:35:TYR:C	0.44	2.88	36	1
1:A:35:TYR:O	1:A:39:PHE:CB	0.44	2.66	34	2
1:A:36:MET:SD	1:A:40:LEU:HD12	0.43	2.53	34	2
1:A:37:LEU:HD12	1:A:37:LEU:N	0.43	2.29	36	1
1:A:41:LEU:HD23	1:A:41:LEU:N	0.43	2.29	4	1
1:A:41:LEU:O	1:A:43:THR:N	0.43	2.52	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:VAL:O	1:A:41:LEU:N	0.42	2.52	39	2
1:A:35:TYR:O	1:A:38:VAL:N	0.42	2.52	37	1
1:A:36:MET:C	1:A:38:VAL:H	0.42	2.18	32	3
1:A:37:LEU:O	1:A:41:LEU:HD23	0.41	2.15	30	1
1:A:38:VAL:C	1:A:40:LEU:H	0.41	2.18	12	1
1:A:41:LEU:C	1:A:43:THR:H	0.41	2.19	10	2
1:A:30:LEU:O	1:A:34:ILE:CD1	0.40	2.65	1	2
1:A:32:PRO:O	1:A:36:MET:SD	0.40	2.80	12	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	17/64 (27%)	6±2 (34±11%)	10±2 (58±13%)	1±1 (8±5%)	1	13
All	All	680/2560 (27%)	233 (34%)	392 (58%)	55 (8%)	1	13

All 11 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	41	LEU	22
1	A	43	THR	17
1	A	39	PHE	4
1	A	27	SER	3
1	A	29	ALA	2
1	A	34	ILE	2
1	A	40	LEU	1
1	A	28	GLY	1
1	A	35	TYR	1
1	A	38	VAL	1
1	A	37	LEU	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	13/53 (25%)	10±1 (75±10%)	3±1 (25±10%)	2	24
All	All	520/2120 (25%)	391 (75%)	129 (25%)	2	24

All 12 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	43	THR	30
1	A	34	ILE	26
1	A	30	LEU	20
1	A	27	SER	10
1	A	35	TYR	9
1	A	39	PHE	9
1	A	41	LEU	8
1	A	38	VAL	5
1	A	31	ILE	4
1	A	37	LEU	4
1	A	40	LEU	3
1	A	36	MET	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry

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 93% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	721
Number of shifts mapped to atoms	721
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	64	-0.43 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	56	0.33 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	58	-0.21 ± 0.07	None needed (< 0.5 ppm)
^{15}N	62	0.52 ± 0.12	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 93%, i.e. 218 atoms were assigned a chemical shift out of a possible 234. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	82/85 (96%)	34/35 (97%)	32/34 (94%)	16/16 (100%)
Sidechain	124/130 (95%)	85/90 (94%)	39/40 (98%)	0/0 (—%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	12/19 (63%)	6/9 (67%)	6/10 (60%)	0/0 (—%)
Overall	218/234 (93%)	125/134 (93%)	77/84 (92%)	16/16 (100%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 721 atoms were assigned a chemical shift out of a possible 846. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	313/326 (96%)	129/135 (96%)	122/128 (95%)	62/63 (98%)
Sidechain	332/388 (86%)	215/253 (85%)	111/125 (89%)	6/10 (60%)
Aromatic	76/132 (58%)	40/67 (60%)	34/57 (60%)	2/8 (25%)
Overall	721/846 (85%)	384/455 (84%)	267/310 (86%)	70/81 (86%)

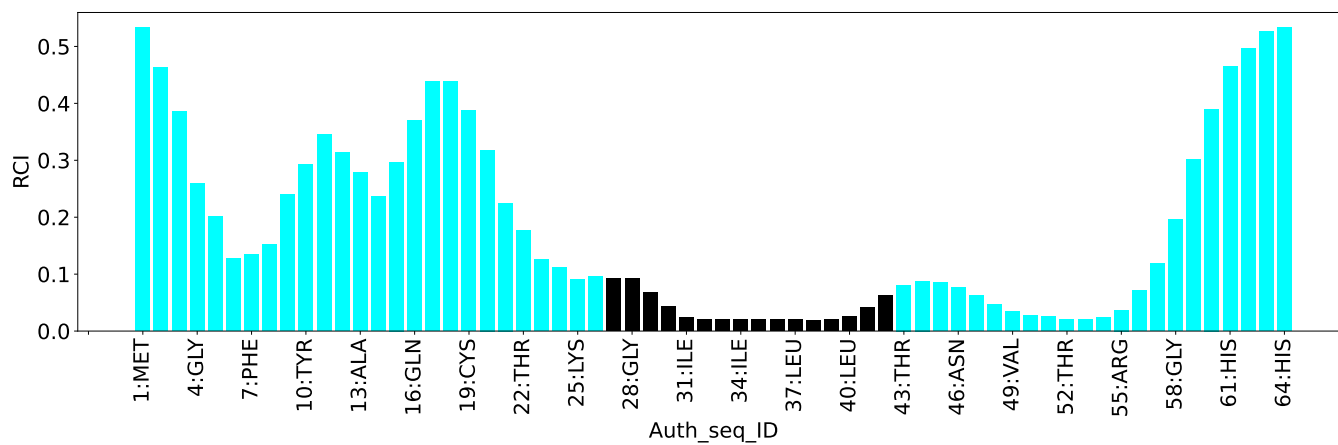
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1489
Intra-residue ($ i-j =0$)	872
Sequential ($ i-j =1$)	353
Medium range ($ i-j >1$ and $ i-j <5$)	264
Long range ($ i-j \geq 5$)	0
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	23.3
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	3.6	0.2
0.2-0.5 (Medium)	4.5	0.5
>0.5 (Large)	2.1	1.37

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

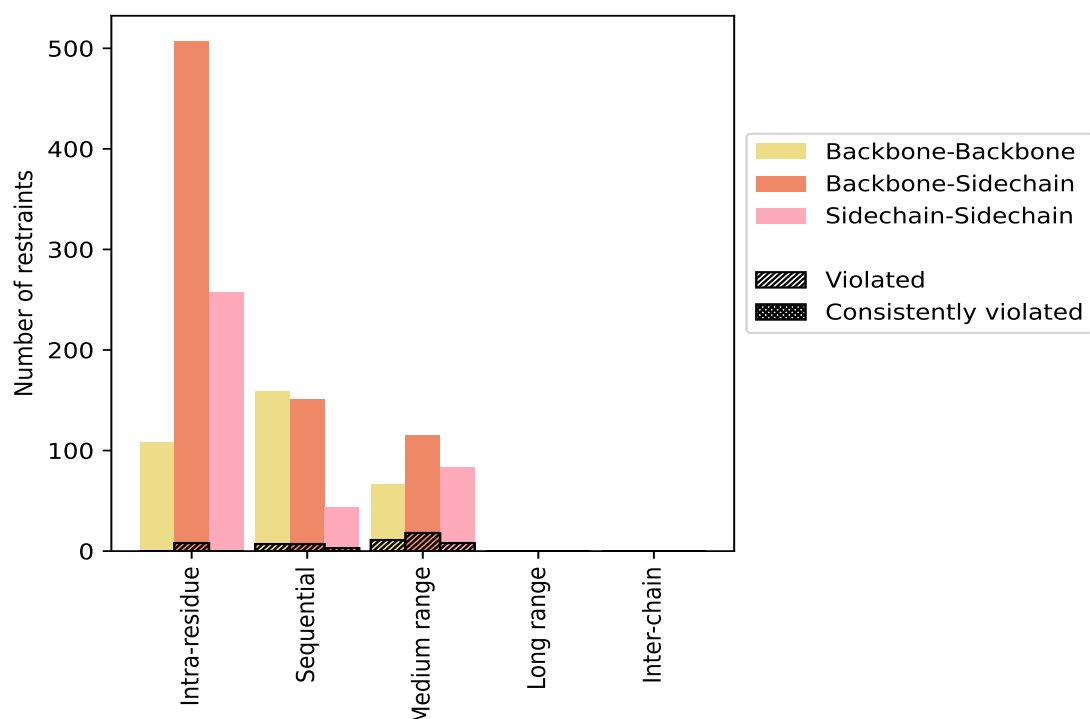
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	872	58.6	8	0.9	0.5	0	0.0	0.0
Backbone-Backbone	108	7.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	507	34.0	8	1.6	0.5	0	0.0	0.0
Sidechain-Sidechain	257	17.3	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	353	23.7	17	4.8	1.1	0	0.0	0.0
Backbone-Backbone	159	10.7	7	4.4	0.5	0	0.0	0.0
Backbone-Sidechain	151	10.1	7	4.6	0.5	0	0.0	0.0
Sidechain-Sidechain	43	2.9	3	7.0	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	264	17.7	37	14.0	2.5	0	0.0	0.0
Backbone-Backbone	66	4.4	11	16.7	0.7	0	0.0	0.0
Backbone-Sidechain	115	7.7	18	15.7	1.2	0	0.0	0.0
Sidechain-Sidechain	83	5.6	8	9.6	0.5	0	0.0	0.0
Long range ($i-j \geq 5$)	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
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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1489	100.0	62	4.2	4.2	0	0.0	0.0
Backbone-Backbone	333	22.4	18	5.4	1.2	0	0.0	0.0
Backbone-Sidechain	773	51.9	33	4.3	2.2	0	0.0	0.0
Sidechain-Sidechain	383	25.7	11	2.9	0.7	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	0	4	3	0	0	7	0.35	0.75	0.21	0.28
2	0	4	5	0	0	9	0.33	0.72	0.18	0.3
3	0	3	8	0	0	11	0.43	0.85	0.21	0.36
4	0	3	3	0	0	6	0.45	0.9	0.28	0.4
5	0	5	5	0	0	10	0.43	1.03	0.27	0.44
6	0	5	9	0	0	14	0.32	1.01	0.25	0.24
7	0	4	8	0	0	12	0.26	0.93	0.22	0.18
8	0	4	7	0	0	11	0.25	0.53	0.12	0.22
9	0	2	4	0	0	6	0.27	0.5	0.14	0.22
10	0	5	10	0	0	15	0.32	0.88	0.21	0.22

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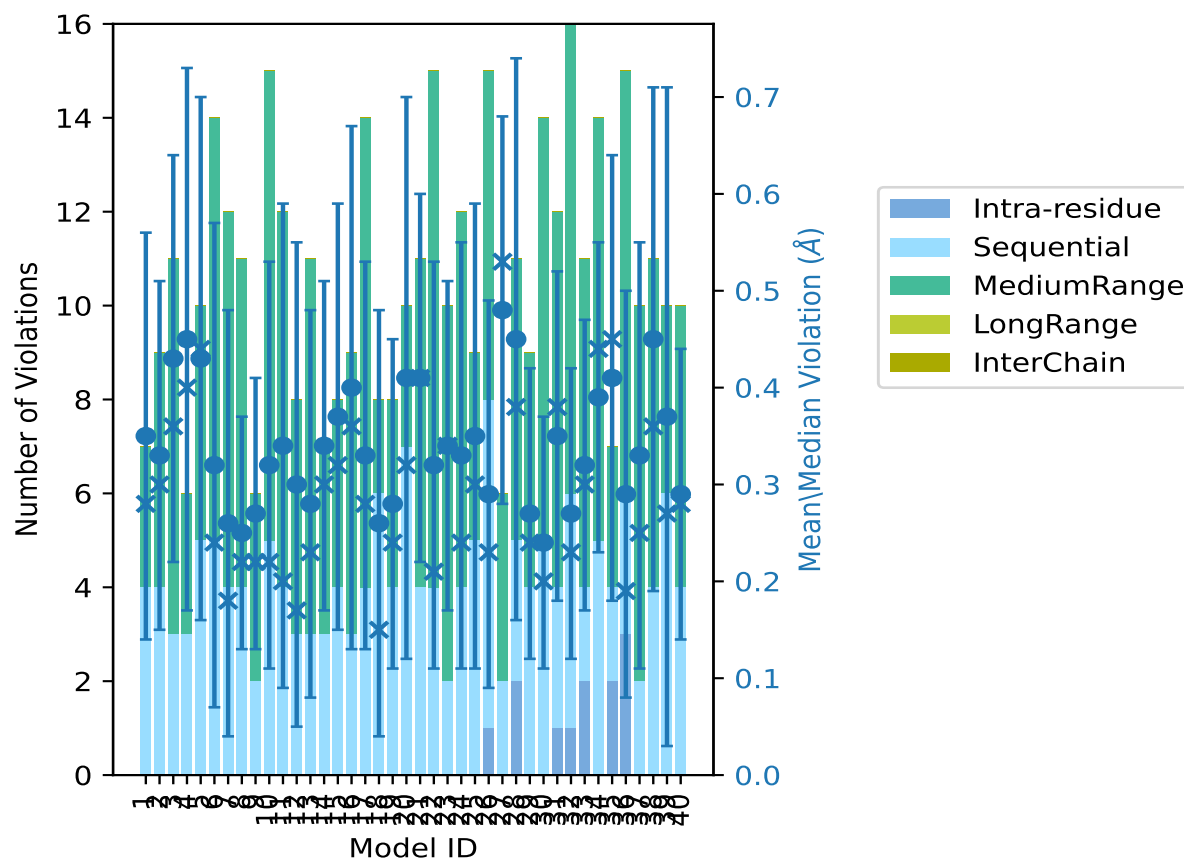
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	4	8	0	0	12	0.34	0.92	0.25	0.2
12	0	3	5	0	0	8	0.3	0.89	0.25	0.17
13	0	3	8	0	0	11	0.28	0.7	0.2	0.23
14	0	3	4	0	0	7	0.34	0.57	0.17	0.3
15	0	4	4	0	0	8	0.37	0.8	0.22	0.32
16	0	3	6	0	0	9	0.4	1.02	0.27	0.36
17	0	4	10	0	0	14	0.33	0.8	0.2	0.28
18	0	6	2	0	0	8	0.26	0.77	0.22	0.15
19	0	4	4	0	0	8	0.28	0.65	0.17	0.24
20	0	7	3	0	0	10	0.41	0.9	0.29	0.32
21	0	4	7	0	0	11	0.41	0.71	0.19	0.41
22	0	4	11	0	0	15	0.32	0.85	0.21	0.21
23	0	2	8	0	0	10	0.34	0.74	0.17	0.34
24	0	4	8	0	0	12	0.33	0.74	0.22	0.24
25	0	5	4	0	0	9	0.35	0.99	0.24	0.3
26	1	7	7	0	0	15	0.29	0.73	0.2	0.23
27	0	2	4	0	0	6	0.48	0.76	0.2	0.53
28	2	3	6	0	0	11	0.45	1.16	0.29	0.38
29	0	4	5	0	0	9	0.27	0.58	0.15	0.24
30	0	5	9	0	0	14	0.24	0.54	0.13	0.2
31	1	3	8	0	0	12	0.35	0.61	0.17	0.38
32	1	5	10	0	0	16	0.27	0.51	0.15	0.23
33	2	2	7	0	0	11	0.32	0.63	0.15	0.3
34	0	5	9	0	0	14	0.39	0.58	0.16	0.44
35	2	2	3	0	0	7	0.41	0.74	0.23	0.45
36	3	3	9	0	0	15	0.29	0.83	0.21	0.19
37	0	2	8	0	0	10	0.33	0.9	0.22	0.25
38	0	4	7	0	0	11	0.45	0.96	0.26	0.36
39	0	6	4	0	0	10	0.37	1.37	0.34	0.27
40	0	4	6	0	0	10	0.29	0.69	0.15	0.28

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 [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1427(IR:864, SQ:336, MR:227, LR:0, 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	%
6	7	9	0	0	22	1	2.5
0	4	3	0	0	7	2	5.0
2	1	2	0	0	5	3	7.5
0	0	0	0	0	0	4	10.0
0	0	2	0	0	2	5	12.5
0	1	2	0	0	3	6	15.0

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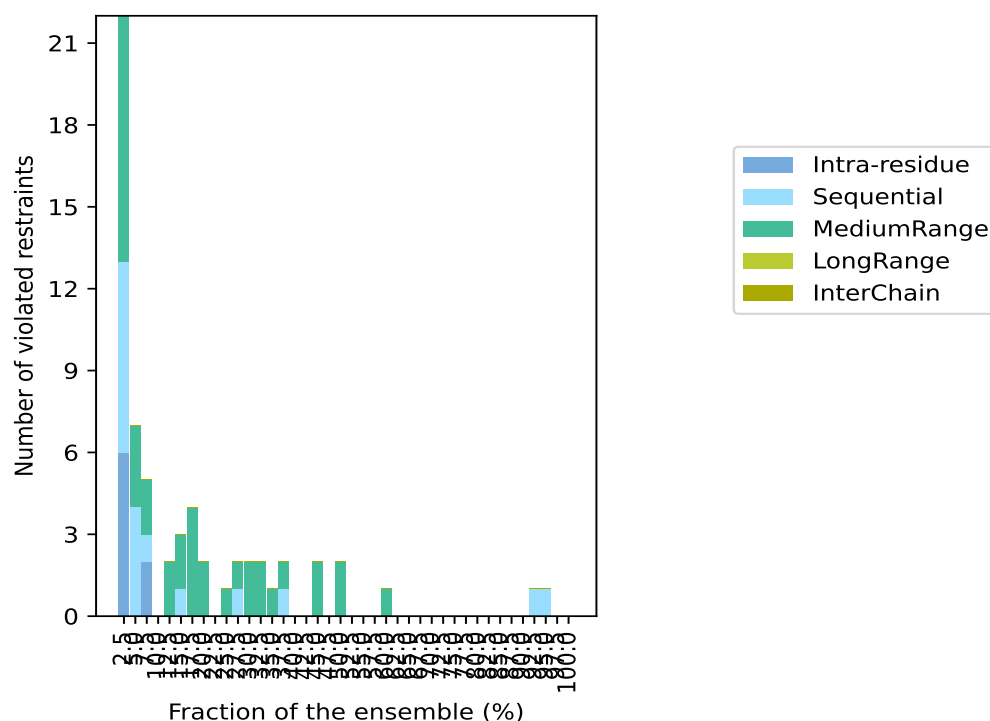
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	4	0	0	4	7	17.5
0	0	2	0	0	2	8	20.0
0	0	0	0	0	0	9	22.5
0	0	1	0	0	1	10	25.0
0	1	1	0	0	2	11	27.5
0	0	2	0	0	2	12	30.0
0	0	2	0	0	2	13	32.5
0	0	1	0	0	1	14	35.0
0	1	1	0	0	2	15	37.5
0	0	0	0	0	0	16	40.0
0	0	0	0	0	0	17	42.5
0	0	2	0	0	2	18	45.0
0	0	0	0	0	0	19	47.5
0	0	2	0	0	2	20	50.0
0	0	0	0	0	0	21	52.5
0	0	0	0	0	0	22	55.0
0	0	0	0	0	0	23	57.5
0	0	1	0	0	1	24	60.0
0	0	0	0	0	0	25	62.5
0	0	0	0	0	0	26	65.0
0	0	0	0	0	0	27	67.5
