



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:01 PM UTC

PDB ID : 2L9L / pdb_00002l9l
BMRB ID : 17477
Title : NMR Structure of the Mouse MFG-E8 C2 Domain
Authors : Ye, H.; Yoon, H.S.
Deposited on : 2011-02-21

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

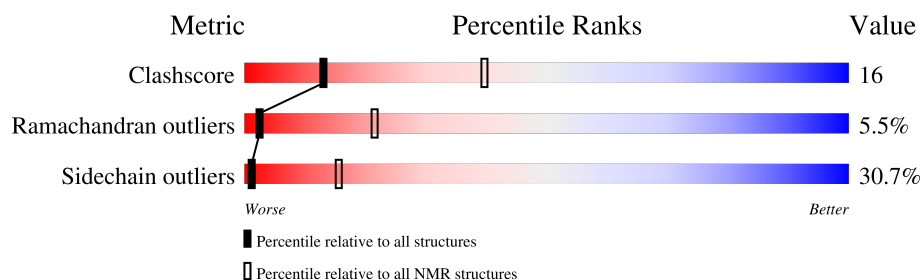
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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	170	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:23, A:34-A:104, A:111-A:158 (142)	1.04	7

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

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

The models can be grouped into 3 clusters and 10 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2379 atoms, of which 1068 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lactadherin.

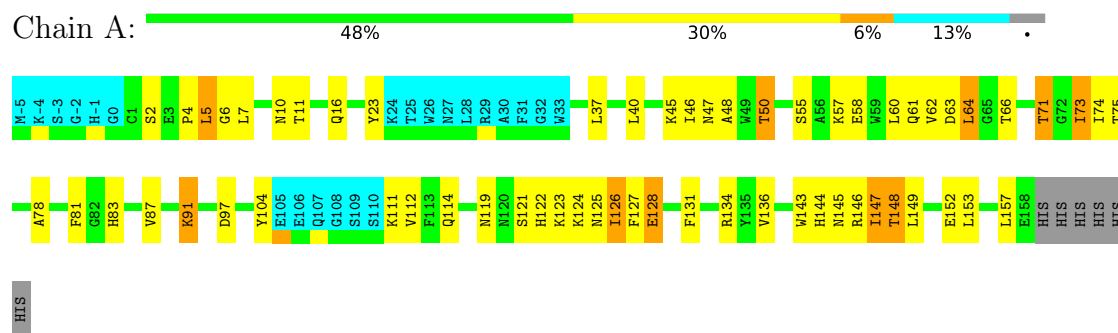
Mol	Chain	Residues	Atoms						Trace
1	A	164	Total	C	H	N	O	S	0
			2379	825	1068	238	243	5	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P21956
A	-4	LYS	-	expression tag	UNP P21956
A	-3	SER	-	expression tag	UNP P21956
A	-2	GLY	-	expression tag	UNP P21956
A	157	LEU	-	expression tag	UNP P21956
A	158	GLU	-	expression tag	UNP P21956
A	159	HIS	-	expression tag	UNP P21956
A	160	HIS	-	expression tag	UNP P21956
A	161	HIS	-	expression tag	UNP P21956
A	162	HIS	-	expression tag	UNP P21956
A	163	HIS	-	expression tag	UNP P21956
A	164	HIS	-	expression tag	UNP P21956

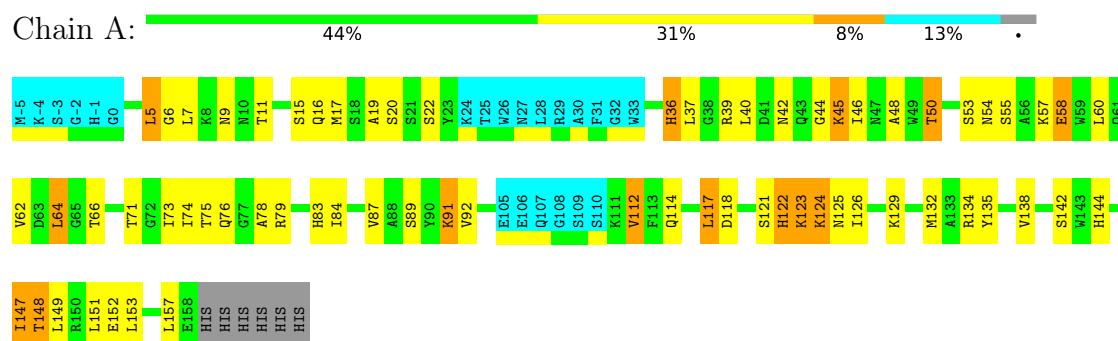
4.2.2 Score per residue for model 2

- Molecule 1: Lactadherin



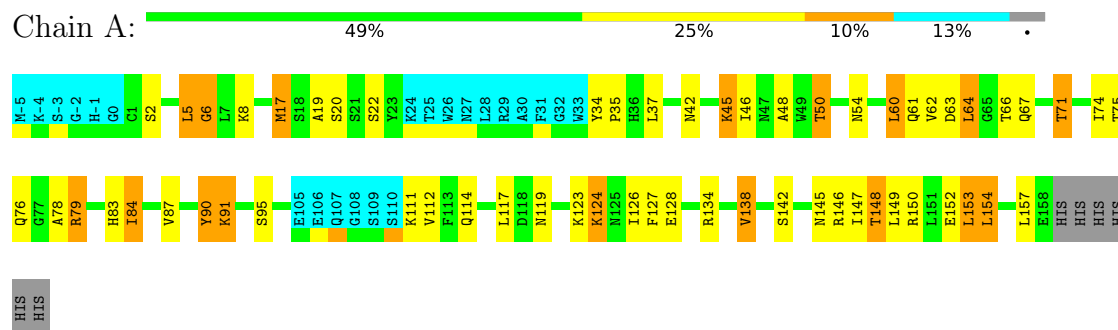
4.2.3 Score per residue for model 3

- Molecule 1: Lactadherin



4.2.4 Score per residue for model 4

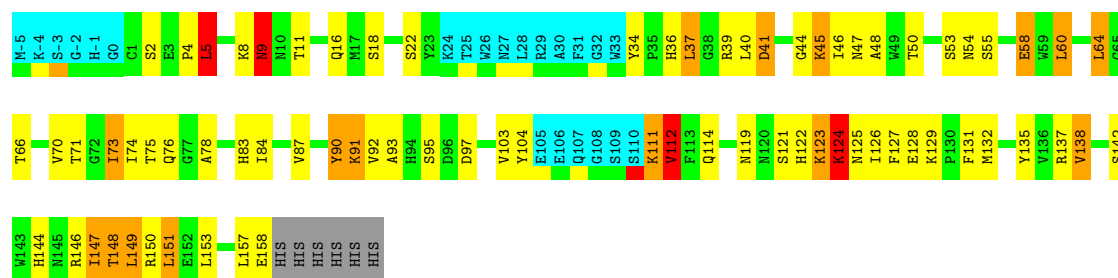
- Molecule 1: Lactadherin



4.2.5 Score per residue for model 5

- Molecule 1: Lactadherin

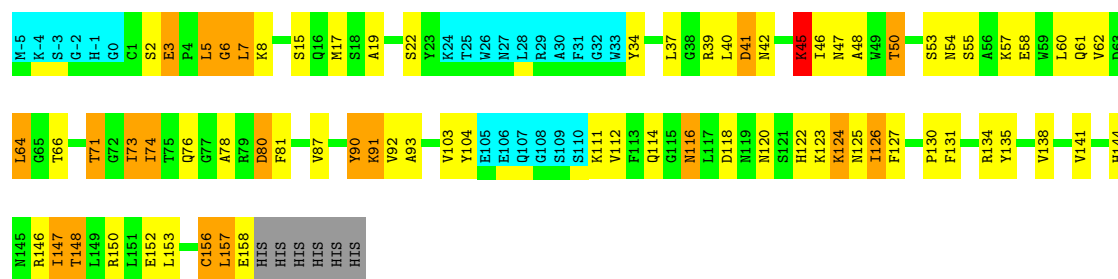




4.2.9 Score per residue for model 9

- Molecule 1: Lactadherin

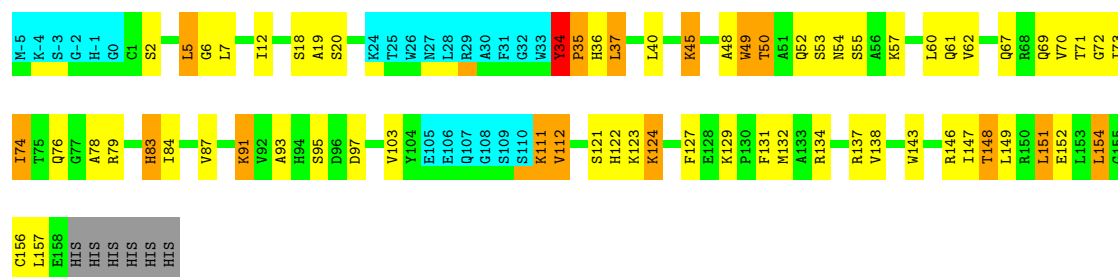
Chain A: 41% 31% 12% 13%



4.2.10 Score per residue for model 10

- Molecule 1: Lactadherin

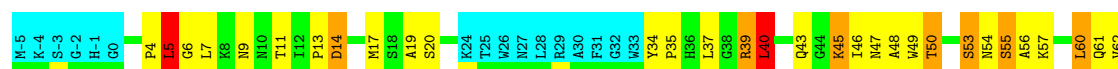
Chain A: 45% 29% 9% 13%



4.2.11 Score per residue for model 11

- Molecule 1: Lactadherin

Chain A: 41% 32% 9% 13%

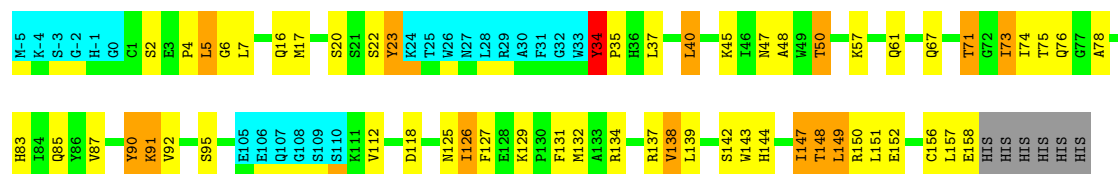




4.2.12 Score per residue for model 12

- Molecule 1: Lactadherin

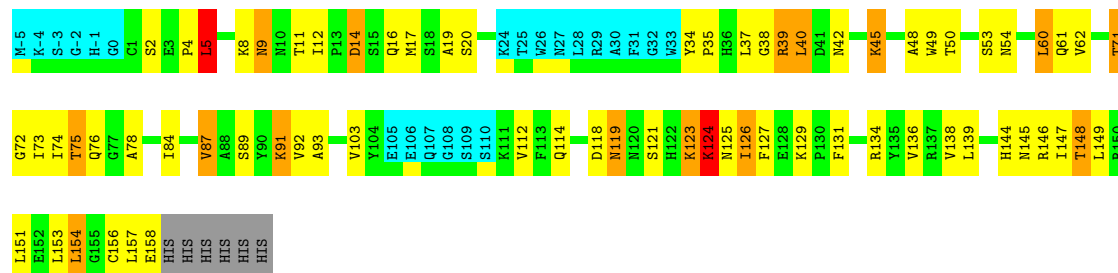
Chain A: 49% 26% 8% 13%



4.2.13 Score per residue for model 13

- Molecule 1: Lactadherin

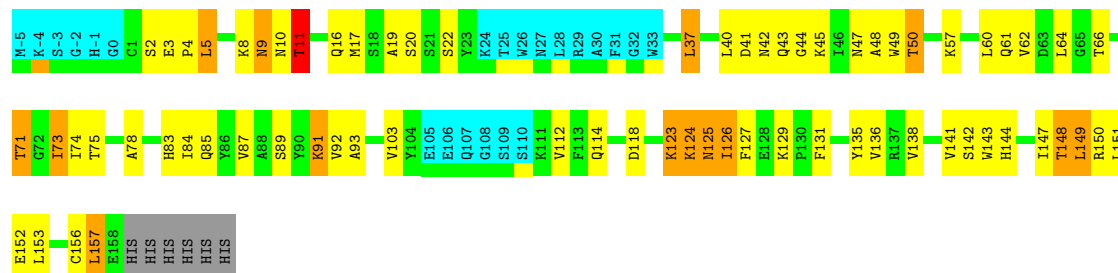
Chain A: 42% 31% 9% 13%



4.2.14 Score per residue for model 14

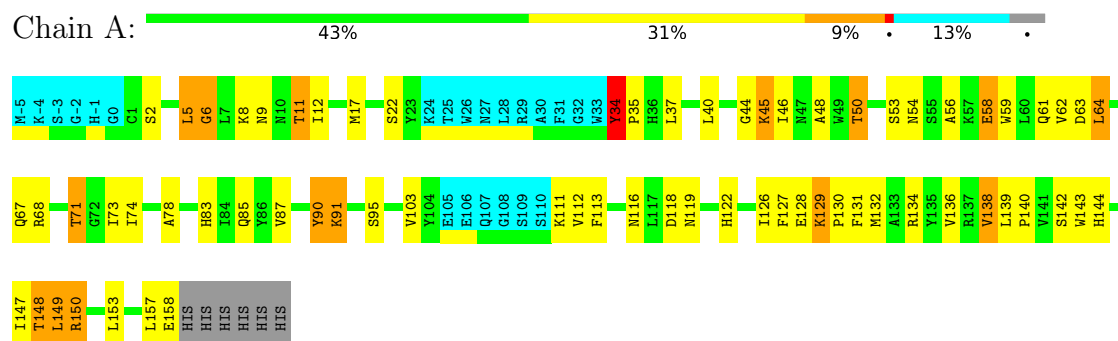
- Molecule 1: Lactadherin

Chain A: 42% 32% 8% 13%



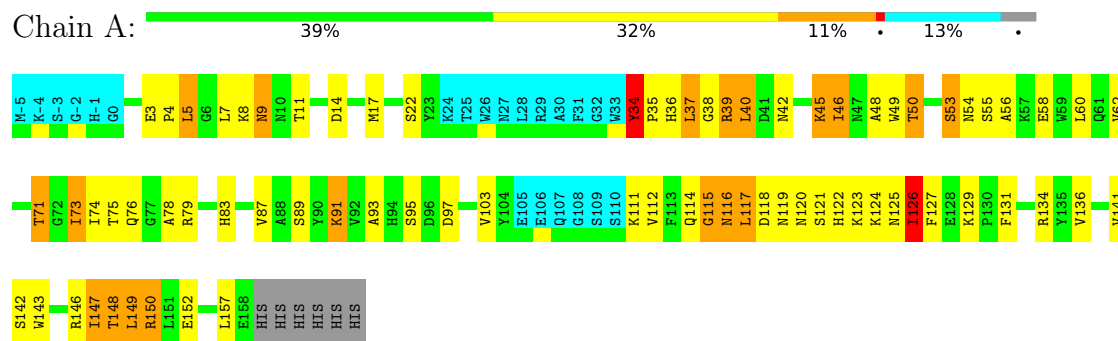
4.2.15 Score per residue for model 15

- Molecule 1: Lactadherin



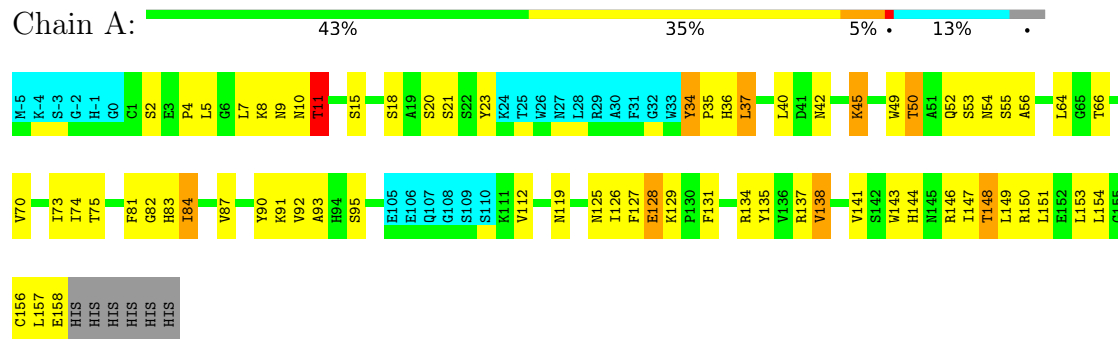
4.2.16 Score per residue for model 16

- Molecule 1: Lactadherin



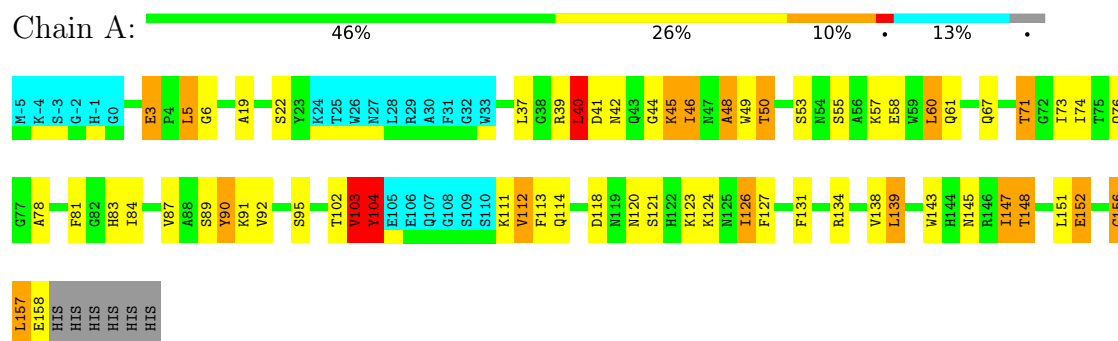
4.2.17 Score per residue for model 17

- Molecule 1: Lactadherin



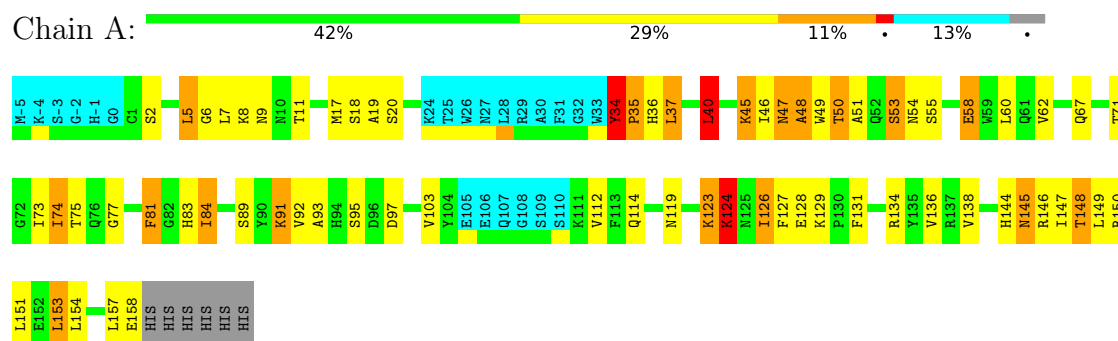
4.2.18 Score per residue for model 18

- Molecule 1: Lactadherin



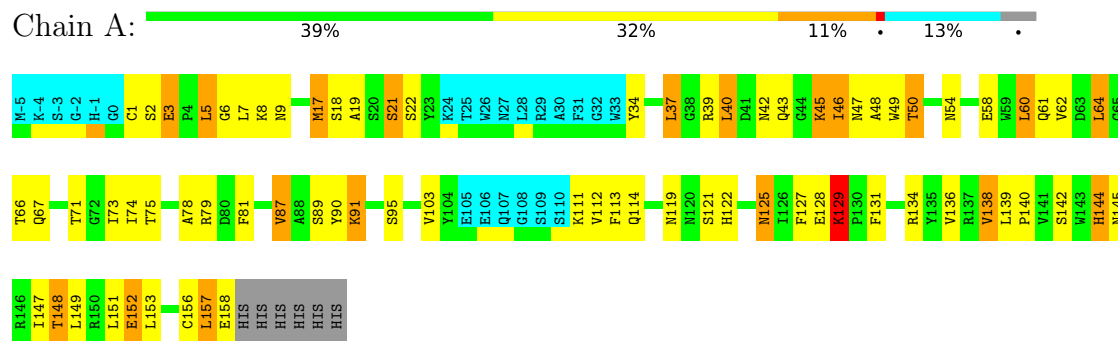
4.2.19 Score per residue for model 19

- Molecule 1: Lactadherin



4.2.20 Score per residue for model 20

- Molecule 1: Lactadherin



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	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	1706
Number of shifts mapped to atoms	1531
Number of unparsed shifts	0
Number of shifts with mapping errors	175
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1136	936	1108	37±5
All	All	22720	18720	22160	735

