



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 05:00 AM UTC

PDB ID : 2LXN / pdb_00002lxn
BMRB ID : 17935
Title : Solution NMR structure of glutamine amido transferase subunit of gaunosine monophosphate synthetase from Methanocaldococcus jannaschii
Authors : Ali, R.; Kumar, S.; Balaram, H.; Sarma, S.P.
Deposited on : 2012-08-30

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

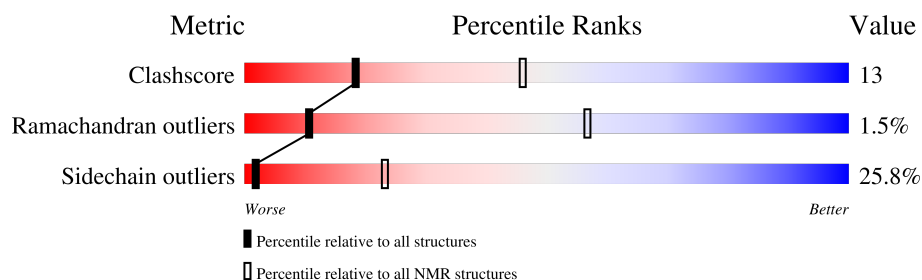
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 56%.

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	188	60% 32% 5% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:163, A:170-A:188 (182)	0.39	18

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 2 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2970 atoms, of which 1491 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GMP synthase [glutamine-hydrolyzing] subunit A.

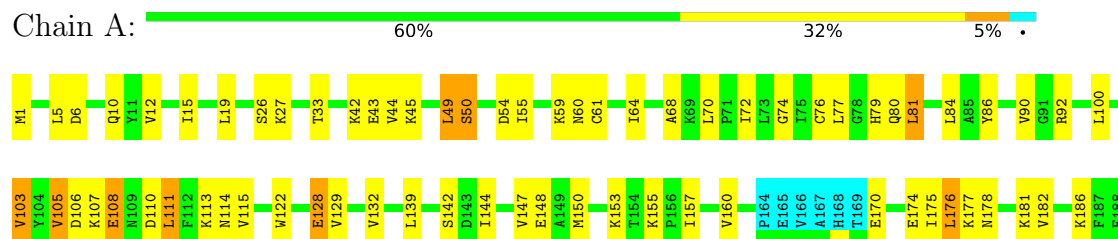
Mol	Chain	Residues	Atoms						Trace
1	A	188	Total	C	H	N	O	S	0
			2970	948	1491	250	274	7	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A

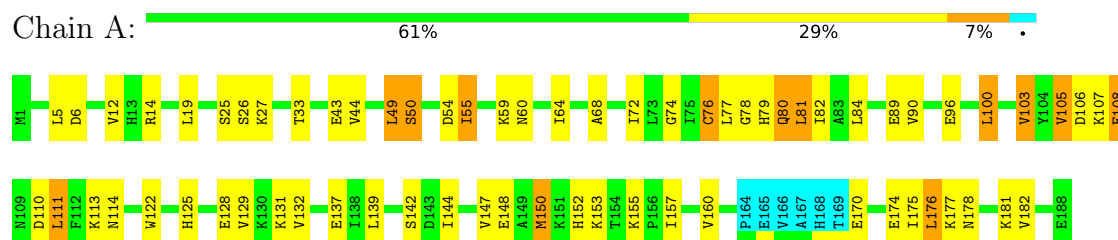


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

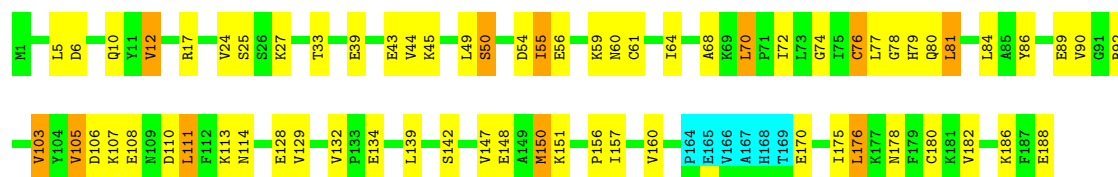
- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



4.2.2 Score per residue for model 2

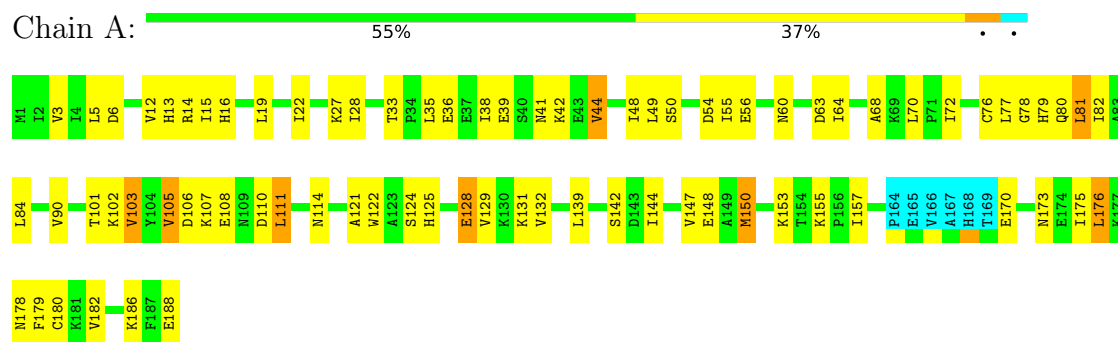
- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A





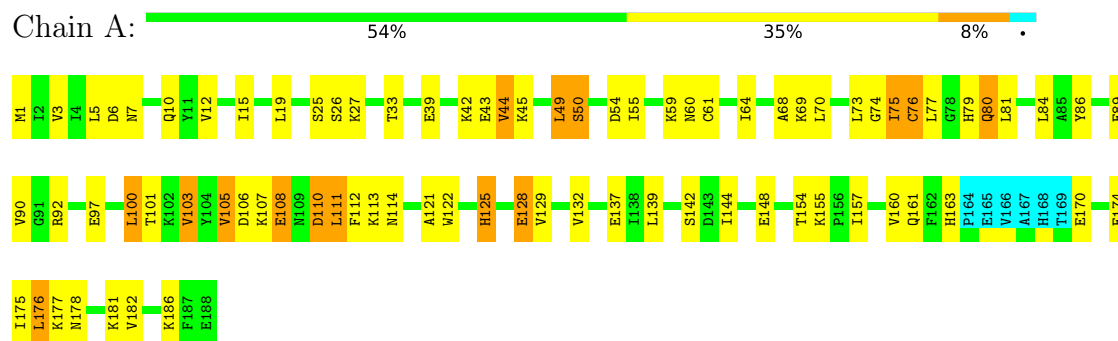
4.2.3 Score per residue for model 3

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



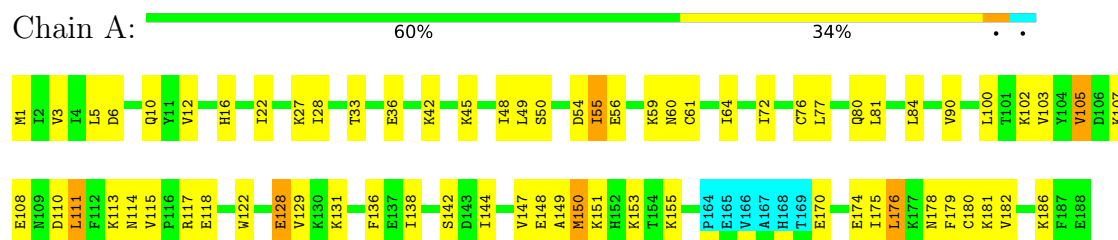
4.2.4 Score per residue for model 4

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



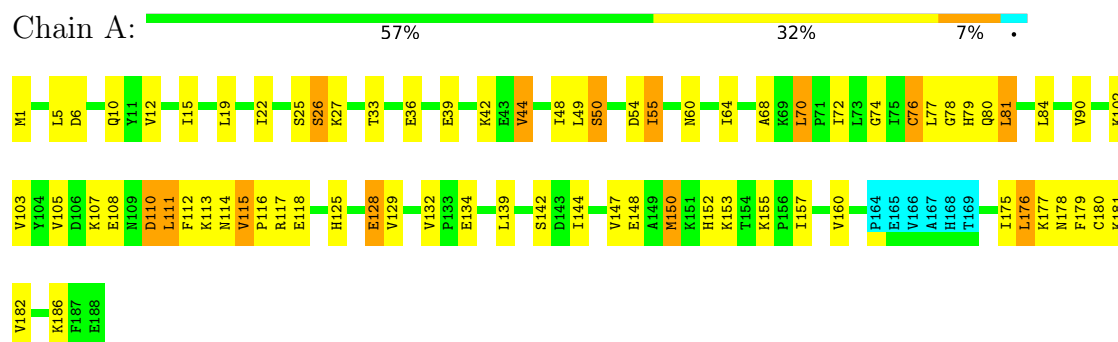
4.2.5 Score per residue for model 5

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



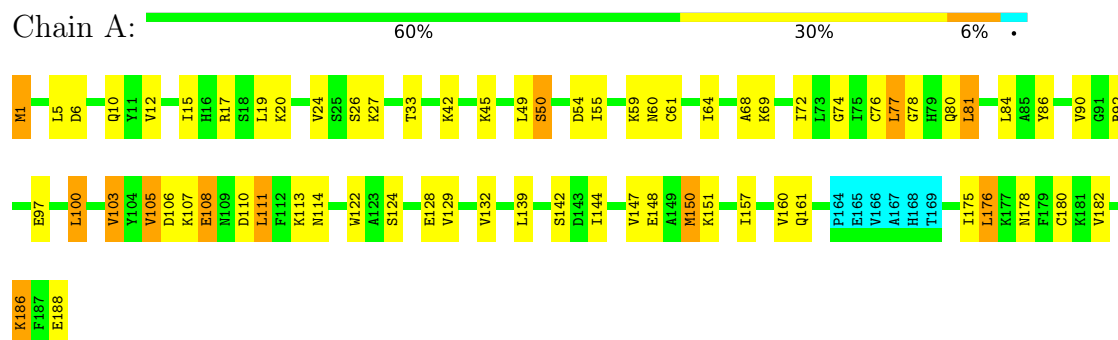
4.2.6 Score per residue for model 6

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



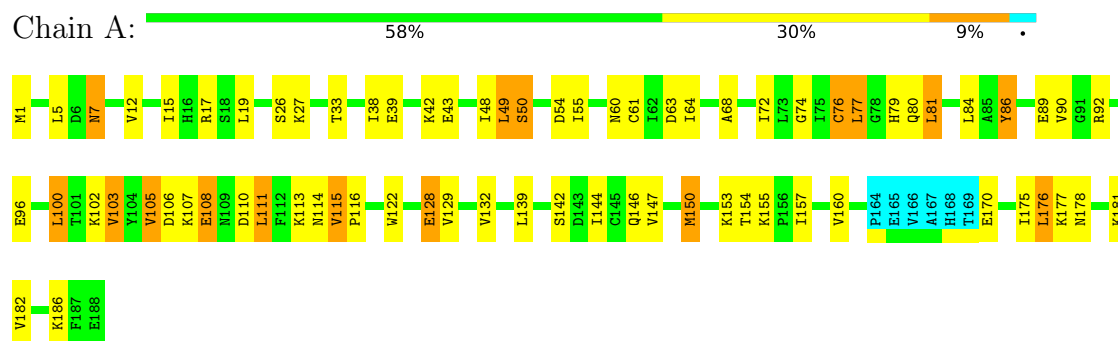
4.2.7 Score per residue for model 7

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



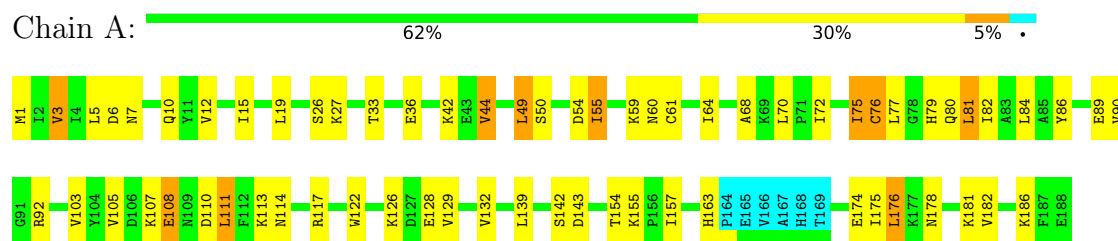
4.2.8 Score per residue for model 8

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



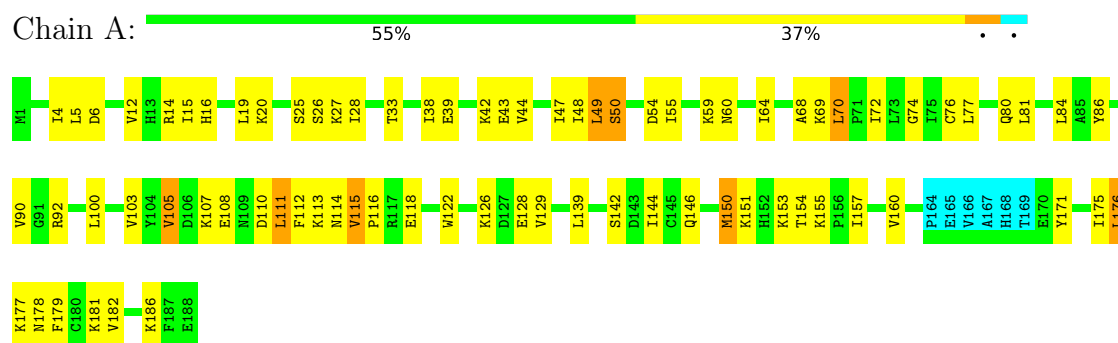
4.2.9 Score per residue for model 9

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



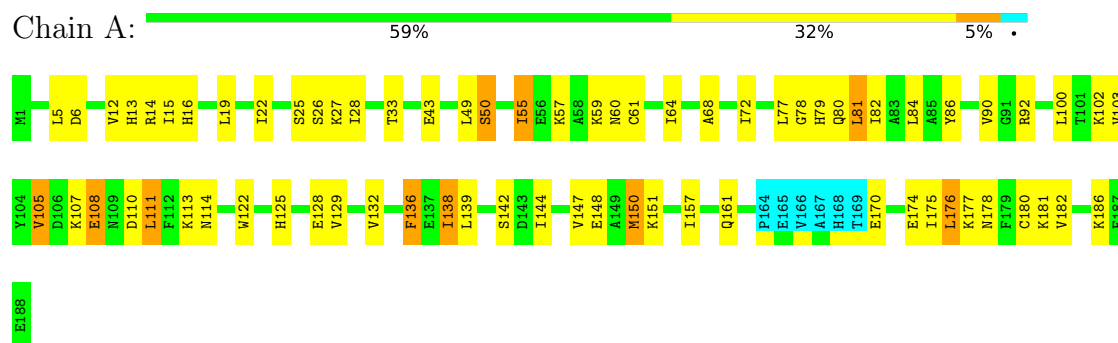
4.2.10 Score per residue for model 10

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



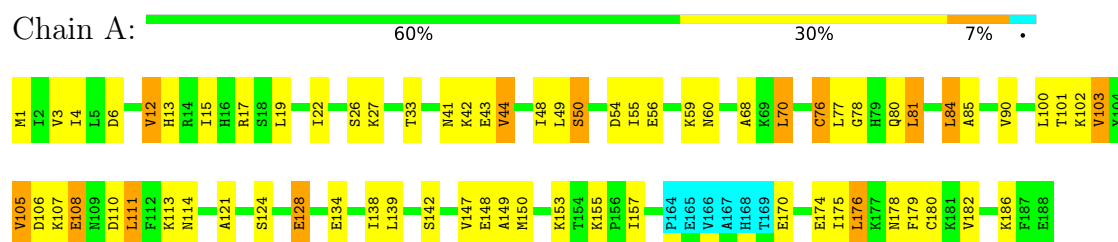
4.2.11 Score per residue for model 11

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



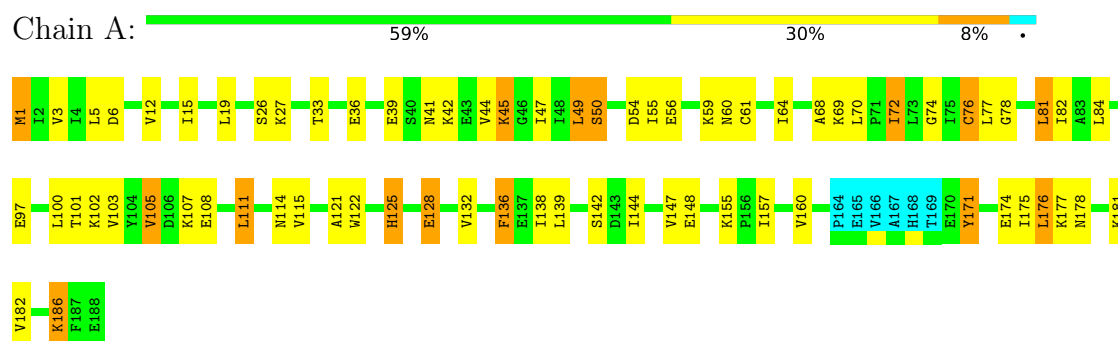
4.2.12 Score per residue for model 12

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



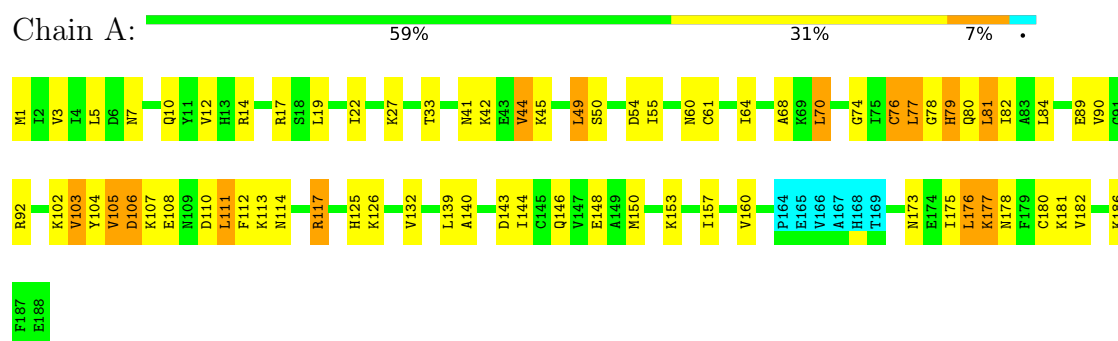
4.2.13 Score per residue for model 13

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



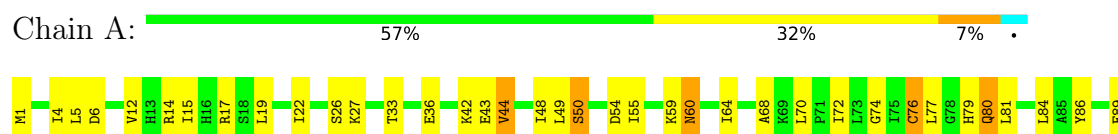
4.2.14 Score per residue for model 14

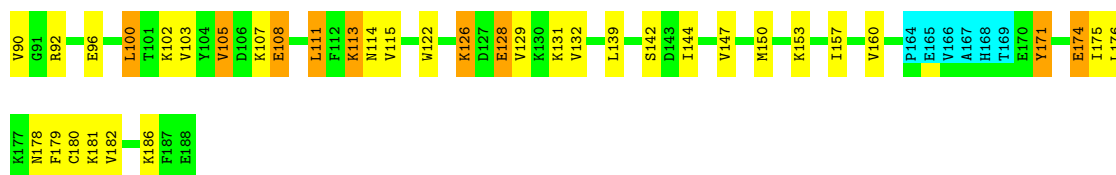
- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



4.2.15 Score per residue for model 15

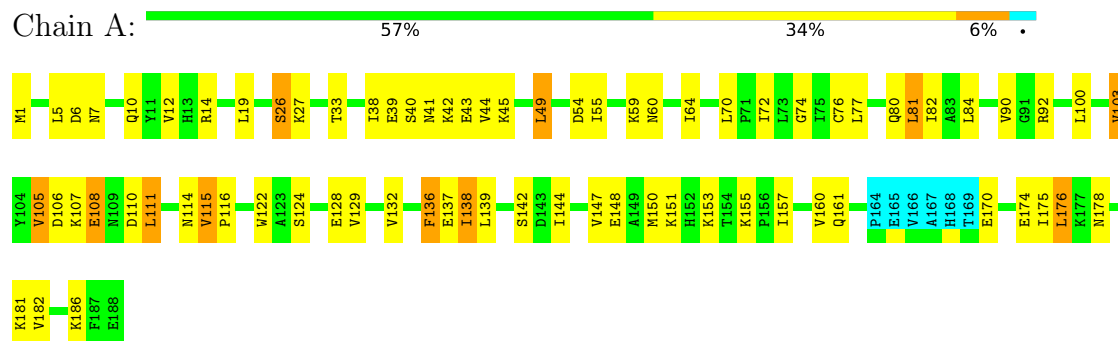
- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A