0	0	0	0	0	0	28	70.0
0	0	0	0	0	0	29	72.5
0	0	0	0	0	0	30	75.0
0	0	0	0	0	0	31	77.5
0	0	0	0	0	0	32	80.0
0	0	0	0	0	0	33	82.5
0	0	0	0	0	0	34	85.0
0	0	0	0	0	0	35	87.5
0	0	0	0	0	0	36	90.0
0	1	0	0	0	1	37	92.5
0	1	0	0	0	1	38	95.0
0	0	0	0	0	0	39	97.5
0	0	0	0	0	0	40	100.0

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

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

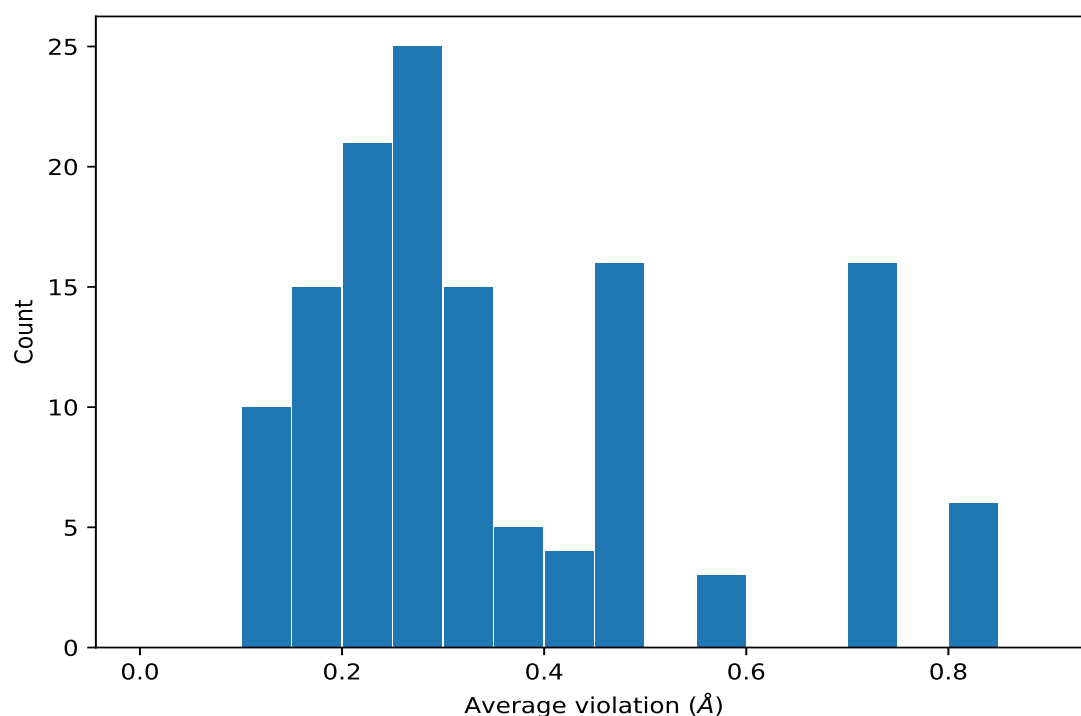
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	38	0.33	0.15	0.34
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	38	0.33	0.15	0.34
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	38	0.33	0.15	0.34
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	37	0.59	0.22	0.6
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	37	0.59	0.22	0.6
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	37	0.59	0.22	0.6
(1,961)	1:36:A:MET:H	1:37:A:LEU:HG	24	0.35	0.15	0.33
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	24	0.35	0.15	0.33
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	24	0.35	0.15	0.33
(1,961)	1:36:A:MET:H	1:32:A:PRO:HB2	24	0.35	0.15	0.33
(1,961)	1:36:A:MET:H	1:32:A:PRO:HB3	24	0.35	0.15	0.33
(1,437)	1:53:A:VAL:HG13	1:56:A:LYS:HB2	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG13	1:56:A:LYS:HB3	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG12	1:56:A:LYS:HB2	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG12	1:56:A:LYS:HB3	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG22	1:56:A:LYS:HB2	20	0.71	0.25	0.71

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,437)	1:53:A:VAL:HG22	1:56:A:LYS:HB3	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB2	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB3	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG13	1:57:A:LYS:HB2	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG13	1:57:A:LYS:HB3	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG23	1:56:A:LYS:HB2	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG23	1:56:A:LYS:HB3	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG21	1:56:A:LYS:HB2	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG21	1:56:A:LYS:HB3	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG12	1:57:A:LYS:HB2	20	0.71	0.25	0.71
(1,437)	1:53:A:VAL:HG12	1:57:A:LYS:HB3	20	0.71	0.25	0.71
(1,303)	1:29:A:ALA:HB2	1:32:A:PRO:HG2	20	0.47	0.22	0.46
(1,303)	1:29:A:ALA:HB2	1:32:A:PRO:HG3	20	0.47	0.22	0.46
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	20	0.47	0.22	0.46
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG3	20	0.47	0.22	0.46
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	20	0.47	0.22	0.46
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG3	20	0.47	0.22	0.46
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB2	18	0.4	0.15	0.42
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB3	18	0.4	0.15	0.42
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	18	0.4	0.15	0.42
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	18	0.4	0.15	0.42
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	18	0.22	0.06	0.22
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	18	0.22	0.06	0.22
(1,981)	1:31:A:ILE:HG12	1:33:A:ALA:H	18	0.22	0.06	0.22
(1,981)	1:31:A:ILE:HG13	1:33:A:ALA:H	18	0.22	0.06	0.22
(1,813)	1:21:A:TYR:HD2	1:19:A:CYS:H	15	0.38	0.18	0.36
(1,813)	1:21:A:TYR:HD1	1:19:A:CYS:H	15	0.38	0.18	0.36
(1,813)	1:21:A:TYR:HD1	1:18:A:GLU:H	15	0.38	0.18	0.36
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	15	0.2	0.08	0.17
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	15	0.2	0.08	0.17
(1,897)	1:32:A:PRO:HB2	1:29:A:ALA:HA	15	0.2	0.08	0.17
(1,897)	1:32:A:PRO:HB3	1:29:A:ALA:HA	15	0.2	0.08	0.17
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	14	0.22	0.11	0.18
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	14	0.22	0.11	0.18
(1,1385)	1:56:A:LYS:HD2	1:58:A:GLY:H	14	0.22	0.11	0.18
(1,1385)	1:56:A:LYS:HD3	1:58:A:GLY:H	14	0.22	0.11	0.18
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD2	13	0.47	0.24	0.48
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD3	13	0.47	0.24	0.48
(1,903)	1:27:A:SER:HB2	1:29:A:ALA:HB1	13	0.47	0.24	0.48
(1,903)	1:27:A:SER:HB2	1:29:A:ALA:HB2	13	0.47	0.24	0.48
(1,903)	1:27:A:SER:HB2	1:29:A:ALA:HB3	13	0.47	0.24	0.48
(1,903)	1:27:A:SER:HB3	1:29:A:ALA:HB1	13	0.47	0.24	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,903)	1:27:A:SER:HB3	1:29:A:ALA:HB2	13	0.47	0.24	0.48
(1,903)	1:27:A:SER:HB3	1:29:A:ALA:HB3	13	0.47	0.24	0.48
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD2	13	0.47	0.24	0.48
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD3	13	0.47	0.24	0.48
(1,1320)	1:11:A:TYR:HB2	1:13:A:ALA:H	13	0.28	0.12	0.24
(1,1320)	1:11:A:TYR:HB3	1:13:A:ALA:H	13	0.28	0.12	0.24
(1,1320)	1:10:A:TYR:HB2	1:13:A:ALA:H	13	0.28	0.12	0.24
(1,1320)	1:10:A:TYR:HB3	1:13:A:ALA:H	13	0.28	0.12	0.24
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	12	0.19	0.06	0.2
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	12	0.19	0.06	0.2
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH11	12	0.19	0.06	0.2
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH12	12	0.19	0.06	0.2
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	12	0.19	0.06	0.2
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	12	0.19	0.06	0.2
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH11	12	0.19	0.06	0.2
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH12	12	0.19	0.06	0.2
(1,608)	1:56:A:LYS:H	1:53:A:VAL:HB	11	0.29	0.12	0.27
(1,608)	1:50:A:LEU:H	1:53:A:VAL:HB	11	0.29	0.12	0.27
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	11	0.15	0.0	0.15
(1,198)	1:36:A:MET:H	1:33:A:ALA:HA	10	0.16	0.03	0.16
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA2	8	0.3	0.18	0.25
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA3	8	0.3	0.18	0.25
(1,1147)	1:38:A:VAL:H	1:42:A:GLY:HA2	8	0.3	0.18	0.25
(1,1147)	1:38:A:VAL:H	1:42:A:GLY:HA3	8	0.3	0.18	0.25
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH21	8	0.3	0.14	0.27
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH22	8	0.3	0.14	0.27
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH11	8	0.3	0.14	0.27
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH12	8	0.3	0.14	0.27
(1,460)	1:53:A:VAL:HG12	1:54:A:PHE:HD1	7	0.82	0.27	0.9
(1,460)	1:53:A:VAL:HG12	1:54:A:PHE:HD2	7	0.82	0.27	0.9
(1,460)	1:53:A:VAL:HG11	1:54:A:PHE:HD1	7	0.82	0.27	0.9
(1,460)	1:53:A:VAL:HG11	1:54:A:PHE:HD2	7	0.82	0.27	0.9
(1,460)	1:53:A:VAL:HG13	1:54:A:PHE:HD1	7	0.82	0.27	0.9
(1,460)	1:53:A:VAL:HG13	1:54:A:PHE:HD2	7	0.82	0.27	0.9
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE1	7	0.29	0.11	0.3
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE2	7	0.29	0.11	0.3