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:HD22	1:A:40:LEU:HD23	0.97	1.35	17	1
1:A:92:VAL:HG22	1:A:138:VAL:HG13	0.89	1.41	18	2
1:A:17:MET:HE3	1:A:60:LEU:HD21	0.88	1.42	3	1
1:A:75:THR:HG23	1:A:149:LEU:HD23	0.87	1.47	12	1
1:A:48:ALA:HB3	1:A:78:ALA:HB2	0.87	1.45	10	17
1:A:92:VAL:HG13	1:A:138:VAL:HG22	0.85	1.49	18	1
1:A:112:VAL:HG11	1:A:141:VAL:HG21	0.84	1.49	9	5
1:A:92:VAL:HG23	1:A:138:VAL:HG22	0.81	1.50	13	5
1:A:37:LEU:HD13	1:A:46:ILE:HG21	0.81	1.51	19	2
1:A:153:LEU:C	1:A:153:LEU:HD22	0.80	2.01	7	1
1:A:78:ALA:HB3	1:A:148:THR:HG22	0.80	1.51	5	4
1:A:60:LEU:HD23	1:A:151:LEU:HD21	0.79	1.53	14	1
1:A:93:ALA:HB2	1:A:103:VAL:HG12	0.79	1.54	13	11
1:A:64:LEU:HD12	1:A:66:THR:HG22	0.79	1.53	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:ALA:HB2	1:A:60:LEU:HD13	0.77	1.56	19	3
1:A:60:LEU:HD12	1:A:151:LEU:HD21	0.75	1.56	10	1
1:A:91:LYS:HG2	1:A:112:VAL:HG12	0.70	1.63	8	9
1:A:83:HIS:O	1:A:84:ILE:C	0.69	2.36	5	10
1:A:19:ALA:HB2	1:A:60:LEU:HD22	0.68	1.64	10	1
1:A:138:VAL:HG21	1:A:151:LEU:HD22	0.67	1.67	1	2
1:A:5:LEU:HD22	1:A:5:LEU:O	0.67	1.89	9	1
1:A:73:ILE:HG22	1:A:153:LEU:HA	0.67	1.66	19	2
1:A:71:THR:HG22	1:A:127:PHE:HB3	0.66	1.64	9	10
1:A:91:LYS:HG3	1:A:112:VAL:HG12	0.66	1.67	13	6
1:A:48:ALA:CB	1:A:78:ALA:HB2	0.66	2.21	7	16
1:A:73:ILE:HD12	1:A:124:LYS:CG	0.65	2.22	8	6
1:A:37:LEU:HD13	1:A:46:ILE:CG2	0.65	2.21	19	1
1:A:5:LEU:HD11	1:A:152:GLU:CD	0.65	2.17	1	2
1:A:54:ASN:HA	1:A:147:ILE:HD13	0.64	1.68	17	8
1:A:90:TYR:CD1	1:A:138:VAL:HG12	0.64	2.28	15	2
1:A:56:ALA:HB2	1:A:143:TRP:CZ3	0.64	2.26	11	6
1:A:71:THR:HG22	1:A:127:PHE:HB2	0.64	1.69	13	2
1:A:91:LYS:CG	1:A:112:VAL:HG12	0.64	2.23	6	11
1:A:78:ALA:HB3	1:A:148:THR:CG2	0.63	2.23	5	4
1:A:73:ILE:HD11	1:A:125:ASN:ND2	0.63	2.09	17	1
1:A:84:ILE:HG23	1:A:119:ASN:ND2	0.63	2.09	19	2
1:A:84:ILE:HD12	1:A:119:ASN:ND2	0.62	2.09	1	1
1:A:64:LEU:CD1	1:A:153:LEU:HD11	0.62	2.24	17	1
1:A:87:VAL:HG13	1:A:149:LEU:HD22	0.62	1.71	7	3
1:A:7:LEU:HD13	1:A:40:LEU:CD2	0.62	2.24	20	1
1:A:112:VAL:HG11	1:A:141:VAL:CG2	0.62	2.23	9	4
1:A:64:LEU:HD23	1:A:66:THR:CG2	0.62	2.25	17	1
1:A:5:LEU:HD13	1:A:16:GLN:OE1	0.62	1.94	14	3
1:A:9:ASN:O	1:A:11:THR:HG23	0.62	1.94	16	6
1:A:73:ILE:HD12	1:A:124:LYS:CD	0.62	2.25	10	2
1:A:87:VAL:HG22	1:A:149:LEU:HD13	0.62	1.70	7	2
1:A:19:ALA:HB2	1:A:60:LEU:CD2	0.62	2.25	10	1
1:A:7:LEU:HD13	1:A:40:LEU:HB2	0.61	1.73	3	3
1:A:7:LEU:HD22	1:A:40:LEU:CB	0.61	2.26	9	1
1:A:74:ILE:HD13	1:A:124:LYS:HB3	0.61	1.72	4	2
1:A:153:LEU:HD13	1:A:153:LEU:N	0.61	2.09	4	1
1:A:17:MET:CG	1:A:60:LEU:HD21	0.61	2.24	9	1
1:A:49:TRP:CE3	1:A:60:LEU:HD13	0.61	2.30	11	1
1:A:149:LEU:HD22	1:A:150:ARG:N	0.61	2.11	15	6
1:A:91:LYS:CE	1:A:112:VAL:HG12	0.60	2.27	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:SER:OG	1:A:112:VAL:HG21	0.60	1.95	19	1
1:A:5:LEU:O	1:A:12:ILE:HD12	0.60	1.96	6	3
1:A:126:ILE:HG23	1:A:127:PHE:N	0.60	2.12	11	7
1:A:73:ILE:HD12	1:A:124:LYS:HD3	0.60	1.72	10	1
1:A:58:GLU:OE2	1:A:147:ILE:HG21	0.59	1.98	3	3
1:A:64:LEU:HD11	1:A:153:LEU:HD11	0.59	1.73	17	1
1:A:92:VAL:HA	1:A:138:VAL:HG12	0.59	1.74	6	6
1:A:73:ILE:HD12	1:A:124:LYS:HG2	0.59	1.74	9	2
1:A:7:LEU:HD21	1:A:39:ARG:HB2	0.59	1.73	20	1
1:A:5:LEU:HD13	1:A:5:LEU:N	0.59	2.13	4	9
1:A:5:LEU:HD22	1:A:5:LEU:C	0.59	2.22	9	1
1:A:50:THR:OG1	1:A:148:THR:HG23	0.59	1.98	20	15
1:A:153:LEU:C	1:A:153:LEU:CD2	0.59	2.75	7	1
1:A:84:ILE:HG23	1:A:119:ASN:OD1	0.58	1.98	13	1
1:A:3:GLU:CD	1:A:157:LEU:HD23	0.58	2.23	9	4
1:A:92:VAL:HG21	1:A:124:LYS:NZ	0.58	2.14	19	1
1:A:75:THR:HG22	1:A:123:LYS:O	0.58	1.99	8	4
1:A:74:ILE:HG23	1:A:152:GLU:HB2	0.58	1.75	3	3
1:A:84:ILE:HG23	1:A:119:ASN:CG	0.58	2.24	19	3
1:A:139:LEU:HD12	1:A:140:PRO:HD2	0.58	1.73	15	1
1:A:92:VAL:CG1	1:A:138:VAL:HG22	0.58	2.26	18	1
1:A:71:THR:HG23	1:A:130:PRO:HB3	0.57	1.75	9	4
1:A:74:ILE:HD11	1:A:122:HIS:HB2	0.57	1.75	5	7
1:A:19:ALA:HB2	1:A:60:LEU:CD1	0.57	2.27	19	2
1:A:111:LYS:O	1:A:112:VAL:C	0.57	2.47	8	2
1:A:6:GLY:O	1:A:7:LEU:HD23	0.57	1.99	19	3
1:A:103:VAL:C	1:A:104:TYR:CG	0.57	2.82	18	1
1:A:37:LEU:HD12	1:A:49:TRP:HA	0.57	1.76	19	2
1:A:74:ILE:HD13	1:A:124:LYS:HB2	0.56	1.75	2	1
1:A:89:SER:HB3	1:A:112:VAL:HG21	0.56	1.76	18	2
1:A:17:MET:HE3	1:A:60:LEU:CD2	0.56	2.25	3	1
1:A:35:PRO:O	1:A:37:LEU:HD22	0.56	1.99	10	1
1:A:149:LEU:C	1:A:149:LEU:HD22	0.56	2.25	14	1
1:A:117:LEU:HD13	1:A:123:LYS:HB3	0.56	1.78	1	1
1:A:5:LEU:HD12	1:A:6:GLY:N	0.56	2.15	3	5
1:A:19:ALA:HB2	1:A:60:LEU:HD12	0.56	1.76	11	4
1:A:6:GLY:C	1:A:7:LEU:HD23	0.56	2.25	9	1
1:A:36:HIS:O	1:A:36:HIS:CG	0.56	2.58	3	1
1:A:127:PHE:O	1:A:129:LYS:N	0.56	2.39	8	2
1:A:49:TRP:CE3	1:A:60:LEU:HD11	0.56	2.36	20	1
1:A:111:LYS:O	1:A:112:VAL:O	0.56	2.24	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:TYR:O	1:A:37:LEU:HD21	0.56	2.01	11	7
1:A:7:LEU:HD13	1:A:40:LEU:HD22	0.56	1.78	16	1
1:A:74:ILE:HD12	1:A:124:LYS:HB2	0.56	1.77	5	1
1:A:62:VAL:HB	1:A:136:VAL:HG22	0.56	1.77	14	10
1:A:35:PRO:O	1:A:36:HIS:CG	0.55	2.60	19	2
1:A:34:TYR:N	1:A:35:PRO:HD2	0.55	2.16	17	8
1:A:17:MET:HG2	1:A:62:VAL:HG22	0.55	1.77	6	2
1:A:64:LEU:HD23	1:A:66:THR:HG22	0.55	1.77	17	1
1:A:50:THR:HG23	1:A:148:THR:HG23	0.55	1.78	12	10
1:A:64:LEU:HD12	1:A:66:THR:CG2	0.55	2.30	2	3
1:A:157:LEU:N	1:A:157:LEU:HD13	0.55	2.16	20	1
1:A:35:PRO:C	1:A:37:LEU:HD22	0.55	2.25	10	3
1:A:74:ILE:HD12	1:A:124:LYS:HB3	0.55	1.79	16	1
1:A:70:VAL:HG22	1:A:131:PHE:O	0.54	2.02	10	1
1:A:17:MET:HE2	1:A:150:ARG:NE	0.54	2.18	5	1
1:A:3:GLU:OE2	1:A:157:LEU:HD23	0.54	2.01	20	1
1:A:50:THR:HA	1:A:147:ILE:O	0.54	2.03	5	4
1:A:87:VAL:HG13	1:A:143:TRP:HB3	0.53	1.79	14	3
1:A:3:GLU:HG2	1:A:157:LEU:HD23	0.53	1.80	14	1
1:A:55:SER:O	1:A:56:ALA:HB3	0.53	2.03	17	3
1:A:63:ASP:C	1:A:64:LEU:HD13	0.53	2.28	15	1
1:A:71:THR:HG22	1:A:127:PHE:CB	0.53	2.32	9	5
1:A:49:TRP:CZ3	1:A:60:LEU:HD11	0.53	2.38	20	1
1:A:17:MET:HE1	1:A:152:GLU:OE2	0.53	2.03	7	1
1:A:34:TYR:HB2	1:A:35:PRO:HD3	0.53	1.80	16	1
1:A:92:VAL:CG2	1:A:138:VAL:HG22	0.53	2.34	14	3
1:A:149:LEU:HD22	1:A:149:LEU:C	0.53	2.28	12	5
1:A:50:THR:HG23	1:A:148:THR:OG1	0.53	2.02	19	1
1:A:91:LYS:O	1:A:138:VAL:HG12	0.53	2.04	4	5
1:A:138:VAL:HG11	1:A:151:LEU:HD22	0.53	1.81	7	1
1:A:49:TRP:CD2	1:A:60:LEU:HD23	0.53	2.38	10	1
1:A:91:LYS:NZ	1:A:103:VAL:HG11	0.53	2.18	15	1
1:A:77:GLY:HA2	1:A:149:LEU:HD23	0.53	1.81	19	1
1:A:37:LEU:HD23	1:A:49:TRP:HA	0.52	1.81	17	3
1:A:87:VAL:HG23	1:A:149:LEU:HD22	0.52	1.82	3	2
1:A:92:VAL:HG21	1:A:124:LYS:HZ1	0.52	1.63	19	1
1:A:91:LYS:HB2	1:A:112:VAL:HG12	0.52	1.80	16	2
1:A:117:LEU:HD13	1:A:123:LYS:CB	0.52	2.34	1	2
1:A:7:LEU:HD22	1:A:40:LEU:HB2	0.52	1.81	9	1
1:A:75:THR:CG2	1:A:149:LEU:HD23	0.52	2.30	12	1
1:A:34:TYR:H	1:A:35:PRO:HD2	0.52	1.65	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:SER:CB	1:A:112:VAL:HG21	0.52	2.34	18	1
1:A:91:LYS:HE3	1:A:112:VAL:HG12	0.52	1.81	18	1
1:A:91:LYS:NZ	1:A:103:VAL:HG21	0.52	2.19	20	1
1:A:87:VAL:CG2	1:A:149:LEU:HD22	0.52	2.33	3	4
1:A:34:TYR:O	1:A:37:LEU:HD11	0.52	2.05	19	3
1:A:143:TRP:CE2	1:A:147:ILE:HD11	0.52	2.39	12	5
1:A:87:VAL:HB	1:A:149:LEU:HD13	0.52	1.81	17	3
1:A:73:ILE:HD11	1:A:125:ASN:HB2	0.52	1.81	7	5
1:A:72:GLY:O	1:A:154:LEU:HD12	0.51	2.04	10	2
1:A:38:GLY:O	1:A:39:ARG:C	0.51	2.54	13	2
1:A:90:TYR:CE1	1:A:138:VAL:HG12	0.51	2.40	20	3
1:A:37:LEU:HG	1:A:46:ILE:HG21	0.51	1.81	18	1
1:A:70:VAL:HG12	1:A:153:LEU:HD13	0.51	1.82	1	1
1:A:73:ILE:HD11	1:A:125:ASN:CB	0.51	2.36	8	4
1:A:87:VAL:HG11	1:A:90:TYR:CD2	0.51	2.41	17	7
1:A:93:ALA:HB2	1:A:103:VAL:CG1	0.51	2.34	1	5
1:A:87:VAL:CG1	1:A:149:LEU:HD22	0.51	2.36	13	1
1:A:17:MET:CG	1:A:62:VAL:HG22	0.51	2.35	3	5
1:A:1:CYS:SG	1:A:71:THR:HG21	0.51	2.46	6	1
1:A:70:VAL:CG1	1:A:153:LEU:HD13	0.50	2.36	1	1
1:A:127:PHE:O	1:A:128:GLU:C	0.50	2.55	4	2
1:A:73:ILE:HD12	1:A:124:LYS:HG3	0.50	1.82	8	1
1:A:60:LEU:HD23	1:A:138:VAL:CG2	0.50	2.35	8	3
1:A:75:THR:CG2	1:A:117:LEU:HD22	0.50	2.37	3	1
1:A:139:LEU:HD23	1:A:139:LEU:O	0.50	2.07	18	2
1:A:49:TRP:CZ3	1:A:60:LEU:HD21	0.50	2.41	20	1
1:A:17:MET:HE2	1:A:60:LEU:HD21	0.50	1.82	20	1
1:A:139:LEU:HD22	1:A:140:PRO:HD2	0.50	1.82	20	1
1:A:153:LEU:O	1:A:154:LEU:HD13	0.50	2.06	4	1
1:A:7:LEU:HG	1:A:40:LEU:HD23	0.50	1.84	7	1
1:A:7:LEU:HD13	1:A:40:LEU:HD13	0.49	1.83	19	3
1:A:3:GLU:CG	1:A:157:LEU:HD23	0.49	2.38	14	1
1:A:10:ASN:C	1:A:11:THR:HG22	0.49	2.31	14	2
1:A:4:PRO:HB3	1:A:7:LEU:HD12	0.49	1.84	12	2
1:A:92:VAL:HG22	1:A:138:VAL:CG1	0.49	2.28	18	1
1:A:149:LEU:N	1:A:149:LEU:CD1	0.49	2.75	8	6
1:A:41:ASP:O	1:A:42:ASN:C	0.49	2.55	18	3
1:A:45:LYS:CD	1:A:45:LYS:N	0.49	2.76	15	1
1:A:126:ILE:HG22	1:A:127:PHE:H	0.49	1.66	16	1
1:A:5:LEU:HD11	1:A:152:GLU:OE2	0.49	2.08	1	1
1:A:74:ILE:HG23	1:A:152:GLU:CG	0.48	2.37	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ILE:HD12	1:A:124:LYS:HB3	0.48	1.84	11	1
1:A:75:THR:HG23	1:A:117:LEU:CD1	0.48	2.38	16	1
1:A:50:THR:CG2	1:A:148:THR:HG23	0.48	2.38	12	8
1:A:139:LEU:HD13	1:A:139:LEU:O	0.48	2.09	20	1
1:A:48:ALA:HB3	1:A:78:ALA:CB	0.48	2.33	1	5
1:A:34:TYR:HB2	1:A:35:PRO:CD	0.48	2.39	16	1
1:A:40:LEU:O	1:A:40:LEU:HD12	0.48	2.08	17	1
1:A:7:LEU:CD1	1:A:40:LEU:HD13	0.48	2.39	16	3
1:A:7:LEU:HD11	1:A:152:GLU:OE2	0.48	2.09	2	1
1:A:127:PHE:O	1:A:127:PHE:CD2	0.48	2.66	11	1
1:A:112:VAL:HG11	1:A:141:VAL:HG23	0.48	1.84	14	1
1:A:60:LEU:HD23	1:A:151:LEU:CD2	0.48	2.35	14	1
1:A:139:LEU:HD13	1:A:139:LEU:C	0.48	2.34	20	1
1:A:34:TYR:CB	1:A:35:PRO:CD	0.47	2.92	19	7
1:A:60:LEU:CD1	1:A:151:LEU:HD21	0.47	2.37	10	1
1:A:19:ALA:HB3	1:A:49:TRP:CZ2	0.47	2.45	20	1
1:A:92:VAL:CG2	1:A:138:VAL:HG13	0.47	2.28	18	1
1:A:7:LEU:HD13	1:A:40:LEU:CB	0.47	2.38	2	1
1:A:46:ILE:HG22	1:A:48:ALA:O	0.47	2.09	8	4
1:A:49:TRP:CE3	1:A:60:LEU:HD22	0.47	2.45	1	2
1:A:75:THR:OG1	1:A:149:LEU:HD23	0.47	2.10	8	2
1:A:47:ASN:O	1:A:48:ALA:HB2	0.46	2.09	19	1
1:A:74:ILE:HD12	1:A:123:LYS:O	0.46	2.11	3	1
1:A:10:ASN:O	1:A:11:THR:C	0.46	2.59	5	2
1:A:49:TRP:CE2	1:A:60:LEU:HD23	0.46	2.44	10	1
1:A:73:ILE:HD12	1:A:74:ILE:N	0.46	2.25	1	1
1:A:56:ALA:HB2	1:A:143:TRP:HZ3	0.46	1.70	15	4
1:A:151:LEU:C	1:A:151:LEU:HD13	0.46	2.35	13	1
1:A:64:LEU:HB2	1:A:66:THR:HG22	0.46	1.88	20	1
1:A:5:LEU:HD12	1:A:153:LEU:O	0.46	2.11	6	2
1:A:5:LEU:HD22	1:A:6:GLY:N	0.46	2.25	19	7
1:A:92:VAL:HG11	1:A:124:LYS:HE3	0.46	1.87	19	1
1:A:74:ILE:HD12	1:A:75:THR:H	0.46	1.71	4	6
1:A:17:MET:HG3	1:A:62:VAL:HG22	0.46	1.87	3	2
1:A:7:LEU:HB3	1:A:40:LEU:HD22	0.46	1.88	9	1
1:A:74:ILE:HD12	1:A:75:THR:N	0.45	2.25	4	5
1:A:80:ASP:O	1:A:81:PHE:C	0.45	2.58	9	1
1:A:5:LEU:HD13	1:A:16:GLN:HE22	0.45	1.70	8	2
1:A:75:THR:HG23	1:A:117:LEU:HD22	0.45	1.87	3	1
1:A:5:LEU:HD11	1:A:36:HIS:CE1	0.45	2.45	8	1
1:A:79:ARG:HB3	1:A:84:ILE:HG23	0.45	1.87	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:VAL:HG11	1:A:90:TYR:CE2	0.45	2.47	18	1
1:A:73:ILE:HD13	1:A:104:TYR:CE2	0.45	2.47	5	1
1:A:70:VAL:CG1	1:A:153:LEU:HD12	0.45	2.41	8	2
1:A:93:ALA:HB3	1:A:137:ARG:O	0.45	2.11	8	2
1:A:34:TYR:N	1:A:35:PRO:CD	0.45	2.79	17	1
1:A:87:VAL:HG21	1:A:149:LEU:HD22	0.45	1.88	17	2
1:A:12:ILE:HG21	1:A:16:GLN:HB3	0.45	1.87	1	1
1:A:5:LEU:CD2	1:A:5:LEU:C	0.45	2.90	7	8
1:A:74:ILE:HG22	1:A:154:LEU:HD11	0.45	1.88	10	1
1:A:88:ALA:HB3	1:A:142:SER:HB3	0.45	1.89	5	1
1:A:153:LEU:HD13	1:A:153:LEU:H	0.44	1.70	4	1
1:A:74:ILE:C	1:A:74:ILE:HD13	0.44	2.37	6	3
1:A:35:PRO:C	1:A:36:HIS:CG	0.44	2.95	19	2
1:A:87:VAL:HG23	1:A:149:LEU:HD23	0.44	1.90	10	1
1:A:126:ILE:HG22	1:A:127:PHE:CD2	0.44	2.47	16	1
1:A:151:LEU:HD12	1:A:151:LEU:O	0.44	2.12	1	1
1:A:147:ILE:HD12	1:A:147:ILE:H	0.44	1.73	17	3
1:A:153:LEU:N	1:A:153:LEU:CD1	0.44	2.80	4	1
1:A:36:HIS:C	1:A:37:LEU:HD13	0.44	2.37	5	2
1:A:5:LEU:HD23	1:A:16:GLN:OE1	0.44	2.13	12	1
1:A:90:TYR:C	1:A:112:VAL:HG12	0.44	2.38	5	1
1:A:54:ASN:CA	1:A:147:ILE:HD13	0.44	2.41	17	2
1:A:60:LEU:HD13	1:A:61:GLN:N	0.44	2.27	10	1
1:A:40:LEU:HD12	1:A:41:ASP:N	0.44	2.28	7	1
1:A:153:LEU:O	1:A:153:LEU:HD12	0.43	2.12	2	1
1:A:48:ALA:HB1	1:A:149:LEU:HA	0.43	1.90	10	1
1:A:153:LEU:O	1:A:153:LEU:HD22	0.43	2.14	4	1
1:A:149:LEU:C	1:A:149:LEU:HD12	0.43	2.37	10	1
1:A:126:ILE:HG23	1:A:128:GLU:H	0.43	1.74	15	2
1:A:45:LYS:HD3	1:A:46:ILE:HD12	0.43	1.90	9	1
1:A:19:ALA:CB	1:A:49:TRP:CZ2	0.43	3.02	20	1
1:A:77:GLY:HA2	1:A:149:LEU:HD12	0.43	1.90	1	1
1:A:46:ILE:O	1:A:47:ASN:C	0.43	2.62	20	7
1:A:7:LEU:HD13	1:A:40:LEU:HD21	0.43	1.88	20	1
1:A:87:VAL:H	1:A:149:LEU:HD13	0.42	1.73	1	1
1:A:73:ILE:HD11	1:A:124:LYS:HD2	0.42	1.91	6	1
1:A:37:LEU:HD23	1:A:49:TRP:CA	0.42	2.44	18	1
1:A:48:ALA:HB1	1:A:149:LEU:CA	0.42	2.44	10	1
1:A:153:LEU:HD23	1:A:153:LEU:H	0.42	1.74	8	1
1:A:91:LYS:CD	1:A:104:TYR:CZ	0.42	3.03	18	1
1:A:46:ILE:C	1:A:47:ASN:CG	0.42	2.87	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:LEU:HD22	1:A:140:PRO:CD	0.42	2.43	20	1
1:A:53:SER:O	1:A:54:ASN:C	0.42	2.63	3	7
1:A:51:ALA:HB2	1:A:147:ILE:HB	0.42	1.91	19	1
1:A:73:ILE:HD11	1:A:125:ASN:OD1	0.42	2.14	1	1
1:A:35:PRO:O	1:A:36:HIS:C	0.42	2.61	10	2
1:A:87:VAL:CG2	1:A:149:LEU:HD13	0.42	2.45	5	2
1:A:46:ILE:HD13	1:A:46:ILE:N	0.42	2.28	15	1
1:A:37:LEU:HD23	1:A:49:TRP:HB2	0.42	1.92	13	1
1:A:66:THR:HG23	1:A:68:ARG:HG2	0.42	1.91	11	1
1:A:126:ILE:C	1:A:128:GLU:H	0.42	2.23	19	1
1:A:51:ALA:HB3	1:A:147:ILE:CG1	0.42	2.45	5	1
1:A:73:ILE:HA	1:A:154:LEU:HD12	0.42	1.90	6	1
1:A:19:ALA:HB2	1:A:60:LEU:HG	0.42	1.92	9	1
1:A:126:ILE:HG23	1:A:128:GLU:N	0.42	2.30	19	1
1:A:128:GLU:O	1:A:129:LYS:CB	0.42	2.68	20	1
1:A:126:ILE:O	1:A:127:PHE:C	0.42	2.62	15	2
1:A:5:LEU:HD11	1:A:152:GLU:HG3	0.42	1.92	6	1
1:A:5:LEU:C	1:A:5:LEU:CD2	0.42	2.93	18	2
1:A:17:MET:HG2	1:A:60:LEU:HD21	0.42	1.90	9	1
1:A:40:LEU:HD23	1:A:41:ASP:N	0.42	2.30	18	1
1:A:5:LEU:HD21	1:A:152:GLU:OE2	0.41	2.15	1	1
1:A:138:VAL:HG21	1:A:151:LEU:HD11	0.41	1.90	5	1
1:A:13:PRO:O	1:A:14:ASP:CB	0.41	2.68	11	1
1:A:62:VAL:CG2	1:A:151:LEU:HD11	0.41	2.45	10	2
1:A:73:ILE:H	1:A:73:ILE:HD13	0.41	1.75	2	1
1:A:71:THR:HG21	1:A:156:CYS:SG	0.41	2.55	9	2
1:A:73:ILE:HD13	1:A:73:ILE:N	0.41	2.29	12	2
1:A:40:LEU:O	1:A:41:ASP:C	0.41	2.62	6	1
1:A:115:GLY:O	1:A:116:ASN:C	0.41	2.63	16	1
1:A:154:LEU:N	1:A:154:LEU:HD22	0.41	2.31	19	1
1:A:91:LYS:HZ3	1:A:103:VAL:HG21	0.41	1.76	20	1
1:A:67:GLN:O	1:A:132:MET:HE2	0.41	2.16	15	1
1:A:73:ILE:HD11	1:A:125:ASN:CG	0.41	2.40	17	1
1:A:138:VAL:C	1:A:139:LEU:HD12	0.41	2.41	6	1
1:A:7:LEU:N	1:A:7:LEU:HD22	0.41	2.29	7	1
1:A:55:SER:O	1:A:56:ALA:CB	0.41	2.69	11	2
1:A:91:LYS:CE	1:A:103:VAL:HG11	0.41	2.46	13	1
1:A:153:LEU:HD22	1:A:153:LEU:O	0.41	2.14	7	1
1:A:73:ILE:HD12	1:A:124:LYS:CB	0.41	2.46	11	1
1:A:154:LEU:HD22	1:A:154:LEU:N	0.41	2.31	11	1
1:A:50:THR:HG23	1:A:148:THR:CG2	0.41	2.46	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ILE:CA	1:A:154:LEU:HD12	0.41	2.45	6	1
1:A:50:THR:CB	1:A:148:THR:HG23	0.41	2.46	10	1
1:A:12:ILE:C	1:A:14:ASP:H	0.41	2.24	13	1
1:A:102:THR:O	1:A:103:VAL:O	0.40	2.39	18	1
1:A:144:HIS:O	1:A:145:ASN:CB	0.40	2.69	6	4
1:A:156:CYS:C	1:A:158:GLU:N	0.40	2.79	20	1
1:A:38:GLY:O	1:A:40:LEU:N	0.40	2.54	16	1
1:A:74:ILE:HG23	1:A:152:GLU:CB	0.40	2.43	3	1
1:A:75:THR:OG1	1:A:151:LEU:HD22	0.40	2.16	8	1
1:A:73:ILE:HD13	1:A:73:ILE:H	0.40	1.76	14	1
1:A:149:LEU:C	1:A:149:LEU:CD2	0.40	2.95	14	1
1:A:88:ALA:HB2	1:A:116:ASN:OD1	0.40	2.17	1	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	141/170 (83%)	105±4 (74±3%)	28±3 (20±2%)	8±3 (6±2%)	2	21
All	All	2820/3400 (83%)	2098 (74%)	566 (20%)	156 (6%)	2	21

All 39 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	45	LYS	19
1	A	147	ILE	13
1	A	124	LYS	9
1	A	118	ASP	7
1	A	81	PHE	6
1	A	44	GLY	6
1	A	34	TYR	6
1	A	67	GLN	6
1	A	9	ASN	6
1	A	126	ILE	6

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Mol	Chain	Res	Type	Models (Total)
1	A	4	PRO	6
1	A	6	GLY	5
1	A	39	ARG	5
1	A	46	ILE	4
1	A	84	ILE	4
1	A	5	LEU	4
1	A	40	LEU	4
1	A	23	TYR	3
1	A	112	VAL	3
1	A	42	ASN	3
1	A	104	TYR	3
1	A	11	THR	3
1	A	82	GLY	2
1	A	115	GLY	2
1	A	128	GLU	2
1	A	116	ASN	2
1	A	35	PRO	2
1	A	129	LYS	2
1	A	21	SER	2
1	A	48	ALA	2
1	A	43	GLN	1
1	A	41	ASP	1
1	A	14	ASP	1
1	A	8	LYS	1
1	A	58	GLU	1
1	A	18	SER	1
1	A	103	VAL	1
1	A	123	LYS	1
1	A	2	SER	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	124/147 (84%)	85±6 (68±5%)	38±4 (30±4%)	1	16
All	All	2449/2940 (83%)	1698 (69%)	751 (31%)	1	15

All 101 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	5	LEU	20
1	A	50	THR	20
1	A	148	THR	20
1	A	157	LEU	20
1	A	91	LYS	18
1	A	45	LYS	17
1	A	71	THR	17
1	A	131	PHE	17
1	A	126	ILE	16
1	A	134	ARG	16
1	A	76	GLN	14
1	A	123	LYS	14
1	A	144	HIS	14
1	A	2	SER	14
1	A	114	GLN	14
1	A	37	LEU	13
1	A	40	LEU	13
1	A	111	LYS	13
1	A	22	SER	13
1	A	95	SER	13
1	A	20	SER	12
1	A	129	LYS	12
1	A	146	ARG	12
1	A	73	ILE	12
1	A	74	ILE	12
1	A	8	LYS	11
1	A	58	GLU	11
1	A	61	GLN	11
1	A	151	LEU	11
1	A	142	SER	10
1	A	156	CYS	10
1	A	119	ASN	9
1	A	121	SER	9
1	A	55	SER	9
1	A	57	LYS	9
1	A	64	LEU	9
1	A	124	LYS	9
1	A	17	MET	9
1	A	150	ARG	9
1	A	53	SER	9
1	A	158	GLU	9
1	A	79	ARG	8

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Mol	Chain	Res	Type	Models (Total)
1	A	60	LEU	8
1	A	83	HIS	8
1	A	125	ASN	8
1	A	153	LEU	8
1	A	138	VAL	8
1	A	152	GLU	8
1	A	149	LEU	7
1	A	118	ASP	7
1	A	90	TYR	7
1	A	34	TYR	7
1	A	9	ASN	6
1	A	89	SER	5
1	A	97	ASP	5
1	A	122	HIS	5
1	A	145	ASN	5
1	A	39	ARG	5
1	A	42	ASN	5
1	A	135	TYR	5
1	A	154	LEU	5
1	A	3	GLU	5
1	A	113	PHE	5
1	A	15	SER	4
1	A	120	ASN	4
1	A	117	LEU	4
1	A	132	MET	4
1	A	139	LEU	4
1	A	137	ARG	4
1	A	18	SER	4
1	A	112	VAL	3
1	A	116	ASN	3
1	A	43	GLN	3
1	A	47	ASN	3
1	A	85	GLN	3
1	A	87	VAL	3
1	A	11	THR	3
1	A	49	TRP	2
1	A	63	ASP	2
1	A	128	GLU	2
1	A	1	CYS	2
1	A	41	ASP	2
1	A	52	GLN	2
1	A	127	PHE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	14	ASP	2
1	A	36	HIS	1
1	A	67	GLN	1
1	A	54	ASN	1
1	A	147	ILE	1
1	A	96	ASP	1
1	A	7	LEU	1
1	A	80	ASP	1
1	A	69	GLN	1
1	A	75	THR	1
1	A	66	THR	1
1	A	59	TRP	1
1	A	68	ARG	1
1	A	103	VAL	1
1	A	104	TYR	1
1	A	81	PHE	1
1	A	21	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 76% 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	1706
Number of shifts mapped to atoms	1531
Number of unparsed shifts	0
Number of shifts with mapping errors	175
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 175 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	-3	SER	HB2	3.73	0.020	2
1	A	-1	HIS	HB2	3.044	0.020	2
1	A	1	CYS	HB2	3.211	0.020	2
1	A	2	SER	HB2	3.547	0.020	2
1	A	3	GLU	HB2	2.226	0.020	2
1	A	3	GLU	HG2	1.922	0.020	2
1	A	4	PRO	HB2	2.168	0.020	2
1	A	4	PRO	HD2	3.621	0.020	2
1	A	4	PRO	HG2	1.903	0.020	2
1	A	5	LEU	HB2	1.507	0.020	2
1	A	7	LEU	HB2	2.375	0.020	2
1	A	8	LYS	HB2	1.871	0.020	2
1	A	9	ASN	HB2	3.153	0.020	2
1	A	10	ASN	HB2	2.91	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	ILE	HG12	1.252	0.020	2
1	A	13	PRO	HB2	2.236	0.020	2
1	A	13	PRO	HD2	3.724	0.020	2
1	A	13	PRO	HG2	1.953	0.020	2
1	A	14	ASP	HB2	2.349	0.020	2
1	A	15	SER	HB2	3.91	0.020	2
1	A	16	GLN	HB2	1.808	0.020	2
1	A	16	GLN	HG2	2.407	0.020	2
1	A	17	MET	HB2	1.818	0.020	2
1	A	17	MET	HG2	2.058	0.020	2
1	A	18	SER	HB2	3.922	0.020	2
1	A	20	SER	HB2	2.865	0.020	2
1	A	21	SER	HB2	4.104	0.020	2
1	A	22	SER	HB2	3.684	0.020	2
1	A	23	TYR	HB2	2.526	0.020	2
1	A	24	LYS	HB2	1.748	0.020	2
1	A	24	LYS	HD2	1.65	0.020	2
1	A	24	LYS	HE2	2.53	0.020	2
1	A	24	LYS	HG2	1.571	0.020	2
1	A	31	PHE	HB2	3.272	0.020	2
1	A	33	TRP	HB2	3.013	0.020	2
1	A	35	PRO	HB2	2.142	0.020	2
1	A	35	PRO	HG2	1.616	0.020	2
1	A	36	HIS	HB2	3.698	0.020	2
1	A	37	LEU	HB2	1.703	0.020	2
1	A	39	ARG	HB2	1.558	0.020	2
1	A	39	ARG	HD2	2.949	0.020	2
1	A	39	ARG	HG2	1.147	0.020	2
1	A	40	LEU	HB2	1.494	0.020	2
1	A	41	ASP	HB2	3.042	0.020	2
1	A	42	ASN	HB2	3.342	0.020	2
1	A	43	GLN	HB2	2.143	0.020	2
1	A	43	GLN	HG2	2.434	0.020	2
1	A	45	LYS	HB2	1.766	0.020	2
1	A	45	LYS	HD2	1.567	0.020	2
1	A	45	LYS	HG2	1.308	0.020	2
1	A	46	ILE	HG12	0.982	0.020	2
1	A	47	ASN	HB2	2.335	0.020	2
1	A	49	TRP	HB2	3.18	0.020	2
1	A	52	GLN	HB2	1.875	0.020	2
1	A	52	GLN	HG2	2.302	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	SER	HB2	3.822	0.020	2
1	A	54	ASN	HB2	2.503	0.020	2
1	A	55	SER	HB2	3.841	0.020	2
1	A	57	LYS	HB2	1.984	0.020	2
1	A	57	LYS	HD2	1.565	0.020	2
1	A	57	LYS	HE2	3.171	0.020	2
1	A	57	LYS	HG2	1.297	0.020	2
1	A	58	GLU	HB2	1.669	0.020	2
1	A	58	GLU	HG2	2.015	0.020	2
1	A	59	TRP	HB2	3.438	0.020	2
1	A	60	LEU	HB2	1.131	0.020	2
1	A	61	GLN	HB2	1.911	0.020	2
1	A	61	GLN	HG2	2.315	0.020	2
1	A	63	ASP	HB2	2.599	0.020	2
1	A	64	LEU	HB2	2.273	0.020	2
1	A	67	GLN	HB2	1.86	0.020	2
1	A	67	GLN	HG2	2.147	0.020	2
1	A	68	ARG	HB2	1.545	0.020	2
1	A	68	ARG	HD2	3.22	0.020	2
1	A	68	ARG	HG2	1.708	0.020	2
1	A	69	GLN	HB2	1.651	0.020	2
1	A	69	GLN	HG2	1.811	0.020	2
1	A	74	ILE	HG12	1.278	0.020	2
1	A	76	GLN	HB2	1.814	0.020	2
1	A	76	GLN	HG2	2.294	0.020	2
1	A	79	ARG	HB2	1.595	0.020	2
1	A	79	ARG	HD2	2.941	0.020	2
1	A	79	ARG	HG2	1.286	0.020	2
1	A	80	ASP	HB2	2.45	0.020	2
1	A	81	PHE	HB2	3.274	0.020	2
1	A	83	HIS	HB2	3.213	0.020	2
1	A	84	ILE	HG12	1.638	0.020	2
1	A	85	GLN	HB2	1.864	0.020	2
1	A	85	GLN	HG2	2.156	0.020	2
1	A	86	TYR	HB2	3.455	0.020	2
1	A	89	SER	HB2	3.528	0.020	2
1	A	90	TYR	HB2	3.056	0.020	2
1	A	91	LYS	HB2	1.762	0.020	2
1	A	91	LYS	HD2	1.64	0.020	2
1	A	91	LYS	HE2	3.078	0.020	2
1	A	94	HIS	HB2	3.105	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	95	SER	HB2	3.698	0.020	2
1	A	96	ASP	HB2	2.63	0.020	2
1	A	97	ASP	HB2	2.74	0.020	2
1	A	100	GLN	HB2	1.86	0.020	2
1	A	100	GLN	HG2	2.232	0.020	2
1	A	101	TRP	HB2	2.694	0.020	2
1	A	104	TYR	HB2	2.472	0.020	2
1	A	105	GLU	HB2	1.526	0.020	2
1	A	105	GLU	HG2	2.157	0.020	2
1	A	106	GLU	HB2	1.938	0.020	2
1	A	106	GLU	HG2	2.314	0.020	2
1	A	107	GLN	HB2	2.009	0.020	2
1	A	107	GLN	HG2	2.252	0.020	2
1	A	109	SER	HB2	3.7	0.020	2
1	A	110	SER	HB2	3.633	0.020	2
1	A	111	LYS	HB2	1.781	0.020	2
1	A	111	LYS	HD2	1.227	0.020	2
1	A	111	LYS	HG2	1.283	0.020	2
1	A	113	PHE	HB2	2.253	0.020	2
1	A	114	GLN	HB2	2.07	0.020	2
1	A	114	GLN	HG2	2.392	0.020	2
1	A	116	ASN	HB2	2.957	0.020	2
1	A	117	LEU	HB2	1.514	0.020	2
1	A	118	ASP	HB2	2.831	0.020	2
1	A	119	ASN	HB2	2.43	0.020	2
1	A	120	ASN	HB2	2.668	0.020	2
1	A	121	SER	HB2	3.697	0.020	2
1	A	122	HIS	HB2	3.003	0.020	2
1	A	123	LYS	HB2	1.791	0.020	2
1	A	123	LYS	HD2	1.666	0.020	2
1	A	123	LYS	HE2	2.885	0.020	2
1	A	123	LYS	HG2	1.276	0.020	2
1	A	124	LYS	HB2	1.728	0.020	2
1	A	124	LYS	HE2	2.685	0.020	2
1	A	124	LYS	HG2	1.453	0.020	2
1	A	125	ASN	HB2	2.307	0.020	2
1	A	126	ILE	HG12	1.229	0.020	2
1	A	127	PHE	HB2	3.199	0.020	2
1	A	128	GLU	HB2	2.091	0.020	2
1	A	128	GLU	HG2	2.454	0.020	2
1	A	129	LYS	HB2	1.925	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	129	LYS	HD2	1.74	0.020	2
1	A	129	LYS	HE2	3.0	0.020	2
1	A	129	LYS	HG2	1.435	0.020	2
1	A	130	PRO	HB2	2.165	0.020	2
1	A	130	PRO	HD2	3.593	0.020	2
1	A	130	PRO	HG2	1.947	0.020	2
1	A	131	PHE	HB2	2.839	0.020	2
1	A	132	MET	HB2	1.926	0.020	2
1	A	132	MET	HG2	2.425	0.020	2
1	A	134	ARG	HD2	2.808	0.020	2
1	A	134	ARG	HG2	1.42	0.020	2
1	A	135	TYR	HB2	2.805	0.020	2
1	A	137	ARG	HB2	1.172	0.020	2
1	A	137	ARG	HG2	1.049	0.020	2
1	A	139	LEU	HB2	1.459	0.020	2
1	A	140	PRO	HB2	1.999	0.020	2
1	A	140	PRO	HD2	3.071	0.020	2
1	A	140	PRO	HG2	1.875	0.020	2
1	A	142	SER	HB2	3.553	0.020	2
1	A	143	TRP	HB2	3.276	0.020	2
1	A	144	HIS	HB2	3.814	0.020	2
1	A	145	ASN	HB2	3.427	0.020	2
1	A	146	ARG	HB2	1.054	0.020	2
1	A	146	ARG	HD2	2.259	0.020	2
1	A	146	ARG	HG2	0.84	0.020	2
1	A	147	ILE	HG12	-0.001	0.020	2
1	A	149	LEU	HB2	1.712	0.020	2
1	A	150	ARG	HB2	1.949	0.020	2
1	A	150	ARG	HG2	1.625	0.020	2
1	A	151	LEU	HB2	1.715	0.020	2
1	A	152	GLU	HB2	1.731	0.020	2
1	A	152	GLU	HG2	2.059	0.020	2
1	A	153	LEU	HB2	1.537	0.020	2
1	A	154	LEU	HB2	1.071	0.020	2
1	A	156	CYS	HB2	3.197	0.020	2
1	A	157	LEU	HB2	1.404	0.020	2
1	A	158	GLU	HB2	1.788	0.020	2
1	A	158	GLU	HG2	2.049	0.020	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	156	2.91 ± 0.14	Should be checked
$^{13}\text{C}_\beta$	142	2.45 ± 0.17	Should be checked
$^{13}\text{C}'$	148	3.28 ± 0.15	Should be applied
^{15}N	149	0.38 ± 0.42	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1581 atoms were assigned a chemical shift out of a possible 1948. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	699/710 (98%)	287/289 (99%)	276/284 (97%)	136/137 (99%)
Sidechain	859/1061 (81%)	597/687 (87%)	255/325 (78%)	7/49 (14%)
Aromatic	23/177 (13%)	20/88 (23%)	0/80 (0%)	3/9 (33%)
Overall	1581/1948 (81%)	904/1064 (85%)	531/689 (77%)	146/195 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1705 atoms were assigned a chemical shift out of a possible 2232. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	772/824 (94%)	319/337 (95%)	304/328 (93%)	149/159 (94%)
Sidechain	908/1190 (76%)	632/769 (82%)	269/365 (74%)	7/56 (12%)
Aromatic	25/218 (11%)	21/109 (19%)	0/97 (0%)	4/12 (33%)
Overall	1705/2232 (76%)	972/1215 (80%)	573/790 (73%)	160/227 (70%)