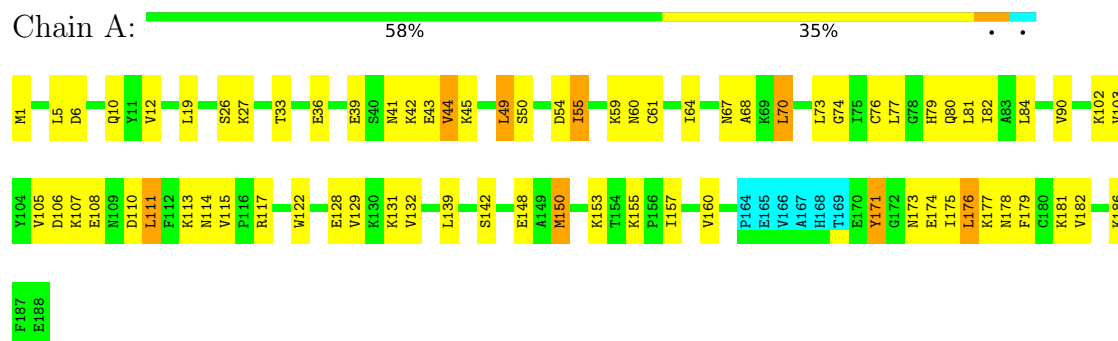
4.2.16 Score per residue for model 16

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



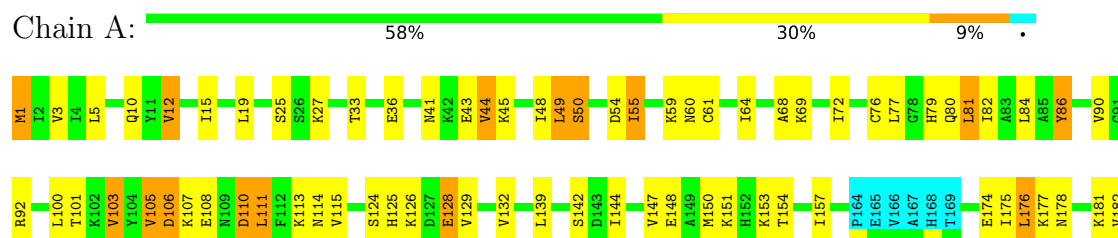
4.2.17 Score per residue for model 17

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



4.2.18 Score per residue for model 18 (medoid)

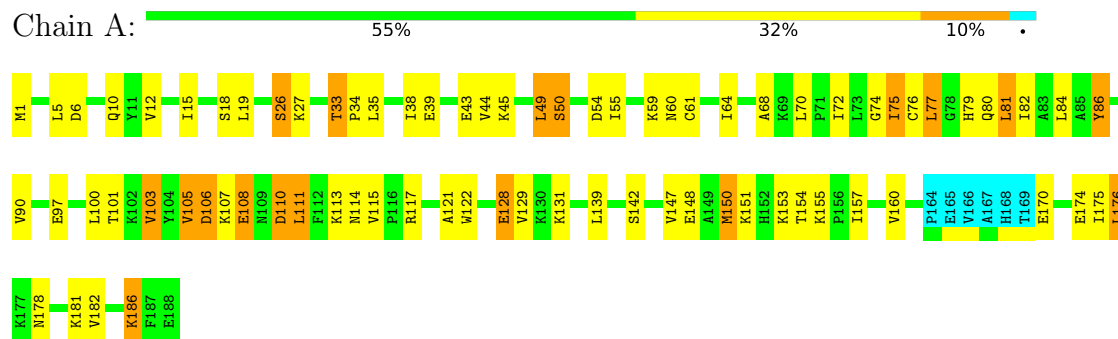
- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A





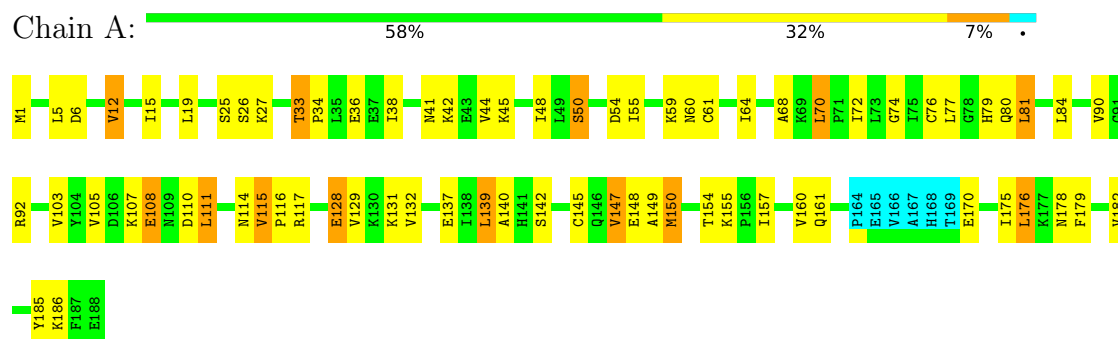
4.2.19 Score per residue for model 19

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



4.2.20 Score per residue for model 20

- Molecule 1: GMP synthase [glutamine-hydrolyzing] subunit A



5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CCPN	structure solution	
Cyana-3.0	structure solution	
TALOS+	geometry optimization	
TALOS+	structure solution	
Procheck	geometry optimization	
Procheck	structure solution	
ProcheckNMR	geometry optimization	
ProcheckNMR	structure solution	
CSI	structure solution	
MOLMOL	structure solution	
PSVS	structure solution	
PSVS	geometry optimization	
Cyana-3.0	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	1455
Number of shifts mapped to atoms	1454
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	56%

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	1434	1450	1452	38±4
All	All	28680	29000	29040	757

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LEU:HD21	1:A:49:LEU:HD22	0.88	1.46	4	4
1:A:55:ILE:HD11	1:A:77:LEU:HD21	0.86	1.47	5	3
1:A:68:ALA:HB1	1:A:157:ILE:HD11	0.85	1.48	20	18
1:A:5:LEU:HD11	1:A:64:ILE:HD11	0.84	1.47	4	17
1:A:84:LEU:C	1:A:84:LEU:HD22	0.84	1.98	12	1
1:A:111:LEU:HD12	1:A:175:ILE:HG23	0.83	1.50	14	20
1:A:44:VAL:HG23	1:A:70:LEU:HD22	0.81	1.52	10	4
1:A:49:LEU:HD11	1:A:81:LEU:HD13	0.79	1.54	11	7
1:A:64:ILE:HG23	1:A:72:ILE:HD13	0.72	1.58	16	13
1:A:55:ILE:HG21	1:A:81:LEU:HD12	0.72	1.61	11	2
1:A:49:LEU:HD21	1:A:81:LEU:HD13	0.67	1.66	13	1
1:A:44:VAL:HG23	1:A:70:LEU:HD13	0.67	1.65	13	6
1:A:55:ILE:HG22	1:A:61:CYS:HB3	0.66	1.68	11	4
1:A:178:ASN:O	1:A:182:VAL:HG23	0.65	1.92	5	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:ALA:HB3	1:A:149:ALA:HB3	0.64	1.68	20	1
1:A:19:LEU:HD13	1:A:26:SER:OG	0.63	1.94	11	2
1:A:132:VAL:HG23	1:A:136:PHE:CE2	0.63	2.29	13	3
1:A:49:LEU:HD22	1:A:78:GLY:HA2	0.63	1.71	1	8
1:A:100:LEU:O	1:A:144:ILE:HD12	0.63	1.93	11	6
1:A:12:VAL:HG22	1:A:50:SER:CB	0.62	2.24	11	13
1:A:68:ALA:CB	1:A:157:ILE:HD11	0.62	2.25	18	11
1:A:55:ILE:CG1	1:A:77:LEU:HD11	0.61	2.26	5	3
1:A:79:HIS:CD2	1:A:129:VAL:HG23	0.60	2.31	6	11
1:A:12:VAL:HG13	1:A:15:ILE:HD12	0.60	1.72	7	8
1:A:55:ILE:HB	1:A:77:LEU:HD11	0.60	1.73	12	1
1:A:67:ASN:O	1:A:70:LEU:HD12	0.60	1.97	17	1
1:A:86:TYR:OH	1:A:154:THR:HG21	0.60	1.96	18	3
1:A:47:ILE:HB	1:A:72:ILE:HD12	0.58	1.75	13	1
1:A:55:ILE:CD1	1:A:77:LEU:HD21	0.58	2.28	17	3
1:A:77:LEU:O	1:A:77:LEU:HD13	0.58	1.98	5	5
1:A:129:VAL:HG21	1:A:150:MET:HE1	0.58	1.75	7	1
1:A:80:GLN:OE1	1:A:90:VAL:HG11	0.58	1.99	14	3
1:A:15:ILE:HD13	1:A:48:ILE:HG21	0.58	1.74	18	3
1:A:112:PHE:CZ	1:A:140:ALA:HB2	0.58	2.33	14	1
1:A:84:LEU:C	1:A:84:LEU:CD2	0.58	2.72	12	1
1:A:5:LEU:CD2	1:A:49:LEU:HD22	0.58	2.29	18	4
1:A:55:ILE:HG12	1:A:77:LEU:HD12	0.57	1.75	7	3
1:A:19:LEU:HD23	1:A:26:SER:HB3	0.57	1.75	20	8
1:A:82:ILE:HG21	1:A:157:ILE:HG21	0.57	1.77	16	2
1:A:108:GLU:HB2	1:A:139:LEU:HD13	0.57	1.76	15	18
1:A:110:ASP:HB3	1:A:111:LEU:HD23	0.56	1.77	1	15
1:A:68:ALA:HB1	1:A:157:ILE:CD1	0.56	2.29	9	2
1:A:171:TYR:O	1:A:171:TYR:CG	0.56	2.59	13	1
1:A:108:GLU:HG2	1:A:139:LEU:HD22	0.56	1.76	15	10
1:A:128:GLU:HB2	1:A:147:VAL:HG21	0.56	1.77	5	12
1:A:5:LEU:HD11	1:A:64:ILE:CG1	0.56	2.30	14	6
1:A:19:LEU:HD23	1:A:26:SER:CB	0.56	2.31	19	8
1:A:111:LEU:HD12	1:A:175:ILE:CG2	0.56	2.30	4	16
1:A:49:LEU:HD22	1:A:78:GLY:CA	0.56	2.31	11	4
1:A:15:ILE:HD13	1:A:48:ILE:CG2	0.55	2.32	18	4
1:A:80:GLN:CG	1:A:90:VAL:HG21	0.55	2.31	20	11
1:A:112:PHE:CE2	1:A:175:ILE:HD11	0.55	2.36	6	1
1:A:171:TYR:CG	1:A:171:TYR:O	0.55	2.60	15	2
1:A:5:LEU:HD11	1:A:64:ILE:CD1	0.55	2.27	4	10
1:A:49:LEU:CD1	1:A:81:LEU:HD13	0.55	2.31	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:VAL:CG2	1:A:150:MET:HE1	0.55	2.32	7	2
1:A:19:LEU:HD22	1:A:180:CYS:CB	0.55	2.32	14	1
1:A:90:VAL:HG13	1:A:128:GLU:C	0.55	2.27	18	12
1:A:103:VAL:HG12	1:A:106:ASP:OD2	0.55	2.02	8	1
1:A:138:ILE:HD11	1:A:147:VAL:HG12	0.55	1.79	16	2
1:A:5:LEU:HD21	1:A:49:LEU:CD2	0.54	2.28	4	6
1:A:12:VAL:HG22	1:A:50:SER:HB2	0.54	1.78	4	4
1:A:61:CYS:HA	1:A:64:ILE:HD12	0.54	1.79	5	10
1:A:55:ILE:HG12	1:A:81:LEU:HD12	0.54	1.78	16	6
1:A:108:GLU:CG	1:A:139:LEU:HD22	0.54	2.33	2	14
1:A:15:ILE:O	1:A:19:LEU:HD13	0.54	2.02	4	6
1:A:55:ILE:HG13	1:A:77:LEU:HD11	0.53	1.80	17	3
1:A:100:LEU:O	1:A:144:ILE:HD13	0.53	2.02	13	4
1:A:139:LEU:HD11	1:A:151:LYS:HB2	0.53	1.79	16	5
1:A:19:LEU:HD22	1:A:180:CYS:HB2	0.53	1.80	14	3
1:A:115:VAL:HG22	1:A:116:PRO:HD2	0.53	1.81	20	5
1:A:81:LEU:HD23	1:A:82:ILE:N	0.53	2.19	1	4
1:A:3:VAL:CG2	1:A:44:VAL:HG11	0.53	2.33	3	6
1:A:125:HIS:CE1	1:A:144:ILE:HG22	0.53	2.39	6	5
1:A:15:ILE:HG21	1:A:48:ILE:HG21	0.53	1.81	20	4
1:A:55:ILE:HG22	1:A:80:GLN:OE1	0.53	2.04	1	1
1:A:74:GLY:O	1:A:160:VAL:HG22	0.53	2.03	19	14
1:A:115:VAL:HG22	1:A:174:GLU:HG2	0.52	1.81	13	2
1:A:68:ALA:CA	1:A:157:ILE:HD11	0.52	2.34	6	3
1:A:68:ALA:HA	1:A:157:ILE:HD11	0.52	1.82	6	3
1:A:139:LEU:HD11	1:A:151:LYS:CB	0.52	2.35	11	5
1:A:129:VAL:HG21	1:A:150:MET:HE2	0.52	1.81	11	4
1:A:55:ILE:HG21	1:A:84:LEU:CD2	0.52	2.34	15	2
1:A:49:LEU:HD23	1:A:50:SER:O	0.52	2.05	2	4
1:A:5:LEU:HD11	1:A:64:ILE:HG12	0.52	1.81	18	2
1:A:1:MET:H1	1:A:186:LYS:HD3	0.51	1.65	19	4
1:A:55:ILE:HD11	1:A:81:LEU:HD12	0.51	1.82	18	3
1:A:55:ILE:HD13	1:A:84:LEU:CD2	0.51	2.36	5	4
1:A:55:ILE:HG21	1:A:84:LEU:HD21	0.51	1.82	15	3
1:A:80:GLN:HG3	1:A:90:VAL:HG21	0.50	1.82	5	9
1:A:79:HIS:HA	1:A:82:ILE:HD12	0.50	1.83	17	1
1:A:41:ASN:O	1:A:44:VAL:HG13	0.50	2.07	17	3
1:A:61:CYS:SG	1:A:84:LEU:HD11	0.50	2.47	20	1
1:A:24:VAL:HG21	1:A:180:CYS:SG	0.50	2.47	2	2
1:A:103:VAL:HG12	1:A:106:ASP:OD1	0.50	2.07	2	10
1:A:80:GLN:CD	1:A:90:VAL:HG11	0.50	2.32	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:LEU:HD21	1:A:64:ILE:HD13	0.49	1.84	4	1
1:A:100:LEU:HD12	1:A:100:LEU:O	0.49	2.06	1	1
1:A:7:ASN:OD1	1:A:49:LEU:HD11	0.49	2.07	14	2
1:A:22:ILE:HD13	1:A:180:CYS:SG	0.49	2.48	11	6
1:A:154:THR:HG23	1:A:155:LYS:HG2	0.49	1.84	10	3
1:A:45:LYS:HG2	1:A:186:LYS:HZ1	0.49	1.68	19	1
1:A:73:LEU:CD2	1:A:176:LEU:HD22	0.48	2.38	4	1
1:A:90:VAL:HG22	1:A:129:VAL:HA	0.48	1.85	9	2
1:A:171:TYR:CE2	1:A:175:ILE:HD11	0.48	2.43	13	1
1:A:5:LEU:HD12	1:A:60:ASN:OD1	0.48	2.07	15	1
1:A:41:ASN:O	1:A:44:VAL:HG22	0.48	2.08	3	2
1:A:82:ILE:CG2	1:A:157:ILE:HG21	0.48	2.38	11	3
1:A:12:VAL:HG22	1:A:50:SER:OG	0.48	2.07	18	6
1:A:47:ILE:CG2	1:A:72:ILE:HD12	0.48	2.39	10	2
1:A:75:ILE:HD12	1:A:163:HIS:CE1	0.48	2.43	4	1
1:A:7:ASN:CG	1:A:55:ILE:HD12	0.48	2.33	9	1
1:A:125:HIS:NE2	1:A:144:ILE:HG22	0.48	2.23	4	3
1:A:5:LEU:CD1	1:A:64:ILE:HD11	0.48	2.36	13	5
1:A:55:ILE:CD1	1:A:81:LEU:HD12	0.48	2.38	12	4
1:A:15:ILE:CG2	1:A:48:ILE:HG21	0.48	2.39	10	1
1:A:82:ILE:HD13	1:A:157:ILE:HG22	0.48	1.86	18	2
1:A:55:ILE:HD11	1:A:77:LEU:CD2	0.47	2.33	5	3
1:A:82:ILE:HD13	1:A:157:ILE:CG2	0.47	2.39	16	2
1:A:147:VAL:HB	1:A:150:MET:HE1	0.47	1.85	1	7
1:A:16:HIS:HB2	1:A:28:ILE:HD11	0.47	1.86	5	4
1:A:80:GLN:HG2	1:A:90:VAL:HG21	0.47	1.87	16	4
1:A:44:VAL:CG2	1:A:70:LEU:HD13	0.47	2.40	12	7
1:A:73:LEU:HD21	1:A:176:LEU:HD22	0.47	1.87	4	1
1:A:80:GLN:HE21	1:A:90:VAL:HG11	0.47	1.70	17	1
1:A:77:LEU:HD13	1:A:77:LEU:C	0.47	2.35	2	5
1:A:84:LEU:C	1:A:84:LEU:HD12	0.46	2.35	2	18
1:A:55:ILE:HD11	1:A:77:LEU:HB3	0.46	1.86	8	2
1:A:140:ALA:HB3	1:A:149:ALA:CB	0.46	2.40	20	1
1:A:176:LEU:O	1:A:176:LEU:HD13	0.46	2.10	7	10
1:A:55:ILE:CG1	1:A:81:LEU:HD12	0.46	2.40	16	2
1:A:7:ASN:CG	1:A:55:ILE:HG23	0.46	2.36	8	1
1:A:73:LEU:HD22	1:A:179:PHE:CG	0.46	2.45	17	1
1:A:4:ILE:HD11	1:A:19:LEU:CD1	0.46	2.41	10	1
1:A:22:ILE:HD13	1:A:177:LYS:CG	0.46	2.41	14	1
1:A:64:ILE:CG2	1:A:81:LEU:HD21	0.46	2.41	16	3
1:A:55:ILE:HG22	1:A:61:CYS:CB	0.45	2.41	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:THR:HG22	1:A:34:PRO:HD2	0.45	1.88	19	2
1:A:44:VAL:CG2	1:A:70:LEU:HD22	0.45	2.37	20	2
1:A:101:THR:O	1:A:121:ALA:HB3	0.45	2.11	12	5
1:A:45:LYS:CD	1:A:186:LYS:HZ1	0.45	2.25	13	1
1:A:111:LEU:CD1	1:A:175:ILE:HG23	0.45	2.38	16	6
1:A:49:LEU:CD2	1:A:81:LEU:HD13	0.45	2.40	13	1
1:A:55:ILE:CG2	1:A:84:LEU:HD21	0.44	2.42	1	1
1:A:48:ILE:HD11	1:A:179:PHE:CE1	0.44	2.47	5	7
1:A:129:VAL:HG23	1:A:150:MET:HE1	0.44	1.89	16	1
1:A:132:VAL:HG13	1:A:132:VAL:O	0.44	2.12	18	12
1:A:49:LEU:HD21	1:A:64:ILE:CD1	0.44	2.43	4	1
1:A:156:PRO:O	1:A:157:ILE:HD13	0.44	2.13	2	1
1:A:104:TYR:C	1:A:117:ARG:O	0.44	2.60	14	1
1:A:5:LEU:HD21	1:A:49:LEU:HD23	0.44	1.88	17	2
1:A:3:VAL:HG23	1:A:44:VAL:HG11	0.43	1.89	3	1
1:A:49:LEU:HD13	1:A:50:SER:O	0.43	2.13	15	2
1:A:84:LEU:HD22	1:A:85:ALA:N	0.43	2.28	12	1
1:A:7:ASN:OD1	1:A:49:LEU:HD21	0.43	2.13	14	1
1:A:12:VAL:HG13	1:A:50:SER:HB2	0.43	1.90	20	1
1:A:79:HIS:CD2	1:A:80:GLN:N	0.43	2.87	14	1
1:A:139:LEU:HD21	1:A:151:LYS:HE2	0.43	1.89	2	1
1:A:105:VAL:O	1:A:105:VAL:HG13	0.43	2.14	14	5
1:A:35:LEU:HD12	1:A:63:ASP:OD1	0.43	2.14	3	1
1:A:55:ILE:HG12	1:A:77:LEU:HD11	0.43	1.91	5	1
1:A:55:ILE:HG23	1:A:84:LEU:HD21	0.43	1.89	1	1
1:A:3:VAL:HG22	1:A:44:VAL:HG11	0.42	1.92	9	1
1:A:138:ILE:HG23	1:A:149:ALA:O	0.42	2.14	5	2
1:A:19:LEU:HD12	1:A:26:SER:OG	0.42	2.14	15	1
1:A:185:TYR:O	1:A:185:TYR:CG	0.42	2.71	20	1
1:A:15:ILE:O	1:A:19:LEU:HD12	0.42	2.14	10	1
1:A:113:LYS:O	1:A:115:VAL:HG23	0.42	2.14	15	1
1:A:129:VAL:CG2	1:A:150:MET:HE2	0.42	2.44	11	1
1:A:4:ILE:HG12	1:A:15:ILE:HG21	0.42	1.91	12	1
1:A:81:LEU:HD23	1:A:82:ILE:HD13	0.42	1.91	13	2
1:A:112:PHE:CE1	1:A:175:ILE:HD11	0.41	2.50	10	1
1:A:55:ILE:HD13	1:A:84:LEU:HD23	0.41	1.91	5	1
1:A:55:ILE:HD13	1:A:84:LEU:HD21	0.41	1.91	11	1
1:A:108:GLU:HG3	1:A:139:LEU:HD22	0.41	1.90	18	1
1:A:112:PHE:CD1	1:A:175:ILE:HD12	0.41	2.51	4	1
1:A:105:VAL:HG13	1:A:105:VAL:O	0.41	2.16	11	10
1:A:64:ILE:HD12	1:A:81:LEU:HD11	0.41	1.93	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:ASN:HB2	1:A:44:VAL:HG13	0.41	1.93	3	1
1:A:47:ILE:CB	1:A:72:ILE:HD12	0.41	2.44	13	1
1:A:81:LEU:HD23	1:A:81:LEU:C	0.41	2.41	13	1
1:A:78:GLY:O	1:A:82:ILE:HD12	0.41	2.16	14	1
1:A:108:GLU:OE1	1:A:139:LEU:HD22	0.41	2.15	17	1
1:A:7:ASN:OD1	1:A:55:ILE:HD12	0.40	2.16	9	1
1:A:55:ILE:HG22	1:A:55:ILE:O	0.40	2.16	8	1
1:A:4:ILE:HG21	1:A:15:ILE:HD12	0.40	1.92	15	1
1:A:132:VAL:O	1:A:132:VAL:HG13	0.40	2.17	1	1
1:A:55:ILE:O	1:A:55:ILE:HG22	0.40	2.17	10	1
1:A:84:LEU:HD12	1:A:84:LEU:C	0.40	2.41	15	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	180/188 (96%)	160±2 (89±1%)	18±2 (10±1%)	3±1 (1±0%)	11	57
All	All	3600/3760 (96%)	3196 (89%)	351 (10%)	53 (1%)	11	57