(1,425)	1:31:A:ILE:HB	1:35:A:TYR:HE1	7	0.29	0.11	0.3
(1,425)	1:31:A:ILE:HB	1:35:A:TYR:HE2	7	0.29	0.11	0.3
(1,410)	1:33:A:ALA:HB2	1:31:A:ILE:H	7	0.24	0.12	0.19
(1,410)	1:33:A:ALA:HB3	1:31:A:ILE:H	7	0.24	0.12	0.19
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB2	7	0.23	0.11	0.21
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB3	7	0.23	0.11	0.21

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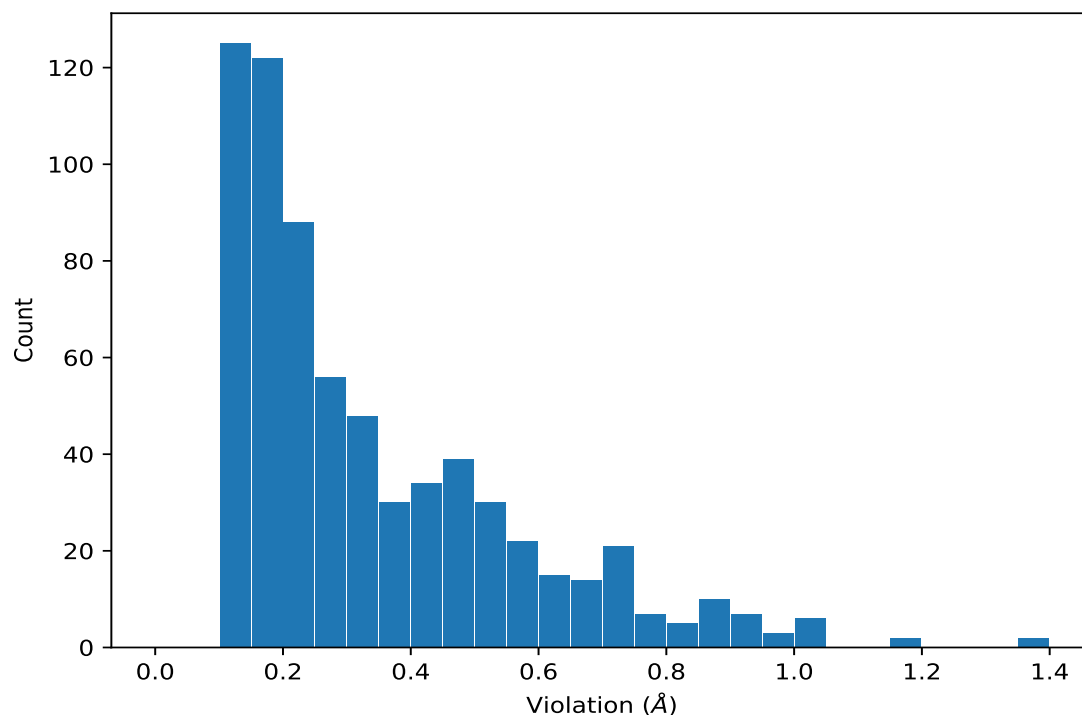
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,207)	1:43:A:THR:HB	1:45:A:GLY:H	6	0.36	0.11	0.32
(1,207)	1:43:A:THR:HB	1:46:A:ASN:H	6	0.36	0.11	0.32
(1,1468)	1:53:A:VAL:H	1:50:A:LEU:HA	6	0.34	0.14	0.4
(1,1468)	1:49:A:VAL:H	1:50:A:LEU:HA	6	0.34	0.14	0.4
(1,1358)	1:42:A:GLY:H	1:43:A:THR:HB	6	0.24	0.09	0.22
(1,1358)	1:42:A:GLY:H	1:39:A:PHE:HA	6	0.24	0.09	0.22
(1,167)	1:34:A:ILE:HG21	1:35:A:TYR:HA	5	0.3	0.11	0.26
(1,167)	1:34:A:ILE:HG22	1:35:A:TYR:HA	5	0.3	0.11	0.26
(1,167)	1:34:A:ILE:HG23	1:35:A:TYR:HA	5	0.3	0.11	0.26
(1,167)	1:31:A:ILE:HG21	1:35:A:TYR:HA	5	0.3	0.11	0.26
(1,167)	1:31:A:ILE:HG22	1:35:A:TYR:HA	5	0.3	0.11	0.26
(1,167)	1:31:A:ILE:HG23	1:35:A:TYR:HA	5	0.3	0.11	0.26
(1,990)	1:46:A:ASN:H	1:44:A:THR:HA	5	0.23	0.05	0.22
(1,199)	1:37:A:LEU:HB2	1:38:A:VAL:H	3	0.32	0.02	0.33
(1,801)	1:20:A:GLU:HB2	1:19:A:CYS:HA	3	0.32	0.12	0.32
(1,801)	1:20:A:GLU:HB3	1:19:A:CYS:HA	3	0.32	0.12	0.32
(1,801)	1:18:A:GLU:HB2	1:19:A:CYS:HA	3	0.32	0.12	0.32
(1,801)	1:18:A:GLU:HB3	1:19:A:CYS:HA	3	0.32	0.12	0.32
(1,415)	1:10:A:TYR:HB2	1:10:A:TYR:H	3	0.16	0.0	0.16
(1,415)	1:10:A:TYR:HB3	1:10:A:TYR:H	3	0.16	0.0	0.16
(1,1194)	1:10:A:TYR:HB2	1:10:A:TYR:H	3	0.16	0.0	0.16
(1,1194)	1:10:A:TYR:HB3	1:10:A:TYR:H	3	0.16	0.0	0.16
(1,705)	1:31:A:ILE:HG21	1:35:A:TYR:HE1	3	0.14	0.04	0.14
(1,705)	1:31:A:ILE:HG21	1:35:A:TYR:HE2	3	0.14	0.04	0.14
(1,705)	1:31:A:ILE:HG22	1:35:A:TYR:HE1	3	0.14	0.04	0.14
(1,705)	1:31:A:ILE:HG22	1:35:A:TYR:HE2	3	0.14	0.04	0.14
(1,705)	1:31:A:ILE:HG23	1:35:A:TYR:HE1	3	0.14	0.04	0.14
(1,705)	1:31:A:ILE:HG23	1:35:A:TYR:HE2	3	0.14	0.04	0.14
(1,412)	1:19:A:CYS:HB3	1:18:A:GLU:HA	2	0.26	0.14	0.26
(1,1465)	1:50:A:LEU:H	1:51:A:TRP:HA	2	0.22	0.04	0.22
(1,1402)	1:46:A:ASN:H	1:44:A:THR:H	2	0.2	0.03	0.2
(1,476)	1:23:A:ASP:HB2	1:22:A:THR:HA	2	0.16	0.01	0.16
(1,476)	1:23:A:ASP:HB3	1:22:A:THR:HA	2	0.16	0.01	0.16
(1,85)	1:50:A:LEU:HG	1:51:A:TRP:H	2	0.14	0.02	0.14
(1,1202)	1:61:A:HIS:HA	1:62:A:HIS:H	2	0.12	0.01	0.12
(1,1433)	1:61:A:HIS:H	1:62:A:HIS:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:53:A:VAL:HG12	1:57:A:LYS:HB2	39	1.37
(1,437)	1:53:A:VAL:HG12	1:57:A:LYS:HB3	39	1.37
(1,460)	1:53:A:VAL:HG11	1:54:A:PHE:HD1	28	1.16
(1,460)	1:53:A:VAL:HG11	1:54:A:PHE:HD2	28	1.16
(1,460)	1:53:A:VAL:HG12	1:54:A:PHE:HD1	5	1.03
(1,460)	1:53:A:VAL:HG12	1:54:A:PHE:HD2	5	1.03
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB2	16	1.02
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB3	16	1.02
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	6	1.01
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG3	6	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	25	0.99
(1,460)	1:53:A:VAL:HG12	1:54:A:PHE:HD1	38	0.96
(1,460)	1:53:A:VAL:HG12	1:54:A:PHE:HD2	38	0.96
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	7	0.93
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	11	0.92
(1,460)	1:53:A:VAL:HG11	1:54:A:PHE:HD1	20	0.9
(1,460)	1:53:A:VAL:HG11	1:54:A:PHE:HD2	20	0.9
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB2	37	0.9
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB3	37	0.9
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	4	0.9
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	12	0.89
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG3	12	0.89
(1,437)	1:53:A:VAL:HG12	1:56:A:LYS:HB2	10	0.88
(1,437)	1:53:A:VAL:HG12	1:56:A:LYS:HB3	10	0.88
(1,903)	1:27:A:SER:HB3	1:29:A:ALA:HB1	38	0.87
(1,903)	1:27:A:SER:HB3	1:29:A:ALA:HB2	38	0.87
(1,903)	1:27:A:SER:HB3	1:29:A:ALA:HB3	38	0.87
(1,437)	1:53:A:VAL:HG12	1:56:A:LYS:HB2	3	0.85
(1,437)	1:53:A:VAL:HG12	1:56:A:LYS:HB3	3	0.85
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	22	0.85
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB2	36	0.83
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB3	36	0.83
(1,437)	1:53:A:VAL:HG23	1:56:A:LYS:HB2	17	0.8
(1,437)	1:53:A:VAL:HG23	1:56:A:LYS:HB3	17	0.8
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	15	0.8
(1,903)	1:27:A:SER:HB3	1:29:A:ALA:HB1	18	0.77
(1,903)	1:27:A:SER:HB3	1:29:A:ALA:HB2	18	0.77
(1,903)	1:27:A:SER:HB3	1:29:A:ALA:HB3	18	0.77
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	17	0.77
(1,813)	1:21:A:TYR:HD1	1:18:A:GLU:H	27	0.76
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	1	0.75
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	20	0.75
(1,460)	1:53:A:VAL:HG13	1:54:A:PHE:HD1	24	0.74
(1,460)	1:53:A:VAL:HG13	1:54:A:PHE:HD2	24	0.74
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB2	35	0.74
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB3	35	0.74
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	23	0.74
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	26	0.73
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD2	3	0.72
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD3	3	0.72
(1,437)	1:53:A:VAL:HG13	1:56:A:LYS:HB2	2	0.72
(1,437)	1:53:A:VAL:HG13	1:56:A:LYS:HB3	2	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:53:A:VAL:HG22	1:56:A:LYS:HB2	4	0.72
(1,437)	1:53:A:VAL:HG22	1:56:A:LYS:HB3	4	0.72
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA2	21	0.71
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA3	21	0.71
(1,903)	1:27:A:SER:HB2	1:29:A:ALA:HB1	5	0.71
(1,903)	1:27:A:SER:HB2	1:29:A:ALA:HB2	5	0.71
(1,903)	1:27:A:SER:HB2	1:29:A:ALA:HB3	5	0.71
(1,437)	1:53:A:VAL:HG13	1:57:A:LYS:HB2	13	0.7
(1,437)	1:53:A:VAL:HG13	1:57:A:LYS:HB3	13	0.7
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	11	0.7
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG3	11	0.7
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	40	0.69
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB2	21	0.68
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB3	21	0.68
(1,437)	1:53:A:VAL:HG13	1:57:A:LYS:HB2	22	0.68
(1,437)	1:53:A:VAL:HG13	1:57:A:LYS:HB3	22	0.68
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	24	0.68
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG3	24	0.68
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	35	0.67
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	35	0.67
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	20	0.66
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	28	0.66
(1,437)	1:53:A:VAL:HG12	1:56:A:LYS:HB2	19	0.65
(1,437)	1:53:A:VAL:HG12	1:56:A:LYS:HB3	19	0.65
