



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 09:53 PM EST

PDB ID : 2MHG
BMRB ID : 19632
Title : NMR structure of protein NP_254181.1 from *Pseudomonas aeruginosa* PA01
Authors : Dutta, S.K.; Serrano, P.; Geralt, M.; Wuthrich, K.; Joint Center for Structural Genomics (JCSG)
Deposited on : 2013-11-22

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

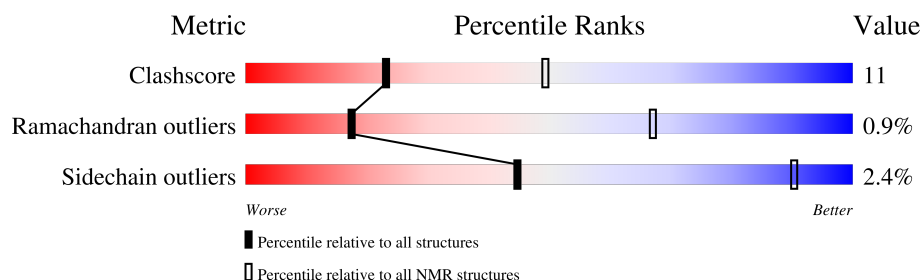
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 42%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	75	<div> <div>67%</div> <div>24%</div> <div>9%</div> </div>
1	B	75	<div> <div>72%</div> <div>19%</div> <div>9%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:75, B:108-B:175 (136)	1.15	1

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2353 atoms, of which 1148 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					Trace
1	A	75	Total	C	H	N	O	0
			1177	384	575	102	116	
1	B	75	Total	C	H	N	O	0
			1176	384	573	102	117	

There are 2 discrepancies between the modelled and reference sequences:

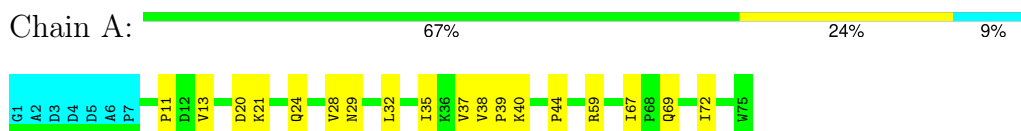
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9HT79
B	101	GLY	-	expression tag	UNP Q9HT79

4 Residue-property plots

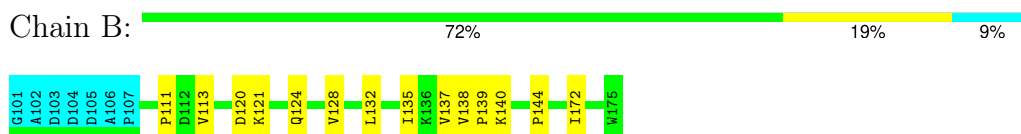
4.1 Average score per residue in the NMR ensemble

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: Uncharacterized protein



- Molecule 1: Uncharacterized protein

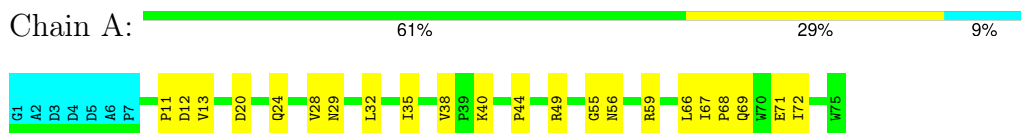


4.2 Scores per residue for each member of the ensemble

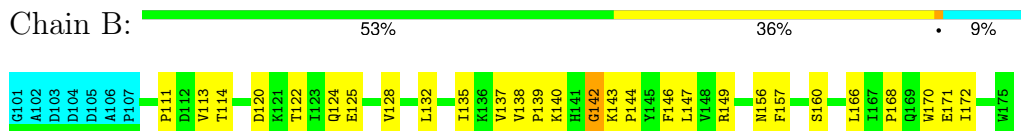
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Uncharacterized protein