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	46	ILE	HG21	-0.90	-0.56 – 2.11	-6.3
1	A	46	ILE	HG22	-0.90	-0.56 – 2.11	-6.3
1	A	46	ILE	HG23	-0.90	-0.56 – 2.11	-6.3

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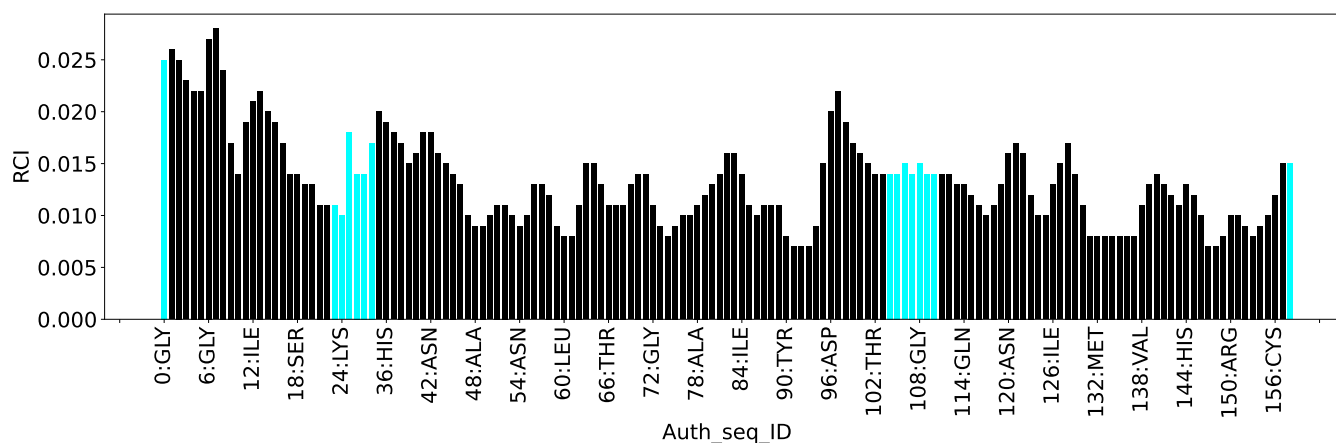
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	98	GLY	HA3	2.02	2.08 – 5.71	-5.2
1	A	24	LYS	HE3	1.89	1.92 – 3.89	-5.2

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	2099
Intra-residue ($ i-j =0$)	400
Sequential ($ i-j =1$)	640
Medium range ($ i-j >1$ and $ i-j <5$)	180
Long range ($ i-j \geq 5$)	729
Inter-chain	0
Hydrogen bond restraints	149
Disulfide bond restraints	1
Total dihedral-angle restraints	110
Number of unmapped restraints	0
Number of restraints per residue	13.0
Number of long range restraints per residue ¹	5.2

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)	40.0	0.2
0.2-0.5 (Medium)	31.5	0.5
>0.5 (Large)	0.9	0.63

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)	11.4	7.86
10.0-20.0 (Medium)	0.1	18.63
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

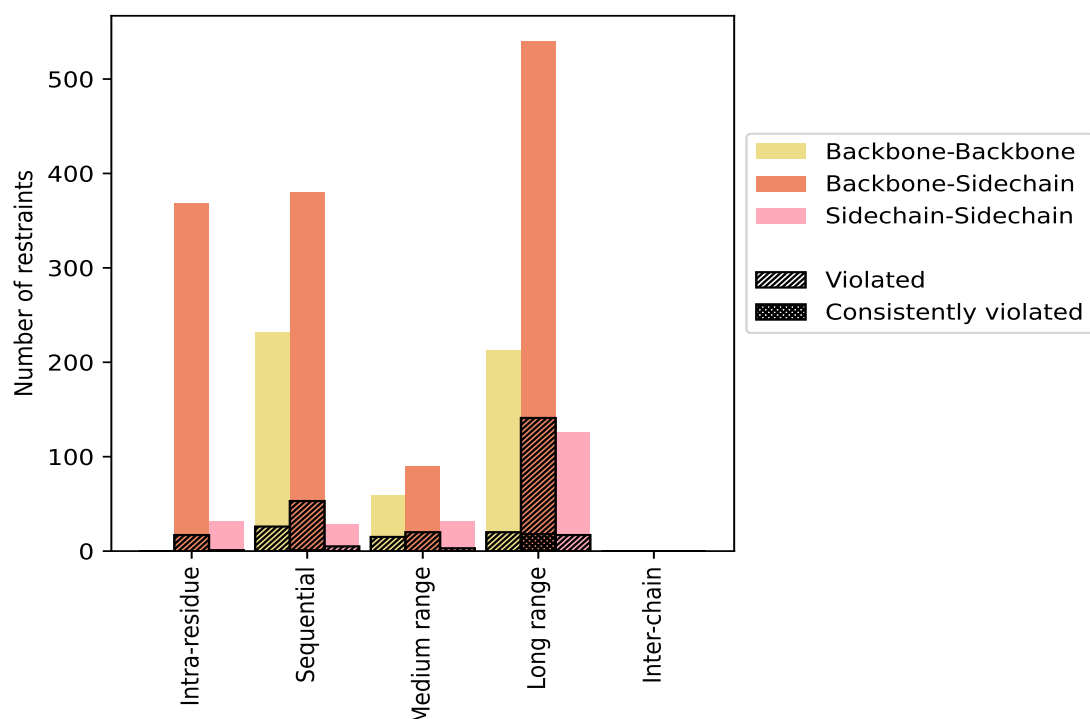
9.1 Summary of distance violations ⓘ

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)	400	19.1	18	4.5	0.9	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	368	17.5	17	4.6	0.8	0	0.0	0.0
Sidechain-Sidechain	31	1.5	1	3.2	0.0	0	0.0	0.0
Sequential (i-j =1)	640	30.5	84	13.1	4.0	1	0.2	0.0
Backbone-Backbone	232	11.1	26	11.2	1.2	0	0.0	0.0
Backbone-Sidechain	380	18.1	53	13.9	2.5	1	0.3	0.0
Sidechain-Sidechain	28	1.3	5	17.9	0.2	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	180	8.6	38	21.1	1.8	0	0.0	0.0
Backbone-Backbone	59	2.8	15	25.4	0.7	0	0.0	0.0
Backbone-Sidechain	90	4.3	20	22.2	1.0	0	0.0	0.0
Sidechain-Sidechain	31	1.5	3	9.7	0.1	0	0.0	0.0
Long range (i-j ≥5)	729	34.7	90	12.3	4.3	1	0.1	0.0
Backbone-Backbone	213	10.1	20	9.4	1.0	0	0.0	0.0
Backbone-Sidechain	391	18.6	53	13.6	2.5	1	0.3	0.0
Sidechain-Sidechain	125	6.0	17	13.6	0.8	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	149	7.1	88	59.1	4.2	17	11.4	0.8
Disulfide bond	1	0.0	0	0.0	0.0	0	0.0	0.0
Total	2099	100.0	318	15.2	15.2	19	0.9	0.9
Backbone-Backbone	505	24.1	61	12.1	2.9	0	0.0	0.0
Backbone-Sidechain	1378	65.7	231	16.8	11.0	19	1.4	0.9
Sidechain-Sidechain	216	10.3	26	12.0	1.2	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	3	4	53	0	60	0.2	0.48	0.09	0.16
2	3	7	4	47	0	61	0.23	0.56	0.1	0.23
3	1	6	2	52	0	61	0.21	0.54	0.1	0.17
4	3	6	5	45	0	59	0.22	0.5	0.1	0.19
5	0	5	3	64	0	72	0.21	0.48	0.09	0.17
6	2	9	4	72	0	87	0.22	0.55	0.1	0.19
7	1	10	4	59	0	74	0.21	0.48	0.09	0.18
8	4	20	2	58	0	84	0.2	0.53	0.09	0.18
9	2	12	2	65	0	81	0.21	0.48	0.09	0.18
10	0	11	1	58	0	70	0.2	0.49	0.09	0.19

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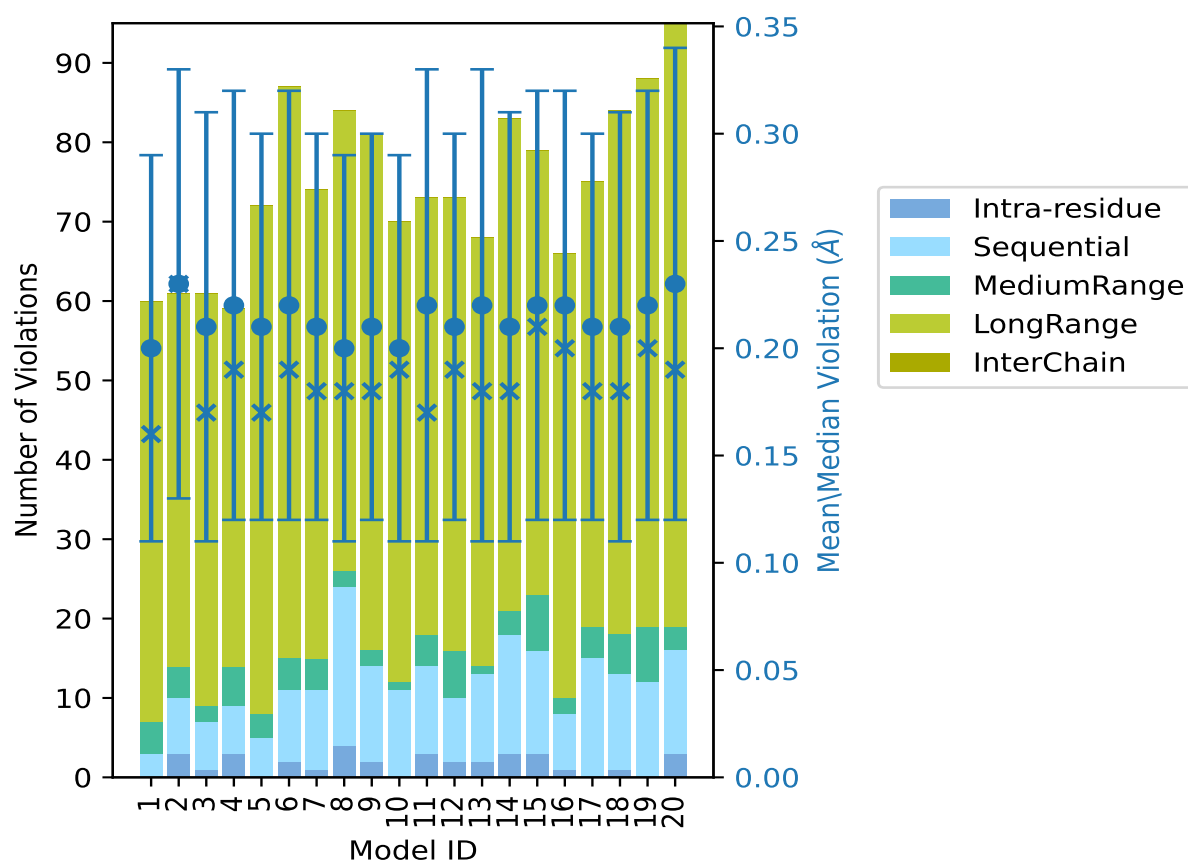
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	11	4	55	0	73	0.22	0.53	0.11	0.17
12	2	8	6	57	0	73	0.21	0.55	0.09	0.19
13	2	11	1	54	0	68	0.22	0.61	0.11	0.18
14	3	15	3	62	0	83	0.21	0.55	0.1	0.18
15	3	13	7	56	0	79	0.22	0.52	0.1	0.21
16	1	7	2	56	0	66	0.22	0.56	0.1	0.2
17	0	15	4	56	0	75	0.21	0.53	0.09	0.18
18	1	12	5	66	0	84	0.21	0.53	0.1	0.18
19	0	12	7	69	0	88	0.22	0.63	0.1	0.2
20	3	13	3	76	0	95	0.23	0.63	0.11	0.19

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

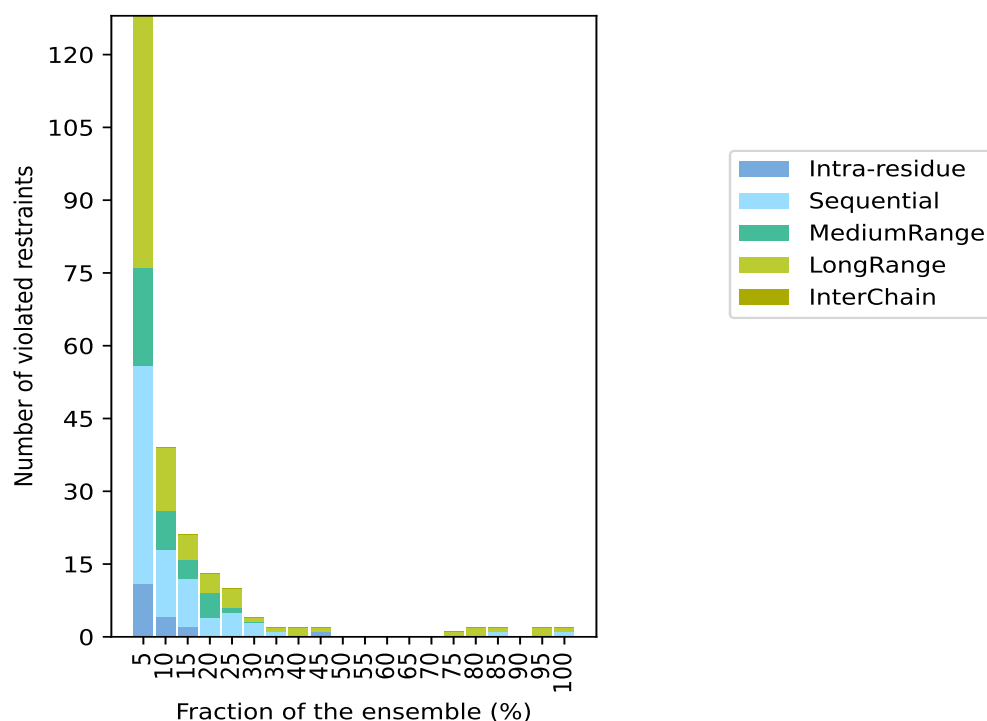
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1719(IR:382, SQ:556, MR:142, LR:639, IC:0) restraints are 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	45	20	52	0	128	1	5.0
4	14	8	13	0	39	2	10.0
2	10	4	5	0	21	3	15.0
0	4	5	4	0	13	4	20.0
0	5	1	4	0	10	5	25.0
0	3	0	1	0	4	6	30.0
0	1	0	1	0	2	7	35.0
0	0	0	2	0	2	8	40.0
1	0	0	1	0	2	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	1	0	1	15	75.0
0	0	0	2	0	2	16	80.0
0	1	0	1	0	2	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	2	0	2	19	95.0
0	1	0	1	0	2	20	100.0