All 5 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	105	VAL	20
1	A	76	CYS	19
1	A	44	VAL	10
1	A	126	LYS	3
1	A	147	VAL	1

6.3.2 Protein sidechains [i](#)

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	155/160 (97%)	115±4 (74±2%)	40±4 (26±2%)	2	23
All	All	3100/3200 (97%)	2300 (74%)	800 (26%)	2	23

All 97 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	27	LYS	20
1	A	33	THR	20
1	A	60	ASN	20
1	A	103	VAL	20
1	A	107	LYS	20
1	A	111	LEU	20
1	A	114	ASN	20
1	A	176	LEU	20
1	A	54	ASP	19
1	A	81	LEU	19
1	A	142	SER	19
1	A	186	LYS	19
1	A	6	ASP	17
1	A	50	SER	17
1	A	59	LYS	16
1	A	113	LYS	16
1	A	148	GLU	16
1	A	150	MET	16
1	A	181	LYS	15
1	A	42	LYS	15
1	A	77	LEU	14
1	A	1	MET	14
1	A	153	LYS	13
1	A	43	GLU	12
1	A	108	GLU	12
1	A	122	TRP	12
1	A	92	ARG	12
1	A	49	LEU	11
1	A	155	LYS	11
1	A	170	GLU	11
1	A	174	GLU	11
1	A	10	GLN	11
1	A	128	GLU	11
1	A	76	CYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	177	LYS	10
1	A	12	VAL	10
1	A	39	GLU	10
1	A	45	LYS	10
1	A	70	LEU	10
1	A	86	TYR	10
1	A	102	LYS	10
1	A	55	ILE	9
1	A	36	GLU	9
1	A	115	VAL	9
1	A	25	SER	8
1	A	14	ARG	7
1	A	89	GLU	7
1	A	100	LEU	7
1	A	131	LYS	7
1	A	110	ASP	7
1	A	117	ARG	7
1	A	17	ARG	6
1	A	38	ILE	6
1	A	56	GLU	5
1	A	124	SER	5
1	A	69	LYS	5
1	A	161	GLN	5
1	A	137	GLU	4
1	A	26	SER	4
1	A	97	GLU	4
1	A	136	PHE	4
1	A	171	TYR	4
1	A	106	ASP	4
1	A	80	GLN	3
1	A	96	GLU	3
1	A	134	GLU	3
1	A	188	GLU	3
1	A	13	HIS	3
1	A	173	ASN	3
1	A	75	ILE	3
1	A	3	VAL	3
1	A	118	GLU	3
1	A	146	GLN	3
1	A	126	LYS	3
1	A	138	ILE	3
1	A	41	ASN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	152	HIS	2
1	A	7	ASN	2
1	A	125	HIS	2
1	A	151	LYS	2
1	A	20	LYS	2
1	A	143	ASP	2
1	A	79	HIS	2
1	A	72	ILE	2
1	A	154	THR	1
1	A	63	ASP	1
1	A	105	VAL	1
1	A	163	HIS	1
1	A	57	LYS	1
1	A	84	LEU	1
1	A	40	SER	1
1	A	44	VAL	1
1	A	101	THR	1
1	A	18	SER	1
1	A	35	LEU	1
1	A	139	LEU	1
1	A	145	CYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 56% for the well-defined parts and 55% 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	1455
Number of shifts mapped to atoms	1454
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	152	HIS	HE2	9.482	.	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	186	-0.28 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	168	-0.01 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	175	0.31 ± 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 56%, i.e. 1400 atoms were assigned a chemical shift out of a possible 2500. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	681/911 (75%)	331/372 (89%)	180/364 (49%)	170/175 (97%)
Sidechain	682/1396 (49%)	471/908 (52%)	203/443 (46%)	8/45 (18%)
Aromatic	37/193 (19%)	36/96 (38%)	0/89 (0%)	1/8 (12%)
Overall	1400/2500 (56%)	838/1376 (61%)	383/896 (43%)	179/228 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 55%, i.e. 1425 atoms were assigned a chemical shift out of a possible 2574. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	698/939 (74%)	338/383 (88%)	186/376 (49%)	174/180 (97%)
Sidechain	690/1435 (48%)	473/934 (51%)	209/456 (46%)	8/45 (18%)
Aromatic	37/200 (18%)	36/100 (36%)	0/91 (0%)	1/9 (11%)
Overall	1425/2574 (55%)	847/1417 (60%)	395/923 (43%)	183/234 (78%)

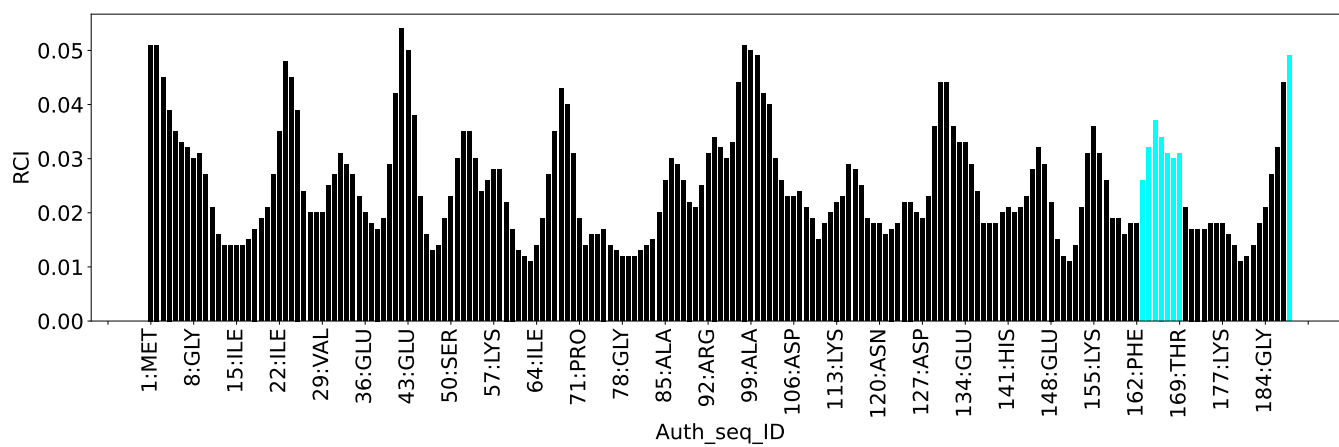
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1762
Intra-residue ($ i-j =0$)	606
Sequential ($ i-j =1$)	496
Medium range ($ i-j >1$ and $ i-j <5$)	196
Long range ($ i-j \geq 5$)	356
Inter-chain	0
Hydrogen bond restraints	108
Disulfide bond restraints	0
Total dihedral-angle restraints	364
Number of unmapped restraints	0
Number of restraints per residue	11.3
Number of long range restraints per residue ¹	2.2

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)	28.9	0.2
0.2-0.5 (Medium)	1.2	0.39
>0.5 (Large)	1.0	1.51

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)	16.8	5.99
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

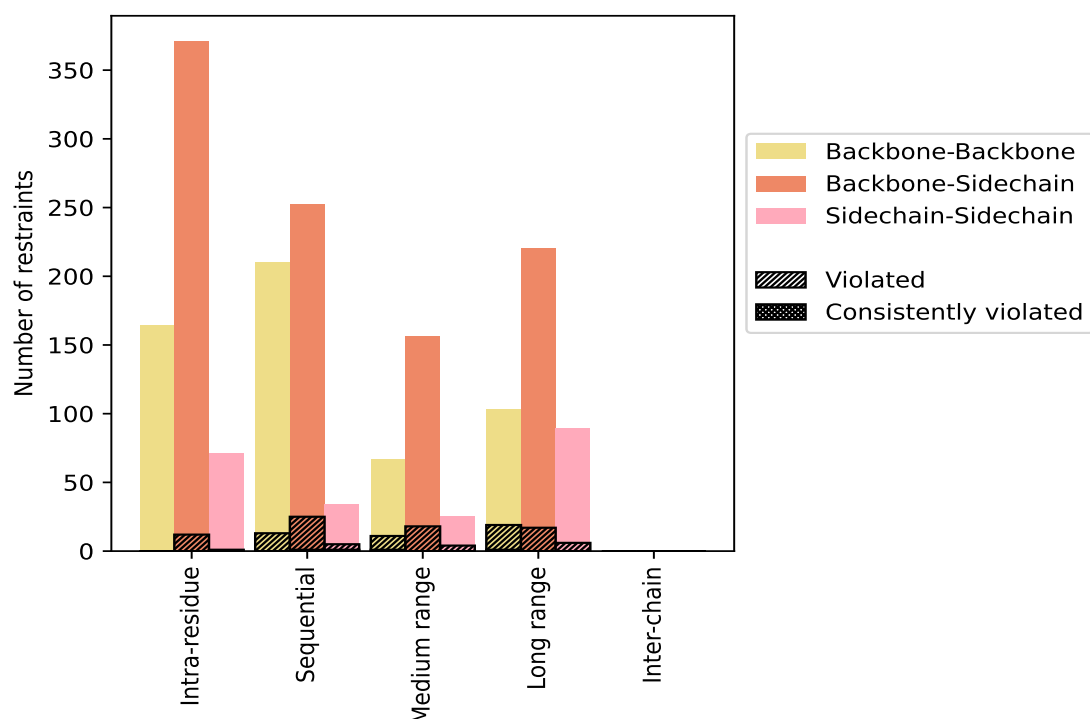
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	606	34.4	13	2.1	0.7	0	0.0	0.0
Backbone-Backbone	164	9.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	371	21.1	12	3.2	0.7	0	0.0	0.0
Sidechain-Sidechain	71	4.0	1	1.4	0.1	0	0.0	0.0
Sequential (i-j =1)	496	28.1	43	8.7	2.4	2	0.4	0.1
Backbone-Backbone	210	11.9	13	6.2	0.7	0	0.0	0.0
Backbone-Sidechain	252	14.3	25	9.9	1.4	1	0.4	0.1
Sidechain-Sidechain	34	1.9	5	14.7	0.3	1	2.9	0.1
Medium range (i-j >1 & i-j <5)	196	11.1	27	13.8	1.5	1	0.5	0.1
Backbone-Backbone	67	3.8	11	16.4	0.6	1	1.5	0.1
Backbone-Sidechain	104	5.9	12	11.5	0.7	0	0.0	0.0
Sidechain-Sidechain	25	1.4	4	16.0	0.2	0	0.0	0.0
Long range (i-j ≥5)	356	20.2	41	11.5	2.3	1	0.3	0.1
Backbone-Backbone	103	5.8	19	18.4	1.1	1	1.0	0.1
Backbone-Sidechain	164	9.3	16	9.8	0.9	0	0.0	0.0
Sidechain-Sidechain	89	5.1	6	6.7	0.3	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	108	6.1	7	6.5	0.4	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1762	100.0	131	7.4	7.4	4	0.2	0.2
Backbone-Backbone	544	30.9	43	7.9	2.4	2	0.4	0.1
Backbone-Sidechain	999	56.7	72	7.2	4.1	1	0.1	0.1
Sidechain-Sidechain	219	12.4	16	7.3	0.9	1	0.5	0.1

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	2	15	6	9	0	32	0.17	1.41	0.22	0.12
2	3	15	6	8	0	32	0.17	1.49	0.24	0.12
3	1	14	10	11	0	36	0.16	1.44	0.22	0.12
4	1	12	5	9	0	27	0.18	1.41	0.24	0.13
5	2	10	4	11	0	27	0.18	1.41	0.24	0.14
6	3	10	8	14	0	35	0.17	1.42	0.22	0.13
7	3	11	8	15	0	37	0.18	1.51	0.23	0.12
8	1	7	9	10	0	27	0.17	1.37	0.24	0.11
9	1	13	10	13	0	37	0.16	1.41	0.21	0.12
10	3	10	10	9	0	32	0.19	1.44	0.24	0.12

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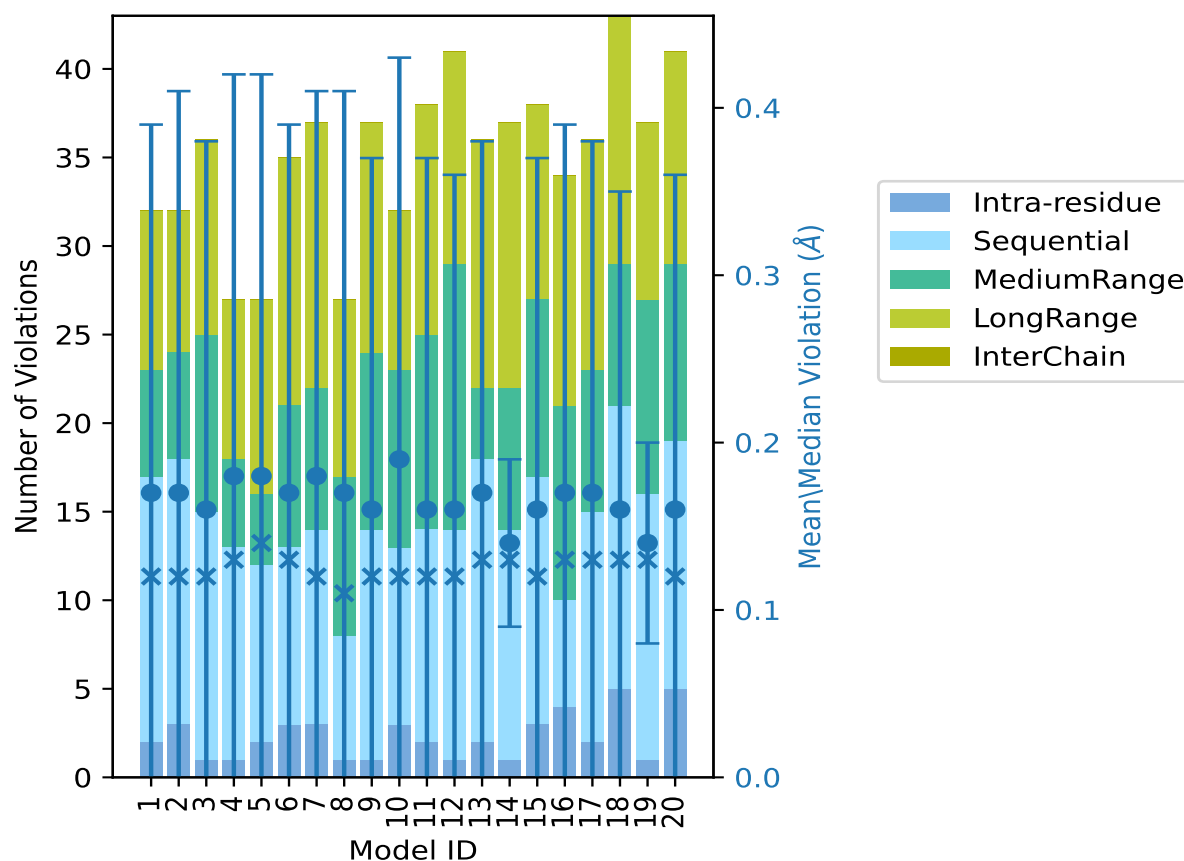
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	2	12	11	13	0	38	0.16	1.4	0.21	0.12
12	1	13	15	12	0	41	0.16	1.41	0.2	0.12
13	2	16	4	14	0	36	0.17	1.39	0.21	0.13
14	1	13	8	15	0	37	0.14	0.39	0.05	0.13
15	3	14	10	11	0	38	0.16	1.42	0.21	0.12
16	4	6	11	13	0	34	0.17	1.42	0.22	0.13
17	2	13	8	13	0	36	0.17	1.41	0.21	0.13
18	5	16	8	14	0	43	0.16	1.37	0.19	0.13
19	1	15	11	10	0	37	0.14	0.38	0.06	0.13
20	5	14	10	12	0	41	0.16	1.4	0.2	0.12

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

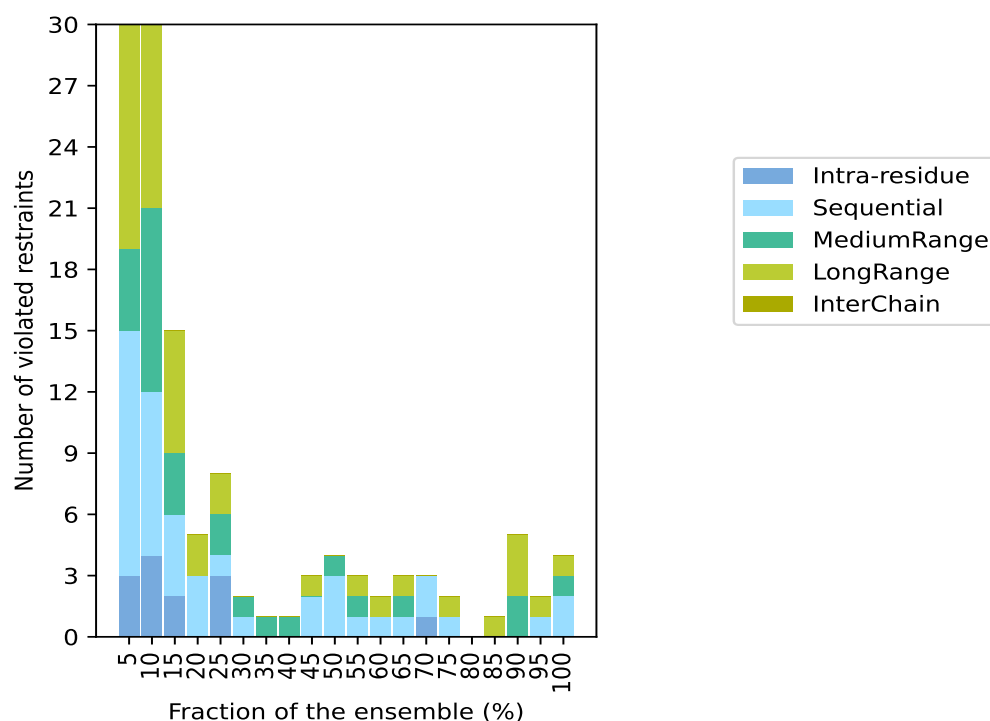
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1530(IR:593, SQ:453, MR:169, LR:315, IC:0) restraints are 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	%
3	12	4	11	0	30	1	5.0
4	8	9	9	0	30	2	10.0
2	4	3	6	0	15	3	15.0
0	3	0	2	0	5	4	20.0
3	1	2	2	0	8	5	25.0
0	1	1	0	0	2	6	30.0
0	0	1	0	0	1	7	35.0
0	0	1	0	0	1	8	40.0
0	2	0	1	0	3	9	45.0
0	3	1	0	0	4	10	50.0
0	1	1	1	0	3	11	55.0
0	1	0	1	0	2	12	60.0
0	1	1	1	0	3	13	65.0
1	2	0	0	0	3	14	70.0
0	1	0	1	0	2	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	1	0	1	17	85.0
0	0	2	3	0	5	18	90.0
0	1	0	1	0	2	19	95.0
0	2	1	1	0	4	20	100.0