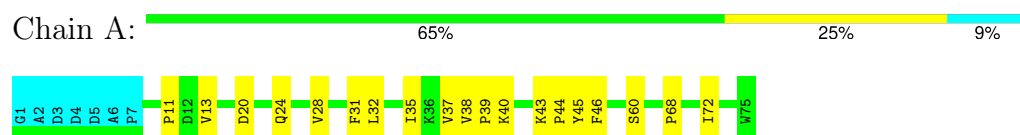


- Molecule 1: Uncharacterized protein

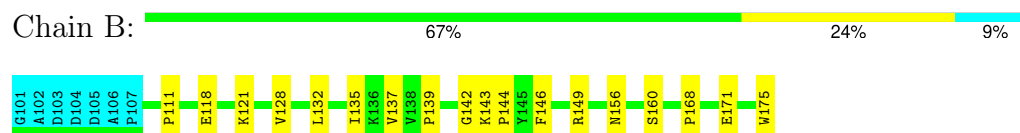


4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein

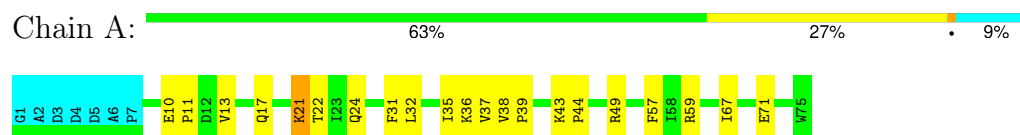


- Molecule 1: Uncharacterized protein

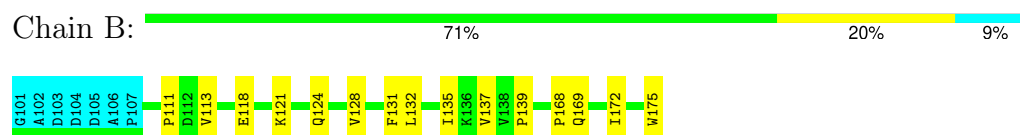


4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein

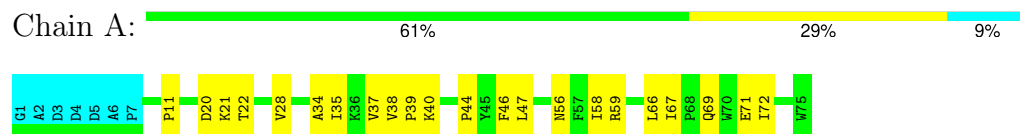


- Molecule 1: Uncharacterized protein

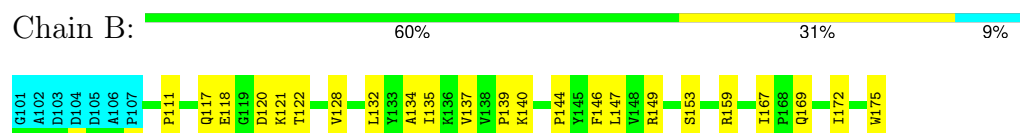


4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein

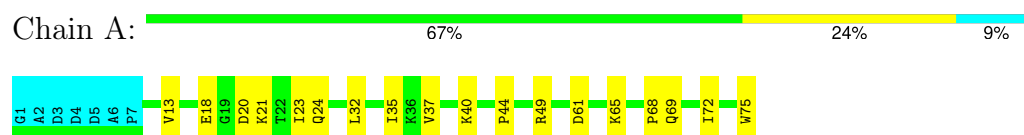


- Molecule 1: Uncharacterized protein

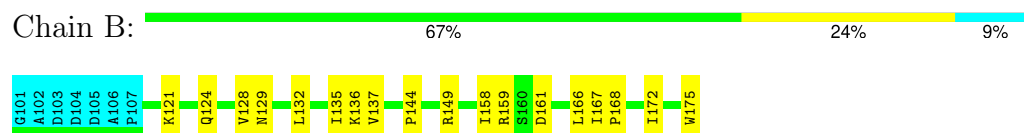


4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein

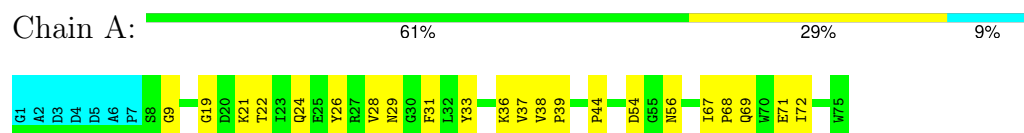


- Molecule 1: Uncharacterized protein

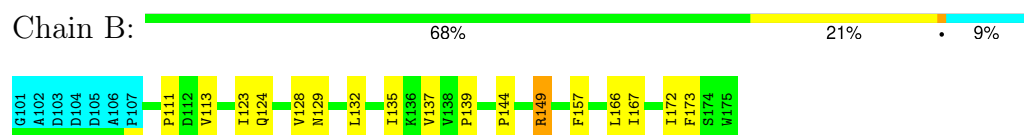


4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein

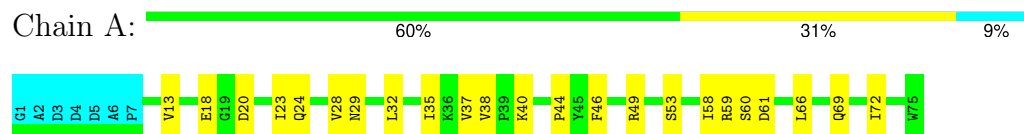


- Molecule 1: Uncharacterized protein

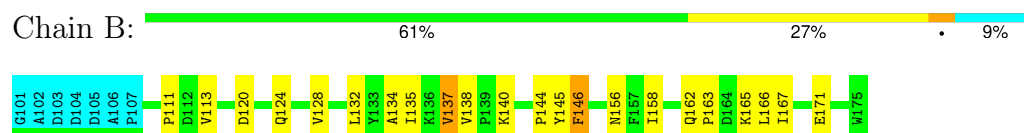


4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein

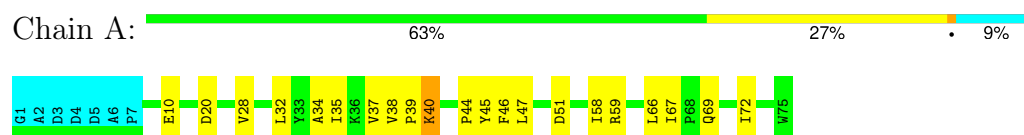


- Molecule 1: Uncharacterized protein

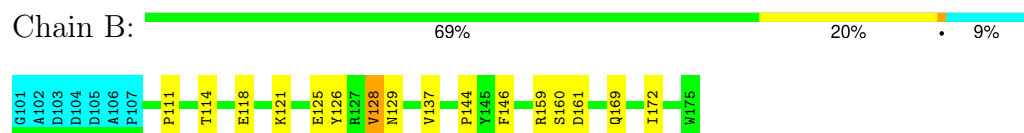


4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein

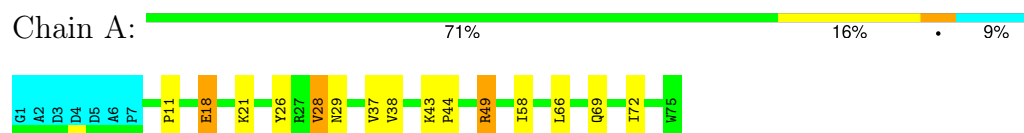


- Molecule 1: Uncharacterized protein

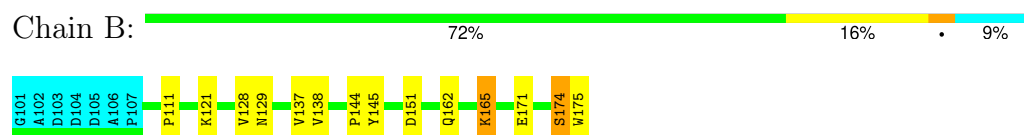


4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein

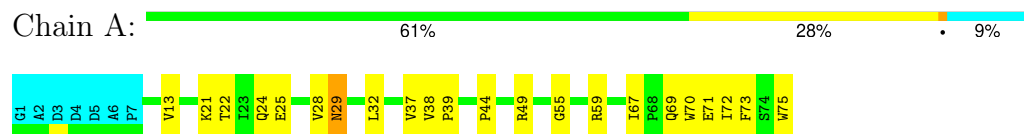


- Molecule 1: Uncharacterized protein

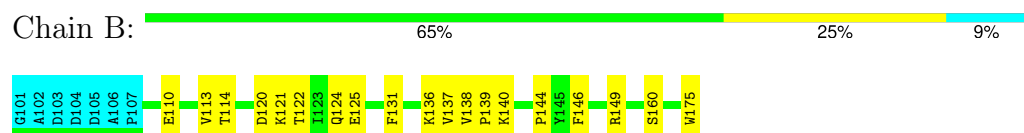


4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein

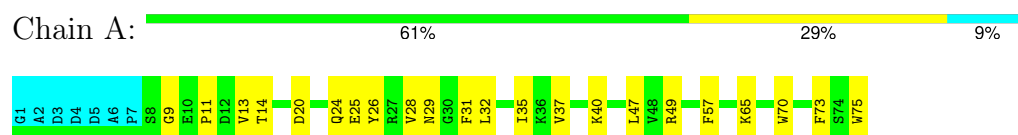


- Molecule 1: Uncharacterized protein

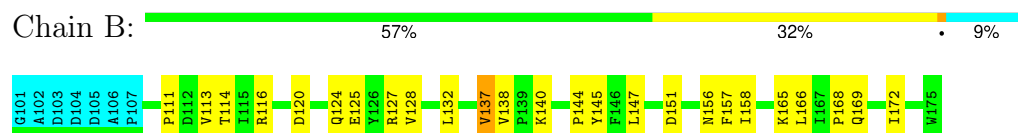


