



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 12:19 PM UTC

PDB ID : 6R0J / pdb_00006r0j
BMRB ID : 34376
Title : The N-terminal domain of rhomboid protease YqgP
Authors : Began, J.; Strisovsky, K.; Veverka, V.
Deposited on : 2019-03-13

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

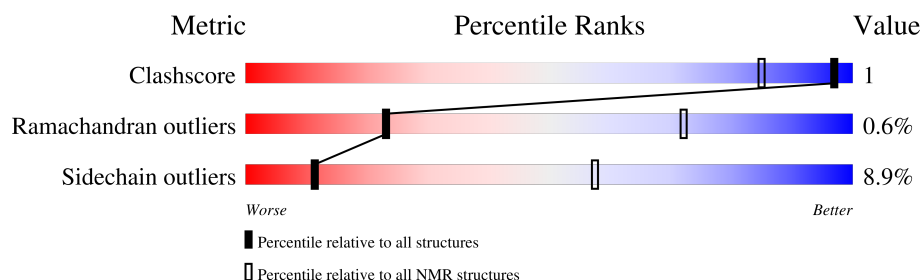
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	185	

2 Ensemble composition and analysis

This entry contains 30 models. Model 27 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:25, A:29-A:133, A:146-A:159 (142)	0.74	27

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

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

The models can be grouped into 3 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 8, 9, 10, 13, 14, 19, 20, 25, 27, 29
2	4, 11, 15, 18, 24, 26, 28
3	7, 16, 17, 22
Single-model clusters	6; 12; 21; 23; 30

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3031 atoms, of which 1494 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Rhomboid family serine protease.

Mol	Chain	Residues	Atoms						Trace
1	A	185	Total	C	H	N	O	S	0
			3031	967	1494	271	293	6	

There are 9 discrepancies between the modelled and reference sequences:

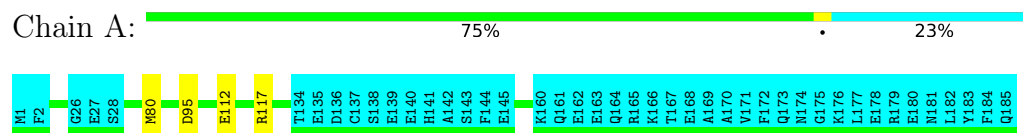
Chain	Residue	Modelled	Actual	Comment	Reference
A	177	LEU	-	expression tag	UNP A0A162T8T3
A	178	GLU	-	expression tag	UNP A0A162T8T3
A	179	ARG	-	expression tag	UNP A0A162T8T3
A	180	GLU	-	expression tag	UNP A0A162T8T3
A	181	ASN	-	expression tag	UNP A0A162T8T3
A	182	LEU	-	expression tag	UNP A0A162T8T3
A	183	TYR	-	expression tag	UNP A0A162T8T3
A	184	PHE	-	expression tag	UNP A0A162T8T3
A	185	GLN	-	expression tag	UNP A0A162T8T3

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: Rhomboid family serine protease

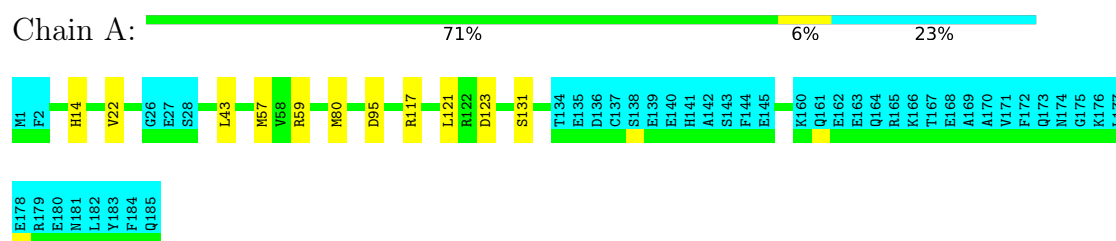


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

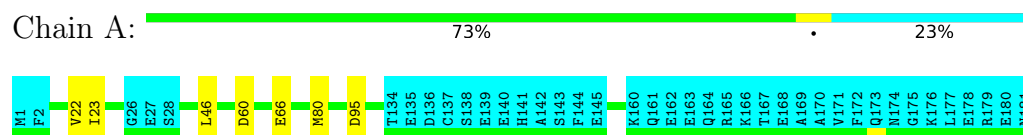
4.2.1 Score per residue for model 1

- Molecule 1: Rhomboid family serine protease



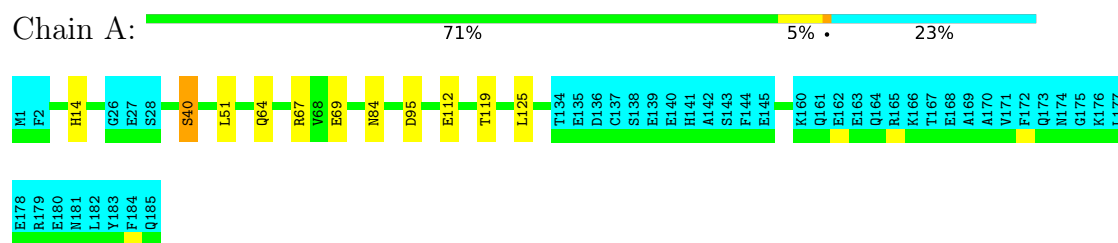
4.2.2 Score per residue for model 2

- Molecule 1: Rhomboid family serine protease



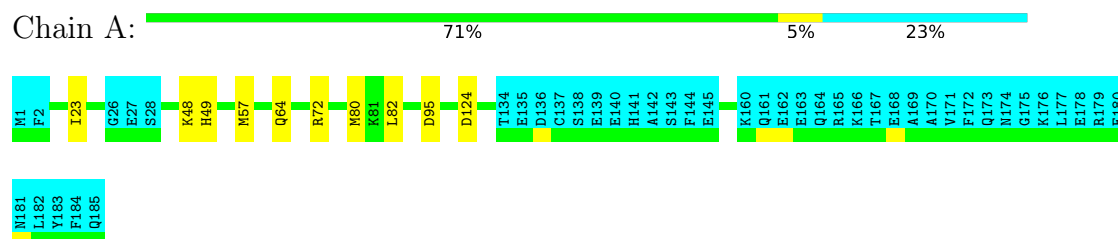
4.2.3 Score per residue for model 3

- Molecule 1: Rhomboid family serine protease



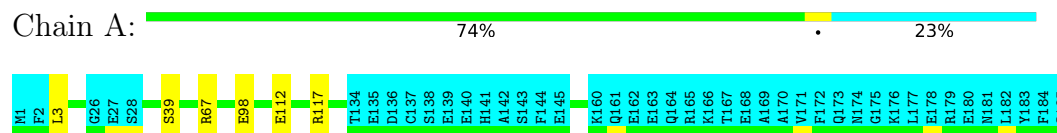
4.2.4 Score per residue for model 4

- Molecule 1: Rhomboid family serine protease



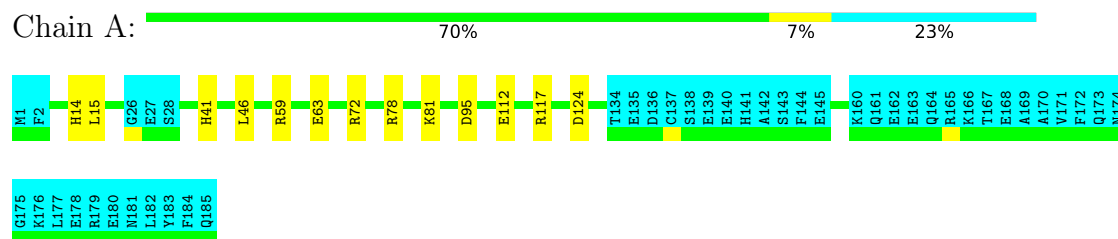
4.2.5 Score per residue for model 5

- Molecule 1: Rhomboid family serine protease



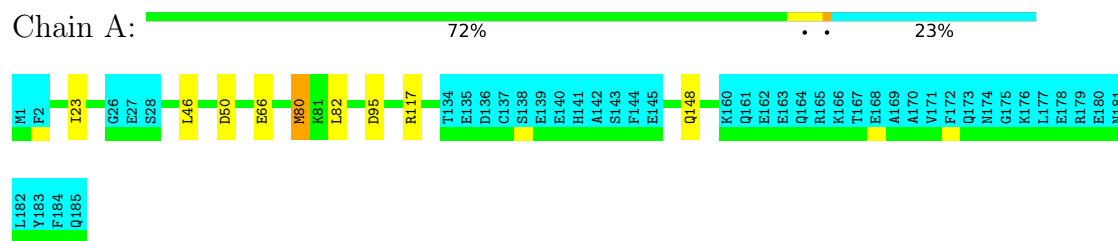
4.2.6 Score per residue for model 6

- Molecule 1: Rhomboid family serine protease



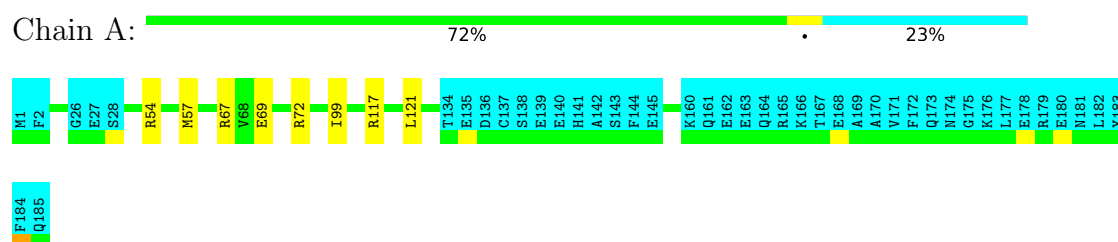
4.2.7 Score per residue for model 7

- Molecule 1: Rhomboid family serine protease



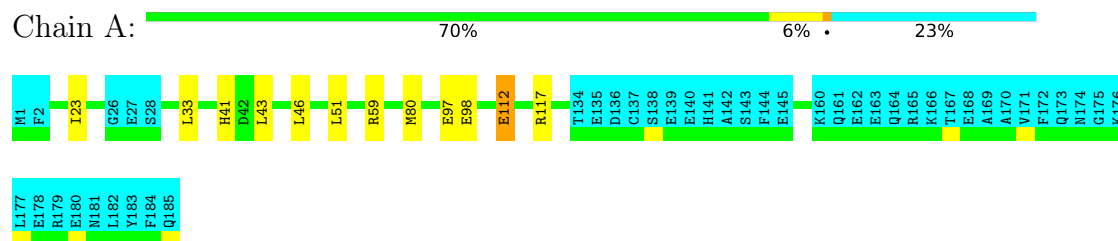
4.2.8 Score per residue for model 8

- Molecule 1: Rhomboid family serine protease



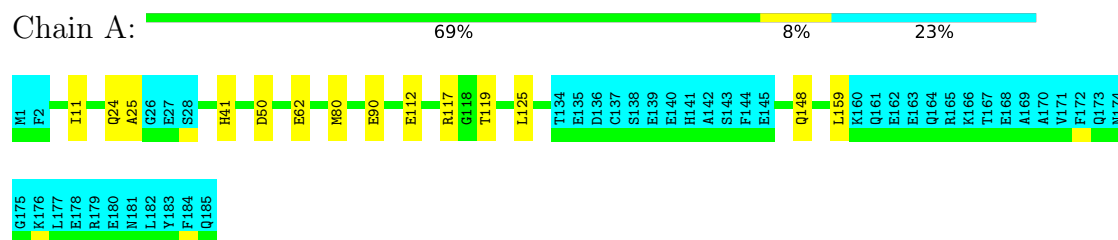
4.2.9 Score per residue for model 9

- Molecule 1: Rhomboid family serine protease



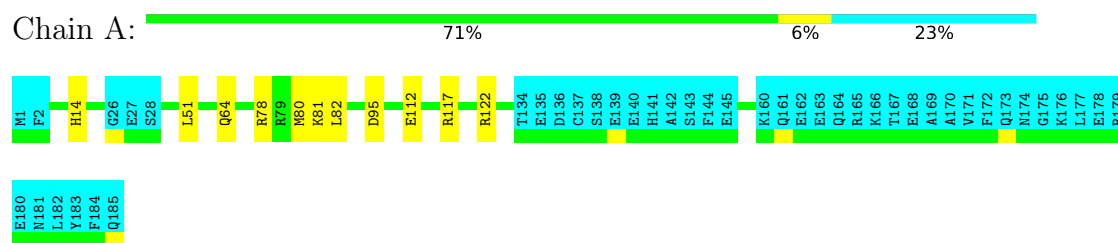
4.2.10 Score per residue for model 10

- Molecule 1: Rhomboid family serine protease



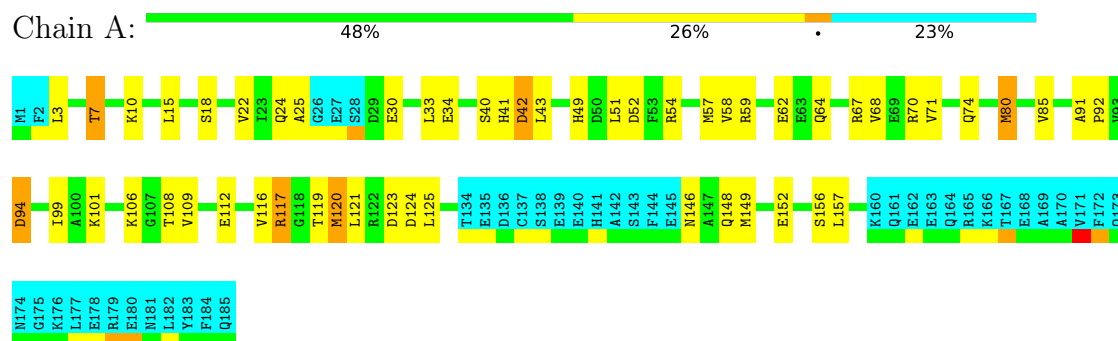
4.2.11 Score per residue for model 11

- Molecule 1: Rhomboid family serine protease



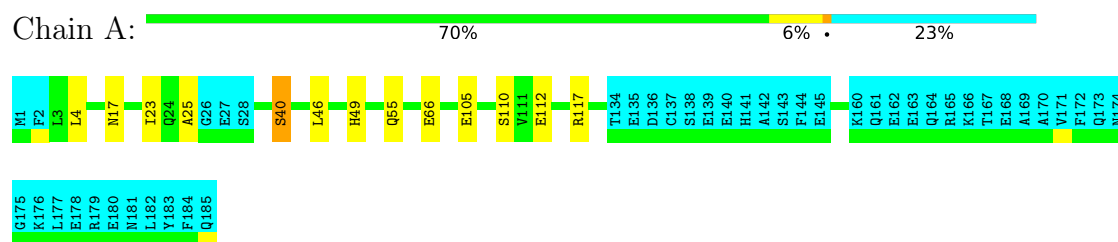
4.2.12 Score per residue for model 12

- Molecule 1: Rhomboid family serine protease



4.2.13 Score per residue for model 13

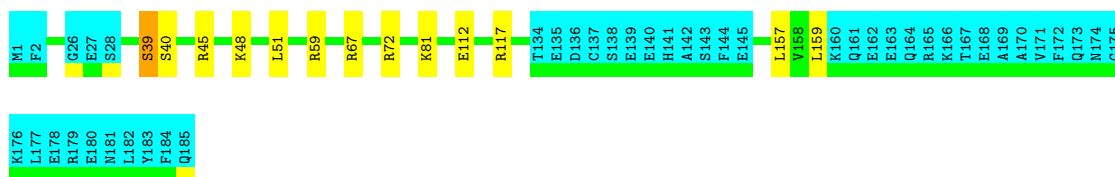
- Molecule 1: Rhomboid family serine protease



4.2.14 Score per residue for model 14

- Molecule 1: Rhomboid family serine protease

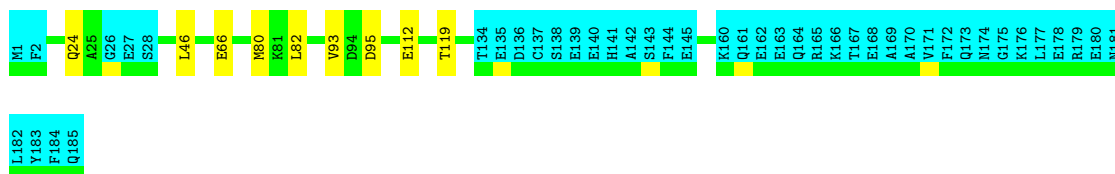




4.2.15 Score per residue for model 15

- Molecule 1: Rhomboid family serine protease

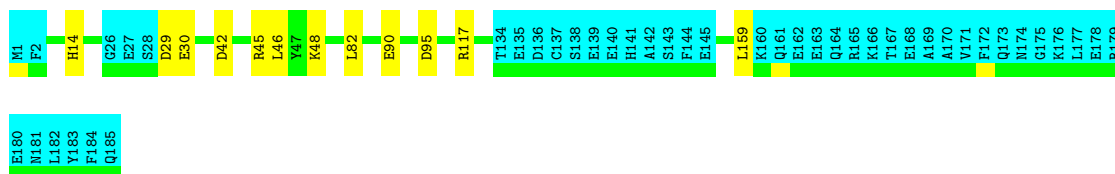
Chain A: 72% 5% 23%



4.2.16 Score per residue for model 16

- Molecule 1: Rhomboid family serine protease

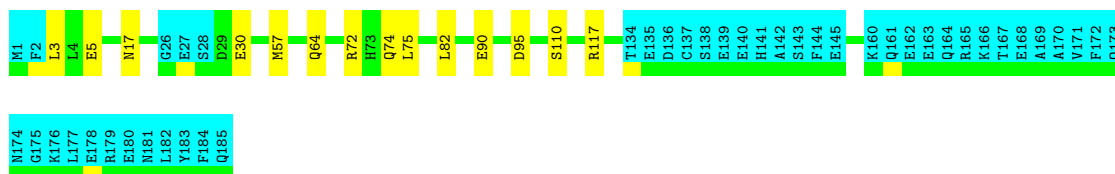
Chain A: 70% 6% 23%



4.2.17 Score per residue for model 17

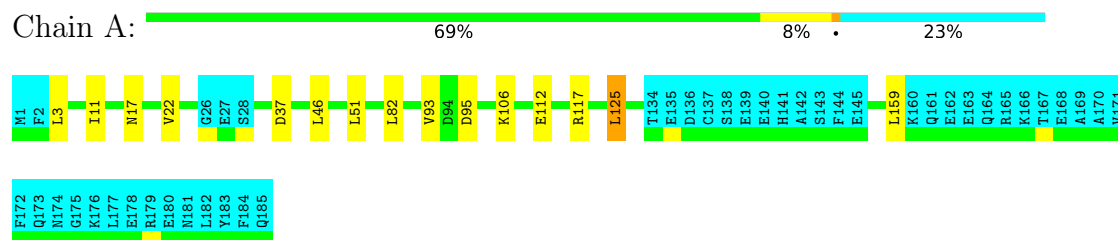
- Molecule 1: Rhomboid family serine protease

