



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2M65 / pdb_00002m65
BMRB ID : 19108
Title : NMR structure of human restriction factor APOBEC3A
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Deposited on : 2013-03-21

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

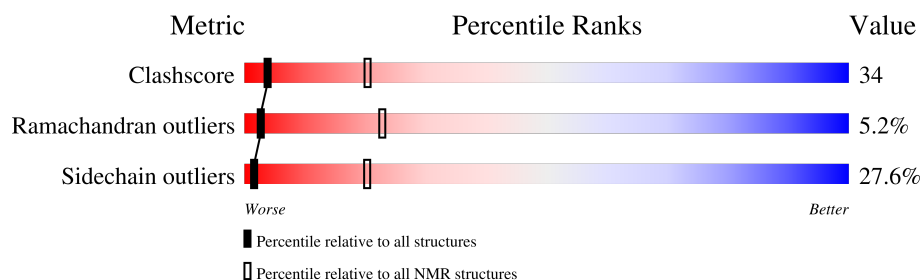
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 67%.

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	207	

2 Ensemble composition and analysis

This entry contains 30 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:11-A:57, A:70-A:194 (172)	0.79	14

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 5 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3160 atoms, of which 1537 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Probable DNA dC->dU-editing enzyme APOBEC-3A.

Mol	Chain	Residues	Atoms						Trace
1	A	199	Total	C	H	N	O	S	0
			3159	1029	1537	292	290	11	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	LEU	-	expression tag	UNP P31941
A	201	GLU	-	expression tag	UNP P31941
A	202	HIS	-	expression tag	UNP P31941
A	203	HIS	-	expression tag	UNP P31941
A	204	HIS	-	expression tag	UNP P31941
A	205	HIS	-	expression tag	UNP P31941
A	206	HIS	-	expression tag	UNP P31941
A	207	HIS	-	expression tag	UNP P31941

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

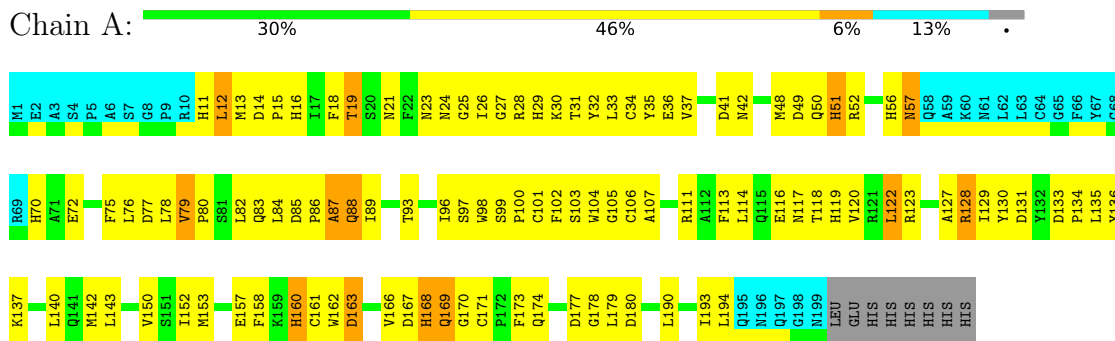
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

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: Probable DNA dC->dU-editing enzyme APOBEC-3A

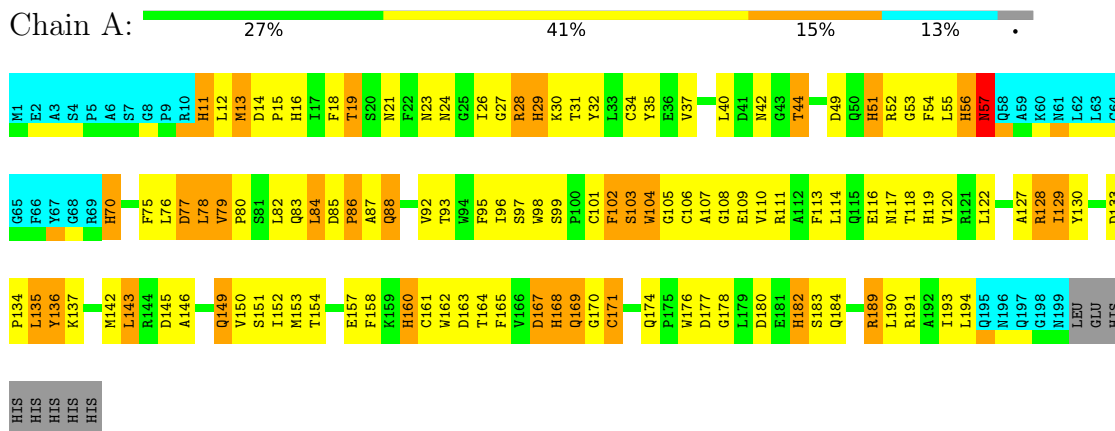


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

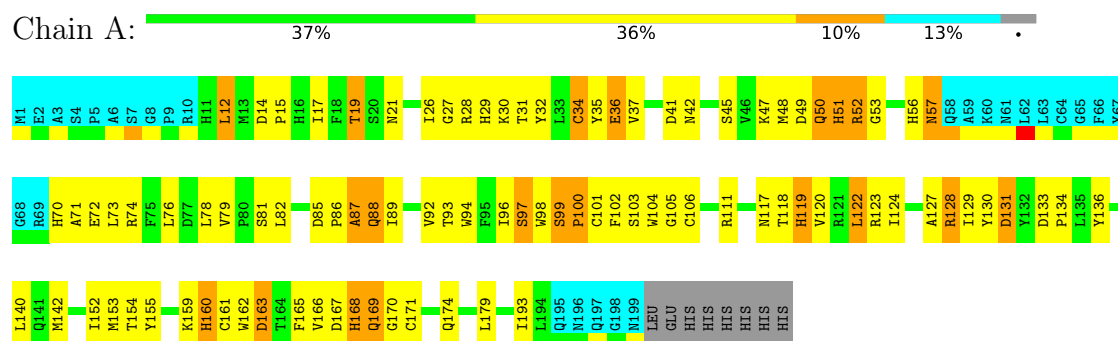
4.2.1 Score per residue for model 1

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



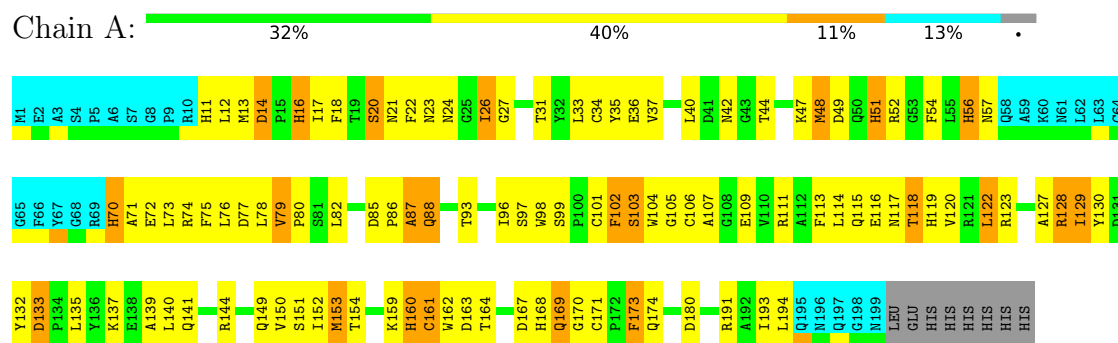
4.2.2 Score per residue for model 2

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



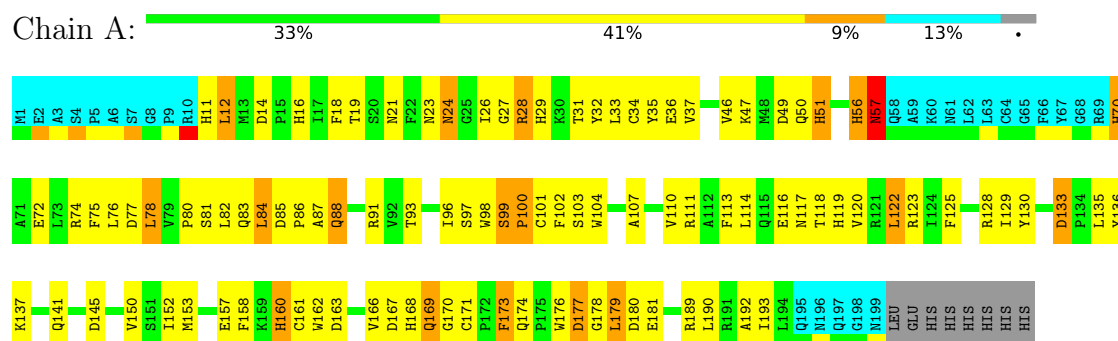
4.2.3 Score per residue for model 3

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



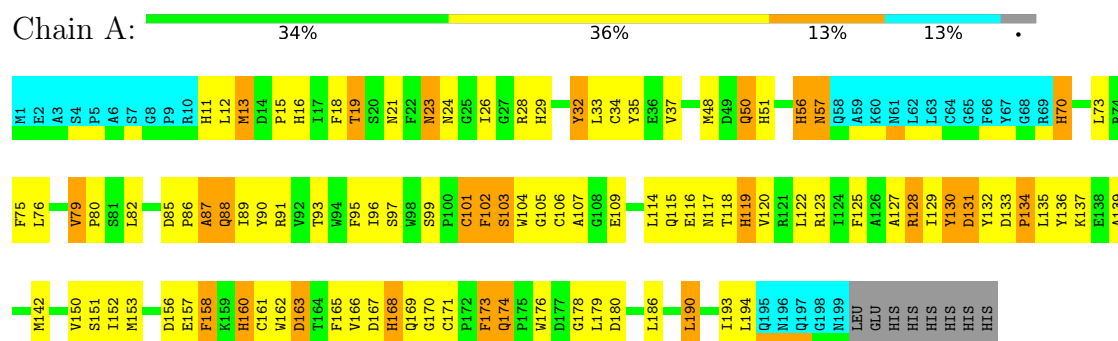
4.2.4 Score per residue for model 4

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



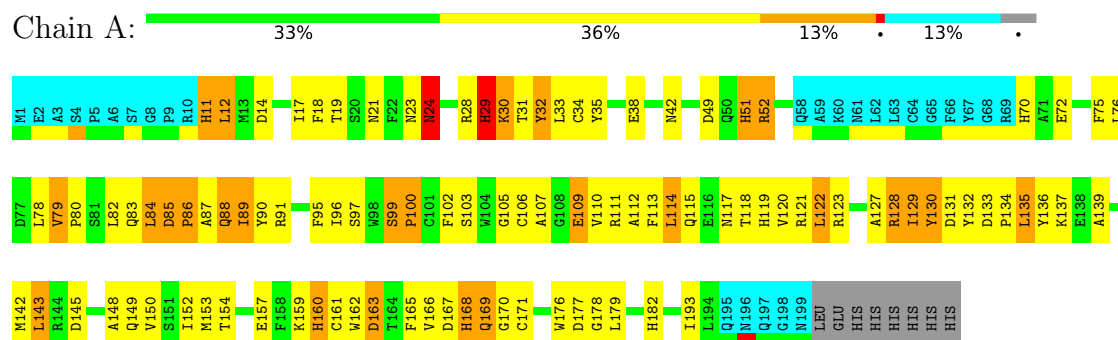
4.2.8 Score per residue for model 8

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



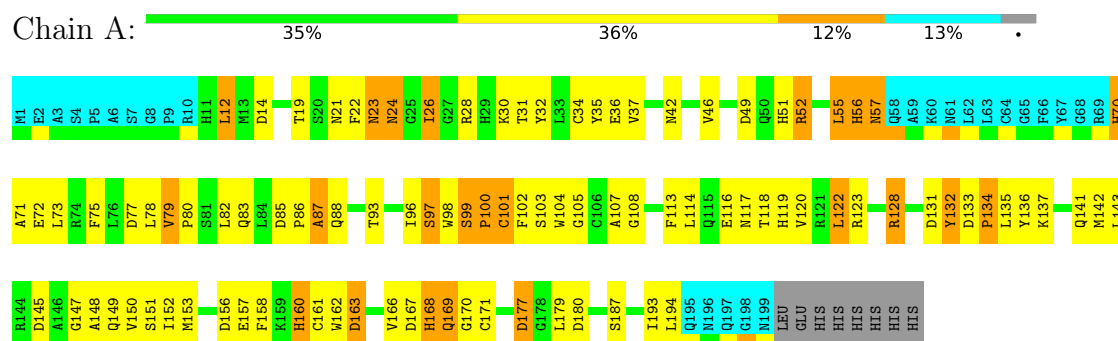
4.2.9 Score per residue for model 9

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



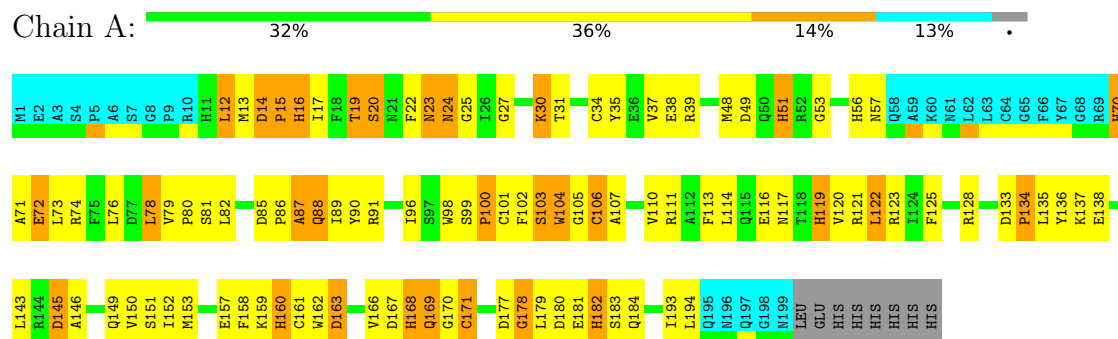
4.2.10 Score per residue for model 10

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



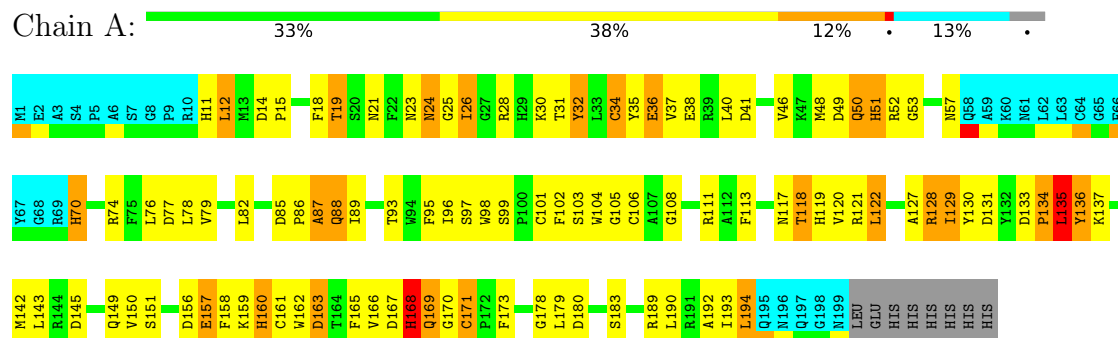
4.2.11 Score per residue for model 11

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



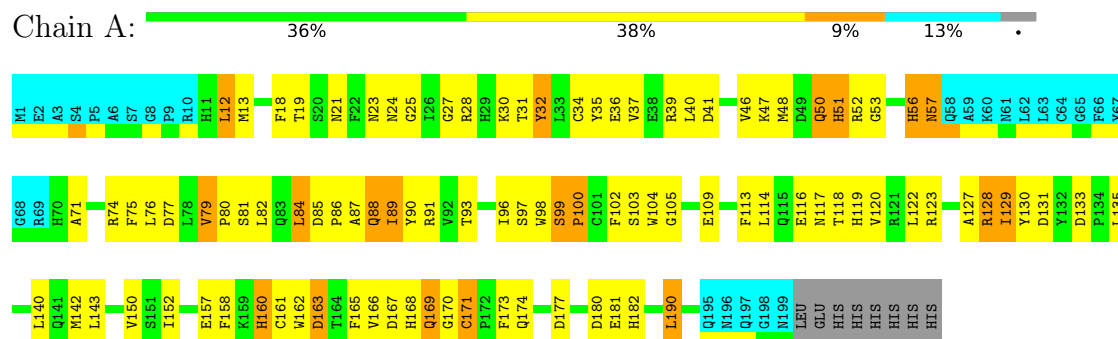
4.2.12 Score per residue for model 12

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



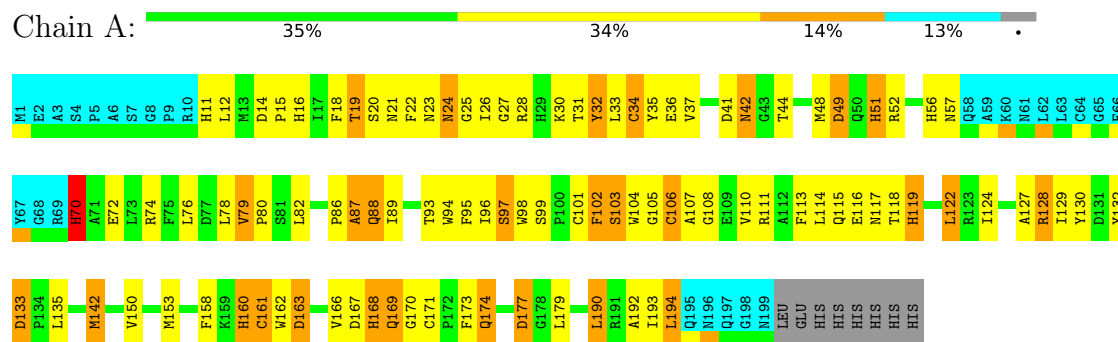
4.2.13 Score per residue for model 13

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



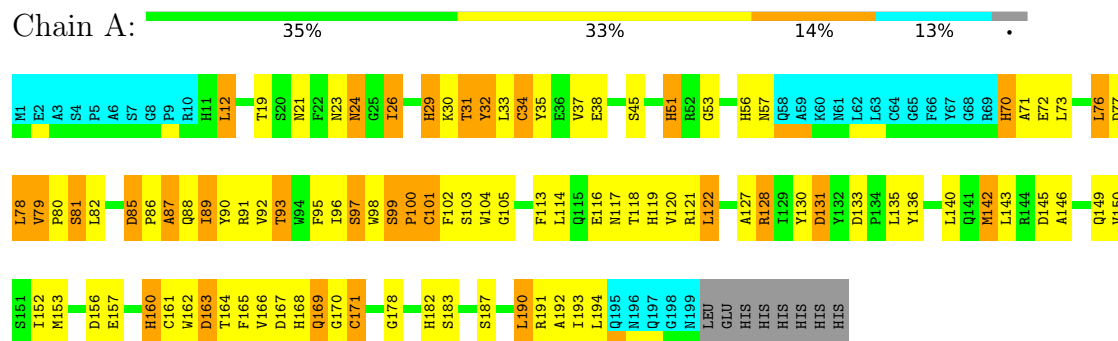
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