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

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

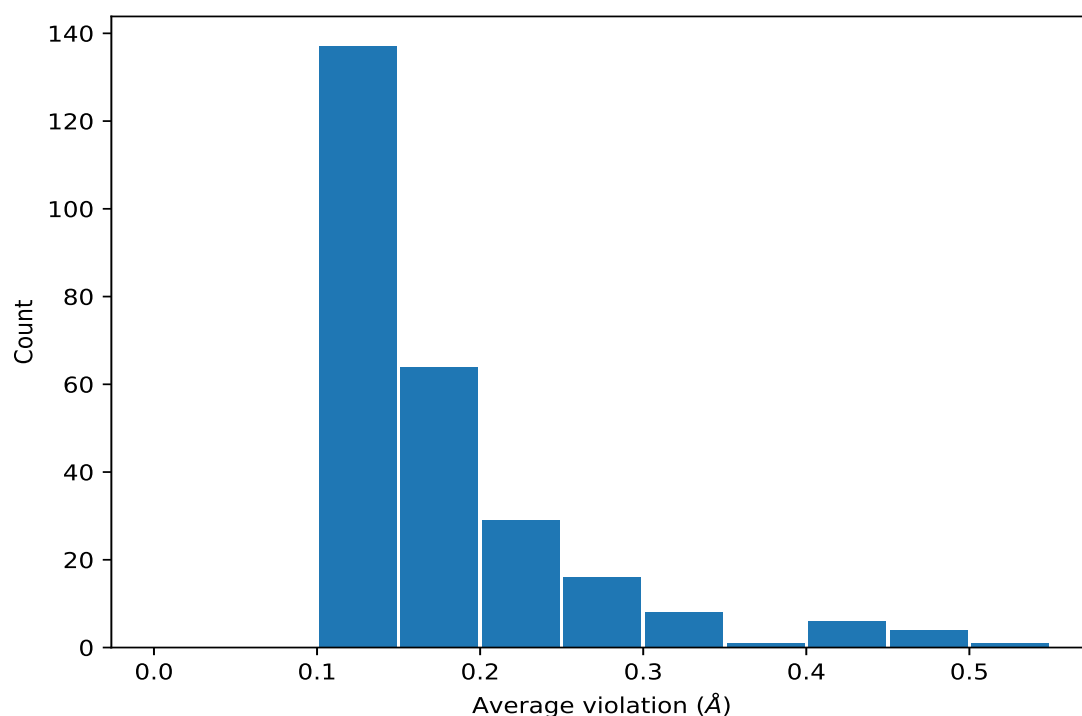
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	20	0.5	0.06	0.5
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	20	0.45	0.05	0.44
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	20	0.43	0.03	0.42
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	20	0.38	0.1	0.4
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	20	0.34	0.03	0.34
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	20	0.33	0.04	0.33
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	20	0.33	0.05	0.32
(2,145)	1:89:A:SER:O	1:142:A:SER:N	20	0.32	0.04	0.32
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	20	0.31	0.05	0.31
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	20	0.31	0.06	0.31
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	20	0.29	0.07	0.29
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	20	0.29	0.06	0.3
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	20	0.27	0.04	0.28
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	20	0.26	0.05	0.26
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	20	0.26	0.05	0.26
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	20	0.26	0.05	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	20	0.21	0.04	0.2
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	20	0.17	0.04	0.16
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	20	0.17	0.02	0.17
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	20	0.17	0.03	0.16
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	20	0.16	0.04	0.16
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	19	0.27	0.09	0.29
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	19	0.26	0.07	0.27
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	19	0.25	0.05	0.26
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	18	0.28	0.03	0.28
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	18	0.26	0.08	0.24
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	18	0.22	0.05	0.22
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	18	0.18	0.05	0.16
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	18	0.15	0.02	0.15
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	17	0.22	0.06	0.22
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	17	0.22	0.04	0.24
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	17	0.21	0.06	0.23
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	17	0.21	0.06	0.21
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	17	0.17	0.04	0.16
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	17	0.16	0.04	0.16
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	17	0.14	0.05	0.12
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	17	0.14	0.03	0.13
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	16	0.25	0.05	0.24
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	16	0.16	0.04	0.16
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	16	0.14	0.03	0.13
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	15	0.23	0.09	0.25
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	15	0.21	0.05	0.21
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	15	0.15	0.05	0.13
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	14	0.19	0.04	0.19
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	13	0.33	0.11	0.35
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	13	0.21	0.06	0.22
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	12	0.28	0.07	0.3
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	12	0.16	0.02	0.15
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	12	0.15	0.04	0.14
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	11	0.21	0.05	0.22
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	11	0.21	0.07	0.21
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	11	0.13	0.03	0.12
(2,132)	1:49:A:TRP:N	1:149:A:LEU:O	10	0.19	0.05	0.19
(2,15)	1:73:A:ILE:N	1:125:A:ASN:O	10	0.16	0.04	0.14
(2,114)	1:93:A:ALA:N	1:137:A:ARG:O	9	0.18	0.05	0.16
(2,105)	1:70:A:VAL:N	1:131:A:PHE:O	9	0.16	0.05	0.15
(1,598)	1:50:A:THR:HG21	1:146:A:ARG:HA	9	0.14	0.02	0.13
(1,598)	1:50:A:THR:HG22	1:146:A:ARG:HA	9	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,598)	1:50:A:THR:HG23	1:146:A:ARG:HA	9	0.14	0.02	0.13
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG11	8	0.19	0.06	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG12	8	0.19	0.06	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG13	8	0.19	0.06	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG21	8	0.19	0.06	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG22	8	0.19	0.06	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG23	8	0.19	0.06	0.18
(2,126)	1:89:A:SER:O	1:141:A:VAL:N	8	0.15	0.04	0.15
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG11	8	0.15	0.06	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG12	8	0.15	0.06	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG13	8	0.15	0.06	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG21	8	0.15	0.06	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG22	8	0.15	0.06	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG23	8	0.15	0.06	0.12
(1,41)	1:122:A:HIS:H	1:123:A:LYS:HA	7	0.21	0.02	0.2
(2,42)	1:95:A:SER:O	1:135:A:TYR:H	7	0.14	0.01	0.14
(2,72)	1:78:A:ALA:O	1:85:A:GLN:H	7	0.13	0.01	0.14
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG21	7	0.13	0.02	0.13
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG22	7	0.13	0.02	0.13
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG23	7	0.13	0.02	0.13
(1,1124)	1:127:A:PHE:HA	1:128:A:GLU:H	6	0.24	0.01	0.24
(2,101)	1:62:A:VAL:N	1:136:A:VAL:O	6	0.2	0.07	0.2
(1,556)	1:71:A:THR:HA	1:127:A:PHE:H	6	0.18	0.08	0.14
(2,80)	1:73:A:ILE:O	1:125:A:ASN:H	6	0.18	0.03	0.18
(2,50)	1:91:A:LYS:O	1:139:A:LEU:H	6	0.17	0.03	0.16
(1,902)	1:73:A:ILE:HD11	1:74:A:ILE:H	6	0.14	0.02	0.14
(1,902)	1:73:A:ILE:HD12	1:74:A:ILE:H	6	0.14	0.02	0.14
(1,902)	1:73:A:ILE:HD13	1:74:A:ILE:H	6	0.14	0.02	0.14
(1,826)	1:95:A:SER:H	1:98:A:GLY:HA2	5	0.22	0.07	0.23
(1,1067)	1:36:A:HIS:H	1:49:A:TRP:HB3	5	0.19	0.04	0.19
(2,78)	1:75:A:THR:O	1:123:A:LYS:H	5	0.19	0.11	0.13
(1,454)	1:122:A:HIS:HD1	1:123:A:LYS:H	5	0.18	0.03	0.17
(1,152)	1:48:A:ALA:H	1:49:A:TRP:H	5	0.18	0.04	0.16
(2,86)	1:3:A:GLU:O	1:155:A:GLY:H	5	0.17	0.03	0.16
(1,1372)	1:38:A:GLY:HA2	1:150:A:ARG:HA	5	0.17	0.05	0.19
(1,1372)	1:38:A:GLY:HA3	1:150:A:ARG:HA	5	0.17	0.05	0.19
(2,130)	1:18:A:SER:N	1:61:A:GLN:O	5	0.15	0.03	0.15
(1,563)	1:147:A:ILE:H	1:148:A:THR:HA	5	0.14	0.02	0.13
(2,81)	1:73:A:ILE:O	1:125:A:ASN:N	5	0.14	0.01	0.14
(1,1570)	1:79:A:ARG:H	1:85:A:GLN:HB3	5	0.13	0.04	0.12
(1,1470)	1:61:A:GLN:HB3	1:138:A:VAL:H	5	0.12	0.02	0.11
(1,193)	1:5:A:LEU:HA	1:6:A:GLY:H	5	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,76)	1:88:A:ALA:O	1:115:A:GLY:H	5	0.11	0.01	0.11
(1,241)	1:106:A:GLU:H	1:110:A:SER:HA	4	0.26	0.08	0.3
(1,1404)	1:45:A:LYS:HG3	1:46:A:ILE:HA	4	0.22	0.08	0.22
(1,1774)	1:116:A:ASN:HB3	1:118:A:ASP:H	4	0.19	0.05	0.21
(2,92)	1:65:A:GLY:H	1:134:A:ARG:O	4	0.16	0.07	0.14
(1,1058)	1:14:A:ASP:H	1:16:A:GLN:H	4	0.15	0.02	0.14
(1,1125)	1:128:A:GLU:H	1:129:A:LYS:H	4	0.15	0.04	0.13
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD11	4	0.15	0.04	0.15
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD12	4	0.15	0.04	0.15
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD13	4	0.15	0.04	0.15
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD21	4	0.15	0.04	0.15
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD22	4	0.15	0.04	0.15
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD23	4	0.15	0.04	0.15
(1,1626)	1:87:A:VAL:HG11	1:141:A:VAL:H	4	0.15	0.04	0.14
(1,1626)	1:87:A:VAL:HG12	1:141:A:VAL:H	4	0.15	0.04	0.14
(1,1626)	1:87:A:VAL:HG13	1:141:A:VAL:H	4	0.15	0.04	0.14
(1,1626)	1:87:A:VAL:HG21	1:141:A:VAL:H	4	0.15	0.04	0.14
(1,1626)	1:87:A:VAL:HG22	1:141:A:VAL:H	4	0.15	0.04	0.14
(1,1626)	1:87:A:VAL:HG23	1:141:A:VAL:H	4	0.15	0.04	0.14
(1,998)	1:37:A:LEU:H	1:49:A:TRP:H	4	0.14	0.01	0.14
(1,1587)	1:79:A:ARG:HG3	1:82:A:GLY:H	4	0.14	0.03	0.14
(2,1)	1:60:A:LEU:H	1:138:A:VAL:O	4	0.13	0.01	0.13
(2,62)	1:20:A:SER:H	1:59:A:TRP:O	4	0.13	0.04	0.11
(1,1206)	1:72:A:GLY:H	1:155:A:GLY:H	4	0.12	0.01	0.12
(1,1406)	1:45:A:LYS:HD3	1:46:A:ILE:HA	4	0.12	0.01	0.12
(1,386)	1:42:A:ASN:HA	1:47:A:ASN:H	4	0.11	0.0	0.11
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG21	3	0.42	0.03	0.43
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG22	3	0.42	0.03	0.43
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG23	3	0.42	0.03	0.43
(1,165)	1:116:A:ASN:HA	1:117:A:LEU:HG	3	0.25	0.0	0.25
(2,138)	1:88:A:ALA:O	1:115:A:GLY:N	3	0.23	0.06	0.25
(2,134)	1:18:A:SER:O	1:61:A:GLN:N	3	0.21	0.03	0.21
(1,1385)	1:42:A:ASN:H	1:47:A:ASN:HB3	3	0.19	0.03	0.19
(1,1637)	1:87:A:VAL:HG11	1:148:A:THR:HB	3	0.19	0.04	0.17
(1,1637)	1:87:A:VAL:HG12	1:148:A:THR:HB	3	0.19	0.04	0.17
(1,1637)	1:87:A:VAL:HG13	1:148:A:THR:HB	3	0.19	0.04	0.17
(1,1637)	1:87:A:VAL:HG21	1:148:A:THR:HB	3	0.19	0.04	0.17
(1,1637)	1:87:A:VAL:HG22	1:148:A:THR:HB	3	0.19	0.04	0.17
(1,1637)	1:87:A:VAL:HG23	1:148:A:THR:HB	3	0.19	0.04	0.17
(1,278)	1:127:A:PHE:HA	1:129:A:LYS:H	3	0.18	0.07	0.19
(1,1050)	1:10:A:ASN:H	1:11:A:THR:H	3	0.18	0.01	0.19
(1,670)	1:73:A:ILE:HD11	1:74:A:ILE:HA	3	0.16	0.05	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,670)	1:73:A:ILE:HD12	1:74:A:ILE:HA	3	0.16	0.05	0.13
(1,670)	1:73:A:ILE:HD13	1:74:A:ILE:HA	3	0.16	0.05	0.13
(2,120)	1:68:A:ARG:O	1:133:A:ALA:N	3	0.16	0.05	0.14
(1,342)	1:116:A:ASN:H	1:118:A:ASP:H	3	0.15	0.06	0.13
(1,1172)	1:40:A:LEU:HG	1:41:A:ASP:H	3	0.15	0.05	0.13
(1,1396)	1:44:A:GLY:H	1:45:A:LYS:HD3	3	0.15	0.03	0.17
(1,1454)	1:58:A:GLU:H	1:147:A:ILE:HG13	3	0.15	0.05	0.13
(1,1392)	1:43:A:GLN:H	1:44:A:GLY:HA2	3	0.14	0.03	0.14
(1,1392)	1:43:A:GLN:H	1:44:A:GLY:HA3	3	0.14	0.03	0.14
(2,24)	1:90:A:TYR:H	1:113:A:PHE:O	3	0.14	0.02	0.16
(2,147)	1:71:A:THR:N	1:154:A:LEU:O	3	0.14	0.03	0.13
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG21	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG22	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG23	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG21	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG22	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG23	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG21	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG22	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG23	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG21	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG22	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG23	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG21	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG22	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG23	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG21	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG22	3	0.14	0.04	0.13
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG23	3	0.14	0.04	0.13
(2,123)	1:93:A:ALA:O	1:137:A:ARG:N	3	0.14	0.02	0.13
(1,1627)	1:87:A:VAL:HG11	1:142:A:SER:H	3	0.13	0.02	0.14
(1,1627)	1:87:A:VAL:HG12	1:142:A:SER:H	3	0.13	0.02	0.14
(1,1627)	1:87:A:VAL:HG13	1:142:A:SER:H	3	0.13	0.02	0.14
(1,1627)	1:87:A:VAL:HG21	1:142:A:SER:H	3	0.13	0.02	0.14
(1,1627)	1:87:A:VAL:HG22	1:142:A:SER:H	3	0.13	0.02	0.14
(1,1627)	1:87:A:VAL:HG23	1:142:A:SER:H	3	0.13	0.02	0.14
(2,127)	1:76:A:GLN:O	1:150:A:ARG:N	3	0.13	0.01	0.13
(1,1049)	1:79:A:ARG:H	1:81:A:PHE:H	3	0.13	0.02	0.13
(1,279)	1:116:A:ASN:H	1:117:A:LEU:H	3	0.12	0.0	0.12
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD11	3	0.12	0.01	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD12	3	0.12	0.01	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD13	3	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD21	3	0.12	0.01	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD22	3	0.12	0.01	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD23	3	0.12	0.01	0.11
(2,90)	1:89:A:SER:O	1:142:A:SER:H	3	0.11	0.0	0.11
(1,1791)	1:122:A:HIS:H	1:123:A:LYS:HB3	3	0.11	0.01	0.11
(1,1147)	1:46:A:ILE:HD11	1:47:A:ASN:H	2	0.46	0.01	0.46
(1,1147)	1:46:A:ILE:HD12	1:47:A:ASN:H	2	0.46	0.01	0.46
(1,1147)	1:46:A:ILE:HD13	1:47:A:ASN:H	2	0.46	0.01	0.46
(1,567)	1:13:A:PRO:HA	1:14:A:ASP:HA	2	0.44	0.17	0.44
(1,1168)	1:13:A:PRO:HA	1:14:A:ASP:H	2	0.4	0.12	0.4
(1,150)	1:106:A:GLU:H	1:109:A:SER:H	2	0.34	0.01	0.34
(1,1722)	1:105:A:GLU:H	1:105:A:GLU:HG3	2	0.27	0.01	0.27
(1,1664)	1:91:A:LYS:HA	1:113:A:PHE:HB3	2	0.24	0.08	0.24
(1,869)	1:111:A:LYS:HA	1:112:A:VAL:H	2	0.22	0.05	0.22
(1,248)	1:41:A:ASP:H	1:42:A:ASN:HA	2	0.22	0.01	0.22
(1,1119)	1:104:A:TYR:HA	1:105:A:GLU:H	2	0.22	0.06	0.22
(1,612)	1:46:A:ILE:HB	1:46:A:ILE:HD11	2	0.22	0.01	0.22
(1,612)	1:46:A:ILE:HB	1:46:A:ILE:HD12	2	0.22	0.01	0.22
(1,612)	1:46:A:ILE:HB	1:46:A:ILE:HD13	2	0.22	0.01	0.22
(1,931)	1:71:A:THR:H	1:156:A:CYS:HA	2	0.22	0.1	0.22
(1,1547)	1:75:A:THR:HA	1:76:A:GLN:HG3	2	0.2	0.04	0.2
(1,997)	1:35:A:PRO:HA	1:49:A:TRP:H	2	0.2	0.0	0.2
(2,111)	1:89:A:SER:N	1:142:A:SER:O	2	0.2	0.08	0.2
(1,72)	1:153:A:LEU:HG	1:154:A:LEU:H	2	0.19	0.03	0.19
(1,1623)	1:87:A:VAL:HG11	1:140:A:PRO:HA	2	0.19	0.04	0.19
(1,1623)	1:87:A:VAL:HG12	1:140:A:PRO:HA	2	0.19	0.04	0.19
(1,1623)	1:87:A:VAL:HG13	1:140:A:PRO:HA	2	0.19	0.04	0.19
(1,1623)	1:87:A:VAL:HG21	1:140:A:PRO:HA	2	0.19	0.04	0.19
(1,1623)	1:87:A:VAL:HG22	1:140:A:PRO:HA	2	0.19	0.04	0.19
(1,1623)	1:87:A:VAL:HG23	1:140:A:PRO:HA	2	0.19	0.04	0.19
(1,949)	1:87:A:VAL:HA	1:148:A:THR:H	2	0.18	0.06	0.18
(2,117)	1:94:A:HIS:O	1:102:A:THR:N	2	0.18	0.04	0.18
(1,1737)	1:107:A:GLN:HG3	1:109:A:SER:H	2	0.18	0.07	0.18
(1,1726)	1:105:A:GLU:HB3	1:109:A:SER:H	2	0.18	0.02	0.18
(1,690)	1:64:A:LEU:HG	1:66:A:THR:HB	2	0.17	0.05	0.17
(1,371)	1:40:A:LEU:HA	1:42:A:ASN:H	2	0.16	0.02	0.16
(1,1012)	1:88:A:ALA:HB1	1:143:A:TRP:H	2	0.16	0.05	0.16
(1,1012)	1:88:A:ALA:HB2	1:143:A:TRP:H	2	0.16	0.05	0.16
(1,1012)	1:88:A:ALA:HB3	1:143:A:TRP:H	2	0.16	0.05	0.16
(1,1137)	1:10:A:ASN:H	1:10:A:ASN:HD22	2	0.16	0.02	0.16
(1,1725)	1:105:A:GLU:HB3	1:108:A:GLY:H	2	0.16	0.02	0.16
(1,202)	1:10:A:ASN:H	1:12:A:ILE:H	2	0.16	0.01	0.16