Chain A: 69% 8% 23%



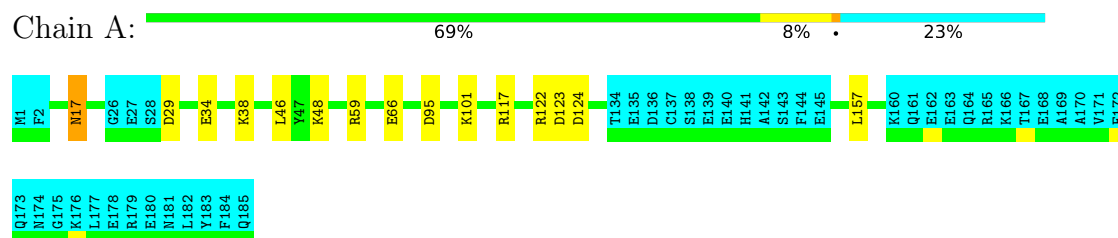
4.2.18 Score per residue for model 18

- Molecule 1: Rhomboid family serine protease



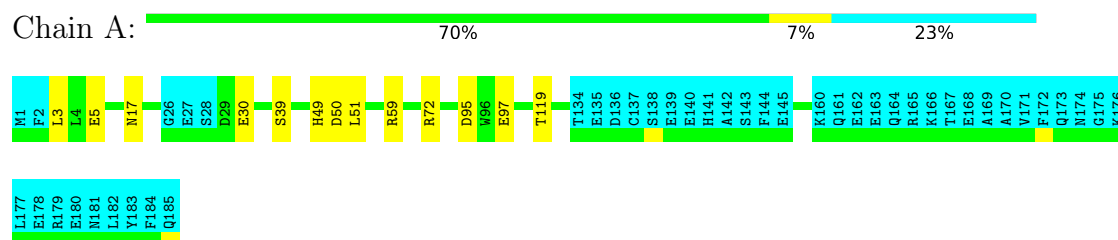
4.2.19 Score per residue for model 19

- Molecule 1: Rhomboid family serine protease



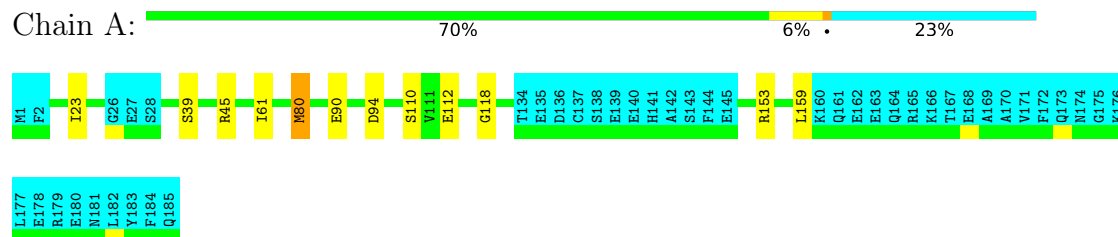
4.2.20 Score per residue for model 20

- Molecule 1: Rhomboid family serine protease



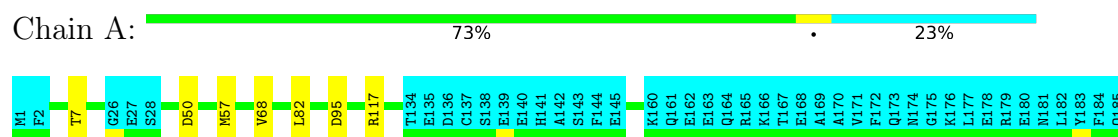
4.2.21 Score per residue for model 21

- Molecule 1: Rhomboid family serine protease



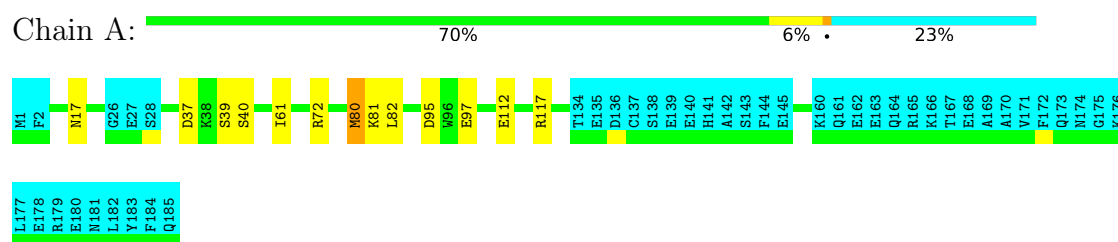
4.2.22 Score per residue for model 22

- Molecule 1: Rhomboid family serine protease



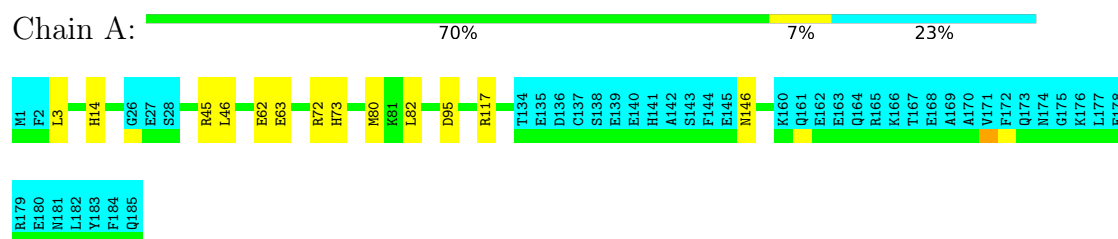
4.2.23 Score per residue for model 23

- Molecule 1: Rhomboid family serine protease



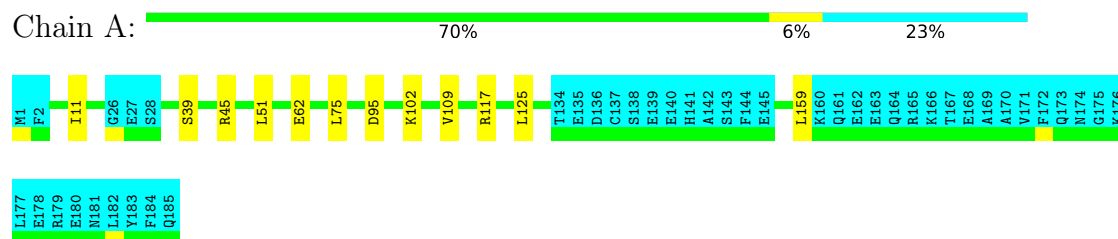
4.2.24 Score per residue for model 24

- Molecule 1: Rhomboid family serine protease



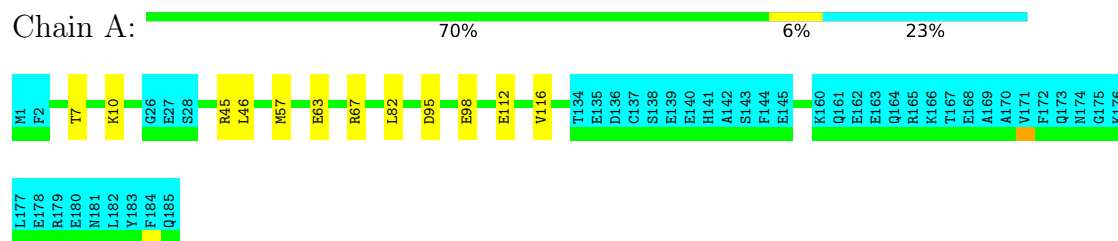
4.2.25 Score per residue for model 25

- Molecule 1: Rhomboid family serine protease



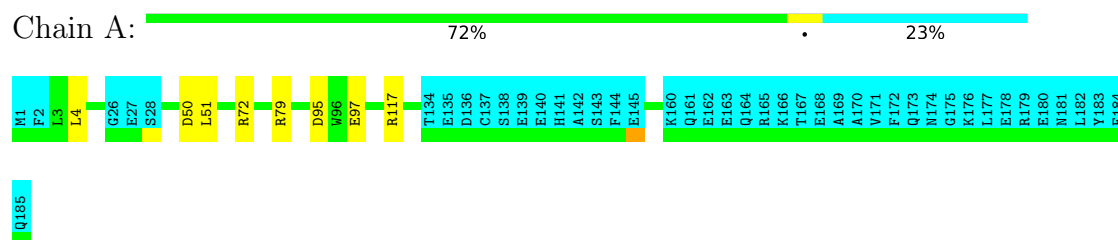
4.2.26 Score per residue for model 26

- Molecule 1: Rhomboid family serine protease



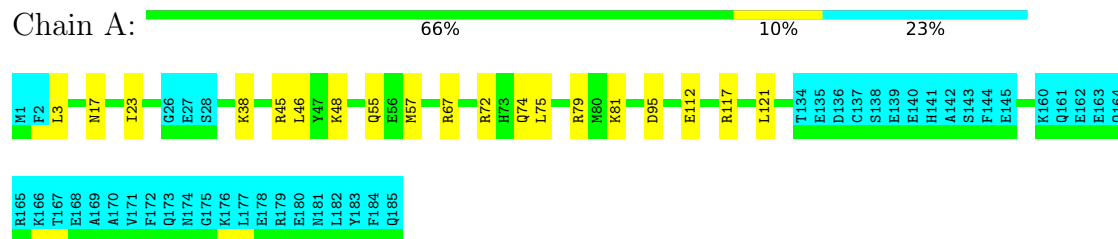
4.2.27 Score per residue for model 27 (medoid)

- Molecule 1: Rhomboid family serine protease



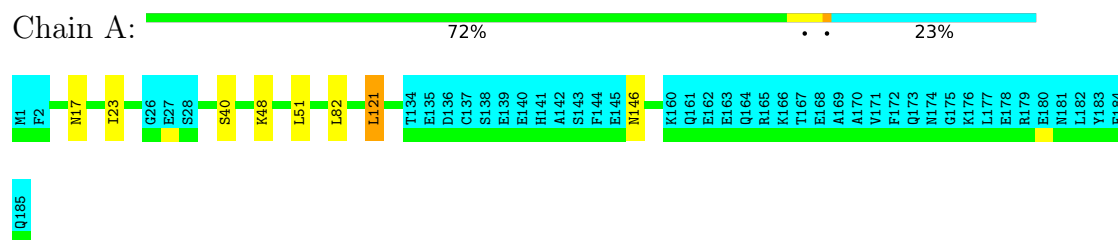
4.2.28 Score per residue for model 28

- Molecule 1: Rhomboid family serine protease



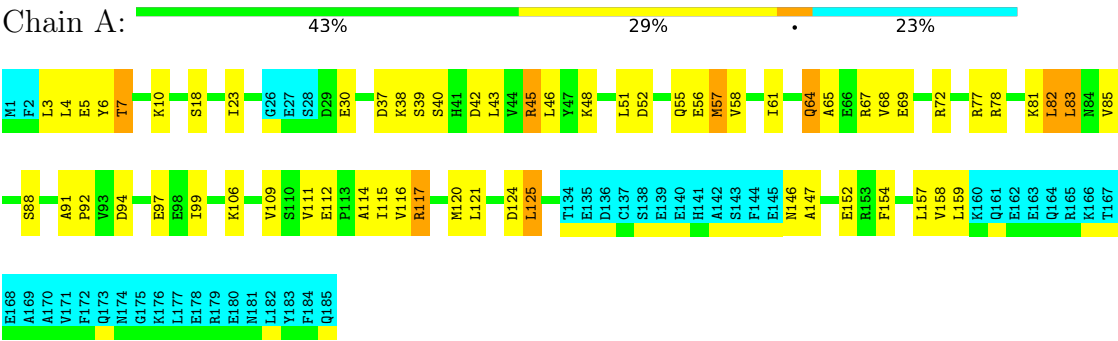
4.2.29 Score per residue for model 29

- Molecule 1: Rhomboid family serine protease



4.2.30 Score per residue for model 30

● Molecule 1: Rhomboid family serine protease



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	
YASARA	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	2244
Number of shifts mapped to atoms	2244
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.72±0.13	0±0/1204 (0.0± 0.0%)	0.90±0.08	1±1/1626 (0.1± 0.1%)
All	All	0.73	10/36120 (0.0%)	0.91	26/48780 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	80	MET	SD-CE	-7.98	1.59	1.79	24	5
1	A	57	MET	SD-CE	-5.41	1.66	1.79	26	5

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	121	LEU	N-CA-C	6.61	119.33	111.33	28	4
1	A	23	ILE	N-CA-C	-6.52	105.95	111.56	29	8
1	A	93	VAL	N-CA-C	6.45	121.18	111.89	18	2
1	A	94	ASP	N-CA-C	5.55	116.37	108.54	21	1
1	A	78	ARG	N-CA-C	5.41	116.86	111.07	11	1
1	A	38	LYS	N-CA-C	-5.30	104.58	111.74	19	1
1	A	25	ALA	N-CA-C	5.30	116.97	107.80	13	2
1	A	40	SER	N-CA-C	5.23	121.94	110.80	13	1
1	A	110	SER	N-CA-C	-5.18	100.26	109.06	21	1
1	A	42	ASP	N-CA-C	-5.09	106.57	112.89	16	1
1	A	112	GLU	CA-C-N	-5.05	115.36	120.31	9	1
1	A	112	GLU	C-N-CA	-5.05	115.36	120.31	9	1
1	A	95	ASP	N-CA-C	5.04	118.55	111.90	24	1
1	A	118	GLY	N-CA-C	-5.04	106.31	113.86	21	1

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	1179	1172	1172	2±6
All	All	35370	35160	35160	52

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:VAL:HG11	1:A:109:VAL:HG13	0.76	1.55	12	2
1:A:7:THR:HG21	1:A:121:LEU:HD21	0.74	1.57	12	1
1:A:64:GLN:O	1:A:68:VAL:HG23	0.63	1.93	12	2
1:A:116:VAL:HG13	1:A:124:ASP:CB	0.63	2.24	12	1
1:A:42:ASP:CB	1:A:80:MET:HE3	0.62	2.25	12	1
1:A:42:ASP:HB2	1:A:80:MET:HE3	0.61	1.71	12	1
1:A:7:THR:CG2	1:A:121:LEU:HD21	0.59	2.26	12	1
1:A:119:THR:HG23	1:A:120:MET:HG2	0.58	1.75	12	1
1:A:42:ASP:O	1:A:43:LEU:HD23	0.58	1.99	12	1
1:A:116:VAL:HG12	1:A:124:ASP:HB3	0.57	1.76	30	1
1:A:116:VAL:HG12	1:A:124:ASP:CB	0.57	2.29	30	1
1:A:91:ALA:HB2	1:A:117:ARG:HD2	0.56	1.77	30	2
1:A:82:LEU:O	1:A:111:VAL:HG13	0.55	2.02	30	1
1:A:159:LEU:HD13	1:A:159:LEU:O	0.54	2.01	30	1
1:A:116:VAL:HG13	1:A:124:ASP:HB2	0.53	1.80	12	1
1:A:82:LEU:HD13	1:A:83:LEU:N	0.53	2.19	30	1
1:A:57:MET:HE1	1:A:115:ILE:CD1	0.52	2.34	30	1
1:A:6:TYR:HB2	1:A:147:ALA:HB2	0.52	1.81	30	1
1:A:45:ARG:CG	1:A:82:LEU:HD11	0.51	2.36	30	1
1:A:22:VAL:HG11	1:A:25:ALA:HB2	0.50	1.84	12	1
1:A:4:LEU:HD11	1:A:88:SER:O	0.49	2.08	30	1
1:A:45:ARG:HG3	1:A:82:LEU:HD11	0.49	1.82	30	1
1:A:119:THR:HG23	1:A:120:MET:CG	0.48	2.38	12	1
1:A:85:VAL:CG1	1:A:116:VAL:HG23	0.47	2.39	12	1
1:A:57:MET:O	1:A:61:ILE:HD12	0.47	2.08	30	1
1:A:57:MET:HE1	1:A:115:ILE:HD12	0.47	1.86	30	1
1:A:154:PHE:O	1:A:158:VAL:HG23	0.47	2.09	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:LEU:HD13	1:A:159:LEU:C	0.46	2.36	30	1
1:A:91:ALA:HB1	1:A:92:PRO:HD2	0.45	1.87	12	2
1:A:85:VAL:HG23	1:A:114:ALA:CB	0.45	2.42	30	1
1:A:23:ILE:HD11	1:A:43:LEU:HD22	0.45	1.89	30	1
1:A:22:VAL:CG1	1:A:25:ALA:HB2	0.44	2.42	12	1
1:A:54:ARG:HD2	1:A:99:ILE:HD11	0.44	1.89	8	1
1:A:68:VAL:CG1	1:A:109:VAL:HG13	0.44	2.34	12	1
1:A:11:ILE:HD11	1:A:125:LEU:HD11	0.44	1.89	25	2
1:A:15:LEU:HG	1:A:33:LEU:HD13	0.44	1.89	12	1
1:A:43:LEU:HD11	1:A:71:VAL:HG11	0.44	1.90	12	1
1:A:58:VAL:HG13	1:A:99:ILE:HG12	0.44	1.90	12	1
1:A:15:LEU:HB3	1:A:33:LEU:HD22	0.43	1.89	12	1
1:A:17:ASN:C	1:A:17:ASN:HD22	0.42	2.22	19	1
1:A:65:ALA:HB1	1:A:106:LYS:CB	0.42	2.44	30	1
1:A:68:VAL:HG13	1:A:80:MET:HB3	0.41	1.91	12	1
1:A:7:THR:CG2	1:A:125:LEU:HD11	0.41	2.46	30	1
1:A:58:VAL:CG1	1:A:99:ILE:HD12	0.41	2.44	30	1
1:A:45:ARG:O	1:A:46:LEU:HD12	0.40	2.15	30	1
1:A:3:LEU:HD12	1:A:3:LEU:O	0.40	2.17	30	1
1:A:157:LEU:C	1:A:157:LEU:HD23	0.40	2.42	30	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	142/185 (77%)	138±2 (97±1%)	3±2 (2±1%)	1±1 (1±0%)	23	72
All	All	4260/5550 (77%)	4138 (97%)	97 (2%)	25 (1%)	23	72

All 4 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	95	ASP	19
1	A	40	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	94	ASP	2
1	A	39	SER	2

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	126/164 (77%)	115±7 (91±6%)	11±7 (9±6%)	11	57
All	All	3780/4920 (77%)	3445 (91%)	335 (9%)	11	57