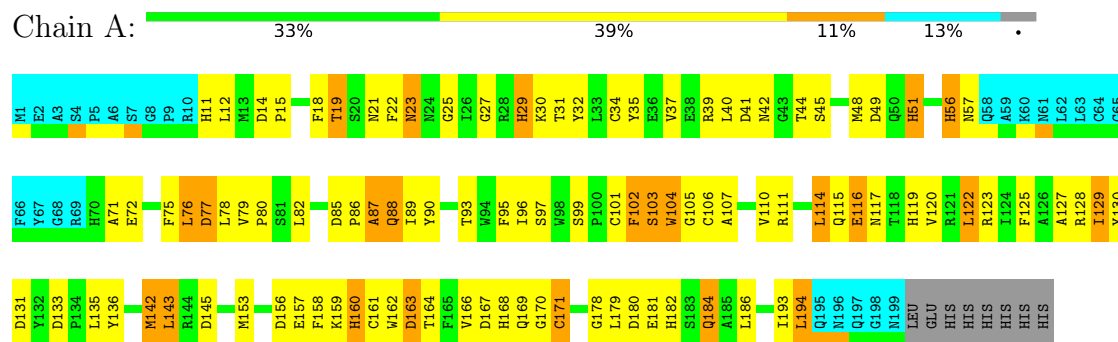
4.2.15 Score per residue for model 15

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



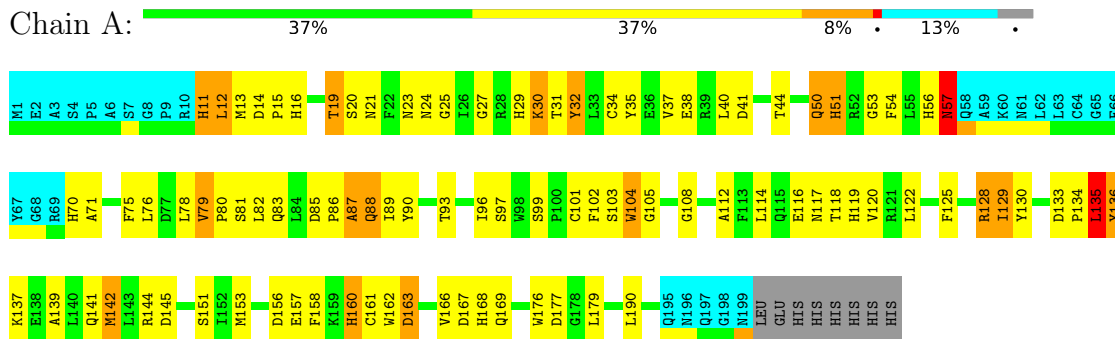
4.2.16 Score per residue for model 16

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



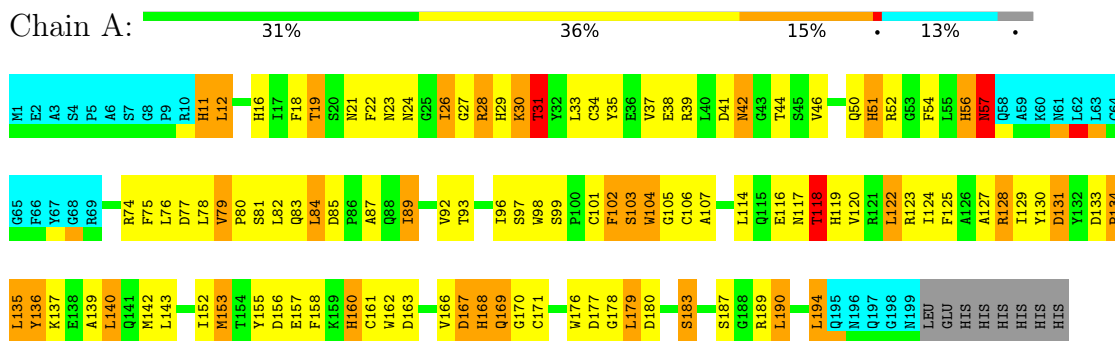
4.2.17 Score per residue for model 17

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



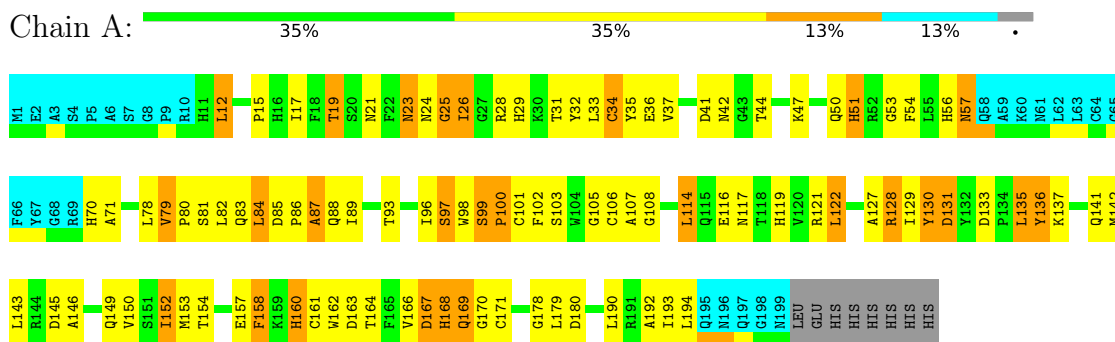
4.2.18 Score per residue for model 18

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



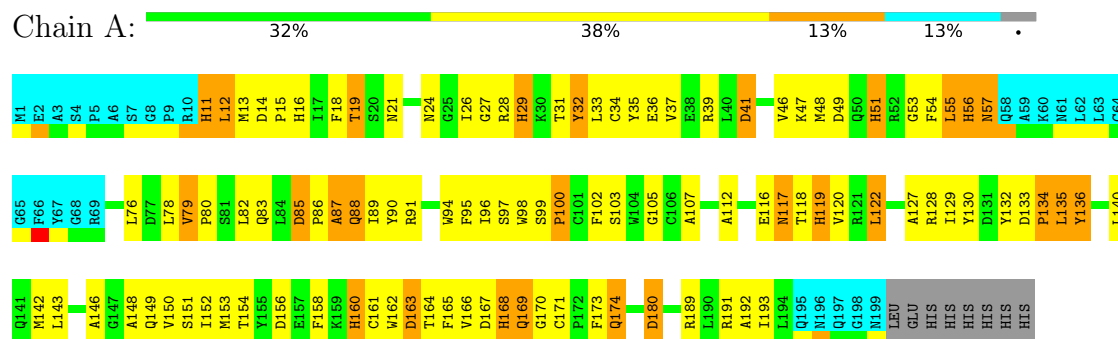
4.2.19 Score per residue for model 19

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



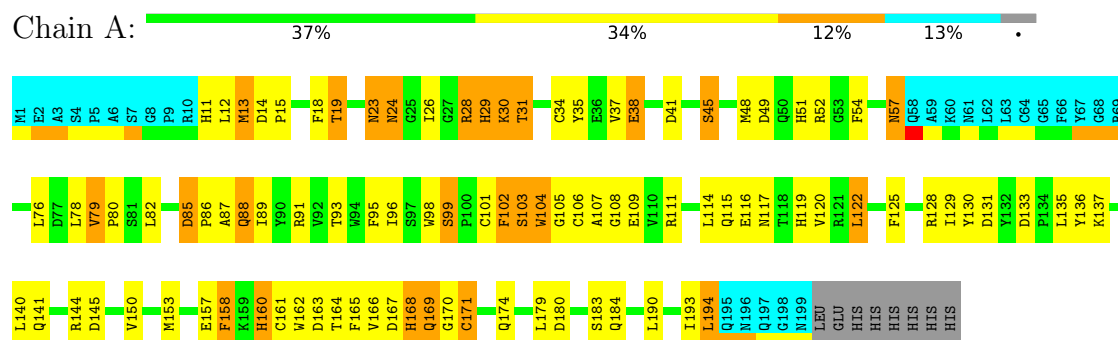
4.2.20 Score per residue for model 20

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



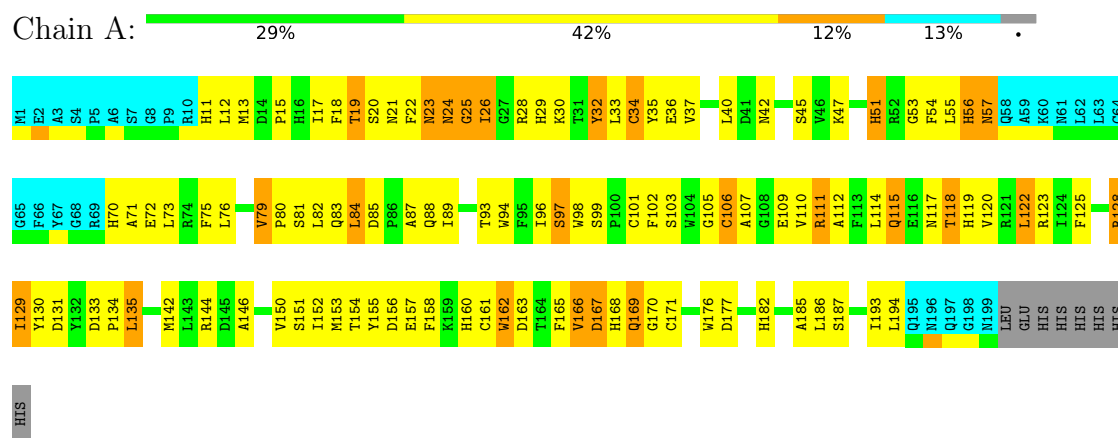
4.2.21 Score per residue for model 21

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



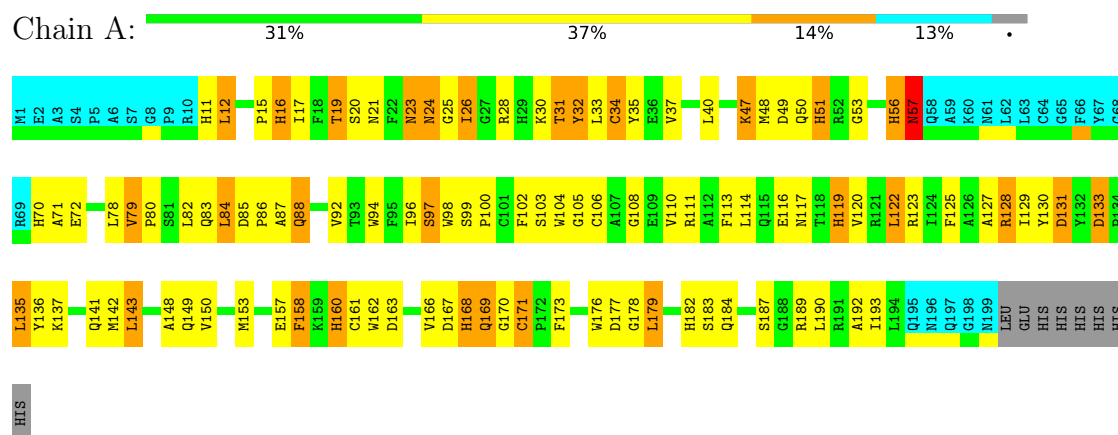
4.2.22 Score per residue for model 22

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



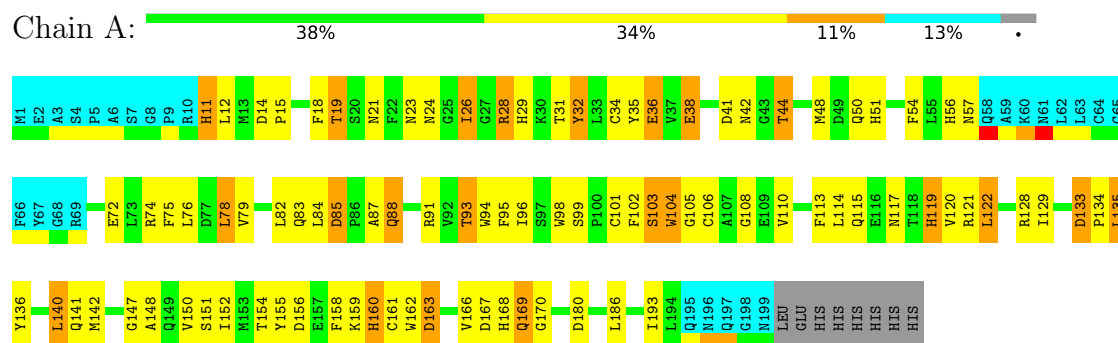
4.2.23 Score per residue for model 23

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



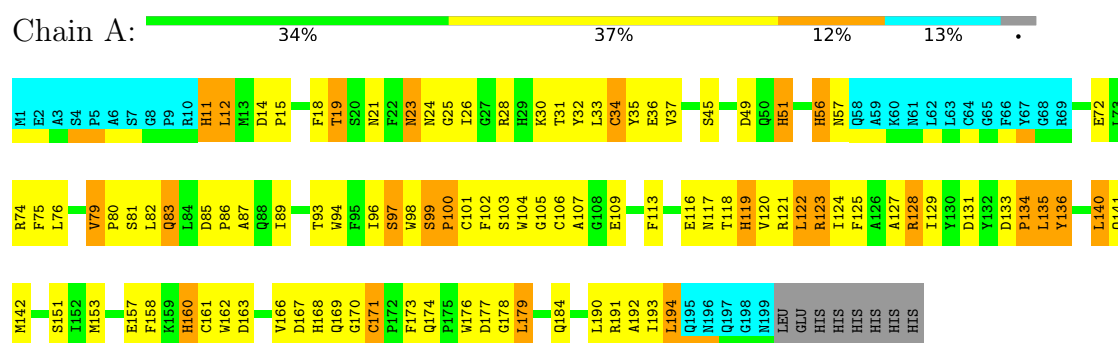
4.2.24 Score per residue for model 24

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



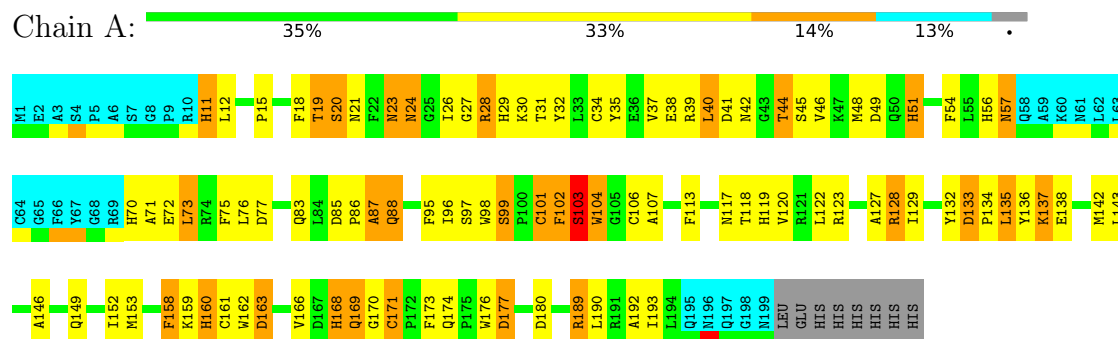
4.2.25 Score per residue for model 25

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



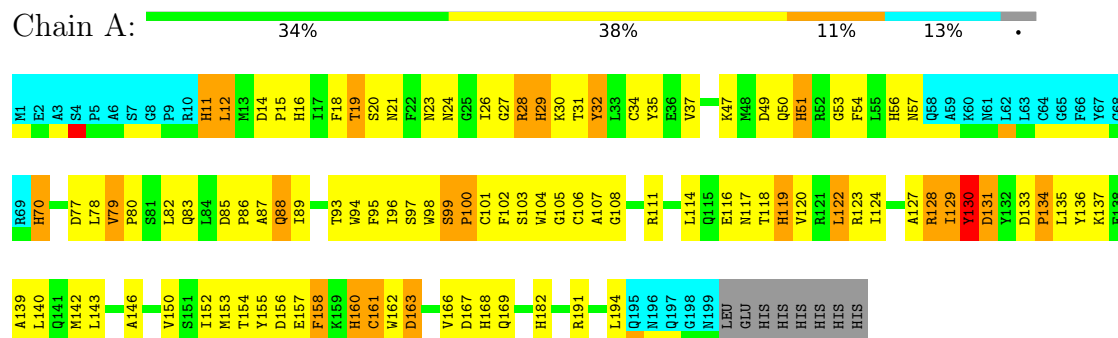
4.2.26 Score per residue for model 26

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



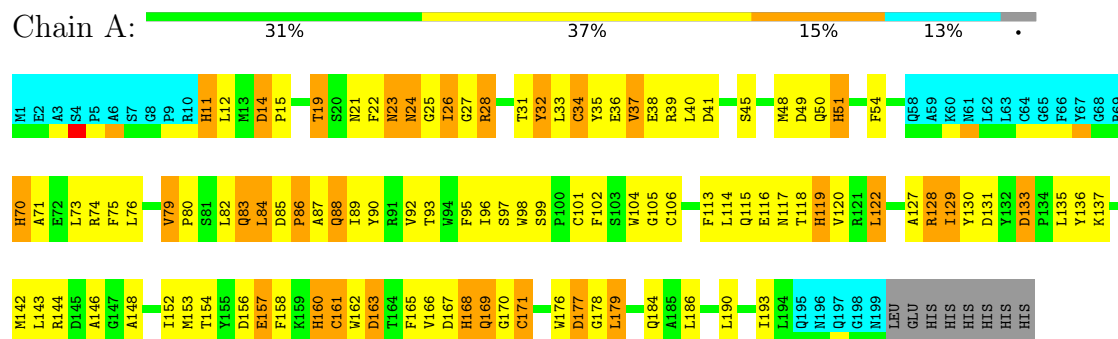
4.2.27 Score per residue for model 27

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



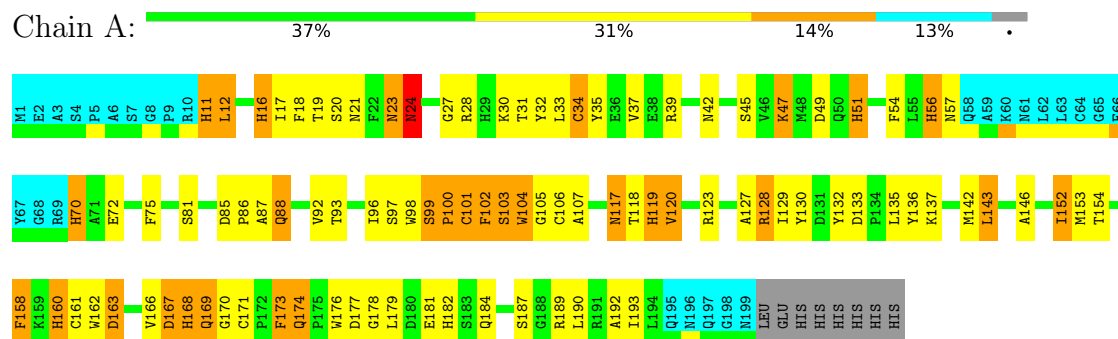
4.2.28 Score per residue for model 28

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



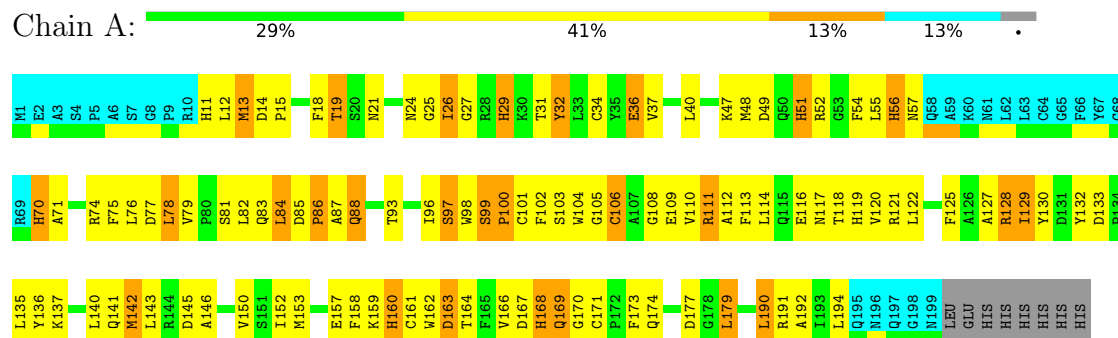
4.2.29 Score per residue for model 29

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



4.2.30 Score per residue for model 30

- Molecule 1: Probable DNA dC->dU-editing enzyme APOBEC-3A



5 Refinement protocol and experimental data overview

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

Of the 512 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	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	1851
Number of shifts mapped to atoms	1851
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	67%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	0.63±0.00	0±0/1466 (0.0± 0.0%)	1.10±0.01	0±0/1991 (0.0± 0.0%)
All	All	0.63	0/43980 (0.0%)	1.10	1/59730 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	HIS	CA-CB-CG	-6.64	107.16	113.80	17	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1421	1343	1343	94±10
All	All	42660	40290	40290	2834

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:HD13	1:A:79:VAL:N	0.87	1.82	30	1
1:A:12:LEU:H	1:A:12:LEU:HD22	0.83	1.33	20	2
1:A:12:LEU:HD23	1:A:12:LEU:N	0.83	1.89	25	3
1:A:12:LEU:HD22	1:A:12:LEU:N	0.81	1.90	12	14
1:A:31:THR:HG1	1:A:98:TRP:CD1	0.81	1.93	25	1
1:A:168:HIS:HD1	1:A:171:CYS:C	0.80	1.85	21	1
1:A:103:SER:O	1:A:107:ALA:HB3	0.79	1.78	22	19
1:A:140:LEU:HD11	1:A:190:LEU:HD21	0.78	1.53	18	1
1:A:78:LEU:HD22	1:A:78:LEU:O	0.78	1.77	30	1
1:A:11:HIS:C	1:A:12:LEU:HD23	0.77	2.05	17	3
1:A:12:LEU:HD12	1:A:166:VAL:O	0.75	1.82	17	2
1:A:78:LEU:HD23	1:A:79:VAL:N	0.75	1.97	1	2
1:A:55:LEU:N	1:A:55:LEU:HD23	0.74	1.97	30	1
1:A:31:THR:HG22	1:A:98:TRP:CD2	0.73	2.18	19	16
1:A:51:HIS:NE2	1:A:82:LEU:HD22	0.73	1.98	12	11
1:A:106:CYS:O	1:A:110:VAL:HG23	0.73	1.82	22	5
1:A:70:HIS:CE1	1:A:73:LEU:HD11	0.72	2.20	3	1
1:A:153:MET:HE2	1:A:157:GLU:CD	0.72	2.10	23	1
1:A:55:LEU:H	1:A:55:LEU:HD12	0.71	1.45	10	1
1:A:51:HIS:NE2	1:A:82:LEU:HD12	0.71	1.99	28	2
1:A:12:LEU:HD22	1:A:12:LEU:H	0.71	1.45	9	5
1:A:11:HIS:C	1:A:12:LEU:HD13	0.71	2.11	12	1
1:A:75:PHE:O	1:A:78:LEU:HD12	0.71	1.84	30	1
1:A:99:SER:OG	1:A:129:ILE:HG23	0.70	1.86	21	3
1:A:117:ASN:O	1:A:120:VAL:HG22	0.70	1.85	16	8
1:A:51:HIS:HE2	1:A:82:LEU:HD22	0.70	1.47	27	6
1:A:129:ILE:HD13	1:A:129:ILE:N	0.70	2.01	22	1
1:A:103:SER:OG	1:A:139:ALA:HB2	0.69	1.86	18	4
1:A:33:LEU:C	1:A:33:LEU:HD13	0.69	2.13	18	3
1:A:55:LEU:HD12	1:A:55:LEU:N	0.68	2.03	10	1
1:A:89:ILE:HD12	1:A:89:ILE:N	0.68	2.04	27	3
1:A:28:ARG:HE	1:A:28:ARG:H	0.67	1.32	5	2
1:A:119:HIS:CD2	1:A:120:VAL:HG23	0.67	2.24	5	5
1:A:37:VAL:HG11	1:A:51:HIS:CE1	0.66	2.24	1	12
1:A:37:VAL:HG21	1:A:51:HIS:ND1	0.66	2.05	27	11
1:A:78:LEU:C	1:A:78:LEU:HD12	0.66	2.16	6	11
1:A:26:ILE:HD12	1:A:98:TRP:NE1	0.66	2.06	4	1
1:A:70:HIS:CD2	1:A:70:HIS:N	0.66	2.64	10	15
1:A:28:ARG:NE	1:A:28:ARG:H	0.65	1.88	28	2
1:A:38:GLU:OE2	1:A:40:LEU:HD12	0.65	1.92	26	1
1:A:168:HIS:CD2	1:A:170:GLY:H	0.65	2.10	19	25
1:A:31:THR:HG22	1:A:98:TRP:CG	0.65	2.26	6	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:C	1:A:33:LEU:HD23	0.65	2.17	7	11
1:A:101:CYS:SG	1:A:102:PHE:N	0.65	2.69	16	14
1:A:82:LEU:HD22	1:A:82:LEU:N	0.65	2.06	10	4
1:A:46:VAL:HG23	1:A:46:VAL:O	0.65	1.92	26	4
1:A:12:LEU:HD12	1:A:166:VAL:C	0.65	2.16	27	4
1:A:12:LEU:N	1:A:12:LEU:HD12	0.64	2.08	8	8
1:A:78:LEU:HD13	1:A:78:LEU:C	0.64	2.16	30	1
1:A:162:TRP:CD1	1:A:163:ASP:N	0.64	2.65	15	28
1:A:28:ARG:HE	1:A:29:HIS:N	0.64	1.91	24	1
1:A:78:LEU:HD22	1:A:78:LEU:C	0.64	2.18	30	1
1:A:88:GLN:NE2	1:A:88:GLN:N	0.64	2.46	13	11
1:A:160:HIS:ND1	1:A:161:CYS:N	0.64	2.45	3	2
1:A:70:HIS:CD2	1:A:70:HIS:H	0.64	2.10	8	12
1:A:70:HIS:CE1	1:A:73:LEU:HD13	0.63	2.28	22	1
1:A:168:HIS:CD2	1:A:169:GLN:N	0.63	2.66	14	22
1:A:56:HIS:C	1:A:71:ALA:HB2	0.63	2.18	13	5
1:A:78:LEU:HD23	1:A:78:LEU:C	0.63	2.18	1	1
1:A:26:ILE:HD11	1:A:98:TRP:HE1	0.63	1.54	24	1
1:A:88:GLN:NE2	1:A:88:GLN:H	0.63	1.92	20	7
1:A:168:HIS:ND1	1:A:171:CYS:N	0.63	2.47	21	17
1:A:150:VAL:O	1:A:150:VAL:HG13	0.63	1.94	15	4
1:A:117:ASN:ND2	1:A:119:HIS:CD2	0.63	2.67	8	1
1:A:35:TYR:CG	1:A:75:PHE:CE1	0.62	2.87	16	14
1:A:136:TYR:CD1	1:A:137:LYS:N	0.62	2.67	4	7
1:A:21:ASN:ND2	1:A:32:TYR:CG	0.62	2.67	27	5
1:A:21:ASN:ND2	1:A:32:TYR:CE1	0.62	2.67	4	12
1:A:12:LEU:N	1:A:12:LEU:CD2	0.62	2.59	25	17
1:A:28:ARG:HE	1:A:28:ARG:N	0.62	1.93	5	2
1:A:21:ASN:ND2	1:A:32:TYR:CD1	0.62	2.68	15	11
1:A:28:ARG:NH2	1:A:29:HIS:ND1	0.62	2.48	24	1
1:A:160:HIS:CD2	1:A:161:CYS:N	0.62	2.67	16	14
1:A:78:LEU:C	1:A:78:LEU:HD23	0.62	2.20	24	1
1:A:91:ARG:NH1	1:A:123:ARG:NH2	0.62	2.48	4	1
1:A:160:HIS:CG	1:A:161:CYS:N	0.61	2.67	9	26
1:A:182:HIS:ND1	1:A:183:SER:N	0.61	2.48	15	3
1:A:21:ASN:ND2	1:A:22:PHE:CD2	0.61	2.68	18	2
1:A:11:HIS:N	1:A:11:HIS:CD2	0.61	2.67	17	4
1:A:98:TRP:CZ3	1:A:130:TYR:CD2	0.61	2.89	2	1
1:A:76:LEU:O	1:A:79:VAL:HG23	0.60	1.96	2	1
1:A:36:GLU:OE1	1:A:164:THR:HG21	0.60	1.96	19	3
1:A:36:GLU:OE2	1:A:164:THR:HG21	0.60	1.96	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:ILE:HD12	1:A:89:ILE:H	0.60	1.56	7	3
1:A:51:HIS:CD2	1:A:82:LEU:HD12	0.60	2.31	28	2
1:A:28:ARG:HE	1:A:29:HIS:H	0.60	1.39	24	1
1:A:98:TRP:CZ3	1:A:130:TYR:CG	0.60	2.90	2	1
1:A:25:GLY:H	1:A:128:ARG:NH1	0.60	1.94	22	3
1:A:28:ARG:H	1:A:28:ARG:NE	0.60	1.93	5	2
1:A:37:VAL:HG21	1:A:51:HIS:CE1	0.60	2.32	14	13
1:A:29:HIS:N	1:A:29:HIS:ND1	0.60	2.47	9	3
1:A:95:PHE:CE1	1:A:161:CYS:SG	0.59	2.96	1	3
1:A:120:VAL:O	1:A:120:VAL:HG13	0.59	1.96	2	2
1:A:33:LEU:HD22	1:A:72:GLU:OE2	0.59	1.97	5	3
1:A:136:TYR:CG	1:A:137:LYS:N	0.59	2.70	29	7
1:A:28:ARG:HH12	1:A:29:HIS:CE1	0.59	2.16	8	1
1:A:79:VAL:N	1:A:80:PRO:CD	0.59	2.65	23	20
1:A:13:MET:SD	1:A:54:PHE:CE2	0.59	2.96	17	2
1:A:153:MET:SD	1:A:158:PHE:CE2	0.59	2.96	4	14
1:A:153:MET:SD	1:A:158:PHE:CZ	0.59	2.96	19	17
1:A:117:ASN:O	1:A:120:VAL:HG12	0.59	1.97	11	8
1:A:51:HIS:NE2	1:A:82:LEU:HD13	0.59	2.12	4	1
1:A:35:TYR:CD2	1:A:75:PHE:CE1	0.59	2.91	16	4
1:A:95:PHE:CD1	1:A:161:CYS:SG	0.59	2.96	16	2
1:A:13:MET:SD	1:A:54:PHE:CZ	0.59	2.96	20	1
1:A:34:CYS:SG	1:A:165:PHE:CE1	0.59	2.95	28	1
1:A:95:PHE:CZ	1:A:161:CYS:SG	0.59	2.96	15	6
1:A:34:CYS:SG	1:A:165:PHE:CG	0.59	2.96	2	2
1:A:95:PHE:CG	1:A:161:CYS:SG	0.59	2.96	16	5
1:A:21:ASN:ND2	1:A:32:TYR:CD2	0.59	2.71	25	3
1:A:42:ASN:N	1:A:42:ASN:HD22	0.59	1.95	7	1
1:A:153:MET:SD	1:A:158:PHE:CE1	0.58	2.95	21	8
1:A:78:LEU:HD23	1:A:81:SER:OG	0.58	1.98	15	1
1:A:28:ARG:NE	1:A:28:ARG:N	0.58	2.52	18	2
1:A:153:MET:SD	1:A:158:PHE:CD1	0.58	2.96	22	2
1:A:28:ARG:N	1:A:28:ARG:HE	0.58	1.95	28	1
1:A:24:ASN:ND2	1:A:176:TRP:CE2	0.58	2.70	29	1
1:A:95:PHE:CE2	1:A:161:CYS:SG	0.58	2.96	27	8
1:A:23:ASN:H	1:A:23:ASN:HD22	0.58	1.40	26	1
1:A:51:HIS:CE1	1:A:82:LEU:HD21	0.58	2.32	30	1
1:A:55:LEU:N	1:A:55:LEU:CD2	0.58	2.66	30	1
1:A:26:ILE:HD12	1:A:98:TRP:HE1	0.58	1.57	4	1
1:A:98:TRP:CZ3	1:A:130:TYR:CD1	0.58	2.91	29	2
1:A:136:TYR:OH	1:A:193:ILE:HD11	0.58	1.98	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ARG:NE	1:A:29:HIS:ND1	0.58	2.51	24	1
1:A:168:HIS:O	1:A:170:GLY:N	0.58	2.37	10	25
1:A:52:ARG:H	1:A:52:ARG:CD	0.58	2.11	10	1
1:A:51:HIS:CE1	1:A:82:LEU:HD22	0.58	2.34	22	1
1:A:158:PHE:CE1	1:A:173:PHE:CE2	0.57	2.91	12	1
1:A:51:HIS:CE1	1:A:82:LEU:HD13	0.57	2.34	14	2
1:A:23:ASN:HD22	1:A:23:ASN:N	0.57	1.97	26	1
1:A:121:ARG:NH1	1:A:149:GLN:NE2	0.57	2.52	6	1
1:A:111:ARG:HH22	1:A:142:MET:HE3	0.57	1.60	12	1
1:A:29:HIS:H	1:A:29:HIS:CD2	0.57	2.18	15	1
1:A:107:ALA:HB1	1:A:143:LEU:HD13	0.57	1.75	10	2
1:A:16:HIS:CG	1:A:17:ILE:N	0.57	2.72	11	4
1:A:176:TRP:HE1	1:A:182:HIS:CD2	0.57	2.18	23	2
1:A:56:HIS:CD2	1:A:56:HIS:N	0.57	2.73	25	5
1:A:95:PHE:CD2	1:A:161:CYS:SG	0.57	2.98	14	9
1:A:182:HIS:C	1:A:182:HIS:ND1	0.57	2.62	1	2
1:A:168:HIS:CE1	1:A:170:GLY:CA	0.57	2.88	2	13
1:A:176:TRP:CE2	1:A:179:LEU:CD2	0.57	2.87	4	1
1:A:119:HIS:NE2	1:A:120:VAL:HG23	0.56	2.15	5	2
1:A:42:ASN:N	1:A:42:ASN:ND2	0.56	2.49	7	2
1:A:13:MET:SD	1:A:54:PHE:CE1	0.56	2.98	20	3
1:A:40:LEU:HD22	1:A:40:LEU:N	0.56	2.15	22	2
1:A:123:ARG:C	1:A:124:ILE:HD12	0.56	2.25	5	4
1:A:128:ARG:NH2	1:A:186:LEU:HD11	0.56	2.16	8	2
1:A:25:GLY:H	1:A:128:ARG:HH12	0.56	1.42	11	1
1:A:168:HIS:CD2	1:A:170:GLY:N	0.56	2.74	9	13
1:A:51:HIS:NE2	1:A:82:LEU:CD1	0.56	2.68	28	2
1:A:28:ARG:H	1:A:28:ARG:HE	0.56	1.41	18	2
1:A:16:HIS:CD2	1:A:16:HIS:C	0.56	2.83	23	4
1:A:153:MET:HE2	1:A:157:GLU:OE1	0.56	2.01	23	1
1:A:111:ARG:NH2	1:A:142:MET:CE	0.56	2.68	23	2
1:A:129:ILE:N	1:A:129:ILE:CD1	0.56	2.67	22	1
1:A:128:ARG:HE	1:A:128:ARG:CA	0.56	2.14	29	3
1:A:28:ARG:HE	1:A:28:ARG:CA	0.56	2.13	28	2
1:A:141:GLN:NE2	1:A:144:ARG:NH2	0.56	2.54	21	1
1:A:136:TYR:OH	1:A:193:ILE:HD12	0.56	2.01	15	2
1:A:158:PHE:CE1	1:A:173:PHE:CZ	0.56	2.94	23	1
1:A:12:LEU:HD23	1:A:166:VAL:N	0.55	2.16	5	1
1:A:89:ILE:N	1:A:89:ILE:CD1	0.55	2.69	27	2
1:A:12:LEU:N	1:A:12:LEU:CD1	0.55	2.70	8	3
1:A:102:PHE:O	1:A:105:GLY:N	0.55	2.40	3	28