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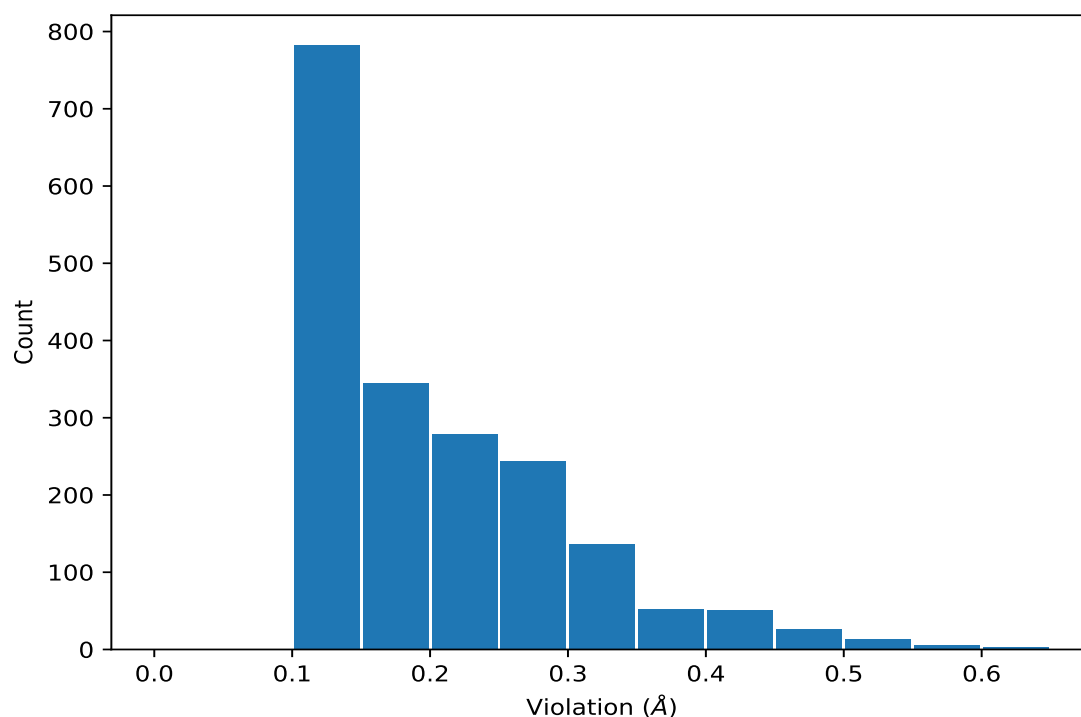
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,259)	1:138:A:VAL:HG21	1:139:A:LEU:H	2	0.15	0.01	0.15
(1,259)	1:138:A:VAL:HG22	1:139:A:LEU:H	2	0.15	0.01	0.15
(1,259)	1:138:A:VAL:HG23	1:139:A:LEU:H	2	0.15	0.01	0.15
(1,158)	1:37:A:LEU:HD11	1:48:A:ALA:H	2	0.15	0.04	0.15
(1,158)	1:37:A:LEU:HD12	1:48:A:ALA:H	2	0.15	0.04	0.15
(1,158)	1:37:A:LEU:HD13	1:48:A:ALA:H	2	0.15	0.04	0.15
(1,1411)	1:46:A:ILE:HA	1:46:A:ILE:HG13	2	0.15	0.0	0.15
(2,93)	1:65:A:GLY:N	1:134:A:ARG:O	2	0.15	0.03	0.15
(2,30)	1:94:A:HIS:H	1:102:A:THR:O	2	0.14	0.04	0.14
(1,585)	1:86:A:TYR:HA	1:148:A:THR:HG21	2	0.13	0.02	0.13
(1,585)	1:86:A:TYR:HA	1:148:A:THR:HG22	2	0.13	0.02	0.13
(1,585)	1:86:A:TYR:HA	1:148:A:THR:HG23	2	0.13	0.02	0.13
(1,1258)	1:5:A:LEU:HD11	1:7:A:LEU:HA	2	0.13	0.02	0.13
(1,1258)	1:5:A:LEU:HD12	1:7:A:LEU:HA	2	0.13	0.02	0.13
(1,1258)	1:5:A:LEU:HD13	1:7:A:LEU:HA	2	0.13	0.02	0.13
(1,1258)	1:5:A:LEU:HD21	1:7:A:LEU:HA	2	0.13	0.02	0.13
(1,1258)	1:5:A:LEU:HD22	1:7:A:LEU:HA	2	0.13	0.02	0.13
(1,1258)	1:5:A:LEU:HD23	1:7:A:LEU:HA	2	0.13	0.02	0.13
(1,1299)	1:17:A:MET:H	1:36:A:HIS:HB3	2	0.13	0.0	0.13
(1,1645)	1:89:A:SER:H	1:90:A:TYR:HB3	2	0.13	0.01	0.13
(2,60)	1:18:A:SER:H	1:61:A:GLN:O	2	0.13	0.03	0.13
(1,472)	1:23:A:TYR:HA	1:24:A:LYS:H	2	0.12	0.01	0.12
(1,1312)	1:18:A:SER:HB3	1:19:A:ALA:H	2	0.12	0.02	0.12
(2,79)	1:75:A:THR:O	1:123:A:LYS:N	2	0.12	0.02	0.12
(1,1801)	1:125:A:ASN:HB3	1:126:A:ILE:HB	2	0.12	0.01	0.12
(2,148)	1:88:A:ALA:N	1:142:A:SER:O	2	0.12	0.0	0.12
(1,767)	1:14:A:ASP:HA	1:36:A:HIS:HA	2	0.12	0.0	0.12
(1,1368)	1:38:A:GLY:H	1:150:A:ARG:HG3	2	0.12	0.0	0.12
(1,1643)	1:88:A:ALA:HB1	1:115:A:GLY:HA2	2	0.11	0.01	0.11
(1,1643)	1:88:A:ALA:HB1	1:115:A:GLY:HA3	2	0.11	0.01	0.11
(1,1643)	1:88:A:ALA:HB2	1:115:A:GLY:HA2	2	0.11	0.01	0.11
(1,1643)	1:88:A:ALA:HB2	1:115:A:GLY:HA3	2	0.11	0.01	0.11
(1,1643)	1:88:A:ALA:HB3	1:115:A:GLY:HA2	2	0.11	0.01	0.11
(1,1643)	1:88:A:ALA:HB3	1:115:A:GLY:HA3	2	0.11	0.01	0.11
(1,1476)	1:62:A:VAL:HG11	1:136:A:VAL:H	2	0.11	0.0	0.11
(1,1476)	1:62:A:VAL:HG12	1:136:A:VAL:H	2	0.11	0.0	0.11
(1,1476)	1:62:A:VAL:HG13	1:136:A:VAL:H	2	0.11	0.0	0.11
(1,1476)	1:62:A:VAL:HG21	1:136:A:VAL:H	2	0.11	0.0	0.11
(1,1476)	1:62:A:VAL:HG22	1:136:A:VAL:H	2	0.11	0.0	0.11
(1,1476)	1:62:A:VAL:HG23	1:136:A:VAL:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	19	0.63
(1,1885)	1:156:A:CYS:HB3	1:157:A:LEU:HB3	20	0.63
(1,567)	1:13:A:PRO:HA	1:14:A:ASP:HA	13	0.61
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	13	0.6
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	2	0.56
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	16	0.56
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	6	0.55
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	12	0.55
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	14	0.55
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	2	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	3	0.54
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	17	0.53
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	8	0.53
(1,1168)	1:13:A:PRO:HA	1:14:A:ASP:H	11	0.53
(1,4)	1:93:A:ALA:HA	1:104:A:TYR:H	18	0.53
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	11	0.52
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	15	0.52
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	2	0.51
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	16	0.5
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	4	0.5
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	20	0.5
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	15	0.5
(1,207)	1:13:A:PRO:HA	1:15:A:SER:H	11	0.5
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	11	0.49
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	10	0.49
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	5	0.48
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	6	0.48
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	9	0.48
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	19	0.48
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	1	0.48
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	5	0.48
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	6	0.48
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	7	0.48
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	14	0.47
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	13	0.47
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	16	0.47
(1,1147)	1:46:A:ILE:HD11	1:47:A:ASN:H	6	0.47
(1,1147)	1:46:A:ILE:HD12	1:47:A:ASN:H	6	0.47
(1,1147)	1:46:A:ILE:HD13	1:47:A:ASN:H	6	0.47
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	14	0.46
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	12	0.46
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	6	0.46
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	17	0.45
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	20	0.45
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	15	0.45
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	9	0.45
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	20	0.45
(1,1147)	1:46:A:ILE:HD11	1:47:A:ASN:H	15	0.45
(1,1147)	1:46:A:ILE:HD12	1:47:A:ASN:H	15	0.45
(1,1147)	1:46:A:ILE:HD13	1:47:A:ASN:H	15	0.45
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	6	0.44
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	10	0.44
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	19	0.44
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	7	0.44
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	8	0.44
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	1	0.44
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	14	0.44
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	3	0.44
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	18	0.44
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG21	15	0.44
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG22	15	0.44
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG23	15	0.44
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	4	0.43
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	14	0.43
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	19	0.43
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	3	0.43
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	8	0.43
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	16	0.43
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG21	17	0.43
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG22	17	0.43
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG23	17	0.43
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	20	0.42
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	7	0.42
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	12	0.42
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	15	0.42
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	12	0.42
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	9	0.41
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	14	0.41
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	3	0.41
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	9	0.41
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	11	0.41
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	18	0.41
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	19	0.41
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	6	0.41
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	7	0.41
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	13	0.41
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	4	0.41
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	5	0.41
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	17	0.41
(2,78)	1:75:A:THR:O	1:123:A:LYS:H	19	0.41
(1,140)	1:55:A:SER:H	1:147:A:ILE:HD11	5	0.41
(1,140)	1:55:A:SER:H	1:147:A:ILE:HD12	5	0.41
(1,140)	1:55:A:SER:H	1:147:A:ILE:HD13	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	11	0.4
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	13	0.4
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	9	0.4
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	18	0.4
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	18	0.4
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	4	0.4
(2,106)	1:72:A:GLY:N	1:154:A:LEU:O	18	0.4
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	17	0.39
(2,145)	1:89:A:SER:O	1:142:A:SER:N	8	0.39
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	19	0.39
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	20	0.39
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	10	0.39
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	5	0.39
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	6	0.39
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	19	0.39
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	15	0.39
(2,145)	1:89:A:SER:O	1:142:A:SER:N	18	0.38
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	16	0.38
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	1	0.38
(2,137)	1:86:A:TYR:N	1:144:A:HIS:O	2	0.38
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	17	0.38
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	1	0.38
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	20	0.38
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	20	0.38
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG21	14	0.38
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG22	14	0.38
(1,205)	1:10:A:ASN:H	1:11:A:THR:HG23	14	0.38
(2,145)	1:89:A:SER:O	1:142:A:SER:N	20	0.37
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	20	0.37
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	5	0.37
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	19	0.37
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	4	0.37
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	13	0.37
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	8	0.37
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	2	0.37
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	8	0.37
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	16	0.37
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	18	0.37
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	11	0.37
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	19	0.37
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	6	0.37
(1,1893)	1:157:A:LEU:HD11	1:158:A:GLU:HA	20	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1893)	1:157:A:LEU:HD12	1:158:A:GLU:HA	20	0.37
(1,1893)	1:157:A:LEU:HD13	1:158:A:GLU:HA	20	0.37
(1,1893)	1:157:A:LEU:HD21	1:158:A:GLU:HA	20	0.37
(1,1893)	1:157:A:LEU:HD22	1:158:A:GLU:HA	20	0.37
(1,1893)	1:157:A:LEU:HD23	1:158:A:GLU:HA	20	0.37
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	15	0.36
(2,145)	1:89:A:SER:O	1:142:A:SER:N	6	0.36
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	2	0.36
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	13	0.36
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	20	0.36
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	6	0.36
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	15	0.36
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	14	0.36
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	4	0.36
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	7	0.36
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	20	0.36
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	2	0.36
(2,145)	1:89:A:SER:O	1:142:A:SER:N	4	0.35
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	10	0.35
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	16	0.35
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	12	0.35
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	9	0.35
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	11	0.35
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	12	0.35
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	19	0.35
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	3	0.35
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	11	0.35
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	20	0.35
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	9	0.35
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	8	0.35
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	18	0.35
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	20	0.35
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	3	0.35
(1,150)	1:106:A:GLU:H	1:109:A:SER:H	12	0.35
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	6	0.34
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	3	0.34
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	4	0.34
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	11	0.34
(2,145)	1:89:A:SER:O	1:142:A:SER:N	12	0.34
(2,145)	1:89:A:SER:O	1:142:A:SER:N	17	0.34
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	4	0.34
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	11	0.34
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	20	0.34
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	17	0.34
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	7	0.34
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	14	0.34
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	1	0.34
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	8	0.34
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	12	0.34
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	17	0.34
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	3	0.34
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	9	0.34
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	4	0.34
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	11	0.34
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	17	0.34
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	20	0.34
(1,665)	1:55:A:SER:HA	1:147:A:ILE:HD11	15	0.34
(1,665)	1:55:A:SER:HA	1:147:A:ILE:HD12	15	0.34
(1,665)	1:55:A:SER:HA	1:147:A:ILE:HD13	15	0.34
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	5	0.34
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	5	0.34
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	5	0.34
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	6	0.34
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	6	0.34
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	6	0.34
(1,241)	1:106:A:GLU:H	1:110:A:SER:HA	12	0.34
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	8	0.33
(2,145)	1:89:A:SER:O	1:142:A:SER:N	9	0.33
(2,145)	1:89:A:SER:O	1:142:A:SER:N	15	0.33
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	7	0.33
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	18	0.33
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	13	0.33
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	9	0.33
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	10	0.33
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	1	0.33
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	13	0.33
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	4	0.33
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	10	0.33
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	16	0.33
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	17	0.33
(2,119)	1:70:A:VAL:O	1:131:A:PHE:N	10	0.33
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	14	0.33
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	13	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	15	0.33
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	9	0.33
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	1	0.33
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	4	0.33
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	9	0.33
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	9	0.33
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	19	0.33
(1,424)	1:51:A:ALA:HB1	1:55:A:SER:H	15	0.33
(1,424)	1:51:A:ALA:HB2	1:55:A:SER:H	15	0.33
(1,424)	1:51:A:ALA:HB3	1:55:A:SER:H	15	0.33
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	7	0.33
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	7	0.33
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	7	0.33
(1,156)	1:21:A:SER:H	1:49:A:TRP:HE1	20	0.33
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	7	0.32
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	20	0.32
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	7	0.32
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	18	0.32
(2,145)	1:89:A:SER:O	1:142:A:SER:N	5	0.32
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	18	0.32
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	19	0.32
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	1	0.32
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	6	0.32
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	1	0.32
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	16	0.32
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	9	0.32
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	3	0.32
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	5	0.32
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	5	0.32
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	9	0.32
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	3	0.32
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	8	0.32
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	16	0.32
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	19	0.32
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	9	0.32
(1,931)	1:71:A:THR:H	1:156:A:CYS:HA	20	0.32
(1,150)	1:106:A:GLU:H	1:109:A:SER:H	4	0.32
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	14	0.31
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	15	0.31
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	1	0.31
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	12	0.31
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	19	0.31
(2,145)	1:89:A:SER:O	1:142:A:SER:N	7	0.31
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	6	0.31
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	9	0.31
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	8	0.31
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	10	0.31
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	11	0.31
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	7	0.31
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	18	0.31
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	18	0.31
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	2	0.31
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	9	0.31
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	19	0.31
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	14	0.31
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	5	0.31
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	6	0.31
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	10	0.31
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	2	0.31
(1,1664)	1:91:A:LYS:HA	1:113:A:PHE:HB3	9	0.31
(1,1420)	1:51:A:ALA:HB1	1:54:A:ASN:HB3	15	0.31
(1,1420)	1:51:A:ALA:HB2	1:54:A:ASN:HB3	15	0.31
(1,1420)	1:51:A:ALA:HB3	1:54:A:ASN:HB3	15	0.31
(1,826)	1:95:A:SER:H	1:98:A:GLY:HA2	18	0.31
(1,556)	1:71:A:THR:HA	1:127:A:PHE:H	19	0.31
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	17	0.31
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	17	0.31
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	17	0.31
(1,241)	1:106:A:GLU:H	1:110:A:SER:HA	4	0.31
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	2	0.3
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	5	0.3
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	6	0.3
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	9	0.3
(2,145)	1:89:A:SER:O	1:142:A:SER:N	11	0.3
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	3	0.3
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	14	0.3
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	2	0.3
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	3	0.3
(2,138)	1:88:A:ALA:O	1:115:A:GLY:N	6	0.3
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	16	0.3
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	4	0.3
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	8	0.3
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	12	0.3
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	7	0.3
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	18	0.3
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	14	0.3
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	11	0.3
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	13	0.3
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	10	0.3
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	14	0.3
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	2	0.3
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	12	0.3
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	4	0.3
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	5	0.3
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	8	0.3
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	18	0.3
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	13	0.3
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG11	18	0.3
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG12	18	0.3
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG13	18	0.3
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG21	18	0.3
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG22	18	0.3
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG23	18	0.3
(1,1404)	1:45:A:LYS:HG3	1:46:A:ILE:HA	13	0.3
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	18	0.3
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	16	0.3
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	16	0.3
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	16	0.3
(1,218)	1:21:A:SER:HA	1:22:A:SER:H	17	0.3
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	8	0.29
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	16	0.29
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	10	0.29
(2,146)	1:65:A:GLY:N	1:134:A:ARG:O	16	0.29
(2,145)	1:89:A:SER:O	1:142:A:SER:N	3	0.29
(2,145)	1:89:A:SER:O	1:142:A:SER:N	10	0.29
(2,145)	1:89:A:SER:O	1:142:A:SER:N	16	0.29
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	5	0.29
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	8	0.29
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	17	0.29
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	19	0.29
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	11	0.29
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	17	0.29
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	10	0.29
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	18	0.29
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	4	0.29
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	18	0.29
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	16	0.29
(2,114)	1:93:A:ALA:N	1:137:A:ARG:O	5	0.29
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	1	0.29
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	15	0.29
(2,101)	1:62:A:VAL:N	1:136:A:VAL:O	5	0.29
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	20	0.29
(2,92)	1:65:A:GLY:H	1:134:A:ARG:O	14	0.29
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	12	0.29
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	14	0.29
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	15	0.29
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG11	10	0.29
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG12	10	0.29
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG13	10	0.29
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG21	10	0.29
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG22	10	0.29
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG23	10	0.29
(1,1404)	1:45:A:LYS:HG3	1:46:A:ILE:HA	16	0.29
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	4	0.29
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	4	0.29
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	4	0.29
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	8	0.29
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	8	0.29
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	8	0.29
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	18	0.29
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	18	0.29
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	18	0.29
(1,67)	1:157:A:LEU:HA	1:158:A:GLU:H	20	0.29
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	4	0.28
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	17	0.28
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	18	0.28
(2,145)	1:89:A:SER:O	1:142:A:SER:N	13	0.28
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	6	0.28
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	2	0.28
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	1	0.28
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	16	0.28
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	19	0.28
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	16	0.28
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	5	0.28
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:76:A:GLN:N	1:150:A:ARG:O	2	0.28
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	18	0.28
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	19	0.28
(2,105)	1:70:A:VAL:N	1:131:A:PHE:O	10	0.28
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	16	0.28
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	7	0.28
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	18	0.28
(2,101)	1:62:A:VAL:N	1:136:A:VAL:O	20	0.28
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	8	0.28
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	19	0.28
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	1	0.28
(1,1722)	1:105:A:GLU:H	1:105:A:GLU:HG3	12	0.28
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	4	0.28
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	14	0.28
(1,1168)	1:13:A:PRO:HA	1:14:A:ASP:H	13	0.28
(1,826)	1:95:A:SER:H	1:98:A:GLY:HA2	6	0.28
(1,241)	1:106:A:GLU:H	1:110:A:SER:HA	7	0.28
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	9	0.27
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	10	0.27
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	19	0.27
(2,145)	1:89:A:SER:O	1:142:A:SER:N	1	0.27
(2,145)	1:89:A:SER:O	1:142:A:SER:N	2	0.27
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	1	0.27
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	14	0.27
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	12	0.27
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	20	0.27
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	6	0.27
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	3	0.27
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	6	0.27
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	5	0.27
(2,132)	1:49:A:TRP:N	1:149:A:LEU:O	8	0.27
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	7	0.27
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	17	0.27
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	19	0.27
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	17	0.27
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	6	0.27
(2,111)	1:89:A:SER:N	1:142:A:SER:O	7	0.27
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	17	0.27
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	20	0.27
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	2	0.27
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	6	0.27
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	19	0.27
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	7	0.27
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	17	0.27
(1,1670)	1:91:A:LYS:HE3	1:111:A:LYS:H	18	0.27
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	17	0.27
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	3	0.27
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	19	0.27
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	20	0.27
(1,1119)	1:104:A:TYR:HA	1:105:A:GLU:H	2	0.27
(1,873)	1:112:A:VAL:H	1:113:A:PHE:HD1	9	0.27
(1,873)	1:112:A:VAL:H	1:113:A:PHE:HD2	9	0.27
(1,869)	1:111:A:LYS:HA	1:112:A:VAL:H	10	0.27
(1,567)	1:13:A:PRO:HA	1:14:A:ASP:HA	11	0.27
(1,426)	1:64:A:LEU:HG	1:66:A:THR:H	15	0.27
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	2	0.26
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	5	0.26
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	11	0.26
(2,145)	1:89:A:SER:O	1:142:A:SER:N	14	0.26
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	7	0.26
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	5	0.26
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	14	0.26
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	2	0.26
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	16	0.26
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	10	0.26
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	12	0.26
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	19	0.26
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	16	0.26
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	17	0.26
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	13	0.26
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	15	0.26
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	5	0.26
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	9	0.26
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	19	0.26
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	9	0.26
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	20	0.26
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	2	0.26
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	2	0.26
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	16	0.26
(1,1722)	1:105:A:GLU:H	1:105:A:GLU:HG3	4	0.26
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG11	6	0.26
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG12	6	0.26
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG13	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG21	6	0.26
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG22	6	0.26
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG23	6	0.26
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	7	0.26
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	10	0.26
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	12	0.26
(1,1124)	1:127:A:PHE:HA	1:128:A:GLU:H	20	0.26
(1,773)	1:74:A:ILE:HD11	1:122:A:HIS:HA	19	0.26
(1,773)	1:74:A:ILE:HD12	1:122:A:HIS:HA	19	0.26
(1,773)	1:74:A:ILE:HD13	1:122:A:HIS:HA	19	0.26
(1,556)	1:71:A:THR:HA	1:127:A:PHE:H	11	0.26
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	9	0.26
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	9	0.26
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	9	0.26
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	20	0.26
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	20	0.26
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	20	0.26
(1,278)	1:127:A:PHE:HA	1:129:A:LYS:H	2	0.26
(1,182)	1:48:A:ALA:H	1:148:A:THR:HG21	20	0.26
(1,182)	1:48:A:ALA:H	1:148:A:THR:HG22	20	0.26
(1,182)	1:48:A:ALA:H	1:148:A:THR:HG23	20	0.26
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	3	0.25
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	17	0.25
(2,138)	1:88:A:ALA:O	1:115:A:GLY:N	5	0.25
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	9	0.25
(2,134)	1:18:A:SER:O	1:61:A:GLN:N	15	0.25
(2,132)	1:49:A:TRP:N	1:149:A:LEU:O	20	0.25
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	10	0.25
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	20	0.25
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	18	0.25
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	2	0.25
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	8	0.25
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	17	0.25
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	16	0.25
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	2	0.25
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	6	0.25
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	7	0.25
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	16	0.25
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	7	0.25
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	6	0.25
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	6	0.25
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	14	0.25
(1,1737)	1:107:A:GLN:HG3	1:109:A:SER:H	7	0.25
(1,1596)	1:80:A:ASP:HB3	1:81:A:PHE:HD1	19	0.25
(1,1596)	1:80:A:ASP:HB3	1:81:A:PHE:HD2	19	0.25
(1,1547)	1:75:A:THR:HA	1:76:A:GLN:HG3	17	0.25
(1,1217)	1:108:A:GLY:H	1:109:A:SER:H	7	0.25
(1,1124)	1:127:A:PHE:HA	1:128:A:GLU:H	2	0.25
(1,1124)	1:127:A:PHE:HA	1:128:A:GLU:H	8	0.25
(1,1067)	1:36:A:HIS:H	1:49:A:TRP:HB3	9	0.25
(1,949)	1:87:A:VAL:HA	1:148:A:THR:H	20	0.25
(1,943)	1:93:A:ALA:HA	1:102:A:THR:H	18	0.25
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	12	0.25
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	12	0.25
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	12	0.25
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	15	0.25
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	15	0.25
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	15	0.25
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	9	0.25
(1,165)	1:116:A:ASN:HA	1:117:A:LEU:HG	2	0.25
(1,165)	1:116:A:ASN:HA	1:117:A:LEU:HG	18	0.25
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	4	0.24
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	17	0.24
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	1	0.24
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	18	0.24
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	1	0.24
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	12	0.24
(2,132)	1:49:A:TRP:N	1:149:A:LEU:O	12	0.24
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	3	0.24
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	5	0.24
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	15	0.24
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	2	0.24
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	10	0.24
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	11	0.24
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	3	0.24
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	13	0.24
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	1	0.24
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	6	0.24
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	10	0.24
(2,114)	1:93:A:ALA:N	1:137:A:ARG:O	7	0.24
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	18	0.24
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	5	0.24
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	10	0.24
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	14	0.24
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	18	0.24
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	12	0.24
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	20	0.24
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	17	0.24
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	19	0.24
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	16	0.24
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	1	0.24
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	2	0.24
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	13	0.24
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	15	0.24
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	3	0.24
(1,1897)	1:1:A:CYS:SG	1:156:A:CYS:CB	20	0.24
(1,1637)	1:87:A:VAL:HG11	1:148:A:THR:HB	7	0.24
(1,1637)	1:87:A:VAL:HG12	1:148:A:THR:HB	7	0.24
(1,1637)	1:87:A:VAL:HG13	1:148:A:THR:HB	7	0.24
(1,1637)	1:87:A:VAL:HG21	1:148:A:THR:HB	7	0.24
(1,1637)	1:87:A:VAL:HG22	1:148:A:THR:HB	7	0.24
(1,1637)	1:87:A:VAL:HG23	1:148:A:THR:HB	7	0.24
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	1	0.24
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	6	0.24
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	8	0.24
(1,1344)	1:35:A:PRO:HG3	1:60:A:LEU:HD11	20	0.24
(1,1344)	1:35:A:PRO:HG3	1:60:A:LEU:HD12	20	0.24
(1,1344)	1:35:A:PRO:HG3	1:60:A:LEU:HD13	20	0.24
(1,1344)	1:35:A:PRO:HG3	1:60:A:LEU:HD21	20	0.24
(1,1344)	1:35:A:PRO:HG3	1:60:A:LEU:HD22	20	0.24
(1,1344)	1:35:A:PRO:HG3	1:60:A:LEU:HD23	20	0.24
(1,1124)	1:127:A:PHE:HA	1:128:A:GLU:H	4	0.24
(1,1124)	1:127:A:PHE:HA	1:128:A:GLU:H	17	0.24
(1,670)	1:73:A:ILE:HD11	1:74:A:ILE:HA	19	0.24
(1,670)	1:73:A:ILE:HD12	1:74:A:ILE:HA	19	0.24
(1,670)	1:73:A:ILE:HD13	1:74:A:ILE:HA	19	0.24
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	13	0.24
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	13	0.24
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	13	0.24
(1,313)	1:51:A:ALA:H	1:147:A:ILE:HD11	5	0.24
(1,313)	1:51:A:ALA:H	1:147:A:ILE:HD12	5	0.24
(1,313)	1:51:A:ALA:H	1:147:A:ILE:HD13	5	0.24
(1,165)	1:116:A:ASN:HA	1:117:A:LEU:HG	12	0.24
(2,145)	1:89:A:SER:O	1:142:A:SER:N	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,144)	1:3:A:GLU:N	1:155:A:GLY:O	20	0.23
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	2	0.23
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	8	0.23
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	15	0.23
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	4	0.23
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	13	0.23
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	17	0.23
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	6	0.23
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	2	0.23
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	3	0.23
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	11	0.23
(2,120)	1:68:A:ARG:O	1:133:A:ALA:N	12	0.23
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	3	0.23
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	15	0.23
(2,117)	1:94:A:HIS:O	1:102:A:THR:N	8	0.23
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	13	0.23
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	15	0.23
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	19	0.23
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	2	0.23
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	13	0.23
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	7	0.23
(2,101)	1:62:A:VAL:N	1:136:A:VAL:O	13	0.23
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	12	0.23
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	5	0.23
(2,15)	1:73:A:ILE:N	1:125:A:ASN:O	17	0.23
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	16	0.23
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	8	0.23
(1,1774)	1:116:A:ASN:HB3	1:118:A:ASP:H	2	0.23
(1,1774)	1:116:A:ASN:HB3	1:118:A:ASP:H	12	0.23
(1,1623)	1:87:A:VAL:HG11	1:140:A:PRO:HA	6	0.23
(1,1623)	1:87:A:VAL:HG12	1:140:A:PRO:HA	6	0.23
(1,1623)	1:87:A:VAL:HG13	1:140:A:PRO:HA	6	0.23
(1,1623)	1:87:A:VAL:HG21	1:140:A:PRO:HA	6	0.23
(1,1623)	1:87:A:VAL:HG22	1:140:A:PRO:HA	6	0.23
(1,1623)	1:87:A:VAL:HG23	1:140:A:PRO:HA	6	0.23
(1,1457)	1:59:A:TRP:HA	1:138:A:VAL:HG11	20	0.23
(1,1457)	1:59:A:TRP:HA	1:138:A:VAL:HG12	20	0.23
(1,1457)	1:59:A:TRP:HA	1:138:A:VAL:HG13	20	0.23
(1,1457)	1:59:A:TRP:HA	1:138:A:VAL:HG21	20	0.23
(1,1457)	1:59:A:TRP:HA	1:138:A:VAL:HG22	20	0.23
(1,1457)	1:59:A:TRP:HA	1:138:A:VAL:HG23	20	0.23
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	2	0.23
(1,1385)	1:42:A:ASN:H	1:47:A:ASN:HB3	18	0.23
(1,1383)	1:41:A:ASP:H	1:42:A:ASN:HD21	19	0.23
(1,1383)	1:41:A:ASP:H	1:42:A:ASN:HD22	19	0.23
(1,1372)	1:38:A:GLY:HA2	1:150:A:ARG:HA	8	0.23
(1,1372)	1:38:A:GLY:HA3	1:150:A:ARG:HA	8	0.23
(1,1124)	1:127:A:PHE:HA	1:128:A:GLU:H	15	0.23
(1,826)	1:95:A:SER:H	1:98:A:GLY:HA2	14	0.23
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	1	0.23
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	1	0.23
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	1	0.23
(1,342)	1:116:A:ASN:H	1:118:A:ASP:H	5	0.23
(1,248)	1:41:A:ASP:H	1:42:A:ASN:HA	9	0.23
(1,152)	1:48:A:ALA:H	1:49:A:TRP:H	12	0.23
(1,41)	1:122:A:HIS:H	1:123:A:LYS:HA	6	0.23
(1,41)	1:122:A:HIS:H	1:123:A:LYS:HA	10	0.23
(2,149)	1:95:A:SER:O	1:134:A:ARG:N	12	0.22
(2,142)	1:49:A:TRP:O	1:149:A:LEU:N	15	0.22
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	16	0.22
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	1	0.22
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	11	0.22
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	5	0.22
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	11	0.22
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	16	0.22
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	3	0.22
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	5	0.22
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	11	0.22
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	13	0.22
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	15	0.22
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	6	0.22
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	7	0.22
(2,80)	1:73:A:ILE:O	1:125:A:ASN:H	14	0.22
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	18	0.22
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	16	0.22
(2,50)	1:91:A:LYS:O	1:139:A:LEU:H	9	0.22
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	11	0.22
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	15	0.22
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	20	0.22
(1,1765)	1:114:A:GLN:HB3	1:115:A:GLY:H	8	0.22
(1,1172)	1:40:A:LEU:HG	1:41:A:ASP:H	19	0.22
(1,1125)	1:128:A:GLU:H	1:129:A:LYS:H	8	0.22
(1,871)	1:111:A:LYS:HD3	1:112:A:VAL:H	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:64:A:LEU:HG	1:66:A:THR:HB	14	0.22
(1,612)	1:46:A:ILE:HB	1:46:A:ILE:HD11	15	0.22
(1,612)	1:46:A:ILE:HB	1:46:A:ILE:HD12	15	0.22
(1,612)	1:46:A:ILE:HB	1:46:A:ILE:HD13	15	0.22
(1,454)	1:122:A:HIS:HD1	1:123:A:LYS:H	6	0.22
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	11	0.22
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	11	0.22
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	11	0.22
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	17	0.22
(1,152)	1:48:A:ALA:H	1:49:A:TRP:H	14	0.22
(1,72)	1:153:A:LEU:HG	1:154:A:LEU:H	15	0.22
(1,41)	1:122:A:HIS:H	1:123:A:LYS:HA	11	0.22
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	15	0.21
(2,134)	1:18:A:SER:O	1:61:A:GLN:N	2	0.21
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	7	0.21
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	18	0.21
(2,132)	1:49:A:TRP:N	1:149:A:LEU:O	14	0.21
(2,132)	1:49:A:TRP:N	1:149:A:LEU:O	19	0.21
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	13	0.21
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	8	0.21
(2,126)	1:89:A:SER:O	1:141:A:VAL:N	10	0.21
(2,126)	1:89:A:SER:O	1:141:A:VAL:N	15	0.21
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	13	0.21
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	13	0.21
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	16	0.21
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	17	0.21
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	3	0.21
(2,114)	1:93:A:ALA:N	1:137:A:ARG:O	6	0.21
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	11	0.21
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	15	0.21
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	8	0.21
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	10	0.21
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	11	0.21
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	4	0.21
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	12	0.21
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	4	0.21
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	10	0.21
(2,86)	1:3:A:GLU:O	1:155:A:GLY:H	13	0.21
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	6	0.21
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	20	0.21
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	11	0.21
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:73:A:ILE:N	1:125:A:ASN:O	2	0.21
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	1	0.21
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	17	0.21
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG11	12	0.21
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG12	12	0.21
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG13	12	0.21
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG21	12	0.21
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG22	12	0.21
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG23	12	0.21
(1,1626)	1:87:A:VAL:HG11	1:141:A:VAL:H	6	0.21
(1,1626)	1:87:A:VAL:HG12	1:141:A:VAL:H	6	0.21
(1,1626)	1:87:A:VAL:HG13	1:141:A:VAL:H	6	0.21
(1,1626)	1:87:A:VAL:HG21	1:141:A:VAL:H	6	0.21
(1,1626)	1:87:A:VAL:HG22	1:141:A:VAL:H	6	0.21
(1,1626)	1:87:A:VAL:HG23	1:141:A:VAL:H	6	0.21
(1,1454)	1:58:A:GLU:H	1:147:A:ILE:HG13	20	0.21
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	11	0.21
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	13	0.21
(1,1012)	1:88:A:ALA:HB1	1:143:A:TRP:H	6	0.21
(1,1012)	1:88:A:ALA:HB2	1:143:A:TRP:H	6	0.21
(1,1012)	1:88:A:ALA:HB3	1:143:A:TRP:H	6	0.21
(1,809)	1:80:A:ASP:HA	1:81:A:PHE:HD1	19	0.21
(1,809)	1:80:A:ASP:HA	1:81:A:PHE:HD2	19	0.21
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	12	0.21
(1,612)	1:46:A:ILE:HB	1:46:A:ILE:HD11	6	0.21
(1,612)	1:46:A:ILE:HB	1:46:A:ILE:HD12	6	0.21
(1,612)	1:46:A:ILE:HB	1:46:A:ILE:HD13	6	0.21
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	15	0.21
(1,454)	1:122:A:HIS:HD1	1:123:A:LYS:H	10	0.21
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	2	0.21
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	2	0.21
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	2	0.21
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	15	0.21
(1,248)	1:41:A:ASP:H	1:42:A:ASN:HA	14	0.21
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	3	0.2
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	2	0.2
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	9	0.2
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	13	0.2
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	10	0.2
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	8	0.2
(2,130)	1:18:A:SER:N	1:61:A:GLN:O	2	0.2
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	5	0.2
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	19	0.2
(2,107)	1:73:A:ILE:N	1:125:A:ASN:O	19	0.2
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	15	0.2
(2,86)	1:3:A:GLU:O	1:155:A:GLY:H	11	0.2
(2,80)	1:73:A:ILE:O	1:125:A:ASN:H	8	0.2
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	16	0.2
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	17	0.2
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	19	0.2
(2,50)	1:91:A:LYS:O	1:139:A:LEU:H	6	0.2
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	4	0.2
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	20	0.2
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	6	0.2
(2,15)	1:73:A:ILE:N	1:125:A:ASN:O	15	0.2
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	18	0.2
(1,1804)	1:127:A:PHE:H	1:128:A:GLU:HB3	10	0.2
(1,1719)	1:103:A:VAL:HG11	1:111:A:LYS:H	18	0.2
(1,1719)	1:103:A:VAL:HG12	1:111:A:LYS:H	18	0.2
(1,1719)	1:103:A:VAL:HG13	1:111:A:LYS:H	18	0.2
(1,1719)	1:103:A:VAL:HG21	1:111:A:LYS:H	18	0.2
(1,1719)	1:103:A:VAL:HG22	1:111:A:LYS:H	18	0.2
(1,1719)	1:103:A:VAL:HG23	1:111:A:LYS:H	18	0.2
(1,1570)	1:79:A:ARG:H	1:85:A:GLN:HB3	5	0.2
(1,1372)	1:38:A:GLY:HA2	1:150:A:ARG:HA	15	0.2
(1,1372)	1:38:A:GLY:HA3	1:150:A:ARG:HA	15	0.2
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD11	16	0.2
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD12	16	0.2
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD13	16	0.2
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD21	16	0.2
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD22	16	0.2
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD23	16	0.2
(1,1067)	1:36:A:HIS:H	1:49:A:TRP:HB3	10	0.2
(1,997)	1:35:A:PRO:HA	1:49:A:TRP:H	19	0.2
(1,997)	1:35:A:PRO:HA	1:49:A:TRP:H	20	0.2
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	4	0.2
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	16	0.2
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	3	0.2
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	3	0.2
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	3	0.2
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	10	0.2
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	10	0.2
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	20	0.2
(1,247)	1:116:A:ASN:HA	1:118:A:ASP:H	19	0.2
(1,230)	1:122:A:HIS:HA	1:123:A:LYS:H	19	0.2
(1,41)	1:122:A:HIS:H	1:123:A:LYS:HA	7	0.2
(1,41)	1:122:A:HIS:H	1:123:A:LYS:HA	13	0.2
(2,147)	1:71:A:THR:N	1:154:A:LEU:O	14	0.19
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	12	0.19
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	3	0.19
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	8	0.19
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	10	0.19
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	14	0.19
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	12	0.19
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	6	0.19
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	6	0.19
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	9	0.19
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	9	0.19
(2,116)	1:95:A:SER:N	1:135:A:TYR:O	6	0.19
(2,114)	1:93:A:ALA:N	1:137:A:ARG:O	12	0.19
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	1	0.19
(2,105)	1:70:A:VAL:N	1:131:A:PHE:O	6	0.19
(2,105)	1:70:A:VAL:N	1:131:A:PHE:O	12	0.19
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	18	0.19
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	8	0.19
(2,80)	1:73:A:ILE:O	1:125:A:ASN:H	10	0.19
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	13	0.19
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	1	0.19
(2,62)	1:20:A:SER:H	1:59:A:TRP:O	20	0.19
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	11	0.19
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	18	0.19
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	3	0.19
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	12	0.19
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	10	0.19
(1,1793)	1:122:A:HIS:HB3	1:123:A:LYS:H	4	0.19
(1,1774)	1:116:A:ASN:HB3	1:118:A:ASP:H	18	0.19
(1,1726)	1:105:A:GLU:HB3	1:109:A:SER:H	4	0.19
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	16	0.19
(1,1385)	1:42:A:ASN:H	1:47:A:ASN:HB3	9	0.19
(1,1372)	1:38:A:GLY:HA2	1:150:A:ARG:HA	18	0.19
(1,1372)	1:38:A:GLY:HA3	1:150:A:ARG:HA	18	0.19
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG21	17	0.19
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG22	17	0.19
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG23	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG21	17	0.19
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG22	17	0.19
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG23	17	0.19
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG21	17	0.19
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG22	17	0.19
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG23	17	0.19
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG21	17	0.19
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG22	17	0.19
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG23	17	0.19
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG21	17	0.19
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG22	17	0.19
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG23	17	0.19
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG21	17	0.19
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG22	17	0.19
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG23	17	0.19
(1,1223)	1:114:A:GLN:HB3	1:115:A:GLY:H	8	0.19
(1,1159)	1:84:A:ILE:HB	1:119:A:ASN:H	19	0.19
(1,1154)	1:115:A:GLY:H	1:116:A:ASN:H	9	0.19
(1,1067)	1:36:A:HIS:H	1:49:A:TRP:HB3	19	0.19
(1,1067)	1:36:A:HIS:H	1:49:A:TRP:HB3	20	0.19
(1,1058)	1:14:A:ASP:H	1:16:A:GLN:H	9	0.19
(1,1050)	1:10:A:ASN:H	1:11:A:THR:H	15	0.19
(1,1050)	1:10:A:ASN:H	1:11:A:THR:H	17	0.19
(1,716)	1:19:A:ALA:HB1	1:35:A:PRO:HB3	20	0.19
(1,716)	1:19:A:ALA:HB2	1:35:A:PRO:HB3	20	0.19
(1,716)	1:19:A:ALA:HB3	1:35:A:PRO:HB3	20	0.19
(1,673)	1:157:A:LEU:HA	1:157:A:LEU:HD21	20	0.19
(1,673)	1:157:A:LEU:HA	1:157:A:LEU:HD22	20	0.19
(1,673)	1:157:A:LEU:HA	1:157:A:LEU:HD23	20	0.19
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	7	0.19
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	9	0.19
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	19	0.19
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	20	0.19
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	14	0.19
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	14	0.19
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	14	0.19
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	14	0.19
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	18	0.19
(1,278)	1:127:A:PHE:HA	1:129:A:LYS:H	15	0.19
(1,158)	1:37:A:LEU:HD11	1:48:A:ALA:H	12	0.19
(1,158)	1:37:A:LEU:HD12	1:48:A:ALA:H	12	0.19
(1,158)	1:37:A:LEU:HD13	1:48:A:ALA:H	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:5:A:LEU:H	1:5:A:LEU:HD21	11	0.19
(1,53)	1:5:A:LEU:H	1:5:A:LEU:HD22	11	0.19
(1,53)	1:5:A:LEU:H	1:5:A:LEU:HD23	11	0.19
(1,41)	1:122:A:HIS:H	1:123:A:LYS:HA	9	0.19
(1,41)	1:122:A:HIS:H	1:123:A:LYS:HA	14	0.19
(2,139)	1:75:A:THR:O	1:123:A:LYS:N	15	0.18
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	4	0.18
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	18	0.18
(2,131)	1:20:A:SER:N	1:59:A:TRP:O	6	0.18
(2,126)	1:89:A:SER:O	1:141:A:VAL:N	5	0.18
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	15	0.18
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	6	0.18
(2,115)	1:94:A:HIS:N	1:102:A:THR:O	7	0.18
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	7	0.18
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	13	0.18
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	15	0.18
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	20	0.18
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	13	0.18