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	13	0.65
(1,460)	1:53:A:VAL:HG11	1:54:A:PHE:HD1	26	0.64
(1,460)	1:53:A:VAL:HG11	1:54:A:PHE:HD2	26	0.64
(1,437)	1:53:A:VAL:HG21	1:56:A:LYS:HB2	20	0.63
(1,437)	1:53:A:VAL:HG21	1:56:A:LYS:HB3	20	0.63
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	33	0.63
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG3	33	0.63
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	36	0.63
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	38	0.63
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	10	0.62
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	31	0.61
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB2	3	0.6
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB3	3	0.6
(1,437)	1:53:A:VAL:HG22	1:56:A:LYS:HB2	28	0.6
(1,437)	1:53:A:VAL:HG22	1:56:A:LYS:HB3	28	0.6
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	24	0.6
(1,813)	1:21:A:TYR:HD2	1:19:A:CYS:H	1	0.59
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB2	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB3	6	0.59
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	21	0.59
(1,207)	1:43:A:THR:HB	1:46:A:ASN:H	26	0.59
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD2	29	0.58
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD3	29	0.58
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB2	34	0.58
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB3	34	0.58
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH21	34	0.57
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH22	34	0.57
(1,813)	1:21:A:TYR:HD1	1:19:A:CYS:H	28	0.57
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	10	0.57
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	14	0.57
(1,437)	1:53:A:VAL:HG22	1:56:A:LYS:HB2	11	0.57
(1,437)	1:53:A:VAL:HG22	1:56:A:LYS:HB3	11	0.57
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	27	0.57
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG3	27	0.57
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	6	0.57
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	27	0.57
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	2	0.55
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	16	0.55
(1,961)	1:36:A:MET:H	1:37:A:LEU:HG	15	0.54
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	34	0.54
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	34	0.54
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	38	0.54
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	38	0.54
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	34	0.54
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG3	34	0.54
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	14	0.54
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	30	0.54
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	37	0.54
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	28	0.53
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	28	0.53
(1,813)	1:21:A:TYR:HD1	1:18:A:GLU:H	8	0.53
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE1	34	0.52
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE2	34	0.52
(1,1320)	1:11:A:TYR:HB2	1:13:A:ALA:H	5	0.51
(1,1320)	1:11:A:TYR:HB3	1:13:A:ALA:H	5	0.51
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB2	32	0.51
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB3	32	0.51
(1,608)	1:50:A:LEU:H	1:53:A:VAL:HB	21	0.51
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	3	0.51
(1,303)	1:29:A:ALA:HB2	1:32:A:PRO:HG2	31	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:29:A:ALA:HB2	1:32:A:PRO:HG3	31	0.51
(1,1468)	1:49:A:VAL:H	1:50:A:LEU:HA	36	0.5
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	34	0.5
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	34	0.5
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	31	0.5
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	31	0.5
(1,813)	1:21:A:TYR:HD1	1:18:A:GLU:H	9	0.5
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	16	0.5
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	27	0.49
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	27	0.49
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	35	0.49
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	5	0.49
(1,961)	1:36:A:MET:H	1:37:A:LEU:HG	5	0.48
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD2	12	0.48
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD3	12	0.48
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD2	31	0.48
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD3	31	0.48
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	11	0.48
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	11	0.48
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	31	0.48
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	31	0.48
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	21	0.48
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG3	21	0.48
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	32	0.47
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	16	0.47
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG3	16	0.47
(1,1320)	1:11:A:TYR:HB2	1:13:A:ALA:H	32	0.46
(1,1320)	1:11:A:TYR:HB3	1:13:A:ALA:H	32	0.46
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH11	15	0.46
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH12	15	0.46
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	20	0.46
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	20	0.46
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD2	23	0.46
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD3	23	0.46
(1,801)	1:20:A:GLU:HB2	1:19:A:CYS:HA	32	0.46
(1,801)	1:20:A:GLU:HB3	1:19:A:CYS:HA	32	0.46
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	18	0.46
(1,1320)	1:10:A:TYR:HB2	1:13:A:ALA:H	3	0.45
(1,1320)	1:10:A:TYR:HB3	1:13:A:ALA:H	3	0.45
(1,410)	1:33:A:ALA:HB2	1:31:A:ILE:H	29	0.45
(1,303)	1:29:A:ALA:HB2	1:32:A:PRO:HG2	38	0.45
(1,303)	1:29:A:ALA:HB2	1:32:A:PRO:HG3	38	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	34	0.45
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	35	0.45
(1,167)	1:34:A:ILE:HG21	1:35:A:TYR:HA	4	0.45
(1,167)	1:34:A:ILE:HG22	1:35:A:TYR:HA	4	0.45
(1,167)	1:34:A:ILE:HG23	1:35:A:TYR:HA	4	0.45
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	14	0.44
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	14	0.44
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	22	0.44
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	22	0.44
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	36	0.44
(1,1468)	1:53:A:VAL:H	1:50:A:LEU:HA	31	0.43
(1,1468)	1:53:A:VAL:H	1:50:A:LEU:HA	33	0.43
(1,961)	1:36:A:MET:H	1:37:A:LEU:HG	22	0.43
(1,961)	1:36:A:MET:H	1:37:A:LEU:HG	30	0.43