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ASN:N	1:A:57:ASN:OD1	0.55	2.40	13	2
1:A:168:HIS:CG	1:A:171:CYS:H	0.55	2.20	5	10
1:A:56:HIS:ND1	1:A:56:HIS:N	0.55	2.55	22	2
1:A:111:ARG:CG	1:A:112:ALA:N	0.55	2.68	22	2
1:A:54:PHE:CD1	1:A:54:PHE:N	0.55	2.74	3	12
1:A:26:ILE:HD13	1:A:26:ILE:H	0.55	1.62	22	1
1:A:25:GLY:N	1:A:128:ARG:HH11	0.55	1.99	23	1
1:A:40:LEU:HD12	1:A:89:ILE:HG21	0.55	1.78	28	1
1:A:103:SER:O	1:A:108:GLY:N	0.55	2.40	24	10
1:A:57:ASN:HD21	1:A:70:HIS:CD2	0.55	2.19	17	1
1:A:28:ARG:N	1:A:28:ARG:CD	0.55	2.70	18	1
1:A:102:PHE:O	1:A:104:TRP:N	0.55	2.40	16	14
1:A:161:CYS:O	1:A:165:PHE:N	0.55	2.40	7	5
1:A:163:ASP:OD1	1:A:168:HIS:ND1	0.55	2.40	1	1
1:A:28:ARG:O	1:A:98:TRP:CZ2	0.55	2.60	4	8
1:A:25:GLY:H	1:A:128:ARG:NH2	0.55	2.00	14	1
1:A:176:TRP:NE1	1:A:179:LEU:CD1	0.55	2.69	17	1
1:A:167:ASP:C	1:A:169:GLN:N	0.54	2.64	12	12
1:A:88:GLN:H	1:A:88:GLN:CD	0.54	2.10	8	6
1:A:115:GLN:CD	1:A:115:GLN:N	0.54	2.62	9	1
1:A:115:GLN:N	1:A:115:GLN:OE1	0.54	2.40	22	1
1:A:111:ARG:O	1:A:115:GLN:NE2	0.54	2.40	9	1
1:A:152:ILE:CD1	1:A:190:LEU:HD12	0.54	2.32	18	1
1:A:12:LEU:HD21	1:A:52:ARG:NH2	0.54	2.17	5	1
1:A:166:VAL:O	1:A:168:HIS:ND1	0.54	2.40	27	3
1:A:168:HIS:C	1:A:170:GLY:N	0.54	2.65	26	27
1:A:101:CYS:O	1:A:103:SER:N	0.54	2.40	26	5
1:A:21:ASN:HD22	1:A:28:ARG:NH2	0.54	1.99	2	2
1:A:168:HIS:ND1	1:A:171:CYS:C	0.54	2.66	28	13
1:A:57:ASN:ND2	1:A:71:ALA:H	0.54	2.00	26	2
1:A:133:ASP:O	1:A:135:LEU:N	0.54	2.41	26	14
1:A:52:ARG:H	1:A:52:ARG:NE	0.54	1.99	10	1
1:A:182:HIS:ND1	1:A:182:HIS:C	0.54	2.65	15	3
1:A:24:ASN:N	1:A:128:ARG:HH21	0.54	2.01	9	1
1:A:119:HIS:CE1	1:A:120:VAL:CG1	0.54	2.90	12	3
1:A:40:LEU:N	1:A:40:LEU:CD2	0.54	2.71	30	2
1:A:97:SER:O	1:A:128:ARG:N	0.54	2.41	29	3
1:A:28:ARG:NE	1:A:29:HIS:H	0.54	2.01	24	1
1:A:34:CYS:SG	1:A:165:PHE:CZ	0.54	2.98	28	1
1:A:24:ASN:ND2	1:A:176:TRP:CZ2	0.54	2.76	29	1
1:A:162:TRP:CD1	1:A:162:TRP:C	0.54	2.86	22	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:PHE:CE1	1:A:157:GLU:OE1	0.54	2.61	12	1
1:A:84:LEU:HD11	1:A:90:TYR:CD1	0.53	2.38	13	1
1:A:173:PHE:CE2	1:A:174:GLN:O	0.53	2.61	4	2
1:A:54:PHE:O	1:A:55:LEU:HD12	0.53	2.02	1	1
1:A:128:ARG:HH21	1:A:186:LEU:HD11	0.53	1.62	8	1
1:A:85:ASP:O	1:A:87:ALA:N	0.53	2.42	30	7
1:A:76:LEU:O	1:A:78:LEU:N	0.53	2.42	16	1
1:A:129:ILE:HD11	1:A:186:LEU:HD12	0.53	1.81	22	1
1:A:11:HIS:O	1:A:11:HIS:CG	0.53	2.61	3	4
1:A:51:HIS:ND1	1:A:51:HIS:O	0.53	2.42	30	9
1:A:14:ASP:O	1:A:16:HIS:N	0.53	2.42	7	2
1:A:127:ALA:O	1:A:128:ARG:NH2	0.53	2.42	25	3
1:A:113:PHE:O	1:A:117:ASN:N	0.53	2.42	15	14
1:A:122:LEU:HD12	1:A:122:LEU:O	0.53	2.04	2	2
1:A:119:HIS:O	1:A:119:HIS:ND1	0.53	2.42	6	12
1:A:131:ASP:OD1	1:A:132:TYR:N	0.53	2.42	10	1
1:A:19:THR:O	1:A:23:ASN:N	0.53	2.42	12	11
1:A:21:ASN:HD21	1:A:32:TYR:CB	0.53	2.17	17	3
1:A:141:GLN:HE22	1:A:144:ARG:NH2	0.53	2.01	21	1
1:A:167:ASP:O	1:A:169:GLN:N	0.53	2.42	12	9
1:A:72:GLU:OE1	1:A:94:TRP:CZ3	0.53	2.62	2	1
1:A:173:PHE:CD1	1:A:173:PHE:O	0.53	2.62	5	2
1:A:143:LEU:HD12	1:A:148:ALA:HB3	0.53	1.81	9	2
1:A:11:HIS:CD2	1:A:11:HIS:O	0.53	2.62	30	2
1:A:88:GLN:N	1:A:88:GLN:CD	0.53	2.66	28	5
1:A:129:ILE:O	1:A:130:TYR:CD2	0.53	2.62	9	10
1:A:82:LEU:N	1:A:82:LEU:CD2	0.53	2.71	10	4
1:A:38:GLU:OE1	1:A:91:ARG:NH2	0.53	2.42	21	1
1:A:85:ASP:N	1:A:85:ASP:OD1	0.53	2.42	28	2
1:A:160:HIS:ND1	1:A:160:HIS:C	0.53	2.67	9	7
1:A:168:HIS:CG	1:A:170:GLY:H	0.53	2.23	19	22
1:A:35:TYR:C	1:A:35:TYR:CD1	0.53	2.87	24	9
1:A:28:ARG:N	1:A:28:ARG:NE	0.53	2.57	5	2
1:A:143:LEU:O	1:A:146:ALA:N	0.53	2.42	29	8
1:A:35:TYR:CE1	1:A:53:GLY:C	0.52	2.88	20	8
1:A:134:PRO:O	1:A:136:TYR:N	0.52	2.42	25	8
1:A:34:CYS:SG	1:A:165:PHE:CD1	0.52	3.02	2	2
1:A:88:GLN:O	1:A:119:HIS:CE1	0.52	2.62	29	1
1:A:21:ASN:OD1	1:A:32:TYR:CD1	0.52	2.62	6	4
1:A:134:PRO:C	1:A:136:TYR:N	0.52	2.67	12	13
1:A:162:TRP:CD1	1:A:163:ASP:OD1	0.52	2.62	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ILE:O	1:A:130:TYR:CD1	0.52	2.62	4	1
1:A:174:GLN:H	1:A:174:GLN:CD	0.52	2.13	7	1
1:A:125:PHE:CD1	1:A:157:GLU:OE1	0.52	2.62	21	3
1:A:24:ASN:HD22	1:A:128:ARG:NH1	0.52	2.03	15	1
1:A:163:ASP:CG	1:A:168:HIS:ND1	0.52	2.67	24	1
1:A:57:ASN:HA	1:A:71:ALA:HB2	0.52	1.80	2	1
1:A:119:HIS:O	1:A:119:HIS:CG	0.52	2.62	29	7
1:A:125:PHE:CE1	1:A:157:GLU:OE2	0.52	2.62	4	5
1:A:11:HIS:H	1:A:11:HIS:CD2	0.52	2.22	27	2
1:A:163:ASP:OD2	1:A:168:HIS:NE2	0.52	2.43	8	2
1:A:193:ILE:HG23	1:A:194:LEU:N	0.52	2.20	5	3
1:A:28:ARG:O	1:A:98:TRP:CH2	0.52	2.62	13	7
1:A:89:ILE:C	1:A:90:TYR:CD1	0.52	2.87	9	4
1:A:21:ASN:CG	1:A:32:TYR:CE1	0.52	2.88	29	3
1:A:168:HIS:ND1	1:A:171:CYS:O	0.52	2.42	11	3
1:A:129:ILE:O	1:A:130:TYR:CG	0.52	2.63	12	3
1:A:189:ARG:HE	1:A:189:ARG:CA	0.52	2.15	1	1
1:A:71:ALA:O	1:A:74:ARG:N	0.52	2.43	2	1
1:A:117:ASN:C	1:A:119:HIS:N	0.52	2.67	22	27
1:A:168:HIS:CE1	1:A:170:GLY:C	0.52	2.88	21	12
1:A:111:ARG:NH2	1:A:115:GLN:OE1	0.52	2.42	3	3
1:A:173:PHE:CE1	1:A:174:GLN:O	0.52	2.63	8	7
1:A:52:ARG:NH1	1:A:164:THR:HG21	0.52	2.18	6	1
1:A:168:HIS:O	1:A:171:CYS:N	0.52	2.42	22	2
1:A:22:PHE:O	1:A:128:ARG:NH2	0.52	2.42	16	1
1:A:29:HIS:O	1:A:29:HIS:CD2	0.52	2.62	24	2
1:A:168:HIS:CE1	1:A:171:CYS:O	0.52	2.62	6	1
1:A:21:ASN:OD1	1:A:32:TYR:CE1	0.52	2.62	29	3
1:A:72:GLU:OE2	1:A:94:TRP:CZ3	0.52	2.62	22	1
1:A:125:PHE:CE1	1:A:157:GLU:OE1	0.52	2.62	25	1
1:A:88:GLN:O	1:A:88:GLN:NE2	0.52	2.43	28	1
1:A:52:ARG:NH2	1:A:164:THR:O	0.52	2.42	1	2
1:A:36:GLU:OE1	1:A:37:VAL:N	0.52	2.43	13	7
1:A:56:HIS:CD2	1:A:56:HIS:H	0.52	2.23	3	1
1:A:87:ALA:C	1:A:88:GLN:NE2	0.52	2.67	5	8
1:A:156:ASP:OD1	1:A:156:ASP:N	0.52	2.42	12	1
1:A:168:HIS:CD2	1:A:169:GLN:H	0.52	2.22	15	3
1:A:28:ARG:NE	1:A:28:ARG:CA	0.52	2.73	21	1
1:A:117:ASN:O	1:A:119:HIS:N	0.52	2.43	12	11
1:A:48:MET:O	1:A:52:ARG:NE	0.52	2.43	6	1
1:A:52:ARG:NH1	1:A:164:THR:O	0.52	2.42	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:HIS:CG	1:A:30:LYS:N	0.52	2.75	16	1
1:A:26:ILE:N	1:A:26:ILE:CD1	0.52	2.73	22	1
1:A:28:ARG:O	1:A:29:HIS:CG	0.52	2.62	19	4
1:A:114:LEU:C	1:A:116:GLU:N	0.52	2.68	16	19
1:A:12:LEU:CD1	1:A:12:LEU:N	0.52	2.72	16	7
1:A:48:MET:O	1:A:52:ARG:NH2	0.52	2.42	3	2
1:A:173:PHE:CD2	1:A:173:PHE:O	0.52	2.62	3	6
1:A:31:THR:OG1	1:A:57:ASN:ND2	0.52	2.42	11	2
1:A:28:ARG:NH2	1:A:98:TRP:CE3	0.52	2.78	21	1
1:A:162:TRP:NE1	1:A:163:ASP:OD1	0.52	2.43	24	1
1:A:113:PHE:O	1:A:117:ASN:ND2	0.52	2.42	3	1
1:A:163:ASP:OD1	1:A:168:HIS:NE2	0.52	2.43	13	1
1:A:85:ASP:O	1:A:119:HIS:CE1	0.52	2.63	15	1
1:A:162:TRP:CE3	1:A:166:VAL:HG21	0.52	2.40	16	4
1:A:40:LEU:CD2	1:A:40:LEU:N	0.52	2.73	17	1
1:A:20:SER:O	1:A:23:ASN:ND2	0.52	2.43	26	1
1:A:166:VAL:C	1:A:168:HIS:H	0.52	2.13	30	26
1:A:28:ARG:NH1	1:A:29:HIS:CE1	0.52	2.77	8	1
1:A:12:LEU:H	1:A:12:LEU:CD2	0.52	2.14	20	2
1:A:87:ALA:O	1:A:88:GLN:NE2	0.52	2.43	27	3
1:A:162:TRP:CG	1:A:163:ASP:N	0.51	2.78	13	15
1:A:190:LEU:C	1:A:192:ALA:N	0.51	2.68	30	3
1:A:76:LEU:C	1:A:78:LEU:N	0.51	2.67	16	2
1:A:26:ILE:HD13	1:A:26:ILE:N	0.51	2.20	22	1
1:A:88:GLN:NE2	1:A:88:GLN:C	0.51	2.68	28	1
1:A:55:LEU:HD23	1:A:55:LEU:H	0.51	1.65	30	1
1:A:102:PHE:C	1:A:104:TRP:N	0.51	2.68	29	15
1:A:155:TYR:C	1:A:155:TYR:CD1	0.51	2.89	22	3
1:A:28:ARG:O	1:A:30:LYS:N	0.51	2.44	26	2
1:A:42:ASN:N	1:A:42:ASN:OD1	0.51	2.43	14	1
1:A:49:ASP:OD1	1:A:49:ASP:N	0.51	2.44	23	2
1:A:26:ILE:CD1	1:A:98:TRP:HE1	0.51	2.18	24	2
1:A:111:ARG:NH2	1:A:142:MET:HE3	0.51	2.20	12	1
1:A:16:HIS:CE1	1:A:20:SER:OG	0.51	2.64	17	1
1:A:163:ASP:OD1	1:A:168:HIS:CD2	0.51	2.63	18	1
1:A:70:HIS:C	1:A:72:GLU:N	0.51	2.67	23	2
1:A:28:ARG:NE	1:A:29:HIS:N	0.51	2.58	24	1
1:A:193:ILE:N	1:A:193:ILE:HD12	0.51	2.19	12	16
1:A:57:ASN:CA	1:A:71:ALA:HB2	0.51	2.34	2	1
1:A:33:LEU:HD23	1:A:34:CYS:N	0.51	2.21	28	10
1:A:117:ASN:OD1	1:A:119:HIS:CD2	0.51	2.62	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ARG:CD	1:A:28:ARG:N	0.51	2.73	26	2
1:A:119:HIS:CE1	1:A:120:VAL:CG2	0.51	2.93	10	5
1:A:57:ASN:ND2	1:A:57:ASN:C	0.51	2.68	1	3
1:A:70:HIS:CE1	1:A:73:LEU:CD1	0.51	2.94	11	1
1:A:91:ARG:NH2	1:A:123:ARG:CZ	0.51	2.74	13	1
1:A:56:HIS:N	1:A:56:HIS:ND1	0.51	2.59	30	2
1:A:11:HIS:O	1:A:52:ARG:NH2	0.51	2.43	18	1
1:A:13:MET:SD	1:A:165:PHE:O	0.51	2.69	21	7
1:A:21:ASN:ND2	1:A:22:PHE:CE2	0.51	2.79	3	2
1:A:24:ASN:OD1	1:A:128:ARG:NH1	0.51	2.44	23	2
1:A:26:ILE:C	1:A:26:ILE:HD12	0.51	2.30	21	9
1:A:39:ARG:NH1	1:A:41:ASP:OD2	0.51	2.42	20	2
1:A:122:LEU:HD13	1:A:123:ARG:N	0.51	2.21	23	10
1:A:76:LEU:HD22	1:A:109:GLU:OE1	0.51	2.06	6	1
1:A:88:GLN:CD	1:A:88:GLN:N	0.51	2.68	8	3
1:A:56:HIS:CE1	1:A:74:ARG:HH22	0.51	2.24	11	1
1:A:176:TRP:NE1	1:A:179:LEU:HD12	0.51	2.20	23	1
1:A:174:GLN:CD	1:A:174:GLN:N	0.50	2.68	20	2
1:A:132:TYR:CD2	1:A:133:ASP:OD1	0.50	2.64	20	1
1:A:152:ILE:HD11	1:A:190:LEU:HD22	0.50	1.83	8	1
1:A:88:GLN:N	1:A:88:GLN:HE21	0.50	2.04	17	3
1:A:25:GLY:N	1:A:128:ARG:NH1	0.50	2.59	23	2
1:A:94:TRP:CD1	1:A:94:TRP:N	0.50	2.78	23	1
1:A:35:TYR:CD1	1:A:35:TYR:C	0.50	2.90	7	9
1:A:140:LEU:HD23	1:A:140:LEU:O	0.50	2.06	24	4
1:A:177:ASP:N	1:A:177:ASP:OD1	0.50	2.42	9	4
1:A:35:TYR:CE2	1:A:53:GLY:C	0.50	2.89	2	4
1:A:91:ARG:HH21	1:A:123:ARG:CZ	0.50	2.20	13	1
1:A:13:MET:SD	1:A:13:MET:N	0.50	2.84	20	1
1:A:136:TYR:CD1	1:A:136:TYR:C	0.50	2.88	9	8
1:A:12:LEU:N	1:A:12:LEU:HD13	0.50	2.21	12	2
1:A:28:ARG:CZ	1:A:29:HIS:ND1	0.50	2.74	24	1
1:A:80:PRO:C	1:A:82:LEU:N	0.50	2.69	11	5
1:A:140:LEU:CD2	1:A:190:LEU:HD21	0.50	2.36	13	1
1:A:11:HIS:CD2	1:A:11:HIS:H	0.50	2.25	30	2
1:A:14:ASP:OD1	1:A:14:ASP:N	0.50	2.44	14	6
1:A:103:SER:O	1:A:142:MET:SD	0.50	2.70	2	5
1:A:33:LEU:C	1:A:33:LEU:CD1	0.50	2.84	18	3
1:A:155:TYR:O	1:A:155:TYR:CD1	0.50	2.65	18	1
1:A:37:VAL:CG2	1:A:51:HIS:ND1	0.50	2.74	27	8
1:A:88:GLN:N	1:A:88:GLN:NE2	0.50	2.60	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:PHE:C	1:A:75:PHE:CD1	0.50	2.90	3	1
1:A:189:ARG:O	1:A:192:ALA:HB3	0.50	2.06	4	6
1:A:101:CYS:O	1:A:102:PHE:C	0.50	2.55	16	9
1:A:111:ARG:O	1:A:114:LEU:N	0.50	2.45	22	2
1:A:38:GLU:OE1	1:A:91:ARG:NH1	0.50	2.44	24	1
1:A:98:TRP:CH2	1:A:130:TYR:CD1	0.50	3.00	29	1
1:A:97:SER:O	1:A:128:ARG:CB	0.49	2.60	15	25
1:A:173:PHE:CD1	1:A:173:PHE:C	0.49	2.88	5	2
1:A:72:GLU:OE1	1:A:106:CYS:SG	0.49	2.70	9	2
1:A:52:ARG:C	1:A:52:ARG:HE	0.49	2.15	9	1
1:A:153:MET:SD	1:A:158:PHE:CD2	0.49	3.05	14	1
1:A:40:LEU:N	1:A:40:LEU:HD22	0.49	2.21	17	1
1:A:123:ARG:NH1	1:A:149:GLN:OE1	0.49	2.46	26	2
1:A:111:ARG:C	1:A:115:GLN:HE21	0.49	2.14	9	1
1:A:180:ASP:CG	1:A:181:GLU:N	0.49	2.70	13	2
1:A:72:GLU:OE2	1:A:106:CYS:SG	0.49	2.70	14	2
1:A:28:ARG:C	1:A:29:HIS:ND1	0.49	2.71	19	1
1:A:117:ASN:C	1:A:119:HIS:H	0.49	2.16	2	25
1:A:20:SER:OG	1:A:21:ASN:N	0.49	2.42	3	1
1:A:28:ARG:H	1:A:28:ARG:CD	0.49	2.21	28	3
1:A:16:HIS:CD2	1:A:17:ILE:HG23	0.49	2.42	11	1
1:A:95:PHE:CE1	1:A:125:PHE:CD2	0.49	3.01	16	1
1:A:167:ASP:OD1	1:A:167:ASP:N	0.49	2.43	16	1
1:A:179:LEU:HD23	1:A:179:LEU:O	0.49	2.08	16	3
1:A:141:GLN:OE1	1:A:144:ARG:NH1	0.49	2.45	17	1
1:A:103:SER:OG	1:A:142:MET:SD	0.49	2.70	19	3
1:A:157:GLU:O	1:A:161:CYS:SG	0.49	2.70	1	1
1:A:173:PHE:O	1:A:173:PHE:CG	0.49	2.63	8	1
1:A:182:HIS:CG	1:A:183:SER:N	0.49	2.79	15	2
1:A:133:ASP:C	1:A:135:LEU:H	0.49	2.15	22	19
1:A:168:HIS:CG	1:A:169:GLN:N	0.49	2.81	27	10
1:A:152:ILE:HD12	1:A:152:ILE:N	0.49	2.23	13	3
1:A:186:LEU:HD12	1:A:186:LEU:N	0.49	2.23	24	1
1:A:11:HIS:CD2	1:A:11:HIS:N	0.49	2.79	27	4
1:A:94:TRP:CD1	1:A:122:LEU:HD21	0.49	2.43	27	4
1:A:89:ILE:HG23	1:A:119:HIS:O	0.49	2.08	15	1
1:A:85:ASP:C	1:A:87:ALA:N	0.49	2.71	30	11
1:A:168:HIS:C	1:A:170:GLY:H	0.49	2.16	23	24
1:A:168:HIS:NE2	1:A:170:GLY:N	0.49	2.61	9	13
1:A:82:LEU:O	1:A:83:GLN:CB	0.49	2.61	5	5
1:A:128:ARG:HH21	1:A:186:LEU:CG	0.49	2.21	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ARG:NH2	1:A:98:TRP:CD2	0.49	2.81	21	1
1:A:12:LEU:HD21	1:A:52:ARG:HH22	0.48	1.67	5	2
1:A:37:VAL:CB	1:A:51:HIS:ND1	0.48	2.76	27	9
1:A:70:HIS:CD2	1:A:70:HIS:O	0.48	2.66	19	2
1:A:190:LEU:O	1:A:192:ALA:N	0.48	2.46	15	3
1:A:163:ASP:CG	1:A:168:HIS:CG	0.48	2.91	24	1
1:A:23:ASN:O	1:A:25:GLY:N	0.48	2.46	28	1
1:A:18:PHE:C	1:A:18:PHE:CD1	0.48	2.91	8	9
1:A:38:GLU:OE2	1:A:91:ARG:NE	0.48	2.46	9	1
1:A:25:GLY:N	1:A:128:ARG:HE	0.48	2.07	12	1
1:A:186:LEU:CD2	1:A:186:LEU:N	0.48	2.76	16	1
1:A:152:ILE:HG21	1:A:187:SER:OG	0.48	2.09	29	1
1:A:35:TYR:CD1	1:A:35:TYR:O	0.48	2.66	18	6
1:A:114:LEU:O	1:A:117:ASN:N	0.48	2.46	8	3
1:A:152:ILE:CD1	1:A:152:ILE:N	0.48	2.77	24	2
1:A:152:ILE:N	1:A:152:ILE:HD12	0.48	2.24	24	1
1:A:167:ASP:C	1:A:169:GLN:H	0.48	2.16	4	12
1:A:78:LEU:C	1:A:78:LEU:CD1	0.48	2.87	17	12
1:A:117:ASN:O	1:A:120:VAL:N	0.48	2.46	25	3
1:A:182:HIS:O	1:A:185:ALA:N	0.48	2.47	22	1
1:A:70:HIS:O	1:A:73:LEU:N	0.48	2.46	28	1
1:A:85:ASP:O	1:A:88:GLN:NE2	0.48	2.46	28	1
1:A:33:LEU:C	1:A:33:LEU:CD2	0.48	2.87	7	11
1:A:86:PRO:C	1:A:88:GLN:N	0.48	2.70	6	5
1:A:152:ILE:HG23	1:A:152:ILE:O	0.48	2.08	6	2
1:A:176:TRP:C	1:A:176:TRP:CD1	0.48	2.91	26	1
1:A:180:ASP:OD1	1:A:180:ASP:N	0.48	2.46	12	6
1:A:33:LEU:HD13	1:A:33:LEU:O	0.48	2.08	9	1
1:A:173:PHE:O	1:A:174:GLN:NE2	0.48	2.46	14	1
1:A:87:ALA:C	1:A:88:GLN:HE21	0.48	2.16	15	2
1:A:186:LEU:N	1:A:186:LEU:HD22	0.48	2.23	16	1
1:A:23:ASN:CG	1:A:24:ASN:N	0.48	2.69	21	2
1:A:119:HIS:CD2	1:A:119:HIS:C	0.48	2.89	2	7
1:A:72:GLU:H	1:A:72:GLU:CD	0.48	2.16	10	3
1:A:75:PHE:CD1	1:A:75:PHE:C	0.48	2.92	9	3
1:A:39:ARG:HH12	1:A:88:GLN:CB	0.48	2.22	29	1
1:A:34:CYS:SG	1:A:165:PHE:CD2	0.48	3.07	2	2
1:A:176:TRP:NE1	1:A:179:LEU:CD2	0.48	2.77	4	1
1:A:162:TRP:CD1	1:A:173:PHE:N	0.48	2.81	6	1
1:A:103:SER:OG	1:A:142:MET:CB	0.48	2.62	15	1
1:A:70:HIS:NE2	1:A:73:LEU:CD1	0.48	2.77	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:PRO:C	1:A:136:TYR:H	0.48	2.17	27	11
1:A:14:ASP:C	1:A:16:HIS:N	0.48	2.70	11	2
1:A:72:GLU:CD	1:A:106:CYS:SG	0.48	2.97	14	2
1:A:22:PHE:C	1:A:24:ASN:N	0.47	2.72	10	1
1:A:31:THR:HG22	1:A:57:ASN:CG	0.47	2.33	13	2
1:A:28:ARG:HH21	1:A:98:TRP:HE1	0.47	1.52	26	1
1:A:88:GLN:O	1:A:119:HIS:ND1	0.47	2.46	29	1
1:A:133:ASP:C	1:A:135:LEU:N	0.47	2.72	9	13
1:A:20:SER:C	1:A:22:PHE:N	0.47	2.73	11	1
1:A:25:GLY:H	1:A:128:ARG:HE	0.47	1.50	12	1
1:A:168:HIS:ND1	1:A:168:HIS:N	0.47	2.63	17	1
1:A:125:PHE:CZ	1:A:157:GLU:OE1	0.47	2.67	25	1
1:A:30:LYS:O	1:A:30:LYS:CG	0.47	2.62	26	1
1:A:176:TRP:O	1:A:178:GLY:N	0.47	2.47	28	4
1:A:16:HIS:C	1:A:16:HIS:ND1	0.47	2.67	11	1
1:A:82:LEU:C	1:A:84:LEU:N	0.47	2.72	13	1
1:A:28:ARG:CD	1:A:28:ARG:C	0.47	2.87	21	1
1:A:114:LEU:O	1:A:118:THR:HG23	0.47	2.09	8	1
1:A:128:ARG:HH21	1:A:186:LEU:CD1	0.47	2.22	8	1
1:A:143:LEU:CD1	1:A:148:ALA:HB3	0.47	2.39	23	1
1:A:29:HIS:O	1:A:29:HIS:CG	0.47	2.67	24	1
1:A:127:ALA:C	1:A:128:ARG:HH21	0.47	2.17	29	3
1:A:40:LEU:HD12	1:A:89:ILE:CG2	0.47	2.39	28	1
1:A:78:LEU:C	1:A:78:LEU:CD2	0.47	2.86	24	2
1:A:131:ASP:N	1:A:131:ASP:OD1	0.47	2.43	2	1
1:A:171:CYS:O	1:A:171:CYS:SG	0.47	2.70	25	1
1:A:28:ARG:O	1:A:29:HIS:CD2	0.47	2.67	27	1
1:A:86:PRO:O	1:A:88:GLN:N	0.47	2.47	6	1
1:A:95:PHE:CD1	1:A:153:MET:HE3	0.47	2.44	8	1
1:A:105:GLY:O	1:A:109:GLU:CG	0.47	2.62	8	2
1:A:52:ARG:CD	1:A:52:ARG:N	0.47	2.77	10	1
1:A:158:PHE:CE1	1:A:173:PHE:CD2	0.47	3.03	12	1
1:A:21:ASN:OD1	1:A:32:TYR:CZ	0.47	2.68	23	1
1:A:123:ARG:NH1	1:A:149:GLN:NE2	0.47	2.63	26	1
1:A:16:HIS:ND1	1:A:16:HIS:C	0.47	2.69	29	1
1:A:75:PHE:O	1:A:75:PHE:CD1	0.47	2.67	30	1
1:A:85:ASP:C	1:A:87:ALA:H	0.47	2.18	28	7
1:A:72:GLU:CD	1:A:72:GLU:N	0.47	2.73	10	3
1:A:163:ASP:N	1:A:163:ASP:OD1	0.47	2.48	4	1
1:A:70:HIS:ND1	1:A:73:LEU:HD13	0.47	2.24	8	1
1:A:49:ASP:O	1:A:52:ARG:NH2	0.47	2.48	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:PHE:O	1:A:173:PHE:CD2	0.47	2.67	8	1
1:A:176:TRP:CD1	1:A:179:LEU:H	0.47	2.28	8	1
1:A:92:VAL:CG1	1:A:122:LEU:HD22	0.47	2.40	15	1
1:A:31:THR:CG2	1:A:57:ASN:ND2	0.47	2.78	17	1
1:A:21:ASN:ND2	1:A:28:ARG:NH1	0.46	2.63	2	1
1:A:167:ASP:O	1:A:168:HIS:C	0.46	2.58	9	14
1:A:114:LEU:O	1:A:116:GLU:N	0.46	2.48	6	12
1:A:48:MET:O	1:A:52:ARG:NH1	0.46	2.48	21	2
1:A:141:GLN:HE22	1:A:144:ARG:HH22	0.46	1.52	21	1
1:A:128:ARG:CA	1:A:128:ARG:NE	0.46	2.78	25	3
1:A:143:LEU:O	1:A:146:ALA:HB3	0.46	2.10	1	4
1:A:193:ILE:N	1:A:193:ILE:CD1	0.46	2.79	19	12
1:A:103:SER:OG	1:A:139:ALA:CB	0.46	2.62	3	2
1:A:121:ARG:NH1	1:A:149:GLN:HE21	0.46	2.06	6	1
1:A:167:ASP:CG	1:A:167:ASP:O	0.46	2.58	7	2
1:A:80:PRO:C	1:A:82:LEU:H	0.46	2.18	11	1
1:A:37:VAL:HG11	1:A:51:HIS:ND1	0.46	2.25	1	6