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	14	0.18
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	17	0.18
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	20	0.18
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	8	0.18
(2,101)	1:62:A:VAL:N	1:136:A:VAL:O	18	0.18
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	1	0.18
(2,80)	1:73:A:ILE:O	1:125:A:ASN:H	6	0.18
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	5	0.18
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	6	0.18
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	4	0.18
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	20	0.18
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	13	0.18
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	8	0.18
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	9	0.18
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	19	0.18
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	6	0.18
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	1	0.18
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	5	0.18
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	6	0.18
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	7	0.18
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	6	0.18
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	19	0.18
(1,1815)	1:129:A:LYS:H	1:129:A:LYS:HG3	20	0.18
(1,1718)	1:103:A:VAL:HG11	1:110:A:SER:HB3	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1718)	1:103:A:VAL:HG12	1:110:A:SER:HB3	8	0.18
(1,1718)	1:103:A:VAL:HG13	1:110:A:SER:HB3	8	0.18
(1,1718)	1:103:A:VAL:HG21	1:110:A:SER:HB3	8	0.18
(1,1718)	1:103:A:VAL:HG22	1:110:A:SER:HB3	8	0.18
(1,1718)	1:103:A:VAL:HG23	1:110:A:SER:HB3	8	0.18
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG11	14	0.18
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG12	14	0.18
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG13	14	0.18
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG21	14	0.18
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG22	14	0.18
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG23	14	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG11	7	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG12	7	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG13	7	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG21	7	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG22	7	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG23	7	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG11	8	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG12	8	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG13	8	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG21	8	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG22	8	0.18
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG23	8	0.18
(1,1587)	1:79:A:ARG:HG3	1:82:A:GLY:H	17	0.18
(1,1513)	1:68:A:ARG:HD3	1:157:A:LEU:HA	20	0.18
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	18	0.18
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	18	0.18
(1,1405)	1:45:A:LYS:HD3	1:46:A:ILE:H	15	0.18
(1,1396)	1:44:A:GLY:H	1:45:A:LYS:HD3	16	0.18
(1,1392)	1:43:A:GLN:H	1:44:A:GLY:HA2	19	0.18
(1,1392)	1:43:A:GLN:H	1:44:A:GLY:HA3	19	0.18
(1,1187)	1:117:A:LEU:H	1:118:A:ASP:H	3	0.18
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	17	0.18
(1,445)	1:37:A:LEU:H	1:39:A:ARG:H	3	0.18
(1,435)	1:91:A:LYS:H	1:112:A:VAL:HG21	8	0.18
(1,435)	1:91:A:LYS:H	1:112:A:VAL:HG22	8	0.18
(1,435)	1:91:A:LYS:H	1:112:A:VAL:HG23	8	0.18
(1,415)	1:50:A:THR:HG21	1:146:A:ARG:H	19	0.18
(1,415)	1:50:A:THR:HG22	1:146:A:ARG:H	19	0.18
(1,415)	1:50:A:THR:HG23	1:146:A:ARG:H	19	0.18
(1,371)	1:40:A:LEU:HA	1:42:A:ASN:H	19	0.18
(1,13)	1:63:A:ASP:HA	1:134:A:ARG:HE	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:22:A:SER:HA	1:49:A:TRP:HE1	9	0.18
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	11	0.17
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	17	0.17
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	7	0.17
(2,134)	1:18:A:SER:O	1:61:A:GLN:N	11	0.17
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	16	0.17
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	17	0.17
(2,132)	1:49:A:TRP:N	1:149:A:LEU:O	15	0.17
(2,130)	1:18:A:SER:N	1:61:A:GLN:O	19	0.17
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	14	0.17
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	20	0.17
(2,123)	1:93:A:ALA:O	1:137:A:ARG:N	5	0.17
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	7	0.17
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	13	0.17
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	5	0.17
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	6	0.17
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	10	0.17
(2,104)	1:68:A:ARG:N	1:133:A:ALA:O	14	0.17
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	17	0.17
(2,93)	1:65:A:GLY:N	1:134:A:ARG:O	14	0.17
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	20	0.17
(2,80)	1:73:A:ILE:O	1:125:A:ASN:H	7	0.17
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	13	0.17
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	8	0.17
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	3	0.17
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	4	0.17
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	6	0.17
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	18	0.17
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	16	0.17
(2,30)	1:94:A:HIS:H	1:102:A:THR:O	18	0.17
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	7	0.17
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	16	0.17
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	5	0.17
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	1	0.17
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	3	0.17
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	19	0.17
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	3	0.17
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	11	0.17
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	19	0.17
(1,1725)	1:105:A:GLU:HB3	1:108:A:GLY:H	7	0.17
(1,1666)	1:91:A:LYS:HG3	1:92:A:VAL:H	18	0.17
(1,1637)	1:87:A:VAL:HG11	1:148:A:THR:HB	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1637)	1:87:A:VAL:HG12	1:148:A:THR:HB	13	0.17
(1,1637)	1:87:A:VAL:HG13	1:148:A:THR:HB	13	0.17
(1,1637)	1:87:A:VAL:HG21	1:148:A:THR:HB	13	0.17
(1,1637)	1:87:A:VAL:HG22	1:148:A:THR:HB	13	0.17
(1,1637)	1:87:A:VAL:HG23	1:148:A:THR:HB	13	0.17
(1,1396)	1:44:A:GLY:H	1:45:A:LYS:HD3	13	0.17
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD11	19	0.17
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD12	19	0.17
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD13	19	0.17
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD21	19	0.17
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD22	19	0.17
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD23	19	0.17
(1,1137)	1:10:A:ASN:H	1:10:A:ASN:HD22	15	0.17
(1,1050)	1:10:A:ASN:H	1:11:A:THR:H	14	0.17
(1,869)	1:111:A:LYS:HA	1:112:A:VAL:H	8	0.17
(1,832)	1:72:A:GLY:H	1:155:A:GLY:HA3	11	0.17
(1,722)	1:51:A:ALA:HB1	1:147:A:ILE:HD11	5	0.17
(1,722)	1:51:A:ALA:HB1	1:147:A:ILE:HD12	5	0.17
(1,722)	1:51:A:ALA:HB1	1:147:A:ILE:HD13	5	0.17
(1,722)	1:51:A:ALA:HB2	1:147:A:ILE:HD11	5	0.17
(1,722)	1:51:A:ALA:HB2	1:147:A:ILE:HD12	5	0.17
(1,722)	1:51:A:ALA:HB2	1:147:A:ILE:HD13	5	0.17
(1,722)	1:51:A:ALA:HB3	1:147:A:ILE:HD11	5	0.17
(1,722)	1:51:A:ALA:HB3	1:147:A:ILE:HD12	5	0.17
(1,722)	1:51:A:ALA:HB3	1:147:A:ILE:HD13	5	0.17
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	2	0.17
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	10	0.17
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	11	0.17
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	15	0.17
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	17	0.17
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	20	0.17
(1,598)	1:50:A:THR:HG21	1:146:A:ARG:HA	14	0.17
(1,598)	1:50:A:THR:HG22	1:146:A:ARG:HA	14	0.17
(1,598)	1:50:A:THR:HG23	1:146:A:ARG:HA	14	0.17
(1,598)	1:50:A:THR:HG21	1:146:A:ARG:HA	15	0.17
(1,598)	1:50:A:THR:HG22	1:146:A:ARG:HA	15	0.17
(1,598)	1:50:A:THR:HG23	1:146:A:ARG:HA	15	0.17
(1,563)	1:147:A:ILE:H	1:148:A:THR:HA	3	0.17
(1,454)	1:122:A:HIS:HD1	1:123:A:LYS:H	11	0.17
(1,446)	1:38:A:GLY:H	1:39:A:ARG:HB3	13	0.17
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	5	0.17
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,206)	1:15:A:SER:H	1:16:A:GLN:H	11	0.17
(1,136)	1:36:A:HIS:H	1:37:A:LEU:HD21	16	0.17
(1,136)	1:36:A:HIS:H	1:37:A:LEU:HD22	16	0.17
(1,136)	1:36:A:HIS:H	1:37:A:LEU:HD23	16	0.17
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	20	0.16
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	5	0.16
(2,136)	1:78:A:ALA:O	1:85:A:GLN:N	20	0.16
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	2	0.16
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	3	0.16
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	4	0.16
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	9	0.16
(2,132)	1:49:A:TRP:N	1:149:A:LEU:O	9	0.16
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	19	0.16
(2,114)	1:93:A:ALA:N	1:137:A:ARG:O	10	0.16
(2,114)	1:93:A:ALA:N	1:137:A:ARG:O	19	0.16
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	4	0.16
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	3	0.16
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	14	0.16
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	16	0.16
(2,86)	1:3:A:GLU:O	1:155:A:GLY:H	20	0.16
(2,81)	1:73:A:ILE:O	1:125:A:ASN:N	14	0.16
(2,78)	1:75:A:THR:O	1:123:A:LYS:H	14	0.16
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	7	0.16
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	12	0.16
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	14	0.16
(2,72)	1:78:A:ALA:O	1:85:A:GLN:H	19	0.16
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	9	0.16
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	17	0.16
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	1	0.16
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	13	0.16
(2,60)	1:18:A:SER:H	1:61:A:GLN:O	1	0.16
(2,50)	1:91:A:LYS:O	1:139:A:LEU:H	8	0.16
(2,50)	1:91:A:LYS:O	1:139:A:LEU:H	12	0.16
(2,42)	1:95:A:SER:O	1:135:A:TYR:H	8	0.16
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	12	0.16
(2,38)	1:70:A:VAL:O	1:131:A:PHE:H	10	0.16
(2,24)	1:90:A:TYR:H	1:113:A:PHE:O	18	0.16
(2,24)	1:90:A:TYR:H	1:113:A:PHE:O	19	0.16
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	1	0.16
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	17	0.16
(2,15)	1:73:A:ILE:N	1:125:A:ASN:O	6	0.16
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	12	0.16
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	18	0.16
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	16	0.16
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	17	0.16
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	9	0.16
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG21	20	0.16
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG22	20	0.16
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG23	20	0.16
(1,1726)	1:105:A:GLU:HB3	1:109:A:SER:H	12	0.16
(1,1664)	1:91:A:LYS:HA	1:113:A:PHE:HB3	14	0.16
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG11	4	0.16
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG12	4	0.16
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG13	4	0.16
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG21	4	0.16
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG22	4	0.16
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG23	4	0.16
(1,1547)	1:75:A:THR:HA	1:76:A:GLN:HG3	8	0.16
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	19	0.16
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	17	0.16
(1,1399)	1:44:A:GLY:HA2	1:46:A:ILE:HD11	6	0.16
(1,1399)	1:44:A:GLY:HA2	1:46:A:ILE:HD12	6	0.16
(1,1399)	1:44:A:GLY:HA2	1:46:A:ILE:HD13	6	0.16
(1,1399)	1:44:A:GLY:HA3	1:46:A:ILE:HD11	6	0.16
(1,1399)	1:44:A:GLY:HA3	1:46:A:ILE:HD12	6	0.16
(1,1399)	1:44:A:GLY:HA3	1:46:A:ILE:HD13	6	0.16
(1,1190)	1:6:A:GLY:H	1:8:A:LYS:H	11	0.16
(1,1119)	1:104:A:TYR:HA	1:105:A:GLU:H	18	0.16
(1,902)	1:73:A:ILE:HD11	1:74:A:ILE:H	14	0.16
(1,902)	1:73:A:ILE:HD12	1:74:A:ILE:H	14	0.16
(1,902)	1:73:A:ILE:HD13	1:74:A:ILE:H	14	0.16
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	1	0.16
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	3	0.16
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	5	0.16
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	8	0.16
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	13	0.16
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	19	0.16
(1,598)	1:50:A:THR:HG21	1:146:A:ARG:HA	11	0.16
(1,598)	1:50:A:THR:HG22	1:146:A:ARG:HA	11	0.16
(1,598)	1:50:A:THR:HG23	1:146:A:ARG:HA	11	0.16
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	4	0.16
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	9	0.16
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	16	0.16
(1,454)	1:122:A:HIS:HD1	1:123:A:LYS:H	14	0.16
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	6	0.16
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	8	0.16
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	16	0.16
(1,259)	1:138:A:VAL:HG21	1:139:A:LEU:H	15	0.16
(1,259)	1:138:A:VAL:HG22	1:139:A:LEU:H	15	0.16
(1,259)	1:138:A:VAL:HG23	1:139:A:LEU:H	15	0.16
(1,202)	1:10:A:ASN:H	1:12:A:ILE:H	17	0.16
(1,152)	1:48:A:ALA:H	1:49:A:TRP:H	8	0.16
(1,152)	1:48:A:ALA:H	1:49:A:TRP:H	17	0.16
(1,72)	1:153:A:LEU:HG	1:154:A:LEU:H	12	0.16
(1,28)	1:7:A:LEU:H	1:7:A:LEU:HG	7	0.16
(1,5)	1:105:A:GLU:H	1:105:A:GLU:HB3	2	0.16
(2,140)	1:73:A:ILE:O	1:125:A:ASN:N	3	0.15
(2,138)	1:88:A:ALA:O	1:115:A:GLY:N	13	0.15
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	2	0.15
(2,135)	1:78:A:ALA:N	1:148:A:THR:O	8	0.15
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	1	0.15
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	12	0.15
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	14	0.15
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	19	0.15
(2,132)	1:49:A:TRP:N	1:149:A:LEU:O	1	0.15
(2,132)	1:49:A:TRP:N	1:149:A:LEU:O	11	0.15
(2,130)	1:18:A:SER:N	1:61:A:GLN:O	1	0.15
(2,127)	1:76:A:GLN:O	1:150:A:ARG:N	9	0.15
(2,126)	1:89:A:SER:O	1:141:A:VAL:N	18	0.15
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	5	0.15
(2,114)	1:93:A:ALA:N	1:137:A:ARG:O	4	0.15
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	8	0.15
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	11	0.15
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	12	0.15
(2,105)	1:70:A:VAL:N	1:131:A:PHE:O	9	0.15
(2,105)	1:70:A:VAL:N	1:131:A:PHE:O	16	0.15
(2,86)	1:3:A:GLU:O	1:155:A:GLY:H	10	0.15
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	9	0.15
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	17	0.15
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	20	0.15
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	9	0.15
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	11	0.15
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	15	0.15
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	8	0.15
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	12	0.15
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	10	0.15
(2,50)	1:91:A:LYS:O	1:139:A:LEU:H	17	0.15
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	15	0.15
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	9	0.15
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	11	0.15
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	13	0.15
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	19	0.15
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	20	0.15
(2,18)	1:75:A:THR:H	1:123:A:LYS:O	19	0.15
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	4	0.15
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	9	0.15
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	20	0.15
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	1	0.15
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	3	0.15
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	9	0.15
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	20	0.15
(1,1748)	1:111:A:LYS:HG3	1:112:A:VAL:H	8	0.15
(1,1721)	1:105:A:GLU:H	1:105:A:GLU:HB3	2	0.15
(1,1646)	1:89:A:SER:H	1:112:A:VAL:HG11	7	0.15
(1,1646)	1:89:A:SER:H	1:112:A:VAL:HG12	7	0.15
(1,1646)	1:89:A:SER:H	1:112:A:VAL:HG13	7	0.15
(1,1646)	1:89:A:SER:H	1:112:A:VAL:HG21	7	0.15
(1,1646)	1:89:A:SER:H	1:112:A:VAL:HG22	7	0.15
(1,1646)	1:89:A:SER:H	1:112:A:VAL:HG23	7	0.15
(1,1637)	1:87:A:VAL:HG11	1:148:A:THR:HB	19	0.15
(1,1637)	1:87:A:VAL:HG12	1:148:A:THR:HB	19	0.15
(1,1637)	1:87:A:VAL:HG13	1:148:A:THR:HB	19	0.15
(1,1637)	1:87:A:VAL:HG21	1:148:A:THR:HB	19	0.15
(1,1637)	1:87:A:VAL:HG22	1:148:A:THR:HB	19	0.15
(1,1637)	1:87:A:VAL:HG23	1:148:A:THR:HB	19	0.15
(1,1627)	1:87:A:VAL:HG11	1:142:A:SER:H	16	0.15
(1,1627)	1:87:A:VAL:HG12	1:142:A:SER:H	16	0.15
(1,1627)	1:87:A:VAL:HG13	1:142:A:SER:H	16	0.15
(1,1627)	1:87:A:VAL:HG21	1:142:A:SER:H	16	0.15
(1,1627)	1:87:A:VAL:HG22	1:142:A:SER:H	16	0.15
(1,1627)	1:87:A:VAL:HG23	1:142:A:SER:H	16	0.15
(1,1626)	1:87:A:VAL:HG11	1:141:A:VAL:H	20	0.15
(1,1626)	1:87:A:VAL:HG12	1:141:A:VAL:H	20	0.15
(1,1626)	1:87:A:VAL:HG13	1:141:A:VAL:H	20	0.15
(1,1626)	1:87:A:VAL:HG21	1:141:A:VAL:H	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:87:A:VAL:HG22	1:141:A:VAL:H	20	0.15
(1,1626)	1:87:A:VAL:HG23	1:141:A:VAL:H	20	0.15
(1,1623)	1:87:A:VAL:HG11	1:140:A:PRO:HA	20	0.15
(1,1623)	1:87:A:VAL:HG12	1:140:A:PRO:HA	20	0.15
(1,1623)	1:87:A:VAL:HG13	1:140:A:PRO:HA	20	0.15
(1,1623)	1:87:A:VAL:HG21	1:140:A:PRO:HA	20	0.15
(1,1623)	1:87:A:VAL:HG22	1:140:A:PRO:HA	20	0.15
(1,1623)	1:87:A:VAL:HG23	1:140:A:PRO:HA	20	0.15
(1,1470)	1:61:A:GLN:HB3	1:138:A:VAL:H	17	0.15
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	13	0.15
(1,1419)	1:51:A:ALA:HA	1:147:A:ILE:HG13	11	0.15
(1,1411)	1:46:A:ILE:HA	1:46:A:ILE:HG13	15	0.15
(1,1404)	1:45:A:LYS:HG3	1:46:A:ILE:HA	17	0.15
(1,1390)	1:42:A:ASN:HB3	1:48:A:ALA:H	19	0.15
(1,1385)	1:42:A:ASN:H	1:47:A:ASN:HB3	14	0.15
(1,1363)	1:37:A:LEU:HD11	1:48:A:ALA:H	18	0.15
(1,1363)	1:37:A:LEU:HD12	1:48:A:ALA:H	18	0.15
(1,1363)	1:37:A:LEU:HD13	1:48:A:ALA:H	18	0.15
(1,1363)	1:37:A:LEU:HD21	1:48:A:ALA:H	18	0.15
(1,1363)	1:37:A:LEU:HD22	1:48:A:ALA:H	18	0.15
(1,1363)	1:37:A:LEU:HD23	1:48:A:ALA:H	18	0.15
(1,1312)	1:18:A:SER:HB3	1:19:A:ALA:H	18	0.15
(1,1258)	1:5:A:LEU:HD11	1:7:A:LEU:HA	11	0.15
(1,1258)	1:5:A:LEU:HD12	1:7:A:LEU:HA	11	0.15
(1,1258)	1:5:A:LEU:HD13	1:7:A:LEU:HA	11	0.15
(1,1258)	1:5:A:LEU:HD21	1:7:A:LEU:HA	11	0.15
(1,1258)	1:5:A:LEU:HD22	1:7:A:LEU:HA	11	0.15
(1,1258)	1:5:A:LEU:HD23	1:7:A:LEU:HA	11	0.15
(1,1068)	1:17:A:MET:H	1:36:A:HIS:H	20	0.15
(1,1058)	1:14:A:ASP:H	1:16:A:GLN:H	1	0.15
(1,1049)	1:79:A:ARG:H	1:81:A:PHE:H	5	0.15
(1,998)	1:37:A:LEU:H	1:49:A:TRP:H	1	0.15
(1,902)	1:73:A:ILE:HD11	1:74:A:ILE:H	9	0.15
(1,902)	1:73:A:ILE:HD12	1:74:A:ILE:H	9	0.15
(1,902)	1:73:A:ILE:HD13	1:74:A:ILE:H	9	0.15
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	18	0.15
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	5	0.15
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	8	0.15
(1,585)	1:86:A:TYR:HA	1:148:A:THR:HG21	18	0.15
(1,585)	1:86:A:TYR:HA	1:148:A:THR:HG22	18	0.15
(1,585)	1:86:A:TYR:HA	1:148:A:THR:HG23	18	0.15
(1,563)	1:147:A:ILE:H	1:148:A:THR:HA	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:122:A:HIS:HD1	1:123:A:LYS:H	7	0.15
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	4	0.15
(1,202)	1:10:A:ASN:H	1:12:A:ILE:H	14	0.15
(1,183)	1:93:A:ALA:HB1	1:101:A:TRP:HD1	18	0.15
(1,183)	1:93:A:ALA:HB2	1:101:A:TRP:HD1	18	0.15
(1,183)	1:93:A:ALA:HB3	1:101:A:TRP:HD1	18	0.15
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	20	0.14
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	1	0.14
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	2	0.14
(2,126)	1:89:A:SER:O	1:141:A:VAL:N	17	0.14
(2,125)	1:91:A:LYS:O	1:139:A:LEU:N	19	0.14
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	15	0.14
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	20	0.14
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	1	0.14
(2,120)	1:68:A:ARG:O	1:133:A:ALA:N	10	0.14
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	20	0.14
(2,117)	1:94:A:HIS:O	1:102:A:THR:N	2	0.14
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	1	0.14
(2,92)	1:65:A:GLY:H	1:134:A:ARG:O	20	0.14
(2,86)	1:3:A:GLU:O	1:155:A:GLY:H	16	0.14
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	5	0.14
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	13	0.14
(2,81)	1:73:A:ILE:O	1:125:A:ASN:N	6	0.14
(2,81)	1:73:A:ILE:O	1:125:A:ASN:N	8	0.14
(2,81)	1:73:A:ILE:O	1:125:A:ASN:N	10	0.14
(2,79)	1:75:A:THR:O	1:123:A:LYS:N	19	0.14
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	7	0.14
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	8	0.14
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	3	0.14
(2,72)	1:78:A:ALA:O	1:85:A:GLN:H	5	0.14
(2,72)	1:78:A:ALA:O	1:85:A:GLN:H	6	0.14
(2,72)	1:78:A:ALA:O	1:85:A:GLN:H	7	0.14
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	11	0.14
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	3	0.14
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	7	0.14
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	12	0.14
(2,42)	1:95:A:SER:O	1:135:A:TYR:H	6	0.14
(2,42)	1:95:A:SER:O	1:135:A:TYR:H	10	0.14
(2,42)	1:95:A:SER:O	1:135:A:TYR:H	16	0.14
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	1	0.14
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	14	0.14
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:73:A:ILE:N	1:125:A:ASN:O	3	0.14
(2,15)	1:73:A:ILE:N	1:125:A:ASN:O	18	0.14
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	8	0.14
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	4	0.14
(2,1)	1:60:A:LEU:H	1:138:A:VAL:O	10	0.14
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	10	0.14
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	15	0.14
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG21	7	0.14
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG22	7	0.14
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG23	7	0.14
(1,1797)	1:124:A:LYS:HG3	1:125:A:ASN:H	14	0.14
(1,1772)	1:116:A:ASN:HB3	1:117:A:LEU:H	16	0.14
(1,1725)	1:105:A:GLU:HB3	1:108:A:GLY:H	12	0.14
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG11	17	0.14
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG12	17	0.14
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG13	17	0.14
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG21	17	0.14
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG22	17	0.14
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG23	17	0.14
(1,1645)	1:89:A:SER:H	1:90:A:TYR:HB3	18	0.14
(1,1627)	1:87:A:VAL:HG11	1:142:A:SER:H	13	0.14
(1,1627)	1:87:A:VAL:HG12	1:142:A:SER:H	13	0.14
(1,1627)	1:87:A:VAL:HG13	1:142:A:SER:H	13	0.14
(1,1627)	1:87:A:VAL:HG21	1:142:A:SER:H	13	0.14
(1,1627)	1:87:A:VAL:HG22	1:142:A:SER:H	13	0.14
(1,1627)	1:87:A:VAL:HG23	1:142:A:SER:H	13	0.14
(1,1609)	1:85:A:GLN:HG3	1:146:A:ARG:H	5	0.14
(1,1587)	1:79:A:ARG:HG3	1:82:A:GLY:H	5	0.14
(1,1570)	1:79:A:ARG:H	1:85:A:GLN:HB3	10	0.14
(1,1411)	1:46:A:ILE:HA	1:46:A:ILE:HG13	6	0.14
(1,1392)	1:43:A:GLN:H	1:44:A:GLY:HA2	9	0.14
(1,1392)	1:43:A:GLN:H	1:44:A:GLY:HA3	9	0.14
(1,1327)	1:21:A:SER:HB3	1:22:A:SER:H	9	0.14
(1,1266)	1:6:A:GLY:HA2	1:11:A:THR:HB	11	0.14
(1,1266)	1:6:A:GLY:HA3	1:11:A:THR:HB	11	0.14
(1,1206)	1:72:A:GLY:H	1:155:A:GLY:H	17	0.14
(1,1137)	1:10:A:ASN:H	1:10:A:ASN:HD22	14	0.14
(1,1125)	1:128:A:GLU:H	1:129:A:LYS:H	9	0.14
(1,1043)	1:103:A:VAL:HA	1:104:A:TYR:H	18	0.14
(1,998)	1:37:A:LEU:H	1:49:A:TRP:H	3	0.14
(1,998)	1:37:A:LEU:H	1:49:A:TRP:H	9	0.14
(1,961)	1:37:A:LEU:HD21	1:48:A:ALA:H	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,961)	1:37:A:LEU:HD22	1:48:A:ALA:H	16	0.14
(1,961)	1:37:A:LEU:HD23	1:48:A:ALA:H	16	0.14
(1,902)	1:73:A:ILE:HD11	1:74:A:ILE:H	7	0.14
(1,902)	1:73:A:ILE:HD12	1:74:A:ILE:H	7	0.14
(1,902)	1:73:A:ILE:HD13	1:74:A:ILE:H	7	0.14
(1,902)	1:73:A:ILE:HD11	1:74:A:ILE:H	8	0.14
(1,902)	1:73:A:ILE:HD12	1:74:A:ILE:H	8	0.14
(1,902)	1:73:A:ILE:HD13	1:74:A:ILE:H	8	0.14
(1,826)	1:95:A:SER:H	1:98:A:GLY:HA2	16	0.14
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	7	0.14
(1,556)	1:71:A:THR:HA	1:127:A:PHE:H	6	0.14
(1,556)	1:71:A:THR:HA	1:127:A:PHE:H	13	0.14
(1,525)	1:74:A:ILE:HD11	1:122:A:HIS:HB3	19	0.14
(1,525)	1:74:A:ILE:HD12	1:122:A:HIS:HB3	19	0.14
(1,525)	1:74:A:ILE:HD13	1:122:A:HIS:HB3	19	0.14
(1,371)	1:40:A:LEU:HA	1:42:A:ASN:H	6	0.14
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	7	0.14
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	12	0.14
(1,259)	1:138:A:VAL:HG21	1:139:A:LEU:H	20	0.14
(1,259)	1:138:A:VAL:HG22	1:139:A:LEU:H	20	0.14
(1,259)	1:138:A:VAL:HG23	1:139:A:LEU:H	20	0.14
(1,148)	1:23:A:TYR:H	1:51:A:ALA:H	1	0.14
(2,147)	1:71:A:THR:N	1:154:A:LEU:O	16	0.13
(2,143)	1:3:A:GLU:O	1:155:A:GLY:N	15	0.13
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	11	0.13
(2,130)	1:18:A:SER:N	1:61:A:GLN:O	3	0.13
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	11	0.13
(2,128)	1:74:A:ILE:O	1:152:A:GLU:N	16	0.13
(2,127)	1:76:A:GLN:O	1:150:A:ARG:N	15	0.13
(2,126)	1:89:A:SER:O	1:141:A:VAL:N	7	0.13
(2,123)	1:93:A:ALA:O	1:137:A:ARG:N	10	0.13
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	19	0.13
(2,114)	1:93:A:ALA:N	1:137:A:ARG:O	16	0.13
(2,105)	1:70:A:VAL:N	1:131:A:PHE:O	1	0.13
(2,105)	1:70:A:VAL:N	1:131:A:PHE:O	17	0.13
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	13	0.13
(2,101)	1:62:A:VAL:N	1:136:A:VAL:O	15	0.13
(2,92)	1:65:A:GLY:H	1:134:A:ARG:O	17	0.13
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	2	0.13
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	12	0.13
(2,78)	1:75:A:THR:O	1:123:A:LYS:H	13	0.13
(2,76)	1:88:A:ALA:O	1:115:A:GLY:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	4	0.13
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	14	0.13
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	19	0.13
(2,72)	1:78:A:ALA:O	1:85:A:GLN:H	2	0.13
(2,71)	1:78:A:ALA:N	1:148:A:THR:O	19	0.13
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	2	0.13
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	5	0.13
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	14	0.13
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	16	0.13
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	13	0.13
(2,50)	1:91:A:LYS:O	1:139:A:LEU:H	4	0.13
(2,42)	1:95:A:SER:O	1:135:A:TYR:H	2	0.13
(2,42)	1:95:A:SER:O	1:135:A:TYR:H	7	0.13
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	3	0.13
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	8	0.13
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	4	0.13
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	5	0.13
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	12	0.13
(2,16)	1:74:A:ILE:H	1:152:A:GLU:O	15	0.13
(2,15)	1:73:A:ILE:N	1:125:A:ASN:O	16	0.13
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	10	0.13
(2,1)	1:60:A:LEU:H	1:138:A:VAL:O	9	0.13
(2,1)	1:60:A:LEU:H	1:138:A:VAL:O	20	0.13
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	6	0.13
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	8	0.13
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	18	0.13
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	18	0.13
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG21	5	0.13
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG22	5	0.13
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG23	5	0.13
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG21	9	0.13
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG22	9	0.13
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG23	9	0.13
(1,1801)	1:125:A:ASN:HB3	1:126:A:ILE:HB	9	0.13
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG11	9	0.13
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG12	9	0.13
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG13	9	0.13
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG21	9	0.13
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG22	9	0.13
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG23	9	0.13
(1,1649)	1:89:A:SER:HB3	1:112:A:VAL:HG11	5	0.13
(1,1649)	1:89:A:SER:HB3	1:112:A:VAL:HG12	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1649)	1:89:A:SER:HB3	1:112:A:VAL:HG13	5	0.13
(1,1649)	1:89:A:SER:HB3	1:112:A:VAL:HG21	5	0.13
(1,1649)	1:89:A:SER:HB3	1:112:A:VAL:HG22	5	0.13
(1,1649)	1:89:A:SER:HB3	1:112:A:VAL:HG23	5	0.13
(1,1626)	1:87:A:VAL:HG11	1:141:A:VAL:H	16	0.13
(1,1626)	1:87:A:VAL:HG12	1:141:A:VAL:H	16	0.13
(1,1626)	1:87:A:VAL:HG13	1:141:A:VAL:H	16	0.13
(1,1626)	1:87:A:VAL:HG21	1:141:A:VAL:H	16	0.13
(1,1626)	1:87:A:VAL:HG22	1:141:A:VAL:H	16	0.13
(1,1626)	1:87:A:VAL:HG23	1:141:A:VAL:H	16	0.13
(1,1587)	1:79:A:ARG:HG3	1:82:A:GLY:H	4	0.13
(1,1552)	1:76:A:GLN:HA	1:76:A:GLN:HE21	14	0.13
(1,1552)	1:76:A:GLN:HA	1:76:A:GLN:HE22	14	0.13
(1,1470)	1:61:A:GLN:HB3	1:138:A:VAL:H	9	0.13
(1,1454)	1:58:A:GLU:H	1:147:A:ILE:HG13	17	0.13
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	6	0.13
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	9	0.13
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	10	0.13
(1,1406)	1:45:A:LYS:HD3	1:46:A:ILE:HA	20	0.13
(1,1404)	1:45:A:LYS:HG3	1:46:A:ILE:HA	4	0.13
(1,1372)	1:38:A:GLY:HA2	1:150:A:ARG:HA	14	0.13
(1,1372)	1:38:A:GLY:HA3	1:150:A:ARG:HA	14	0.13
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG21	8	0.13
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG22	8	0.13
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG23	8	0.13
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG21	8	0.13
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG22	8	0.13
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG23	8	0.13
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG21	8	0.13
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG22	8	0.13
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG23	8	0.13
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG21	8	0.13
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG22	8	0.13
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG23	8	0.13
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG21	8	0.13
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG22	8	0.13
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG23	8	0.13
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG21	8	0.13
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG22	8	0.13
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG23	8	0.13
(1,1299)	1:17:A:MET:H	1:36:A:HIS:HB3	1	0.13
(1,1299)	1:17:A:MET:H	1:36:A:HIS:HB3	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD11	8	0.13
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD12	8	0.13
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD13	8	0.13
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD21	8	0.13
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD22	8	0.13
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD23	8	0.13
(1,1239)	1:3:A:GLU:HB3	1:157:A:LEU:HD11	20	0.13
(1,1239)	1:3:A:GLU:HB3	1:157:A:LEU:HD12	20	0.13
(1,1239)	1:3:A:GLU:HB3	1:157:A:LEU:HD13	20	0.13
(1,1239)	1:3:A:GLU:HB3	1:157:A:LEU:HD21	20	0.13
(1,1239)	1:3:A:GLU:HB3	1:157:A:LEU:HD22	20	0.13
(1,1239)	1:3:A:GLU:HB3	1:157:A:LEU:HD23	20	0.13
(1,1206)	1:72:A:GLY:H	1:155:A:GLY:H	6	0.13
(1,1172)	1:40:A:LEU:HG	1:41:A:ASP:H	8	0.13
(1,1067)	1:36:A:HIS:H	1:49:A:TRP:HB3	1	0.13
(1,1058)	1:14:A:ASP:H	1:16:A:GLN:H	10	0.13
(1,1058)	1:14:A:ASP:H	1:16:A:GLN:H	19	0.13
(1,1049)	1:79:A:ARG:H	1:81:A:PHE:H	19	0.13
(1,998)	1:37:A:LEU:H	1:49:A:TRP:H	17	0.13
(1,811)	1:6:A:GLY:HA2	1:11:A:THR:HG21	14	0.13
(1,811)	1:6:A:GLY:HA2	1:11:A:THR:HG22	14	0.13
(1,811)	1:6:A:GLY:HA2	1:11:A:THR:HG23	14	0.13
(1,696)	1:71:A:THR:HA	1:127:A:PHE:HD1	11	0.13
(1,696)	1:71:A:THR:HA	1:127:A:PHE:HD2	11	0.13
(1,670)	1:73:A:ILE:HD11	1:74:A:ILE:HA	13	0.13
(1,670)	1:73:A:ILE:HD12	1:74:A:ILE:HA	13	0.13
(1,670)	1:73:A:ILE:HD13	1:74:A:ILE:HA	13	0.13
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	6	0.13
(1,598)	1:50:A:THR:HG21	1:146:A:ARG:HA	5	0.13
(1,598)	1:50:A:THR:HG22	1:146:A:ARG:HA	5	0.13
(1,598)	1:50:A:THR:HG23	1:146:A:ARG:HA	5	0.13
(1,598)	1:50:A:THR:HG21	1:146:A:ARG:HA	17	0.13
(1,598)	1:50:A:THR:HG22	1:146:A:ARG:HA	17	0.13
(1,598)	1:50:A:THR:HG23	1:146:A:ARG:HA	17	0.13
(1,598)	1:50:A:THR:HG21	1:146:A:ARG:HA	18	0.13
(1,598)	1:50:A:THR:HG22	1:146:A:ARG:HA	18	0.13
(1,598)	1:50:A:THR:HG23	1:146:A:ARG:HA	18	0.13
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	12	0.13
(1,566)	1:7:A:LEU:HA	1:8:A:LYS:HA	14	0.13
(1,563)	1:147:A:ILE:H	1:148:A:THR:HA	8	0.13
(1,563)	1:147:A:ILE:H	1:148:A:THR:HA	10	0.13
(1,472)	1:23:A:TYR:HA	1:24:A:LYS:H	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,342)	1:116:A:ASN:H	1:118:A:ASP:H	7	0.13
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	10	0.13
(1,309)	1:59:A:TRP:HB3	1:60:A:LEU:H	14	0.13
(1,241)	1:106:A:GLU:H	1:110:A:SER:HA	18	0.13
(1,193)	1:5:A:LEU:HA	1:6:A:GLY:H	8	0.13
(1,130)	1:10:A:ASN:HD21	1:11:A:THR:HG21	15	0.13
(1,130)	1:10:A:ASN:HD21	1:11:A:THR:HG22	15	0.13
(1,130)	1:10:A:ASN:HD21	1:11:A:THR:HG23	15	0.13
(1,114)	1:9:A:ASN:H	1:10:A:ASN:HA	15	0.13
(2,148)	1:88:A:ALA:N	1:142:A:SER:O	10	0.12
(2,148)	1:88:A:ALA:N	1:142:A:SER:O	14	0.12
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	10	0.12
(2,133)	1:51:A:ALA:N	1:147:A:ILE:O	15	0.12
(2,132)	1:49:A:TRP:N	1:149:A:LEU:O	3	0.12
(2,130)	1:18:A:SER:N	1:61:A:GLN:O	5	0.12
(2,127)	1:76:A:GLN:O	1:150:A:ARG:N	5	0.12
(2,123)	1:93:A:ALA:O	1:137:A:ARG:N	7	0.12
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	11	0.12
(2,118)	1:90:A:TYR:O	1:113:A:PHE:N	7	0.12
(2,114)	1:93:A:ALA:N	1:137:A:ARG:O	13	0.12
(2,111)	1:89:A:SER:N	1:142:A:SER:O	5	0.12
(2,109)	1:75:A:THR:N	1:123:A:LYS:O	1	0.12
(2,108)	1:74:A:ILE:N	1:152:A:GLU:O	1	0.12
(2,105)	1:70:A:VAL:N	1:131:A:PHE:O	5	0.12
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	1	0.12
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	11	0.12
(2,98)	1:95:A:SER:O	1:134:A:ARG:H	6	0.12
(2,93)	1:65:A:GLY:N	1:134:A:ARG:O	20	0.12
(2,90)	1:89:A:SER:O	1:142:A:SER:H	5	0.12
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	4	0.12
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	16	0.12
(2,81)	1:73:A:ILE:O	1:125:A:ASN:N	7	0.12
(2,78)	1:75:A:THR:O	1:123:A:LYS:H	4	0.12
(2,78)	1:75:A:THR:O	1:123:A:LYS:H	9	0.12
(2,76)	1:88:A:ALA:O	1:115:A:GLY:H	18	0.12
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	12	0.12
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	15	0.12
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	1	0.12
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	2	0.12
(2,74)	1:86:A:TYR:H	1:144:A:HIS:O	10	0.12
(2,72)	1:78:A:ALA:O	1:85:A:GLN:H	12	0.12
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	15	0.12
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	3	0.12
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	5	0.12
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	6	0.12
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	9	0.12
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	4	0.12
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	6	0.12
(2,54)	1:76:A:GLN:O	1:150:A:ARG:H	1	0.12
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	3	0.12
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	10	0.12
(2,15)	1:73:A:ILE:N	1:125:A:ASN:O	12	0.12
(2,14)	1:73:A:ILE:H	1:125:A:ASN:O	13	0.12
(2,5)	1:16:A:GLN:O	1:63:A:ASP:H	20	0.12
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	2	0.12
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	5	0.12
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	2	0.12
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	4	0.12
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	8	0.12
(1,1898)	1:1:A:CYS:CB	1:156:A:CYS:SG	20	0.12
(1,1865)	1:147:A:ILE:HA	1:149:A:LEU:HB3	19	0.12
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG21	12	0.12
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG22	12	0.12
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG23	12	0.12
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG21	14	0.12
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG22	14	0.12
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG23	14	0.12
(1,1791)	1:122:A:HIS:H	1:123:A:LYS:HB3	12	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG11	6	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG12	6	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG13	6	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG21	6	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG22	6	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG23	6	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG11	7	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG12	7	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG13	7	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG21	7	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG22	7	0.12
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG23	7	0.12
(1,1645)	1:89:A:SER:H	1:90:A:TYR:HB3	17	0.12
(1,1643)	1:88:A:ALA:HB1	1:115:A:GLY:HA2	14	0.12
(1,1643)	1:88:A:ALA:HB1	1:115:A:GLY:HA3	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1643)	1:88:A:ALA:HB2	1:115:A:GLY:HA2	14	0.12
(1,1643)	1:88:A:ALA:HB2	1:115:A:GLY:HA3	14	0.12
(1,1643)	1:88:A:ALA:HB3	1:115:A:GLY:HA2	14	0.12
(1,1643)	1:88:A:ALA:HB3	1:115:A:GLY:HA3	14	0.12
(1,1570)	1:79:A:ARG:H	1:85:A:GLN:HB3	11	0.12
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	3	0.12
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	14	0.12
(1,1406)	1:45:A:LYS:HD3	1:46:A:ILE:HA	19	0.12
(1,1368)	1:38:A:GLY:H	1:150:A:ARG:HG3	1	0.12
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD11	1	0.12
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD12	1	0.12
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD13	1	0.12
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD21	1	0.12
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD22	1	0.12
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD23	1	0.12
(1,1289)	1:16:A:GLN:H	1:62:A:VAL:HG11	11	0.12
(1,1289)	1:16:A:GLN:H	1:62:A:VAL:HG12	11	0.12
(1,1289)	1:16:A:GLN:H	1:62:A:VAL:HG13	11	0.12
(1,1289)	1:16:A:GLN:H	1:62:A:VAL:HG21	11	0.12
(1,1289)	1:16:A:GLN:H	1:62:A:VAL:HG22	11	0.12
(1,1289)	1:16:A:GLN:H	1:62:A:VAL:HG23	11	0.12
(1,1245)	1:4:A:PRO:HA	1:153:A:LEU:HD11	3	0.12
(1,1245)	1:4:A:PRO:HA	1:153:A:LEU:HD12	3	0.12
(1,1245)	1:4:A:PRO:HA	1:153:A:LEU:HD13	3	0.12
(1,1245)	1:4:A:PRO:HA	1:153:A:LEU:HD21	3	0.12
(1,1245)	1:4:A:PRO:HA	1:153:A:LEU:HD22	3	0.12
(1,1245)	1:4:A:PRO:HA	1:153:A:LEU:HD23	3	0.12
(1,1125)	1:128:A:GLU:H	1:129:A:LYS:H	11	0.12
(1,1125)	1:128:A:GLU:H	1:129:A:LYS:H	17	0.12
(1,1117)	1:109:A:SER:H	1:111:A:LYS:H	8	0.12
(1,1116)	1:105:A:GLU:H	1:111:A:LYS:H	12	0.12
(1,1033)	1:126:A:ILE:HG21	1:127:A:PHE:H	10	0.12
(1,1033)	1:126:A:ILE:HG22	1:127:A:PHE:H	10	0.12
(1,1033)	1:126:A:ILE:HG23	1:127:A:PHE:H	10	0.12
(1,966)	1:38:A:GLY:H	1:48:A:ALA:H	20	0.12
(1,955)	1:90:A:TYR:H	1:112:A:VAL:HB	5	0.12
(1,949)	1:87:A:VAL:HA	1:148:A:THR:H	6	0.12
(1,826)	1:95:A:SER:H	1:98:A:GLY:HA2	2	0.12
(1,767)	1:14:A:ASP:HA	1:36:A:HIS:HA	16	0.12
(1,739)	1:127:A:PHE:HD1	1:129:A:LYS:HA	19	0.12
(1,739)	1:127:A:PHE:HD2	1:129:A:LYS:HA	19	0.12
(1,690)	1:64:A:LEU:HG	1:66:A:THR:HB	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:73:A:ILE:HD11	1:74:A:ILE:HA	11	0.12
(1,670)	1:73:A:ILE:HD12	1:74:A:ILE:HA	11	0.12
(1,670)	1:73:A:ILE:HD13	1:74:A:ILE:HA	11	0.12
(1,598)	1:50:A:THR:HG21	1:146:A:ARG:HA	2	0.12
(1,598)	1:50:A:THR:HG22	1:146:A:ARG:HA	2	0.12
(1,598)	1:50:A:THR:HG23	1:146:A:ARG:HA	2	0.12
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	1	0.12
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	6	0.12
(1,563)	1:147:A:ILE:H	1:148:A:THR:HA	7	0.12
(1,556)	1:71:A:THR:HA	1:127:A:PHE:H	9	0.12
(1,472)	1:23:A:TYR:HA	1:24:A:LYS:H	17	0.12
(1,465)	1:19:A:ALA:HB1	1:22:A:SER:H	20	0.12
(1,465)	1:19:A:ALA:HB2	1:22:A:SER:H	20	0.12
(1,465)	1:19:A:ALA:HB3	1:22:A:SER:H	20	0.12
(1,386)	1:42:A:ASN:HA	1:47:A:ASN:H	6	0.12
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	2	0.12
(1,279)	1:116:A:ASN:H	1:117:A:LEU:H	2	0.12
(1,279)	1:116:A:ASN:H	1:117:A:LEU:H	12	0.12
(1,279)	1:116:A:ASN:H	1:117:A:LEU:H	18	0.12
(1,193)	1:5:A:LEU:HA	1:6:A:GLY:H	11	0.12
(1,193)	1:5:A:LEU:HA	1:6:A:GLY:H	13	0.12
(2,147)	1:71:A:THR:N	1:154:A:LEU:O	12	0.11
(2,126)	1:89:A:SER:O	1:141:A:VAL:N	11	0.11
(2,122)	1:62:A:VAL:O	1:136:A:VAL:N	8	0.11
(2,121)	1:95:A:SER:O	1:135:A:TYR:N	12	0.11
(2,113)	1:91:A:LYS:N	1:139:A:LEU:O	7	0.11
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	3	0.11
(2,112)	1:90:A:TYR:N	1:113:A:PHE:O	4	0.11
(2,105)	1:70:A:VAL:N	1:131:A:PHE:O	7	0.11
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	14	0.11
(2,103)	1:64:A:LEU:N	1:134:A:ARG:O	19	0.11
(2,102)	1:16:A:GLN:O	1:63:A:ASP:N	16	0.11
(2,101)	1:62:A:VAL:N	1:136:A:VAL:O	19	0.11
(2,90)	1:89:A:SER:O	1:142:A:SER:H	8	0.11
(2,90)	1:89:A:SER:O	1:142:A:SER:H	18	0.11
(2,85)	1:49:A:TRP:O	1:149:A:LEU:N	9	0.11
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	7	0.11
(2,84)	1:49:A:TRP:O	1:149:A:LEU:H	10	0.11
(2,82)	1:86:A:TYR:O	1:144:A:HIS:H	6	0.11
(2,80)	1:73:A:ILE:O	1:125:A:ASN:H	9	0.11
(2,79)	1:75:A:THR:O	1:123:A:LYS:N	14	0.11
(2,76)	1:88:A:ALA:O	1:115:A:GLY:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	3	0.11
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	9	0.11
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	11	0.11
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	18	0.11
(2,75)	1:86:A:TYR:N	1:144:A:HIS:O	19	0.11
(2,72)	1:78:A:ALA:O	1:85:A:GLN:H	9	0.11
(2,70)	1:78:A:ALA:H	1:148:A:THR:O	10	0.11
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	12	0.11
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	14	0.11
(2,62)	1:20:A:SER:H	1:59:A:TRP:O	7	0.11
(2,62)	1:20:A:SER:H	1:59:A:TRP:O	18	0.11
(2,43)	1:95:A:SER:O	1:135:A:TYR:N	6	0.11
(2,42)	1:95:A:SER:O	1:135:A:TYR:H	15	0.11
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	7	0.11
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	13	0.11
(2,24)	1:90:A:TYR:H	1:113:A:PHE:O	5	0.11
(2,20)	1:76:A:GLN:H	1:150:A:ARG:O	15	0.11
(2,15)	1:73:A:ILE:N	1:125:A:ASN:O	4	0.11
(2,15)	1:73:A:ILE:N	1:125:A:ASN:O	5	0.11
(2,13)	1:72:A:GLY:N	1:154:A:LEU:O	17	0.11
(2,9)	1:68:A:ARG:H	1:133:A:ALA:O	5	0.11
(2,7)	1:64:A:LEU:H	1:134:A:ARG:O	20	0.11
(2,1)	1:60:A:LEU:H	1:138:A:VAL:O	6	0.11
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	7	0.11
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	11	0.11
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	15	0.11
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	5	0.11
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	12	0.11
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	13	0.11
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	14	0.11
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	17	0.11
(1,1869)	1:148:A:THR:HA	1:149:A:LEU:HB3	19	0.11
(1,1807)	1:127:A:PHE:HB3	1:129:A:LYS:H	8	0.11
(1,1801)	1:125:A:ASN:HB3	1:126:A:ILE:HB	8	0.11
(1,1791)	1:122:A:HIS:H	1:123:A:LYS:HB3	18	0.11
(1,1737)	1:107:A:GLN:HG3	1:109:A:SER:H	12	0.11
(1,1735)	1:107:A:GLN:HB3	1:109:A:SER:H	18	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG11	4	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG12	4	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG13	4	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG21	4	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG22	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG23	4	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG11	17	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG12	17	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG13	17	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG21	17	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG22	17	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG23	17	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG11	19	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG12	19	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG13	19	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG21	19	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG22	19	0.11
(1,1687)	1:94:A:HIS:HA	1:138:A:VAL:HG23	19	0.11
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG11	9	0.11
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG12	9	0.11
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG13	9	0.11
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG21	9	0.11
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG22	9	0.11
(1,1661)	1:91:A:LYS:H	1:138:A:VAL:HG23	9	0.11
(1,1654)	1:90:A:TYR:HB3	1:91:A:LYS:H	20	0.11
(1,1641)	1:88:A:ALA:H	1:143:A:TRP:HB3	7	0.11
(1,1627)	1:87:A:VAL:HG11	1:142:A:SER:H	6	0.11
(1,1627)	1:87:A:VAL:HG12	1:142:A:SER:H	6	0.11
(1,1627)	1:87:A:VAL:HG13	1:142:A:SER:H	6	0.11
(1,1627)	1:87:A:VAL:HG21	1:142:A:SER:H	6	0.11
(1,1627)	1:87:A:VAL:HG22	1:142:A:SER:H	6	0.11
(1,1627)	1:87:A:VAL:HG23	1:142:A:SER:H	6	0.11
(1,1626)	1:87:A:VAL:HG11	1:141:A:VAL:H	13	0.11
(1,1626)	1:87:A:VAL:HG12	1:141:A:VAL:H	13	0.11
(1,1626)	1:87:A:VAL:HG13	1:141:A:VAL:H	13	0.11
(1,1626)	1:87:A:VAL:HG21	1:141:A:VAL:H	13	0.11
(1,1626)	1:87:A:VAL:HG22	1:141:A:VAL:H	13	0.11
(1,1626)	1:87:A:VAL:HG23	1:141:A:VAL:H	13	0.11
(1,1587)	1:79:A:ARG:HG3	1:82:A:GLY:H	11	0.11
(1,1570)	1:79:A:ARG:H	1:85:A:GLN:HB3	8	0.11
(1,1530)	1:71:A:THR:HG21	1:156:A:CYS:HB3	20	0.11
(1,1530)	1:71:A:THR:HG22	1:156:A:CYS:HB3	20	0.11
(1,1530)	1:71:A:THR:HG23	1:156:A:CYS:HB3	20	0.11
(1,1476)	1:62:A:VAL:HG11	1:136:A:VAL:H	18	0.11
(1,1476)	1:62:A:VAL:HG12	1:136:A:VAL:H	18	0.11
(1,1476)	1:62:A:VAL:HG13	1:136:A:VAL:H	18	0.11
(1,1476)	1:62:A:VAL:HG21	1:136:A:VAL:H	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1476)	1:62:A:VAL:HG22	1:136:A:VAL:H	18	0.11
(1,1476)	1:62:A:VAL:HG23	1:136:A:VAL:H	18	0.11
(1,1470)	1:61:A:GLN:HB3	1:138:A:VAL:H	10	0.11
(1,1470)	1:61:A:GLN:HB3	1:138:A:VAL:H	12	0.11
(1,1470)	1:61:A:GLN:HB3	1:138:A:VAL:H	20	0.11
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	4	0.11
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	8	0.11
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	12	0.11
(1,1435)	1:55:A:SER:H	1:147:A:ILE:HG13	20	0.11
(1,1406)	1:45:A:LYS:HD3	1:46:A:ILE:HA	8	0.11
(1,1406)	1:45:A:LYS:HD3	1:46:A:ILE:HA	11	0.11
(1,1396)	1:44:A:GLY:H	1:45:A:LYS:HD3	17	0.11
(1,1392)	1:43:A:GLN:H	1:44:A:GLY:HA2	6	0.11
(1,1392)	1:43:A:GLN:H	1:44:A:GLY:HA3	6	0.11
(1,1376)	1:39:A:ARG:HD3	1:40:A:LEU:H	10	0.11
(1,1368)	1:38:A:GLY:H	1:150:A:ARG:HG3	17	0.11
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD11	20	0.11
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD12	20	0.11
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD13	20	0.11
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD21	20	0.11
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD22	20	0.11
(1,1346)	1:36:A:HIS:H	1:37:A:LEU:HD23	20	0.11
(1,1258)	1:5:A:LEU:HD11	1:7:A:LEU:HA	19	0.11
(1,1258)	1:5:A:LEU:HD12	1:7:A:LEU:HA	19	0.11
(1,1258)	1:5:A:LEU:HD13	1:7:A:LEU:HA	19	0.11
(1,1258)	1:5:A:LEU:HD21	1:7:A:LEU:HA	19	0.11
(1,1258)	1:5:A:LEU:HD22	1:7:A:LEU:HA	19	0.11
(1,1258)	1:5:A:LEU:HD23	1:7:A:LEU:HA	19	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD11	11	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD12	11	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD13	11	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD21	11	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD22	11	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD23	11	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD11	13	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD12	13	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD13	13	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD21	13	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD22	13	0.11
(1,1250)	1:5:A:LEU:H	1:5:A:LEU:HD23	13	0.11
(1,1206)	1:72:A:GLY:H	1:155:A:GLY:H	2	0.11
(1,1206)	1:72:A:GLY:H	1:155:A:GLY:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:40:A:LEU:HG	1:41:A:ASP:H	6	0.11
(1,1080)	1:122:A:HIS:H	1:122:A:HIS:HD1	9	0.11
(1,1049)	1:79:A:ARG:H	1:81:A:PHE:H	17	0.11
(1,1012)	1:88:A:ALA:HB1	1:143:A:TRP:H	18	0.11
(1,1012)	1:88:A:ALA:HB2	1:143:A:TRP:H	18	0.11
(1,1012)	1:88:A:ALA:HB3	1:143:A:TRP:H	18	0.11
(1,931)	1:71:A:THR:H	1:156:A:CYS:HA	17	0.11
(1,902)	1:73:A:ILE:HD11	1:74:A:ILE:H	6	0.11
(1,902)	1:73:A:ILE:HD12	1:74:A:ILE:H	6	0.11
(1,902)	1:73:A:ILE:HD13	1:74:A:ILE:H	6	0.11
(1,902)	1:73:A:ILE:HD11	1:74:A:ILE:H	19	0.11
(1,902)	1:73:A:ILE:HD12	1:74:A:ILE:H	19	0.11
(1,902)	1:73:A:ILE:HD13	1:74:A:ILE:H	19	0.11
(1,767)	1:14:A:ASP:HA	1:36:A:HIS:HA	19	0.11
(1,642)	1:136:A:VAL:HG21	1:137:A:ARG:H	10	0.11
(1,642)	1:136:A:VAL:HG22	1:137:A:ARG:H	10	0.11
(1,642)	1:136:A:VAL:HG23	1:137:A:ARG:H	10	0.11
(1,641)	1:135:A:TYR:HA	1:136:A:VAL:HB	14	0.11
(1,598)	1:50:A:THR:HG21	1:146:A:ARG:HA	3	0.11
(1,598)	1:50:A:THR:HG22	1:146:A:ARG:HA	3	0.11
(1,598)	1:50:A:THR:HG23	1:146:A:ARG:HA	3	0.11
(1,598)	1:50:A:THR:HG21	1:146:A:ARG:HA	16	0.11
(1,598)	1:50:A:THR:HG22	1:146:A:ARG:HA	16	0.11
(1,598)	1:50:A:THR:HG23	1:146:A:ARG:HA	16	0.11
(1,592)	1:90:A:TYR:HA	1:139:A:LEU:HA	13	0.11
(1,585)	1:86:A:TYR:HA	1:148:A:THR:HG21	9	0.11
(1,585)	1:86:A:TYR:HA	1:148:A:THR:HG22	9	0.11
(1,585)	1:86:A:TYR:HA	1:148:A:THR:HG23	9	0.11
(1,574)	1:133:A:ALA:HB1	1:136:A:VAL:HA	18	0.11
(1,574)	1:133:A:ALA:HB2	1:136:A:VAL:HA	18	0.11
(1,574)	1:133:A:ALA:HB3	1:136:A:VAL:HA	18	0.11
(1,556)	1:71:A:THR:HA	1:127:A:PHE:H	14	0.11
(1,487)	1:101:A:TRP:HD1	1:102:A:THR:H	18	0.11
(1,418)	1:51:A:ALA:HA	1:53:A:SER:H	1	0.11
(1,386)	1:42:A:ASN:HA	1:47:A:ASN:H	3	0.11
(1,386)	1:42:A:ASN:HA	1:47:A:ASN:H	7	0.11
(1,386)	1:42:A:ASN:HA	1:47:A:ASN:H	19	0.11
(1,340)	1:88:A:ALA:HA	1:116:A:ASN:H	5	0.11
(1,193)	1:5:A:LEU:HA	1:6:A:GLY:H	14	0.11
(1,193)	1:5:A:LEU:HA	1:6:A:GLY:H	17	0.11
(1,152)	1:48:A:ALA:H	1:49:A:TRP:H	6	0.11
(1,94)	1:94:A:HIS:H	1:101:A:TRP:HA	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:146:A:ARG:H	1:147:A:ILE:HD11	13	0.11
(1,70)	1:146:A:ARG:H	1:147:A:ILE:HD12	13	0.11
(1,70)	1:146:A:ARG:H	1:147:A:ILE:HD13	13	0.11
(2,126)	1:89:A:SER:O	1:141:A:VAL:N	3	0.1
(2,120)	1:68:A:ARG:O	1:133:A:ALA:N	15	0.1
(2,100)	1:60:A:LEU:N	1:138:A:VAL:O	13	0.1
(2,92)	1:65:A:GLY:H	1:134:A:ARG:O	15	0.1
(2,87)	1:3:A:GLU:O	1:155:A:GLY:N	11	0.1
(2,76)	1:88:A:ALA:O	1:115:A:GLY:H	5	0.1
(2,76)	1:88:A:ALA:O	1:115:A:GLY:H	9	0.1
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	10	0.1
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	16	0.1
(2,66)	1:51:A:ALA:H	1:147:A:ILE:O	18	0.1
(2,64)	1:49:A:TRP:H	1:149:A:LEU:O	5	0.1
(2,62)	1:20:A:SER:H	1:59:A:TRP:O	9	0.1
(2,60)	1:18:A:SER:H	1:61:A:GLN:O	9	0.1
(2,39)	1:70:A:VAL:O	1:131:A:PHE:N	18	0.1
(2,30)	1:94:A:HIS:H	1:102:A:THR:O	14	0.1
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	12	0.1
(1,1900)	1:1:A:CYS:CB	1:156:A:CYS:SG	14	0.1
(1,1899)	1:1:A:CYS:SG	1:156:A:CYS:CB	1	0.1
(1,1886)	1:156:A:CYS:HB3	1:158:A:GLU:H	20	0.1
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG21	13	0.1
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG22	13	0.1
(1,1843)	1:140:A:PRO:HD3	1:147:A:ILE:HG23	13	0.1
(1,1817)	1:129:A:LYS:H	1:130:A:PRO:HD3	10	0.1
(1,1791)	1:122:A:HIS:H	1:123:A:LYS:HB3	5	0.1
(1,1774)	1:116:A:ASN:HB3	1:118:A:ASP:H	16	0.1
(1,1745)	1:111:A:LYS:HA	1:111:A:LYS:HG3	8	0.1
(1,1693)	1:94:A:HIS:HB3	1:137:A:ARG:H	18	0.1
(1,1643)	1:88:A:ALA:HB1	1:115:A:GLY:HA2	16	0.1
(1,1643)	1:88:A:ALA:HB1	1:115:A:GLY:HA3	16	0.1
(1,1643)	1:88:A:ALA:HB2	1:115:A:GLY:HA2	16	0.1
(1,1643)	1:88:A:ALA:HB2	1:115:A:GLY:HA3	16	0.1
(1,1643)	1:88:A:ALA:HB3	1:115:A:GLY:HA2	16	0.1
(1,1643)	1:88:A:ALA:HB3	1:115:A:GLY:HA3	16	0.1
(1,1570)	1:79:A:ARG:H	1:85:A:GLN:HB3	3	0.1
(1,1569)	1:79:A:ARG:H	1:79:A:ARG:HD3	4	0.1
(1,1476)	1:62:A:VAL:HG11	1:136:A:VAL:H	17	0.1
(1,1476)	1:62:A:VAL:HG12	1:136:A:VAL:H	17	0.1
(1,1476)	1:62:A:VAL:HG13	1:136:A:VAL:H	17	0.1
(1,1476)	1:62:A:VAL:HG21	1:136:A:VAL:H	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1476)	1:62:A:VAL:HG22	1:136:A:VAL:H	17	0.1
(1,1476)	1:62:A:VAL:HG23	1:136:A:VAL:H	17	0.1
(1,1454)	1:58:A:GLU:H	1:147:A:ILE:HG13	8	0.1
(1,1442)	1:55:A:SER:HB3	1:58:A:GLU:H	15	0.1
(1,1431)	1:54:A:ASN:HB3	1:146:A:ARG:HE	12	0.1
(1,1372)	1:38:A:GLY:HA2	1:150:A:ARG:HA	6	0.1
(1,1372)	1:38:A:GLY:HA3	1:150:A:ARG:HA	6	0.1
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG21	10	0.1
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG22	10	0.1
(1,1360)	1:37:A:LEU:HD11	1:46:A:ILE:HG23	10	0.1
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG21	10	0.1
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG22	10	0.1
(1,1360)	1:37:A:LEU:HD12	1:46:A:ILE:HG23	10	0.1
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG21	10	0.1
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG22	10	0.1
(1,1360)	1:37:A:LEU:HD13	1:46:A:ILE:HG23	10	0.1
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG21	10	0.1
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG22	10	0.1
(1,1360)	1:37:A:LEU:HD21	1:46:A:ILE:HG23	10	0.1
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG21	10	0.1
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG22	10	0.1
(1,1360)	1:37:A:LEU:HD22	1:46:A:ILE:HG23	10	0.1
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG21	10	0.1
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG22	10	0.1
(1,1360)	1:37:A:LEU:HD23	1:46:A:ILE:HG23	10	0.1
(1,1312)	1:18:A:SER:HB3	1:19:A:ALA:H	9	0.1
(1,923)	1:66:A:THR:H	1:134:A:ARG:HE	14	0.1
(1,666)	1:143:A:TRP:HA	1:147:A:ILE:HD11	15	0.1
(1,666)	1:143:A:TRP:HA	1:147:A:ILE:HD12	15	0.1
(1,666)	1:143:A:TRP:HA	1:147:A:ILE:HD13	15	0.1
(1,342)	1:116:A:ASN:H	1:118:A:ASP:H	13	0.1
(1,337)	1:148:A:THR:H	1:149:A:LEU:HA	3	0.1
(1,278)	1:127:A:PHE:HA	1:129:A:LYS:H	4	0.1
(1,158)	1:37:A:LEU:HD11	1:48:A:ALA:H	15	0.1
(1,158)	1:37:A:LEU:HD12	1:48:A:ALA:H	15	0.1
(1,158)	1:37:A:LEU:HD13	1:48:A:ALA:H	15	0.1
(1,127)	1:72:A:GLY:H	1:154:A:LEU:HA	6	0.1
(1,91)	1:73:A:ILE:H	1:73:A:ILE:HD11	8	0.1
(1,91)	1:73:A:ILE:H	1:73:A:ILE:HD12	8	0.1
(1,91)	1:73:A:ILE:H	1:73:A:ILE:HD13	8	0.1