4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein

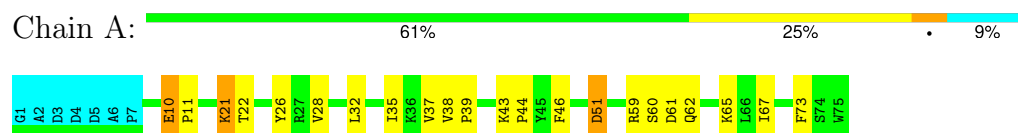


- Molecule 1: Uncharacterized protein

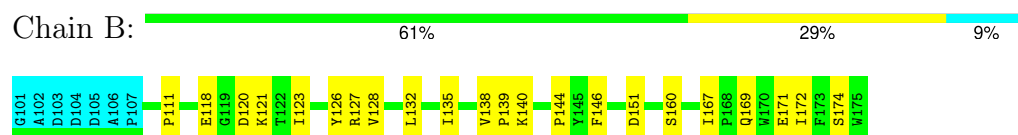


4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein

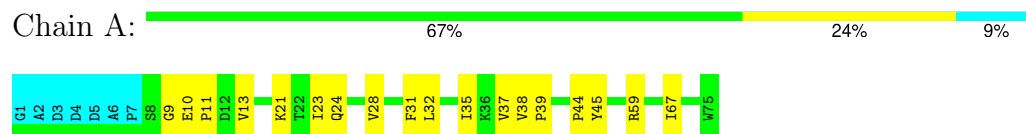


- Molecule 1: Uncharacterized protein

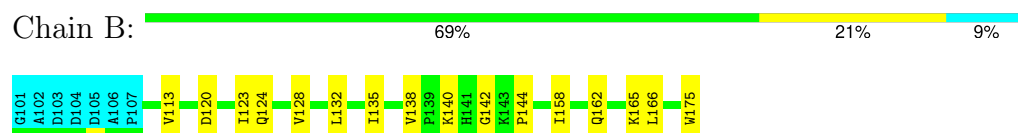


4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein

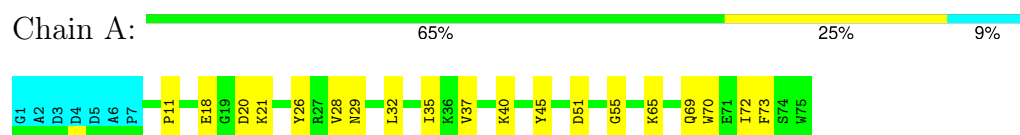


- Molecule 1: Uncharacterized protein

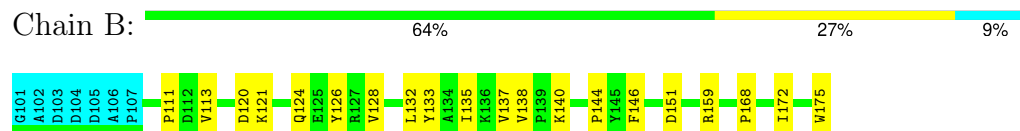


4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein

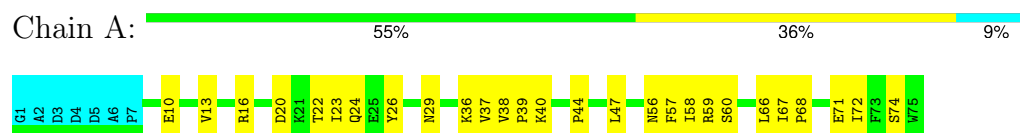


- Molecule 1: Uncharacterized protein

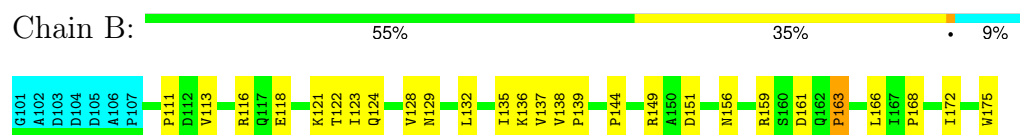


4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein

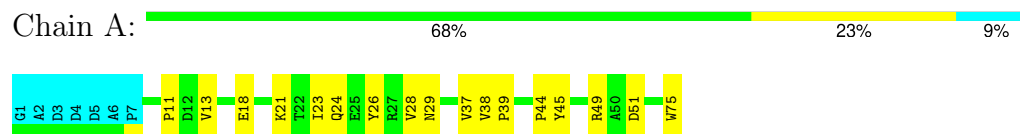


- Molecule 1: Uncharacterized protein