1:A:24:ASN:HD21	1:A:182:HIS:CD2	0.46	2.28	13	1
1:A:38:GLU:N	1:A:38:GLU:OE2	0.46	2.48	18	1
1:A:25:GLY:H	1:A:128:ARG:HH11	0.46	1.54	23	1
1:A:46:VAL:O	1:A:46:VAL:CG2	0.46	2.63	26	2
1:A:157:GLU:N	1:A:157:GLU:CD	0.46	2.73	19	2
1:A:39:ARG:HH22	1:A:88:GLN:CD	0.46	2.19	11	1
1:A:23:ASN:CG	1:A:24:ASN:H	0.46	2.18	21	1
1:A:124:ILE:HD12	1:A:143:LEU:HD21	0.46	1.86	18	1
1:A:29:HIS:ND1	1:A:29:HIS:N	0.46	2.64	4	2
1:A:89:ILE:O	1:A:90:TYR:CD1	0.46	2.69	13	1
1:A:111:ARG:NH1	1:A:115:GLN:NE2	0.46	2.64	14	1
1:A:124:ILE:HD12	1:A:124:ILE:N	0.46	2.26	5	5
1:A:176:TRP:NE1	1:A:179:LEU:HD22	0.46	2.26	4	1
1:A:157:GLU:OE1	1:A:157:GLU:CA	0.46	2.64	6	1
1:A:12:LEU:HD23	1:A:167:ASP:HA	0.46	1.88	7	2
1:A:75:PHE:C	1:A:77:ASP:N	0.46	2.73	4	2
1:A:72:GLU:CB	1:A:106:CYS:SG	0.46	3.04	11	1
1:A:158:PHE:CD1	1:A:173:PHE:CE2	0.46	3.04	12	1
1:A:55:LEU:C	1:A:56:HIS:CD2	0.46	2.94	20	1
1:A:153:MET:SD	1:A:158:PHE:CG	0.46	3.09	22	1
1:A:70:HIS:O	1:A:72:GLU:N	0.46	2.48	23	1
1:A:57:ASN:N	1:A:57:ASN:HD22	0.46	2.09	19	1
1:A:186:LEU:HD22	1:A:186:LEU:N	0.46	2.26	22	1
1:A:101:CYS:O	1:A:133:ASP:CB	0.45	2.63	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:LEU:N	1:A:179:LEU:HD12	0.45	2.26	11	1
1:A:82:LEU:CD1	1:A:82:LEU:N	0.45	2.79	20	2
1:A:115:GLN:CD	1:A:115:GLN:H	0.45	2.18	22	1
1:A:88:GLN:C	1:A:88:GLN:HE21	0.45	2.19	28	1
1:A:117:ASN:CG	1:A:119:HIS:CD2	0.45	2.95	2	1
1:A:168:HIS:CE1	1:A:170:GLY:N	0.45	2.84	10	12
1:A:186:LEU:N	1:A:186:LEU:CD2	0.45	2.79	22	1
1:A:21:ASN:CG	1:A:32:TYR:CD1	0.45	2.95	1	2
1:A:51:HIS:CD2	1:A:82:LEU:HD22	0.45	2.47	1	1
1:A:168:HIS:O	1:A:169:GLN:C	0.45	2.59	6	6
1:A:32:TYR:CZ	1:A:56:HIS:ND1	0.45	2.85	22	1
1:A:97:SER:HA	1:A:127:ALA:HB3	0.45	1.89	5	21
1:A:18:PHE:CD1	1:A:18:PHE:C	0.45	2.95	20	10
1:A:150:VAL:O	1:A:150:VAL:CG1	0.45	2.62	15	3
1:A:29:HIS:O	1:A:31:THR:HG23	0.45	2.12	24	1
1:A:166:VAL:HG12	1:A:168:HIS:N	0.45	2.26	24	2
1:A:88:GLN:CD	1:A:88:GLN:H	0.45	2.20	28	1
1:A:25:GLY:H	1:A:128:ARG:HH22	0.45	1.53	14	1
1:A:21:ASN:OD1	1:A:32:TYR:CG	0.45	2.70	16	1
1:A:144:ARG:C	1:A:146:ALA:H	0.45	2.20	7	2
1:A:50:GLN:O	1:A:50:GLN:CG	0.45	2.64	12	1
1:A:168:HIS:N	1:A:168:HIS:HD1	0.45	2.10	17	1
1:A:57:ASN:N	1:A:71:ALA:HB2	0.45	2.26	2	3
1:A:13:MET:CG	1:A:54:PHE:CZ	0.45	3.00	3	1
1:A:158:PHE:CD1	1:A:159:LYS:N	0.45	2.85	12	1
1:A:178:GLY:O	1:A:179:LEU:C	0.44	2.60	11	9
1:A:24:ASN:ND2	1:A:182:HIS:CD2	0.44	2.85	13	1
1:A:152:ILE:N	1:A:152:ILE:CD1	0.44	2.80	13	2
1:A:79:VAL:O	1:A:80:PRO:C	0.44	2.59	16	1
1:A:47:LYS:CD	1:A:47:LYS:H	0.44	2.23	23	1
1:A:29:HIS:C	1:A:31:THR:H	0.44	2.20	24	1
1:A:88:GLN:NE2	1:A:90:TYR:CD2	0.44	2.85	28	1
1:A:89:ILE:HG22	1:A:90:TYR:N	0.44	2.27	11	4
1:A:13:MET:SD	1:A:54:PHE:CD2	0.44	3.11	17	1
1:A:32:TYR:OH	1:A:56:HIS:CE1	0.44	2.70	22	1
1:A:166:VAL:O	1:A:168:HIS:N	0.44	2.50	22	2
1:A:78:LEU:CD2	1:A:82:LEU:HD13	0.44	2.42	30	1
1:A:15:PRO:O	1:A:19:THR:OG1	0.44	2.35	8	21
1:A:102:PHE:O	1:A:103:SER:C	0.44	2.60	1	22
1:A:131:ASP:C	1:A:133:ASP:H	0.44	2.20	9	5
1:A:21:ASN:HD21	1:A:30:LYS:CE	0.44	2.26	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ILE:C	1:A:26:ILE:CD1	0.44	2.90	21	8
1:A:48:MET:O	1:A:52:ARG:CZ	0.44	2.66	6	1
1:A:21:ASN:HD21	1:A:30:LYS:NZ	0.44	2.09	9	1
1:A:35:TYR:O	1:A:35:TYR:CG	0.44	2.70	21	1
1:A:111:ARG:NE	1:A:115:GLN:HE21	0.44	2.09	22	1
1:A:99:SER:HB3	1:A:129:ILE:HG23	0.44	1.88	25	1
1:A:137:LYS:O	1:A:141:GLN:NE2	0.44	2.50	4	1
1:A:152:ILE:CD1	1:A:190:LEU:HD22	0.44	2.42	8	1
1:A:29:HIS:ND1	1:A:30:LYS:N	0.44	2.66	21	1
1:A:113:PHE:CD2	1:A:117:ASN:ND2	0.44	2.86	14	1
1:A:123:ARG:NH1	1:A:149:GLN:CD	0.44	2.76	26	1
1:A:31:THR:OG1	1:A:57:ASN:CG	0.44	2.61	26	4
1:A:76:LEU:O	1:A:79:VAL:CG2	0.44	2.65	2	1
1:A:166:VAL:CG1	1:A:167:ASP:N	0.44	2.80	2	7
1:A:157:GLU:OE1	1:A:157:GLU:N	0.44	2.51	6	1
1:A:122:LEU:HD13	1:A:122:LEU:C	0.44	2.37	9	1
1:A:163:ASP:OD1	1:A:163:ASP:O	0.44	2.36	13	1
1:A:132:TYR:CE2	1:A:133:ASP:OD1	0.44	2.70	20	1
1:A:135:LEU:C	1:A:137:LYS:N	0.44	2.76	8	5
1:A:133:ASP:OD1	1:A:133:ASP:N	0.44	2.46	4	1
1:A:87:ALA:HB1	1:A:88:GLN:NE2	0.44	2.27	26	3
1:A:99:SER:O	1:A:100:PRO:O	0.44	2.36	11	14
1:A:166:VAL:HG12	1:A:167:ASP:N	0.44	2.27	9	7
1:A:11:HIS:CD2	1:A:12:LEU:O	0.44	2.71	14	1
1:A:35:TYR:CG	1:A:75:PHE:CZ	0.44	3.06	16	1
1:A:112:ALA:C	1:A:114:LEU:N	0.44	2.74	17	1
1:A:86:PRO:O	1:A:87:ALA:C	0.43	2.61	21	21
1:A:128:ARG:NH2	1:A:182:HIS:ND1	0.43	2.66	5	1
1:A:182:HIS:CE1	1:A:183:SER:OG	0.43	2.71	23	1
1:A:97:SER:O	1:A:128:ARG:O	0.43	2.36	23	13
1:A:72:GLU:N	1:A:72:GLU:CD	0.43	2.76	4	1
1:A:35:TYR:CD1	1:A:53:GLY:O	0.43	2.71	11	1
1:A:140:LEU:CD1	1:A:190:LEU:HD21	0.43	2.36	18	1
1:A:32:TYR:CE1	1:A:56:HIS:ND1	0.43	2.86	22	1
1:A:73:LEU:HD11	1:A:109:GLU:HG3	0.43	1.88	22	1
1:A:186:LEU:N	1:A:186:LEU:CD1	0.43	2.80	24	1
1:A:72:GLU:OE1	1:A:101:CYS:SG	0.43	2.76	26	1
1:A:132:TYR:O	1:A:132:TYR:CG	0.43	2.70	29	1
1:A:42:ASN:C	1:A:44:THR:H	0.43	2.22	19	6
1:A:83:GLN:O	1:A:84:LEU:C	0.43	2.61	1	11
1:A:114:LEU:C	1:A:116:GLU:H	0.43	2.21	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ASN:O	1:A:24:ASN:C	0.43	2.61	8	13
1:A:12:LEU:HD13	1:A:164:THR:O	0.43	2.13	6	1
1:A:152:ILE:O	1:A:152:ILE:CG2	0.43	2.65	6	1
1:A:31:THR:N	1:A:57:ASN:OD1	0.43	2.51	3	1
1:A:21:ASN:O	1:A:21:ASN:OD1	0.43	2.36	27	2
1:A:167:ASP:O	1:A:167:ASP:CG	0.43	2.60	5	2
1:A:73:LEU:HD11	1:A:109:GLU:OE1	0.43	2.12	7	1
1:A:78:LEU:O	1:A:79:VAL:C	0.43	2.62	11	1
1:A:73:LEU:O	1:A:76:LEU:N	0.43	2.51	15	1
1:A:28:ARG:C	1:A:29:HIS:CG	0.43	2.96	19	1
1:A:29:HIS:C	1:A:30:LYS:CG	0.43	2.91	21	1
1:A:23:ASN:N	1:A:23:ASN:ND2	0.43	2.64	26	1
1:A:120:VAL:O	1:A:120:VAL:HG23	0.43	2.12	29	1
1:A:109:GLU:OE1	1:A:109:GLU:C	0.43	2.61	6	2
1:A:111:ARG:CG	1:A:115:GLN:NE2	0.43	2.81	9	1
1:A:159:LYS:O	1:A:163:ASP:OD2	0.43	2.36	11	2
1:A:179:LEU:O	1:A:183:SER:OG	0.43	2.36	12	1
1:A:167:ASP:O	1:A:167:ASP:OD1	0.43	2.37	14	1
1:A:134:PRO:O	1:A:135:LEU:C	0.43	2.62	25	2
1:A:18:PHE:C	1:A:20:SER:N	0.43	2.75	22	1
1:A:88:GLN:H	1:A:88:GLN:NE2	0.43	2.11	24	1
1:A:163:ASP:OD1	1:A:171:CYS:O	0.43	2.37	1	1
1:A:50:GLN:CD	1:A:50:GLN:O	0.43	2.62	17	3
1:A:70:HIS:O	1:A:71:ALA:C	0.43	2.62	28	3
1:A:24:ASN:O	1:A:25:GLY:O	0.43	2.37	19	1
1:A:143:LEU:C	1:A:145:ASP:N	0.43	2.75	30	1
1:A:174:GLN:CD	1:A:174:GLN:C	0.43	2.87	1	1
1:A:86:PRO:O	1:A:87:ALA:O	0.43	2.37	20	3
1:A:167:ASP:OD1	1:A:167:ASP:C	0.43	2.61	14	4
1:A:23:ASN:O	1:A:24:ASN:O	0.43	2.37	12	3
1:A:157:GLU:CD	1:A:157:GLU:C	0.43	2.86	12	2
1:A:56:HIS:O	1:A:57:ASN:O	0.43	2.37	18	5
1:A:160:HIS:O	1:A:164:THR:OG1	0.43	2.37	16	7
1:A:17:ILE:O	1:A:21:ASN:OD1	0.43	2.37	23	4
1:A:70:HIS:NE2	1:A:73:LEU:HD12	0.43	2.29	2	2
1:A:152:ILE:O	1:A:153:MET:C	0.43	2.62	28	9
1:A:31:THR:HG22	1:A:98:TRP:CE2	0.43	2.49	5	4
1:A:113:PHE:CE1	1:A:117:ASN:OD1	0.43	2.72	9	1
1:A:130:TYR:O	1:A:131:ASP:CG	0.43	2.62	9	1
1:A:20:SER:C	1:A:22:PHE:H	0.43	2.20	11	1
1:A:130:TYR:C	1:A:131:ASP:OD1	0.43	2.61	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:SER:O	1:A:187:SER:OG	0.43	2.37	18	1
1:A:70:HIS:C	1:A:72:GLU:H	0.43	2.21	23	1
1:A:103:SER:OG	1:A:139:ALA:CA	0.43	2.67	27	1
1:A:120:VAL:O	1:A:120:VAL:CG2	0.43	2.66	29	1
1:A:122:LEU:C	1:A:122:LEU:CD1	0.43	2.91	9	14
1:A:141:GLN:NE2	1:A:193:ILE:CG2	0.43	2.81	3	1
1:A:26:ILE:HD11	1:A:128:ARG:CB	0.43	2.44	4	1
1:A:12:LEU:CD1	1:A:52:ARG:NH1	0.43	2.81	9	1
1:A:52:ARG:C	1:A:52:ARG:NE	0.43	2.77	9	1
1:A:38:GLU:OE1	1:A:93:THR:OG1	0.43	2.36	15	2
1:A:130:TYR:O	1:A:131:ASP:O	0.43	2.37	15	1
1:A:130:TYR:O	1:A:131:ASP:OD2	0.43	2.36	18	1
1:A:168:HIS:CE1	1:A:171:CYS:N	0.43	2.87	18	3
1:A:72:GLU:OE2	1:A:94:TRP:CE3	0.43	2.71	22	1
1:A:38:GLU:OE2	1:A:39:ARG:O	0.43	2.37	26	1
1:A:20:SER:O	1:A:23:ASN:OD1	0.43	2.37	27	1
1:A:56:HIS:O	1:A:57:ASN:C	0.43	2.62	26	4
1:A:31:THR:HG1	1:A:98:TRP:CG	0.43	2.31	4	2
1:A:52:ARG:CZ	1:A:164:THR:O	0.43	2.67	5	1
1:A:154:THR:O	1:A:155:TYR:C	0.43	2.62	5	2
1:A:155:TYR:CD1	1:A:155:TYR:C	0.43	2.92	18	2
1:A:70:HIS:CD2	1:A:72:GLU:OE2	0.43	2.72	9	1
1:A:178:GLY:C	1:A:180:ASP:N	0.43	2.76	11	1
1:A:131:ASP:OD2	1:A:133:ASP:O	0.43	2.37	25	1
1:A:176:TRP:O	1:A:176:TRP:CD1	0.43	2.72	25	1
1:A:55:LEU:N	1:A:55:LEU:CD1	0.42	2.68	10	1
1:A:166:VAL:C	1:A:168:HIS:N	0.42	2.77	30	6
1:A:83:GLN:OE1	1:A:83:GLN:O	0.42	2.36	20	1
1:A:26:ILE:CD1	1:A:26:ILE:C	0.42	2.92	23	1
1:A:136:TYR:O	1:A:139:ALA:HB3	0.42	2.14	9	2
1:A:87:ALA:HB1	1:A:88:GLN:HE21	0.42	1.74	15	1
1:A:94:TRP:CH2	1:A:110:VAL:CG2	0.42	3.02	24	1
1:A:87:ALA:O	1:A:88:GLN:CD	0.42	2.62	29	1
1:A:149:GLN:O	1:A:149:GLN:OE1	0.42	2.38	1	1
1:A:71:ALA:O	1:A:72:GLU:C	0.42	2.63	2	4
1:A:13:MET:CG	1:A:54:PHE:CE2	0.42	3.03	3	1
1:A:22:PHE:O	1:A:23:ASN:O	0.42	2.37	22	1
1:A:36:GLU:O	1:A:38:GLU:OE2	0.42	2.37	24	1
1:A:24:ASN:HD22	1:A:182:HIS:CD2	0.42	2.33	27	1
1:A:38:GLU:OE2	1:A:93:THR:OG1	0.42	2.37	28	1
1:A:16:HIS:ND1	1:A:20:SER:OG	0.42	2.45	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:O	1:A:83:GLN:C	0.42	2.62	18	5
1:A:116:GLU:C	1:A:117:ASN:HD22	0.42	2.22	1	1
1:A:91:ARG:NH1	1:A:123:ARG:HH11	0.42	2.12	11	1
1:A:131:ASP:OD1	1:A:131:ASP:C	0.42	2.63	16	1
1:A:38:GLU:OE1	1:A:45:SER:OG	0.42	2.37	21	1
1:A:130:TYR:C	1:A:131:ASP:CG	0.42	2.87	23	1
1:A:110:VAL:O	1:A:111:ARG:C	0.42	2.63	16	6
1:A:13:MET:O	1:A:167:ASP:OD1	0.42	2.37	13	2
1:A:85:ASP:OD1	1:A:85:ASP:N	0.42	2.52	19	3
1:A:89:ILE:CG2	1:A:90:TYR:N	0.42	2.81	20	3
1:A:131:ASP:OD1	1:A:133:ASP:OD2	0.42	2.37	10	1
1:A:50:GLN:O	1:A:50:GLN:OE1	0.42	2.37	13	1
1:A:88:GLN:NE2	1:A:88:GLN:CA	0.42	2.82	13	1
1:A:21:ASN:OD1	1:A:21:ASN:O	0.42	2.38	16	3
1:A:90:TYR:HB2	1:A:120:VAL:HG12	0.42	1.92	16	1
1:A:28:ARG:O	1:A:29:HIS:ND1	0.42	2.52	19	1
1:A:29:HIS:CG	1:A:29:HIS:O	0.42	2.71	19	1
1:A:83:GLN:OE1	1:A:85:ASP:OD1	0.42	2.37	20	1
1:A:94:TRP:CH2	1:A:110:VAL:HG22	0.42	2.49	23	1
1:A:83:GLN:O	1:A:83:GLN:CD	0.42	2.62	25	1
1:A:107:ALA:O	1:A:108:GLY:C	0.42	2.62	14	3
1:A:35:TYR:CE2	1:A:53:GLY:CA	0.42	3.03	2	1
1:A:105:GLY:O	1:A:109:GLU:OE2	0.42	2.38	3	1
1:A:18:PHE:CZ	1:A:22:PHE:CD2	0.42	3.07	14	1
1:A:142:MET:O	1:A:143:LEU:C	0.42	2.63	16	1
1:A:157:GLU:O	1:A:158:PHE:C	0.42	2.62	16	3
1:A:28:ARG:O	1:A:29:HIS:C	0.42	2.62	19	1
1:A:162:TRP:NE1	1:A:171:CYS:O	0.42	2.50	23	2
1:A:114:LEU:CD2	1:A:120:VAL:O	0.42	2.67	23	1
1:A:28:ARG:NH2	1:A:98:TRP:HE1	0.42	2.12	26	1
1:A:85:ASP:O	1:A:88:GLN:OE1	0.42	2.37	28	1
1:A:132:TYR:O	1:A:133:ASP:OD1	0.42	2.38	3	1
1:A:50:GLN:CD	1:A:50:GLN:C	0.42	2.88	4	3
1:A:160:HIS:O	1:A:163:ASP:OD1	0.42	2.37	4	3
1:A:193:ILE:CG2	1:A:194:LEU:N	0.42	2.82	25	3
1:A:190:LEU:C	1:A:192:ALA:H	0.42	2.21	15	2
1:A:136:TYR:O	1:A:137:LYS:C	0.42	2.62	26	1
1:A:97:SER:O	1:A:128:ARG:CA	0.42	2.67	29	1
1:A:45:SER:O	1:A:45:SER:OG	0.42	2.37	25	3
1:A:23:ASN:ND2	1:A:23:ASN:C	0.42	2.78	28	2
1:A:91:ARG:NH1	1:A:123:ARG:NH1	0.42	2.68	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ASN:OD1	1:A:57:ASN:C	0.42	2.62	10	1
1:A:21:ASN:OD1	1:A:21:ASN:C	0.42	2.62	17	2
1:A:12:LEU:CD1	1:A:52:ARG:HH22	0.42	2.28	2	1
1:A:120:VAL:O	1:A:120:VAL:CG1	0.42	2.67	2	2
1:A:144:ARG:C	1:A:146:ALA:N	0.42	2.76	7	2
1:A:130:TYR:O	1:A:131:ASP:OD1	0.42	2.38	8	1
1:A:98:TRP:CD1	1:A:98:TRP:N	0.42	2.88	10	1
1:A:14:ASP:C	1:A:16:HIS:H	0.42	2.23	11	1
1:A:183:SER:OG	1:A:184:GLN:N	0.42	2.52	11	1
1:A:111:ARG:HH22	1:A:142:MET:CE	0.42	2.27	23	1
1:A:116:GLU:O	1:A:117:ASN:OD1	0.42	2.37	23	1
1:A:177:ASP:OD1	1:A:177:ASP:N	0.42	2.53	28	1
1:A:76:LEU:HD12	1:A:109:GLU:OE1	0.42	2.15	30	1
1:A:23:ASN:O	1:A:23:ASN:CG	0.42	2.63	26	4
1:A:35:TYR:CG	1:A:35:TYR:O	0.42	2.71	25	2
1:A:135:LEU:O	1:A:136:TYR:C	0.42	2.63	12	8
1:A:23:ASN:O	1:A:23:ASN:OD1	0.42	2.38	9	1
1:A:39:ARG:NH2	1:A:88:GLN:CD	0.42	2.78	11	1
1:A:22:PHE:O	1:A:23:ASN:C	0.42	2.63	28	1
1:A:122:LEU:C	1:A:122:LEU:HD13	0.41	2.40	10	8
1:A:72:GLU:CD	1:A:72:GLU:H	0.41	2.23	4	1
1:A:50:GLN:OE1	1:A:50:GLN:N	0.41	2.53	8	1
1:A:128:ARG:HE	1:A:186:LEU:HD21	0.41	1.75	8	1
1:A:181:GLU:O	1:A:182:HIS:C	0.41	2.63	16	3
1:A:81:SER:C	1:A:82:LEU:HD12	0.41	2.40	15	1
1:A:35:TYR:CD2	1:A:75:PHE:CD1	0.41	3.08	18	1
1:A:78:LEU:O	1:A:78:LEU:HD23	0.41	2.14	20	1
1:A:176:TRP:CD1	1:A:176:TRP:C	0.41	2.98	22	1
1:A:11:HIS:C	1:A:12:LEU:HD22	0.41	2.40	4	2
1:A:111:ARG:O	1:A:112:ALA:C	0.41	2.63	22	2
1:A:147:GLY:O	1:A:148:ALA:C	0.41	2.62	10	2
1:A:168:HIS:CE1	1:A:170:GLY:H	0.41	2.33	19	2
1:A:24:ASN:OD1	1:A:128:ARG:NH2	0.41	2.53	11	1
1:A:145:ASP:OD1	1:A:145:ASP:N	0.41	2.50	11	1
1:A:75:PHE:CE1	1:A:79:VAL:CG2	0.41	3.03	6	1
1:A:178:GLY:O	1:A:180:ASP:N	0.41	2.53	11	1
1:A:168:HIS:CD2	1:A:168:HIS:C	0.41	2.97	12	5
1:A:30:LYS:O	1:A:31:THR:C	0.41	2.64	21	1
1:A:119:HIS:CD2	1:A:120:VAL:HG13	0.41	2.49	29	1
1:A:125:PHE:CZ	1:A:157:GLU:OE2	0.41	2.73	30	1
1:A:189:ARG:CA	1:A:189:ARG:NE	0.41	2.83	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:TYR:CZ	1:A:53:GLY:N	0.41	2.88	2	2
1:A:91:ARG:HH12	1:A:149:GLN:HE22	0.41	1.57	5	1
1:A:55:LEU:C	1:A:56:HIS:ND1	0.41	2.78	6	1
1:A:157:GLU:OE1	1:A:157:GLU:O	0.41	2.37	12	1
1:A:82:LEU:C	1:A:84:LEU:H	0.41	2.24	13	1
1:A:23:ASN:C	1:A:23:ASN:OD1	0.41	2.63	18	1
1:A:52:ARG:HH11	1:A:52:ARG:C	0.41	2.24	18	1
1:A:169:GLN:N	1:A:169:GLN:CD	0.41	2.78	28	1
1:A:47:LYS:NZ	1:A:47:LYS:CB	0.41	2.83	29	1
1:A:76:LEU:C	1:A:78:LEU:H	0.41	2.21	16	1
1:A:112:ALA:O	1:A:116:GLU:OE1	0.41	2.39	20	1
1:A:84:LEU:O	1:A:85:ASP:C	0.41	2.64	24	1
1:A:124:ILE:N	1:A:124:ILE:CD1	0.41	2.84	25	1
1:A:152:ILE:O	1:A:152:ILE:HG23	0.41	2.15	2	1
1:A:119:HIS:CE1	1:A:120:VAL:HG13	0.41	2.50	16	1
1:A:111:ARG:O	1:A:115:GLN:CD	0.41	2.63	22	1
1:A:137:LYS:CG	1:A:138:GLU:N	0.41	2.83	11	1
1:A:116:GLU:C	1:A:116:GLU:CD	0.41	2.88	16	1
1:A:38:GLU:OE1	1:A:91:ARG:CZ	0.41	2.69	21	1
1:A:111:ARG:O	1:A:115:GLN:OE1	0.41	2.39	22	1
1:A:180:ASP:O	1:A:184:GLN:CG	0.41	2.68	1	1
1:A:37:VAL:CG1	1:A:48:MET:SD	0.41	3.09	6	1
1:A:75:PHE:CE2	1:A:79:VAL:CG2	0.41	3.04	7	1
1:A:57:ASN:ND2	1:A:57:ASN:H	0.41	2.13	8	1
1:A:70:HIS:CE1	1:A:73:LEU:HD22	0.41	2.51	10	1
1:A:79:VAL:CG1	1:A:113:PHE:CZ	0.41	3.03	12	1
1:A:181:GLU:O	1:A:184:GLN:N	0.41	2.54	16	1
1:A:141:GLN:C	1:A:143:LEU:N	0.41	2.77	19	1
1:A:51:HIS:O	1:A:51:HIS:ND1	0.41	2.53	24	1
1:A:101:CYS:O	1:A:102:PHE:CB	0.41	2.68	4	1
1:A:177:ASP:OD1	1:A:177:ASP:C	0.41	2.63	4	1
1:A:166:VAL:CG1	1:A:168:HIS:ND1	0.41	2.84	6	1
1:A:42:ASN:O	1:A:42:ASN:ND2	0.41	2.53	9	1
1:A:22:PHE:C	1:A:24:ASN:H	0.41	2.24	10	1
1:A:179:LEU:HD12	1:A:179:LEU:H	0.41	1.74	11	1
1:A:118:THR:C	1:A:120:VAL:H	0.41	2.23	18	3
1:A:100:PRO:O	1:A:131:ASP:CG	0.41	2.63	15	1
1:A:180:ASP:O	1:A:183:SER:OG	0.41	2.37	21	1
1:A:49:ASP:OD1	1:A:49:ASP:C	0.41	2.62	26	1
1:A:131:ASP:OD1	1:A:131:ASP:N	0.41	2.54	28	1
1:A:176:TRP:CZ2	1:A:179:LEU:CD1	0.41	3.04	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:ARG:CZ	1:A:123:ARG:HE	0.41	2.28	9	1
1:A:119:HIS:CD2	1:A:120:VAL:CG1	0.41	3.03	29	1
1:A:12:LEU:HD23	1:A:166:VAL:O	0.41	2.16	30	1
1:A:49:ASP:OD1	1:A:50:GLN:N	0.40	2.53	2	1
1:A:35:TYR:O	1:A:35:TYR:CD1	0.40	2.74	9	1
1:A:26:ILE:O	1:A:130:TYR:CZ	0.40	2.74	20	1
1:A:92:VAL:O	1:A:122:LEU:HD23	0.40	2.16	28	1
1:A:21:ASN:HD22	1:A:28:ARG:CZ	0.40	2.29	2	1
1:A:72:GLU:OE1	1:A:72:GLU:N	0.40	2.54	5	1
1:A:13:MET:HB2	1:A:17:ILE:HD11	0.40	1.91	11	1
1:A:24:ASN:O	1:A:25:GLY:C	0.40	2.64	13	1
1:A:140:LEU:HD21	1:A:190:LEU:CD1	0.40	2.45	21	1
1:A:13:MET:O	1:A:167:ASP:CG	0.40	2.64	22	1
1:A:47:LYS:CD	1:A:47:LYS:N	0.40	2.84	23	1
1:A:78:LEU:O	1:A:81:SER:OG	0.40	2.37	4	1
1:A:189:ARG:O	1:A:190:LEU:C	0.40	2.64	7	1
1:A:73:LEU:HD12	1:A:73:LEU:N	0.40	2.31	10	1
1:A:23:ASN:ND2	1:A:24:ASN:N	0.40	2.70	21	1
1:A:123:ARG:CD	1:A:123:ARG:N	0.40	2.83	25	1
1:A:24:ASN:ND2	1:A:24:ASN:H	0.40	2.13	29	1
1:A:190:LEU:HD23	1:A:190:LEU:O	0.40	2.17	1	1
1:A:57:ASN:OD1	1:A:57:ASN:N	0.40	2.53	12	1
1:A:105:GLY:O	1:A:109:GLU:OE1	0.40	2.38	25	1
1:A:87:ALA:HB1	1:A:88:GLN:HE22	0.40	1.77	26	1
1:A:190:LEU:HD23	1:A:190:LEU:C	0.40	2.42	1	1
1:A:79:VAL:N	1:A:80:PRO:HD2	0.40	2.31	5	1
1:A:72:GLU:O	1:A:73:LEU:C	0.40	2.64	6	1
1:A:163:ASP:C	1:A:165:PHE:N	0.40	2.79	15	1
1:A:99:SER:CB	1:A:129:ILE:HG23	0.40	2.46	20	1
1:A:73:LEU:C	1:A:75:PHE:N	0.40	2.79	22	1
1:A:38:GLU:OE2	1:A:39:ARG:C	0.40	2.65	26	1
1:A:14:ASP:O	1:A:15:PRO:C	0.40	2.65	28	1
1:A:28:ARG:HE	1:A:28:ARG:C	0.40	2.25	28	1
1:A:167:ASP:OD1	1:A:169:GLN:OE1	0.40	2.40	28	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	172/207 (83%)	138±3 (80±2%)	25±4 (15±2%)	9±3 (5±2%)	3	23
All	All	5160/6210 (83%)	4135 (80%)	757 (15%)	268 (5%)	3	23