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

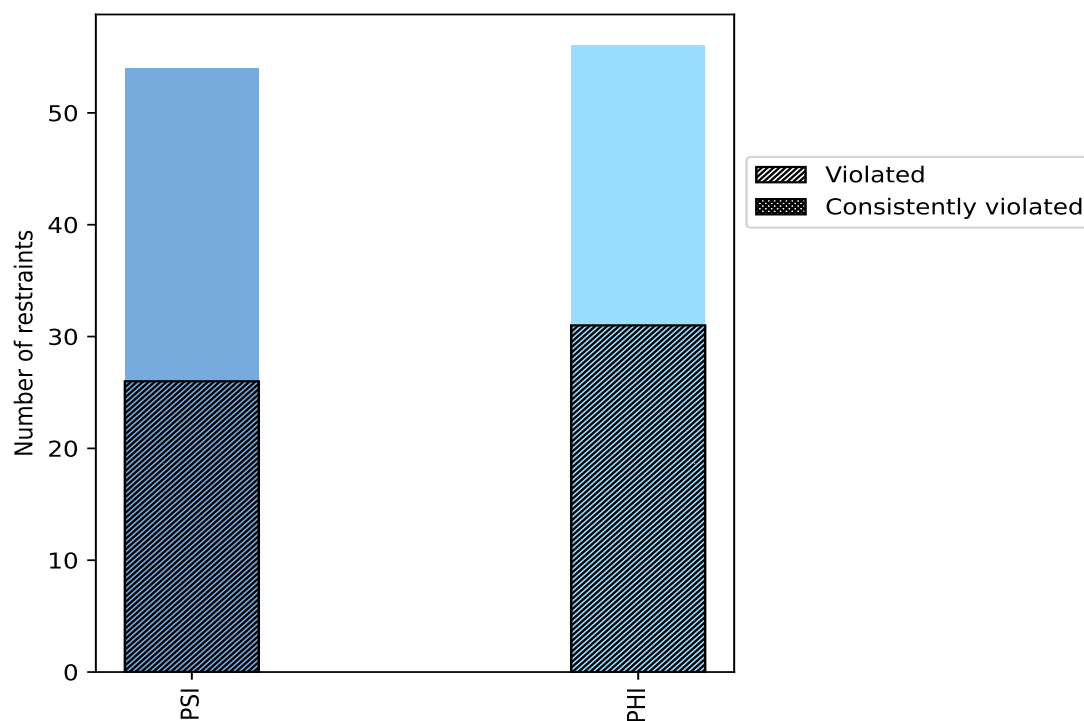
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	54	49.1	26	48.1	23.6	0	0.0	0.0
PHI	56	50.9	31	55.4	28.2	0	0.0	0.0
Total	110	100.0	57	51.8	51.8	0	0.0	0.0