All 87 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	117	ARG	22
1	A	112	GLU	16
1	A	82	LEU	13
1	A	46	LEU	12
1	A	51	LEU	11
1	A	72	ARG	11
1	A	80	MET	10
1	A	67	ARG	8
1	A	17	ASN	8
1	A	45	ARG	8
1	A	59	ARG	7
1	A	48	LYS	7
1	A	3	LEU	7
1	A	14	HIS	6
1	A	40	SER	6
1	A	39	SER	6
1	A	81	LYS	6
1	A	159	LEU	6
1	A	66	GLU	5
1	A	64	GLN	5
1	A	125	LEU	5
1	A	50	ASP	5
1	A	97	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	30	GLU	5
1	A	119	THR	4
1	A	49	HIS	4
1	A	57	MET	4
1	A	41	HIS	4
1	A	62	GLU	4
1	A	90	GLU	4
1	A	7	THR	4
1	A	146	ASN	4
1	A	22	VAL	3
1	A	123	ASP	3
1	A	69	GLU	3
1	A	124	ASP	3
1	A	98	GLU	3
1	A	63	GLU	3
1	A	148	GLN	3
1	A	24	GLN	3
1	A	10	LYS	3
1	A	74	GLN	3
1	A	157	LEU	3
1	A	55	GLN	3
1	A	5	GLU	3
1	A	75	LEU	3
1	A	37	ASP	3
1	A	43	LEU	2
1	A	78	ARG	2
1	A	122	ARG	2
1	A	18	SER	2
1	A	34	GLU	2
1	A	42	ASP	2
1	A	52	ASP	2
1	A	101	LYS	2
1	A	106	LYS	2
1	A	120	MET	2
1	A	152	GLU	2
1	A	4	LEU	2
1	A	110	SER	2
1	A	29	ASP	2
1	A	61	ILE	2
1	A	79	ARG	2
1	A	38	LYS	2
1	A	121	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	131	SER	1
1	A	60	ASP	1
1	A	84	ASN	1
1	A	15	LEU	1
1	A	33	LEU	1
1	A	11	ILE	1
1	A	54	ARG	1
1	A	70	ARG	1
1	A	94	ASP	1
1	A	108	THR	1
1	A	149	MET	1
1	A	156	SER	1
1	A	105	GLU	1
1	A	153	ARG	1
1	A	68	VAL	1
1	A	73	HIS	1
1	A	102	LYS	1
1	A	109	VAL	1
1	A	116	VAL	1
1	A	56	GLU	1
1	A	77	ARG	1
1	A	83	LEU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% 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: *starch_output*

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	2244
Number of shifts mapped to atoms	2244
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
$^{13}\text{C}_\alpha$	184	-0.51 ± 0.14	Should be checked
$^{13}\text{C}_\beta$	177	0.03 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	183	-0.11 ± 0.08	None needed (< 0.5 ppm)
^{15}N	176	-0.20 ± 0.23	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 1775 atoms were assigned a chemical shift out of a possible 2067. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	702/707 (99%)	283/285 (99%)	283/284 (100%)	136/138 (99%)
Sidechain	953/1190 (80%)	662/769 (86%)	282/363 (78%)	9/58 (16%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	120/170 (71%)	72/85 (85%)	45/78 (58%)	3/7 (43%)
Overall	1775/2067 (86%)	1017/1139 (89%)	610/725 (84%)	148/203 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 2244 atoms were assigned a chemical shift out of a possible 2643. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	910/924 (98%)	367/373 (98%)	367/370 (99%)	176/181 (97%)
Sidechain	1187/1493 (80%)	822/958 (86%)	352/462 (76%)	13/73 (18%)
Aromatic	147/226 (65%)	90/113 (80%)	54/105 (51%)	3/8 (38%)
Overall	2244/2643 (85%)	1279/1444 (89%)	773/937 (82%)	192/262 (73%)

7.1.4 Statistically unusual chemical shifts ⓘ

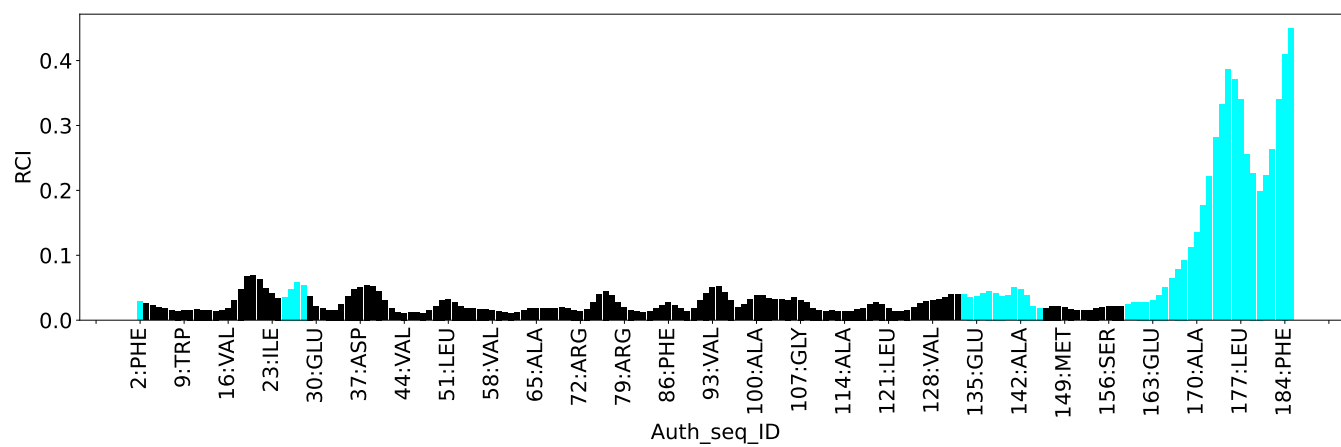
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	38	LYS	HD2	3.11	0.58 – 2.64	7.3
1	A	151	ARG	HG3	-0.48	0.15 – 2.94	-7.3
1	A	38	LYS	HD3	3.11	0.54 – 2.65	7.2
1	A	45	ARG	HB3	-0.02	0.43 – 3.11	-6.7
1	A	151	ARG	HB3	0.06	0.43 – 3.11	-6.4
1	A	97	GLU	HG3	0.97	1.20 – 3.30	-6.1
1	A	48	LYS	HB3	0.23	0.46 – 3.04	-5.9
1	A	48	LYS	HD3	0.35	0.54 – 2.65	-5.9

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2522
Intra-residue ($ i-j =0$)	295
Sequential ($ i-j =1$)	690
Medium range ($ i-j >1$ and $ i-j <5$)	542
Long range ($ i-j \geq 5$)	995
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	300
Number of unmapped restraints	0
Number of restraints per residue	15.3
Number of long range restraints per residue ¹	5.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	3.3	0.2
0.2-0.5 (Medium)	1.5	0.49
>0.5 (Large)	None	None

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)	2.9	5.08
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

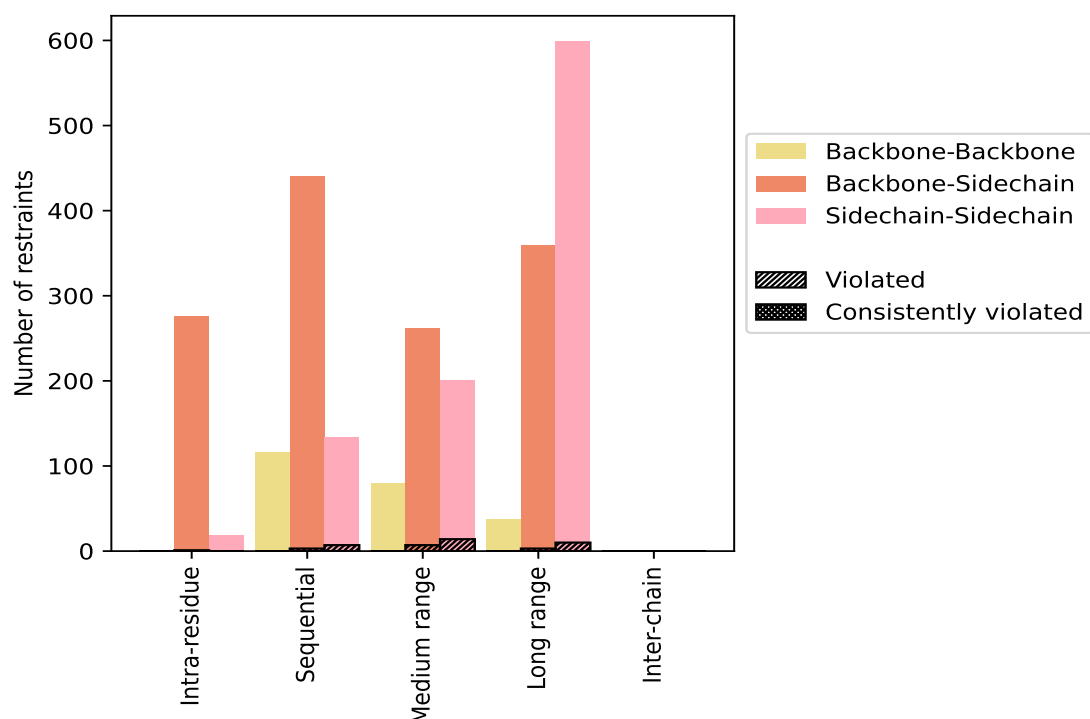
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	295	11.7	1	0.3	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	276	10.9	1	0.4	0.0	0	0.0	0.0
Sidechain-Sidechain	19	0.8	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	690	27.4	10	1.4	0.4	0	0.0	0.0
Backbone-Backbone	116	4.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	440	17.4	3	0.7	0.1	0	0.0	0.0
Sidechain-Sidechain	134	5.3	7	5.2	0.3	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	542	21.5	21	3.9	0.8	0	0.0	0.0
Backbone-Backbone	79	3.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	262	10.4	7	2.7	0.3	0	0.0	0.0
Sidechain-Sidechain	201	8.0	14	7.0	0.6	0	0.0	0.0
Long range ($i-j \geq 5$)	995	39.5	13	1.3	0.5	0	0.0	0.0
Backbone-Backbone	37	1.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	359	14.2	3	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	599	23.8	10	1.7	0.4	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	2522	100.0	45	1.8	1.8	0	0.0	0.0
Backbone-Backbone	232	9.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1337	53.0	14	1.0	0.6	0	0.0	0.0
Sidechain-Sidechain	953	37.8	31	3.3	1.2	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	1	3	2	0	6	0.18	0.23	0.03	0.19
2	0	0	7	3	0	10	0.14	0.22	0.04	0.12
3	0	0	3	2	0	5	0.19	0.27	0.05	0.18
4	1	1	8	4	0	14	0.16	0.3	0.05	0.15
5	0	2	2	2	0	6	0.18	0.33	0.08	0.15
6	0	1	4	3	0	8	0.15	0.3	0.06	0.12
7	1	1	2	1	0	5	0.2	0.35	0.1	0.14
8	0	1	4	1	0	6	0.19	0.32	0.08	0.16
9	0	1	1	0	0	2	0.16	0.2	0.05	0.16
10	0	0	2	3	0	5	0.16	0.23	0.04	0.16

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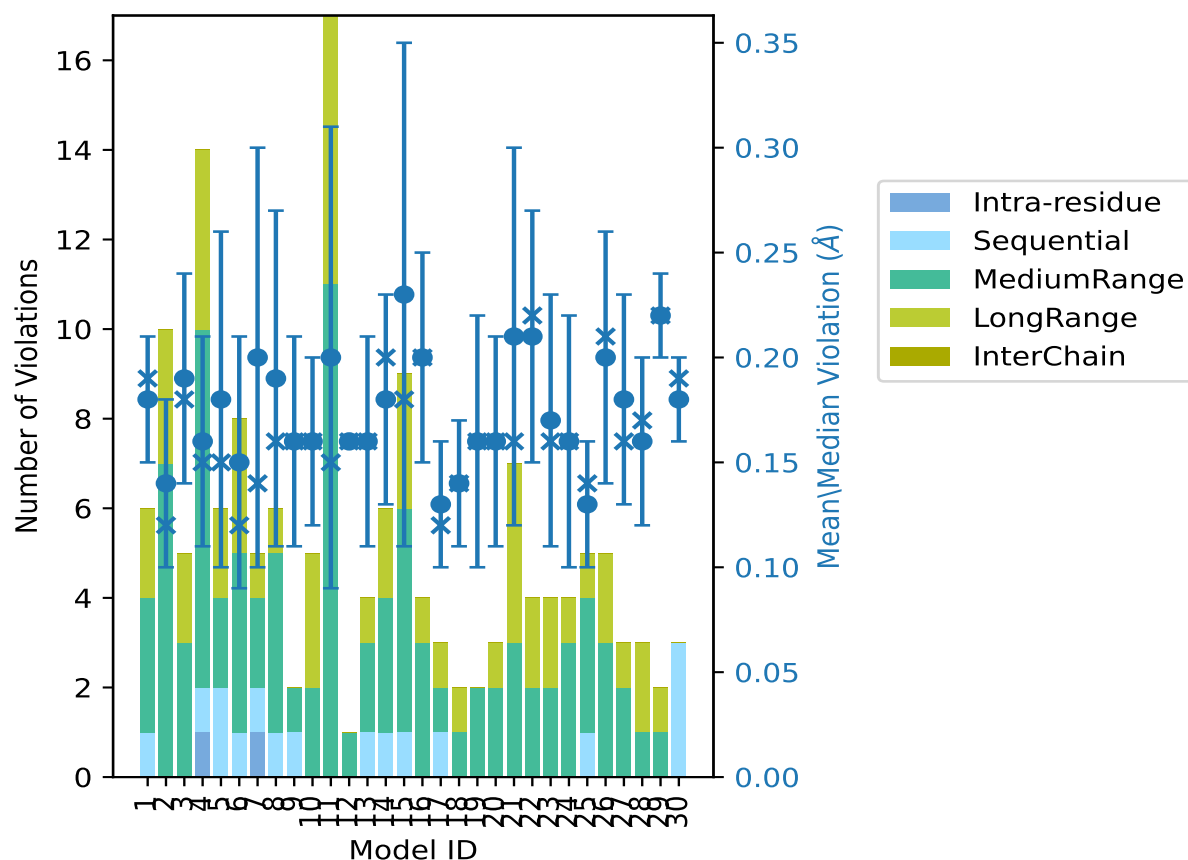
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	11	6	0	17	0.2	0.49	0.11	0.15
12	0	0	1	0	0	1	0.16	0.16	0.0	0.16
13	0	1	2	1	0	4	0.16	0.23	0.05	0.16
14	0	1	3	2	0	6	0.18	0.25	0.05	0.2
15	0	1	5	3	0	9	0.23	0.42	0.12	0.18
16	0	0	3	1	0	4	0.2	0.26	0.05	0.2
17	0	1	1	1	0	3	0.13	0.17	0.03	0.12
18	0	0	1	1	0	2	0.14	0.17	0.03	0.14
19	0	0	2	0	0	2	0.16	0.22	0.06	0.16
20	0	0	2	1	0	3	0.16	0.23	0.05	0.16
21	0	0	3	4	0	7	0.21	0.34	0.09	0.16
22	0	0	2	2	0	4	0.21	0.26	0.06	0.22
23	0	0	2	2	0	4	0.17	0.25	0.06	0.16
24	0	0	3	1	0	4	0.16	0.23	0.06	0.16
25	0	1	3	1	0	5	0.13	0.17	0.03	0.14
26	0	0	3	2	0	5	0.2	0.27	0.06	0.21
27	0	0	2	1	0	3	0.18	0.25	0.05	0.16
28	0	0	1	2	0	3	0.16	0.2	0.04	0.17
29	0	0	1	1	0	2	0.22	0.24	0.02	0.22
30	0	3	0	0	0	3	0.18	0.21	0.02	0.19

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, 2477(IR:294, SQ:680, MR:521, LR:982, 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	%
0	5	8	8	0	21	1	3.3
1	4	6	1	0	12	2	6.7
0	1	2	1	0	4	3	10.0
0	0	1	0	0	1	4	13.3
0	0	1	1	0	2	5	16.7
0	0	1	0	0	1	6	20.0

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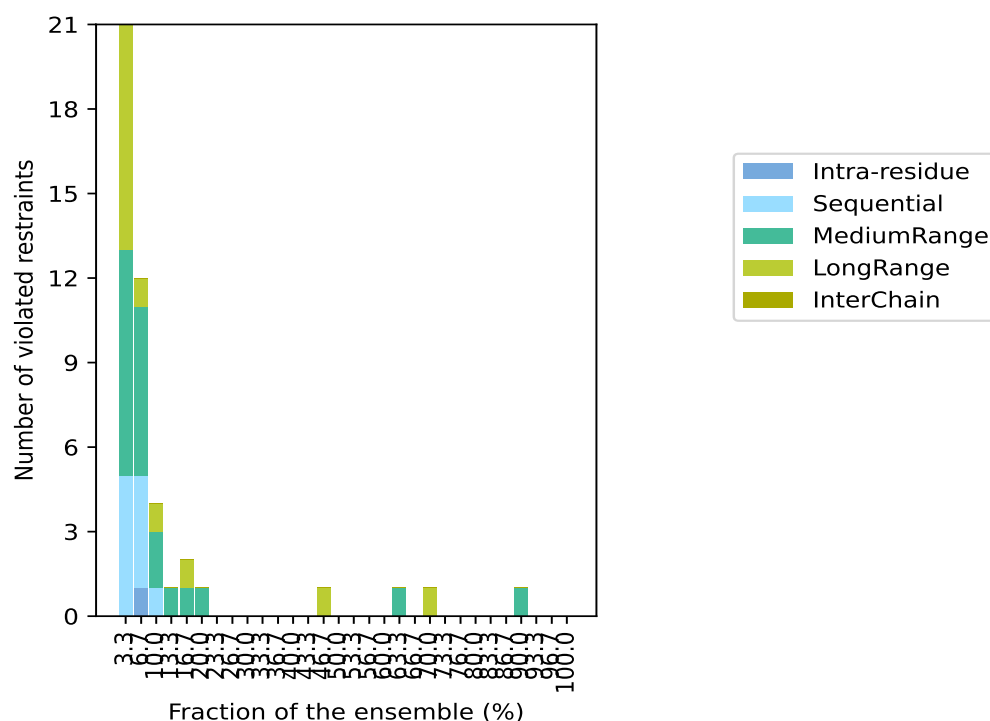
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	7	23.3
0	0	0	0	0	0	8	26.7
0	0	0	0	0	0	9	30.0
0	0	0	0	0	0	10	33.3
0	0	0	0	0	0	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	1	0	1	14	46.7
0	0	0	0	0	0	15	50.0
0	0	0	0	0	0	16	53.3
0	0	0	0	0	0	17	56.7
0	0	0	0	0	0	18	60.0
0	0	1	0	0	1	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	1	0	1	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	26	86.7
0	0	1	0	0	1	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	29	96.7
0	0	0	0	0	0	30	100.0