All 37 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	51	HIS	25
1	A	169	GLN	24
1	A	27	GLY	18
1	A	87	ALA	16
1	A	30	LYS	15
1	A	100	PRO	15
1	A	103	SER	13
1	A	134	PRO	13
1	A	29	HIS	10
1	A	102	PHE	10
1	A	24	ASN	10
1	A	84	LEU	9
1	A	118	THR	9
1	A	57	ASN	8
1	A	25	GLY	7
1	A	86	PRO	6
1	A	168	HIS	6
1	A	177	ASP	6
1	A	178	GLY	5
1	A	11	HIS	5
1	A	135	LEU	5
1	A	31	THR	5
1	A	115	GLN	4
1	A	23	ASN	3
1	A	26	ILE	2
1	A	153	MET	2
1	A	83	GLN	2
1	A	131	ASP	2
1	A	15	PRO	2
1	A	130	TYR	2
1	A	191	ARG	2
1	A	167	ASP	2
1	A	70	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	77	ASP	1
1	A	117	ASN	1
1	A	148	ALA	1
1	A	71	ALA	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	151/179 (84%)	109±4 (72±3%)	42±4 (28±3%)	1	20
All	All	4530/5370 (84%)	3281 (72%)	1249 (28%)	1	20

All 120 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	34	CYS	30
1	A	96	ILE	30
1	A	160	HIS	30
1	A	122	LEU	29
1	A	19	THR	28
1	A	99	SER	28
1	A	88	GLN	26
1	A	128	ARG	26
1	A	93	THR	23
1	A	104	TRP	22
1	A	76	LEU	21
1	A	79	VAL	21
1	A	106	CYS	21
1	A	129	ILE	21
1	A	163	ASP	21
1	A	26	ILE	20
1	A	56	HIS	20
1	A	85	ASP	20
1	A	142	MET	20
1	A	12	LEU	18
1	A	49	ASP	16

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Mol	Chain	Res	Type	Models (Total)
1	A	133	ASP	16
1	A	14	ASP	16
1	A	150	VAL	16
1	A	70	HIS	15
1	A	118	THR	15
1	A	135	LEU	15
1	A	194	LEU	15
1	A	32	TYR	15
1	A	190	LEU	15
1	A	41	ASP	14
1	A	168	HIS	14
1	A	179	LEU	14
1	A	57	ASN	13
1	A	151	SER	13
1	A	48	MET	13
1	A	89	ILE	13
1	A	101	CYS	13
1	A	119	HIS	13
1	A	11	HIS	12
1	A	24	ASN	12
1	A	28	ARG	12
1	A	77	ASP	12
1	A	145	ASP	12
1	A	171	CYS	12
1	A	47	LYS	12
1	A	140	LEU	12
1	A	23	ASN	12
1	A	156	ASP	12
1	A	16	HIS	11
1	A	152	ILE	11
1	A	154	THR	11
1	A	177	ASP	11
1	A	50	GLN	11
1	A	81	SER	11
1	A	97	SER	11
1	A	78	LEU	10
1	A	149	GLN	10
1	A	131	ASP	10
1	A	158	PHE	10
1	A	40	LEU	9
1	A	45	SER	9
1	A	174	GLN	9

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Mol	Chain	Res	Type	Models (Total)
1	A	30	LYS	8
1	A	74	ARG	8
1	A	180	ASP	8
1	A	121	ARG	8
1	A	44	THR	7
1	A	136	TYR	7
1	A	143	LEU	7
1	A	36	GLU	7
1	A	42	ASN	7
1	A	159	LYS	7
1	A	38	GLU	7
1	A	130	TYR	7
1	A	132	TYR	7
1	A	141	GLN	7
1	A	92	VAL	6
1	A	167	ASP	6
1	A	137	LYS	6
1	A	161	CYS	6
1	A	173	PHE	6
1	A	37	VAL	6
1	A	157	GLU	6
1	A	184	GLN	6
1	A	13	MET	5
1	A	52	ARG	5
1	A	20	SER	5
1	A	114	LEU	5
1	A	46	VAL	4
1	A	83	GLN	4
1	A	55	LEU	4
1	A	29	HIS	4
1	A	187	SER	4
1	A	109	GLU	3
1	A	189	ARG	3
1	A	17	ILE	3
1	A	116	GLU	3
1	A	39	ARG	3
1	A	111	ARG	3
1	A	182	HIS	2
1	A	144	ARG	2
1	A	183	SER	2
1	A	31	THR	2
1	A	72	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	91	ARG	2
1	A	115	GLN	2
1	A	123	ARG	2
1	A	176	TRP	1
1	A	191	ARG	1
1	A	84	LEU	1
1	A	193	ILE	1
1	A	162	TRP	1
1	A	166	VAL	1
1	A	125	PHE	1
1	A	73	LEU	1
1	A	103	SER	1
1	A	138	GLU	1
1	A	117	ASN	1
1	A	120	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 67% for the well-defined parts and 67% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1851
Number of shifts mapped to atoms	1851
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	197	-0.39 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	180	0.31 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	183	0.17 ± 0.32	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 67%, i.e. 1619 atoms were assigned a chemical shift out of a possible 2415. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	664/856 (78%)	331/347 (95%)	171/344 (50%)	162/165 (98%)
Sidechain	862/1256 (69%)	594/815 (73%)	257/386 (67%)	11/55 (20%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	93/303 (31%)	80/153 (52%)	8/135 (6%)	5/15 (33%)
Overall	1619/2415 (67%)	1005/1315 (76%)	436/865 (50%)	178/235 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 67%, i.e. 1843 atoms were assigned a chemical shift out of a possible 2757. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	760/991 (77%)	380/403 (94%)	197/398 (49%)	183/190 (96%)
Sidechain	986/1444 (68%)	676/935 (72%)	295/441 (67%)	15/68 (22%)
Aromatic	97/322 (30%)	82/162 (51%)	10/145 (7%)	5/15 (33%)
Overall	1843/2757 (67%)	1138/1500 (76%)	502/984 (51%)	203/273 (74%)

7.1.4 Statistically unusual chemical shifts [i](#)

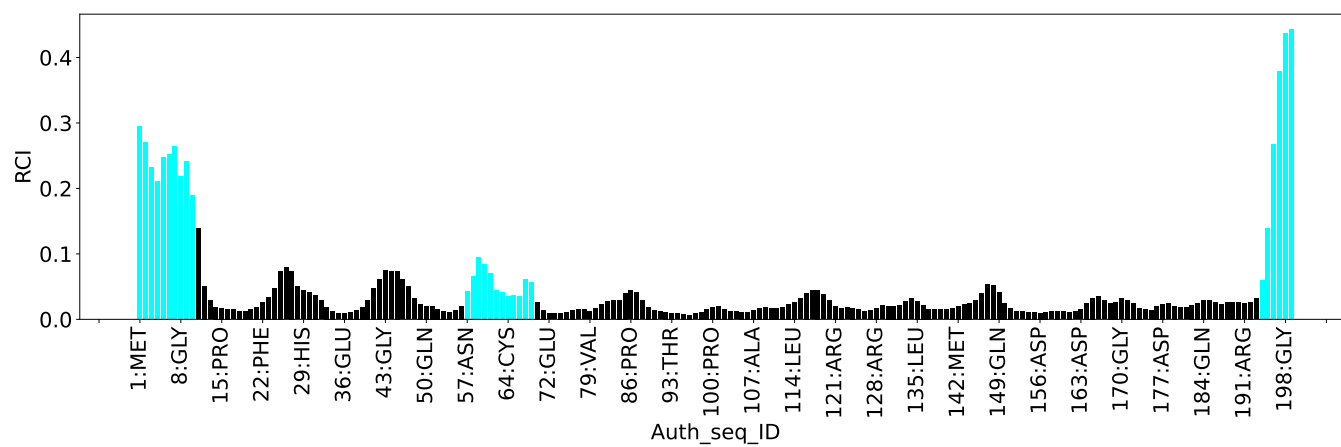
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	72	GLU	H	12.69	5.45 – 11.20	7.6
1	A	94	TRP	HE1	5.54	6.88 – 13.28	-7.1
1	A	97	SER	HB2	2.45	2.61 – 5.13	-5.6
1	A	170	GLY	H	11.56	5.23 – 11.42	5.2
1	A	179	LEU	HG	-0.20	-0.13 – 3.16	-5.2

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2979
Intra-residue ($ i-j =0$)	1124
Sequential ($ i-j =1$)	656
Medium range ($ i-j >1$ and $ i-j <5$)	308
Long range ($ i-j \geq 5$)	739
Inter-chain	0
Hydrogen bond restraints	152
Disulfide bond restraints	0
Total dihedral-angle restraints	300
Number of unmapped restraints	0
Number of restraints per residue	15.8
Number of long range restraints per residue ¹	3.8

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)	8.8	0.2
0.2-0.5 (Medium)	4.5	0.5
>0.5 (Large)	1.5	1.47

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)	5.7	4.03
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

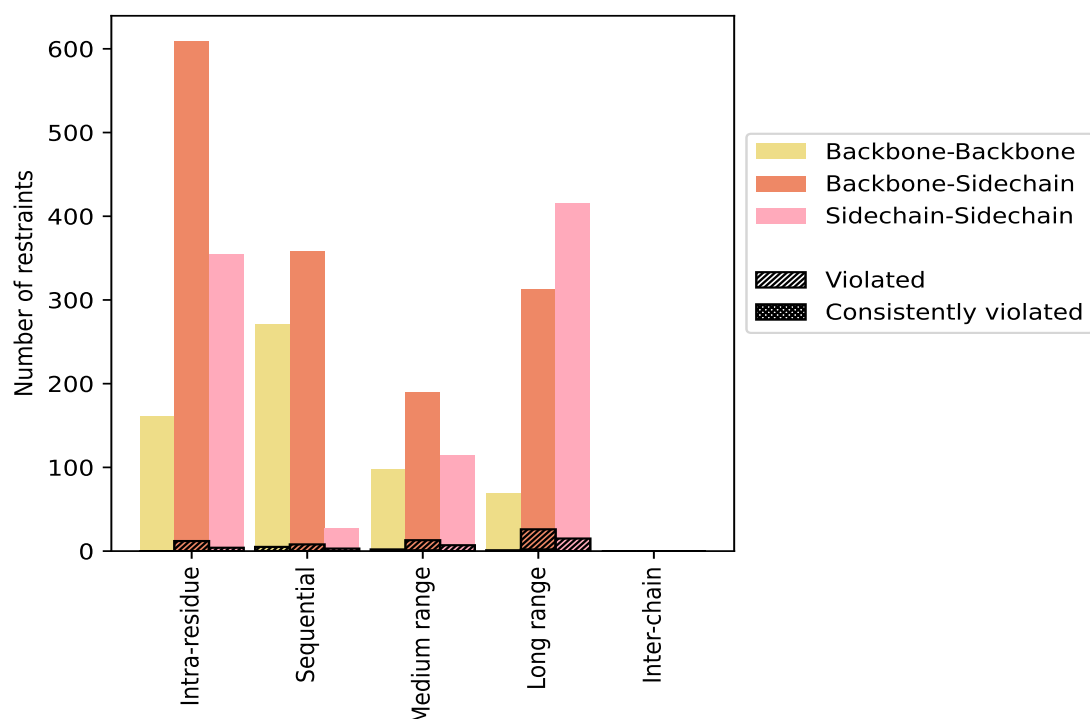
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1124	37.7	16	1.4	0.5	0	0.0	0.0
Backbone-Backbone	161	5.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	609	20.4	12	2.0	0.4	0	0.0	0.0
Sidechain-Sidechain	354	11.9	4	1.1	0.1	0	0.0	0.0
Sequential ($i-j =1$)	656	22.0	16	2.4	0.5	0	0.0	0.0
Backbone-Backbone	271	9.1	5	1.8	0.2	0	0.0	0.0
Backbone-Sidechain	358	12.0	8	2.2	0.3	0	0.0	0.0
Sidechain-Sidechain	27	0.9	3	11.1	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	308	10.3	17	5.5	0.6	1	0.3	0.0
Backbone-Backbone	98	3.3	2	2.0	0.1	0	0.0	0.0
Backbone-Sidechain	96	3.2	8	8.3	0.3	1	1.0	0.0
Sidechain-Sidechain	114	3.8	7	6.1	0.2	0	0.0	0.0
Long range ($i-j \geq 5$)	739	24.8	37	5.0	1.2	2	0.3	0.1
Backbone-Backbone	69	2.3	1	1.4	0.0	0	0.0	0.0
Backbone-Sidechain	255	8.6	21	8.2	0.7	2	0.8	0.1
Sidechain-Sidechain	415	13.9	15	3.6	0.5	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	152	5.1	10	6.6	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2979	100.0	96	3.2	3.2	3	0.1	0.1
Backbone-Backbone	599	20.1	8	1.3	0.3	0	0.0	0.0
Backbone-Sidechain	1470	49.3	59	4.0	2.0	3	0.2	0.1
Sidechain-Sidechain	910	30.5	29	3.2	1.0	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	1	4	10	0	16	0.26	1.32	0.29	0.16
2	0	1	7	11	0	19	0.18	0.62	0.11	0.15
3	1	2	3	8	0	14	0.17	0.26	0.05	0.17
4	0	0	3	12	0	15	0.21	0.79	0.16	0.16
5	0	1	4	9	0	14	0.2	0.65	0.14	0.14
6	0	2	2	8	0	12	0.36	1.32	0.32	0.28
7	1	2	4	12	0	19	0.24	1.02	0.22	0.17
8	1	2	3	5	0	11	0.17	0.3	0.06	0.16
9	3	2	9	10	0	24	0.25	1.35	0.29	0.14
10	0	2	4	10	0	16	0.27	1.23	0.29	0.18

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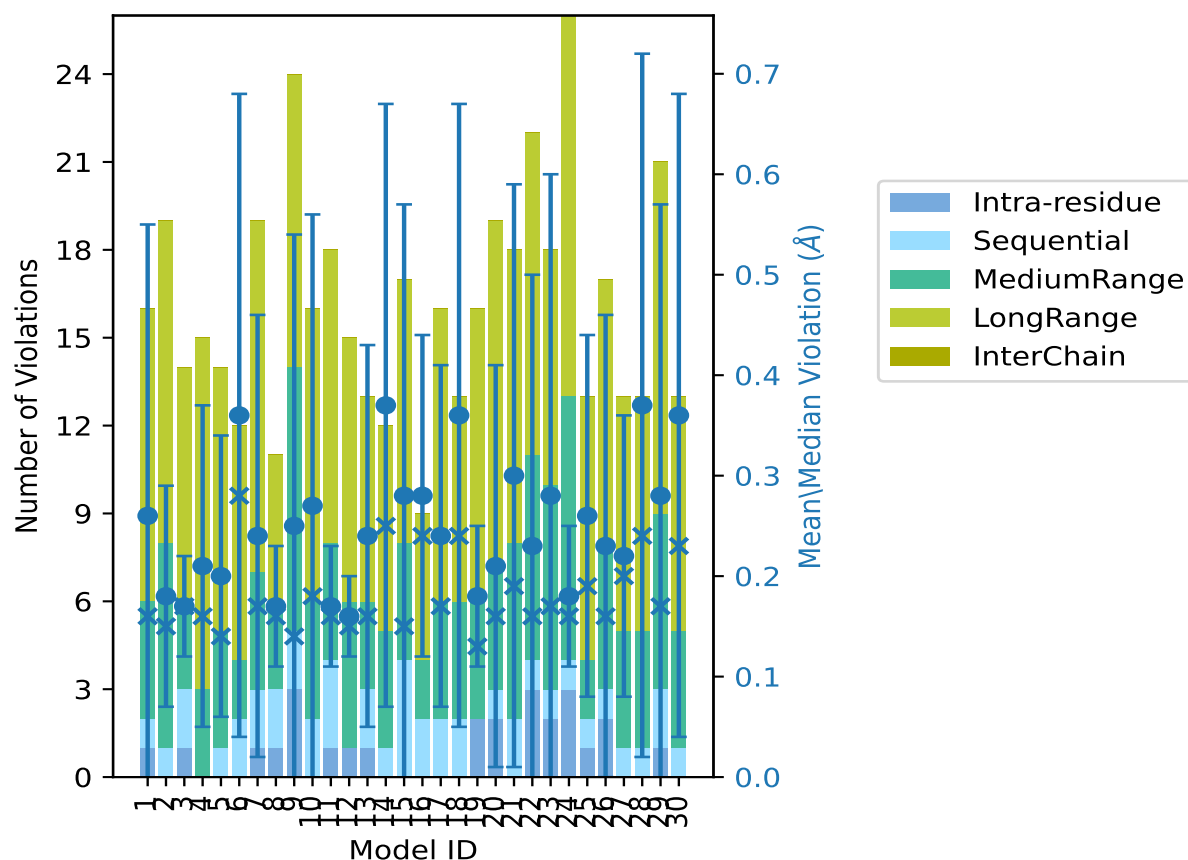
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	3	4	10	0	18	0.17	0.31	0.06	0.16
12	1	0	5	9	0	15	0.16	0.26	0.04	0.15
13	1	2	3	7	0	13	0.24	0.85	0.19	0.16
14	0	1	4	7	0	12	0.37	1.19	0.3	0.25
15	0	4	4	9	0	17	0.28	1.32	0.29	0.15
16	0	2	2	5	0	9	0.28	0.72	0.16	0.24
17	0	2	4	10	0	16	0.24	0.77	0.17	0.17
18	0	2	4	7	0	13	0.36	1.18	0.31	0.24
19	2	0	4	10	0	16	0.18	0.34	0.07	0.13
20	2	1	4	12	0	19	0.21	1.02	0.2	0.16
21	0	2	6	10	0	18	0.3	1.03	0.29	0.19
22	3	1	7	11	0	22	0.23	1.39	0.27	0.16
23	2	1	7	8	0	18	0.28	1.47	0.32	0.17
24	3	1	9	13	0	26	0.18	0.37	0.07	0.16
25	1	1	2	9	0	13	0.26	0.74	0.18	0.19
26	2	1	5	9	0	17	0.23	1.13	0.23	0.16
27	0	1	4	8	0	13	0.22	0.67	0.14	0.2
28	0	1	4	8	0	13	0.37	1.41	0.35	0.24
29	1	2	6	12	0	21	0.28	1.35	0.29	0.17
30	0	1	4	8	0	13	0.36	1.19	0.32	0.23

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, 2741(IR:1108, SQ:640, MR:291, LR:702, 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	%
11	8	8	16	0	43	1	3.3
3	3	2	4	0	12	2	6.7
0	1	3	2	0	6	3	10.0
1	3	0	2	0	6	4	13.3
1	0	0	1	0	2	5	16.7
0	0	0	0	0	0	6	20.0

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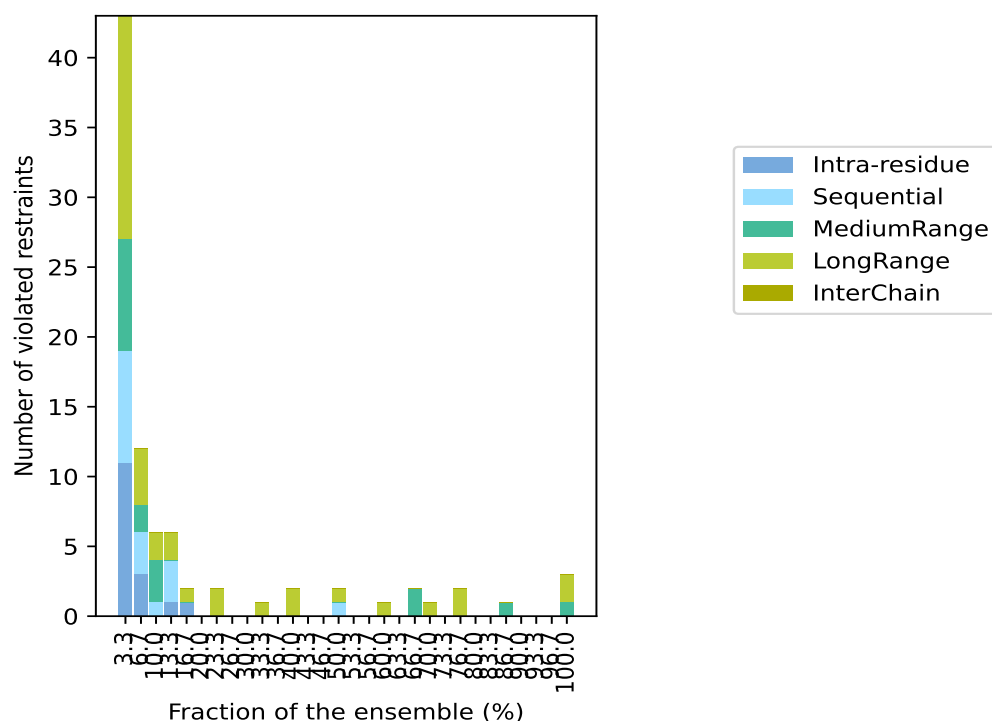
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	2	0	2	7	23.3
0	0	0	0	0	0	8	26.7
0	0	0	0	0	0	9	30.0
0	0	0	1	0	1	10	33.3
0	0	0	0	0	0	11	36.7
0	0	0	2	0	2	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	0	0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