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

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



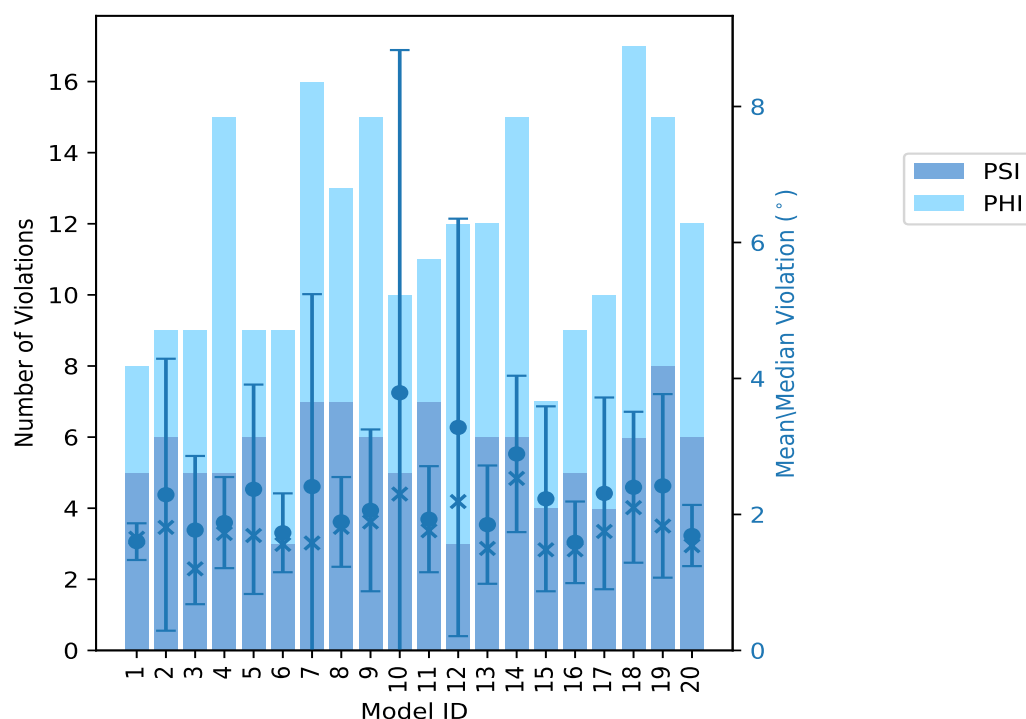
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	5	3	8	1.6	1.96	0.27	1.65
2	6	3	9	2.29	7.86	2.0	1.81
3	5	4	9	1.77	4.09	1.09	1.2
4	5	10	15	1.88	3.12	0.67	1.72
5	6	3	9	2.37	5.93	1.54	1.69
6	3	6	9	1.73	2.91	0.58	1.56
7	7	9	16	2.41	13.13	2.83	1.58
8	7	6	13	1.89	3.24	0.66	1.81
9	6	9	15	2.06	6.09	1.19	1.89
10	5	5	10	3.79	18.63	5.04	2.3
11	7	4	11	1.93	3.88	0.78	1.76
12	3	9	12	3.28	11.99	3.07	2.19
13	6	6	12	1.85	4.34	0.87	1.5
14	6	9	15	2.89	5.61	1.15	2.53
15	4	3	7	2.23	5.22	1.36	1.48
16	5	4	9	1.59	2.78	0.6	1.48
17	4	6	10	2.31	6.0	1.41	1.75
18	6	11	17	2.4	5.32	1.11	2.1
19	8	7	15	2.42	4.88	1.35	1.83
20	6	6	12	1.69	2.58	0.45	1.54

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
10	12	22	1	5.0
3	2	5	2	10.0
2	6	8	3	15.0
4	0	4	4	20.0
1	1	2	5	25.0
1	5	6	6	30.0
0	0	0	7	35.0
0	1	1	8	40.0
0	0	0	9	45.0
1	2	3	10	50.0
1	0	1	11	55.0

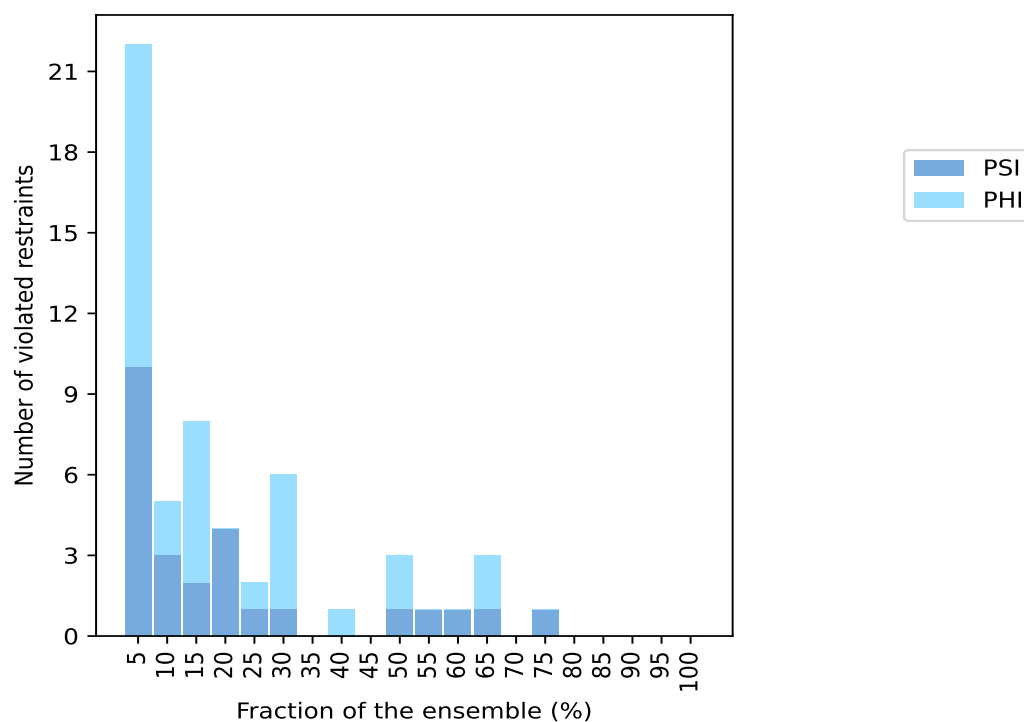
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
1	0	1	12	60.0
1	2	3	13	65.0
0	0	0	14	70.0
1	0	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

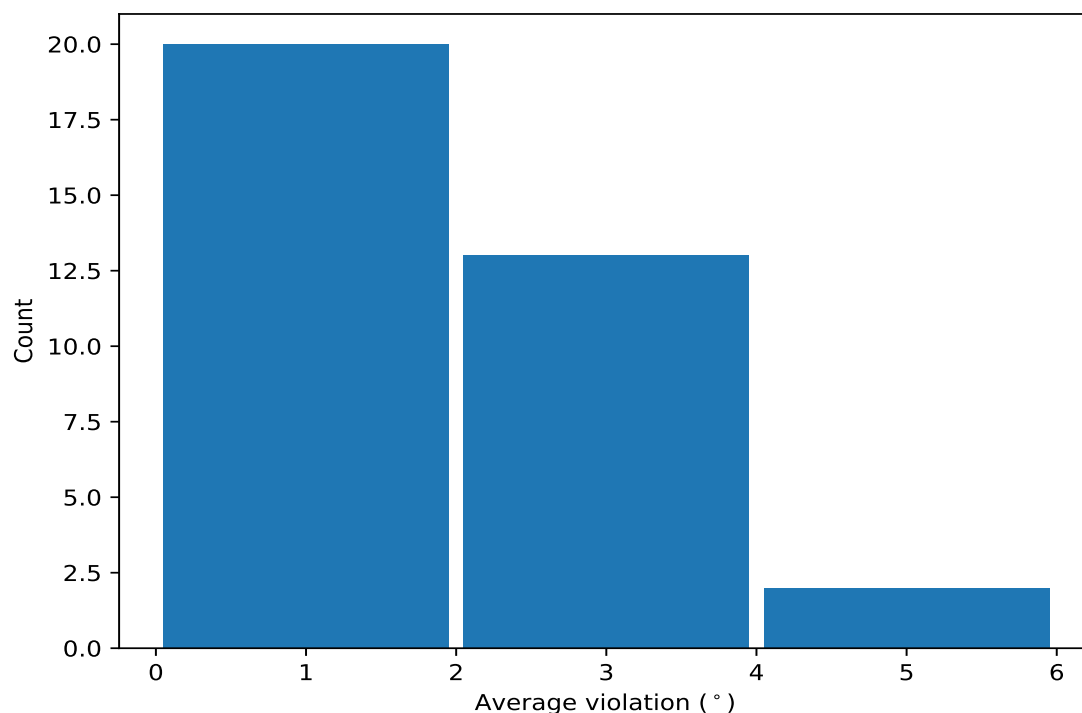


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	15	1.47	0.23	1.39
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	13	2.35	1.53	1.67
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	13	2.23	0.97	1.81
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	13	2.09	0.57	2.19
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	12	2.24	0.7	2.09
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	11	1.41	0.25	1.47
(1,52)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ILE:N	10	3.78	0.96	3.36
(1,28)	1:59:A:TRP:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	10	1.43	0.27	1.38
(1,94)	1:136:A:VAL:C	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	10	1.31	0.36	1.15
(1,44)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	8	1.74	0.33	1.62
(1,106)	1:153:A:LEU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	6	2.17	0.36	2.13
(1,87)	1:125:A:ASN:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	6	2.16	0.61	2.34
(1,50)	1:79:A:ARG:C	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	6	1.93	0.68	1.7
(1,43)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	6	1.53	0.54	1.24
(1,61)	1:92:A:VAL:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	6	1.34	0.19	1.34
(1,24)	1:49:A:TRP:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	6	1.3	0.24	1.27
(1,76)	1:108:A:GLY:C	1:109:A:SER:N	1:109:A:SER:CA	1:109:A:SER:C	5	4.98	4.23	3.1
(1,56)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:TYR:N	5	1.84	0.6	1.87
(1,19)	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	1:43:A:GLN:N	4	3.59	1.55	3.89
(1,42)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:ILE:N	4	2.74	0.44	2.77

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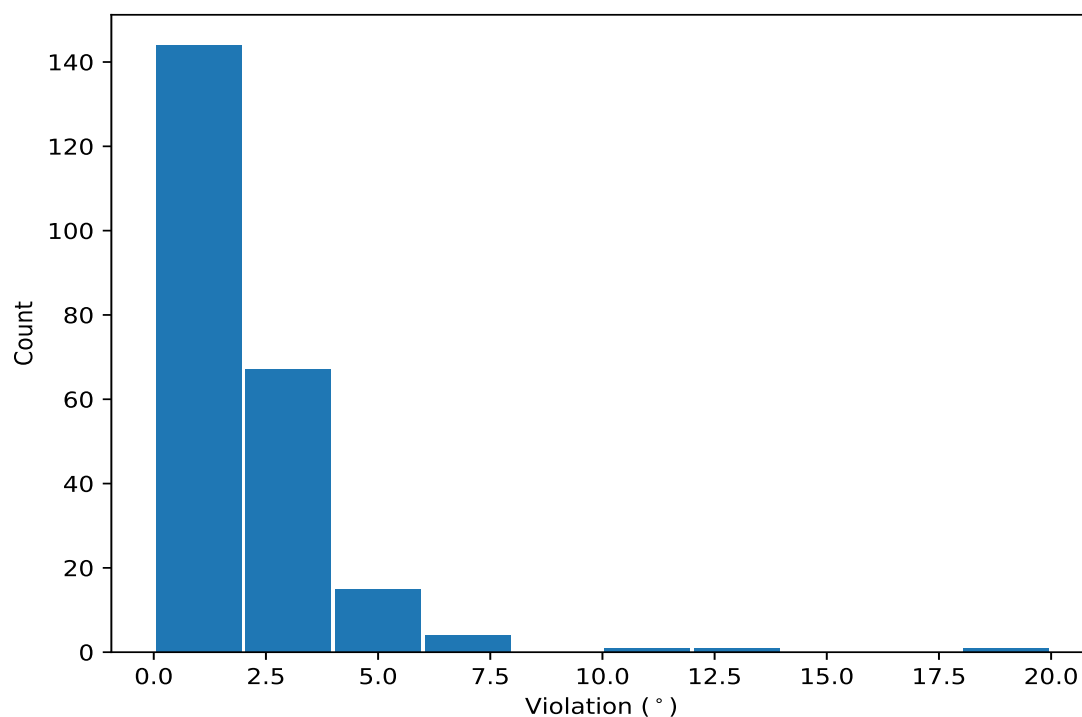
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,98)	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	1:141:A:VAL:N	4	1.8	0.56	1.85
(1,49)	1:79:A:ARG:N	1:79:A:ARG:CA	1:79:A:ARG:C	1:80:A:ASP:N	4	1.61	0.56	1.4
(1,18)	1:41:A:ASP:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	3	5.46	0.59	5.61
(1,103)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:LEU:N	3	2.75	1.48	1.93
(1,104)	1:152:A:GLU:C	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	3	2.13	0.83	1.69
(1,105)	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	1:154:A:LEU:N	3	1.8	0.29	1.95
(1,78)	1:110:A:SER:C	1:111:A:LYS:N	1:111:A:LYS:CA	1:111:A:LYS:C	3	1.79	0.82	1.28
(1,57)	1:86:A:TYR:C	1:87:A:VAL:N	1:87:A:VAL:CA	1:87:A:VAL:C	3	1.48	0.33	1.46
(1,66)	1:96:A:ASP:C	1:97:A:ASP:N	1:97:A:ASP:CA	1:97:A:ASP:C	3	1.38	0.48	1.09
(1,84)	1:121:A:SER:C	1:122:A:HIS:N	1:122:A:HIS:CA	1:122:A:HIS:C	3	1.32	0.19	1.41
(1,54)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:GLN:N	2	2.52	1.4	2.52
(1,36)	1:67:A:GLN:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	2	2.23	0.03	2.23
(1,34)	1:65:A:GLY:C	1:66:A:THR:N	1:66:A:THR:CA	1:66:A:THR:C	2	1.72	0.06	1.72
(1,62)	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	1:94:A:HIS:N	2	1.72	0.26	1.72
(1,37)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:GLN:N	2	1.54	0.42	1.54

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 (°)
(1,80)	1:111:A:LYS:C	1:112:A:VAL:N	1:112:A:VAL:CA	1:112:A:VAL:C	10	18.63
(1,76)	1:108:A:GLY:C	1:109:A:SER:N	1:109:A:SER:CA	1:109:A:SER:C	7	13.13
(1,12)	1:23:A:TYR:C	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	12	11.99
(1,74)	1:104:A:TYR:C	1:105:A:GLU:N	1:105:A:GLU:CA	1:105:A:GLU:C	2	7.86
(1,13)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:THR:N	12	6.68
(1,18)	1:41:A:ASP:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	9	6.09
(1,52)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ILE:N	17	6.0
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	5	5.93
(1,18)	1:41:A:ASP:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	14	5.61
(1,19)	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	1:43:A:GLN:N	18	5.32
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	15	5.22
(1,52)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ILE:N	19	4.88
(1,103)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:LEU:N	19	4.82
(1,76)	1:108:A:GLY:C	1:109:A:SER:N	1:109:A:SER:CA	1:109:A:SER:C	12	4.82
(1,18)	1:41:A:ASP:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	18	4.68
(1,19)	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	1:43:A:GLN:N	14	4.57
(1,7)	1:13:A:PRO:N	1:13:A:PRO:CA	1:13:A:PRO:C	1:14:A:ASP:N	13	4.34
(1,52)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ILE:N	5	4.26
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	14	4.21
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	19	4.19
(1,89)	1:126:A:ILE:C	1:127:A:PHE:N	1:127:A:PHE:CA	1:127:A:PHE:C	10	4.14
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	3	4.09
(1,54)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:GLN:N	19	3.91
(1,52)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ILE:N	11	3.88
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	17	3.76
(1,52)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ILE:N	3	3.43
(1,104)	1:152:A:GLU:C	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	19	3.29
(1,52)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ILE:N	14	3.29
(1,50)	1:79:A:ARG:C	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	14	3.28
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	14	3.27
(1,52)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ILE:N	10	3.26
(1,42)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:ILE:N	8	3.24
(1,19)	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	1:43:A:GLN:N	9	3.21
(1,52)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ILE:N	4	3.12
(1,76)	1:108:A:GLY:C	1:109:A:SER:N	1:109:A:SER:CA	1:109:A:SER:C	4	3.1
(1,42)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:ILE:N	7	3.08
(1,87)	1:125:A:ASN:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	14	2.98
(1,68)	1:98:A:GLY:C	1:99:A:VAL:N	1:99:A:VAL:CA	1:99:A:VAL:C	18	2.97
(1,78)	1:110:A:SER:C	1:111:A:LYS:N	1:111:A:LYS:CA	1:111:A:LYS:C	18	2.95
(1,106)	1:153:A:LEU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	15	2.91
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	6	2.91
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	18	2.88
(1,52)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ILE:N	18	2.87
(1,52)	1:83:A:HIS:N	1:83:A:HIS:CA	1:83:A:HIS:C	1:84:A:ILE:N	8	2.86
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	12	2.82
(1,77)	1:109:A:SER:N	1:109:A:SER:CA	1:109:A:SER:C	1:110:A:SER:N	7	2.81
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	16	2.78

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,76)	1:108:A:GLY:C	1:109:A:SER:N	1:109:A:SER:CA	1:109:A:SER:C	8	2.66
(1,43)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	4	2.6
(1,56)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:TYR:N	13	2.59
(1,109)	1:156:A:CYS:N	1:156:A:CYS:CA	1:156:A:CYS:C	1:157:A:LEU:N	20	2.58
(1,49)	1:79:A:ARG:N	1:79:A:ARG:CA	1:79:A:ARG:C	1:80:A:ASP:N	14	2.53
(1,42)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:ILE:N	10	2.46
(1,98)	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	1:141:A:VAL:N	7	2.44
(1,87)	1:125:A:ASN:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	10	2.44
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	6	2.42
(1,87)	1:125:A:ASN:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	19	2.4
(1,56)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:TYR:N	16	2.39
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	11	2.39
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	14	2.33
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	20	2.31
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	4	2.31
(1,44)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	18	2.31
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	11	2.3
(1,87)	1:125:A:ASN:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	13	2.28
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	11	2.28
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	12	2.28
(1,36)	1:67:A:GLN:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	17	2.26
(1,33)	1:63:A:ASP:N	1:63:A:ASP:CA	1:63:A:ASP:C	1:64:A:LEU:N	14	2.26
(1,98)	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	1:141:A:VAL:N	5	2.24
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	4	2.24
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	18	2.22
(1,6)	1:11:A:THR:C	1:12:A:ILE:N	1:12:A:ILE:CA	1:12:A:ILE:C	14	2.22
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	15	2.21
(1,36)	1:67:A:GLN:C	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	20	2.2
(1,106)	1:153:A:LEU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	12	2.19
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	12	2.19
(1,44)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	4	2.19
(1,94)	1:136:A:VAL:C	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	10	2.17
(1,42)	1:73:A:ILE:N	1:73:A:ILE:CA	1:73:A:ILE:C	1:74:A:ILE:N	11	2.17
(1,106)	1:153:A:LEU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	9	2.15
(1,50)	1:79:A:ARG:C	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	8	2.15
(1,106)	1:153:A:LEU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	2	2.12
(1,75)	1:105:A:GLU:N	1:105:A:GLU:CA	1:105:A:GLU:C	1:106:A:GLU:N	18	2.1
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	9	2.08
(1,105)	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	1:154:A:LEU:N	2	2.05
(1,66)	1:96:A:ASP:C	1:97:A:ASP:N	1:97:A:ASP:CA	1:97:A:ASP:C	14	2.05
(1,92)	1:135:A:TYR:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	14	2.03
(1,28)	1:59:A:TRP:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	9	2.02
(1,62)	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	1:94:A:HIS:N	6	1.97
(1,79)	1:111:A:LYS:N	1:111:A:LYS:CA	1:111:A:LYS:C	1:112:A:VAL:N	8	1.96
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	1	1.96
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	5	1.96
(1,37)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:GLN:N	19	1.96
(1,105)	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	1:154:A:LEU:N	9	1.95
(1,50)	1:79:A:ARG:C	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	18	1.95
(1,103)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:LEU:N	9	1.93
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	17	1.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	13	1.9
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	9	1.89
(1,57)	1:86:A:TYR:C	1:87:A:VAL:N	1:87:A:VAL:CA	1:87:A:VAL:C	16	1.89
(1,45)	1:76:A:GLN:N	1:76:A:GLN:CA	1:76:A:GLN:C	1:77:A:GLY:N	8	1.88
(1,56)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:TYR:N	7	1.87
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	20	1.85
(1,87)	1:125:A:ASN:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	7	1.84
(1,44)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	17	1.84
(1,43)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	1	1.84
(1,106)	1:153:A:LEU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	4	1.83
(1,106)	1:153:A:LEU:C	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	7	1.83
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	19	1.83
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	2	1.82
(1,30)	1:60:A:LEU:C	1:61:A:GLN:N	1:61:A:GLN:CA	1:61:A:GLN:C	20	1.82
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	2	1.81
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	8	1.81
(1,34)	1:65:A:GLY:C	1:66:A:THR:N	1:66:A:THR:CA	1:66:A:THR:C	18	1.78
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	11	1.76
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	1	1.76
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	6	1.73
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	4	1.72
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	13	1.71
(1,104)	1:152:A:GLU:C	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	4	1.69
(1,24)	1:49:A:TRP:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	5	1.69
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	1	1.67
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	11	1.67
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	3	1.67
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	18	1.67
(1,34)	1:65:A:GLY:C	1:66:A:THR:N	1:66:A:THR:CA	1:66:A:THR:C	17	1.66
(1,60)	1:91:A:LYS:C	1:92:A:VAL:N	1:92:A:VAL:CA	1:92:A:VAL:C	18	1.65
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	8	1.64
(1,44)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	1	1.64
(1,94)	1:136:A:VAL:C	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	17	1.62
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	5	1.6
(1,61)	1:92:A:VAL:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	9	1.6
(1,44)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	7	1.6
(1,28)	1:59:A:TRP:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	14	1.6
(1,94)	1:136:A:VAL:C	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	12	1.57
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	1	1.57
(1,28)	1:59:A:TRP:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	7	1.57
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	20	1.56
(1,49)	1:79:A:ARG:N	1:79:A:ARG:CA	1:79:A:ARG:C	1:80:A:ASP:N	8	1.56
(1,28)	1:59:A:TRP:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	6	1.56
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	18	1.55
(1,61)	1:92:A:VAL:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	20	1.53
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	13	1.52
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	19	1.52
(1,44)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	20	1.51
(1,103)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:LEU:N	16	1.49
(1,84)	1:121:A:SER:C	1:122:A:HIS:N	1:122:A:HIS:CA	1:122:A:HIS:C	13	1.49
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	12	1.49

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	15	1.48
(1,24)	1:49:A:TRP:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	16	1.48
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	13	1.47
(1,62)	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	1:94:A:HIS:N	9	1.46
(1,57)	1:86:A:TYR:C	1:87:A:VAL:N	1:87:A:VAL:CA	1:87:A:VAL:C	18	1.46
(1,98)	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	1:141:A:VAL:N	20	1.45
(1,50)	1:79:A:ARG:C	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	10	1.45
(1,44)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	9	1.44
(1,61)	1:92:A:VAL:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	17	1.42
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	13	1.42
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	4	1.42
(1,84)	1:121:A:SER:C	1:122:A:HIS:N	1:122:A:HIS:CA	1:122:A:HIS:C	9	1.41
(1,105)	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	1:154:A:LEU:N	17	1.4
(1,104)	1:152:A:GLU:C	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	7	1.4
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	11	1.39
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	15	1.39
(1,28)	1:59:A:TRP:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	19	1.39
(1,64)	1:94:A:HIS:N	1:94:A:HIS:CA	1:94:A:HIS:C	1:95:A:SER:N	19	1.38
(1,50)	1:79:A:ARG:C	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	3	1.38
(1,28)	1:59:A:TRP:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	18	1.38
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	9	1.37
(1,28)	1:59:A:TRP:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	15	1.37
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	7	1.36
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	13	1.36
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	2	1.35
(1,50)	1:79:A:ARG:C	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	11	1.35
(1,44)	1:74:A:ILE:C	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	6	1.35
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	1	1.35
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	8	1.35
(1,28)	1:59:A:TRP:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	12	1.32
(1,24)	1:49:A:TRP:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	19	1.32
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	5	1.29
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	6	1.29
(1,94)	1:136:A:VAL:C	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	4	1.28
(1,78)	1:110:A:SER:C	1:111:A:LYS:N	1:111:A:LYS:CA	1:111:A:LYS:C	4	1.28
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	5	1.27
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	8	1.27
(1,56)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:TYR:N	20	1.27
(1,82)	1:119:A:ASN:C	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	9	1.25
(1,61)	1:92:A:VAL:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	6	1.25
(1,19)	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	1:43:A:GLN:N	2	1.25
(1,43)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	19	1.24
(1,43)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	20	1.24
(1,49)	1:79:A:ARG:N	1:79:A:ARG:CA	1:79:A:ARG:C	1:80:A:ASP:N	10	1.23
(1,43)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	17	1.23
(1,61)	1:92:A:VAL:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	4	1.22
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	7	1.21
(1,24)	1:49:A:TRP:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	2	1.21
(1,76)	1:108:A:GLY:C	1:109:A:SER:N	1:109:A:SER:CA	1:109:A:SER:C	3	1.2
(1,94)	1:136:A:VAL:C	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	7	1.19
(1,65)	1:94:A:HIS:C	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	19	1.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,78)	1:110:A:SER:C	1:111:A:LYS:N	1:111:A:LYS:CA	1:111:A:LYS:C	14	1.15
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	7	1.13
(1,54)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:GLN:N	5	1.12
(1,49)	1:79:A:ARG:N	1:79:A:ARG:CA	1:79:A:ARG:C	1:80:A:ASP:N	18	1.12
(1,94)	1:136:A:VAL:C	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	8	1.11
(1,83)	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	1:121:A:SER:N	4	1.11
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	10	1.11
(1,37)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:GLN:N	2	1.11
(1,16)	1:38:A:GLY:C	1:39:A:ARG:N	1:39:A:ARG:CA	1:39:A:ARG:C	16	1.11
(1,66)	1:96:A:ASP:C	1:97:A:ASP:N	1:97:A:ASP:CA	1:97:A:ASP:C	7	1.09
(1,57)	1:86:A:TYR:C	1:87:A:VAL:N	1:87:A:VAL:CA	1:87:A:VAL:C	13	1.09
(1,39)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:VAL:N	16	1.09
(1,98)	1:140:A:PRO:N	1:140:A:PRO:CA	1:140:A:PRO:C	1:141:A:VAL:N	3	1.07
(1,55)	1:84:A:ILE:C	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	7	1.07
(1,56)	1:85:A:GLN:N	1:85:A:GLN:CA	1:85:A:GLN:C	1:86:A:TYR:N	11	1.06
(1,28)	1:59:A:TRP:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	8	1.06
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	16	1.05
(1,84)	1:121:A:SER:C	1:122:A:HIS:N	1:122:A:HIS:CA	1:122:A:HIS:C	6	1.05
(1,94)	1:136:A:VAL:C	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	1	1.04
(1,94)	1:136:A:VAL:C	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	19	1.04
(1,91)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:ARG:N	3	1.04
(1,61)	1:92:A:VAL:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	12	1.04
(1,24)	1:49:A:TRP:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	4	1.04
(1,94)	1:136:A:VAL:C	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	11	1.03
(1,94)	1:136:A:VAL:C	1:137:A:ARG:N	1:137:A:ARG:CA	1:137:A:ARG:C	13	1.03
(1,28)	1:59:A:TRP:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	3	1.03
(1,24)	1:49:A:TRP:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	12	1.03
(1,29)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:GLN:N	10	1.02
(1,107)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:GLY:N	20	1.01
(1,87)	1:125:A:ASN:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	9	1.01
(1,43)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:THR:N	15	1.01
(1,66)	1:96:A:ASP:C	1:97:A:ASP:N	1:97:A:ASP:CA	1:97:A:ASP:C	16	1.0
(1,26)	1:54:A:ASN:C	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	3	1.0