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	32	0.43
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	32	0.43
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	33	0.43
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	34	0.43
(1,437)	1:53:A:VAL:HG12	1:57:A:LYS:HB2	23	0.43
(1,437)	1:53:A:VAL:HG12	1:57:A:LYS:HB3	23	0.43
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	33	0.43
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	6	0.42
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	26	0.42
(1,410)	1:33:A:ALA:HB2	1:31:A:ILE:H	9	0.42
(1,813)	1:21:A:TYR:HD1	1:19:A:CYS:H	19	0.41
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB2	39	0.41
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB3	39	0.41
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	24	0.41
(1,412)	1:19:A:CYS:HB3	1:18:A:GLU:HA	7	0.41
(1,167)	1:34:A:ILE:HG21	1:35:A:TYR:HA	21	0.41
(1,167)	1:34:A:ILE:HG22	1:35:A:TYR:HA	21	0.41
(1,167)	1:34:A:ILE:HG23	1:35:A:TYR:HA	21	0.41
(1,813)	1:21:A:TYR:HD1	1:19:A:CYS:H	33	0.4
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	40	0.4
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	40	0.4
(1,608)	1:50:A:LEU:H	1:53:A:VAL:HB	23	0.4
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	27	0.4
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB2	39	0.4
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB3	39	0.4
(1,608)	1:56:A:LYS:H	1:53:A:VAL:HB	22	0.39
(1,608)	1:56:A:LYS:H	1:53:A:VAL:HB	32	0.39
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG3	5	0.39
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA2	25	0.38
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA3	25	0.38
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA2	30	0.38
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA3	30	0.38
(1,897)	1:32:A:PRO:HB2	1:29:A:ALA:HA	10	0.38
(1,897)	1:32:A:PRO:HB3	1:29:A:ALA:HA	10	0.38
(1,608)	1:56:A:LYS:H	1:53:A:VAL:HB	15	0.38
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	28	0.38
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	8	0.38
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG3	8	0.38
(1,1358)	1:42:A:GLY:H	1:39:A:PHE:HA	22	0.37
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	25	0.37
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	25	0.37
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	17	0.37
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	17	0.37
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	10	0.37
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG3	10	0.37
(1,1468)	1:53:A:VAL:H	1:50:A:LEU:HA	28	0.36
(1,961)	1:36:A:MET:H	1:37:A:LEU:HG	38	0.36
(1,813)	1:21:A:TYR:HD2	1:19:A:CYS:H	16	0.36
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB2	23	0.36
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB3	23	0.36
(1,437)	1:53:A:VAL:HG13	1:56:A:LYS:HB2	34	0.36
(1,437)	1:53:A:VAL:HG13	1:56:A:LYS:HB3	34	0.36
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	3	0.36
(1,207)	1:43:A:THR:HB	1:45:A:GLY:H	2	0.36
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	7	0.34
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	7	0.34
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD2	17	0.34
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD3	17	0.34
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	2	0.34
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	4	0.34
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	25	0.34
(1,207)	1:43:A:THR:HB	1:46:A:ASN:H	24	0.34
(1,199)	1:37:A:LEU:HB2	1:38:A:VAL:H	10	0.34
(1,1385)	1:56:A:LYS:HD2	1:58:A:GLY:H	17	0.33
(1,1385)	1:56:A:LYS:HD3	1:58:A:GLY:H	17	0.33
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	8	0.33
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	8	0.33
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	7	0.33
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	13	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	39	0.33
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE1	31	0.33
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE2	31	0.33
(1,199)	1:37:A:LEU:HB2	1:38:A:VAL:H	1	0.33
(1,1358)	1:42:A:GLY:H	1:43:A:THR:HB	3	0.32
(1,1320)	1:11:A:TYR:HB2	1:13:A:ALA:H	21	0.32
(1,1320)	1:11:A:TYR:HB3	1:13:A:ALA:H	21	0.32
(1,1147)	1:38:A:VAL:H	1:42:A:GLY:HA2	23	0.32
(1,1147)	1:38:A:VAL:H	1:42:A:GLY:HA3	23	0.32
(1,801)	1:20:A:GLU:HB2	1:19:A:CYS:HA	8	0.32
(1,801)	1:20:A:GLU:HB3	1:19:A:CYS:HA	8	0.32
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	37	0.32
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH11	21	0.31
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH12	21	0.31
(1,990)	1:46:A:ASN:H	1:44:A:THR:HA	37	0.31
(1,813)	1:21:A:TYR:HD1	1:19:A:CYS:H	40	0.31
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	21	0.31
(1,425)	1:31:A:ILE:HB	1:35:A:TYR:HE1	6	0.31
(1,425)	1:31:A:ILE:HB	1:35:A:TYR:HE2	6	0.31
(1,961)	1:36:A:MET:H	1:37:A:LEU:HG	6	0.3
(1,961)	1:36:A:MET:H	1:37:A:LEU:HG	11	0.3
(1,813)	1:21:A:TYR:HD1	1:19:A:CYS:H	14	0.3
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB2	33	0.3
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB3	33	0.3
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	38	0.3
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE1	13	0.3
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE2	13	0.3
(1,303)	1:29:A:ALA:HB2	1:32:A:PRO:HG2	2	0.3
(1,303)	1:29:A:ALA:HB2	1:32:A:PRO:HG3	2	0.3
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	19	0.3
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG3	19	0.3
(1,207)	1:43:A:THR:HB	1:45:A:GLY:H	17	0.3
(1,207)	1:43:A:THR:HB	1:45:A:GLY:H	25	0.3
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	6	0.29
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	6	0.29
(1,1174)	1:34:A:ILE:H	1:36:A:MET:HB2	33	0.29
(1,1174)	1:34:A:ILE:H	1:36:A:MET:HB3	33	0.29
(1,460)	1:53:A:VAL:HG12	1:54:A:PHE:HD1	30	0.29
(1,460)	1:53:A:VAL:HG12	1:54:A:PHE:HD2	30	0.29
(1,199)	1:37:A:LEU:HB2	1:38:A:VAL:H	29	0.29
(1,1320)	1:11:A:TYR:HB2	1:13:A:ALA:H	2	0.28
(1,1320)	1:11:A:TYR:HB3	1:13:A:ALA:H	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH11	22	0.28
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH12	22	0.28
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	17	0.28
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	17	0.28
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	40	0.28
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	40	0.28
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	17	0.28
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	17	0.28
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	40	0.28
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	40	0.28