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

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

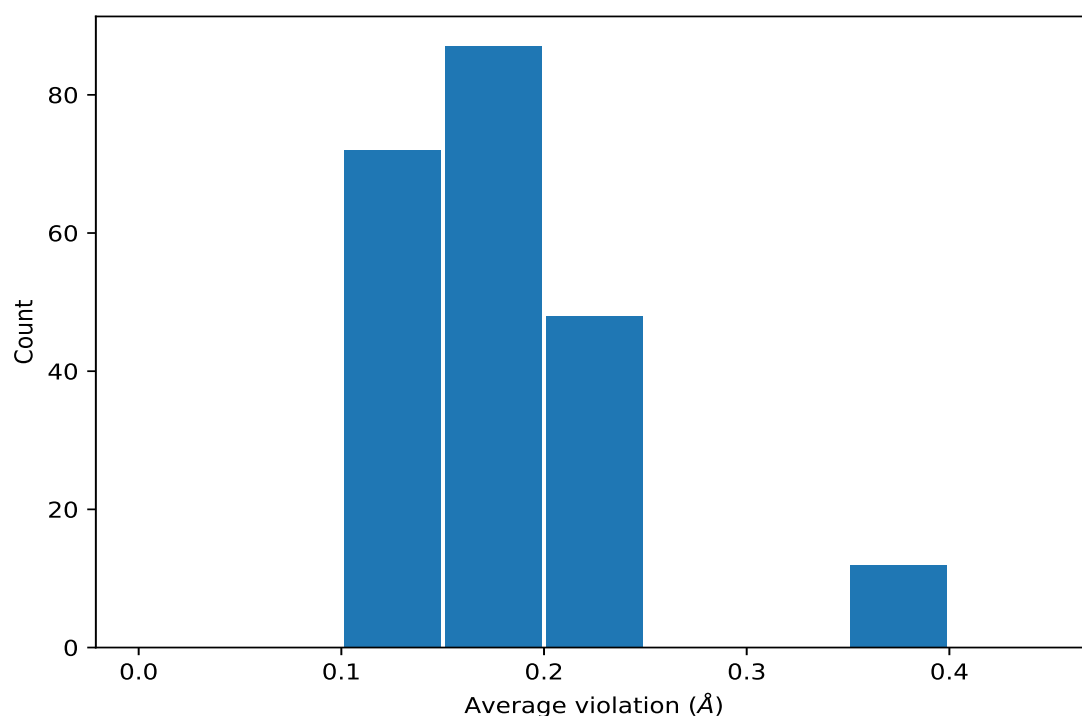
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	27	0.24	0.07	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	27	0.24	0.07	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	27	0.24	0.07	0.23
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	21	0.19	0.06	0.18
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	21	0.19	0.06	0.18
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	21	0.19	0.06	0.18
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	21	0.19	0.06	0.18
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	21	0.19	0.06	0.18
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	21	0.19	0.06	0.18
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	21	0.19	0.06	0.18
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	21	0.19	0.06	0.18
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	21	0.19	0.06	0.18
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	21	0.19	0.06	0.18
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	21	0.19	0.06	0.18
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	21	0.19	0.06	0.18
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	19	0.23	0.08	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	19	0.23	0.08	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	19	0.23	0.08	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	19	0.23	0.08	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	19	0.23	0.08	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	19	0.23	0.08	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	19	0.23	0.08	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	19	0.23	0.08	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	19	0.23	0.08	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	19	0.23	0.08	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	19	0.23	0.08	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	19	0.23	0.08	0.22
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	14	0.14	0.04	0.13
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	14	0.14	0.04	0.13
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	14	0.14	0.04	0.13
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	14	0.14	0.04	0.13
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	14	0.14	0.04	0.13
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	14	0.14	0.04	0.13
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	14	0.14	0.04	0.13
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	14	0.14	0.04	0.13
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	14	0.14	0.04	0.13
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG21	6	0.13	0.02	0.12
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG22	6	0.13	0.02	0.12
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG23	6	0.13	0.02	0.12
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG2	5	0.22	0.11	0.16
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG3	5	0.22	0.11	0.16
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG2	5	0.22	0.11	0.16
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG3	5	0.22	0.11	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG2	5	0.22	0.11	0.16
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG3	5	0.22	0.11	0.16
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG2	5	0.22	0.11	0.16
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG3	5	0.22	0.11	0.16
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG2	5	0.22	0.11	0.16
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG3	5	0.22	0.11	0.16
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG2	5	0.22	0.11	0.16
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG3	5	0.22	0.11	0.16
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG21	5	0.12	0.01	0.12
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG22	5	0.12	0.01	0.12
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG23	5	0.12	0.01	0.12
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD11	4	0.16	0.03	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD12	4	0.16	0.03	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD13	4	0.16	0.03	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD21	4	0.16	0.03	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD22	4	0.16	0.03	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD23	4	0.16	0.03	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD11	4	0.16	0.03	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD12	4	0.16	0.03	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD13	4	0.16	0.03	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD21	4	0.16	0.03	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD22	4	0.16	0.03	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD23	4	0.16	0.03	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG11	3	0.17	0.07	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG12	3	0.17	0.07	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG13	3	0.17	0.07	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG21	3	0.17	0.07	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG22	3	0.17	0.07	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG23	3	0.17	0.07	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG11	3	0.17	0.07	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG12	3	0.17	0.07	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG13	3	0.17	0.07	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG21	3	0.17	0.07	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG22	3	0.17	0.07	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG23	3	0.17	0.07	0.16
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG11	3	0.12	0.01	0.12
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG12	3	0.12	0.01	0.12
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG13	3	0.12	0.01	0.12
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG11	3	0.12	0.01	0.12
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG12	3	0.12	0.01	0.12
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG13	3	0.12	0.01	0.12
(1,1112)	1:89:A:THR:HG21	1:91:A:ALA:H	3	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1112)	1:89:A:THR:HG22	1:91:A:ALA:H	3	0.12	0.02	0.11
(1,1112)	1:89:A:THR:HG23	1:91:A:ALA:H	3	0.12	0.02	0.11
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD11	3	0.11	0.01	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD12	3	0.11	0.01	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD13	3	0.11	0.01	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD21	3	0.11	0.01	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD22	3	0.11	0.01	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD23	3	0.11	0.01	0.1
(1,2491)	1:157:A:LEU:HD11	1:161:A:GLN:HE21	2	0.38	0.03	0.38
(1,2491)	1:157:A:LEU:HD11	1:161:A:GLN:HE22	2	0.38	0.03	0.38
(1,2491)	1:157:A:LEU:HD12	1:161:A:GLN:HE21	2	0.38	0.03	0.38
(1,2491)	1:157:A:LEU:HD12	1:161:A:GLN:HE22	2	0.38	0.03	0.38
(1,2491)	1:157:A:LEU:HD13	1:161:A:GLN:HE21	2	0.38	0.03	0.38
(1,2491)	1:157:A:LEU:HD13	1:161:A:GLN:HE22	2	0.38	0.03	0.38
(1,2491)	1:157:A:LEU:HD21	1:161:A:GLN:HE21	2	0.38	0.03	0.38
(1,2491)	1:157:A:LEU:HD21	1:161:A:GLN:HE22	2	0.38	0.03	0.38
(1,2491)	1:157:A:LEU:HD22	1:161:A:GLN:HE21	2	0.38	0.03	0.38
(1,2491)	1:157:A:LEU:HD22	1:161:A:GLN:HE22	2	0.38	0.03	0.38
(1,2491)	1:157:A:LEU:HD23	1:161:A:GLN:HE21	2	0.38	0.03	0.38
(1,2491)	1:157:A:LEU:HD23	1:161:A:GLN:HE22	2	0.38	0.03	0.38
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG11	2	0.2	0.06	0.2
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG12	2	0.2	0.06	0.2
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG13	2	0.2	0.06	0.2
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG21	2	0.2	0.06	0.2
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG22	2	0.2	0.06	0.2
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG23	2	0.2	0.06	0.2
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG11	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG12	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG13	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG21	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG22	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG23	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG11	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG12	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG13	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG21	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG22	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG23	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG11	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG12	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG13	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG21	2	0.19	0.0	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG22	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG23	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG11	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG12	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG13	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG21	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG22	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG23	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG11	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG12	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG13	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG21	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG22	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG23	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG11	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG12	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG13	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG21	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG22	2	0.19	0.0	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG23	2	0.19	0.0	0.19
(1,1994)	1:16:A:VAL:HG11	1:17:A:ASN:HD21	2	0.18	0.04	0.18
(1,1994)	1:16:A:VAL:HG11	1:17:A:ASN:HD22	2	0.18	0.04	0.18
(1,1994)	1:16:A:VAL:HG12	1:17:A:ASN:HD21	2	0.18	0.04	0.18
(1,1994)	1:16:A:VAL:HG12	1:17:A:ASN:HD22	2	0.18	0.04	0.18
(1,1994)	1:16:A:VAL:HG13	1:17:A:ASN:HD21	2	0.18	0.04	0.18
(1,1994)	1:16:A:VAL:HG13	1:17:A:ASN:HD22	2	0.18	0.04	0.18
(1,1994)	1:16:A:VAL:HG21	1:17:A:ASN:HD21	2	0.18	0.04	0.18
(1,1994)	1:16:A:VAL:HG21	1:17:A:ASN:HD22	2	0.18	0.04	0.18
(1,1994)	1:16:A:VAL:HG22	1:17:A:ASN:HD21	2	0.18	0.04	0.18
(1,1994)	1:16:A:VAL:HG22	1:17:A:ASN:HD22	2	0.18	0.04	0.18
(1,1994)	1:16:A:VAL:HG23	1:17:A:ASN:HD21	2	0.18	0.04	0.18
(1,1994)	1:16:A:VAL:HG23	1:17:A:ASN:HD22	2	0.18	0.04	0.18
(1,905)	1:61:A:ILE:HD11	1:63:A:GLU:H	2	0.16	0.04	0.16
(1,905)	1:61:A:ILE:HD12	1:63:A:GLU:H	2	0.16	0.04	0.16
(1,905)	1:61:A:ILE:HD13	1:63:A:GLU:H	2	0.16	0.04	0.16
(1,1017)	1:80:A:MET:H	1:80:A:MET:HE1	2	0.15	0.03	0.15
(1,1017)	1:80:A:MET:H	1:80:A:MET:HE2	2	0.15	0.03	0.15
(1,1017)	1:80:A:MET:H	1:80:A:MET:HE3	2	0.15	0.03	0.15
(1,1882)	1:154:A:PHE:HE1	1:157:A:LEU:HD21	2	0.14	0.01	0.14
(1,1882)	1:154:A:PHE:HE1	1:157:A:LEU:HD22	2	0.14	0.01	0.14
(1,1882)	1:154:A:PHE:HE1	1:157:A:LEU:HD23	2	0.14	0.01	0.14
(1,1882)	1:154:A:PHE:HE2	1:157:A:LEU:HD21	2	0.14	0.01	0.14