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

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

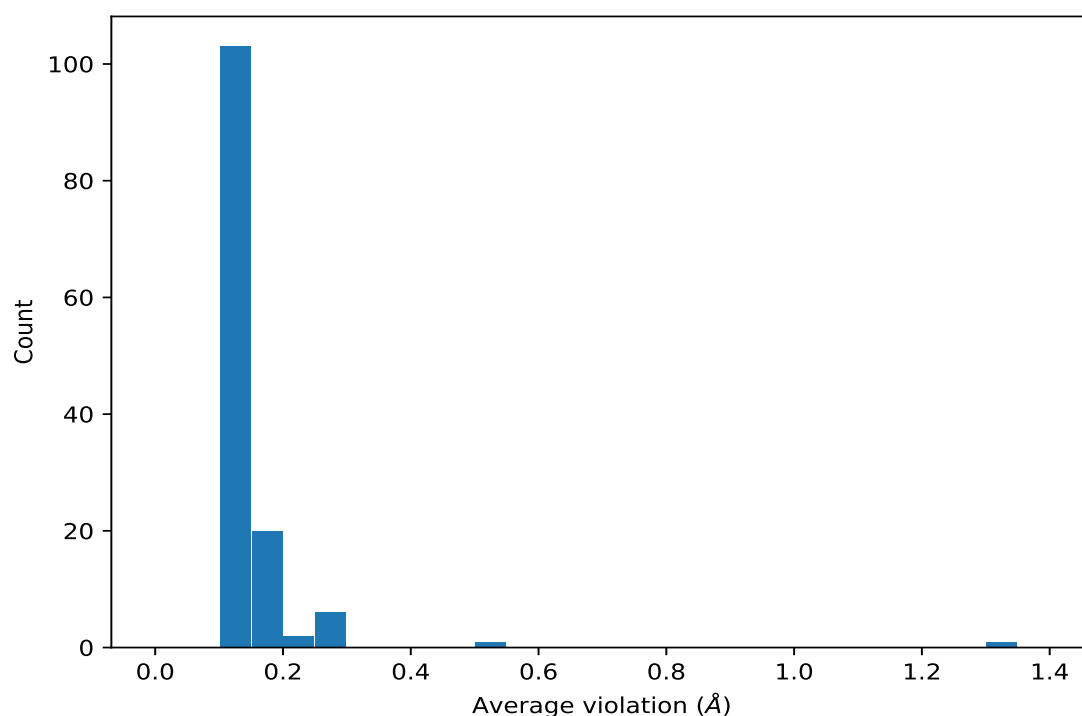
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	20	1.31	0.31	1.41
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	20	0.16	0.02	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	20	0.16	0.01	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	20	0.16	0.01	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	20	0.16	0.01	0.16
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	20	0.13	0.01	0.13
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	19	0.14	0.01	0.14
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	19	0.14	0.01	0.14
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	18	0.14	0.03	0.15
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	18	0.13	0.02	0.14
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	18	0.12	0.02	0.12
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	18	0.12	0.02	0.12
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	18	0.12	0.02	0.12
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	18	0.12	0.01	0.12
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	18	0.11	0.01	0.11
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	17	0.13	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	17	0.13	0.01	0.12
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	17	0.13	0.01	0.12
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	15	0.15	0.02	0.15
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	15	0.12	0.02	0.11
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	14	0.13	0.02	0.13
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	14	0.12	0.01	0.12
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	14	0.11	0.0	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	14	0.11	0.0	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	14	0.11	0.0	0.11
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	13	0.13	0.02	0.12
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	13	0.12	0.02	0.11
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	13	0.11	0.01	0.11
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	12	0.12	0.01	0.13
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	12	0.12	0.02	0.12
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	12	0.12	0.02	0.12
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	11	0.15	0.01	0.14
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	11	0.14	0.02	0.14
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	11	0.11	0.01	0.11
(1,372)	1:42:A:LYS:HA	1:43:A:GLU:H	10	0.14	0.03	0.15
(1,695)	1:79:A:HIS:HB3	1:81:A:LEU:H	10	0.13	0.04	0.12
(1,1283)	1:141:A:HIS:H	1:142:A:SER:H	10	0.11	0.01	0.11
(1,793)	1:89:A:GLU:H	1:90:A:VAL:H	10	0.11	0.01	0.11
(1,487)	1:55:A:ILE:HB	1:81:A:LEU:HA	9	0.13	0.01	0.13
(1,247)	1:27:A:LYS:H	1:28:A:ILE:H	9	0.12	0.01	0.11
(1,715)	1:81:A:LEU:HB2	1:82:A:ILE:H	9	0.12	0.01	0.12
(1,1296)	1:142:A:SER:H	1:146:A:GLN:HA	8	0.13	0.01	0.13
(1,344)	1:38:A:ILE:HD11	1:40:A:SER:H	7	0.11	0.01	0.11
(1,344)	1:38:A:ILE:HD12	1:40:A:SER:H	7	0.11	0.01	0.11
(1,344)	1:38:A:ILE:HD13	1:40:A:SER:H	7	0.11	0.01	0.11
(1,314)	1:35:A:LEU:H	1:38:A:ILE:H	6	0.15	0.02	0.16
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD11	6	0.14	0.03	0.14
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD12	6	0.14	0.03	0.14
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD13	6	0.14	0.03	0.14
(1,474)	1:54:A:ASP:HA	1:56:A:GLU:H	5	0.16	0.05	0.15
(1,732)	1:83:A:ALA:H	1:84:A:LEU:H	5	0.12	0.01	0.12
(2,40)	1:90:A:VAL:HG21	1:133:A:PRO:HD3	5	0.12	0.01	0.11
(2,40)	1:90:A:VAL:HG22	1:133:A:PRO:HD3	5	0.12	0.01	0.11
(2,40)	1:90:A:VAL:HG23	1:133:A:PRO:HD3	5	0.12	0.01	0.11
(1,926)	1:102:A:LYS:HE2	1:102:A:LYS:H	5	0.12	0.0	0.12
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG21	5	0.11	0.01	0.12
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG22	5	0.11	0.01	0.12
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG23	5	0.11	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,826)	1:92:A:ARG:H	1:92:A:ARG:HD3	5	0.11	0.0	0.11
(1,827)	1:92:A:ARG:HA	1:92:A:ARG:HD2	5	0.11	0.0	0.11
(1,44)	1:3:A:VAL:H	1:46:A:GLY:H	5	0.11	0.01	0.1
(1,1190)	1:131:A:LYS:HG3	1:132:A:VAL:HA	4	0.19	0.01	0.2
(1,707)	1:80:A:GLN:HB3	1:81:A:LEU:HA	4	0.11	0.01	0.11
(1,1046)	1:111:A:LEU:HB2	1:175:A:ILE:H	4	0.11	0.01	0.11
(1,1401)	1:156:A:PRO:HD3	1:157:A:ILE:H	4	0.11	0.01	0.11
(1,27)	1:2:A:ILE:HD11	1:185:A:TYR:HE1	4	0.11	0.01	0.11
(1,27)	1:2:A:ILE:HD11	1:185:A:TYR:HE2	4	0.11	0.01	0.11
(1,27)	1:2:A:ILE:HD12	1:185:A:TYR:HE1	4	0.11	0.01	0.11
(1,27)	1:2:A:ILE:HD12	1:185:A:TYR:HE2	4	0.11	0.01	0.11
(1,27)	1:2:A:ILE:HD13	1:185:A:TYR:HE1	4	0.11	0.01	0.11
(1,27)	1:2:A:ILE:HD13	1:185:A:TYR:HE2	4	0.11	0.01	0.11
(1,1127)	1:119:A:PHE:H	1:119:A:PHE:HD1	3	0.25	0.03	0.24
(1,1127)	1:119:A:PHE:H	1:119:A:PHE:HD2	3	0.25	0.03	0.24
(1,1105)	1:116:A:PRO:HG3	1:119:A:PHE:HB3	3	0.17	0.01	0.17
(1,970)	1:104:A:TYR:HA	1:119:A:PHE:H	3	0.15	0.01	0.14
(2,59)	1:116:A:PRO:HG3	1:117:A:ARG:HD2	3	0.15	0.02	0.16
(1,179)	1:20:A:LYS:HG3	1:20:A:LYS:H	3	0.14	0.0	0.14
(1,425)	1:47:A:ILE:H	1:71:A:PRO:HD2	3	0.14	0.0	0.14
(1,63)	1:4:A:ILE:HG13	1:15:A:ILE:HG12	3	0.13	0.03	0.12
(1,63)	1:4:A:ILE:HG13	1:15:A:ILE:HG13	3	0.13	0.03	0.12
(1,1203)	1:132:A:VAL:HG21	1:136:A:PHE:HD1	3	0.13	0.0	0.13
(1,1203)	1:132:A:VAL:HG22	1:136:A:PHE:HD1	3	0.13	0.0	0.13
(1,1203)	1:132:A:VAL:HG23	1:136:A:PHE:HD1	3	0.13	0.0	0.13
(1,806)	1:90:A:VAL:H	1:91:A:GLY:H	3	0.13	0.0	0.13
(1,1436)	1:169:A:THR:HA	1:172:A:GLY:H	3	0.13	0.01	0.13
(1,1252)	1:138:A:ILE:HA	1:149:A:ALA:H	3	0.12	0.0	0.12
(1,786)	1:88:A:GLY:H	1:89:A:GLU:HB2	3	0.11	0.0	0.11
(1,1348)	1:150:A:MET:H	1:151:A:LYS:H	3	0.11	0.01	0.11
(2,3)	1:8:A:GLY:HA3	1:52:A:GLY:H	3	0.11	0.0	0.11
(1,650)	1:72:A:ILE:HA	1:183:A:CYS:HG	3	0.11	0.0	0.11
(1,176)	1:20:A:LYS:HB3	1:20:A:LYS:HE3	2	0.51	0.0	0.51
(1,160)	1:18:A:SER:HA	1:20:A:LYS:HE3	2	0.28	0.0	0.28
(1,396)	1:46:A:GLY:HA3	1:47:A:ILE:HD11	2	0.26	0.02	0.26
(1,396)	1:46:A:GLY:HA3	1:47:A:ILE:HD12	2	0.26	0.02	0.26
(1,396)	1:46:A:GLY:HA3	1:47:A:ILE:HD13	2	0.26	0.02	0.26
(1,1446)	1:173:A:ASN:H	1:173:A:ASN:HD22	2	0.22	0.01	0.22
(1,1514)	1:181:A:LYS:H	1:181:A:LYS:HE2	2	0.22	0.01	0.22
(1,727)	1:82:A:ILE:HG21	1:84:A:LEU:H	2	0.18	0.06	0.18
(1,727)	1:82:A:ILE:HG22	1:84:A:LEU:H	2	0.18	0.06	0.18
(1,727)	1:82:A:ILE:HG23	1:84:A:LEU:H	2	0.18	0.06	0.18