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

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

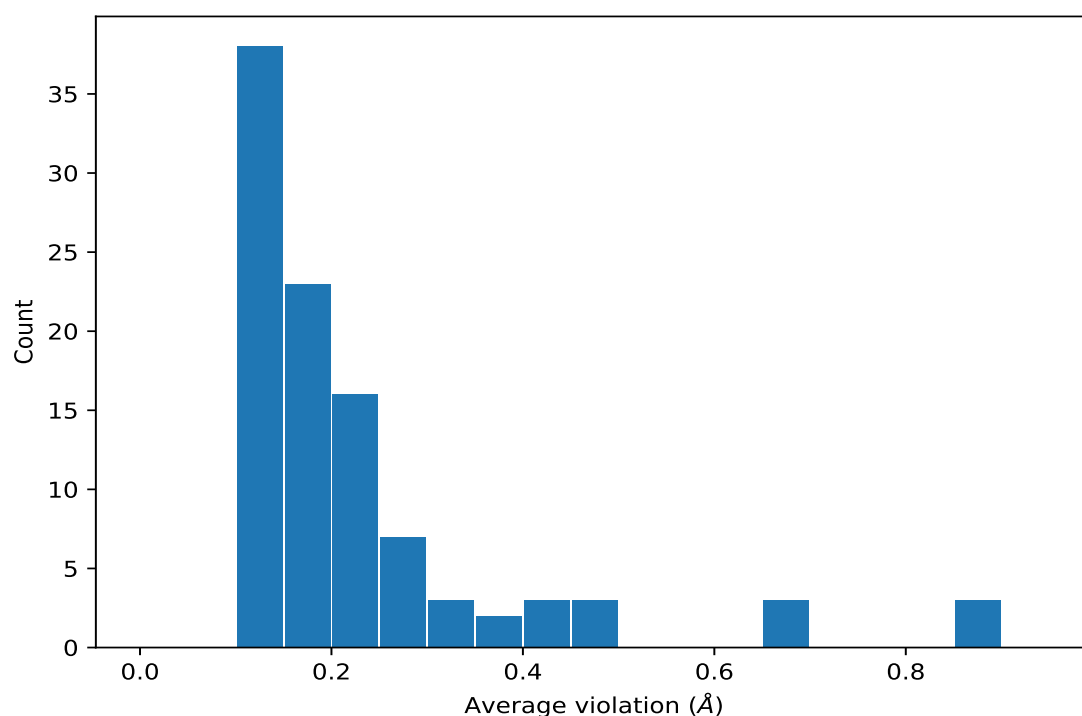
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	30	0.37	0.26	0.18
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	30	0.27	0.03	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	30	0.27	0.03	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	30	0.27	0.03	0.26
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	30	0.22	0.03	0.22
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	30	0.22	0.03	0.22
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	30	0.22	0.03	0.22
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	26	0.18	0.04	0.16
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	26	0.18	0.04	0.16
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	26	0.18	0.04	0.16
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	23	0.67	0.38	0.62
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	23	0.67	0.38	0.62
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	23	0.67	0.38	0.62
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	23	0.23	0.05	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	23	0.23	0.05	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	23	0.23	0.05	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	21	0.89	0.42	1.02
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	21	0.89	0.42	1.02
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	21	0.89	0.42	1.02
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	20	0.16	0.03	0.17
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	20	0.16	0.03	0.17
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	20	0.16	0.04	0.16
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	18	0.15	0.05	0.13
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	18	0.15	0.05	0.13
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	16	0.12	0.02	0.12
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	15	0.24	0.05	0.25
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	15	0.17	0.15	0.12
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	12	0.24	0.05	0.26
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	12	0.24	0.05	0.26
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	12	0.24	0.05	0.26
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	12	0.14	0.02	0.14
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	12	0.14	0.02	0.14
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	12	0.14	0.02	0.14
(1,124)	1:12:A:LEU:HD11	1:168:A:HIS:HD2	10	0.14	0.02	0.14
(1,124)	1:12:A:LEU:HD12	1:168:A:HIS:HD2	10	0.14	0.02	0.14
(1,124)	1:12:A:LEU:HD13	1:168:A:HIS:HD2	10	0.14	0.02	0.14
(1,124)	1:12:A:LEU:HD21	1:168:A:HIS:HD2	10	0.14	0.02	0.14
(1,124)	1:12:A:LEU:HD22	1:168:A:HIS:HD2	10	0.14	0.02	0.14
(1,124)	1:12:A:LEU:HD23	1:168:A:HIS:HD2	10	0.14	0.02	0.14
(2,100)	1:114:A:LEU:O	1:118:A:THR:N	9	0.12	0.01	0.12
(1,619)	1:37:A:VAL:HA	1:51:A:HIS:HE1	7	0.14	0.02	0.15
(2,35)	1:32:A:TYR:O	1:97:A:SER:H	7	0.12	0.01	0.11
(1,1564)	1:98:A:TRP:HZ3	1:130:A:TYR:HA	7	0.12	0.02	0.11
(1,104)	1:12:A:LEU:HD21	1:12:A:LEU:H	5	0.13	0.03	0.12
(1,104)	1:12:A:LEU:HD22	1:12:A:LEU:H	5	0.13	0.03	0.12
(1,104)	1:12:A:LEU:HD23	1:12:A:LEU:H	5	0.13	0.03	0.12
(1,206)	1:15:A:PRO:HA	1:162:A:TRP:HE1	5	0.12	0.02	0.12
(1,1193)	1:78:A:LEU:HG	1:78:A:LEU:H	4	0.37	0.0	0.37
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG21	4	0.26	0.1	0.26
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG22	4	0.26	0.1	0.26
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG23	4	0.26	0.1	0.26
(1,126)	1:12:A:LEU:HD21	1:168:A:HIS:H	4	0.22	0.12	0.18
(1,126)	1:12:A:LEU:HD22	1:168:A:HIS:H	4	0.22	0.12	0.18
(1,126)	1:12:A:LEU:HD23	1:168:A:HIS:H	4	0.22	0.12	0.18
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD21	4	0.2	0.03	0.2
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD22	4	0.2	0.03	0.2
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD23	4	0.2	0.03	0.2
(1,1383)	1:89:A:ILE:HD11	1:90:A:TYR:H	4	0.18	0.03	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1383)	1:89:A:ILE:HD12	1:90:A:TYR:H	4	0.18	0.03	0.19
(1,1383)	1:89:A:ILE:HD13	1:90:A:TYR:H	4	0.18	0.03	0.19
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD11	4	0.14	0.05	0.11
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD12	4	0.14	0.05	0.11
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD13	4	0.14	0.05	0.11
(2,99)	1:114:A:LEU:O	1:118:A:THR:H	4	0.12	0.01	0.12
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD21	3	0.17	0.02	0.17
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD22	3	0.17	0.02	0.17
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD23	3	0.17	0.02	0.17
(1,1685)	1:111:A:ARG:HD2	1:115:A:GLN:HG3	3	0.16	0.02	0.17
(1,2568)	1:179:A:LEU:HG	1:182:A:HIS:HB2	3	0.15	0.01	0.15
(1,2568)	1:179:A:LEU:HG	1:182:A:HIS:HB3	3	0.15	0.01	0.15
(1,2557)	1:178:A:GLY:H	1:182:A:HIS:HD2	3	0.13	0.02	0.12
(2,83)	1:105:A:GLY:O	1:109:A:GLU:H	3	0.12	0.02	0.11
(1,2366)	1:162:A:TRP:HZ2	1:171:A:CYS:H	3	0.12	0.01	0.11
(1,1389)	1:89:A:ILE:HG13	1:90:A:TYR:H	3	0.11	0.01	0.11
(1,91)	1:11:A:HIS:HD2	1:12:A:LEU:HD11	2	0.46	0.05	0.46
(1,91)	1:11:A:HIS:HD2	1:12:A:LEU:HD12	2	0.46	0.05	0.46
(1,91)	1:11:A:HIS:HD2	1:12:A:LEU:HD13	2	0.46	0.05	0.46
(1,1703)	1:112:A:ALA:HB1	1:115:A:GLN:HE22	2	0.42	0.15	0.42
(1,1703)	1:112:A:ALA:HB2	1:115:A:GLN:HE22	2	0.42	0.15	0.42
(1,1703)	1:112:A:ALA:HB3	1:115:A:GLN:HE22	2	0.42	0.15	0.42
(1,230)	1:16:A:HIS:HD2	1:17:A:ILE:HD11	2	0.3	0.16	0.3
(1,230)	1:16:A:HIS:HD2	1:17:A:ILE:HD12	2	0.3	0.16	0.3
(1,230)	1:16:A:HIS:HD2	1:17:A:ILE:HD13	2	0.3	0.16	0.3
(1,1060)	1:73:A:LEU:HG	1:73:A:LEU:H	2	0.25	0.09	0.25
(1,415)	1:30:A:LYS:H	1:98:A:TRP:HD1	2	0.18	0.02	0.18
(1,630)	1:37:A:VAL:HB	1:82:A:LEU:HD11	2	0.18	0.04	0.18
(1,630)	1:37:A:VAL:HB	1:82:A:LEU:HD12	2	0.18	0.04	0.18
(1,630)	1:37:A:VAL:HB	1:82:A:LEU:HD13	2	0.18	0.04	0.18
(1,229)	1:16:A:HIS:HD2	1:16:A:HIS:H	2	0.17	0.0	0.17
(1,145)	1:13:A:MET:HA	1:166:A:VAL:HG11	2	0.14	0.02	0.14
(1,145)	1:13:A:MET:HA	1:166:A:VAL:HG12	2	0.14	0.02	0.14
(1,145)	1:13:A:MET:HA	1:166:A:VAL:HG13	2	0.14	0.02	0.14
(1,226)	1:16:A:HIS:HB2	1:17:A:ILE:HG21	2	0.13	0.02	0.13
(1,226)	1:16:A:HIS:HB2	1:17:A:ILE:HG22	2	0.13	0.02	0.13
(1,226)	1:16:A:HIS:HB2	1:17:A:ILE:HG23	2	0.13	0.02	0.13
(1,226)	1:16:A:HIS:HB3	1:17:A:ILE:HG21	2	0.13	0.02	0.13
(1,226)	1:16:A:HIS:HB3	1:17:A:ILE:HG22	2	0.13	0.02	0.13
(1,226)	1:16:A:HIS:HB3	1:17:A:ILE:HG23	2	0.13	0.02	0.13
(1,685)	1:39:A:ARG:HA	1:90:A:TYR:H	2	0.12	0.02	0.12
(1,1978)	1:129:A:ILE:HB	1:131:A:ASP:H	2	0.12	0.02	0.12