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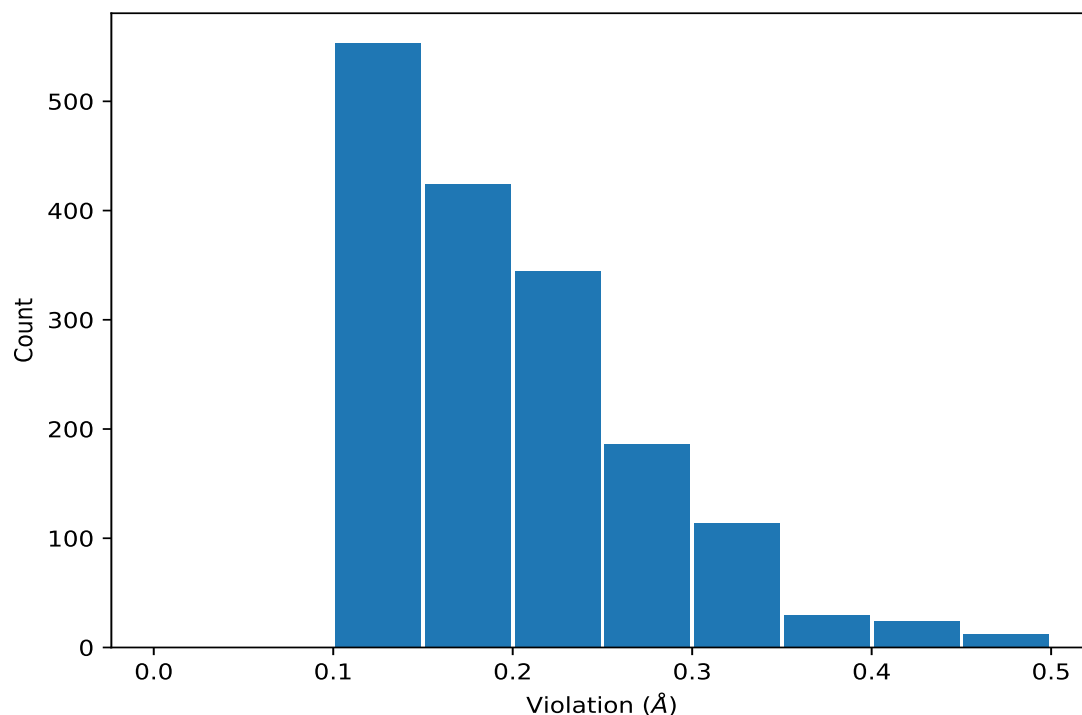
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1882)	1:154:A:PHE:HE2	1:157:A:LEU:HD22	2	0.14	0.01	0.14
(1,1882)	1:154:A:PHE:HE2	1:157:A:LEU:HD23	2	0.14	0.01	0.14
(1,1182)	1:96:A:TRP:H	1:99:A:ILE:HD11	2	0.13	0.03	0.13
(1,1182)	1:96:A:TRP:H	1:99:A:ILE:HD12	2	0.13	0.03	0.13
(1,1182)	1:96:A:TRP:H	1:99:A:ILE:HD13	2	0.13	0.03	0.13
(1,2395)	1:116:A:VAL:HG11	1:117:A:ARG:HD2	2	0.13	0.02	0.13
(1,2395)	1:116:A:VAL:HG11	1:117:A:ARG:HD3	2	0.13	0.02	0.13
(1,2395)	1:116:A:VAL:HG12	1:117:A:ARG:HD2	2	0.13	0.02	0.13
(1,2395)	1:116:A:VAL:HG12	1:117:A:ARG:HD3	2	0.13	0.02	0.13
(1,2395)	1:116:A:VAL:HG13	1:117:A:ARG:HD2	2	0.13	0.02	0.13
(1,2395)	1:116:A:VAL:HG13	1:117:A:ARG:HD3	2	0.13	0.02	0.13
(1,2395)	1:116:A:VAL:HG21	1:117:A:ARG:HD2	2	0.13	0.02	0.13
(1,2395)	1:116:A:VAL:HG21	1:117:A:ARG:HD3	2	0.13	0.02	0.13
(1,2395)	1:116:A:VAL:HG22	1:117:A:ARG:HD2	2	0.13	0.02	0.13
(1,2395)	1:116:A:VAL:HG22	1:117:A:ARG:HD3	2	0.13	0.02	0.13
(1,2395)	1:116:A:VAL:HG23	1:117:A:ARG:HD2	2	0.13	0.02	0.13
(1,2395)	1:116:A:VAL:HG23	1:117:A:ARG:HD3	2	0.13	0.02	0.13
(1,2391)	1:115:A:ILE:HD11	1:117:A:ARG:HB2	2	0.12	0.02	0.12
(1,2391)	1:115:A:ILE:HD11	1:117:A:ARG:HB3	2	0.12	0.02	0.12
(1,2391)	1:115:A:ILE:HD12	1:117:A:ARG:HB2	2	0.12	0.02	0.12
(1,2391)	1:115:A:ILE:HD12	1:117:A:ARG:HB3	2	0.12	0.02	0.12
(1,2391)	1:115:A:ILE:HD13	1:117:A:ARG:HB2	2	0.12	0.02	0.12
(1,2391)	1:115:A:ILE:HD13	1:117:A:ARG:HB3	2	0.12	0.02	0.12
(1,817)	1:182:A:LEU:HD21	1:183:A:TYR:HD1	2	0.11	0.0	0.11
(1,817)	1:182:A:LEU:HD21	1:183:A:TYR:HD2	2	0.11	0.0	0.11
(1,817)	1:182:A:LEU:HD22	1:183:A:TYR:HD1	2	0.11	0.0	0.11
(1,817)	1:182:A:LEU:HD22	1:183:A:TYR:HD2	2	0.11	0.0	0.11
(1,817)	1:182:A:LEU:HD23	1:183:A:TYR:HD1	2	0.11	0.0	0.11
(1,817)	1:182:A:LEU:HD23	1:183:A:TYR:HD2	2	0.11	0.0	0.11
(1,909)	1:61:A:ILE:HD11	1:104:A:PHE:HE1	2	0.11	0.01	0.11
(1,909)	1:61:A:ILE:HD11	1:104:A:PHE:HE2	2	0.11	0.01	0.11
(1,909)	1:61:A:ILE:HD12	1:104:A:PHE:HE1	2	0.11	0.01	0.11
(1,909)	1:61:A:ILE:HD12	1:104:A:PHE:HE2	2	0.11	0.01	0.11
(1,909)	1:61:A:ILE:HD13	1:104:A:PHE:HE1	2	0.11	0.01	0.11
(1,909)	1:61:A:ILE:HD13	1:104:A:PHE:HE2	2	0.11	0.01	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)
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	11	0.49
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	11	0.49
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	11	0.49
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	11	0.49
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	11	0.49
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	11	0.49
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	11	0.49
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	11	0.49
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	11	0.49
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	11	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	11	0.49
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	11	0.49
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG2	15	0.42
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG3	15	0.42
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG2	15	0.42
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG3	15	0.42
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG2	15	0.42
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG3	15	0.42
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG2	15	0.42
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG3	15	0.42
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG2	15	0.42
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG3	15	0.42
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG2	15	0.42
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG3	15	0.42
(1,2491)	1:157:A:LEU:HD11	1:161:A:GLN:HE21	15	0.4
(1,2491)	1:157:A:LEU:HD11	1:161:A:GLN:HE22	15	0.4
(1,2491)	1:157:A:LEU:HD12	1:161:A:GLN:HE21	15	0.4
(1,2491)	1:157:A:LEU:HD12	1:161:A:GLN:HE22	15	0.4
(1,2491)	1:157:A:LEU:HD13	1:161:A:GLN:HE21	15	0.4
(1,2491)	1:157:A:LEU:HD13	1:161:A:GLN:HE22	15	0.4
(1,2491)	1:157:A:LEU:HD21	1:161:A:GLN:HE21	15	0.4
(1,2491)	1:157:A:LEU:HD21	1:161:A:GLN:HE22	15	0.4
(1,2491)	1:157:A:LEU:HD22	1:161:A:GLN:HE21	15	0.4
(1,2491)	1:157:A:LEU:HD22	1:161:A:GLN:HE22	15	0.4
(1,2491)	1:157:A:LEU:HD23	1:161:A:GLN:HE21	15	0.4
(1,2491)	1:157:A:LEU:HD23	1:161:A:GLN:HE22	15	0.4
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	11	0.38
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	11	0.38
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	11	0.38
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	11	0.38
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	11	0.38
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	11	0.38
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	11	0.38
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	11	0.38
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	11	0.38
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	11	0.38
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	11	0.38
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	11	0.38
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	15	0.36
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	15	0.36
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	15	0.36
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	15	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	15	0.36
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	15	0.36
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	15	0.36
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	15	0.36
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	15	0.36
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	15	0.36
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	15	0.36
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	15	0.36
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	15	0.36
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	15	0.36
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	15	0.36
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	15	0.36
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	15	0.36
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	15	0.36
(1,2491)	1:157:A:LEU:HD11	1:161:A:GLN:HE21	11	0.35
(1,2491)	1:157:A:LEU:HD11	1:161:A:GLN:HE22	11	0.35
(1,2491)	1:157:A:LEU:HD12	1:161:A:GLN:HE21	11	0.35
(1,2491)	1:157:A:LEU:HD12	1:161:A:GLN:HE22	11	0.35
(1,2491)	1:157:A:LEU:HD13	1:161:A:GLN:HE21	11	0.35
(1,2491)	1:157:A:LEU:HD13	1:161:A:GLN:HE22	11	0.35
(1,2491)	1:157:A:LEU:HD21	1:161:A:GLN:HE21	11	0.35
(1,2491)	1:157:A:LEU:HD21	1:161:A:GLN:HE22	11	0.35
(1,2491)	1:157:A:LEU:HD22	1:161:A:GLN:HE21	11	0.35
(1,2491)	1:157:A:LEU:HD22	1:161:A:GLN:HE22	11	0.35
(1,2491)	1:157:A:LEU:HD23	1:161:A:GLN:HE21	11	0.35
(1,2491)	1:157:A:LEU:HD23	1:161:A:GLN:HE22	11	0.35
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	7	0.35
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	7	0.35
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	7	0.35
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	7	0.35
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	7	0.35
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	7	0.35
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	7	0.35
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	7	0.35
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	7	0.35
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	7	0.35
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	7	0.35
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	7	0.35
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	7	0.35
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	7	0.35
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	7	0.35
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	7	0.35
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	7	0.35
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	21	0.34
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	21	0.34
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	21	0.34
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	21	0.34
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	21	0.34
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	21	0.34
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	21	0.34
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	21	0.34
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	21	0.34
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	21	0.34
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	21	0.34
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	21	0.34
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	21	0.34
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	21	0.34
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	21	0.34
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	21	0.34
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	21	0.34
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	21	0.34
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	5	0.33
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	5	0.33
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	5	0.33
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	5	0.33
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	5	0.33
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	5	0.33
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	5	0.33
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	5	0.33
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	5	0.33
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	5	0.33
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	5	0.33
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	5	0.33
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	5	0.33
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	5	0.33
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	5	0.33
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	5	0.33
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	5	0.33
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	5	0.33
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	21	0.32
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	21	0.32
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	21	0.32
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	21	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	21	0.32
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	21	0.32
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	21	0.32
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	21	0.32
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	21	0.32
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	21	0.32
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	21	0.32
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	21	0.32
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	8	0.32
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	8	0.32
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	8	0.32
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	8	0.32
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	8	0.32
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	8	0.32
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	8	0.32
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	8	0.32
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	8	0.32
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	8	0.32
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	8	0.32
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	8	0.32
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	8	0.32
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	8	0.32
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	8	0.32
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	8	0.32
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	8	0.32
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	8	0.32
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	11	0.31
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	11	0.31
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	11	0.31
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	11	0.31
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	11	0.31
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	11	0.31
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	11	0.31
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	11	0.31
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	11	0.31
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	11	0.31
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	11	0.31
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	11	0.31
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	11	0.31
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	11	0.31
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	11	0.31
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	11	0.31
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	11	0.31
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	6	0.3
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	6	0.3
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	6	0.3
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	6	0.3
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	6	0.3
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	6	0.3
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	6	0.3
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	6	0.3
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	6	0.3
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	6	0.3
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	6	0.3
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	6	0.3
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	4	0.3
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	4	0.3
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	4	0.3
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	4	0.3
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	4	0.3
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	4	0.3
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	4	0.3
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	4	0.3
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	4	0.3
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	4	0.3
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	4	0.3
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	4	0.3
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	4	0.3
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	4	0.3
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	4	0.3
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	4	0.3
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	4	0.3
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	4	0.3
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG2	3	0.27
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG3	3	0.27
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG2	3	0.27
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG3	3	0.27
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG2	3	0.27
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG3	3	0.27
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG2	3	0.27
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG3	3	0.27
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG2	3	0.27
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG3	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG2	3	0.27
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG3	3	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	7	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	7	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	7	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	7	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	7	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	7	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	7	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	7	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	7	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	7	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	7	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	7	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	8	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	8	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	8	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	8	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	8	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	8	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	8	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	8	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	8	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	8	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	8	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	8	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	26	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	26	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	26	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	26	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	26	0.27
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	26	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	26	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	26	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	26	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	26	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	26	0.27
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	26	0.27
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG11	26	0.26
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG12	26	0.26
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG13	26	0.26
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG21	26	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG22	26	0.26
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG23	26	0.26
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG11	22	0.26
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG12	22	0.26
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG13	22	0.26
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG21	22	0.26
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG22	22	0.26
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG23	22	0.26
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG11	22	0.26
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG12	22	0.26
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG13	22	0.26
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG21	22	0.26
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG22	22	0.26
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG23	22	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	16	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	16	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	16	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	16	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	16	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	16	0.26
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	16	0.26
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	16	0.26
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	16	0.26
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	16	0.26
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	16	0.26
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	16	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	16	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	16	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	16	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	16	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	16	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	16	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	22	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	22	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	22	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	22	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	22	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	22	0.26
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	22	0.26
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	22	0.26
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	22	0.26
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	22	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	22	0.26
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	22	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	22	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	22	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	22	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	22	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	22	0.26
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	22	0.26
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	14	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	14	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	14	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	14	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	14	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	14	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	14	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	14	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	14	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	14	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	14	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	14	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	14	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	14	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	14	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	14	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	14	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	14	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	23	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	23	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	23	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	23	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	23	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	23	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	23	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	23	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	23	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	23	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	23	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	23	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	23	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	23	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	23	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	23	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	23	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	23	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	27	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	27	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	27	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	27	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	27	0.25
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	27	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	27	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	27	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	27	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	27	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	27	0.25
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	27	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	27	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	27	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	27	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	27	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	27	0.25
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	27	0.25
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	21	0.24
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	21	0.24
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	21	0.24
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	21	0.24
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	21	0.24
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	21	0.24
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	21	0.24
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	21	0.24
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	21	0.24
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	21	0.24
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	21	0.24
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	21	0.24
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	29	0.24
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	29	0.24
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	29	0.24
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	29	0.24
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	29	0.24
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	29	0.24
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	29	0.24
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	29	0.24
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	29	0.24
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	29	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	29	0.24
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	29	0.24
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	29	0.24
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	29	0.24
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	29	0.24
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	29	0.24
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	29	0.24
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	29	0.24
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	10	0.23
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	10	0.23
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	10	0.23
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	10	0.23
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	10	0.23
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	10	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	10	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	10	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	10	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	10	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	10	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	10	0.23
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	24	0.23
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	24	0.23
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	24	0.23
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	24	0.23
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	24	0.23
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	24	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	24	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	24	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	24	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	24	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	24	0.23
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	24	0.23
(1,1994)	1:16:A:VAL:HG11	1:17:A:ASN:HD21	5	0.23
(1,1994)	1:16:A:VAL:HG11	1:17:A:ASN:HD22	5	0.23
(1,1994)	1:16:A:VAL:HG12	1:17:A:ASN:HD21	5	0.23
(1,1994)	1:16:A:VAL:HG12	1:17:A:ASN:HD22	5	0.23
(1,1994)	1:16:A:VAL:HG13	1:17:A:ASN:HD21	5	0.23
(1,1994)	1:16:A:VAL:HG13	1:17:A:ASN:HD22	5	0.23
(1,1994)	1:16:A:VAL:HG21	1:17:A:ASN:HD21	5	0.23
(1,1994)	1:16:A:VAL:HG21	1:17:A:ASN:HD22	5	0.23
(1,1994)	1:16:A:VAL:HG22	1:17:A:ASN:HD21	5	0.23
(1,1994)	1:16:A:VAL:HG22	1:17:A:ASN:HD22	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1994)	1:16:A:VAL:HG23	1:17:A:ASN:HD21	5	0.23
(1,1994)	1:16:A:VAL:HG23	1:17:A:ASN:HD22	5	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	1	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	1	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	1	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	1	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	1	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	1	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	1	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	1	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	1	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	1	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	1	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	1	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	1	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	1	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	1	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	1	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	1	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	1	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	13	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	13	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	13	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	13	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	13	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	13	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	13	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	13	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	13	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	13	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	13	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	13	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	13	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	13	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	13	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	13	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	13	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	13	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	20	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	20	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	20	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	20	0.23
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	20	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	20	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	20	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	20	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	20	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	20	0.23
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	20	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	20	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	20	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	20	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	20	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	20	0.23
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	20	0.23
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	16	0.22
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	16	0.22
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	16	0.22
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	16	0.22
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	16	0.22
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	16	0.22
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	16	0.22
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	16	0.22
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	16	0.22
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	16	0.22
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	16	0.22
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	16	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	2	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	2	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	2	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	2	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	2	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	2	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	2	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	2	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	2	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	2	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	2	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	2	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	19	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	19	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	19	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	19	0.22
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	19	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	19	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	19	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	19	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	19	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	19	0.22
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	19	0.22
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	4	0.22
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	4	0.22
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	4	0.22
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	4	0.22
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	4	0.22
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	4	0.22
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	4	0.22
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	4	0.22
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	4	0.22
(1,2514)	1:171:A:VAL:HG11	1:173:A:GLN:HG2	14	0.21
(1,2514)	1:171:A:VAL:HG11	1:173:A:GLN:HG3	14	0.21
(1,2514)	1:171:A:VAL:HG12	1:173:A:GLN:HG2	14	0.21
(1,2514)	1:171:A:VAL:HG12	1:173:A:GLN:HG3	14	0.21
(1,2514)	1:171:A:VAL:HG13	1:173:A:GLN:HG2	14	0.21
(1,2514)	1:171:A:VAL:HG13	1:173:A:GLN:HG3	14	0.21
(1,2514)	1:171:A:VAL:HG21	1:173:A:GLN:HG2	14	0.21
(1,2514)	1:171:A:VAL:HG21	1:173:A:GLN:HG3	14	0.21
(1,2514)	1:171:A:VAL:HG22	1:173:A:GLN:HG2	14	0.21
(1,2514)	1:171:A:VAL:HG22	1:173:A:GLN:HG3	14	0.21
(1,2514)	1:171:A:VAL:HG23	1:173:A:GLN:HG2	14	0.21
(1,2514)	1:171:A:VAL:HG23	1:173:A:GLN:HG3	14	0.21
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD11	1	0.21
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD12	1	0.21
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD13	1	0.21
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD21	1	0.21
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD22	1	0.21
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD23	1	0.21
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD11	1	0.21
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD12	1	0.21
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD13	1	0.21
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD21	1	0.21
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD22	1	0.21
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD23	1	0.21
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	29	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	29	0.21
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	29	0.21
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	29	0.21
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	29	0.21
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	29	0.21
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	29	0.21
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	29	0.21
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	29	0.21
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	29	0.21
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	29	0.21
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	29	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	14	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	14	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	14	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	14	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	14	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	14	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	14	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	14	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	14	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	14	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	14	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	14	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	23	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	23	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	23	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	23	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	23	0.21
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	23	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	23	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	23	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	23	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	23	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	23	0.21
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	23	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	24	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	24	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	24	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	24	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	24	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	24	0.21
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	24	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	24	0.21
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	24	0.21
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	24	0.21
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	24	0.21
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	24	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	24	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	24	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	24	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	24	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	24	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	24	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	26	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	26	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	26	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	26	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	26	0.21
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	26	0.21
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	26	0.21
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	26	0.21
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	26	0.21
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	26	0.21
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	26	0.21
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	26	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	26	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	26	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	26	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	26	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	26	0.21
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	26	0.21
(1,1452)	1:120:A:MET:HE1	1:121:A:LEU:H	30	0.21
(1,1452)	1:120:A:MET:HE2	1:121:A:LEU:H	30	0.21
(1,1452)	1:120:A:MET:HE3	1:121:A:LEU:H	30	0.21
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	2	0.21
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	2	0.21
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	2	0.21
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	2	0.21
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	2	0.21
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	2	0.21
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	2	0.21
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	2	0.21
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	2	0.21
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	4	0.2
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	4	0.2
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	4	0.2
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	4	0.2
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	4	0.2
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	4	0.2
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	4	0.2
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	4	0.2
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	4	0.2
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	4	0.2
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	4	0.2
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	13	0.2
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	13	0.2
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	13	0.2
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	13	0.2
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	13	0.2
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	13	0.2
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	13	0.2
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	13	0.2
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	13	0.2
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	13	0.2
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	13	0.2
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	13	0.2
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	3	0.2
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	3	0.2
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	3	0.2
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	3	0.2
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	3	0.2
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	3	0.2
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	3	0.2
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	3	0.2
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	3	0.2
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	3	0.2
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	3	0.2
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	3	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	9	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	9	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	9	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	9	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	9	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	9	0.2
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	9	0.2
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	9	0.2
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	9	0.2
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	9	0.2
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	9	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	9	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	9	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	9	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	9	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	9	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	9	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	28	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	28	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	28	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	28	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	28	0.2
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	28	0.2
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	28	0.2
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	28	0.2
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	28	0.2
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	28	0.2
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	28	0.2
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	28	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	28	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	28	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	28	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	28	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	28	0.2
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	28	0.2
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	1	0.19
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	1	0.19
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	1	0.19
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	1	0.19
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	1	0.19
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	1	0.19
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	1	0.19
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	1	0.19
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	1	0.19
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	1	0.19
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	1	0.19
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	1	0.19
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	2	0.19
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	2	0.19
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	2	0.19
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	2	0.19
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	2	0.19
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	2	0.19
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	2	0.19
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	2	0.19
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	2	0.19
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	2	0.19
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	2	0.19
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	14	0.19
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	14	0.19
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	14	0.19
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	14	0.19
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	14	0.19
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	14	0.19
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	14	0.19
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	14	0.19
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	14	0.19
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	14	0.19
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	14	0.19
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	14	0.19
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	4	0.19
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	4	0.19
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	4	0.19
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	4	0.19
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	4	0.19
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	4	0.19
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	4	0.19
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	4	0.19
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	4	0.19
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	4	0.19
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	4	0.19
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	4	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG11	1	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG12	1	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG13	1	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG21	1	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG22	1	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG23	1	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG11	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG12	1	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG13	1	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG21	1	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG22	1	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG23	1	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG11	1	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG12	1	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG13	1	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG21	1	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG22	1	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG23	1	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG11	1	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG12	1	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG13	1	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG21	1	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG22	1	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG23	1	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG11	1	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG12	1	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG13	1	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG21	1	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG22	1	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG23	1	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG11	1	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG12	1	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG13	1	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG21	1	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG22	1	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG23	1	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG11	8	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG12	8	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG13	8	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG21	8	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG22	8	0.19
(1,1981)	1:15:A:LEU:HD11	1:16:A:VAL:HG23	8	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG11	8	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG12	8	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG13	8	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG21	8	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG22	8	0.19
(1,1981)	1:15:A:LEU:HD12	1:16:A:VAL:HG23	8	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG11	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG12	8	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG13	8	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG21	8	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG22	8	0.19