(1,981)	1:31:A:ILE:HG12	1:33:A:ALA:H	1	0.28
(1,981)	1:31:A:ILE:HG13	1:33:A:ALA:H	1	0.28
(1,981)	1:31:A:ILE:HG12	1:33:A:ALA:H	36	0.28
(1,981)	1:31:A:ILE:HG13	1:33:A:ALA:H	36	0.28
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	40	0.28
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	40	0.28
(1,961)	1:36:A:MET:H	1:37:A:LEU:HG	39	0.28
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	30	0.28
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	30	0.28
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	19	0.28
(1,897)	1:32:A:PRO:HB2	1:29:A:ALA:HA	26	0.27
(1,897)	1:32:A:PRO:HB3	1:29:A:ALA:HA	26	0.27
(1,608)	1:50:A:LEU:H	1:53:A:VAL:HB	37	0.27
(1,1465)	1:50:A:LEU:H	1:51:A:TRP:HA	39	0.26
(1,1423)	1:9:A:ASN:HB2	1:9:A:ASN:H	31	0.26
(1,1423)	1:9:A:ASN:HB3	1:9:A:ASN:H	31	0.26
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	25	0.26
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	25	0.26
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH11	3	0.26
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH12	3	0.26
(1,897)	1:32:A:PRO:HB2	1:29:A:ALA:HA	29	0.26
(1,897)	1:32:A:PRO:HB3	1:29:A:ALA:HA	29	0.26
(1,167)	1:34:A:ILE:HG21	1:35:A:TYR:HA	12	0.26
(1,167)	1:34:A:ILE:HG22	1:35:A:TYR:HA	12	0.26
(1,167)	1:34:A:ILE:HG23	1:35:A:TYR:HA	12	0.26
(1,1320)	1:11:A:TYR:HB2	1:13:A:ALA:H	10	0.25
(1,1320)	1:11:A:TYR:HB3	1:13:A:ALA:H	10	0.25
(1,990)	1:46:A:ASN:H	1:44:A:THR:HA	34	0.25
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	15	0.25
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	15	0.25
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	38	0.25
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	38	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB2	15	0.25
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB3	15	0.25
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	26	0.25
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG3	26	0.25
(1,207)	1:43:A:THR:HB	1:46:A:ASN:H	16	0.25
(1,1320)	1:11:A:TYR:HB2	1:13:A:ALA:H	8	0.24
(1,1320)	1:11:A:TYR:HB3	1:13:A:ALA:H	8	0.24
(1,1320)	1:10:A:TYR:HB2	1:13:A:ALA:H	17	0.24
(1,1320)	1:10:A:TYR:HB3	1:13:A:ALA:H	17	0.24
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH11	38	0.24
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH12	38	0.24
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH11	24	0.24
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH12	24	0.24
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH11	24	0.24
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH12	24	0.24
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	32	0.24
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	32	0.24
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	26	0.24
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	26	0.24
(1,303)	1:29:A:ALA:HB2	1:32:A:PRO:HG2	29	0.24
(1,303)	1:29:A:ALA:HB2	1:32:A:PRO:HG3	29	0.24
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	39	0.24
(1,1402)	1:46:A:ASN:H	1:44:A:THR:H	37	0.23
(1,1358)	1:42:A:GLY:H	1:39:A:PHE:HA	29	0.23
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	3	0.23
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	3	0.23
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	32	0.23
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	32	0.23
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	3	0.23
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	3	0.23
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	32	0.23
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	32	0.23
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	13	0.23
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	13	0.23
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	13	0.23
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	13	0.23
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB2	26	0.23
(1,756)	1:38:A:VAL:HB	1:35:A:TYR:HB3	26	0.23
(1,608)	1:50:A:LEU:H	1:53:A:VAL:HB	36	0.23
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	11	0.23
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE1	33	0.23
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE2	33	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1358)	1:42:A:GLY:H	1:39:A:PHE:HA	10	0.22
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	10	0.22
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	10	0.22
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	10	0.22
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	10	0.22
(1,990)	1:46:A:ASN:H	1:44:A:THR:HA	8	0.22
(1,990)	1:46:A:ASN:H	1:44:A:THR:HA	17	0.22
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	9	0.22
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	9	0.22
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	30	0.22
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	30	0.22
(1,961)	1:36:A:MET:H	1:37:A:LEU:HG	17	0.22
(1,198)	1:36:A:MET:H	1:33:A:ALA:HA	10	0.22
(1,167)	1:31:A:ILE:HG21	1:35:A:TYR:HA	24	0.22
(1,167)	1:31:A:ILE:HG22	1:35:A:TYR:HA	24	0.22
(1,167)	1:31:A:ILE:HG23	1:35:A:TYR:HA	24	0.22
(1,1468)	1:53:A:VAL:H	1:50:A:LEU:HA	37	0.21
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	1	0.21
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	1	0.21
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	4	0.21
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	4	0.21
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	23	0.21
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	23	0.21
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	25	0.21
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	25	0.21
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD2	9	0.21
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD3	9	0.21
(1,813)	1:21:A:TYR:HD1	1:19:A:CYS:H	30	0.21
(1,798)	1:31:A:ILE:H	1:32:A:PRO:HB2	40	0.21
(1,798)	1:31:A:ILE:H	1:32:A:PRO:HB3	40	0.21
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB2	22	0.21
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB3	22	0.21
(1,226)	1:31:A:ILE:H	1:32:A:PRO:HB2	40	0.21
(1,226)	1:31:A:ILE:H	1:32:A:PRO:HB3	40	0.21
(1,1320)	1:11:A:TYR:HB2	1:13:A:ALA:H	36	0.2
(1,1320)	1:11:A:TYR:HB3	1:13:A:ALA:H	36	0.2
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	5	0.2
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	5	0.2
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	17	0.2
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	17	0.2
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	37	0.2
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	37	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,961)	1:36:A:MET:H	1:32:A:PRO:HB2	37	0.2
(1,961)	1:36:A:MET:H	1:32:A:PRO:HB3	37	0.2
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD2	14	0.2