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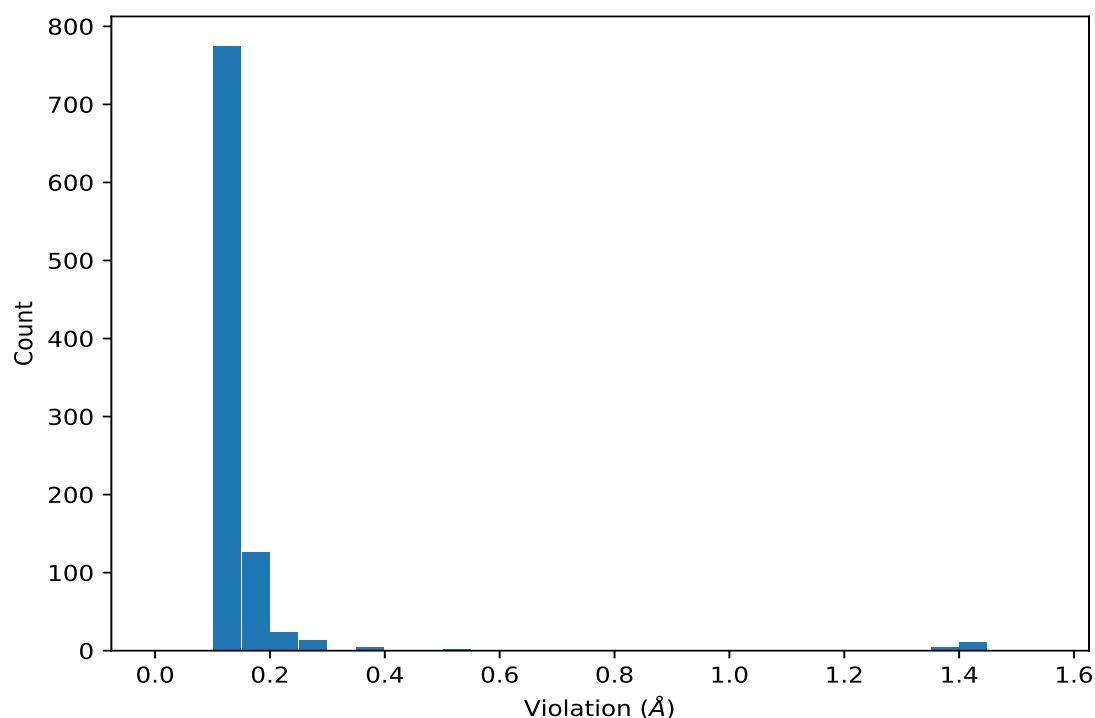
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,167)	1:19:A:LEU:H	1:22:A:ILE:HG13	2	0.16	0.01	0.16
(1,364)	1:41:A:ASN:H	1:43:A:GLU:H	2	0.16	0.06	0.16
(3,21)	1:21:A:TYR:H	1:17:A:ARG:O	2	0.15	0.01	0.15
(1,186)	1:20:A:LYS:HG3	1:23:A:GLY:H	2	0.15	0.0	0.15
(1,885)	1:97:A:GLU:HA	1:98:A:TYR:H	2	0.15	0.0	0.15
(1,983)	1:105:A:VAL:H	1:118:A:GLU:HA	2	0.14	0.03	0.14
(1,1451)	1:173:A:ASN:HB2	1:174:A:GLU:H	2	0.13	0.01	0.13
(3,54)	1:83:A:ALA:H	1:79:A:HIS:O	2	0.12	0.02	0.12
(1,1235)	1:137:A:GLU:H	1:152:A:HIS:HB2	2	0.12	0.02	0.12
(2,76)	1:153:A:LYS:H	1:157:A:ILE:HB	2	0.12	0.02	0.12
(3,11)	1:16:A:HIS:H	1:12:A:VAL:O	2	0.12	0.01	0.12
(1,41)	1:3:A:VAL:HG21	1:27:A:LYS:H	2	0.12	0.02	0.12
(1,41)	1:3:A:VAL:HG22	1:27:A:LYS:H	2	0.12	0.02	0.12
(1,41)	1:3:A:VAL:HG23	1:27:A:LYS:H	2	0.12	0.02	0.12
(1,471)	1:54:A:ASP:H	1:55:A:ILE:HG21	2	0.12	0.02	0.12
(1,471)	1:54:A:ASP:H	1:55:A:ILE:HG22	2	0.12	0.02	0.12
(1,471)	1:54:A:ASP:H	1:55:A:ILE:HG23	2	0.12	0.02	0.12
(1,687)	1:78:A:GLY:H	1:80:A:GLN:HB3	2	0.12	0.0	0.12
(1,950)	1:103:A:VAL:H	1:119:A:PHE:HA	2	0.12	0.0	0.12
(2,61)	1:123:A:ALA:H	1:125:A:HIS:H	2	0.12	0.0	0.12
(1,541)	1:61:A:CYS:HB3	1:64:A:ILE:HB	2	0.11	0.0	0.11
(1,799)	1:89:A:GLU:H	1:132:A:VAL:H	2	0.11	0.01	0.11
(1,935)	1:102:A:LYS:HA	1:119:A:PHE:HA	2	0.11	0.01	0.11
(1,1364)	1:151:A:LYS:HB3	1:152:A:HIS:H	2	0.11	0.01	0.11
(1,899)	1:100:A:LEU:H	1:100:A:LEU:HG	2	0.11	0.0	0.11
(1,1044)	1:111:A:LEU:H	1:175:A:ILE:HA	2	0.11	0.0	0.11
(1,1223)	1:136:A:PHE:HB3	1:137:A:GLU:H	2	0.11	0.0	0.11
(1,59)	1:4:A:ILE:HB	1:5:A:LEU:HD21	2	0.1	0.0	0.1
(1,59)	1:4:A:ILE:HB	1:5:A:LEU:HD22	2	0.1	0.0	0.1
(1,59)	1:4:A:ILE:HB	1:5:A:LEU:HD23	2	0.1	0.0	0.1
(1,64)	1:4:A:ILE:H	1:26:A:SER:HA	2	0.1	0.0	0.1
(1,856)	1:94:A:GLU:HB2	1:95:A:ALA:H	2	0.1	0.0	0.1
(2,47)	1:102:A:LYS:HA	1:142:A:SER:HB3	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	7	1.51
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	2	1.49
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	3	1.44
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	10	1.44
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	6	1.42
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	15	1.42
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	16	1.42
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	1	1.41
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	4	1.41
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	5	1.41
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	9	1.41
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	12	1.41
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	17	1.41
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	11	1.4
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	20	1.4
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	13	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	8	1.37
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	18	1.37
(1,176)	1:20:A:LYS:HB3	1:20:A:LYS:HE3	7	0.51
(1,176)	1:20:A:LYS:HB3	1:20:A:LYS:HE3	10	0.51
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	14	0.39
(1,312)	1:35:A:LEU:HD21	1:36:A:GLU:H	19	0.38
(1,312)	1:35:A:LEU:HD22	1:36:A:GLU:H	19	0.38
(1,312)	1:35:A:LEU:HD23	1:36:A:GLU:H	19	0.38
(1,199)	1:21:A:TYR:HD1	1:22:A:ILE:H	19	0.37
(1,1127)	1:119:A:PHE:H	1:119:A:PHE:HD1	17	0.29
(1,1127)	1:119:A:PHE:H	1:119:A:PHE:HD2	17	0.29
(1,160)	1:18:A:SER:HA	1:20:A:LYS:HE3	7	0.28
(1,160)	1:18:A:SER:HA	1:20:A:LYS:HE3	10	0.28
(1,396)	1:46:A:GLY:HA3	1:47:A:ILE:HD11	5	0.27
(1,396)	1:46:A:GLY:HA3	1:47:A:ILE:HD12	5	0.27
(1,396)	1:46:A:GLY:HA3	1:47:A:ILE:HD13	5	0.27
(1,1365)	1:151:A:LYS:HG3	1:152:A:HIS:H	18	0.26
(1,474)	1:54:A:ASP:HA	1:56:A:GLU:H	11	0.26
(1,384)	1:44:A:VAL:HG21	1:44:A:VAL:H	16	0.26
(1,384)	1:44:A:VAL:HG22	1:44:A:VAL:H	16	0.26
(1,384)	1:44:A:VAL:HG23	1:44:A:VAL:H	16	0.26
(1,251)	1:27:A:LYS:HE2	1:28:A:ILE:H	18	0.26
(1,695)	1:79:A:HIS:HB3	1:81:A:LEU:H	12	0.25
(1,1393)	1:154:A:THR:HG21	1:155:A:LYS:H	4	0.24
(1,1393)	1:154:A:THR:HG22	1:155:A:LYS:H	4	0.24
(1,1393)	1:154:A:THR:HG23	1:155:A:LYS:H	4	0.24
(1,1127)	1:119:A:PHE:H	1:119:A:PHE:HD1	6	0.24
(1,1127)	1:119:A:PHE:H	1:119:A:PHE:HD2	6	0.24
(1,396)	1:46:A:GLY:HA3	1:47:A:ILE:HD11	13	0.24
(1,396)	1:46:A:GLY:HA3	1:47:A:ILE:HD12	13	0.24
(1,396)	1:46:A:GLY:HA3	1:47:A:ILE:HD13	13	0.24
(1,1127)	1:119:A:PHE:H	1:119:A:PHE:HD1	20	0.23
(1,1127)	1:119:A:PHE:H	1:119:A:PHE:HD2	20	0.23
(1,727)	1:82:A:ILE:HG21	1:84:A:LEU:H	9	0.23
(1,727)	1:82:A:ILE:HG22	1:84:A:LEU:H	9	0.23
(1,727)	1:82:A:ILE:HG23	1:84:A:LEU:H	9	0.23
(1,1514)	1:181:A:LYS:H	1:181:A:LYS:HE2	7	0.22
(1,1446)	1:173:A:ASN:H	1:173:A:ASN:HD22	13	0.22
(1,364)	1:41:A:ASN:H	1:43:A:GLU:H	16	0.22
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	16	0.22
(1,1514)	1:181:A:LYS:H	1:181:A:LYS:HE2	2	0.21
(1,1446)	1:173:A:ASN:H	1:173:A:ASN:HD22	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD11	14	0.21
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD12	14	0.21
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD13	14	0.21
(1,1190)	1:131:A:LYS:HG3	1:132:A:VAL:HA	1	0.2
(1,1190)	1:131:A:LYS:HG3	1:132:A:VAL:HA	5	0.2
(1,1190)	1:131:A:LYS:HG3	1:132:A:VAL:HA	15	0.19
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	10	0.19
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	13	0.19
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	14	0.19
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	15	0.19
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	12	0.18
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	15	0.18
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	20	0.18
(1,1105)	1:116:A:PRO:HG3	1:119:A:PHE:HB3	20	0.18
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	9	0.18
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	15	0.18
(1,372)	1:42:A:LYS:HA	1:43:A:GLU:H	13	0.18
(1,372)	1:42:A:LYS:HA	1:43:A:GLU:H	14	0.18
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	3	0.18
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	6	0.18
(1,314)	1:35:A:LEU:H	1:38:A:ILE:H	16	0.18
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	4	0.17
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	6	0.17
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	7	0.17
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	17	0.17
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	18	0.17
(1,1555)	1:186:A:LYS:H	1:186:A:LYS:HG3	20	0.17
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	11	0.17
(1,1190)	1:131:A:LYS:HG3	1:132:A:VAL:HA	19	0.17
(1,1105)	1:116:A:PRO:HG3	1:119:A:PHE:HB3	6	0.17
(1,983)	1:105:A:VAL:H	1:118:A:GLU:HA	9	0.17
(1,969)	1:104:A:TYR:HA	1:118:A:GLU:HA	14	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	6	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	6	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	6	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	10	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	10	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	10	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	15	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	15	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	15	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	16	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	16	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	18	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	18	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	18	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	20	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	20	0.17
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	20	0.17
(1,757)	1:84:A:LEU:HB2	1:85:A:ALA:H	12	0.17
(1,694)	1:79:A:HIS:HB3	1:80:A:GLN:H	14	0.17
(1,372)	1:42:A:LYS:HA	1:43:A:GLU:H	17	0.17
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	2	0.17
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	7	0.17
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	11	0.17
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	18	0.17
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	15	0.17
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	17	0.17
(1,314)	1:35:A:LEU:H	1:38:A:ILE:H	8	0.17
(1,311)	1:35:A:LEU:HG	1:36:A:GLU:H	19	0.17
(1,167)	1:19:A:LEU:H	1:22:A:ILE:HG13	14	0.17
(1,63)	1:4:A:ILE:HG13	1:15:A:ILE:HG12	12	0.17
(1,63)	1:4:A:ILE:HG13	1:15:A:ILE:HG13	12	0.17
(3,21)	1:21:A:TYR:H	1:17:A:ARG:O	7	0.16
(2,59)	1:116:A:PRO:HG3	1:117:A:ARG:HD2	6	0.16
(2,59)	1:116:A:PRO:HG3	1:117:A:ARG:HD2	20	0.16
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	1	0.16
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	8	0.16
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	12	0.16
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	4	0.16
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	9	0.16
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	4	0.16
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	9	0.16
(1,970)	1:104:A:TYR:HA	1:119:A:PHE:H	14	0.16
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	8	0.16
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	8	0.16
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	8	0.16
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	17	0.16
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	17	0.16
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	17	0.16
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	4	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	1	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	1	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	2	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	2	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	2	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	3	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	3	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	3	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	4	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	4	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	4	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	5	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	5	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	5	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	7	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	7	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	7	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	8	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	8	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	8	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	11	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	11	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	11	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	12	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	12	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	12	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	13	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	13	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	13	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	17	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	17	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	17	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	19	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	19	0.16
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	19	0.16
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	5	0.16
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	17	0.16
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	20	0.16
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	4	0.16
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	16	0.16
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	6	0.16
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	12	0.16
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	2	0.16
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	9	0.16
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	19	0.16
(1,314)	1:35:A:LEU:H	1:38:A:ILE:H	10	0.16
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	5	0.16
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	17	0.15
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	4	0.15
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	7	0.15
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	10	0.15
(1,1105)	1:116:A:PRO:HG3	1:119:A:PHE:HB3	17	0.15
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	17	0.15
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	17	0.15
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	17	0.15
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	6	0.15
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	6	0.15
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	6	0.15
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	2	0.15
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	6	0.15
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	13	0.15
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	14	0.15
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	20	0.15
(1,885)	1:97:A:GLU:HA	1:98:A:TYR:H	1	0.15
(1,885)	1:97:A:GLU:HA	1:98:A:TYR:H	19	0.15
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	9	0.15
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	9	0.15
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	9	0.15
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB1	14	0.15
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB2	14	0.15
(1,859)	1:94:A:GLU:HB3	1:95:A:ALA:HB3	14	0.15
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	5	0.15
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	8	0.15
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	1	0.15
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	5	0.15
(1,740)	1:83:A:ALA:HA	1:86:A:TYR:H	12	0.15
(1,715)	1:81:A:LEU:HB2	1:82:A:ILE:H	12	0.15
(1,487)	1:55:A:ILE:HB	1:81:A:LEU:HA	3	0.15
(1,474)	1:54:A:ASP:HA	1:56:A:GLU:H	2	0.15
(1,474)	1:54:A:ASP:HA	1:56:A:GLU:H	5	0.15
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	1	0.15
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	6	0.15
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	14	0.15
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	17	0.15
(1,372)	1:42:A:LYS:HA	1:43:A:GLU:H	3	0.15
(1,372)	1:42:A:LYS:HA	1:43:A:GLU:H	18	0.15
(1,372)	1:42:A:LYS:HA	1:43:A:GLU:H	20	0.15
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	1	0.15
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	10	0.15
(1,345)	1:38:A:ILE:HA	1:41:A:ASN:H	16	0.15
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	4	0.15
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	11	0.15
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	12	0.15
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	18	0.15
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	20	0.15
(1,314)	1:35:A:LEU:H	1:38:A:ILE:H	3	0.15
(1,314)	1:35:A:LEU:H	1:38:A:ILE:H	19	0.15
(1,247)	1:27:A:LYS:H	1:28:A:ILE:H	18	0.15
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD11	2	0.15
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD12	2	0.15
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD13	2	0.15
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD11	19	0.15
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD12	19	0.15
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD13	19	0.15
(1,186)	1:20:A:LYS:HG3	1:23:A:GLY:H	14	0.15
(1,186)	1:20:A:LYS:HG3	1:23:A:GLY:H	19	0.15
(1,167)	1:19:A:LEU:H	1:22:A:ILE:HG13	19	0.15
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	3	0.15
(3,54)	1:83:A:ALA:H	1:79:A:HIS:O	12	0.14
(3,21)	1:21:A:TYR:H	1:17:A:ARG:O	10	0.14
(2,76)	1:153:A:LYS:H	1:157:A:ILE:HB	18	0.14
(2,40)	1:90:A:VAL:HG21	1:133:A:PRO:HD3	5	0.14
(2,40)	1:90:A:VAL:HG22	1:133:A:PRO:HD3	5	0.14
(2,40)	1:90:A:VAL:HG23	1:133:A:PRO:HD3	5	0.14
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	11	0.14
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	15	0.14
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	18	0.14
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	1	0.14
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	12	0.14
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	16	0.14
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	3	0.14
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	20	0.14
(1,1451)	1:173:A:ASN:HB2	1:174:A:GLU:H	6	0.14
(1,1436)	1:169:A:THR:HA	1:172:A:GLY:H	20	0.14
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	7	0.14
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	13	0.14
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	16	0.14
(1,1296)	1:142:A:SER:H	1:146:A:GLN:HA	8	0.14
(1,1296)	1:142:A:SER:H	1:146:A:GLN:HA	15	0.14
(1,1296)	1:142:A:SER:H	1:146:A:GLN:HA	16	0.14
(1,1283)	1:141:A:HIS:H	1:142:A:SER:H	6	0.14
(1,1235)	1:137:A:GLU:H	1:152:A:HIS:HB2	18	0.14
(1,1203)	1:132:A:VAL:HG21	1:136:A:PHE:HD1	16	0.14
(1,1203)	1:132:A:VAL:HG22	1:136:A:PHE:HD1	16	0.14
(1,1203)	1:132:A:VAL:HG23	1:136:A:PHE:HD1	16	0.14
(1,1147)	1:123:A:ALA:HA	1:162:A:PHE:HA	11	0.14
(1,970)	1:104:A:TYR:HA	1:119:A:PHE:H	6	0.14
(1,970)	1:104:A:TYR:HA	1:119:A:PHE:H	20	0.14
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	1	0.14
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	1	0.14
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	1	0.14
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	10	0.14
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	10	0.14
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	10	0.14
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	14	0.14
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	14	0.14
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	14	0.14
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	10	0.14
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	10	0.14
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	10	0.14
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	16	0.14
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	16	0.14
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	16	0.14
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	20	0.14
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	20	0.14
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	20	0.14
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	3	0.14
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	5	0.14
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	7	0.14
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	10	0.14
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	12	0.14
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	17	0.14
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	18	0.14
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	2	0.14
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	4	0.14
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	15	0.14
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	19	0.14
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	7	0.14
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	13	0.14
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	16	0.14
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	18	0.14
(1,732)	1:83:A:ALA:H	1:84:A:LEU:H	18	0.14
(1,487)	1:55:A:ILE:HB	1:81:A:LEU:HA	6	0.14
(1,487)	1:55:A:ILE:HB	1:81:A:LEU:HA	18	0.14
(1,474)	1:54:A:ASP:HA	1:56:A:GLU:H	17	0.14
(1,425)	1:47:A:ILE:H	1:71:A:PRO:HD2	5	0.14
(1,425)	1:47:A:ILE:H	1:71:A:PRO:HD2	13	0.14
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	9	0.14
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	19	0.14
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	3	0.14
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	4	0.14
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	5	0.14
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	9	0.14
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	12	0.14
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	13	0.14
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	18	0.14
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	4	0.14
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	8	0.14
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	19	0.14
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	5	0.14
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	7	0.14
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	8	0.14
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	2	0.14
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	3	0.14
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	7	0.14
(1,179)	1:20:A:LYS:HG3	1:20:A:LYS:H	14	0.14
(1,179)	1:20:A:LYS:HG3	1:20:A:LYS:H	19	0.14
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	2	0.14
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	7	0.14
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	12	0.14
(1,38)	1:3:A:VAL:HG21	1:4:A:ILE:H	9	0.14
(1,38)	1:3:A:VAL:HG22	1:4:A:ILE:H	9	0.14
(1,38)	1:3:A:VAL:HG23	1:4:A:ILE:H	9	0.14
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	1	0.13
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	4	0.13
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	9	0.13
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	12	0.13
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	18	0.13
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	19	0.13
(3,52)	1:82:A:ILE:H	1:78:A:GLY:O	12	0.13
(3,11)	1:16:A:HIS:H	1:12:A:VAL:O	15	0.13
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	1	0.13
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	4	0.13
(2,40)	1:90:A:VAL:HG21	1:133:A:PRO:HD3	16	0.13
(2,40)	1:90:A:VAL:HG22	1:133:A:PRO:HD3	16	0.13
(2,40)	1:90:A:VAL:HG23	1:133:A:PRO:HD3	16	0.13
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	10	0.13
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	19	0.13
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	3	0.13
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	5	0.13
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	18	0.13
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	19	0.13
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	11	0.13
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	13	0.13
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	14	0.13
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	17	0.13
(1,1436)	1:169:A:THR:HA	1:172:A:GLY:H	17	0.13
(1,1401)	1:156:A:PRO:HD3	1:157:A:ILE:H	2	0.13
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	15	0.13
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	19	0.13
(1,1348)	1:150:A:MET:H	1:151:A:LYS:H	13	0.13
(1,1296)	1:142:A:SER:H	1:146:A:GLN:HA	10	0.13
(1,1296)	1:142:A:SER:H	1:146:A:GLN:HA	14	0.13
(1,1296)	1:142:A:SER:H	1:146:A:GLN:HA	19	0.13
(1,1283)	1:141:A:HIS:H	1:142:A:SER:H	13	0.13
(1,1273)	1:140:A:ALA:H	1:141:A:HIS:H	9	0.13
(1,1203)	1:132:A:VAL:HG21	1:136:A:PHE:HD1	11	0.13
(1,1203)	1:132:A:VAL:HG22	1:136:A:PHE:HD1	11	0.13
(1,1203)	1:132:A:VAL:HG23	1:136:A:PHE:HD1	11	0.13
(1,1203)	1:132:A:VAL:HG21	1:136:A:PHE:HD1	13	0.13
(1,1203)	1:132:A:VAL:HG22	1:136:A:PHE:HD1	13	0.13
(1,1203)	1:132:A:VAL:HG23	1:136:A:PHE:HD1	13	0.13
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	15	0.13
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	15	0.13
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	15	0.13
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	14	0.13
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	14	0.13
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	18	0.13
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	18	0.13
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	18	0.13
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	19	0.13
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	19	0.13
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	19	0.13
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	1	0.13
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	9	0.13
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	16	0.13
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	19	0.13
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	3	0.13
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	6	0.13
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	9	0.13
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	13	0.13
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	14	0.13
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	17	0.13
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	18	0.13
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	20	0.13
(1,806)	1:90:A:VAL:H	1:91:A:GLY:H	4	0.13
(1,806)	1:90:A:VAL:H	1:91:A:GLY:H	9	0.13
(1,806)	1:90:A:VAL:H	1:91:A:GLY:H	14	0.13
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	11	0.13
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	16	0.13
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	3	0.13
(1,725)	1:82:A:ILE:HG21	1:83:A:ALA:HA	9	0.13
(1,725)	1:82:A:ILE:HG22	1:83:A:ALA:HA	9	0.13
(1,725)	1:82:A:ILE:HG23	1:83:A:ALA:HA	9	0.13
(1,707)	1:80:A:GLN:HB3	1:81:A:LEU:HA	20	0.13
(1,596)	1:65:A:ALA:HA	1:72:A:ILE:HG21	17	0.13
(1,596)	1:65:A:ALA:HA	1:72:A:ILE:HG22	17	0.13
(1,596)	1:65:A:ALA:HA	1:72:A:ILE:HG23	17	0.13
(1,487)	1:55:A:ILE:HB	1:81:A:LEU:HA	1	0.13
(1,487)	1:55:A:ILE:HB	1:81:A:LEU:HA	16	0.13
(1,487)	1:55:A:ILE:HB	1:81:A:LEU:HA	20	0.13
(1,476)	1:54:A:ASP:H	1:77:A:LEU:HG	11	0.13
(1,471)	1:54:A:ASP:H	1:55:A:ILE:HG21	2	0.13
(1,471)	1:54:A:ASP:H	1:55:A:ILE:HG22	2	0.13
(1,471)	1:54:A:ASP:H	1:55:A:ILE:HG23	2	0.13
(1,425)	1:47:A:ILE:H	1:71:A:PRO:HD2	6	0.13
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	17	0.13
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	19	0.13
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	14	0.13
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	8	0.13
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	19	0.13
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	9	0.13
(1,344)	1:38:A:ILE:HD11	1:40:A:SER:H	18	0.13
(1,344)	1:38:A:ILE:HD12	1:40:A:SER:H	18	0.13
(1,344)	1:38:A:ILE:HD13	1:40:A:SER:H	18	0.13
(1,247)	1:27:A:LYS:H	1:28:A:ILE:H	5	0.13
(1,247)	1:27:A:LYS:H	1:28:A:ILE:H	13	0.13
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	10	0.13
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	13	0.13
(1,179)	1:20:A:LYS:HG3	1:20:A:LYS:H	2	0.13
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	14	0.13
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG21	8	0.13
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG22	8	0.13
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG23	8	0.13
(1,41)	1:3:A:VAL:HG21	1:27:A:LYS:H	13	0.13
(1,41)	1:3:A:VAL:HG22	1:27:A:LYS:H	13	0.13
(1,41)	1:3:A:VAL:HG23	1:27:A:LYS:H	13	0.13