(1,1981)	1:15:A:LEU:HD13	1:16:A:VAL:HG23	8	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG11	8	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG12	8	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG13	8	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG21	8	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG22	8	0.19
(1,1981)	1:15:A:LEU:HD21	1:16:A:VAL:HG23	8	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG11	8	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG12	8	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG13	8	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG21	8	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG22	8	0.19
(1,1981)	1:15:A:LEU:HD22	1:16:A:VAL:HG23	8	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG11	8	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG12	8	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG13	8	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG21	8	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG22	8	0.19
(1,1981)	1:15:A:LEU:HD23	1:16:A:VAL:HG23	8	0.19
(1,905)	1:61:A:ILE:HD11	1:63:A:GLU:H	11	0.19
(1,905)	1:61:A:ILE:HD12	1:63:A:GLU:H	11	0.19
(1,905)	1:61:A:ILE:HD13	1:63:A:GLU:H	11	0.19
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	15	0.19
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	15	0.19
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	15	0.19
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	15	0.19
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	15	0.19
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	15	0.19
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	15	0.19
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	15	0.19
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	15	0.19
(1,11)	1:9:A:TRP:H	1:10:A:LYS:HG2	30	0.19
(1,11)	1:9:A:TRP:H	1:10:A:LYS:HG3	30	0.19
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	15	0.18
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	15	0.18
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	15	0.18
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	15	0.18
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	15	0.18
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	15	0.18
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	15	0.18
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	15	0.18
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	15	0.18
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	15	0.18
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	15	0.18
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	22	0.18
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	22	0.18
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	22	0.18
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	22	0.18
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	22	0.18
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	22	0.18
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	22	0.18
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	22	0.18
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	22	0.18
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	22	0.18
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	22	0.18
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	22	0.18
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	3	0.18
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	3	0.18
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	3	0.18
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	3	0.18
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	3	0.18
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	3	0.18
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	3	0.18
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	3	0.18
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	3	0.18
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	3	0.18
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	3	0.18
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	3	0.18
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	3	0.18
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	3	0.18
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	3	0.18
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	3	0.18
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	3	0.18
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	3	0.18
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG21	11	0.18
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG22	11	0.18
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG23	11	0.18
(1,1017)	1:80:A:MET:H	1:80:A:MET:HE1	4	0.18
(1,1017)	1:80:A:MET:H	1:80:A:MET:HE2	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:80:A:MET:H	1:80:A:MET:HE3	4	0.18
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	17	0.17
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	17	0.17
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	17	0.17
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	17	0.17
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	17	0.17
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	17	0.17
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	17	0.17
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	17	0.17
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	17	0.17
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	17	0.17
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	17	0.17
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	17	0.17
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	28	0.17
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	28	0.17
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	28	0.17
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	28	0.17
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	28	0.17
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	28	0.17
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	28	0.17
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	28	0.17
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	28	0.17
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	28	0.17
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	28	0.17
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	28	0.17
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	16	0.17
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	16	0.17
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	16	0.17
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	16	0.17
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	16	0.17
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	16	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	16	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	16	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	16	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	16	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	16	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	16	0.17
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	25	0.17
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	25	0.17
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	25	0.17
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	25	0.17
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	25	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	25	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	25	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	25	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	25	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	25	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	25	0.17
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	25	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	10	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	10	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	10	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	10	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	10	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	10	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	10	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	10	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	10	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	10	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	10	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	10	0.17
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	10	0.17
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	10	0.17
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	10	0.17
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	10	0.17
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	10	0.17
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	10	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	18	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	18	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	18	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	18	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	18	0.17
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	18	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	18	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	18	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	18	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	18	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	18	0.17
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	18	0.17
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	18	0.17
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	18	0.17
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	18	0.17
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	18	0.17
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	18	0.17
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG2	4	0.16
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG3	4	0.16
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG2	4	0.16
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG3	4	0.16
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG2	4	0.16
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG3	4	0.16
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG2	4	0.16
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG3	4	0.16
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG2	4	0.16
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG3	4	0.16
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG2	4	0.16
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG3	4	0.16
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG2	27	0.16
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG3	27	0.16
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG2	27	0.16
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG3	27	0.16
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG2	27	0.16
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG3	27	0.16
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG2	27	0.16
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG3	27	0.16
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG2	27	0.16
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG3	27	0.16
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG2	27	0.16
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG3	27	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD11	5	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD12	5	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD13	5	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD21	5	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD22	5	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD23	5	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD11	5	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD12	5	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD13	5	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD21	5	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD22	5	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD23	5	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD11	11	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD12	11	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD13	11	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD21	11	0.16
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD22	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD23	11	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD11	11	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD12	11	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD13	11	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD21	11	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD22	11	0.16
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD23	11	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG11	21	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG12	21	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG13	21	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG21	21	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG22	21	0.16
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG23	21	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG11	21	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG12	21	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG13	21	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG21	21	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG22	21	0.16
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG23	21	0.16
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	6	0.16
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	6	0.16
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	6	0.16
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	6	0.16
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	6	0.16
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	6	0.16
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	6	0.16
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	6	0.16
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	6	0.16
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	6	0.16
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	6	0.16
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	6	0.16
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	10	0.16
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	10	0.16
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	10	0.16
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	10	0.16
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	10	0.16
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	10	0.16
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	10	0.16
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	10	0.16
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	10	0.16
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	10	0.16
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	10	0.16
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	26	0.16
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	26	0.16
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	26	0.16
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	26	0.16
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	26	0.16
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	26	0.16
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	26	0.16
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	26	0.16
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	26	0.16
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	26	0.16
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	26	0.16
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	26	0.16
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	20	0.16
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	20	0.16
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	20	0.16
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	20	0.16
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	20	0.16
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	20	0.16
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	20	0.16
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	20	0.16
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	20	0.16
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	20	0.16
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	20	0.16
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	20	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	6	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	6	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	6	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	6	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	6	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	6	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	6	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	6	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	6	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	6	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	6	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	6	0.16
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	6	0.16
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	6	0.16
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	6	0.16
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	6	0.16
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	6	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	25	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	25	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	25	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	25	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	25	0.16
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	25	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	25	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	25	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	25	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	25	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	25	0.16
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	25	0.16
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	25	0.16
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	25	0.16
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	25	0.16
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	25	0.16
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	25	0.16
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	25	0.16
(1,1266)	1:170:A:ALA:HA	1:172:A:PHE:HD1	12	0.16
(1,1266)	1:170:A:ALA:HA	1:172:A:PHE:HD2	12	0.16
(1,1182)	1:96:A:TRP:H	1:99:A:ILE:HD11	11	0.16
(1,1182)	1:96:A:TRP:H	1:99:A:ILE:HD12	11	0.16
(1,1182)	1:96:A:TRP:H	1:99:A:ILE:HD13	11	0.16
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	1	0.16
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	1	0.16
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	1	0.16
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	1	0.16
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	1	0.16
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	1	0.16
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	1	0.16
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	1	0.16
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	1	0.16
(1,2395)	1:116:A:VAL:HG11	1:117:A:ARG:HD2	4	0.15
(1,2395)	1:116:A:VAL:HG11	1:117:A:ARG:HD3	4	0.15
(1,2395)	1:116:A:VAL:HG12	1:117:A:ARG:HD2	4	0.15
(1,2395)	1:116:A:VAL:HG12	1:117:A:ARG:HD3	4	0.15
(1,2395)	1:116:A:VAL:HG13	1:117:A:ARG:HD2	4	0.15
(1,2395)	1:116:A:VAL:HG13	1:117:A:ARG:HD3	4	0.15
(1,2395)	1:116:A:VAL:HG21	1:117:A:ARG:HD2	4	0.15
(1,2395)	1:116:A:VAL:HG21	1:117:A:ARG:HD3	4	0.15
(1,2395)	1:116:A:VAL:HG22	1:117:A:ARG:HD2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2395)	1:116:A:VAL:HG22	1:117:A:ARG:HD3	4	0.15
(1,2395)	1:116:A:VAL:HG23	1:117:A:ARG:HD2	4	0.15
(1,2395)	1:116:A:VAL:HG23	1:117:A:ARG:HD3	4	0.15
(1,2279)	1:75:A:LEU:HD11	1:80:A:MET:HG2	21	0.15
(1,2279)	1:75:A:LEU:HD11	1:80:A:MET:HG3	21	0.15
(1,2279)	1:75:A:LEU:HD12	1:80:A:MET:HG2	21	0.15
(1,2279)	1:75:A:LEU:HD12	1:80:A:MET:HG3	21	0.15
(1,2279)	1:75:A:LEU:HD13	1:80:A:MET:HG2	21	0.15
(1,2279)	1:75:A:LEU:HD13	1:80:A:MET:HG3	21	0.15
(1,2279)	1:75:A:LEU:HD21	1:80:A:MET:HG2	21	0.15
(1,2279)	1:75:A:LEU:HD21	1:80:A:MET:HG3	21	0.15
(1,2279)	1:75:A:LEU:HD22	1:80:A:MET:HG2	21	0.15
(1,2279)	1:75:A:LEU:HD22	1:80:A:MET:HG3	21	0.15
(1,2279)	1:75:A:LEU:HD23	1:80:A:MET:HG2	21	0.15
(1,2279)	1:75:A:LEU:HD23	1:80:A:MET:HG3	21	0.15
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	3	0.15
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	3	0.15
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	3	0.15
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	3	0.15
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	3	0.15
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	3	0.15
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	3	0.15
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	3	0.15
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	3	0.15
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	3	0.15
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	3	0.15
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	3	0.15
(1,1945)	1:9:A:TRP:HB2	1:10:A:LYS:HG2	30	0.15
(1,1945)	1:9:A:TRP:HB2	1:10:A:LYS:HG3	30	0.15
(1,1945)	1:9:A:TRP:HB3	1:10:A:LYS:HG2	30	0.15
(1,1945)	1:9:A:TRP:HB3	1:10:A:LYS:HG3	30	0.15
(1,1882)	1:154:A:PHE:HE1	1:157:A:LEU:HD21	15	0.15
(1,1882)	1:154:A:PHE:HE1	1:157:A:LEU:HD22	15	0.15
(1,1882)	1:154:A:PHE:HE1	1:157:A:LEU:HD23	15	0.15
(1,1882)	1:154:A:PHE:HE2	1:157:A:LEU:HD21	15	0.15
(1,1882)	1:154:A:PHE:HE2	1:157:A:LEU:HD22	15	0.15
(1,1882)	1:154:A:PHE:HE2	1:157:A:LEU:HD23	15	0.15
(1,1112)	1:89:A:THR:HG21	1:91:A:ALA:H	11	0.15
(1,1112)	1:89:A:THR:HG22	1:91:A:ALA:H	11	0.15
(1,1112)	1:89:A:THR:HG23	1:91:A:ALA:H	11	0.15
(1,2391)	1:115:A:ILE:HD11	1:117:A:ARG:HB2	4	0.14
(1,2391)	1:115:A:ILE:HD11	1:117:A:ARG:HB3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2391)	1:115:A:ILE:HD12	1:117:A:ARG:HB2	4	0.14
(1,2391)	1:115:A:ILE:HD12	1:117:A:ARG:HB3	4	0.14
(1,2391)	1:115:A:ILE:HD13	1:117:A:ARG:HB2	4	0.14
(1,2391)	1:115:A:ILE:HD13	1:117:A:ARG:HB3	4	0.14
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	7	0.14
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	7	0.14
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	7	0.14
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	7	0.14
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	7	0.14
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	7	0.14
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	7	0.14
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	7	0.14
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	7	0.14
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	7	0.14
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	7	0.14
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	7	0.14
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	27	0.14
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	27	0.14
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	27	0.14
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	27	0.14
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	27	0.14
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	27	0.14
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	27	0.14
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	27	0.14
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	27	0.14
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	27	0.14
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	27	0.14
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	27	0.14
(1,1994)	1:16:A:VAL:HG11	1:17:A:ASN:HD21	25	0.14
(1,1994)	1:16:A:VAL:HG11	1:17:A:ASN:HD22	25	0.14
(1,1994)	1:16:A:VAL:HG12	1:17:A:ASN:HD21	25	0.14
(1,1994)	1:16:A:VAL:HG12	1:17:A:ASN:HD22	25	0.14
(1,1994)	1:16:A:VAL:HG13	1:17:A:ASN:HD21	25	0.14
(1,1994)	1:16:A:VAL:HG13	1:17:A:ASN:HD22	25	0.14
(1,1994)	1:16:A:VAL:HG21	1:17:A:ASN:HD21	25	0.14
(1,1994)	1:16:A:VAL:HG21	1:17:A:ASN:HD22	25	0.14
(1,1994)	1:16:A:VAL:HG22	1:17:A:ASN:HD21	25	0.14
(1,1994)	1:16:A:VAL:HG22	1:17:A:ASN:HD22	25	0.14
(1,1994)	1:16:A:VAL:HG23	1:17:A:ASN:HD21	25	0.14
(1,1994)	1:16:A:VAL:HG23	1:17:A:ASN:HD22	25	0.14
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG21	4	0.14
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG22	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG23	4	0.14
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	3	0.14
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	3	0.14
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	3	0.14
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	3	0.14
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	3	0.14
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	3	0.14
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	3	0.14
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	3	0.14
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	3	0.14
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	10	0.14
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	10	0.14
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	10	0.14
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	10	0.14
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	10	0.14
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	10	0.14
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	10	0.14
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	10	0.14
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	10	0.14
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG11	16	0.13
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG12	16	0.13
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG13	16	0.13
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG21	16	0.13
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG22	16	0.13
(1,2511)	1:169:A:ALA:HA	1:171:A:VAL:HG23	16	0.13
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD11	8	0.13
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD12	8	0.13
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD13	8	0.13
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD21	8	0.13
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD22	8	0.13
(1,2470)	1:153:A:ARG:HD2	1:157:A:LEU:HD23	8	0.13
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD11	8	0.13
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD12	8	0.13
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD13	8	0.13
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD21	8	0.13
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD22	8	0.13
(1,2470)	1:153:A:ARG:HD3	1:157:A:LEU:HD23	8	0.13
(1,2461)	1:151:A:ARG:H	1:155:A:LEU:HD11	2	0.13
(1,2461)	1:151:A:ARG:H	1:155:A:LEU:HD12	2	0.13
(1,2461)	1:151:A:ARG:H	1:155:A:LEU:HD13	2	0.13
(1,2461)	1:151:A:ARG:H	1:155:A:LEU:HD21	2	0.13
(1,2461)	1:151:A:ARG:H	1:155:A:LEU:HD22	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2461)	1:151:A:ARG:H	1:155:A:LEU:HD23	2	0.13
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD11	5	0.13
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD12	5	0.13
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD13	5	0.13
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD21	5	0.13
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD22	5	0.13
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD23	5	0.13
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	22	0.13
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	22	0.13
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	22	0.13
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	22	0.13
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	22	0.13
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	22	0.13
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	22	0.13
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	22	0.13
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	22	0.13
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	22	0.13
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	22	0.13
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	22	0.13
(1,2158)	1:51:A:LEU:HD11	1:96:A:TRP:HE3	11	0.13
(1,2158)	1:51:A:LEU:HD12	1:96:A:TRP:HE3	11	0.13
(1,2158)	1:51:A:LEU:HD13	1:96:A:TRP:HE3	11	0.13
(1,2158)	1:51:A:LEU:HD21	1:96:A:TRP:HE3	11	0.13
(1,2158)	1:51:A:LEU:HD22	1:96:A:TRP:HE3	11	0.13
(1,2158)	1:51:A:LEU:HD23	1:96:A:TRP:HE3	11	0.13
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	2	0.13
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	2	0.13
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	2	0.13
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	2	0.13
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	2	0.13
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	2	0.13
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	2	0.13
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	2	0.13
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	2	0.13
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	2	0.13
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	2	0.13
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	2	0.13
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	2	0.13
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	2	0.13
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	2	0.13
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	2	0.13
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	2	0.13
(1,1882)	1:154:A:PHE:HE1	1:157:A:LEU:HD21	1	0.13
(1,1882)	1:154:A:PHE:HE1	1:157:A:LEU:HD22	1	0.13
(1,1882)	1:154:A:PHE:HE1	1:157:A:LEU:HD23	1	0.13
(1,1882)	1:154:A:PHE:HE2	1:157:A:LEU:HD21	1	0.13
(1,1882)	1:154:A:PHE:HE2	1:157:A:LEU:HD22	1	0.13
(1,1882)	1:154:A:PHE:HE2	1:157:A:LEU:HD23	1	0.13
(1,1240)	1:103:A:THR:HG21	1:106:A:LYS:H	11	0.13
(1,1240)	1:103:A:THR:HG22	1:106:A:LYS:H	11	0.13
(1,1240)	1:103:A:THR:HG23	1:106:A:LYS:H	11	0.13
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG21	11	0.13
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG22	11	0.13
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG23	11	0.13
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG21	21	0.13
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG22	21	0.13
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG23	21	0.13
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG11	6	0.13
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG12	6	0.13
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG13	6	0.13
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG11	6	0.13
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG12	6	0.13
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG13	6	0.13
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	11	0.13
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	11	0.13
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	11	0.13
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	11	0.13
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	11	0.13
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	11	0.13
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	11	0.13
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	11	0.13
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	11	0.13
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	14	0.13
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	14	0.13
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	14	0.13
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	14	0.13
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	14	0.13
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	14	0.13
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	14	0.13
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	14	0.13
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	14	0.13
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	23	0.12
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	23	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	23	0.12
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	23	0.12
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	23	0.12
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	23	0.12
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	23	0.12
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	23	0.12
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	23	0.12
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	23	0.12
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	23	0.12
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	23	0.12
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG11	13	0.12
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG12	13	0.12
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG13	13	0.12
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG21	13	0.12
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG22	13	0.12
(1,2191)	1:55:A:GLN:HE21	1:58:A:VAL:HG23	13	0.12
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG11	13	0.12
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG12	13	0.12
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG13	13	0.12
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG21	13	0.12
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG22	13	0.12
(1,2191)	1:55:A:GLN:HE22	1:58:A:VAL:HG23	13	0.12
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD11	17	0.12
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD12	17	0.12
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD13	17	0.12
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD21	17	0.12
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD22	17	0.12
(1,1971)	1:13:A:ALA:HB1	1:15:A:LEU:HD23	17	0.12
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD11	17	0.12
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD12	17	0.12
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD13	17	0.12
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD21	17	0.12
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD22	17	0.12
(1,1971)	1:13:A:ALA:HB2	1:15:A:LEU:HD23	17	0.12
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD11	17	0.12
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD12	17	0.12
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD13	17	0.12
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD21	17	0.12
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD22	17	0.12
(1,1971)	1:13:A:ALA:HB3	1:15:A:LEU:HD23	17	0.12
(1,1322)	1:69:A:GLU:HG2	1:109:A:VAL:HG11	11	0.12
(1,1322)	1:69:A:GLU:HG2	1:109:A:VAL:HG12	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1322)	1:69:A:GLU:HG2	1:109:A:VAL:HG13	11	0.12
(1,1322)	1:69:A:GLU:HG3	1:109:A:VAL:HG11	11	0.12
(1,1322)	1:69:A:GLU:HG3	1:109:A:VAL:HG12	11	0.12
(1,1322)	1:69:A:GLU:HG3	1:109:A:VAL:HG13	11	0.12
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG21	6	0.12
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG22	6	0.12
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG23	6	0.12
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG21	15	0.12
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG22	15	0.12
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG23	15	0.12
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG21	6	0.12
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG22	6	0.12
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG23	6	0.12
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG21	15	0.12
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG22	15	0.12
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG23	15	0.12
(1,1017)	1:80:A:MET:H	1:80:A:MET:HE1	7	0.12
(1,1017)	1:80:A:MET:H	1:80:A:MET:HE2	7	0.12
(1,1017)	1:80:A:MET:H	1:80:A:MET:HE3	7	0.12
(1,909)	1:61:A:ILE:HD11	1:104:A:PHE:HE1	10	0.12
(1,909)	1:61:A:ILE:HD11	1:104:A:PHE:HE2	10	0.12
(1,909)	1:61:A:ILE:HD12	1:104:A:PHE:HE1	10	0.12
(1,909)	1:61:A:ILE:HD12	1:104:A:PHE:HE2	10	0.12
(1,909)	1:61:A:ILE:HD13	1:104:A:PHE:HE1	10	0.12
(1,909)	1:61:A:ILE:HD13	1:104:A:PHE:HE2	10	0.12
(1,905)	1:61:A:ILE:HD11	1:63:A:GLU:H	4	0.12
(1,905)	1:61:A:ILE:HD12	1:63:A:GLU:H	4	0.12
(1,905)	1:61:A:ILE:HD13	1:63:A:GLU:H	4	0.12
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG11	11	0.12
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG12	11	0.12
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG13	11	0.12
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG11	11	0.12
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG12	11	0.12
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG13	11	0.12
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	8	0.12
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	8	0.12
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	8	0.12
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	8	0.12
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	8	0.12
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	8	0.12
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	8	0.12
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	8	0.12
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	26	0.12
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	26	0.12
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	26	0.12
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	26	0.12
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	26	0.12
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	26	0.12
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	26	0.12
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	26	0.12
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	26	0.12
(1,609)	1:23:A:ILE:HG21	1:34:A:GLU:HG2	6	0.12
(1,609)	1:23:A:ILE:HG21	1:34:A:GLU:HG3	6	0.12
(1,609)	1:23:A:ILE:HG22	1:34:A:GLU:HG2	6	0.12
(1,609)	1:23:A:ILE:HG22	1:34:A:GLU:HG3	6	0.12
(1,609)	1:23:A:ILE:HG23	1:34:A:GLU:HG2	6	0.12
(1,609)	1:23:A:ILE:HG23	1:34:A:GLU:HG3	6	0.12
(1,2517)	1:182:A:LEU:HD11	1:183:A:TYR:HB2	14	0.11
(1,2517)	1:182:A:LEU:HD11	1:183:A:TYR:HB3	14	0.11
(1,2517)	1:182:A:LEU:HD12	1:183:A:TYR:HB2	14	0.11
(1,2517)	1:182:A:LEU:HD12	1:183:A:TYR:HB3	14	0.11
(1,2517)	1:182:A:LEU:HD13	1:183:A:TYR:HB2	14	0.11
(1,2517)	1:182:A:LEU:HD13	1:183:A:TYR:HB3	14	0.11
(1,2517)	1:182:A:LEU:HD21	1:183:A:TYR:HB2	14	0.11
(1,2517)	1:182:A:LEU:HD21	1:183:A:TYR:HB3	14	0.11
(1,2517)	1:182:A:LEU:HD22	1:183:A:TYR:HB2	14	0.11
(1,2517)	1:182:A:LEU:HD22	1:183:A:TYR:HB3	14	0.11
(1,2517)	1:182:A:LEU:HD23	1:183:A:TYR:HB2	14	0.11
(1,2517)	1:182:A:LEU:HD23	1:183:A:TYR:HB3	14	0.11
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG2	19	0.11
(1,2496)	1:158:A:VAL:HG11	1:162:A:GLU:HG3	19	0.11
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG2	19	0.11
(1,2496)	1:158:A:VAL:HG12	1:162:A:GLU:HG3	19	0.11
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG2	19	0.11
(1,2496)	1:158:A:VAL:HG13	1:162:A:GLU:HG3	19	0.11
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG2	19	0.11
(1,2496)	1:158:A:VAL:HG21	1:162:A:GLU:HG3	19	0.11
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG2	19	0.11
(1,2496)	1:158:A:VAL:HG22	1:162:A:GLU:HG3	19	0.11
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG2	19	0.11
(1,2496)	1:158:A:VAL:HG23	1:162:A:GLU:HG3	19	0.11
(1,2489)	1:157:A:LEU:HD11	1:160:A:LYS:HE2	24	0.11
(1,2489)	1:157:A:LEU:HD11	1:160:A:LYS:HE3	24	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2489)	1:157:A:LEU:HD12	1:160:A:LYS:HE2	24	0.11
(1,2489)	1:157:A:LEU:HD12	1:160:A:LYS:HE3	24	0.11
(1,2489)	1:157:A:LEU:HD13	1:160:A:LYS:HE2	24	0.11
(1,2489)	1:157:A:LEU:HD13	1:160:A:LYS:HE3	24	0.11
(1,2489)	1:157:A:LEU:HD21	1:160:A:LYS:HE2	24	0.11
(1,2489)	1:157:A:LEU:HD21	1:160:A:LYS:HE3	24	0.11
(1,2489)	1:157:A:LEU:HD22	1:160:A:LYS:HE2	24	0.11
(1,2489)	1:157:A:LEU:HD22	1:160:A:LYS:HE3	24	0.11
(1,2489)	1:157:A:LEU:HD23	1:160:A:LYS:HE2	24	0.11
(1,2489)	1:157:A:LEU:HD23	1:160:A:LYS:HE3	24	0.11
(1,2395)	1:116:A:VAL:HG11	1:117:A:ARG:HD2	7	0.11
(1,2395)	1:116:A:VAL:HG11	1:117:A:ARG:HD3	7	0.11
(1,2395)	1:116:A:VAL:HG12	1:117:A:ARG:HD2	7	0.11
(1,2395)	1:116:A:VAL:HG12	1:117:A:ARG:HD3	7	0.11
(1,2395)	1:116:A:VAL:HG13	1:117:A:ARG:HD2	7	0.11
(1,2395)	1:116:A:VAL:HG13	1:117:A:ARG:HD3	7	0.11
(1,2395)	1:116:A:VAL:HG21	1:117:A:ARG:HD2	7	0.11
(1,2395)	1:116:A:VAL:HG21	1:117:A:ARG:HD3	7	0.11
(1,2395)	1:116:A:VAL:HG22	1:117:A:ARG:HD2	7	0.11
(1,2395)	1:116:A:VAL:HG22	1:117:A:ARG:HD3	7	0.11
(1,2395)	1:116:A:VAL:HG23	1:117:A:ARG:HD2	7	0.11
(1,2395)	1:116:A:VAL:HG23	1:117:A:ARG:HD3	7	0.11
(1,2391)	1:115:A:ILE:HD11	1:117:A:ARG:HB2	2	0.11
(1,2391)	1:115:A:ILE:HD11	1:117:A:ARG:HB3	2	0.11
(1,2391)	1:115:A:ILE:HD12	1:117:A:ARG:HB2	2	0.11
(1,2391)	1:115:A:ILE:HD12	1:117:A:ARG:HB3	2	0.11
(1,2391)	1:115:A:ILE:HD13	1:117:A:ARG:HB2	2	0.11
(1,2391)	1:115:A:ILE:HD13	1:117:A:ARG:HB3	2	0.11
(1,2359)	1:104:A:PHE:HA	1:111:A:VAL:HG11	2	0.11
(1,2359)	1:104:A:PHE:HA	1:111:A:VAL:HG12	2	0.11
(1,2359)	1:104:A:PHE:HA	1:111:A:VAL:HG13	2	0.11
(1,2359)	1:104:A:PHE:HA	1:111:A:VAL:HG21	2	0.11
(1,2359)	1:104:A:PHE:HA	1:111:A:VAL:HG22	2	0.11
(1,2359)	1:104:A:PHE:HA	1:111:A:VAL:HG23	2	0.11
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD1	5	0.11
(1,2253)	1:68:A:VAL:HG11	1:104:A:PHE:HD2	5	0.11
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD1	5	0.11
(1,2253)	1:68:A:VAL:HG12	1:104:A:PHE:HD2	5	0.11
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD1	5	0.11
(1,2253)	1:68:A:VAL:HG13	1:104:A:PHE:HD2	5	0.11
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD1	5	0.11
(1,2253)	1:68:A:VAL:HG21	1:104:A:PHE:HD2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD1	5	0.11
(1,2253)	1:68:A:VAL:HG22	1:104:A:PHE:HD2	5	0.11
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD1	5	0.11
(1,2253)	1:68:A:VAL:HG23	1:104:A:PHE:HD2	5	0.11
(1,2240)	1:67:A:ARG:HD2	1:68:A:VAL:HG11	17	0.11
(1,2240)	1:67:A:ARG:HD2	1:68:A:VAL:HG12	17	0.11
(1,2240)	1:67:A:ARG:HD2	1:68:A:VAL:HG13	17	0.11
(1,2240)	1:67:A:ARG:HD2	1:68:A:VAL:HG21	17	0.11
(1,2240)	1:67:A:ARG:HD2	1:68:A:VAL:HG22	17	0.11
(1,2240)	1:67:A:ARG:HD2	1:68:A:VAL:HG23	17	0.11
(1,2240)	1:67:A:ARG:HD3	1:68:A:VAL:HG11	17	0.11
(1,2240)	1:67:A:ARG:HD3	1:68:A:VAL:HG12	17	0.11
(1,2240)	1:67:A:ARG:HD3	1:68:A:VAL:HG13	17	0.11
(1,2240)	1:67:A:ARG:HD3	1:68:A:VAL:HG21	17	0.11
(1,2240)	1:67:A:ARG:HD3	1:68:A:VAL:HG22	17	0.11
(1,2240)	1:67:A:ARG:HD3	1:68:A:VAL:HG23	17	0.11
(1,1613)	1:154:A:PHE:HE1	1:157:A:LEU:HD11	11	0.11
(1,1613)	1:154:A:PHE:HE1	1:157:A:LEU:HD12	11	0.11
(1,1613)	1:154:A:PHE:HE1	1:157:A:LEU:HD13	11	0.11
(1,1613)	1:154:A:PHE:HE2	1:157:A:LEU:HD11	11	0.11
(1,1613)	1:154:A:PHE:HE2	1:157:A:LEU:HD12	11	0.11
(1,1613)	1:154:A:PHE:HE2	1:157:A:LEU:HD13	11	0.11
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG21	4	0.11
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG22	4	0.11
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG23	4	0.11
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG21	2	0.11
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG22	2	0.11
(1,1211)	1:96:A:TRP:HZ3	1:99:A:ILE:HG23	2	0.11
(1,1112)	1:89:A:THR:HG21	1:91:A:ALA:H	4	0.11
(1,1112)	1:89:A:THR:HG22	1:91:A:ALA:H	4	0.11
(1,1112)	1:89:A:THR:HG23	1:91:A:ALA:H	4	0.11
(1,1029)	1:75:A:LEU:HD11	1:80:A:MET:HE1	4	0.11
(1,1029)	1:75:A:LEU:HD11	1:80:A:MET:HE2	4	0.11
(1,1029)	1:75:A:LEU:HD11	1:80:A:MET:HE3	4	0.11
(1,1029)	1:75:A:LEU:HD12	1:80:A:MET:HE1	4	0.11
(1,1029)	1:75:A:LEU:HD12	1:80:A:MET:HE2	4	0.11
(1,1029)	1:75:A:LEU:HD12	1:80:A:MET:HE3	4	0.11
(1,1029)	1:75:A:LEU:HD13	1:80:A:MET:HE1	4	0.11
(1,1029)	1:75:A:LEU:HD13	1:80:A:MET:HE2	4	0.11
(1,1029)	1:75:A:LEU:HD13	1:80:A:MET:HE3	4	0.11
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG11	4	0.11
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG12	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:55:A:GLN:HG2	1:58:A:VAL:HG13	4	0.11
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG11	4	0.11
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG12	4	0.11
(1,892)	1:55:A:GLN:HG3	1:58:A:VAL:HG13	4	0.11
(1,817)	1:182:A:LEU:HD21	1:183:A:TYR:HD1	9	0.11
(1,817)	1:182:A:LEU:HD21	1:183:A:TYR:HD2	9	0.11
(1,817)	1:182:A:LEU:HD22	1:183:A:TYR:HD1	9	0.11
(1,817)	1:182:A:LEU:HD22	1:183:A:TYR:HD2	9	0.11
(1,817)	1:182:A:LEU:HD23	1:183:A:TYR:HD1	9	0.11
(1,817)	1:182:A:LEU:HD23	1:183:A:TYR:HD2	9	0.11
(1,817)	1:182:A:LEU:HD21	1:183:A:TYR:HD1	15	0.11
(1,817)	1:182:A:LEU:HD21	1:183:A:TYR:HD2	15	0.11
(1,817)	1:182:A:LEU:HD22	1:183:A:TYR:HD1	15	0.11
(1,817)	1:182:A:LEU:HD22	1:183:A:TYR:HD2	15	0.11
(1,817)	1:182:A:LEU:HD23	1:183:A:TYR:HD1	15	0.11
(1,817)	1:182:A:LEU:HD23	1:183:A:TYR:HD2	15	0.11
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	5	0.11
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	5	0.11
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	5	0.11
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	5	0.11
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	5	0.11
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	5	0.11
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	5	0.11
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	5	0.11
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	5	0.11
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	18	0.11
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	18	0.11
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	18	0.11
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	18	0.11
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	18	0.11
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	18	0.11
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	18	0.11
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	18	0.11
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	18	0.11
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD11	6	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD12	6	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD13	6	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD21	6	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD22	6	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD23	6	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD11	13	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD12	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD13	13	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD21	13	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD22	13	0.1
(1,2421)	1:120:A:MET:HA	1:121:A:LEU:HD23	13	0.1
(1,2365)	1:105:A:GLU:HG2	1:111:A:VAL:HG11	23	0.1
(1,2365)	1:105:A:GLU:HG2	1:111:A:VAL:HG12	23	0.1
(1,2365)	1:105:A:GLU:HG2	1:111:A:VAL:HG13	23	0.1
(1,2365)	1:105:A:GLU:HG2	1:111:A:VAL:HG21	23	0.1
(1,2365)	1:105:A:GLU:HG2	1:111:A:VAL:HG22	23	0.1
(1,2365)	1:105:A:GLU:HG2	1:111:A:VAL:HG23	23	0.1
(1,2365)	1:105:A:GLU:HG3	1:111:A:VAL:HG11	23	0.1
(1,2365)	1:105:A:GLU:HG3	1:111:A:VAL:HG12	23	0.1
(1,2365)	1:105:A:GLU:HG3	1:111:A:VAL:HG13	23	0.1
(1,2365)	1:105:A:GLU:HG3	1:111:A:VAL:HG21	23	0.1
(1,2365)	1:105:A:GLU:HG3	1:111:A:VAL:HG22	23	0.1
(1,2365)	1:105:A:GLU:HG3	1:111:A:VAL:HG23	23	0.1
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG11	28	0.1
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG12	28	0.1
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG13	28	0.1
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG21	28	0.1
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG22	28	0.1
(1,2267)	1:72:A:ARG:HD2	1:109:A:VAL:HG23	28	0.1
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG11	28	0.1
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG12	28	0.1
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG13	28	0.1
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG21	28	0.1
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG22	28	0.1
(1,2267)	1:72:A:ARG:HD3	1:109:A:VAL:HG23	28	0.1
(1,2208)	1:58:A:VAL:HG11	1:62:A:GLU:HG2	25	0.1
(1,2208)	1:58:A:VAL:HG11	1:62:A:GLU:HG3	25	0.1
(1,2208)	1:58:A:VAL:HG12	1:62:A:GLU:HG2	25	0.1
(1,2208)	1:58:A:VAL:HG12	1:62:A:GLU:HG3	25	0.1
(1,2208)	1:58:A:VAL:HG13	1:62:A:GLU:HG2	25	0.1
(1,2208)	1:58:A:VAL:HG13	1:62:A:GLU:HG3	25	0.1
(1,2208)	1:58:A:VAL:HG21	1:62:A:GLU:HG2	25	0.1
(1,2208)	1:58:A:VAL:HG21	1:62:A:GLU:HG3	25	0.1
(1,2208)	1:58:A:VAL:HG22	1:62:A:GLU:HG2	25	0.1
(1,2208)	1:58:A:VAL:HG22	1:62:A:GLU:HG3	25	0.1
(1,2208)	1:58:A:VAL:HG23	1:62:A:GLU:HG2	25	0.1
(1,2208)	1:58:A:VAL:HG23	1:62:A:GLU:HG3	25	0.1
(1,1973)	1:13:A:ALA:HB1	1:17:A:ASN:HD21	8	0.1
(1,1973)	1:13:A:ALA:HB1	1:17:A:ASN:HD22	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1973)	1:13:A:ALA:HB2	1:17:A:ASN:HD21	8	0.1
(1,1973)	1:13:A:ALA:HB2	1:17:A:ASN:HD22	8	0.1
(1,1973)	1:13:A:ALA:HB3	1:17:A:ASN:HD21	8	0.1
(1,1973)	1:13:A:ALA:HB3	1:17:A:ASN:HD22	8	0.1
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG21	24	0.1
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG22	24	0.1
(1,1213)	1:59:A:ARG:H	1:99:A:ILE:HG23	24	0.1
(1,1182)	1:96:A:TRP:H	1:99:A:ILE:HD11	2	0.1
(1,1182)	1:96:A:TRP:H	1:99:A:ILE:HD12	2	0.1
(1,1182)	1:96:A:TRP:H	1:99:A:ILE:HD13	2	0.1
(1,1112)	1:89:A:THR:HG21	1:91:A:ALA:H	2	0.1
(1,1112)	1:89:A:THR:HG22	1:91:A:ALA:H	2	0.1
(1,1112)	1:89:A:THR:HG23	1:91:A:ALA:H	2	0.1
(1,909)	1:61:A:ILE:HD11	1:104:A:PHE:HE1	25	0.1
(1,909)	1:61:A:ILE:HD11	1:104:A:PHE:HE2	25	0.1
(1,909)	1:61:A:ILE:HD12	1:104:A:PHE:HE1	25	0.1
(1,909)	1:61:A:ILE:HD12	1:104:A:PHE:HE2	25	0.1
(1,909)	1:61:A:ILE:HD13	1:104:A:PHE:HE1	25	0.1
(1,909)	1:61:A:ILE:HD13	1:104:A:PHE:HE2	25	0.1
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	20	0.1
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	20	0.1
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	20	0.1
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	20	0.1
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	20	0.1
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	20	0.1
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	20	0.1
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	20	0.1
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	20	0.1
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE1	21	0.1
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE2	21	0.1
(1,702)	1:35:A:ALA:HB1	1:80:A:MET:HE3	21	0.1
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE1	21	0.1
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE2	21	0.1
(1,702)	1:35:A:ALA:HB2	1:80:A:MET:HE3	21	0.1
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE1	21	0.1
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE2	21	0.1
(1,702)	1:35:A:ALA:HB3	1:80:A:MET:HE3	21	0.1
(1,684)	1:16:A:VAL:HA	1:33:A:LEU:HD11	11	0.1
(1,684)	1:16:A:VAL:HA	1:33:A:LEU:HD12	11	0.1
(1,684)	1:16:A:VAL:HA	1:33:A:LEU:HD13	11	0.1