(1,903)	1:27:A:SER:HB2	1:25:A:LYS:HD3	14	0.2
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	34	0.2
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	34	0.2
(1,608)	1:50:A:LEU:H	1:53:A:VAL:HB	6	0.2
(1,410)	1:33:A:ALA:HB3	1:31:A:ILE:H	19	0.2
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	8	0.2
(1,1320)	1:11:A:TYR:HB2	1:13:A:ALA:H	1	0.19
(1,1320)	1:11:A:TYR:HB3	1:13:A:ALA:H	1	0.19
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	36	0.19
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	36	0.19
(1,897)	1:32:A:PRO:HB2	1:29:A:ALA:HA	7	0.19
(1,897)	1:32:A:PRO:HB3	1:29:A:ALA:HA	7	0.19
(1,813)	1:21:A:TYR:HD1	1:19:A:CYS:H	10	0.19
(1,813)	1:21:A:TYR:HD1	1:19:A:CYS:H	26	0.19
(1,705)	1:31:A:ILE:HG21	1:35:A:TYR:HE1	23	0.19
(1,705)	1:31:A:ILE:HG21	1:35:A:TYR:HE2	23	0.19
(1,705)	1:31:A:ILE:HG22	1:35:A:TYR:HE1	23	0.19
(1,705)	1:31:A:ILE:HG22	1:35:A:TYR:HE2	23	0.19
(1,705)	1:31:A:ILE:HG23	1:35:A:TYR:HE1	23	0.19
(1,705)	1:31:A:ILE:HG23	1:35:A:TYR:HE2	23	0.19
(1,410)	1:33:A:ALA:HB2	1:31:A:ILE:H	28	0.19
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	18	0.18
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	18	0.18
(1,1320)	1:10:A:TYR:HB2	1:13:A:ALA:H	20	0.18
(1,1320)	1:10:A:TYR:HB3	1:13:A:ALA:H	20	0.18
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH11	39	0.18
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH12	39	0.18
(1,1217)	1:9:A:ASN:H	1:11:A:TYR:H	31	0.18
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA2	7	0.18
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA3	7	0.18
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA2	36	0.18
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA3	36	0.18
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	22	0.18
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	22	0.18
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	28	0.18
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	28	0.18
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	24	0.18
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	24	0.18
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:31:A:ILE:HB	1:35:A:TYR:HE1	30	0.18
(1,425)	1:31:A:ILE:HB	1:35:A:TYR:HE2	30	0.18
(1,239)	1:33:A:ALA:HB2	1:34:A:ILE:HB	12	0.18
(1,198)	1:36:A:MET:H	1:33:A:ALA:HA	2	0.18
(1,1465)	1:50:A:LEU:H	1:51:A:TRP:HA	22	0.17
(1,1402)	1:46:A:ASN:H	1:44:A:THR:H	34	0.17
(1,1385)	1:56:A:LYS:HD2	1:58:A:GLY:H	3	0.17
(1,1385)	1:56:A:LYS:HD3	1:58:A:GLY:H	3	0.17
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	26	0.17
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	26	0.17
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	11	0.17
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	11	0.17
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	11	0.17
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	11	0.17
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	23	0.17
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	23	0.17
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	11	0.17
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	11	0.17
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	31	0.17
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	31	0.17
(1,801)	1:18:A:GLU:HB2	1:19:A:CYS:HA	20	0.17
(1,801)	1:18:A:GLU:HB3	1:19:A:CYS:HA	20	0.17
(1,776)	1:31:A:ILE:HA	1:35:A:TYR:HE1	36	0.17
(1,776)	1:31:A:ILE:HA	1:35:A:TYR:HE2	36	0.17
(1,608)	1:56:A:LYS:H	1:53:A:VAL:HB	35	0.17
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	22	0.17
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	23	0.17
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE1	8	0.17
(1,425)	1:38:A:VAL:HB	1:35:A:TYR:HE2	8	0.17
(1,410)	1:33:A:ALA:HB2	1:31:A:ILE:H	13	0.17
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	7	0.17
(1,303)	1:29:A:ALA:HB3	1:32:A:PRO:HG3	7	0.17
(1,198)	1:36:A:MET:H	1:33:A:ALA:HA	38	0.17
(1,1270)	1:8:A:ASP:HB2	1:8:A:ASP:H	26	0.16
(1,1270)	1:8:A:ASP:HB3	1:8:A:ASP:H	26	0.16
(1,1194)	1:10:A:TYR:HB2	1:10:A:TYR:H	28	0.16
(1,1194)	1:10:A:TYR:HB3	1:10:A:TYR:H	28	0.16
(1,1194)	1:10:A:TYR:HB2	1:10:A:TYR:H	35	0.16
(1,1194)	1:10:A:TYR:HB3	1:10:A:TYR:H	35	0.16
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	2	0.16
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	2	0.16
(1,813)	1:21:A:TYR:HD1	1:19:A:CYS:H	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:55:A:ARG:HA	1:55:A:ARG:HD2	36	0.16
(1,639)	1:55:A:ARG:HA	1:55:A:ARG:HD3	36	0.16
(1,476)	1:23:A:ASP:HB2	1:22:A:THR:HA	32	0.16
(1,476)	1:23:A:ASP:HB3	1:22:A:THR:HA	32	0.16
(1,415)	1:10:A:TYR:HB2	1:10:A:TYR:H	28	0.16
(1,415)	1:10:A:TYR:HB3	1:10:A:TYR:H	28	0.16
(1,415)	1:10:A:TYR:HB2	1:10:A:TYR:H	35	0.16
(1,415)	1:10:A:TYR:HB3	1:10:A:TYR:H	35	0.16
(1,410)	1:33:A:ALA:HB3	1:31:A:ILE:H	5	0.16
(1,322)	1:32:A:PRO:HA	1:35:A:TYR:HB2	36	0.16
(1,322)	1:32:A:PRO:HA	1:35:A:TYR:HB3	36	0.16
(1,215)	1:55:A:ARG:HA	1:55:A:ARG:HD2	36	0.16
(1,215)	1:55:A:ARG:HA	1:55:A:ARG:HD3	36	0.16
(1,198)	1:36:A:MET:H	1:33:A:ALA:HA	14	0.16
(1,198)	1:36:A:MET:H	1:33:A:ALA:HA	32	0.16
(1,85)	1:50:A:LEU:HG	1:51:A:TRP:H	39	0.16
(1,1320)	1:11:A:TYR:HB2	1:13:A:ALA:H	11	0.15
(1,1320)	1:11:A:TYR:HB3	1:13:A:ALA:H	11	0.15
(1,1320)	1:11:A:TYR:HB2	1:13:A:ALA:H	38	0.15
(1,1320)	1:11:A:TYR:HB3	1:13:A:ALA:H	38	0.15
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	14	0.15
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	15	0.15
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	17	0.15
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	18	0.15
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	19	0.15
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	25	0.15
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	30	0.15
(1,1194)	1:10:A:TYR:HB2	1:10:A:TYR:H	33	0.15
(1,1194)	1:10:A:TYR:HB3	1:10:A:TYR:H	33	0.15
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD2	22	0.15
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD3	22	0.15
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	5	0.15
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	5	0.15
(1,813)	1:21:A:TYR:HD1	1:19:A:CYS:H	37	0.15
(1,608)	1:50:A:LEU:H	1:53:A:VAL:HB	18	0.15
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	12	0.15
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB2	6	0.15
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB3	6	0.15
(1,476)	1:23:A:ASP:HB2	1:22:A:THR:HA	29	0.15
(1,476)	1:23:A:ASP:HB3	1:22:A:THR:HA	29	0.15
(1,415)	1:10:A:TYR:HB2	1:10:A:TYR:H	33	0.15
(1,415)	1:10:A:TYR:HB3	1:10:A:TYR:H	33	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,198)	1:36:A:MET:H	1:33:A:ALA:HA	11	0.15
(1,198)	1:36:A:MET:H	1:33:A:ALA:HA	30	0.15
(1,167)	1:31:A:ILE:HG21	1:35:A:TYR:HA	7	0.15