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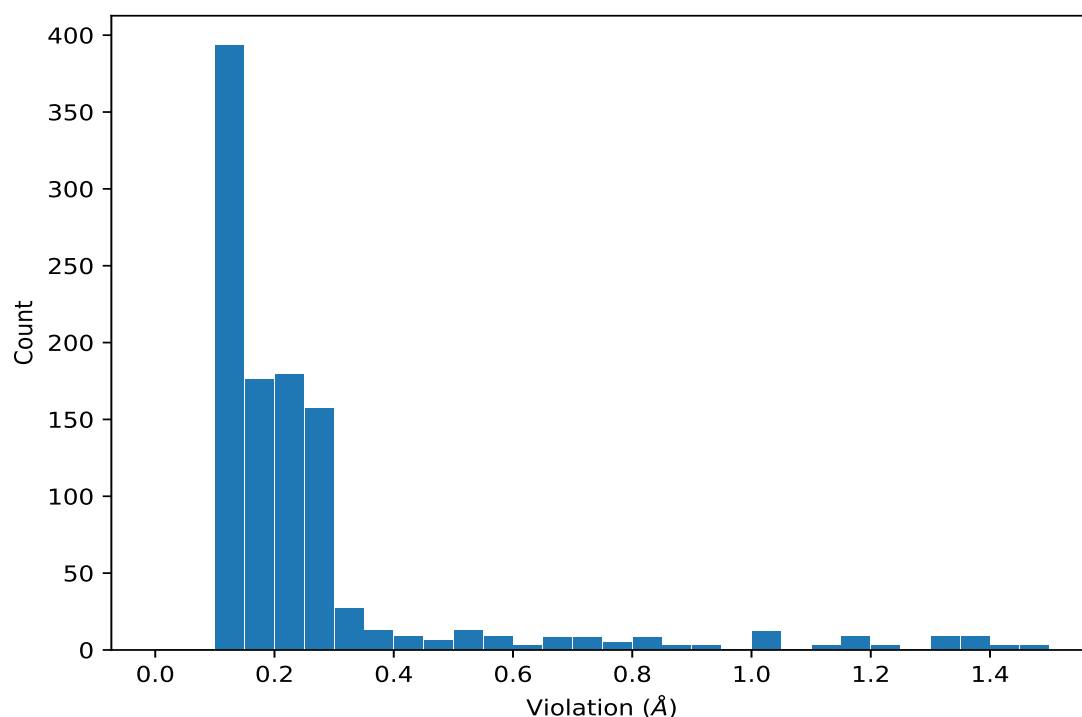
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1778)	1:115:A:GLN:HE21	1:115:A:GLN:HE22	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	23	1.47
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	23	1.47
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	23	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	28	1.41
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	28	1.41
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	28	1.41
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	22	1.39
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	22	1.39
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	22	1.39
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	9	1.35
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	9	1.35
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	9	1.35
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	29	1.35
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	29	1.35
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	29	1.35
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	6	1.32
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	6	1.32
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	6	1.32
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	1	1.32
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	1	1.32
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	1	1.32
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	15	1.32
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	15	1.32
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	15	1.32
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	10	1.23
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	10	1.23
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	10	1.23
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	14	1.19
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	14	1.19
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	14	1.19
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	30	1.19
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	30	1.19
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	30	1.19
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	18	1.18
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	18	1.18
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	18	1.18
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	26	1.13
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	26	1.13
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	26	1.13
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	21	1.03
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	21	1.03
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	21	1.03
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	7	1.02
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	7	1.02
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	7	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	20	1.02
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	20	1.02
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	20	1.02
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	21	1.02
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	21	1.02
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	21	1.02
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	9	0.94
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	9	0.94
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	9	0.94
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	29	0.87
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	29	0.87
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	29	0.87
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	13	0.85
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	30	0.82
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	30	0.82
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	30	0.82
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	28	0.81
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	18	0.8
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	18	0.8
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	18	0.8
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	4	0.79
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	4	0.79
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	4	0.79
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	17	0.77
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	14	0.76
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	25	0.74
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	25	0.74
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	25	0.74
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	21	0.73
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	16	0.72
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	10	0.72
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	10	0.72
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	10	0.72
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	30	0.7
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	23	0.7
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	23	0.7
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	23	0.7
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	27	0.67
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	15	0.66
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	5	0.65
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	18	0.65
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	2	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	2	0.62
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	2	0.62
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	28	0.59
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	28	0.59
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	28	0.59
(1,1703)	1:112:A:ALA:HB1	1:115:A:GLN:HE22	9	0.57
(1,1703)	1:112:A:ALA:HB2	1:115:A:GLN:HE22	9	0.57
(1,1703)	1:112:A:ALA:HB3	1:115:A:GLN:HE22	9	0.57
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	22	0.57
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	22	0.57
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	22	0.57
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	7	0.53
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	7	0.53
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	7	0.53
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	29	0.52
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	25	0.52
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	25	0.52
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	25	0.52
(1,91)	1:11:A:HIS:HD2	1:12:A:LEU:HD11	6	0.51
(1,91)	1:11:A:HIS:HD2	1:12:A:LEU:HD12	6	0.51
(1,91)	1:11:A:HIS:HD2	1:12:A:LEU:HD13	6	0.51
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	1	0.5
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	1	0.5
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	1	0.5
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	14	0.49
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	14	0.49
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	14	0.49
(1,230)	1:16:A:HIS:HD2	1:17:A:ILE:HD11	7	0.46
(1,230)	1:16:A:HIS:HD2	1:17:A:ILE:HD12	7	0.46
(1,230)	1:16:A:HIS:HD2	1:17:A:ILE:HD13	7	0.46
(1,126)	1:12:A:LEU:HD21	1:168:A:HIS:H	6	0.42
(1,126)	1:12:A:LEU:HD22	1:168:A:HIS:H	6	0.42
(1,126)	1:12:A:LEU:HD23	1:168:A:HIS:H	6	0.42
(1,91)	1:11:A:HIS:HD2	1:12:A:LEU:HD11	17	0.42
(1,91)	1:11:A:HIS:HD2	1:12:A:LEU:HD12	17	0.42
(1,91)	1:11:A:HIS:HD2	1:12:A:LEU:HD13	17	0.42
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG21	6	0.41
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG22	6	0.41
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG23	6	0.41
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	15	0.39
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	15	0.39
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	15	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	17	0.39
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	17	0.39
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	17	0.39
(1,1193)	1:78:A:LEU:HG	1:78:A:LEU:H	20	0.37
(1,1193)	1:78:A:LEU:HG	1:78:A:LEU:H	24	0.37
(1,1193)	1:78:A:LEU:HG	1:78:A:LEU:H	25	0.37
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	9	0.36
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	9	0.36
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	9	0.36
(1,1193)	1:78:A:LEU:HG	1:78:A:LEU:H	13	0.36
(1,1060)	1:73:A:LEU:HG	1:73:A:LEU:H	19	0.34
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	13	0.33
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	13	0.33
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	13	0.33
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	18	0.33
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	18	0.33
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	18	0.33
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	24	0.32
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	18	0.32
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	18	0.32
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	18	0.32
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	6	0.32
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	6	0.32
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	6	0.32
(1,406)	1:28:A:ARG:H	1:98:A:TRP:HE1	21	0.32
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	11	0.31
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	11	0.31
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	11	0.31
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	19	0.31
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	19	0.31
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	19	0.31
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	23	0.31
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	23	0.31
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	23	0.31
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG21	17	0.31
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG22	17	0.31
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG23	17	0.31
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	27	0.3
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	8	0.3
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	8	0.3
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	8	0.3
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	14	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	14	0.3
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	14	0.3
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	17	0.3
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	17	0.3
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	17	0.3
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	6	0.29
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	25	0.29
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	25	0.29
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	25	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	1	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	1	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	1	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	5	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	5	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	5	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	16	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	16	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	16	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	28	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	28	0.29
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	28	0.29
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	17	0.28
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	11	0.28
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	11	0.28
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	11	0.28
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	15	0.28
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	15	0.28
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	15	0.28
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	26	0.28
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	26	0.28
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	26	0.28
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	10	0.28
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	10	0.28
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	10	0.28
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	26	0.28
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	26	0.28
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	26	0.28
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	14	0.27
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	14	0.27
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	14	0.27
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	15	0.27
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	15	0.27
(1,1703)	1:112:A:ALA:HB1	1:115:A:GLN:HE22	22	0.27
(1,1703)	1:112:A:ALA:HB2	1:115:A:GLN:HE22	22	0.27
(1,1703)	1:112:A:ALA:HB3	1:115:A:GLN:HE22	22	0.27
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	11	0.27
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	23	0.27
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	23	0.27
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	4	0.27
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	4	0.27
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	4	0.27
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	30	0.27
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	30	0.27
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	30	0.27
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	30	0.27
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	30	0.27
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	30	0.27
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	15	0.26
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	15	0.26
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	15	0.26
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	4	0.26
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	4	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	3	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	3	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	3	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	6	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	6	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	6	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	12	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	12	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	12	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	16	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	16	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	16	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	22	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	22	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	22	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	24	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	24	0.26
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	24	0.26
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	24	0.26
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	24	0.26
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	24	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	24	0.26
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	24	0.26
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	24	0.26
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	24	0.26
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	24	0.26
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	24	0.26
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	3	0.26
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	3	0.26
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	3	0.26
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	28	0.25
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	28	0.25
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	28	0.25
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	7	0.25
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	18	0.25
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	21	0.25
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	13	0.25
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	13	0.25
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	13	0.25
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	14	0.25
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	14	0.25
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	14	0.25
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	22	0.25
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	22	0.25
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	22	0.25
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	26	0.25
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	26	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	2	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	2	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	2	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	5	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	5	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	5	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	10	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	10	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	10	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	19	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	19	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	19	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	20	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	20	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	20	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	27	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	27	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	27	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	28	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	28	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	28	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	29	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	29	0.25
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	29	0.25
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD21	30	0.25
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD22	30	0.25
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD23	30	0.25
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	4	0.25
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	4	0.25
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	4	0.25
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	11	0.25
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	11	0.25
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	11	0.25
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	29	0.25
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	29	0.25
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	29	0.25
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	8	0.25
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	8	0.25
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	8	0.25
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	14	0.25
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	14	0.25
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	14	0.25
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	16	0.24
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	5	0.24
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	5	0.24
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	5	0.24
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	16	0.24
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	16	0.24
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	16	0.24
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	18	0.24
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	18	0.24
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	18	0.24
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	28	0.24
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	28	0.24
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	28	0.24
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	29	0.24
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	29	0.24
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	29	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	27	0.24
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	27	0.24
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	27	0.24
(1,998)	1:62:A:LEU:HD11	1:67:A:TYR:HE1	29	0.24
(1,998)	1:62:A:LEU:HD11	1:67:A:TYR:HE2	29	0.24
(1,998)	1:62:A:LEU:HD12	1:67:A:TYR:HE1	29	0.24
(1,998)	1:62:A:LEU:HD12	1:67:A:TYR:HE2	29	0.24
(1,998)	1:62:A:LEU:HD13	1:67:A:TYR:HE1	29	0.24
(1,998)	1:62:A:LEU:HD13	1:67:A:TYR:HE2	29	0.24
(1,998)	1:62:A:LEU:HD21	1:67:A:TYR:HE1	29	0.24
(1,998)	1:62:A:LEU:HD21	1:67:A:TYR:HE2	29	0.24
(1,998)	1:62:A:LEU:HD22	1:67:A:TYR:HE1	29	0.24
(1,998)	1:62:A:LEU:HD22	1:67:A:TYR:HE2	29	0.24
(1,998)	1:62:A:LEU:HD23	1:67:A:TYR:HE1	29	0.24
(1,998)	1:62:A:LEU:HD23	1:67:A:TYR:HE2	29	0.24
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	26	0.24
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	26	0.24
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	26	0.24
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	24	0.24
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	24	0.24
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	24	0.24
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	27	0.23
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	27	0.23
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	27	0.23
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	26	0.23
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	2	0.23
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	2	0.23
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	2	0.23
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	17	0.23
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	17	0.23
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	17	0.23
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	25	0.23
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	25	0.23
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	25	0.23
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	30	0.23
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	30	0.23
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	30	0.23
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	7	0.23
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	7	0.23
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	7	0.23
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	23	0.23
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	23	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	23	0.23
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD11	16	0.23
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD12	16	0.23
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD13	16	0.23
(1,1225)	1:79:A:VAL:HG21	1:120:A:VAL:HG21	19	0.23
(1,1225)	1:79:A:VAL:HG22	1:120:A:VAL:HG21	19	0.23
(1,1225)	1:79:A:VAL:HG23	1:120:A:VAL:HG21	19	0.23
(1,630)	1:37:A:VAL:HB	1:82:A:LEU:HD11	30	0.23
(1,630)	1:37:A:VAL:HB	1:82:A:LEU:HD12	30	0.23
(1,630)	1:37:A:VAL:HB	1:82:A:LEU:HD13	30	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	2	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	2	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	2	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	5	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	5	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	5	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	12	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	12	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	12	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	13	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	13	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	13	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	15	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	15	0.23
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	15	0.23
(1,126)	1:12:A:LEU:HD21	1:168:A:HIS:H	25	0.23
(1,126)	1:12:A:LEU:HD22	1:168:A:HIS:H	25	0.23
(1,126)	1:12:A:LEU:HD23	1:168:A:HIS:H	25	0.23
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	2	0.22
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	2	0.22
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	2	0.22
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	10	0.22
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	10	0.22
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	10	0.22
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	19	0.22
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	19	0.22
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	19	0.22
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	1	0.22
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	14	0.22
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	7	0.22
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	7	0.22
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	19	0.22
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	19	0.22
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	19	0.22
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	23	0.22
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	23	0.22
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	23	0.22
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	9	0.22
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	23	0.22
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	21	0.22
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	21	0.22
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	21	0.22
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD21	29	0.22
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD22	29	0.22
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD23	29	0.22
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	14	0.22
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	14	0.22
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	14	0.22
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	19	0.21
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	19	0.21
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	20	0.21
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	20	0.21
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	29	0.21
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	1	0.21
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	1	0.21
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	1	0.21
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	20	0.21
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	20	0.21
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	20	0.21
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	21	0.21
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	21	0.21
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	21	0.21
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	24	0.21
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	24	0.21
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	24	0.21
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG21	1	0.21
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG22	1	0.21
(1,1467)	1:94:A:TRP:HA	1:96:A:ILE:HG23	1	0.21
(1,1383)	1:89:A:ILE:HD11	1:90:A:TYR:H	2	0.21
(1,1383)	1:89:A:ILE:HD12	1:90:A:TYR:H	2	0.21
(1,1383)	1:89:A:ILE:HD13	1:90:A:TYR:H	2	0.21
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	27	0.21
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	27	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	27	0.21
(1,415)	1:30:A:LYS:H	1:98:A:TRP:HD1	21	0.21
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	16	0.21
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	16	0.21
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	16	0.21
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	28	0.21
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	28	0.21
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	28	0.21
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	9	0.2
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	9	0.2
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	9	0.2
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	3	0.2
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	14	0.2
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	3	0.2
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	3	0.2
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	3	0.2
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	9	0.2
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	9	0.2
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	9	0.2
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	26	0.2
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	26	0.2
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	26	0.2
(1,1383)	1:89:A:ILE:HD11	1:90:A:TYR:H	22	0.2
(1,1383)	1:89:A:ILE:HD12	1:90:A:TYR:H	22	0.2
(1,1383)	1:89:A:ILE:HD13	1:90:A:TYR:H	22	0.2
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD21	28	0.2
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD22	28	0.2
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD23	28	0.2
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	4	0.2
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	4	0.2
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	4	0.2
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	21	0.2
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	21	0.2
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	21	0.2
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG21	27	0.2
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG22	27	0.2
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG23	27	0.2
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	7	0.19
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	7	0.19
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	10	0.19
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	10	0.19
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	29	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	29	0.19
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	12	0.19
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	12	0.19
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	12	0.19
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	30	0.19
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	30	0.19
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	30	0.19
(1,1760)	1:115:A:GLN:HA	1:115:A:GLN:HG3	22	0.19
(1,1685)	1:111:A:ARG:HD2	1:115:A:GLN:HG3	24	0.19
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	8	0.19
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	8	0.19
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	4	0.19
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	4	0.19
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	4	0.19
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	6	0.19
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	6	0.19
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	6	0.19
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	12	0.19
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	12	0.19
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	12	0.19
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	25	0.19
(1,1057)	1:73:A:LEU:HD21	1:106:A:CYS:H	26	0.19
(1,1057)	1:73:A:LEU:HD22	1:106:A:CYS:H	26	0.19
(1,1057)	1:73:A:LEU:HD23	1:106:A:CYS:H	26	0.19
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	1	0.19
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	1	0.19
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	1	0.19
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	3	0.19
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	3	0.19
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	3	0.19
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	11	0.18
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	11	0.18
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	14	0.18
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	14	0.18
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	28	0.18
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	28	0.18
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	10	0.18
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	10	0.18
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	10	0.18
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	11	0.18
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	11	0.18
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	27	0.18
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	27	0.18
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	27	0.18
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	2	0.18
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	7	0.18
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	8	0.18
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	22	0.18
(1,1383)	1:89:A:ILE:HD11	1:90:A:TYR:H	18	0.18
(1,1383)	1:89:A:ILE:HD12	1:90:A:TYR:H	18	0.18
(1,1383)	1:89:A:ILE:HD13	1:90:A:TYR:H	18	0.18
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD21	20	0.18
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD22	20	0.18
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD23	20	0.18
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	13	0.18
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	13	0.18
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	13	0.18
(1,986)	1:61:A:ASN:HA	1:62:A:LEU:H	10	0.18
(1,619)	1:37:A:VAL:HA	1:51:A:HIS:HE1	2	0.18
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	17	0.18
(1,200)	1:14:A:ASP:H	1:17:A:ILE:HB	7	0.18
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	21	0.18
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	21	0.18
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	21	0.18
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	22	0.18
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	22	0.18
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	22	0.18
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	1	0.17
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	1	0.17
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	12	0.17
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	12	0.17
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	23	0.17
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	23	0.17
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	11	0.17
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	11	0.17
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	11	0.17
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	18	0.17
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	18	0.17
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	18	0.17
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	21	0.17
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	21	0.17
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	21	0.17
(1,1685)	1:111:A:ARG:HD2	1:115:A:GLN:HG3	22	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	6	0.17
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	7	0.17
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	16	0.17
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	18	0.17
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	28	0.17
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	29	0.17
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	3	0.17
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	9	0.17
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	9	0.17
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	10	0.17
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	10	0.17
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	11	0.17
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	11	0.17
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	3	0.17
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	4	0.17
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	12	0.17
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	24	0.17
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD21	15	0.17
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD22	15	0.17
(1,1235)	1:81:A:SER:HA	1:82:A:LEU:HD23	15	0.17
(1,989)	1:61:A:ASN:H	1:63:A:LEU:HD11	29	0.17
(1,989)	1:61:A:ASN:H	1:63:A:LEU:HD12	29	0.17
(1,989)	1:61:A:ASN:H	1:63:A:LEU:HD13	29	0.17
(1,989)	1:61:A:ASN:H	1:63:A:LEU:HD21	29	0.17
(1,989)	1:61:A:ASN:H	1:63:A:LEU:HD22	29	0.17
(1,989)	1:61:A:ASN:H	1:63:A:LEU:HD23	29	0.17
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD21	24	0.17
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD22	24	0.17
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD23	24	0.17
(1,229)	1:16:A:HIS:HD2	1:16:A:HIS:H	3	0.17
(1,229)	1:16:A:HIS:HD2	1:16:A:HIS:H	23	0.17
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	22	0.17
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	22	0.17
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	22	0.17
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	23	0.17
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	23	0.17
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	23	0.17
(1,124)	1:12:A:LEU:HD11	1:168:A:HIS:HD2	7	0.17
(1,124)	1:12:A:LEU:HD12	1:168:A:HIS:HD2	7	0.17
(1,124)	1:12:A:LEU:HD13	1:168:A:HIS:HD2	7	0.17
(1,124)	1:12:A:LEU:HD21	1:168:A:HIS:HD2	7	0.17
(1,124)	1:12:A:LEU:HD22	1:168:A:HIS:HD2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:12:A:LEU:HD23	1:168:A:HIS:HD2	7	0.17
(1,104)	1:12:A:LEU:HD21	1:12:A:LEU:H	20	0.17
(1,104)	1:12:A:LEU:HD22	1:12:A:LEU:H	20	0.17
(1,104)	1:12:A:LEU:HD23	1:12:A:LEU:H	20	0.17
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	11	0.16
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	26	0.16
(1,2568)	1:179:A:LEU:HG	1:182:A:HIS:HB2	23	0.16
(1,2568)	1:179:A:LEU:HG	1:182:A:HIS:HB3	23	0.16
(1,2557)	1:178:A:GLY:H	1:182:A:HIS:HD2	23	0.16
(1,2556)	1:178:A:GLY:H	1:179:A:LEU:H	11	0.16
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	2	0.16
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	2	0.16
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	9	0.16
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	9	0.16
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	24	0.16
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	24	0.16
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	24	0.16
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	26	0.16
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	26	0.16
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	26	0.16
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	4	0.16
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	24	0.16
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	1	0.16
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	6	0.16
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	20	0.16
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	21	0.16
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	26	0.16
(1,1060)	1:73:A:LEU:HG	1:73:A:LEU:H	22	0.16
(1,619)	1:37:A:VAL:HA	1:51:A:HIS:HE1	12	0.16
(1,619)	1:37:A:VAL:HA	1:51:A:HIS:HE1	20	0.16
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	13	0.16
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	20	0.16
(1,415)	1:30:A:LYS:H	1:98:A:TRP:HD1	4	0.16
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	5	0.16
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	5	0.16
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	5	0.16
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	8	0.16
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	8	0.16
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	8	0.16
(1,124)	1:12:A:LEU:HD11	1:168:A:HIS:HD2	17	0.16
(1,124)	1:12:A:LEU:HD12	1:168:A:HIS:HD2	17	0.16
(1,124)	1:12:A:LEU:HD13	1:168:A:HIS:HD2	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:12:A:LEU:HD21	1:168:A:HIS:HD2	17	0.16
(1,124)	1:12:A:LEU:HD22	1:168:A:HIS:HD2	17	0.16
(1,124)	1:12:A:LEU:HD23	1:168:A:HIS:HD2	17	0.16
(2,100)	1:114:A:LEU:O	1:118:A:THR:N	2	0.15
(2,83)	1:105:A:GLY:O	1:109:A:GLU:H	27	0.15
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	1	0.15
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	4	0.15
(1,2568)	1:179:A:LEU:HG	1:182:A:HIS:HB2	15	0.15
(1,2568)	1:179:A:LEU:HG	1:182:A:HIS:HB3	15	0.15
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	3	0.15
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	3	0.15
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	3	0.15
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	4	0.15
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	4	0.15
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	4	0.15
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	8	0.15
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	8	0.15
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	8	0.15
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	13	0.15
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	13	0.15
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	13	0.15
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	17	0.15
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	17	0.15
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	17	0.15
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	25	0.15
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	25	0.15
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	25	0.15
(1,1978)	1:129:A:ILE:HB	1:131:A:ASP:H	29	0.15
(1,1761)	1:115:A:GLN:HA	1:115:A:GLN:HG2	24	0.15
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	21	0.15
(1,1564)	1:98:A:TRP:HZ3	1:130:A:TYR:HA	24	0.15
(1,1194)	1:78:A:LEU:HG	1:79:A:VAL:H	15	0.15
(1,738)	1:40:A:LEU:HD11	1:89:A:ILE:HB	12	0.15
(1,738)	1:40:A:LEU:HD12	1:89:A:ILE:HB	12	0.15
(1,738)	1:40:A:LEU:HD13	1:89:A:ILE:HB	12	0.15
(1,738)	1:40:A:LEU:HD21	1:89:A:ILE:HB	12	0.15
(1,738)	1:40:A:LEU:HD22	1:89:A:ILE:HB	12	0.15
(1,738)	1:40:A:LEU:HD23	1:89:A:ILE:HB	12	0.15
(1,685)	1:39:A:ARG:HA	1:90:A:TYR:H	29	0.15
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD21	5	0.15
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD22	5	0.15
(1,631)	1:37:A:VAL:HB	1:82:A:LEU:HD23	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:37:A:VAL:HA	1:51:A:HIS:HE1	15	0.15
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	9	0.15
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	10	0.15
(1,226)	1:16:A:HIS:HB2	1:17:A:ILE:HG21	3	0.15
(1,226)	1:16:A:HIS:HB2	1:17:A:ILE:HG22	3	0.15
(1,226)	1:16:A:HIS:HB2	1:17:A:ILE:HG23	3	0.15
(1,226)	1:16:A:HIS:HB3	1:17:A:ILE:HG21	3	0.15
(1,226)	1:16:A:HIS:HB3	1:17:A:ILE:HG22	3	0.15
(1,226)	1:16:A:HIS:HB3	1:17:A:ILE:HG23	3	0.15
(1,145)	1:13:A:MET:HA	1:166:A:VAL:HG11	22	0.15
(1,145)	1:13:A:MET:HA	1:166:A:VAL:HG12	22	0.15
(1,145)	1:13:A:MET:HA	1:166:A:VAL:HG13	22	0.15
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	1	0.15
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	1	0.15
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	1	0.15
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	2	0.14
(1,2568)	1:179:A:LEU:HG	1:182:A:HIS:HB2	9	0.14
(1,2568)	1:179:A:LEU:HG	1:182:A:HIS:HB3	9	0.14
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	18	0.14
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	18	0.14
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	23	0.14
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	23	0.14
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	23	0.14
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	29	0.14
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	29	0.14
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	29	0.14
(1,2366)	1:162:A:TRP:HZ2	1:171:A:CYS:H	7	0.14
(1,2115)	1:143:A:LEU:HD12	1:143:A:LEU:H	23	0.14
(1,1543)	1:96:A:ILE:HG21	1:128:A:ARG:H	8	0.14
(1,1543)	1:96:A:ILE:HG22	1:128:A:ARG:H	8	0.14
(1,1543)	1:96:A:ILE:HG23	1:128:A:ARG:H	8	0.14
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	1	0.14
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	1	0.14
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	10	0.14
(1,990)	1:61:A:ASN:H	1:66:A:PHE:HB2	26	0.14
(1,990)	1:61:A:ASN:H	1:66:A:PHE:HB3	26	0.14
(1,895)	1:51:A:HIS:HE1	1:84:A:LEU:HG	24	0.14
(1,630)	1:37:A:VAL:HB	1:82:A:LEU:HD11	29	0.14
(1,630)	1:37:A:VAL:HB	1:82:A:LEU:HD12	29	0.14
(1,630)	1:37:A:VAL:HB	1:82:A:LEU:HD13	29	0.14
(1,230)	1:16:A:HIS:HD2	1:17:A:ILE:HD11	11	0.14
(1,230)	1:16:A:HIS:HD2	1:17:A:ILE:HD12	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:16:A:HIS:HD2	1:17:A:ILE:HD13	11	0.14
(1,206)	1:15:A:PRO:HA	1:162:A:TRP:HE1	1	0.14
(1,206)	1:15:A:PRO:HA	1:162:A:TRP:HE1	7	0.14
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	9	0.14
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	9	0.14
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	9	0.14
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG21	25	0.14
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG22	25	0.14
(1,134)	1:12:A:LEU:HG	1:166:A:VAL:HG23	25	0.14
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	7	0.14
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	7	0.14
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	7	0.14
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	29	0.14
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	29	0.14
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	29	0.14
(1,124)	1:12:A:LEU:HD11	1:168:A:HIS:HD2	10	0.14
(1,124)	1:12:A:LEU:HD12	1:168:A:HIS:HD2	10	0.14
(1,124)	1:12:A:LEU:HD13	1:168:A:HIS:HD2	10	0.14
(1,124)	1:12:A:LEU:HD21	1:168:A:HIS:HD2	10	0.14
(1,124)	1:12:A:LEU:HD22	1:168:A:HIS:HD2	10	0.14
(1,124)	1:12:A:LEU:HD23	1:168:A:HIS:HD2	10	0.14
(1,124)	1:12:A:LEU:HD11	1:168:A:HIS:HD2	11	0.14
(1,124)	1:12:A:LEU:HD12	1:168:A:HIS:HD2	11	0.14
(1,124)	1:12:A:LEU:HD13	1:168:A:HIS:HD2	11	0.14
(1,124)	1:12:A:LEU:HD21	1:168:A:HIS:HD2	11	0.14
(1,124)	1:12:A:LEU:HD22	1:168:A:HIS:HD2	11	0.14
(1,124)	1:12:A:LEU:HD23	1:168:A:HIS:HD2	11	0.14
(1,124)	1:12:A:LEU:HD11	1:168:A:HIS:HD2	20	0.14
(1,124)	1:12:A:LEU:HD12	1:168:A:HIS:HD2	20	0.14
(1,124)	1:12:A:LEU:HD13	1:168:A:HIS:HD2	20	0.14
(1,124)	1:12:A:LEU:HD21	1:168:A:HIS:HD2	20	0.14
(1,124)	1:12:A:LEU:HD22	1:168:A:HIS:HD2	20	0.14
(1,124)	1:12:A:LEU:HD23	1:168:A:HIS:HD2	20	0.14
(1,104)	1:12:A:LEU:HD21	1:12:A:LEU:H	12	0.14
(1,104)	1:12:A:LEU:HD22	1:12:A:LEU:H	12	0.14
(1,104)	1:12:A:LEU:HD23	1:12:A:LEU:H	12	0.14
(2,100)	1:114:A:LEU:O	1:118:A:THR:N	23	0.13
(2,99)	1:114:A:LEU:O	1:118:A:THR:H	24	0.13
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	9	0.13
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	25	0.13
(2,43)	1:92:A:VAL:O	1:123:A:ARG:H	5	0.13
(2,35)	1:32:A:TYR:O	1:97:A:SER:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:32:A:TYR:O	1:97:A:SER:H	23	0.13
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	13	0.13
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	13	0.13
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	21	0.13
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	21	0.13
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	26	0.13
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	26	0.13
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	30	0.13
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	30	0.13
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	20	0.13
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	20	0.13
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	20	0.13
(1,1685)	1:111:A:ARG:HD2	1:115:A:GLN:HG3	9	0.13
(1,1639)	1:108:A:GLY:HA3	1:112:A:ALA:H	2	0.13
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	1	0.13
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	22	0.13
(1,1583)	1:102:A:PHE:HE1	1:142:A:MET:HE1	4	0.13
(1,1583)	1:102:A:PHE:HE1	1:142:A:MET:HE2	4	0.13
(1,1583)	1:102:A:PHE:HE1	1:142:A:MET:HE3	4	0.13
(1,1583)	1:102:A:PHE:HE2	1:142:A:MET:HE1	4	0.13
(1,1583)	1:102:A:PHE:HE2	1:142:A:MET:HE2	4	0.13
(1,1583)	1:102:A:PHE:HE2	1:142:A:MET:HE3	4	0.13
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	8	0.13
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	8	0.13
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	12	0.13
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	12	0.13
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	15	0.13
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	15	0.13
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	11	0.13
(1,1389)	1:89:A:ILE:HG13	1:90:A:TYR:H	15	0.13
(1,1383)	1:89:A:ILE:HD11	1:90:A:TYR:H	13	0.13
(1,1383)	1:89:A:ILE:HD12	1:90:A:TYR:H	13	0.13
(1,1383)	1:89:A:ILE:HD13	1:90:A:TYR:H	13	0.13
(1,1284)	1:83:A:GLN:HG2	1:83:A:GLN:H	1	0.13
(1,1284)	1:83:A:GLN:HG3	1:83:A:GLN:H	1	0.13
(1,1224)	1:79:A:VAL:HG11	1:120:A:VAL:HG21	19	0.13
(1,1224)	1:79:A:VAL:HG12	1:120:A:VAL:HG21	19	0.13
(1,1224)	1:79:A:VAL:HG13	1:120:A:VAL:HG21	19	0.13
(1,748)	1:40:A:LEU:H	1:89:A:ILE:HB	12	0.13
(1,619)	1:37:A:VAL:HA	1:51:A:HIS:HE1	19	0.13
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	29	0.13
(1,386)	1:26:A:ILE:HD11	1:28:A:ARG:HE	21	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:26:A:ILE:HD12	1:28:A:ARG:HE	21	0.13
(1,386)	1:26:A:ILE:HD13	1:28:A:ARG:HE	21	0.13
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG21	20	0.13
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG22	20	0.13
(1,136)	1:12:A:LEU:H	1:166:A:VAL:HG23	20	0.13
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG11	30	0.13
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG12	30	0.13
(1,133)	1:12:A:LEU:HG	1:166:A:VAL:HG13	30	0.13
(1,126)	1:12:A:LEU:HD21	1:168:A:HIS:H	27	0.13
(1,126)	1:12:A:LEU:HD22	1:168:A:HIS:H	27	0.13
(1,126)	1:12:A:LEU:HD23	1:168:A:HIS:H	27	0.13
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	4	0.13
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	4	0.13
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	4	0.13
(1,124)	1:12:A:LEU:HD11	1:168:A:HIS:HD2	2	0.13
(1,124)	1:12:A:LEU:HD12	1:168:A:HIS:HD2	2	0.13
(1,124)	1:12:A:LEU:HD13	1:168:A:HIS:HD2	2	0.13
(1,124)	1:12:A:LEU:HD21	1:168:A:HIS:HD2	2	0.13
(1,124)	1:12:A:LEU:HD22	1:168:A:HIS:HD2	2	0.13
(1,124)	1:12:A:LEU:HD23	1:168:A:HIS:HD2	2	0.13
(1,124)	1:12:A:LEU:HD11	1:168:A:HIS:HD2	19	0.13
(1,124)	1:12:A:LEU:HD12	1:168:A:HIS:HD2	19	0.13
(1,124)	1:12:A:LEU:HD13	1:168:A:HIS:HD2	19	0.13
(1,124)	1:12:A:LEU:HD21	1:168:A:HIS:HD2	19	0.13
(1,124)	1:12:A:LEU:HD22	1:168:A:HIS:HD2	19	0.13
(1,124)	1:12:A:LEU:HD23	1:168:A:HIS:HD2	19	0.13
(1,124)	1:12:A:LEU:HD11	1:168:A:HIS:HD2	27	0.13
(1,124)	1:12:A:LEU:HD12	1:168:A:HIS:HD2	27	0.13
(1,124)	1:12:A:LEU:HD13	1:168:A:HIS:HD2	27	0.13
(1,124)	1:12:A:LEU:HD21	1:168:A:HIS:HD2	27	0.13
(1,124)	1:12:A:LEU:HD22	1:168:A:HIS:HD2	27	0.13
(1,124)	1:12:A:LEU:HD23	1:168:A:HIS:HD2	27	0.13
(2,100)	1:114:A:LEU:O	1:118:A:THR:N	9	0.12
(2,100)	1:114:A:LEU:O	1:118:A:THR:N	12	0.12
(2,100)	1:114:A:LEU:O	1:118:A:THR:N	24	0.12
(2,100)	1:114:A:LEU:O	1:118:A:THR:N	26	0.12
(2,99)	1:114:A:LEU:O	1:118:A:THR:H	2	0.12
(2,99)	1:114:A:LEU:O	1:118:A:THR:H	5	0.12
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	10	0.12
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	19	0.12
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	20	0.12
(2,37)	1:119:A:HIS:O	1:90:A:TYR:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:32:A:TYR:O	1:97:A:SER:H	17	0.12
(1,2785)	1:195:A:GLN:HG2	1:195:A:GLN:H	19	0.12
(1,2785)	1:195:A:GLN:HG3	1:195:A:GLN:H	19	0.12
(1,2557)	1:178:A:GLY:H	1:182:A:HIS:HD2	15	0.12
(1,2429)	1:168:A:HIS:H	1:169:A:GLN:H	28	0.12
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	5	0.12
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	5	0.12
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	5	0.12
(1,1785)	1:115:A:GLN:HG3	1:116:A:GLU:H	9	0.12
(1,1599)	1:104:A:TRP:HE1	1:108:A:GLY:HA2	24	0.12
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	19	0.12
(1,1564)	1:98:A:TRP:HZ3	1:130:A:TYR:HA	17	0.12
(1,1564)	1:98:A:TRP:HZ3	1:130:A:TYR:HA	19	0.12
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	3	0.12
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	3	0.12
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	21	0.12
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	21	0.12
(1,1486)	1:94:A:TRP:HE3	1:125:A:PHE:H	19	0.12
(1,1111)	1:75:A:PHE:HZ	1:122:A:LEU:HD21	29	0.12
(1,1111)	1:75:A:PHE:HZ	1:122:A:LEU:HD22	29	0.12
(1,1111)	1:75:A:PHE:HZ	1:122:A:LEU:HD23	29	0.12
(1,859)	1:48:A:MET:HA	1:48:A:MET:HE1	29	0.12
(1,859)	1:48:A:MET:HA	1:48:A:MET:HE2	29	0.12
(1,859)	1:48:A:MET:HA	1:48:A:MET:HE3	29	0.12
(1,619)	1:37:A:VAL:HA	1:51:A:HIS:HE1	24	0.12
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	18	0.12
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	25	0.12
(1,425)	1:31:A:THR:HG21	1:98:A:TRP:HD1	17	0.12
(1,425)	1:31:A:THR:HG22	1:98:A:TRP:HD1	17	0.12
(1,425)	1:31:A:THR:HG23	1:98:A:TRP:HD1	17	0.12
(1,419)	1:31:A:THR:HG21	1:31:A:THR:H	9	0.12
(1,419)	1:31:A:THR:HG22	1:31:A:THR:H	9	0.12
(1,419)	1:31:A:THR:HG23	1:31:A:THR:H	9	0.12
(1,206)	1:15:A:PRO:HA	1:162:A:TRP:HE1	13	0.12
(1,145)	1:13:A:MET:HA	1:166:A:VAL:HG11	9	0.12
(1,145)	1:13:A:MET:HA	1:166:A:VAL:HG12	9	0.12
(1,145)	1:13:A:MET:HA	1:166:A:VAL:HG13	9	0.12
(1,126)	1:12:A:LEU:HD21	1:168:A:HIS:H	17	0.12
(1,126)	1:12:A:LEU:HD22	1:168:A:HIS:H	17	0.12
(1,126)	1:12:A:LEU:HD23	1:168:A:HIS:H	17	0.12
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	13	0.12
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	13	0.12
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	16	0.12
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	16	0.12
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	16	0.12
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	20	0.12
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	20	0.12
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	20	0.12
(1,124)	1:12:A:LEU:HD11	1:168:A:HIS:HD2	15	0.12
(1,124)	1:12:A:LEU:HD12	1:168:A:HIS:HD2	15	0.12
(1,124)	1:12:A:LEU:HD13	1:168:A:HIS:HD2	15	0.12
(1,124)	1:12:A:LEU:HD21	1:168:A:HIS:HD2	15	0.12
(1,124)	1:12:A:LEU:HD22	1:168:A:HIS:HD2	15	0.12
(1,124)	1:12:A:LEU:HD23	1:168:A:HIS:HD2	15	0.12
(1,104)	1:12:A:LEU:HD21	1:12:A:LEU:H	9	0.12
(1,104)	1:12:A:LEU:HD22	1:12:A:LEU:H	9	0.12
(1,104)	1:12:A:LEU:HD23	1:12:A:LEU:H	9	0.12
(2,100)	1:114:A:LEU:O	1:118:A:THR:N	11	0.11
(2,100)	1:114:A:LEU:O	1:118:A:THR:N	22	0.11
(2,83)	1:105:A:GLY:O	1:109:A:GLU:H	17	0.11
(2,83)	1:105:A:GLY:O	1:109:A:GLU:H	24	0.11
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	6	0.11
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	12	0.11
(2,35)	1:32:A:TYR:O	1:97:A:SER:H	10	0.11
(2,35)	1:32:A:TYR:O	1:97:A:SER:H	20	0.11
(2,35)	1:32:A:TYR:O	1:97:A:SER:H	28	0.11
(2,35)	1:32:A:TYR:O	1:97:A:SER:H	29	0.11
(1,2789)	1:195:A:GLN:H	1:196:A:ASN:H	15	0.11
(1,2366)	1:162:A:TRP:HZ2	1:171:A:CYS:H	6	0.11
(1,2366)	1:162:A:TRP:HZ2	1:171:A:CYS:H	30	0.11
(1,1778)	1:115:A:GLN:HE21	1:115:A:GLN:HE22	9	0.11
(1,1687)	1:111:A:ARG:HD2	1:142:A:MET:HE1	2	0.11
(1,1687)	1:111:A:ARG:HD2	1:142:A:MET:HE2	2	0.11
(1,1687)	1:111:A:ARG:HD2	1:142:A:MET:HE3	2	0.11
(1,1684)	1:111:A:ARG:HD3	1:115:A:GLN:HG3	22	0.11
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	10	0.11
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	27	0.11
(1,1584)	1:102:A:PHE:H	1:103:A:SER:H	26	0.11
(1,1564)	1:98:A:TRP:HZ3	1:130:A:TYR:HA	3	0.11
(1,1564)	1:98:A:TRP:HZ3	1:130:A:TYR:HA	22	0.11
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	5	0.11
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	5	0.11
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	20	0.11
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	22	0.11
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	22	0.11
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	25	0.11
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	25	0.11
(1,1480)	1:94:A:TRP:HH2	1:96:A:ILE:HD11	23	0.11
(1,1480)	1:94:A:TRP:HH2	1:96:A:ILE:HD12	23	0.11
(1,1480)	1:94:A:TRP:HH2	1:96:A:ILE:HD13	23	0.11
(1,1389)	1:89:A:ILE:HG13	1:90:A:TYR:H	9	0.11
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD11	8	0.11
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD12	8	0.11
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD13	8	0.11
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD11	13	0.11
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD12	13	0.11
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD13	13	0.11
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD11	21	0.11
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD12	21	0.11
(1,1234)	1:81:A:SER:HA	1:82:A:LEU:HD13	21	0.11
(1,751)	1:40:A:LEU:H	1:89:A:ILE:HG21	12	0.11
(1,751)	1:40:A:LEU:H	1:89:A:ILE:HG22	12	0.11
(1,751)	1:40:A:LEU:H	1:89:A:ILE:HG23	12	0.11
(1,619)	1:37:A:VAL:HA	1:51:A:HIS:HE1	7	0.11
(1,509)	1:33:A:LEU:HG	1:72:A:GLU:H	2	0.11
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	5	0.11
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	19	0.11
(1,405)	1:28:A:ARG:HE	1:31:A:THR:HG21	24	0.11
(1,405)	1:28:A:ARG:HE	1:31:A:THR:HG22	24	0.11
(1,405)	1:28:A:ARG:HE	1:31:A:THR:HG23	24	0.11
(1,360)	1:24:A:ASN:HB2	1:24:A:ASN:HD22	26	0.11
(1,226)	1:16:A:HIS:HB2	1:17:A:ILE:HG21	23	0.11
(1,226)	1:16:A:HIS:HB2	1:17:A:ILE:HG22	23	0.11
(1,226)	1:16:A:HIS:HB2	1:17:A:ILE:HG23	23	0.11
(1,226)	1:16:A:HIS:HB3	1:17:A:ILE:HG21	23	0.11
(1,226)	1:16:A:HIS:HB3	1:17:A:ILE:HG22	23	0.11
(1,226)	1:16:A:HIS:HB3	1:17:A:ILE:HG23	23	0.11
(1,206)	1:15:A:PRO:HA	1:162:A:TRP:HE1	20	0.11
(1,125)	1:12:A:LEU:HD11	1:168:A:HIS:H	3	0.11
(1,125)	1:12:A:LEU:HD12	1:168:A:HIS:H	3	0.11
(1,125)	1:12:A:LEU:HD13	1:168:A:HIS:H	3	0.11
(2,123)	1:159:A:LYS:O	1:163:A:ASP:H	12	0.1
(2,100)	1:114:A:LEU:O	1:118:A:THR:N	17	0.1
(2,99)	1:114:A:LEU:O	1:118:A:THR:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,96)	1:111:A:ARG:O	1:115:A:GLN:N	2	0.1
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	3	0.1
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	7	0.1
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	22	0.1
(2,47)	1:94:A:TRP:O	1:125:A:PHE:H	24	0.1
(2,19)	1:31:A:THR:O	1:57:A:ASN:H	2	0.1
(1,2557)	1:178:A:GLY:H	1:182:A:HIS:HD2	9	0.1
(1,2447)	1:169:A:GLN:HE22	1:169:A:GLN:HG2	24	0.1
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	5	0.1
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	5	0.1
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA2	22	0.1
(1,2426)	1:168:A:HIS:HD2	1:170:A:GLY:HA3	22	0.1
(1,2412)	1:166:A:VAL:HG21	1:169:A:GLN:H	1	0.1
(1,2412)	1:166:A:VAL:HG22	1:169:A:GLN:H	1	0.1
(1,2412)	1:166:A:VAL:HG23	1:169:A:GLN:H	1	0.1
(1,1978)	1:129:A:ILE:HB	1:131:A:ASP:H	21	0.1
(1,1778)	1:115:A:GLN:HE21	1:115:A:GLN:HE22	22	0.1
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	20	0.1
(1,1585)	1:102:A:PHE:H	1:104:A:TRP:H	30	0.1
(1,1564)	1:98:A:TRP:HZ3	1:130:A:TYR:HA	7	0.1
(1,1564)	1:98:A:TRP:HZ3	1:130:A:TYR:HA	27	0.1
(1,1558)	1:98:A:TRP:HE3	1:130:A:TYR:HA	4	0.1
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	2	0.1
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	2	0.1
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE1	7	0.1
(1,1506)	1:95:A:PHE:HA	1:125:A:PHE:HE2	7	0.1
(1,1390)	1:89:A:ILE:HG12	1:90:A:TYR:H	10	0.1
(1,1389)	1:89:A:ILE:HG13	1:90:A:TYR:H	25	0.1
(1,1242)	1:81:A:SER:H	1:82:A:LEU:HD11	5	0.1
(1,1242)	1:81:A:SER:H	1:82:A:LEU:HD12	5	0.1
(1,1242)	1:81:A:SER:H	1:82:A:LEU:HD13	5	0.1
(1,999)	1:63:A:LEU:HA	1:63:A:LEU:HD11	26	0.1
(1,999)	1:63:A:LEU:HA	1:63:A:LEU:HD12	26	0.1
(1,999)	1:63:A:LEU:HA	1:63:A:LEU:HD13	26	0.1
(1,685)	1:39:A:ARG:HA	1:90:A:TYR:H	24	0.1
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	4	0.1
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	11	0.1
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	14	0.1
(1,433)	1:31:A:THR:H	1:98:A:TRP:HZ3	22	0.1
(1,361)	1:24:A:ASN:HD21	1:24:A:ASN:HD22	8	0.1
(1,206)	1:15:A:PRO:HA	1:162:A:TRP:HE1	11	0.1
(1,185)	1:13:A:MET:HE1	1:167:A:ASP:H	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:13:A:MET:HE2	1:167:A:ASP:H	11	0.1
(1,185)	1:13:A:MET:HE3	1:167:A:ASP:H	11	0.1
(1,154)	1:13:A:MET:HB2	1:54:A:PHE:HD1	24	0.1
(1,154)	1:13:A:MET:HB2	1:54:A:PHE:HD2	24	0.1
(1,154)	1:13:A:MET:HB3	1:54:A:PHE:HD1	24	0.1
(1,154)	1:13:A:MET:HB3	1:54:A:PHE:HD2	24	0.1
(1,124)	1:12:A:LEU:HD11	1:168:A:HIS:HD2	18	0.1
(1,124)	1:12:A:LEU:HD12	1:168:A:HIS:HD2	18	0.1
(1,124)	1:12:A:LEU:HD13	1:168:A:HIS:HD2	18	0.1
(1,124)	1:12:A:LEU:HD21	1:168:A:HIS:HD2	18	0.1
(1,124)	1:12:A:LEU:HD22	1:168:A:HIS:HD2	18	0.1
(1,124)	1:12:A:LEU:HD23	1:168:A:HIS:HD2	18	0.1
(1,104)	1:12:A:LEU:HD21	1:12:A:LEU:H	7	0.1
(1,104)	1:12:A:LEU:HD22	1:12:A:LEU:H	7	0.1
(1,104)	1:12:A:LEU:HD23	1:12:A:LEU:H	7	0.1
(1,104)	1:12:A:LEU:HD21	1:12:A:LEU:H	11	0.1
(1,104)	1:12:A:LEU:HD22	1:12:A:LEU:H	11	0.1
(1,104)	1:12:A:LEU:HD23	1:12:A:LEU:H	11	0.1