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

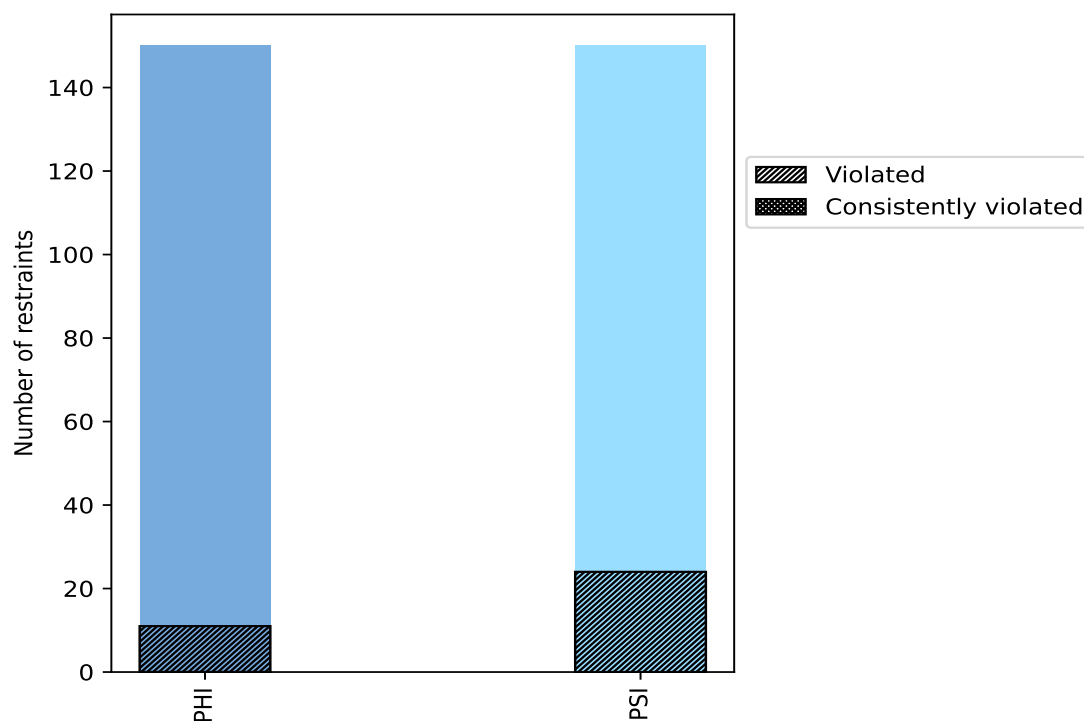
10.1 Summary of dihedral-angle violations [i](#)

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
PHI	150	50.0	11	7.3	3.7	0	0.0	0.0
PSI	150	50.0	24	16.0	8.0	0	0.0	0.0
Total	300	100.0	35	11.7	11.7	0	0.0	0.0