(1,167)	1:31:A:ILE:HG22	1:35:A:TYR:HA	7	0.15
(1,167)	1:31:A:ILE:HG23	1:35:A:TYR:HA	7	0.15
(1,1358)	1:42:A:GLY:H	1:43:A:THR:HB	20	0.14
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	10	0.14
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	32	0.14
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	34	0.14
(1,1271)	1:64:A:HIS:H	1:63:A:HIS:HA	40	0.14
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA2	16	0.14
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA3	16	0.14
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA2	34	0.14
(1,1147)	1:14:A:ASP:H	1:12:A:GLY:HA3	34	0.14
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	22	0.14
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	22	0.14
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	22	0.14
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	22	0.14
(1,990)	1:46:A:ASN:H	1:44:A:THR:HA	16	0.14
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	12	0.14
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	12	0.14
(1,705)	1:31:A:ILE:HG21	1:35:A:TYR:HE1	26	0.14
(1,705)	1:31:A:ILE:HG21	1:35:A:TYR:HE2	26	0.14
(1,705)	1:31:A:ILE:HG22	1:35:A:TYR:HE1	26	0.14
(1,705)	1:31:A:ILE:HG22	1:35:A:TYR:HE2	26	0.14
(1,705)	1:31:A:ILE:HG23	1:35:A:TYR:HE1	26	0.14
(1,705)	1:31:A:ILE:HG23	1:35:A:TYR:HE2	26	0.14
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	17	0.14
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	30	0.14
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	10	0.13
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	10	0.13
(1,1358)	1:42:A:GLY:H	1:39:A:PHE:HA	30	0.13
(1,1202)	1:61:A:HIS:HA	1:62:A:HIS:H	18	0.13
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	8	0.13
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	8	0.13
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	8	0.13
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	8	0.13
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	31	0.13
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	31	0.13
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	6	0.13
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	6	0.13
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	16	0.13
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	19	0.13
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	19	0.13
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	7	0.13
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	7	0.13
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB2	21	0.13
(1,756)	1:31:A:ILE:HB	1:35:A:TYR:HB3	21	0.13
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	1	0.13
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	9	0.13
(1,198)	1:36:A:MET:H	1:33:A:ALA:HA	22	0.13
(1,198)	1:36:A:MET:H	1:33:A:ALA:HA	24	0.13
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	9	0.12
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	9	0.12
(1,1367)	1:24:A:TRP:H	1:22:A:THR:H	27	0.12
(1,1259)	1:12:A:GLY:HA2	1:13:A:ALA:H	26	0.12
(1,1259)	1:12:A:GLY:HA3	1:13:A:ALA:H	26	0.12
(1,1207)	1:11:A:TYR:HA	1:12:A:GLY:H	26	0.12
(1,1202)	1:61:A:HIS:HA	1:62:A:HIS:H	20	0.12
(1,1120)	1:19:A:CYS:HA	1:23:A:ASP:H	40	0.12
(1,928)	1:21:A:TYR:H	1:19:A:CYS:HA	33	0.12
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB2	13	0.12
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB3	13	0.12
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB2	36	0.12
(1,514)	1:53:A:VAL:HA	1:56:A:LYS:HB3	36	0.12
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB2	6	0.12
(1,437)	1:53:A:VAL:HG11	1:57:A:LYS:HB3	6	0.12
(1,419)	1:38:A:VAL:HB	1:39:A:PHE:HB2	32	0.12
(1,419)	1:38:A:VAL:HB	1:39:A:PHE:HB3	32	0.12
(1,412)	1:19:A:CYS:HB3	1:18:A:GLU:HA	25	0.12
(1,378)	1:35:A:TYR:HA	1:35:A:TYR:HE1	36	0.12
(1,378)	1:35:A:TYR:HA	1:35:A:TYR:HE2	36	0.12
(1,294)	1:11:A:TYR:HA	1:12:A:GLY:H	26	0.12
(1,267)	1:50:A:LEU:HA	1:53:A:VAL:HB	12	0.12
(1,85)	1:50:A:LEU:HG	1:51:A:TRP:H	29	0.12
(1,1433)	1:61:A:HIS:H	1:62:A:HIS:H	18	0.11
(1,1433)	1:61:A:HIS:H	1:62:A:HIS:H	20	0.11
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	2	0.11
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	2	0.11
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	6	0.11
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	6	0.11
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	7	0.11
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	6	0.11
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	6	0.11
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	7	0.11
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	7	0.11
(1,608)	1:50:A:LEU:H	1:53:A:VAL:HB	13	0.11
(1,567)	1:33:A:ALA:HB3	1:32:A:PRO:HA	8	0.11
(1,567)	1:33:A:ALA:HB2	1:32:A:PRO:HA	29	0.11
(1,567)	1:33:A:ALA:HB1	1:32:A:PRO:HA	31	0.11
(1,410)	1:33:A:ALA:HB2	1:31:A:ILE:H	32	0.11
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	4	0.11
(1,303)	1:29:A:ALA:HB1	1:32:A:PRO:HG3	4	0.11
(1,254)	1:50:A:LEU:HB2	1:49:A:VAL:HB	39	0.11
(1,254)	1:50:A:LEU:HB3	1:49:A:VAL:HB	39	0.11
(1,239)	1:33:A:ALA:HB1	1:34:A:ILE:HB	18	0.11
(1,198)	1:36:A:MET:H	1:33:A:ALA:HA	6	0.11
(1,1468)	1:53:A:VAL:H	1:50:A:LEU:HA	32	0.1
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	13	0.1
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	13	0.1
(1,1385)	1:57:A:LYS:HD2	1:58:A:GLY:H	15	0.1
(1,1385)	1:57:A:LYS:HD3	1:58:A:GLY:H	15	0.1
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH11	10	0.1
(1,1302)	1:51:A:TRP:HE1	1:55:A:ARG:HH12	10	0.1
(1,1246)	1:45:A:GLY:H	1:47:A:GLY:HA2	24	0.1
(1,1246)	1:45:A:GLY:H	1:47:A:GLY:HA3	24	0.1
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH21	30	0.1
(1,1038)	1:59:A:HIS:HA	1:55:A:ARG:HH22	30	0.1
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH21	30	0.1
(1,992)	1:59:A:HIS:HA	1:55:A:ARG:HH22	30	0.1
(1,981)	1:30:A:LEU:HB2	1:33:A:ALA:H	13	0.1
(1,981)	1:30:A:LEU:HB3	1:33:A:ALA:H	13	0.1
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG12	7	0.1
(1,961)	1:36:A:MET:H	1:34:A:ILE:HG13	7	0.1
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD2	11	0.1
(1,903)	1:27:A:SER:HB3	1:25:A:LYS:HD3	11	0.1
(1,897)	1:30:A:LEU:HB2	1:29:A:ALA:HA	21	0.1
(1,897)	1:30:A:LEU:HB3	1:29:A:ALA:HA	21	0.1
(1,705)	1:31:A:ILE:HG21	1:35:A:TYR:HE1	24	0.1
(1,705)	1:31:A:ILE:HG21	1:35:A:TYR:HE2	24	0.1
(1,705)	1:31:A:ILE:HG22	1:35:A:TYR:HE1	24	0.1
(1,705)	1:31:A:ILE:HG22	1:35:A:TYR:HE2	24	0.1
(1,705)	1:31:A:ILE:HG23	1:35:A:TYR:HE1	24	0.1
(1,705)	1:31:A:ILE:HG23	1:35:A:TYR:HE2	24	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:33:A:ALA:HB3	1:34:A:ILE:HB	19	0.1
(1,181)	1:34:A:ILE:HD11	1:34:A:ILE:HA	32	0.1
(1,181)	1:34:A:ILE:HD12	1:34:A:ILE:HA	32	0.1
(1,181)	1:34:A:ILE:HD13	1:34:A:ILE:HA	32	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found