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	6	0.13
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	2	0.12
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	7	0.12
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	8	0.12
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	9	0.12
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	12	0.12
(2,61)	1:123:A:ALA:H	1:125:A:HIS:H	1	0.12
(2,59)	1:116:A:PRO:HG3	1:117:A:ARG:HD2	17	0.12
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	1	0.12
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	2	0.12
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	3	0.12
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	7	0.12
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	9	0.12
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	17	0.12
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	18	0.12
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	19	0.12
(2,17)	1:42:A:LYS:HA	1:43:A:GLU:HB3	2	0.12
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	2	0.12
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	7	0.12
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	11	0.12
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	17	0.12
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	3	0.12
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	11	0.12
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	19	0.12
(2,9)	1:24:A:VAL:H	1:181:A:LYS:HZ1	7	0.12
(2,9)	1:24:A:VAL:H	1:181:A:LYS:HZ2	7	0.12
(2,9)	1:24:A:VAL:H	1:181:A:LYS:HZ3	7	0.12
(2,3)	1:8:A:GLY:HA3	1:52:A:GLY:H	20	0.12
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	2	0.12
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	15	0.12
(1,1451)	1:173:A:ASN:HB2	1:174:A:GLU:H	13	0.12
(1,1436)	1:169:A:THR:HA	1:172:A:GLY:H	6	0.12
(1,1364)	1:151:A:LYS:HB3	1:152:A:HIS:H	9	0.12
(1,1363)	1:151:A:LYS:HA	1:152:A:HIS:H	18	0.12
(1,1296)	1:142:A:SER:H	1:146:A:GLN:HA	11	0.12
(1,1295)	1:142:A:SER:H	1:145:A:CYS:HB3	20	0.12
(1,1283)	1:141:A:HIS:H	1:142:A:SER:H	5	0.12
(1,1283)	1:141:A:HIS:H	1:142:A:SER:H	20	0.12
(1,1252)	1:138:A:ILE:HA	1:149:A:ALA:H	5	0.12
(1,1252)	1:138:A:ILE:HA	1:149:A:ALA:H	20	0.12
(1,1046)	1:111:A:LEU:HB2	1:175:A:ILE:H	7	0.12
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	4	0.12
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	4	0.12
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	4	0.12
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	6	0.12
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	6	0.12
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	6	0.12
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	9	0.12
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	9	0.12
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	9	0.12
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	11	0.12
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	11	0.12
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	11	0.12
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	12	0.12
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	12	0.12
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	12	0.12
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	16	0.12
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	16	0.12
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	16	0.12
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	18	0.12
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	18	0.12
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	18	0.12
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	19	0.12
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	19	0.12
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	1	0.12
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	1	0.12
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	1	0.12
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	12	0.12
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	12	0.12
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	12	0.12
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	15	0.12
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	15	0.12
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	15	0.12
(1,950)	1:103:A:VAL:H	1:119:A:PHE:HA	17	0.12
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	15	0.12
(1,935)	1:102:A:LYS:HA	1:119:A:PHE:HA	14	0.12
(1,926)	1:102:A:LYS:HE2	1:102:A:LYS:H	1	0.12
(1,926)	1:102:A:LYS:HE2	1:102:A:LYS:H	7	0.12
(1,926)	1:102:A:LYS:HE2	1:102:A:LYS:H	20	0.12
(1,827)	1:92:A:ARG:HA	1:92:A:ARG:HD2	11	0.12
(1,826)	1:92:A:ARG:H	1:92:A:ARG:HD3	10	0.12
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	7	0.12
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	11	0.12
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	12	0.12
(1,799)	1:89:A:GLU:H	1:132:A:VAL:H	11	0.12
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	2	0.12
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	6	0.12
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	18	0.12
(1,793)	1:89:A:GLU:H	1:90:A:VAL:H	10	0.12
(1,793)	1:89:A:GLU:H	1:90:A:VAL:H	18	0.12
(1,793)	1:89:A:GLU:H	1:90:A:VAL:H	20	0.12
(1,786)	1:88:A:GLY:H	1:89:A:GLU:HB2	16	0.12
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	10	0.12
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	19	0.12
(1,732)	1:83:A:ALA:H	1:84:A:LEU:H	1	0.12
(1,732)	1:83:A:ALA:H	1:84:A:LEU:H	3	0.12
(1,727)	1:82:A:ILE:HG21	1:84:A:LEU:H	12	0.12
(1,727)	1:82:A:ILE:HG22	1:84:A:LEU:H	12	0.12
(1,727)	1:82:A:ILE:HG23	1:84:A:LEU:H	12	0.12
(1,715)	1:81:A:LEU:HB2	1:82:A:ILE:H	5	0.12
(1,715)	1:81:A:LEU:HB2	1:82:A:ILE:H	15	0.12
(1,715)	1:81:A:LEU:HB2	1:82:A:ILE:H	16	0.12
(1,715)	1:81:A:LEU:HB2	1:82:A:ILE:H	20	0.12
(1,695)	1:79:A:HIS:HB3	1:81:A:LEU:H	13	0.12
(1,695)	1:79:A:HIS:HB3	1:81:A:LEU:H	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,695)	1:79:A:HIS:HB3	1:81:A:LEU:H	16	0.12
(1,695)	1:79:A:HIS:HB3	1:81:A:LEU:H	18	0.12
(1,687)	1:78:A:GLY:H	1:80:A:GLN:HB3	15	0.12
(1,487)	1:55:A:ILE:HB	1:81:A:LEU:HA	15	0.12
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	7	0.12
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	17	0.12
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	7	0.12
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	10	0.12
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	20	0.12
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	20	0.12
(1,344)	1:38:A:ILE:HD11	1:40:A:SER:H	8	0.12
(1,344)	1:38:A:ILE:HD12	1:40:A:SER:H	8	0.12
(1,344)	1:38:A:ILE:HD13	1:40:A:SER:H	8	0.12
(1,344)	1:38:A:ILE:HD11	1:40:A:SER:H	19	0.12
(1,344)	1:38:A:ILE:HD12	1:40:A:SER:H	19	0.12
(1,344)	1:38:A:ILE:HD13	1:40:A:SER:H	19	0.12
(1,321)	1:36:A:GLU:H	1:39:A:GLU:H	1	0.12
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD11	7	0.12
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD12	7	0.12
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD13	7	0.12
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD11	15	0.12
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD12	15	0.12
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD13	15	0.12
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	16	0.12
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG21	15	0.12
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG22	15	0.12
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG23	15	0.12
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG21	18	0.12
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG22	18	0.12
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG23	18	0.12
(1,63)	1:4:A:ILE:HG13	1:15:A:ILE:HG12	10	0.12
(1,63)	1:4:A:ILE:HG13	1:15:A:ILE:HG13	10	0.12
(1,44)	1:3:A:VAL:H	1:46:A:GLY:H	3	0.12
(1,44)	1:3:A:VAL:H	1:46:A:GLY:H	14	0.12
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	13	0.12
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	14	0.12
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	19	0.12
(1,27)	1:2:A:ILE:HD11	1:185:A:TYR:HE1	6	0.12
(1,27)	1:2:A:ILE:HD11	1:185:A:TYR:HE2	6	0.12
(1,27)	1:2:A:ILE:HD12	1:185:A:TYR:HE1	6	0.12
(1,27)	1:2:A:ILE:HD12	1:185:A:TYR:HE2	6	0.12
(1,27)	1:2:A:ILE:HD13	1:185:A:TYR:HE1	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:2:A:ILE:HD13	1:185:A:TYR:HE2	6	0.12
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	3	0.12
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	12	0.12
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	14	0.12
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	18	0.12
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	20	0.12
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	3	0.11
(3,92)	1:176:A:LEU:H	1:172:A:GLY:O	16	0.11
(3,56)	1:84:A:LEU:H	1:80:A:GLN:O	12	0.11
(3,54)	1:83:A:ALA:H	1:79:A:HIS:O	9	0.11
(3,11)	1:16:A:HIS:H	1:12:A:VAL:O	3	0.11
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	3	0.11
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	6	0.11
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	11	0.11
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	15	0.11
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	20	0.11
(2,61)	1:123:A:ALA:H	1:125:A:HIS:H	7	0.11
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	4	0.11
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	11	0.11
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	12	0.11
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	13	0.11
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	14	0.11
(2,40)	1:90:A:VAL:HG21	1:133:A:PRO:HD3	13	0.11
(2,40)	1:90:A:VAL:HG22	1:133:A:PRO:HD3	13	0.11
(2,40)	1:90:A:VAL:HG23	1:133:A:PRO:HD3	13	0.11
(2,40)	1:90:A:VAL:HG21	1:133:A:PRO:HD3	15	0.11
(2,40)	1:90:A:VAL:HG22	1:133:A:PRO:HD3	15	0.11
(2,40)	1:90:A:VAL:HG23	1:133:A:PRO:HD3	15	0.11
(2,40)	1:90:A:VAL:HG21	1:133:A:PRO:HD3	18	0.11
(2,40)	1:90:A:VAL:HG22	1:133:A:PRO:HD3	18	0.11
(2,40)	1:90:A:VAL:HG23	1:133:A:PRO:HD3	18	0.11
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	4	0.11
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	6	0.11
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	9	0.11
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	10	0.11
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	14	0.11
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	1	0.11
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	2	0.11
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	8	0.11
(2,3)	1:8:A:GLY:HA3	1:52:A:GLY:H	8	0.11
(2,3)	1:8:A:GLY:HA3	1:52:A:GLY:H	18	0.11
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	12	0.11
(1,1401)	1:156:A:PRO:HD3	1:157:A:ILE:H	19	0.11
(1,1348)	1:150:A:MET:H	1:151:A:LYS:H	9	0.11
(1,1283)	1:141:A:HIS:H	1:142:A:SER:H	3	0.11
(1,1283)	1:141:A:HIS:H	1:142:A:SER:H	4	0.11
(1,1283)	1:141:A:HIS:H	1:142:A:SER:H	7	0.11
(1,1252)	1:138:A:ILE:HA	1:149:A:ALA:H	18	0.11
(1,1223)	1:136:A:PHE:HB3	1:137:A:GLU:H	11	0.11
(1,1046)	1:111:A:LEU:HB2	1:175:A:ILE:H	2	0.11
(1,1046)	1:111:A:LEU:HB2	1:175:A:ILE:H	20	0.11
(1,1044)	1:111:A:LEU:H	1:175:A:ILE:HA	13	0.11
(1,983)	1:105:A:VAL:H	1:118:A:GLU:HA	11	0.11
(1,982)	1:105:A:VAL:HG21	1:117:A:ARG:HG2	14	0.11
(1,982)	1:105:A:VAL:HG22	1:117:A:ARG:HG2	14	0.11
(1,982)	1:105:A:VAL:HG23	1:117:A:ARG:HG2	14	0.11
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	3	0.11
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	3	0.11
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	3	0.11
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	7	0.11
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	7	0.11
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	7	0.11
(1,959)	1:103:A:VAL:HG21	1:143:A:ASP:H	20	0.11
(1,959)	1:103:A:VAL:HG22	1:143:A:ASP:H	20	0.11
(1,959)	1:103:A:VAL:HG23	1:143:A:ASP:H	20	0.11
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	3	0.11
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	3	0.11
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	3	0.11
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	4	0.11
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	4	0.11
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	4	0.11
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	5	0.11
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	5	0.11
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	5	0.11
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	7	0.11
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	7	0.11
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	7	0.11
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	11	0.11
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	11	0.11
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	11	0.11
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	13	0.11
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	13	0.11
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:103:A:VAL:H	1:119:A:PHE:HA	6	0.11
(1,941)	1:102:A:LYS:HG3	1:142:A:SER:HA	11	0.11
(1,936)	1:102:A:LYS:HG3	1:119:A:PHE:H	8	0.11
(1,926)	1:102:A:LYS:HE2	1:102:A:LYS:H	2	0.11
(1,926)	1:102:A:LYS:HE2	1:102:A:LYS:H	18	0.11
(1,899)	1:100:A:LEU:H	1:100:A:LEU:HG	20	0.11
(1,827)	1:92:A:ARG:HA	1:92:A:ARG:HD2	10	0.11
(1,827)	1:92:A:ARG:HA	1:92:A:ARG:HD2	15	0.11
(1,827)	1:92:A:ARG:HA	1:92:A:ARG:HD2	16	0.11
(1,827)	1:92:A:ARG:HA	1:92:A:ARG:HD2	18	0.11
(1,826)	1:92:A:ARG:H	1:92:A:ARG:HD3	11	0.11
(1,826)	1:92:A:ARG:H	1:92:A:ARG:HD3	15	0.11
(1,826)	1:92:A:ARG:H	1:92:A:ARG:HD3	16	0.11
(1,826)	1:92:A:ARG:H	1:92:A:ARG:HD3	18	0.11
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	1	0.11
(1,819)	1:91:A:GLY:H	1:127:A:ASP:HA	16	0.11
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	1	0.11
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	3	0.11
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	8	0.11
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	13	0.11
(1,798)	1:89:A:GLU:H	1:130:A:LYS:H	14	0.11
(1,793)	1:89:A:GLU:H	1:90:A:VAL:H	6	0.11
(1,793)	1:89:A:GLU:H	1:90:A:VAL:H	7	0.11
(1,793)	1:89:A:GLU:H	1:90:A:VAL:H	12	0.11
(1,793)	1:89:A:GLU:H	1:90:A:VAL:H	17	0.11
(1,786)	1:88:A:GLY:H	1:89:A:GLU:HB2	11	0.11
(1,786)	1:88:A:GLY:H	1:89:A:GLU:HB2	13	0.11
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	6	0.11
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	8	0.11
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	12	0.11
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	17	0.11
(1,732)	1:83:A:ALA:H	1:84:A:LEU:H	6	0.11
(1,732)	1:83:A:ALA:H	1:84:A:LEU:H	12	0.11
(1,715)	1:81:A:LEU:HB2	1:82:A:ILE:H	9	0.11
(1,715)	1:81:A:LEU:HB2	1:82:A:ILE:H	11	0.11
(1,715)	1:81:A:LEU:HB2	1:82:A:ILE:H	17	0.11
(1,707)	1:80:A:GLN:HB3	1:81:A:LEU:HA	7	0.11
(1,707)	1:80:A:GLN:HB3	1:81:A:LEU:HA	18	0.11
(1,695)	1:79:A:HIS:HB3	1:81:A:LEU:H	10	0.11
(1,695)	1:79:A:HIS:HB3	1:81:A:LEU:H	11	0.11
(1,695)	1:79:A:HIS:HB3	1:81:A:LEU:H	17	0.11
(1,695)	1:79:A:HIS:HB3	1:81:A:LEU:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,687)	1:78:A:GLY:H	1:80:A:GLN:HB3	11	0.11
(1,650)	1:72:A:ILE:HA	1:183:A:CYS:HG	5	0.11
(1,650)	1:72:A:ILE:HA	1:183:A:CYS:HG	13	0.11
(1,541)	1:61:A:CYS:HB3	1:64:A:ILE:HB	15	0.11
(1,541)	1:61:A:CYS:HB3	1:64:A:ILE:HB	20	0.11
(1,487)	1:55:A:ILE:HB	1:81:A:LEU:HA	9	0.11
(1,487)	1:55:A:ILE:HB	1:81:A:LEU:HA	13	0.11
(1,474)	1:54:A:ASP:HA	1:56:A:GLU:H	16	0.11
(1,444)	1:48:A:ILE:HA	1:74:A:GLY:HA2	12	0.11
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	1	0.11
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	2	0.11
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	6	0.11
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	8	0.11
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	11	0.11
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	12	0.11
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	13	0.11
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	14	0.11
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	16	0.11
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	3	0.11
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	6	0.11
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	8	0.11
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	9	0.11
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	11	0.11
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	18	0.11
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	2	0.11
(1,386)	1:44:A:VAL:H	1:45:A:LYS:H	11	0.11
(1,372)	1:42:A:LYS:HA	1:43:A:GLU:H	10	0.11
(1,372)	1:42:A:LYS:HA	1:43:A:GLU:H	15	0.11
(1,357)	1:40:A:SER:H	1:41:A:ASN:HB3	5	0.11
(1,344)	1:38:A:ILE:HD11	1:40:A:SER:H	3	0.11
(1,344)	1:38:A:ILE:HD12	1:40:A:SER:H	3	0.11
(1,344)	1:38:A:ILE:HD13	1:40:A:SER:H	3	0.11
(1,314)	1:35:A:LEU:H	1:38:A:ILE:H	20	0.11
(1,248)	1:27:A:LYS:HA	1:28:A:ILE:H	18	0.11
(1,247)	1:27:A:LYS:H	1:28:A:ILE:H	1	0.11
(1,247)	1:27:A:LYS:H	1:28:A:ILE:H	2	0.11
(1,247)	1:27:A:LYS:H	1:28:A:ILE:H	3	0.11
(1,247)	1:27:A:LYS:H	1:28:A:ILE:H	11	0.11
(1,247)	1:27:A:LYS:H	1:28:A:ILE:H	19	0.11
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	1	0.11
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	15	0.11
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	20	0.11
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD11	3	0.11
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD12	3	0.11
(1,195)	1:21:A:TYR:HB2	1:22:A:ILE:HD13	3	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	3	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	3	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	3	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	5	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	5	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	5	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	6	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	6	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	6	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	8	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	8	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	8	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	12	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	12	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	12	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	13	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	13	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	13	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	15	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	15	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	15	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	16	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	16	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	16	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	17	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	17	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	17	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	18	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	18	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	18	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	20	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	20	0.11
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	20	0.11
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	5	0.11
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	6	0.11
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	9	0.11
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	11	0.11
(1,63)	1:4:A:ILE:HG13	1:15:A:ILE:HG12	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:4:A:ILE:HG13	1:15:A:ILE:HG13	4	0.11
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	4	0.11
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	7	0.11
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	8	0.11
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	9	0.11
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	10	0.11
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	11	0.11
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	12	0.11
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	17	0.11
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	18	0.11
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	20	0.11
(1,27)	1:2:A:ILE:HD11	1:185:A:TYR:HE1	10	0.11
(1,27)	1:2:A:ILE:HD11	1:185:A:TYR:HE2	10	0.11
(1,27)	1:2:A:ILE:HD12	1:185:A:TYR:HE1	10	0.11
(1,27)	1:2:A:ILE:HD12	1:185:A:TYR:HE2	10	0.11
(1,27)	1:2:A:ILE:HD13	1:185:A:TYR:HE1	10	0.11
(1,27)	1:2:A:ILE:HD13	1:185:A:TYR:HE2	10	0.11
(1,27)	1:2:A:ILE:HD11	1:185:A:TYR:HE1	14	0.11
(1,27)	1:2:A:ILE:HD11	1:185:A:TYR:HE2	14	0.11
(1,27)	1:2:A:ILE:HD12	1:185:A:TYR:HE1	14	0.11
(1,27)	1:2:A:ILE:HD12	1:185:A:TYR:HE2	14	0.11
(1,27)	1:2:A:ILE:HD13	1:185:A:TYR:HE1	14	0.11
(1,27)	1:2:A:ILE:HD13	1:185:A:TYR:HE2	14	0.11
(1,23)	1:2:A:ILE:HD11	1:179:A:PHE:HD1	12	0.11
(1,23)	1:2:A:ILE:HD11	1:179:A:PHE:HD2	12	0.11
(1,23)	1:2:A:ILE:HD12	1:179:A:PHE:HD1	12	0.11
(1,23)	1:2:A:ILE:HD12	1:179:A:PHE:HD2	12	0.11
(1,23)	1:2:A:ILE:HD13	1:179:A:PHE:HD1	12	0.11
(1,23)	1:2:A:ILE:HD13	1:179:A:PHE:HD2	12	0.11
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	1	0.11
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	8	0.11
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	10	0.11
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	11	0.11
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	17	0.11
(3,71)	1:119:A:PHE:H	1:103:A:VAL:O	8	0.1
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	8	0.1
(2,82)	1:181:A:LYS:H	1:185:A:TYR:H	10	0.1
(2,76)	1:153:A:LYS:H	1:157:A:ILE:HB	6	0.1
(2,56)	1:114:A:ASN:HD22	1:115:A:VAL:H	15	0.1
(2,47)	1:102:A:LYS:HA	1:142:A:SER:HB3	9	0.1
(2,47)	1:102:A:LYS:HA	1:142:A:SER:HB3	20	0.1
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	13	0.1
(2,14)	1:35:A:LEU:HA	1:37:A:GLU:HA	15	0.1
(2,11)	1:27:A:LYS:HD2	1:29:A:VAL:H	14	0.1
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	10	0.1
(1,1483)	1:177:A:LYS:H	1:178:A:ASN:HB2	19	0.1
(1,1401)	1:156:A:PRO:HD3	1:157:A:ILE:H	1	0.1
(1,1401)	1:156:A:PRO:HD3	1:157:A:ILE:H	14	0.1
(1,1368)	1:151:A:LYS:HA	1:158:A:TYR:HA	17	0.1
(1,1364)	1:151:A:LYS:HB3	1:152:A:HIS:H	16	0.1
(1,1359)	1:151:A:LYS:H	1:151:A:LYS:HE2	18	0.1
(1,1348)	1:150:A:MET:H	1:151:A:LYS:H	16	0.1
(1,1296)	1:142:A:SER:H	1:146:A:GLN:HA	9	0.1
(1,1283)	1:141:A:HIS:H	1:142:A:SER:H	1	0.1
(1,1283)	1:141:A:HIS:H	1:142:A:SER:H	2	0.1
(1,1283)	1:141:A:HIS:H	1:142:A:SER:H	12	0.1
(1,1235)	1:137:A:GLU:H	1:152:A:HIS:HB2	7	0.1
(1,1223)	1:136:A:PHE:HB3	1:137:A:GLU:H	13	0.1
(1,1046)	1:111:A:LEU:HB2	1:175:A:ILE:H	1	0.1
(1,1044)	1:111:A:LEU:H	1:175:A:ILE:HA	15	0.1
(1,951)	1:103:A:VAL:HG21	1:119:A:PHE:H	2	0.1
(1,951)	1:103:A:VAL:HG22	1:119:A:PHE:H	2	0.1
(1,951)	1:103:A:VAL:HG23	1:119:A:PHE:H	2	0.1
(1,935)	1:102:A:LYS:HA	1:119:A:PHE:HA	3	0.1
(1,899)	1:100:A:LEU:H	1:100:A:LEU:HG	5	0.1
(1,856)	1:94:A:GLU:HB2	1:95:A:ALA:H	9	0.1
(1,856)	1:94:A:GLU:HB2	1:95:A:ALA:H	14	0.1
(1,799)	1:89:A:GLU:H	1:132:A:VAL:H	19	0.1
(1,793)	1:89:A:GLU:H	1:90:A:VAL:H	3	0.1
(1,793)	1:89:A:GLU:H	1:90:A:VAL:H	13	0.1
(1,793)	1:89:A:GLU:H	1:90:A:VAL:H	15	0.1
(1,772)	1:85:A:ALA:HB1	1:87:A:GLY:H	12	0.1
(1,772)	1:85:A:ALA:HB2	1:87:A:GLY:H	12	0.1
(1,772)	1:85:A:ALA:HB3	1:87:A:GLY:H	12	0.1
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	2	0.1
(1,742)	1:83:A:ALA:HA	1:88:A:GLY:HA2	14	0.1
(1,715)	1:81:A:LEU:HB2	1:82:A:ILE:H	4	0.1
(1,707)	1:80:A:GLN:HB3	1:81:A:LEU:HA	13	0.1
(1,695)	1:79:A:HIS:HB3	1:81:A:LEU:H	3	0.1
(1,650)	1:72:A:ILE:HA	1:183:A:CYS:HG	15	0.1
(1,471)	1:54:A:ASP:H	1:55:A:ILE:HG21	17	0.1
(1,471)	1:54:A:ASP:H	1:55:A:ILE:HG22	17	0.1
(1,471)	1:54:A:ASP:H	1:55:A:ILE:HG23	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:49:A:LEU:H	1:75:A:ILE:H	16	0.1
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	7	0.1
(1,404)	1:46:A:GLY:HA2	1:179:A:PHE:HZ	18	0.1
(1,397)	1:46:A:GLY:HA2	1:70:A:LEU:HA	12	0.1
(1,372)	1:42:A:LYS:HA	1:43:A:GLU:H	2	0.1
(1,372)	1:42:A:LYS:HA	1:43:A:GLU:H	19	0.1
(1,364)	1:41:A:ASN:H	1:43:A:GLU:H	20	0.1
(1,344)	1:38:A:ILE:HD11	1:40:A:SER:H	10	0.1
(1,344)	1:38:A:ILE:HD12	1:40:A:SER:H	10	0.1
(1,344)	1:38:A:ILE:HD13	1:40:A:SER:H	10	0.1
(1,344)	1:38:A:ILE:HD11	1:40:A:SER:H	12	0.1
(1,344)	1:38:A:ILE:HD12	1:40:A:SER:H	12	0.1
(1,344)	1:38:A:ILE:HD13	1:40:A:SER:H	12	0.1
(1,344)	1:38:A:ILE:HD11	1:40:A:SER:H	17	0.1
(1,344)	1:38:A:ILE:HD12	1:40:A:SER:H	17	0.1
(1,344)	1:38:A:ILE:HD13	1:40:A:SER:H	17	0.1
(1,247)	1:27:A:LYS:H	1:28:A:ILE:H	14	0.1
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	6	0.1
(1,242)	1:26:A:SER:HA	1:27:A:LYS:H	8	0.1
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	1	0.1
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	1	0.1
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	1	0.1
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	4	0.1
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	4	0.1
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	4	0.1
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ1	9	0.1
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ2	9	0.1
(1,174)	1:20:A:LYS:H	1:20:A:LYS:HZ3	9	0.1
(1,147)	1:15:A:ILE:HG12	1:48:A:ILE:HG12	7	0.1
(1,147)	1:15:A:ILE:HG12	1:48:A:ILE:HG13	7	0.1
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	19	0.1
(1,127)	1:12:A:VAL:HB	1:15:A:ILE:HG13	20	0.1
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG21	9	0.1
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG22	9	0.1
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG23	9	0.1
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG21	12	0.1
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG22	12	0.1
(1,111)	1:8:A:GLY:H	1:12:A:VAL:HG23	12	0.1
(1,64)	1:4:A:ILE:H	1:26:A:SER:HA	7	0.1
(1,64)	1:4:A:ILE:H	1:26:A:SER:HA	9	0.1
(1,59)	1:4:A:ILE:HB	1:5:A:LEU:HD21	3	0.1
(1,59)	1:4:A:ILE:HB	1:5:A:LEU:HD22	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:4:A:ILE:HB	1:5:A:LEU:HD23	3	0.1
(1,59)	1:4:A:ILE:HB	1:5:A:LEU:HD21	20	0.1
(1,59)	1:4:A:ILE:HB	1:5:A:LEU:HD22	20	0.1
(1,59)	1:4:A:ILE:HB	1:5:A:LEU:HD23	20	0.1
(1,44)	1:3:A:VAL:H	1:46:A:GLY:H	7	0.1
(1,44)	1:3:A:VAL:H	1:46:A:GLY:H	9	0.1
(1,44)	1:3:A:VAL:H	1:46:A:GLY:H	12	0.1
(1,41)	1:3:A:VAL:HG21	1:27:A:LYS:H	5	0.1
(1,41)	1:3:A:VAL:HG22	1:27:A:LYS:H	5	0.1
(1,41)	1:3:A:VAL:HG23	1:27:A:LYS:H	5	0.1
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	3	0.1
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	5	0.1
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	15	0.1
(1,28)	1:2:A:ILE:H	1:186:A:LYS:HB2	16	0.1
(1,27)	1:2:A:ILE:HD11	1:185:A:TYR:HE1	17	0.1
(1,27)	1:2:A:ILE:HD11	1:185:A:TYR:HE2	17	0.1
(1,27)	1:2:A:ILE:HD12	1:185:A:TYR:HE1	17	0.1
(1,27)	1:2:A:ILE:HD12	1:185:A:TYR:HE2	17	0.1
(1,27)	1:2:A:ILE:HD13	1:185:A:TYR:HE1	17	0.1
(1,27)	1:2:A:ILE:HD13	1:185:A:TYR:HE2	17	0.1
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	2	0.1
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	4	0.1
(1,10)	1:2:A:ILE:HG12	1:3:A:VAL:HG23	15	0.1