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

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



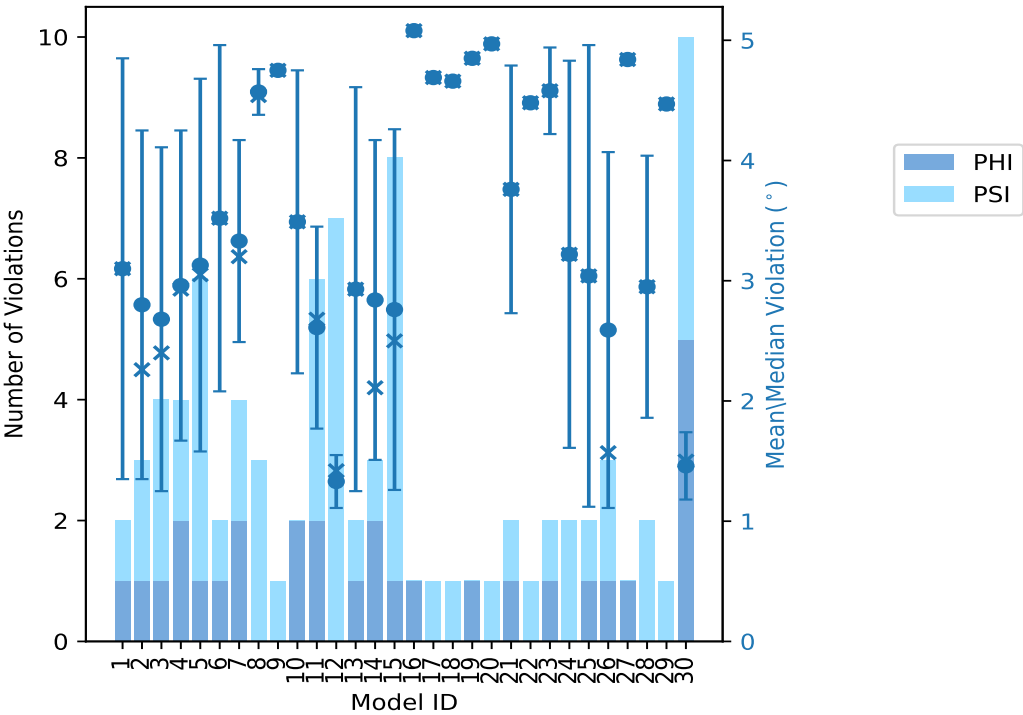
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	1	1	2	3.1	4.85	1.75	3.1
2	1	2	3	2.8	4.78	1.45	2.26
3	1	3	4	2.68	4.88	1.43	2.4
4	2	2	4	2.96	4.67	1.29	2.93
5	1	5	6	3.13	4.96	1.55	3.05
6	1	1	2	3.52	4.95	1.44	3.52
7	2	2	4	3.33	4.64	0.84	3.2
8	0	3	3	4.57	4.81	0.19	4.54
9	0	1	1	4.75	4.75	0.0	4.75
10	2	0	2	3.49	4.74	1.26	3.49
11	2	4	6	2.61	3.96	0.84	2.68
12	0	7	7	1.33	1.61	0.22	1.42
13	1	1	2	2.93	4.61	1.68	2.93
14	2	1	3	2.84	4.71	1.33	2.11
15	1	7	8	2.76	4.91	1.5	2.5
16	1	0	1	5.08	5.08	0.0	5.08
17	0	1	1	4.69	4.69	0.0	4.69
18	0	1	1	4.66	4.66	0.0	4.66
19	1	0	1	4.85	4.85	0.0	4.85
20	0	1	1	4.97	4.97	0.0	4.97
21	1	1	2	3.76	4.8	1.03	3.76
22	0	1	1	4.48	4.48	0.0	4.48
23	1	1	2	4.58	4.94	0.36	4.58
24	0	2	2	3.22	4.82	1.61	3.22
25	1	1	2	3.04	4.96	1.92	3.04
26	1	2	3	2.59	4.69	1.48	1.57
27	1	0	1	4.84	4.84	0.0	4.84
28	0	2	2	2.95	4.04	1.09	2.95
29	0	1	1	4.47	4.47	0.0	4.47
30	5	5	10	1.46	1.99	0.28	1.5

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
7	11	18	1	3.3
1	5	6	2	6.7
1	5	6	3	10.0
1	1	2	4	13.3
0	0	0	5	16.7
0	1	1	6	20.0
0	0	0	7	23.3
0	0	0	8	26.7
0	0	0	9	30.0
0	0	0	10	33.3
0	0	0	11	36.7

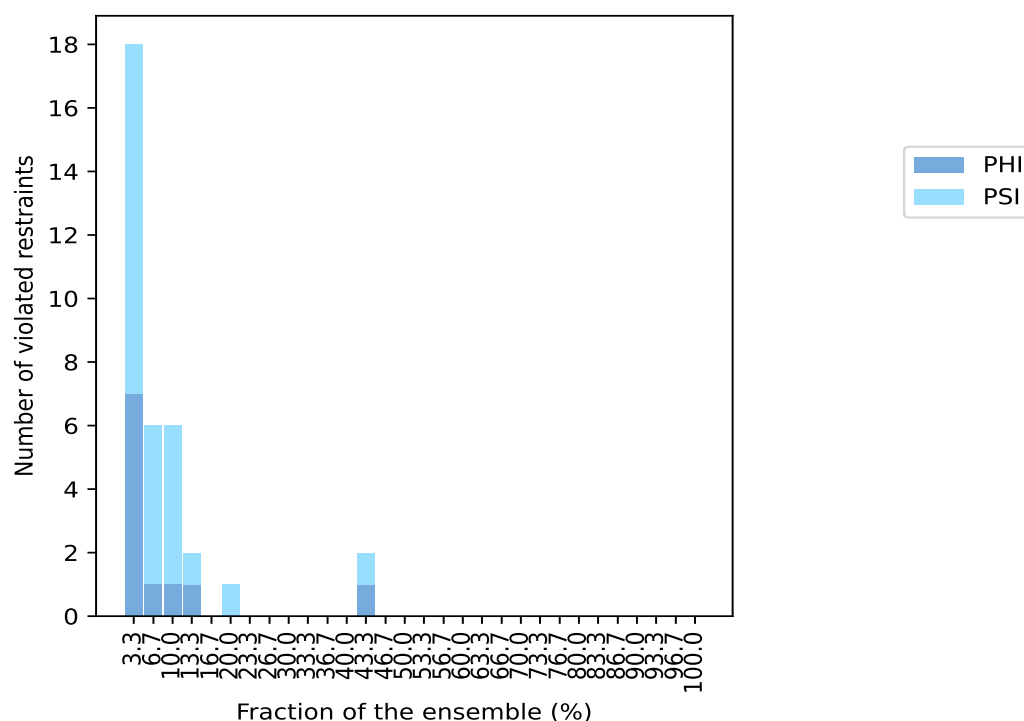
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	40.0
1	1	2	13	43.3
0	0	0	14	46.7
0	0	0	15	50.0
0	0	0	16	53.3
0	0	0	17	56.7
0	0	0	18	60.0
0	0	0	19	63.3
0	0	0	20	66.7
0	0	0	21	70.0
0	0	0	22	73.3
0	0	0	23	76.7
0	0	0	24	80.0
0	0	0	25	83.3
0	0	0	26	86.7
0	0	0	27	90.0
0	0	0	28	93.3
0	0	0	29	96.7
0	0	0	30	100.0

¹ Number of models with violations

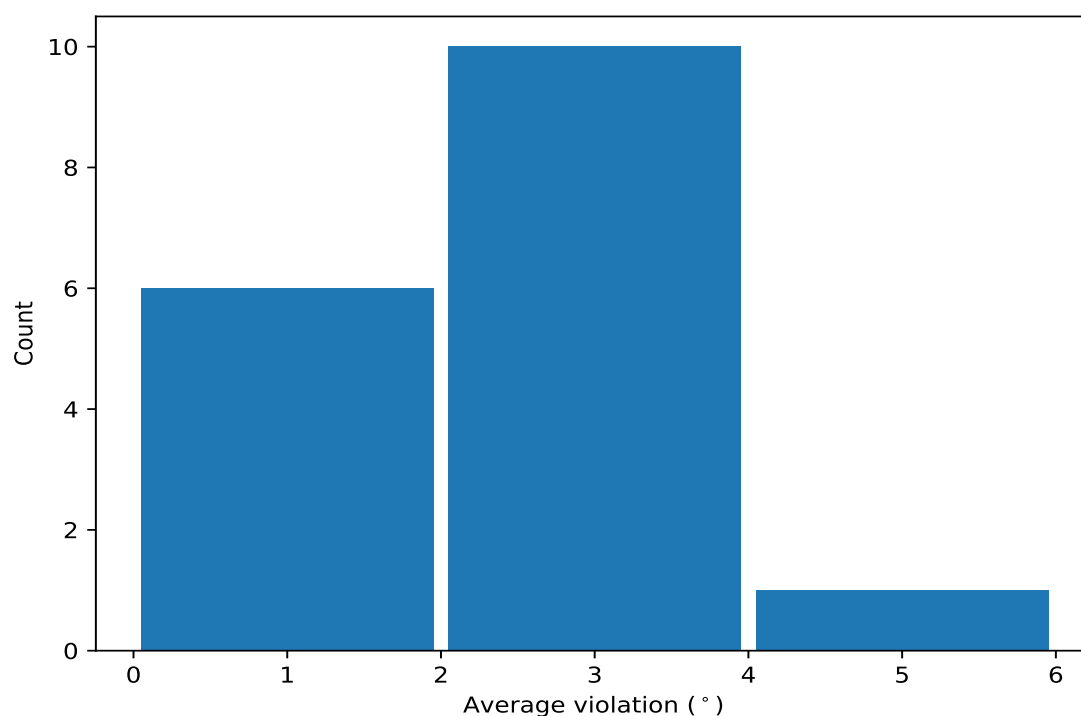
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

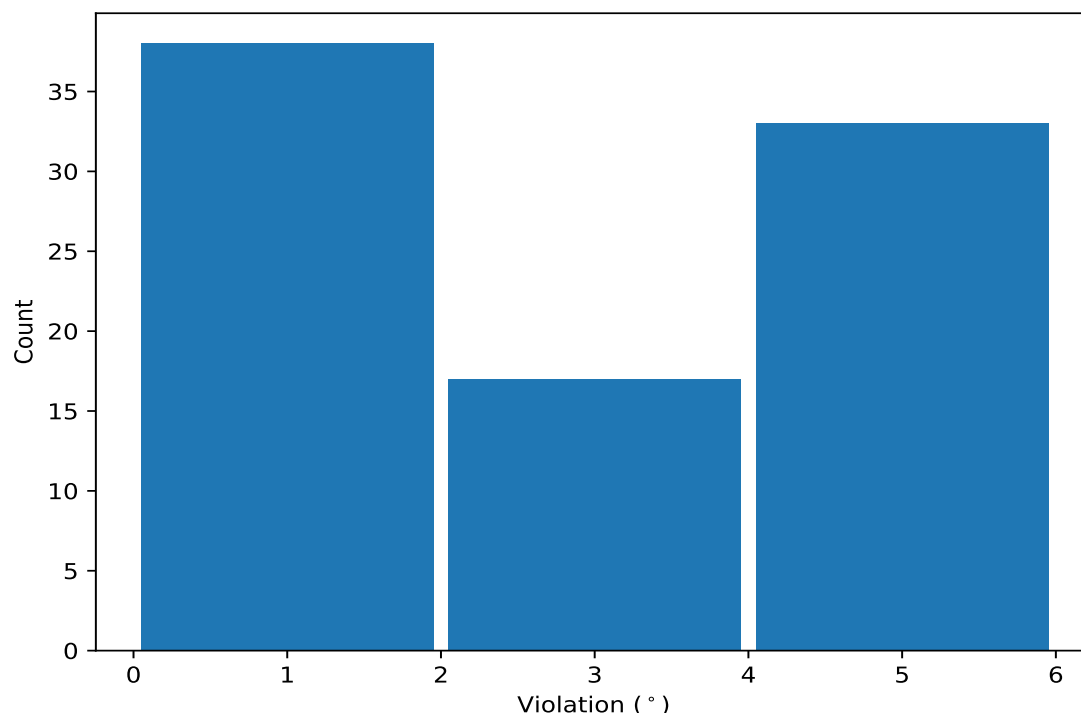
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	13	3.95	1.47	4.84
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	13	3.69	1.46	4.48
(1,188)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:THR:N	6	2.92	1.08	2.71
(1,295)	1:166:A:LYS:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	4	3.85	1.12	4.2
(1,298)	1:168:A:GLU:N	1:168:A:GLU:CA	1:168:A:GLU:C	1:169:A:ALA:N	4	3.54	1.34	3.9
(1,282)	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	1:161:A:GLN:N	3	4.39	0.31	4.54
(1,4)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:GLU:N	3	3.24	1.11	2.89
(1,284)	1:161:A:GLN:N	1:161:A:GLN:CA	1:161:A:GLN:C	1:162:A:GLU:N	3	3.09	1.19	2.73
(1,13)	1:8:A:TYR:C	1:9:A:TRP:N	1:9:A:TRP:CA	1:9:A:TRP:C	3	2.79	1.52	1.73
(1,92)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLU:N	3	2.69	1.56	2.26
(1,254)	1:146:A:ASN:N	1:146:A:ASN:CA	1:146:A:ASN:C	1:147:A:ALA:N	3	2.57	1.56	1.86
(1,251)	1:144:A:PHE:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	2	1.86	0.43	1.86
(1,170)	1:97:A:GLU:N	1:97:A:GLU:CA	1:97:A:GLU:C	1:98:A:GLU:N	2	1.74	0.11	1.74
(1,132)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:GLY:N	2	1.62	0.01	1.62
(1,56)	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	1:36:A:PRO:N	2	1.52	0.04	1.52
(1,230)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:PHE:N	2	1.28	0.14	1.28
(1,248)	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	1:142:A:ALA:N	2	1.2	0.12	1.2

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 (°)
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	16	5.08
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	20	4.97
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	5	4.96
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	25	4.96
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	6	4.95
(1,13)	1:8:A:TYR:C	1:9:A:TRP:N	1:9:A:TRP:CA	1:9:A:TRP:C	23	4.94
(1,278)	1:158:A:VAL:N	1:158:A:VAL:CA	1:158:A:VAL:C	1:159:A:LEU:N	15	4.91
(1,295)	1:166:A:LYS:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	3	4.88
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	1	4.85
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	19	4.85
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	27	4.84
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	24	4.82
(1,298)	1:168:A:GLU:N	1:168:A:GLU:CA	1:168:A:GLU:C	1:169:A:ALA:N	8	4.81
(1,295)	1:166:A:LYS:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	21	4.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,92)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLU:N	2	4.78
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	9	4.75
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	10	4.74
(1,4)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:GLU:N	15	4.74
(1,254)	1:146:A:ASN:N	1:146:A:ASN:CA	1:146:A:ASN:C	1:147:A:ALA:N	5	4.73
(1,298)	1:168:A:GLU:N	1:168:A:GLU:CA	1:168:A:GLU:C	1:169:A:ALA:N	14	4.71
(1,284)	1:161:A:GLN:N	1:161:A:GLN:CA	1:161:A:GLN:C	1:162:A:GLU:N	26	4.69
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	17	4.69
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	4	4.67
(1,282)	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	1:161:A:GLN:N	18	4.66
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	7	4.64
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	13	4.61
(1,282)	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	1:161:A:GLN:N	8	4.54
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	22	4.48
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	29	4.47
(1,188)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:THR:N	8	4.35
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	5	4.26
(1,188)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:THR:N	23	4.22
(1,296)	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	1:168:A:GLU:N	28	4.04
(1,282)	1:160:A:LYS:N	1:160:A:LYS:CA	1:160:A:LYS:C	1:161:A:GLN:N	11	3.96
(1,288)	1:163:A:GLU:N	1:163:A:GLU:CA	1:163:A:GLU:C	1:164:A:GLN:N	15	3.82
(1,295)	1:166:A:LYS:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	4	3.61
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	7	3.29
(1,188)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:THR:N	15	3.16
(1,137)	1:77:A:ARG:C	1:78:A:ARG:N	1:78:A:ARG:CA	1:78:A:ARG:C	11	3.16
(1,298)	1:168:A:GLU:N	1:168:A:GLU:CA	1:168:A:GLU:C	1:169:A:ALA:N	7	3.1
(1,4)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:GLU:N	3	2.89
(1,243)	1:138:A:SER:C	1:139:A:GLU:N	1:139:A:GLU:CA	1:139:A:GLU:C	11	2.79
(1,284)	1:161:A:GLN:N	1:161:A:GLN:CA	1:161:A:GLN:C	1:162:A:GLU:N	21	2.73
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	11	2.56
(1,251)	1:144:A:PHE:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	7	2.29
(1,188)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:THR:N	2	2.26
(1,92)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLU:N	4	2.26
(1,287)	1:162:A:GLU:C	1:163:A:GLU:N	1:163:A:GLU:CA	1:163:A:GLU:C	10	2.23
(1,295)	1:166:A:LYS:C	1:167:A:THR:N	1:167:A:THR:CA	1:167:A:THR:C	14	2.11
(1,4)	1:4:A:LEU:N	1:4:A:LEU:CA	1:4:A:LEU:C	1:5:A:GLU:N	6	2.08
(1,43)	1:28:A:SER:C	1:29:A:ASP:N	1:29:A:ASP:CA	1:29:A:ASP:C	30	1.99
(1,188)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:THR:N	3	1.9
(1,254)	1:146:A:ASN:N	1:146:A:ASN:CA	1:146:A:ASN:C	1:147:A:ALA:N	28	1.86
(1,284)	1:161:A:GLN:N	1:161:A:GLN:CA	1:161:A:GLN:C	1:162:A:GLU:N	5	1.84
(1,170)	1:97:A:GLU:N	1:97:A:GLU:CA	1:97:A:GLU:C	1:98:A:GLU:N	15	1.84
(1,120)	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	1:70:A:ARG:N	5	1.8
(1,13)	1:8:A:TYR:C	1:9:A:TRP:N	1:9:A:TRP:CA	1:9:A:TRP:C	30	1.73
(1,13)	1:8:A:TYR:C	1:9:A:TRP:N	1:9:A:TRP:CA	1:9:A:TRP:C	14	1.7
(1,170)	1:97:A:GLU:N	1:97:A:GLU:CA	1:97:A:GLU:C	1:98:A:GLU:N	11	1.63
(1,132)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:GLY:N	30	1.63
(1,188)	1:107:A:GLY:N	1:107:A:GLY:CA	1:107:A:GLY:C	1:108:A:THR:N	24	1.61
(1,132)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:GLY:N	12	1.61
(1,290)	1:164:A:GLN:N	1:164:A:GLN:CA	1:164:A:GLN:C	1:165:A:ARG:N	26	1.57
(1,45)	1:29:A:ASP:C	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	30	1.57
(1,56)	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	1:36:A:PRO:N	30	1.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,298)	1:168:A:GLU:N	1:168:A:GLU:CA	1:168:A:GLU:C	1:169:A:ALA:N	11	1.54
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	26	1.52
(1,56)	1:35:A:ALA:N	1:35:A:ALA:CA	1:35:A:ALA:C	1:36:A:PRO:N	12	1.49
(1,236)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:GLU:N	12	1.44
(1,251)	1:144:A:PHE:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	30	1.43
(1,230)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:PHE:N	12	1.42
(1,279)	1:158:A:VAL:C	1:159:A:LEU:N	1:159:A:LEU:CA	1:159:A:LEU:C	30	1.35
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	2	1.35
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	1	1.34
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	15	1.32
(1,248)	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	1:142:A:ALA:N	12	1.31
(1,260)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:ALA:N	4	1.29
(1,215)	1:122:A:ARG:C	1:123:A:ASP:N	1:123:A:ASP:CA	1:123:A:ASP:C	13	1.25
(1,257)	1:147:A:ALA:C	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	15	1.2
(1,2)	1:3:A:LEU:N	1:3:A:LEU:CA	1:3:A:LEU:C	1:4:A:LEU:N	5	1.17
(1,230)	1:131:A:SER:N	1:131:A:SER:CA	1:131:A:SER:C	1:132:A:PHE:N	30	1.14
(1,254)	1:146:A:ASN:N	1:146:A:ASN:CA	1:146:A:ASN:C	1:147:A:ALA:N	25	1.12
(1,248)	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	1:142:A:ALA:N	30	1.08
(1,62)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:SER:N	30	1.08
(1,98)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:ARG:N	15	1.06
(1,92)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:GLU:N	3	1.04
(1,190)	1:108:A:THR:N	1:108:A:THR:CA	1:108:A:THR:C	1:109:A:VAL:N	12	1.01
(1,96)	1:57:A:MET:N	1:57:A:MET:CA	1:57:A:MET:C	1:58:A:VAL:N	12	1.01