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

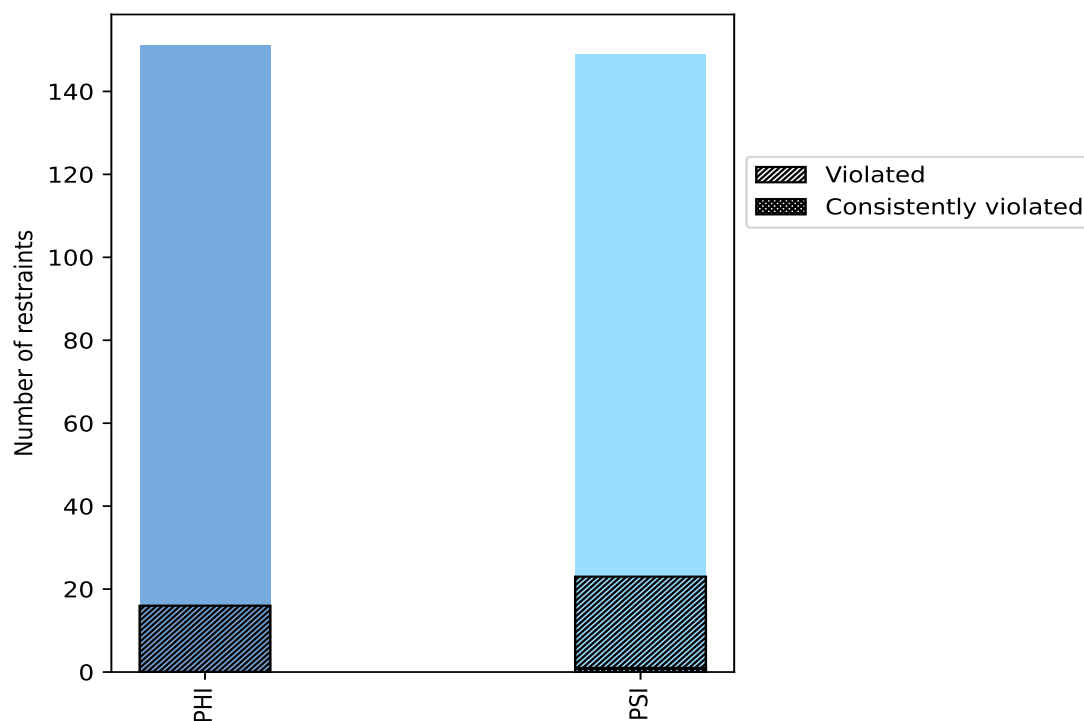
10.1 Summary of dihedral-angle violations [i](#)

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	151	50.3	16	10.6	5.3	0	0.0	0.0
PSI	149	49.7	23	15.4	7.7	1	0.7	0.3
Total	300	100.0	39	13.0	13.0	1	0.3	0.3

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](#)



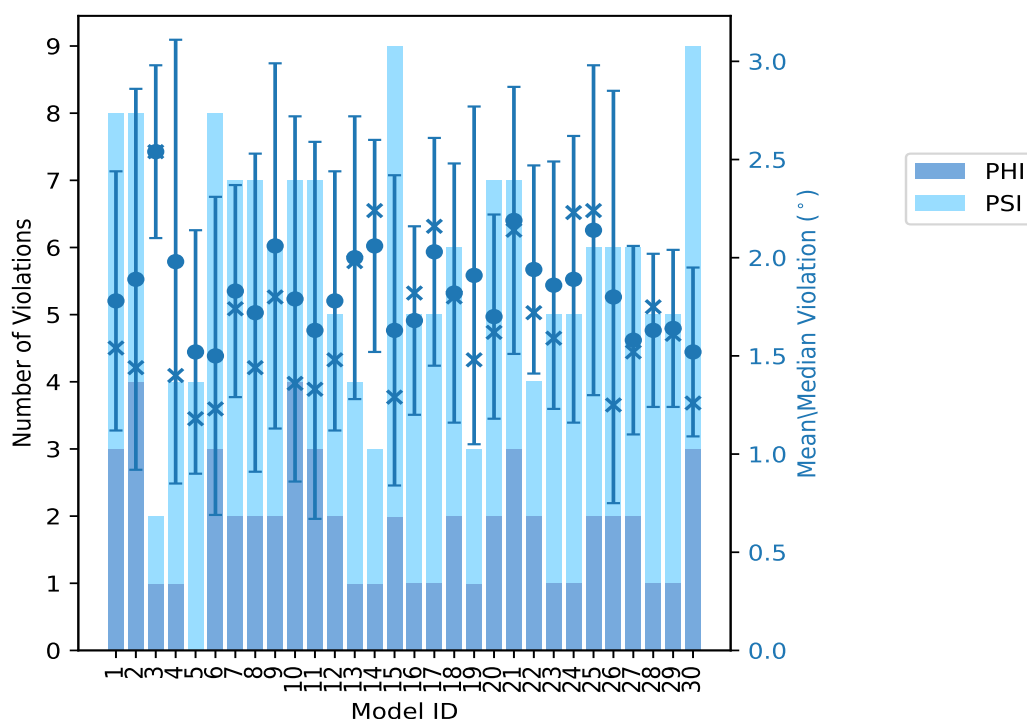
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	3	5	8	1.78	3.3	0.66	1.54
2	4	4	8	1.89	3.83	0.97	1.44
3	1	1	2	2.54	2.97	0.44	2.54
4	1	3	4	1.98	3.94	1.13	1.4
5	0	4	4	1.52	2.59	0.62	1.18
6	3	5	8	1.5	3.63	0.81	1.23
7	2	5	7	1.83	2.91	0.54	1.74
8	2	5	7	1.72	3.63	0.81	1.44
9	2	4	6	2.06	3.97	0.93	1.8
10	4	3	7	1.79	3.84	0.93	1.36
11	3	4	7	1.63	3.96	0.96	1.33
12	2	3	5	1.78	3.08	0.66	1.48
13	1	3	4	2.0	2.84	0.72	1.98
14	1	2	3	2.06	2.62	0.54	2.24
15	2	7	9	1.63	3.62	0.79	1.29
16	1	4	5	1.68	2.31	0.48	1.82
17	1	4	5	2.03	2.82	0.58	2.16
18	2	4	6	1.82	2.91	0.66	1.8
19	1	2	3	1.91	3.11	0.86	1.48
20	2	5	7	1.7	2.89	0.52	1.62
21	3	4	7	2.19	3.14	0.68	2.14
22	2	2	4	1.94	2.82	0.53	1.72
23	1	4	5	1.86	2.83	0.63	1.59
24	1	4	5	1.89	2.84	0.73	2.23
25	2	4	6	2.14	3.39	0.84	2.24
26	2	4	6	1.8	4.03	1.05	1.25
27	2	4	6	1.58	2.49	0.48	1.52
28	1	4	5	1.63	2.08	0.39	1.75
29	1	4	5	1.64	2.23	0.4	1.61
30	3	6	9	1.52	2.24	0.43	1.26

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
8	13	21	1	3.3
1	3	4	2	6.7
1	0	1	3	10.0
1	0	1	4	13.3
3	1	4	5	16.7
0	0	0	6	20.0
0	1	1	7	23.3
1	1	2	8	26.7
0	0	0	9	30.0
0	1	1	10	33.3
0	0	0	11	36.7

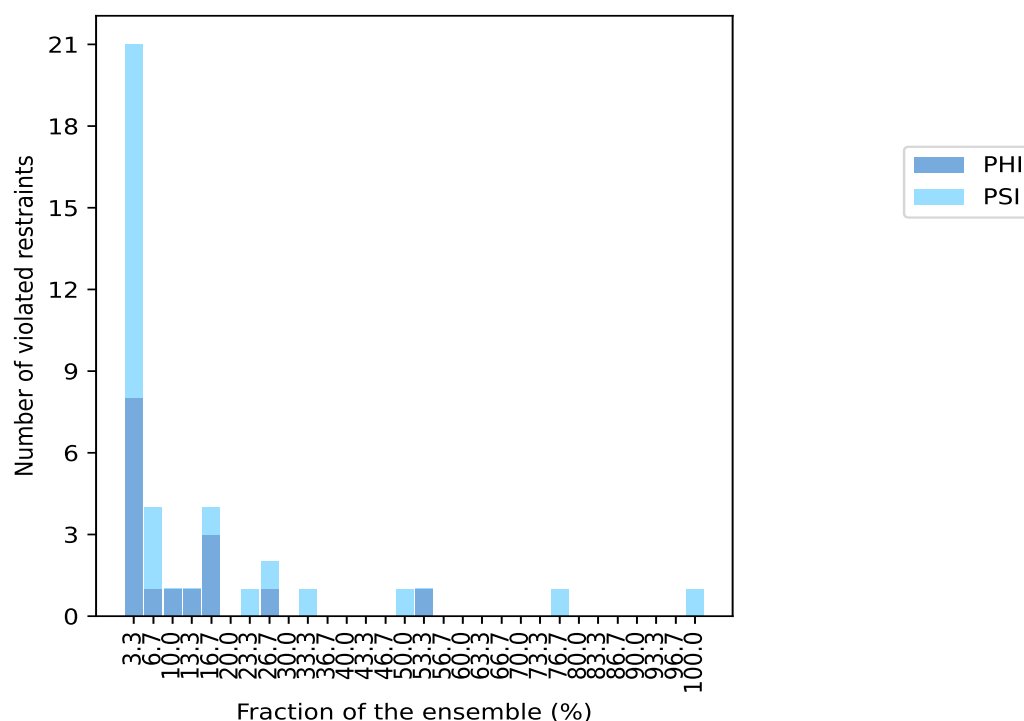
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	40.0
0	0	0	13	43.3
0	0	0	14	46.7
0	1	1	15	50.0
1	0	1	16	53.3
0	0	0	17	56.7
0	0	0	18	60.0
0	0	0	19	63.3
0	0	0	20	66.7
0	0	0	21	70.0
0	0	0	22	73.3
0	1	1	23	76.7
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	1	1	30	100.0

¹ Number of models with violations

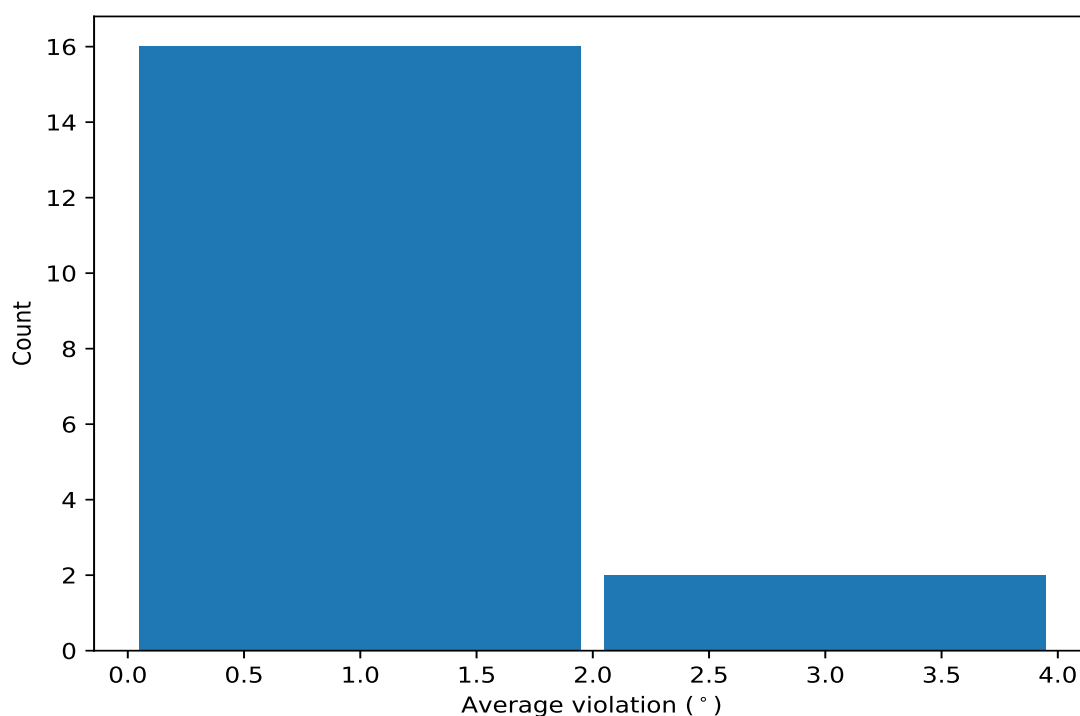
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

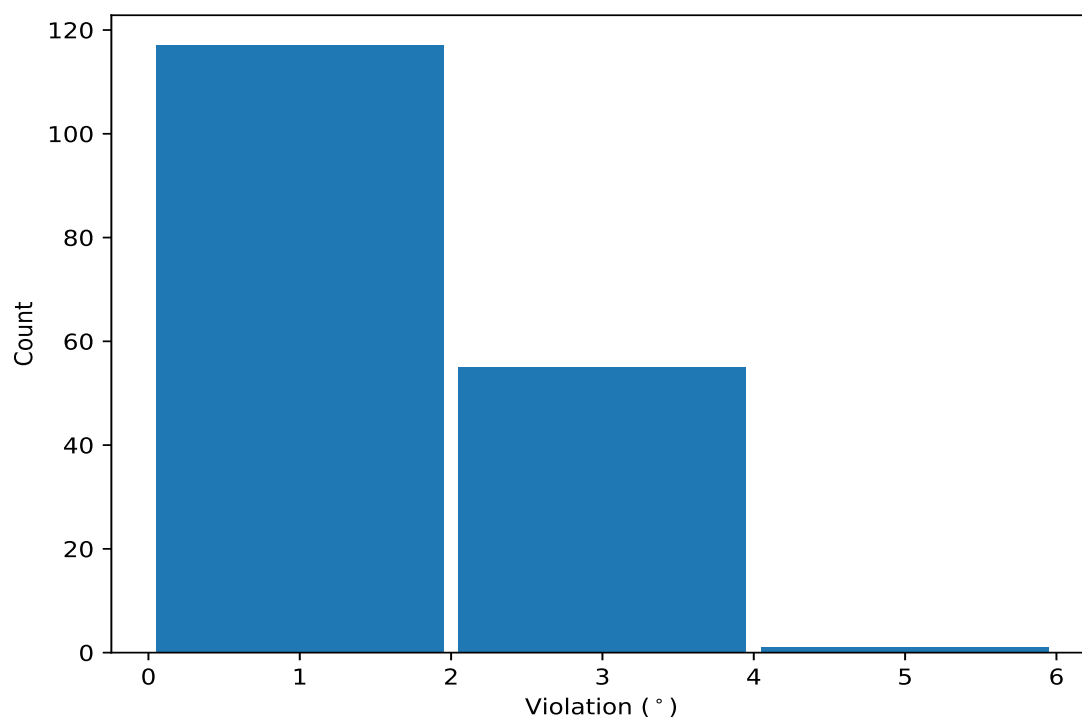
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	30	3.04	0.6	2.94
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	23	1.32	0.15	1.33
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	16	1.57	0.38	1.48
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	15	2.08	0.6	2.23
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:MET:N	10	1.64	0.43	1.61
(1,3)	1:12:A:LEU:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	8	1.83	0.63	1.52
(1,144)	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	1:104:A:TRP:N	8	1.69	0.39	1.9
(1,99)	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	1:78:A:LEU:N	7	1.96	0.43	2.13
(1,147)	1:104:A:TRP:C	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	5	1.44	0.15	1.36
(1,137)	1:97:A:SER:C	1:98:A:TRP:N	1:98:A:TRP:CA	1:98:A:TRP:C	5	1.36	0.24	1.33
(1,149)	1:105:A:GLY:C	1:106:A:CYS:N	1:106:A:CYS:CA	1:106:A:CYS:C	5	1.17	0.14	1.12
(1,252)	1:165:A:PHE:N	1:165:A:PHE:CA	1:165:A:PHE:C	1:166:A:VAL:N	5	1.12	0.14	1.05
(1,181)	1:123:A:ARG:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	4	1.27	0.22	1.18
(1,27)	1:30:A:LYS:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	3	1.71	0.83	1.19
(1,4)	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	1:14:A:ASP:N	2	1.68	0.55	1.68
(1,73)	1:62:A:LEU:N	1:62:A:LEU:CA	1:62:A:LEU:C	1:63:A:LEU:N	2	1.51	0.28	1.51
(1,74)	1:62:A:LEU:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	2	1.5	0.24	1.5
(1,75)	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	1:64:A:CYS:N	2	1.2	0.02	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 (°)
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	26	4.03
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	9	3.97
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	11	3.96
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	4	3.94
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	10	3.84
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	2	3.83
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	6	3.63
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	8	3.63
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	15	3.62
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	25	3.39
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	1	3.3
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	2	3.22
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	21	3.14
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	19	3.11

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	12	3.08
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	3	2.97
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	7	2.91
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	18	2.91
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	20	2.89
(1,27)	1:30:A:LYS:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	21	2.88
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	13	2.84
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	24	2.84
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	23	2.83
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	22	2.82
(1,3)	1:12:A:LEU:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	17	2.82
(1,3)	1:12:A:LEU:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	25	2.8
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	14	2.62
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	5	2.59
(1,99)	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	1:78:A:LEU:N	13	2.58
(1,25)	1:27:A:GLY:C	1:28:A:ARG:N	1:28:A:ARG:CA	1:28:A:ARG:C	21	2.56
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	27	2.49
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	17	2.41
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	10	2.39
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:MET:N	25	2.34
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	9	2.32
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	16	2.31
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	24	2.3
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	23	2.29
(1,99)	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	1:78:A:LEU:N	1	2.28
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	18	2.27
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	30	2.24
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	14	2.24
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	24	2.23
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	29	2.23
(1,4)	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	1:14:A:ASP:N	7	2.23
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	30	2.19
(1,99)	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	1:78:A:LEU:N	15	2.17
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:MET:N	17	2.16
(1,3)	1:12:A:LEU:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	21	2.14
(1,99)	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	1:78:A:LEU:N	25	2.13
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	3	2.1
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	28	2.08
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:MET:N	21	2.08
(1,144)	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	1:104:A:TRP:N	18	2.04
(1,144)	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	1:104:A:TRP:N	26	2.03
(1,144)	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	1:104:A:TRP:N	16	2.01
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	28	1.96
(1,160)	1:111:A:ARG:N	1:111:A:ARG:CA	1:111:A:ARG:C	1:112:A:ALA:N	9	1.94
(1,144)	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	1:104:A:TRP:N	29	1.92
(1,144)	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	1:104:A:TRP:N	8	1.88
(1,247)	1:162:A:TRP:C	1:163:A:ASP:N	1:163:A:ASP:CA	1:163:A:ASP:C	22	1.83
(1,130)	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	1:95:A:PHE:N	16	1.82
(1,73)	1:62:A:LEU:N	1:62:A:LEU:CA	1:62:A:LEU:C	1:63:A:LEU:N	7	1.79
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	27	1.77
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:MET:N	1	1.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	28	1.75
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:MET:N	30	1.75
(1,74)	1:62:A:LEU:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	7	1.74
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	20	1.73
(1,122)	1:90:A:TYR:N	1:90:A:TYR:CA	1:90:A:TYR:C	1:91:A:ARG:N	15	1.7
(1,99)	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	1:78:A:LEU:N	20	1.68
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	12	1.67
(1,147)	1:104:A:TRP:C	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	2	1.67
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	7	1.66
(1,137)	1:97:A:SER:C	1:98:A:TRP:N	1:98:A:TRP:CA	1:98:A:TRP:C	9	1.66
(1,99)	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	1:78:A:LEU:N	30	1.66
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	27	1.65
(1,181)	1:123:A:ARG:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	20	1.62
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	22	1.61
(1,137)	1:97:A:SER:C	1:98:A:TRP:N	1:98:A:TRP:CA	1:98:A:TRP:C	29	1.61
(1,3)	1:12:A:LEU:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	1	1.6
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	23	1.59
(1,147)	1:104:A:TRP:C	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	23	1.55
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	18	1.55
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	17	1.51
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	15	1.5
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	1	1.48
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	12	1.48
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	19	1.48
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	22	1.48
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:MET:N	8	1.47
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	20	1.45
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	1	1.45
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	20	1.45
(1,88)	1:71:A:ALA:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	2	1.45
(1,149)	1:105:A:GLY:C	1:106:A:CYS:N	1:106:A:CYS:CA	1:106:A:CYS:C	2	1.44
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	11	1.44
(1,3)	1:12:A:LEU:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	8	1.44
(1,97)	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	1:77:A:ASP:N	4	1.41
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:MET:N	11	1.41
(1,252)	1:165:A:PHE:N	1:165:A:PHE:CA	1:165:A:PHE:C	1:166:A:VAL:N	12	1.4
(1,3)	1:12:A:LEU:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	27	1.4
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	13	1.39
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	4	1.38
(1,147)	1:104:A:TRP:C	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	9	1.36
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	10	1.36
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	10	1.36
(1,147)	1:104:A:TRP:C	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	10	1.34
(1,144)	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	1:104:A:TRP:N	6	1.34
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	7	1.34
(1,137)	1:97:A:SER:C	1:98:A:TRP:N	1:98:A:TRP:CA	1:98:A:TRP:C	11	1.33
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	8	1.33
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	14	1.33
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	28	1.33
(1,255)	1:167:A:ASP:C	1:168:A:HIS:N	1:168:A:HIS:CA	1:168:A:HIS:C	6	1.29
(1,249)	1:163:A:ASP:C	1:164:A:THR:N	1:164:A:THR:CA	1:164:A:THR:C	12	1.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,181)	1:123:A:ARG:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	1	1.29
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	15	1.29
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	29	1.29
(1,144)	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	1:104:A:TRP:N	21	1.27
(1,74)	1:62:A:LEU:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	26	1.27
(1,147)	1:104:A:TRP:C	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	30	1.26
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	21	1.26
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	2	1.25
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	6	1.25
(1,148)	1:105:A:GLY:N	1:105:A:GLY:CA	1:105:A:GLY:C	1:106:A:CYS:N	17	1.24
(1,3)	1:12:A:LEU:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	30	1.24
(1,84)	1:69:A:ARG:C	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	2	1.23
(1,73)	1:62:A:LEU:N	1:62:A:LEU:CA	1:62:A:LEU:C	1:63:A:LEU:N	26	1.23
(1,99)	1:77:A:ASP:N	1:77:A:ASP:CA	1:77:A:ASP:C	1:78:A:LEU:N	16	1.22
(1,75)	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	1:64:A:CYS:N	8	1.22
(1,3)	1:12:A:LEU:C	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	6	1.21
(1,246)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:ASP:N	30	1.2
(1,75)	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	1:64:A:CYS:N	5	1.19
(1,27)	1:30:A:LYS:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	4	1.19
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	13	1.18
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	27	1.18
(1,264)	1:174:A:GLN:N	1:174:A:GLN:CA	1:174:A:GLN:C	1:175:A:PRO:N	5	1.17
(1,149)	1:105:A:GLY:C	1:106:A:CYS:N	1:106:A:CYS:CA	1:106:A:CYS:C	10	1.17
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:MET:N	7	1.17
(1,258)	1:171:A:CYS:N	1:171:A:CYS:CA	1:171:A:CYS:C	1:172:A:PRO:N	29	1.15
(1,137)	1:97:A:SER:C	1:98:A:TRP:N	1:98:A:TRP:CA	1:98:A:TRP:C	26	1.15
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	19	1.15
(1,129)	1:93:A:THR:C	1:94:A:TRP:N	1:94:A:TRP:CA	1:94:A:TRP:C	15	1.15
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:MET:N	9	1.14
(1,105)	1:80:A:PRO:N	1:80:A:PRO:CA	1:80:A:PRO:C	1:81:A:SER:N	5	1.13
(1,26)	1:28:A:ARG:N	1:28:A:ARG:CA	1:28:A:ARG:C	1:29:A:HIS:N	6	1.13
(1,269)	1:178:A:GLY:C	1:179:A:LEU:N	1:179:A:LEU:CA	1:179:A:LEU:C	11	1.12
(1,149)	1:105:A:GLY:C	1:106:A:CYS:N	1:106:A:CYS:CA	1:106:A:CYS:C	30	1.12
(1,4)	1:13:A:MET:N	1:13:A:MET:CA	1:13:A:MET:C	1:14:A:ASP:N	6	1.12
(1,262)	1:173:A:PHE:N	1:173:A:PHE:CA	1:173:A:PHE:C	1:174:A:GLN:N	1	1.11
(1,149)	1:105:A:GLY:C	1:106:A:CYS:N	1:106:A:CYS:CA	1:106:A:CYS:C	18	1.11
(1,252)	1:165:A:PHE:N	1:165:A:PHE:CA	1:165:A:PHE:C	1:166:A:VAL:N	20	1.1
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	11	1.1
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	15	1.1
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	25	1.09
(1,181)	1:123:A:ARG:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	8	1.08
(1,181)	1:123:A:ARG:C	1:124:A:ILE:N	1:124:A:ILE:CA	1:124:A:ILE:C	25	1.08
(1,2)	1:12:A:LEU:N	1:12:A:LEU:CA	1:12:A:LEU:C	1:13:A:MET:N	15	1.08
(1,137)	1:97:A:SER:C	1:98:A:TRP:N	1:98:A:TRP:CA	1:98:A:TRP:C	18	1.07
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	24	1.06
(1,132)	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	1:96:A:ILE:N	26	1.06
(1,252)	1:165:A:PHE:N	1:165:A:PHE:CA	1:165:A:PHE:C	1:166:A:VAL:N	2	1.05
(1,27)	1:30:A:LYS:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	10	1.05
(1,101)	1:78:A:LEU:N	1:78:A:LEU:CA	1:78:A:LEU:C	1:79:A:VAL:N	28	1.04
(1,252)	1:165:A:PHE:N	1:165:A:PHE:CA	1:165:A:PHE:C	1:166:A:VAL:N	11	1.03
(1,252)	1:165:A:PHE:N	1:165:A:PHE:CA	1:165:A:PHE:C	1:166:A:VAL:N	15	1.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,268)	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	1:178:A:GLY:N	23	1.02
(1,149)	1:105:A:GLY:C	1:106:A:CYS:N	1:106:A:CYS:CA	1:106:A:CYS:C	16	1.02
(1,107)	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	1:82:A:LEU:N	30	1.02
(1,8)	1:15:A:PRO:N	1:15:A:PRO:CA	1:15:A:PRO:C	1:16:A:HIS:N	27	1.02
(1,145)	1:103:A:SER:C	1:104:A:TRP:N	1:104:A:TRP:CA	1:104:A:TRP:C	6	1.01
(1,144)	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	1:104:A:TRP:N	24	1.0