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

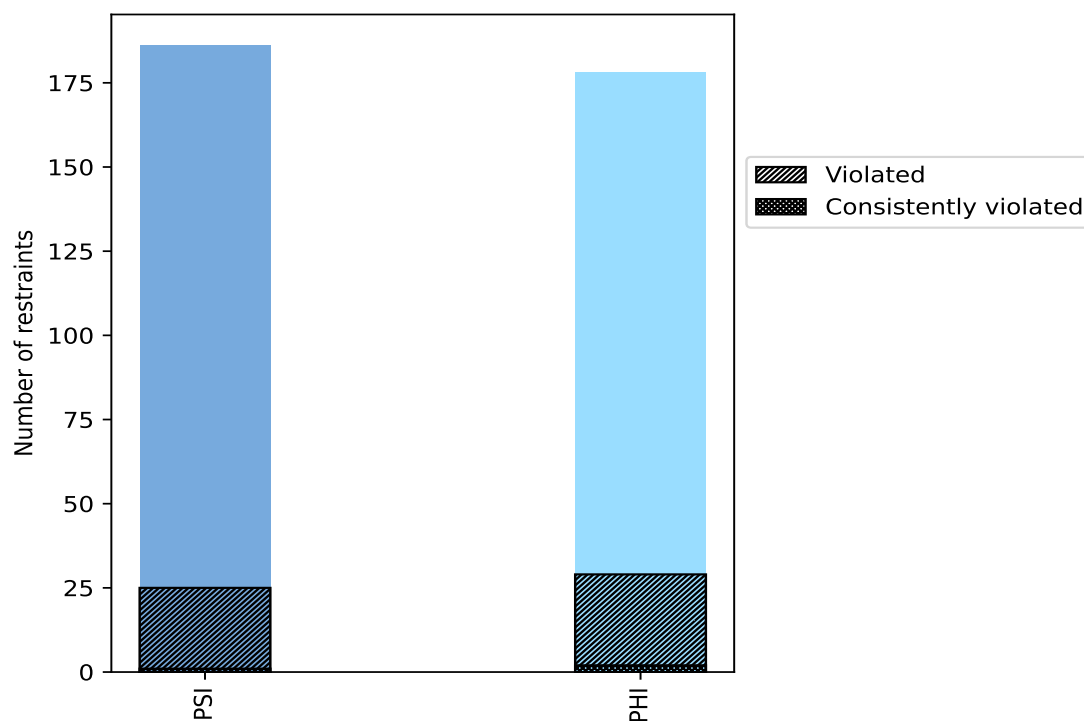
10.1 Summary of dihedral-angle violations [i](#)

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	186	51.1	25	13.4	6.9	1	0.5	0.3
PHI	178	48.9	29	16.3	8.0	2	1.1	0.5
Total	364	100.0	54	14.8	14.8	3	0.8	0.8

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](#)



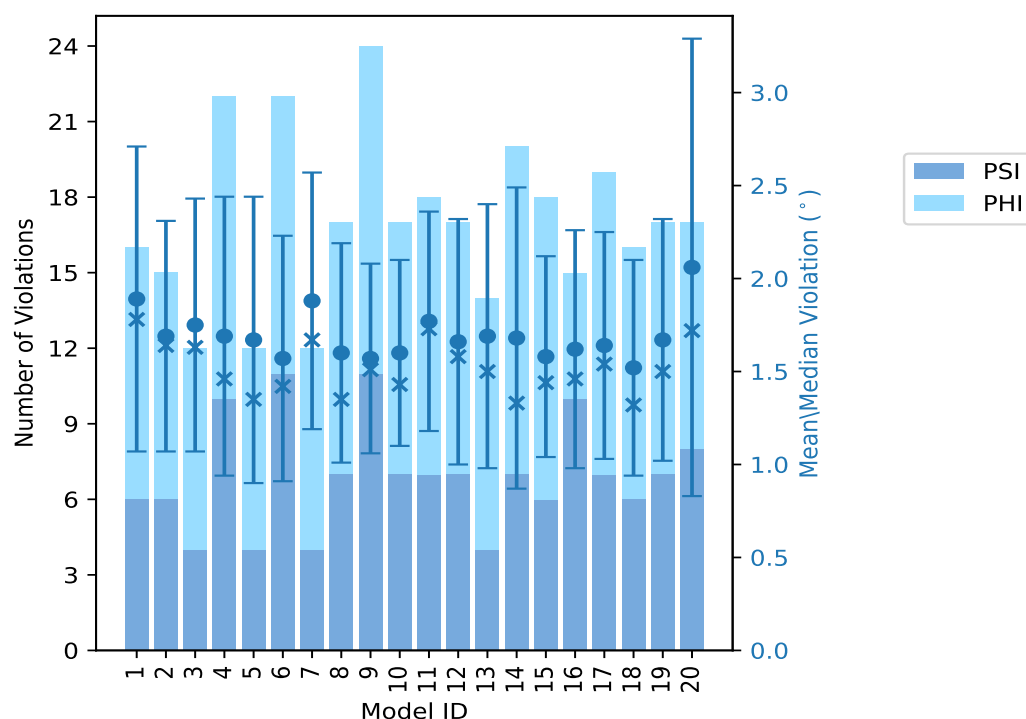
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	6	10	16	1.89	3.77	0.82	1.78
2	6	9	15	1.69	3.49	0.62	1.64
3	4	8	12	1.75	3.56	0.68	1.63
4	10	12	22	1.69	3.81	0.75	1.46
5	4	8	12	1.67	3.68	0.77	1.35
6	11	11	22	1.57	3.73	0.66	1.42
7	4	8	12	1.88	3.55	0.69	1.67
8	7	10	17	1.6	3.46	0.59	1.35
9	11	13	24	1.57	3.65	0.51	1.51
10	7	10	17	1.6	2.95	0.5	1.43
11	7	11	18	1.77	3.53	0.59	1.73
12	7	10	17	1.66	3.81	0.66	1.58
13	4	10	14	1.69	3.31	0.71	1.5
14	7	13	20	1.68	3.76	0.81	1.33
15	6	12	18	1.58	3.07	0.54	1.44
16	10	5	15	1.62	3.24	0.64	1.46
17	7	12	19	1.64	3.79	0.61	1.54
18	6	10	16	1.52	3.13	0.58	1.32
19	7	10	17	1.67	3.81	0.65	1.5
20	8	9	17	2.06	5.99	1.23	1.72

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	%
7	3	10	1	5.0
1	5	6	2	10.0
6	6	12	3	15.0
3	1	4	4	20.0
3	2	5	5	25.0
0	0	0	6	30.0
0	2	2	7	35.0
0	0	0	8	40.0
0	2	2	9	45.0
0	0	0	10	50.0
0	2	2	11	55.0

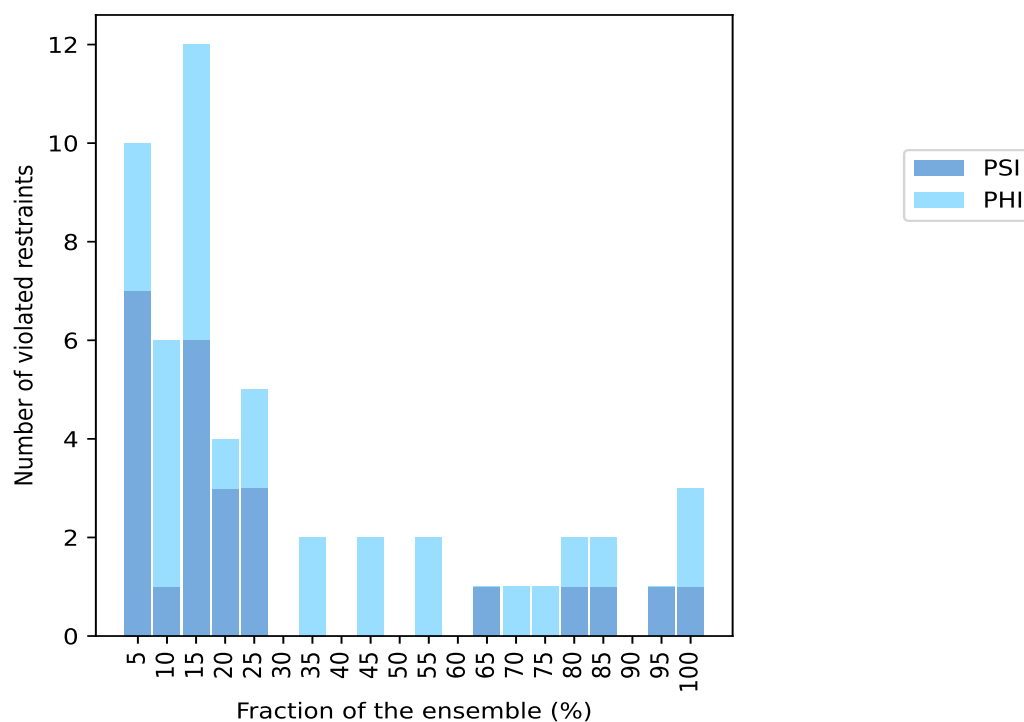
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
1	0	1	13	65.0
0	1	1	14	70.0
0	1	1	15	75.0
1	1	2	16	80.0
1	1	2	17	85.0
0	0	0	18	90.0
1	0	1	19	95.0
1	2	3	20	100.0

¹ Number of models with violations

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

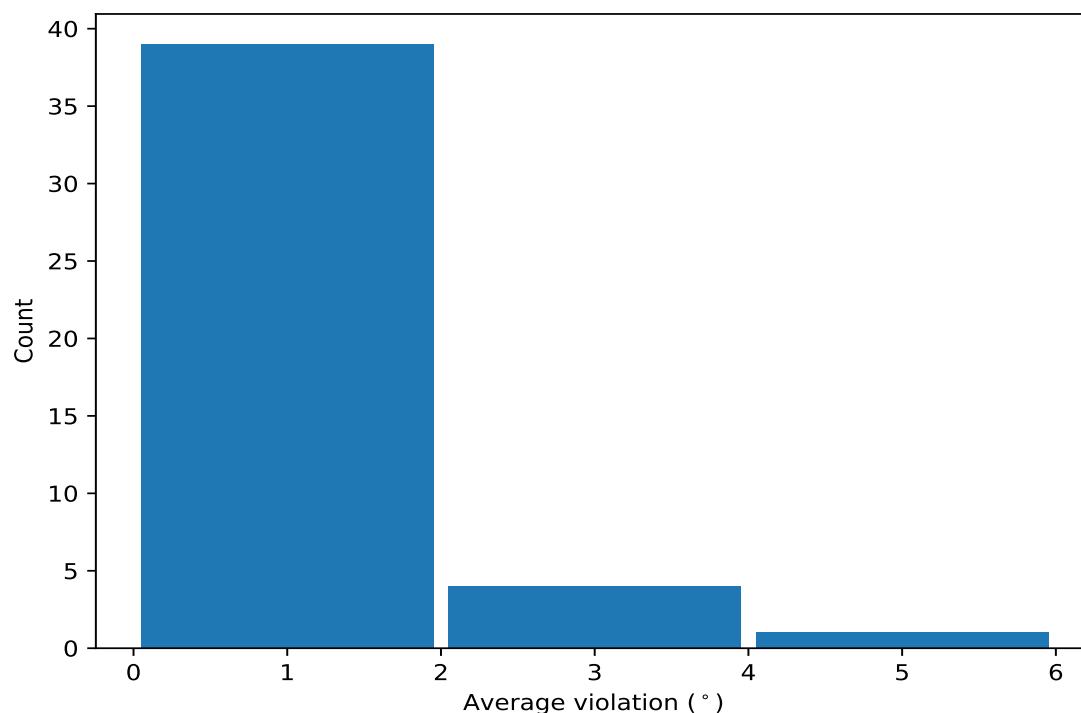


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	20	3.47	0.25	3.52
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	20	2.08	0.38	2.07
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	20	1.73	0.13	1.72
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	19	1.55	0.31	1.49
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	17	2.02	0.5	1.99
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	17	1.69	0.37	1.71
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	16	1.85	0.32	1.86
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	16	1.64	0.33	1.69
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	15	1.56	0.4	1.47
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	14	1.46	0.49	1.18
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	13	1.46	0.36	1.35
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	11	1.3	0.25	1.28
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	11	1.11	0.09	1.1
(1,308)	1:158:A:TYR:C	1:159:A:GLY:N	1:159:A:GLY:CA	1:159:A:GLY:C	9	1.34	0.25	1.46
(1,267)	1:137:A:GLU:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	9	1.27	0.19	1.2
(1,11)	1:6:A:ASP:C	1:7:A:ASN:N	1:7:A:ASN:CA	1:7:A:ASN:C	7	1.33	0.25	1.36
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	7	1.25	0.36	1.1
(1,300)	1:154:A:THR:N	1:154:A:THR:CA	1:154:A:THR:C	1:155:A:LYS:N	5	1.9	0.98	1.44
(1,220)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:ASN:N	5	1.55	0.33	1.46
(1,13)	1:7:A:ASN:C	1:8:A:GLY:N	1:8:A:GLY:CA	1:8:A:GLY:C	5	1.32	0.15	1.33

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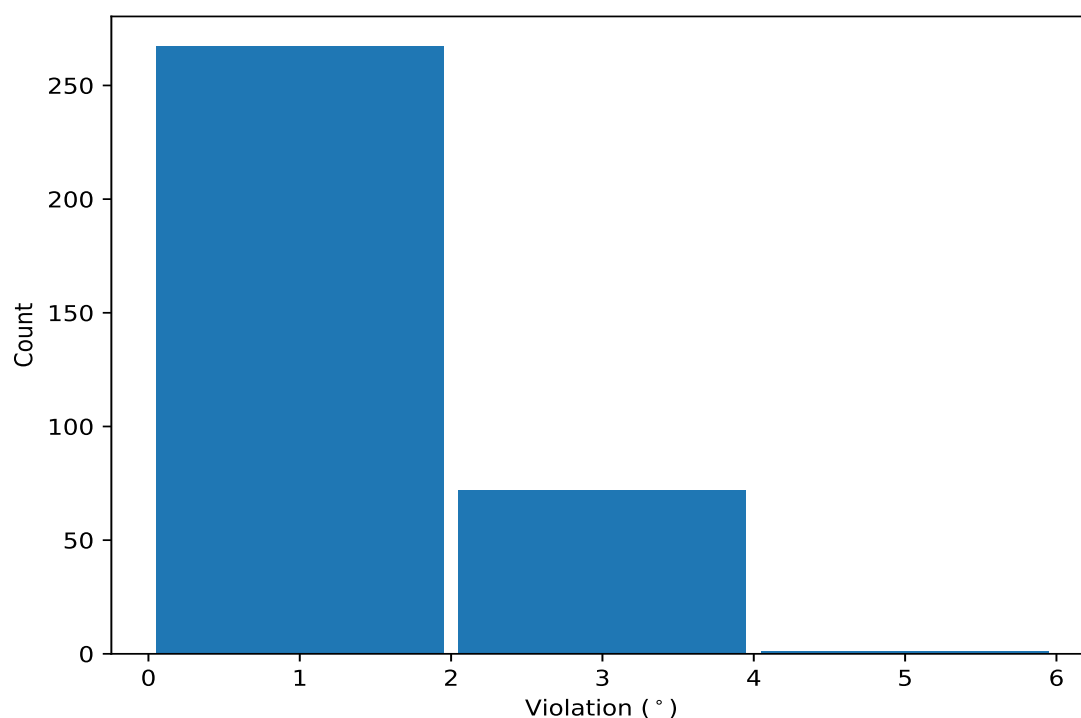
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,143)	1:74:A:GLY:C	1:75:A:ILE:N	1:75:A:ILE:CA	1:75:A:ILE:C	5	1.3	0.14	1.25
(1,356)	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	1:184:A:GLY:N	5	1.17	0.08	1.14
(1,332)	1:171:A:TYR:N	1:171:A:TYR:CA	1:171:A:TYR:C	1:172:A:GLY:N	4	2.34	0.85	1.99
(1,147)	1:76:A:CYS:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	4	1.92	1.02	1.5
(1,57)	1:30:A:PRO:N	1:30:A:PRO:CA	1:30:A:PRO:C	1:31:A:ASN:N	4	1.22	0.17	1.2
(1,10)	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	1:7:A:ASN:N	4	1.17	0.07	1.15
(1,239)	1:123:A:ALA:N	1:123:A:ALA:CA	1:123:A:ALA:C	1:124:A:SER:N	3	1.84	0.75	1.56
(1,189)	1:97:A:GLU:C	1:98:A:TYR:N	1:98:A:TYR:CA	1:98:A:TYR:C	3	1.41	0.05	1.41
(1,202)	1:104:A:TYR:N	1:104:A:TYR:CA	1:104:A:TYR:C	1:105:A:VAL:N	3	1.37	0.28	1.43
(1,225)	1:116:A:PRO:N	1:116:A:PRO:CA	1:116:A:PRO:C	1:117:A:ARG:N	3	1.35	0.16	1.4
(1,134)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	3	1.32	0.23	1.25
(1,282)	1:145:A:CYS:N	1:145:A:CYS:CA	1:145:A:CYS:C	1:146:A:GLN:N	3	1.31	0.15	1.4
(1,177)	1:91:A:GLY:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	3	1.29	0.07	1.3
(1,129)	1:67:A:ASN:N	1:67:A:ASN:CA	1:67:A:ASN:C	1:68:A:ALA:N	3	1.19	0.07	1.15
(1,60)	1:31:A:ASN:C	1:32:A:THR:N	1:32:A:THR:CA	1:32:A:THR:C	3	1.13	0.06	1.09
(1,359)	1:184:A:GLY:C	1:185:A:TYR:N	1:185:A:TYR:CA	1:185:A:TYR:C	3	1.07	0.04	1.1
(1,362)	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	1:187:A:PHE:N	3	1.06	0.04	1.06
(1,141)	1:73:A:LEU:C	1:74:A:GLY:N	1:74:A:GLY:CA	1:74:A:GLY:C	3	1.06	0.05	1.03
(1,333)	1:171:A:TYR:C	1:172:A:GLY:N	1:172:A:GLY:CA	1:172:A:GLY:C	2	4.86	1.13	4.86
(1,329)	1:169:A:THR:C	1:170:A:GLU:N	1:170:A:GLU:CA	1:170:A:GLU:C	2	1.48	0.44	1.48
(1,232)	1:119:A:PHE:C	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	2	1.38	0.08	1.38
(1,213)	1:109:A:ASN:C	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	2	1.34	0.28	1.34
(1,136)	1:71:A:PRO:N	1:71:A:PRO:CA	1:71:A:PRO:C	1:72:A:ILE:N	2	1.1	0.06	1.1
(1,357)	1:183:A:CYS:C	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	2	1.04	0.02	1.04

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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 (°)
(1,333)	1:171:A:TYR:C	1:172:A:GLY:N	1:172:A:GLY:CA	1:172:A:GLY:C	20	5.99
(1,300)	1:154:A:THR:N	1:154:A:THR:CA	1:154:A:THR:C	1:155:A:LYS:N	4	3.81
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	12	3.81
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	19	3.81
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	17	3.79
(1,332)	1:171:A:TYR:N	1:171:A:TYR:CA	1:171:A:TYR:C	1:172:A:GLY:N	20	3.77
(1,240)	1:123:A:ALA:C	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1	3.77
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	14	3.76
(1,333)	1:171:A:TYR:C	1:172:A:GLY:N	1:172:A:GLY:CA	1:172:A:GLY:C	6	3.73
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	5	3.68
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	9	3.65
(1,147)	1:76:A:CYS:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	14	3.61
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	1	3.59
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	3	3.56
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	7	3.55
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	11	3.53
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	4	3.51
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	2	3.49
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	8	3.46
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	13	3.31
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	6	3.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	20	3.29
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	16	3.24
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	18	3.13
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	15	3.07
(1,182)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:ALA:N	10	2.95
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	4	2.88
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	16	2.87
(1,239)	1:123:A:ALA:N	1:123:A:ALA:CA	1:123:A:ALA:C	1:124:A:SER:N	1	2.87
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	5	2.76
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	13	2.76
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	14	2.64
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	7	2.6
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	19	2.56
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	11	2.46
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	14	2.43
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	15	2.39
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	2	2.38
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	20	2.34
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	13	2.32
(1,104)	1:54:A:ASP:C	1:55:A:ILE:N	1:55:A:ILE:CA	1:55:A:ILE:C	11	2.32
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	18	2.3
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	10	2.29
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	7	2.28
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	7	2.27
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	13	2.27
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	12	2.25
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	18	2.23
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	8	2.23
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	8	2.2
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	4	2.2
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	10	2.2
(1,332)	1:171:A:TYR:N	1:171:A:TYR:CA	1:171:A:TYR:C	1:172:A:GLY:N	17	2.16
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	3	2.15
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	3	2.14
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	10	2.13
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	16	2.13
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	9	2.12
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	7	2.09
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	15	2.06
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	1	2.05
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	3	2.04
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	12	2.03
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	19	2.03
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	12	2.02
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	12	2.02
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	5	2.02
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	20	2.02
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	2	2.01
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	17	2.0
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	11	2.0
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	17	2.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	15	2.0
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	3	1.99
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	11	1.99
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	8	1.98
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	11	1.97
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	19	1.97
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	18	1.96
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	20	1.96
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	1	1.96
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	20	1.95
(1,220)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:ASN:N	6	1.94
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	14	1.94
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	15	1.93
(1,220)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:ASN:N	20	1.93
(1,329)	1:169:A:THR:C	1:170:A:GLU:N	1:170:A:GLU:CA	1:170:A:GLU:C	13	1.92
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	1	1.91
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	17	1.89
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	1	1.89
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	2	1.89
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	1	1.88
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	16	1.88
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	2	1.86
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	8	1.85
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	4	1.84
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	6	1.83
(1,332)	1:171:A:TYR:N	1:171:A:TYR:CA	1:171:A:TYR:C	1:172:A:GLY:N	15	1.82
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	17	1.82
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	14	1.82
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	8	1.82
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	9	1.81
(1,147)	1:76:A:CYS:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	11	1.81
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	17	1.8
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	9	1.79
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	2	1.78
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	2	1.78
(1,300)	1:154:A:THR:N	1:154:A:THR:CA	1:154:A:THR:C	1:155:A:LYS:N	11	1.77
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	11	1.77
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	12	1.77
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	9	1.76
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	14	1.76
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	10	1.75
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	7	1.75
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	13	1.75
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	9	1.74
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	12	1.73
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	4	1.73
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	20	1.72
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	4	1.72
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	14	1.71
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	3	1.71
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	6	1.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	13	1.7
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	19	1.7
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	9	1.7
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	1	1.69
(1,202)	1:104:A:TYR:N	1:104:A:TYR:CA	1:104:A:TYR:C	1:105:A:VAL:N	9	1.69
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	11	1.69
(1,308)	1:158:A:TYR:C	1:159:A:GLY:N	1:159:A:GLY:CA	1:159:A:GLY:C	11	1.68
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	12	1.68
(1,11)	1:6:A:ASP:C	1:7:A:ASN:N	1:7:A:ASN:CA	1:7:A:ASN:C	9	1.68
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	11	1.67
(1,267)	1:137:A:GLU:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	10	1.66
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	9	1.66
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	4	1.66
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	6	1.66
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	19	1.65
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	19	1.65
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	17	1.65
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	2	1.64
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	15	1.63
(1,134)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	17	1.63
(1,82)	1:43:A:GLU:N	1:43:A:GLU:CA	1:43:A:GLU:C	1:44:A:VAL:N	16	1.63
(1,11)	1:6:A:ASP:C	1:7:A:ASN:N	1:7:A:ASN:CA	1:7:A:ASN:C	19	1.63
(1,213)	1:109:A:ASN:C	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	5	1.62
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	15	1.61
(1,332)	1:171:A:TYR:N	1:171:A:TYR:CA	1:171:A:TYR:C	1:172:A:GLY:N	6	1.6
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	7	1.59
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	4	1.58
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	12	1.58
(1,308)	1:158:A:TYR:C	1:159:A:GLY:N	1:159:A:GLY:CA	1:159:A:GLY:C	2	1.56
(1,239)	1:123:A:ALA:N	1:123:A:ALA:CA	1:123:A:ALA:C	1:124:A:SER:N	4	1.56
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	1	1.56
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	5	1.56
(1,143)	1:74:A:GLY:C	1:75:A:ILE:N	1:75:A:ILE:CA	1:75:A:ILE:C	11	1.56
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	1	1.55
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	3	1.55
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	18	1.55
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	17	1.54
(1,308)	1:158:A:TYR:C	1:159:A:GLY:N	1:159:A:GLY:CA	1:159:A:GLY:C	9	1.53
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	10	1.53
(1,225)	1:116:A:PRO:N	1:116:A:PRO:CA	1:116:A:PRO:C	1:117:A:ARG:N	20	1.52
(1,308)	1:158:A:TYR:C	1:159:A:GLY:N	1:159:A:GLY:CA	1:159:A:GLY:C	4	1.51
(1,264)	1:136:A:PHE:N	1:136:A:PHE:CA	1:136:A:PHE:C	1:137:A:GLU:N	9	1.51
(1,183)	1:94:A:GLU:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	16	1.51
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	7	1.51
(1,13)	1:7:A:ASN:C	1:8:A:GLY:N	1:8:A:GLY:CA	1:8:A:GLY:C	9	1.51
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	7	1.5
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	19	1.5
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	16	1.49
(1,355)	1:182:A:VAL:C	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	6	1.48
(1,57)	1:30:A:PRO:N	1:30:A:PRO:CA	1:30:A:PRO:C	1:31:A:ASN:N	19	1.48
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	6	1.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	6	1.47
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	18	1.47
(1,189)	1:97:A:GLU:C	1:98:A:TYR:N	1:98:A:TYR:CA	1:98:A:TYR:C	15	1.47
(1,308)	1:158:A:TYR:C	1:159:A:GLY:N	1:159:A:GLY:CA	1:159:A:GLY:C	10	1.46
(1,232)	1:119:A:PHE:C	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	17	1.46
(1,220)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:ASN:N	16	1.46
(1,267)	1:137:A:GLU:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	14	1.45
(1,300)	1:154:A:THR:N	1:154:A:THR:CA	1:154:A:THR:C	1:155:A:LYS:N	20	1.44
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	9	1.44
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	20	1.44
(1,282)	1:145:A:CYS:N	1:145:A:CYS:CA	1:145:A:CYS:C	1:146:A:GLN:N	16	1.43
(1,202)	1:104:A:TYR:N	1:104:A:TYR:CA	1:104:A:TYR:C	1:105:A:VAL:N	10	1.43
(1,11)	1:6:A:ASP:C	1:7:A:ASN:N	1:7:A:ASN:CA	1:7:A:ASN:C	6	1.43
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	19	1.42
(1,13)	1:7:A:ASN:C	1:8:A:GLY:N	1:8:A:GLY:CA	1:8:A:GLY:C	18	1.42
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	8	1.41
(1,189)	1:97:A:GLU:C	1:98:A:TYR:N	1:98:A:TYR:CA	1:98:A:TYR:C	8	1.41
(1,282)	1:145:A:CYS:N	1:145:A:CYS:CA	1:145:A:CYS:C	1:146:A:GLN:N	11	1.4
(1,267)	1:137:A:GLU:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	15	1.4
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	4	1.4
(1,225)	1:116:A:PRO:N	1:116:A:PRO:CA	1:116:A:PRO:C	1:117:A:ARG:N	6	1.4
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	2	1.39
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	10	1.39
(1,300)	1:154:A:THR:N	1:154:A:THR:CA	1:154:A:THR:C	1:155:A:LYS:N	10	1.38
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	4	1.38
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	10	1.37
(1,177)	1:91:A:GLY:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	20	1.37
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	9	1.36
(1,11)	1:6:A:ASP:C	1:7:A:ASN:N	1:7:A:ASN:CA	1:7:A:ASN:C	4	1.36
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	8	1.35
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	5	1.35
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	3	1.35
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	9	1.35
(1,189)	1:97:A:GLU:C	1:98:A:TYR:N	1:98:A:TYR:CA	1:98:A:TYR:C	9	1.35
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	5	1.34
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	14	1.34
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	18	1.34
(1,13)	1:7:A:ASN:C	1:8:A:GLY:N	1:8:A:GLY:CA	1:8:A:GLY:C	8	1.33
(1,267)	1:137:A:GLU:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	19	1.32
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	14	1.32
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	3	1.31
(1,143)	1:74:A:GLY:C	1:75:A:ILE:N	1:75:A:ILE:CA	1:75:A:ILE:C	12	1.31
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	6	1.3
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	16	1.3
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	13	1.3
(1,177)	1:91:A:GLY:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	17	1.3
(1,232)	1:119:A:PHE:C	1:120:A:ASN:N	1:120:A:ASN:CA	1:120:A:ASN:C	6	1.29
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	18	1.29
(1,356)	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	1:184:A:GLY:N	5	1.28
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	17	1.28
(1,129)	1:67:A:ASN:N	1:67:A:ASN:CA	1:67:A:ASN:C	1:68:A:ALA:N	12	1.28

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	17	1.27
(1,57)	1:30:A:PRO:N	1:30:A:PRO:CA	1:30:A:PRO:C	1:31:A:ASN:N	8	1.27
(1,10)	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	1:7:A:ASN:N	8	1.27
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	4	1.26
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	15	1.26
(1,220)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:ASN:N	10	1.25
(1,180)	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	1:94:A:GLU:N	9	1.25
(1,143)	1:74:A:GLY:C	1:75:A:ILE:N	1:75:A:ILE:CA	1:75:A:ILE:C	9	1.25
(1,134)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	11	1.25
(1,13)	1:7:A:ASN:C	1:8:A:GLY:N	1:8:A:GLY:CA	1:8:A:GLY:C	10	1.25
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	12	1.24
(1,143)	1:74:A:GLY:C	1:75:A:ILE:N	1:75:A:ILE:CA	1:75:A:ILE:C	17	1.23
(1,356)	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	1:184:A:GLY:N	4	1.22
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	12	1.22
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	8	1.22
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	19	1.21
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	6	1.21
(1,177)	1:91:A:GLY:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	6	1.21
(1,60)	1:31:A:ASN:C	1:32:A:THR:N	1:32:A:THR:CA	1:32:A:THR:C	15	1.21
(1,267)	1:137:A:GLU:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	4	1.2
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	19	1.2
(1,308)	1:158:A:TYR:C	1:159:A:GLY:N	1:159:A:GLY:CA	1:159:A:GLY:C	7	1.19
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	2	1.19
(1,231)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:ASN:N	15	1.19
(1,147)	1:76:A:CYS:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	18	1.19
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	14	1.19
(1,11)	1:6:A:ASP:C	1:7:A:ASN:N	1:7:A:ASN:CA	1:7:A:ASN:C	1	1.19
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	14	1.18
(1,10)	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	1:7:A:ASN:N	18	1.18
(1,267)	1:137:A:GLU:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	2	1.17
(1,143)	1:74:A:GLY:C	1:75:A:ILE:N	1:75:A:ILE:CA	1:75:A:ILE:C	5	1.17
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	8	1.17
(1,136)	1:71:A:PRO:N	1:71:A:PRO:CA	1:71:A:PRO:C	1:72:A:ILE:N	14	1.16
(1,220)	1:113:A:LYS:N	1:113:A:LYS:CA	1:113:A:LYS:C	1:114:A:ASN:N	8	1.15
(1,129)	1:67:A:ASN:N	1:67:A:ASN:CA	1:67:A:ASN:C	1:68:A:ALA:N	6	1.15
(1,356)	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	1:184:A:GLY:N	12	1.14
(1,356)	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	1:184:A:GLY:N	16	1.14
(1,267)	1:137:A:GLU:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	9	1.14
(1,242)	1:124:A:SER:C	1:125:A:HIS:N	1:125:A:HIS:CA	1:125:A:HIS:C	1	1.14
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	8	1.14
(1,214)	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	1:111:A:LEU:N	19	1.14
(1,225)	1:116:A:PRO:N	1:116:A:PRO:CA	1:116:A:PRO:C	1:117:A:ARG:N	9	1.13
(1,141)	1:73:A:LEU:C	1:74:A:GLY:N	1:74:A:GLY:CA	1:74:A:GLY:C	6	1.13
(1,129)	1:67:A:ASN:N	1:67:A:ASN:CA	1:67:A:ASN:C	1:68:A:ALA:N	17	1.13
(1,57)	1:30:A:PRO:N	1:30:A:PRO:CA	1:30:A:PRO:C	1:31:A:ASN:N	4	1.13
(1,10)	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	1:7:A:ASN:N	2	1.13
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	17	1.12
(1,362)	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	1:187:A:PHE:N	4	1.11
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	10	1.11
(1,300)	1:154:A:THR:N	1:154:A:THR:CA	1:154:A:THR:C	1:155:A:LYS:N	9	1.11
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	20	1.11

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	6	1.11
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	5	1.11
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	9	1.11
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	13	1.11
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	12	1.1
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	15	1.1
(1,359)	1:184:A:GLY:C	1:185:A:TYR:N	1:185:A:TYR:CA	1:185:A:TYR:C	1	1.1
(1,359)	1:184:A:GLY:C	1:185:A:TYR:N	1:185:A:TYR:CA	1:185:A:TYR:C	19	1.1
(1,267)	1:137:A:GLU:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	7	1.1
(1,239)	1:123:A:ALA:N	1:123:A:ALA:CA	1:123:A:ALA:C	1:124:A:SER:N	16	1.1
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1	1.1
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	5	1.1
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	6	1.1
(1,282)	1:145:A:CYS:N	1:145:A:CYS:CA	1:145:A:CYS:C	1:146:A:GLN:N	19	1.09
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	15	1.09
(1,60)	1:31:A:ASN:C	1:32:A:THR:N	1:32:A:THR:CA	1:32:A:THR:C	12	1.09
(1,10)	1:6:A:ASP:N	1:6:A:ASP:CA	1:6:A:ASP:C	1:7:A:ASN:N	16	1.09
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	14	1.09
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	2	1.08
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	3	1.08
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	13	1.08
(1,205)	1:105:A:VAL:C	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	20	1.08
(1,60)	1:31:A:ASN:C	1:32:A:THR:N	1:32:A:THR:CA	1:32:A:THR:C	20	1.08
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	18	1.08
(1,309)	1:159:A:GLY:N	1:159:A:GLY:CA	1:159:A:GLY:C	1:160:A:VAL:N	13	1.07
(1,308)	1:158:A:TYR:C	1:159:A:GLY:N	1:159:A:GLY:CA	1:159:A:GLY:C	15	1.07
(1,241)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:HIS:N	18	1.07
(1,134)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	7	1.07
(1,74)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	3	1.07
(1,13)	1:7:A:ASN:C	1:8:A:GLY:N	1:8:A:GLY:CA	1:8:A:GLY:C	15	1.07
(1,362)	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	1:187:A:PHE:N	6	1.06
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	14	1.06
(1,356)	1:183:A:CYS:N	1:183:A:CYS:CA	1:183:A:CYS:C	1:184:A:GLY:N	1	1.06
(1,213)	1:109:A:ASN:C	1:110:A:ASP:N	1:110:A:ASP:CA	1:110:A:ASP:C	13	1.06
(1,357)	1:183:A:CYS:C	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	4	1.05
(1,257)	1:132:A:VAL:N	1:132:A:VAL:CA	1:132:A:VAL:C	1:133:A:PRO:N	18	1.05
(1,147)	1:76:A:CYS:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	10	1.05
(1,80)	1:42:A:LYS:N	1:42:A:LYS:CA	1:42:A:LYS:C	1:43:A:GLU:N	16	1.05
(1,1)	1:1:A:MET:C	1:2:A:ILE:N	1:2:A:ILE:CA	1:2:A:ILE:C	17	1.05
(1,308)	1:158:A:TYR:C	1:159:A:GLY:N	1:159:A:GLY:CA	1:159:A:GLY:C	20	1.04
(1,215)	1:110:A:ASP:C	1:111:A:LEU:N	1:111:A:LEU:CA	1:111:A:LEU:C	18	1.04
(1,179)	1:92:A:ARG:C	1:93:A:ALA:N	1:93:A:ALA:CA	1:93:A:ALA:C	18	1.04
(1,136)	1:71:A:PRO:N	1:71:A:PRO:CA	1:71:A:PRO:C	1:72:A:ILE:N	6	1.04
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	14	1.04
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	17	1.04
(1,329)	1:169:A:THR:C	1:170:A:GLU:N	1:170:A:GLU:CA	1:170:A:GLU:C	4	1.03
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	3	1.03
(1,141)	1:73:A:LEU:C	1:74:A:GLY:N	1:74:A:GLY:CA	1:74:A:GLY:C	14	1.03
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	15	1.03
(1,11)	1:6:A:ASP:C	1:7:A:ASN:N	1:7:A:ASN:CA	1:7:A:ASN:C	13	1.03
(1,362)	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	1:187:A:PHE:N	9	1.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,359)	1:184:A:GLY:C	1:185:A:TYR:N	1:185:A:TYR:CA	1:185:A:TYR:C	11	1.02
(1,357)	1:183:A:CYS:C	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	5	1.02
(1,71)	1:37:A:GLU:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	4	1.02
(1,11)	1:6:A:ASP:C	1:7:A:ASN:N	1:7:A:ASN:CA	1:7:A:ASN:C	10	1.02
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	13	1.01
(1,267)	1:137:A:GLU:C	1:138:A:ILE:N	1:138:A:ILE:CA	1:138:A:ILE:C	8	1.01
(1,141)	1:73:A:LEU:C	1:74:A:GLY:N	1:74:A:GLY:CA	1:74:A:GLY:C	12	1.01
(1,57)	1:30:A:PRO:N	1:30:A:PRO:CA	1:30:A:PRO:C	1:31:A:ASN:N	16	1.01
(1,361)	1:185:A:TYR:C	1:186:A:LYS:N	1:186:A:LYS:CA	1:186:A:LYS:C	11	1.0
(1,308)	1:158:A:TYR:C	1:159:A:GLY:N	1:159:A:GLY:CA	1:159:A:GLY:C	14	1.0
(1,259)	1:133:A:PRO:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	2	1.0
(1,208)	1:107:A:LYS:N	1:107:A:LYS:CA	1:107:A:LYS:C	1:108:A:GLU:N	14	1.0
(1,202)	1:104:A:TYR:N	1:104:A:TYR:CA	1:104:A:TYR:C	1:105:A:VAL:N	11	1.0