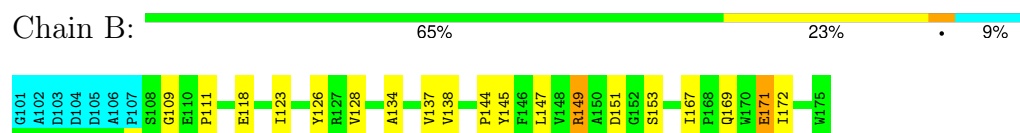


4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein

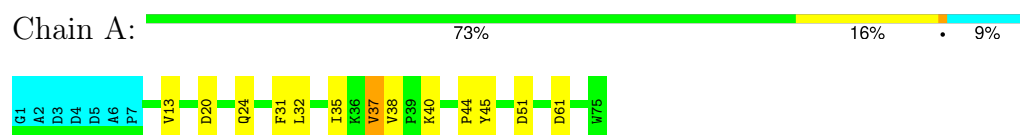


- Molecule 1: Uncharacterized protein

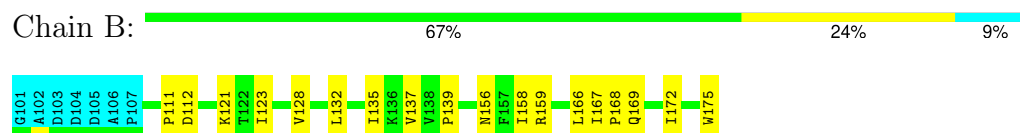


4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein

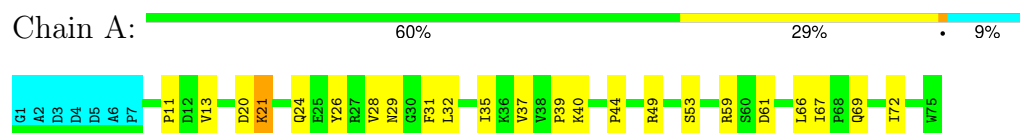


- Molecule 1: Uncharacterized protein

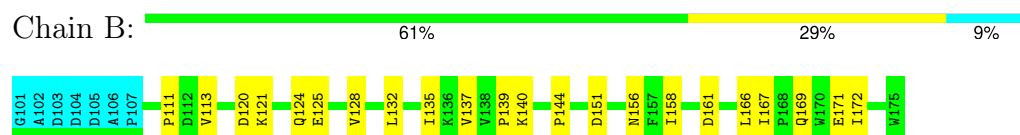


4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein

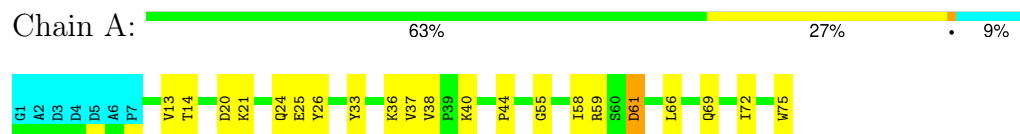


- Molecule 1: Uncharacterized protein

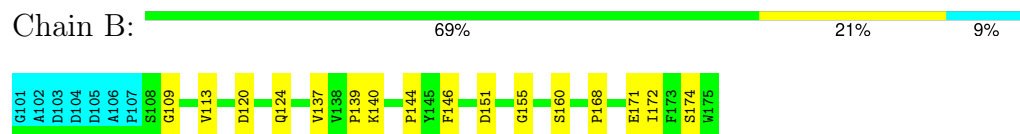


4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein

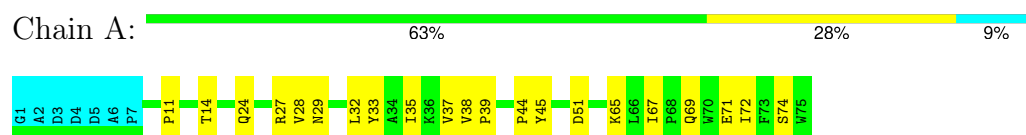


- Molecule 1: Uncharacterized protein

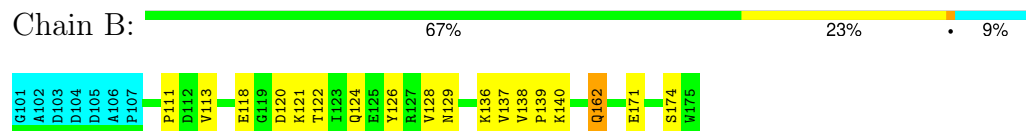


4.2.20 Score per residue for model 20

• Molecule 1: Uncharacterized protein



• Molecule 1: Uncharacterized protein



5 Refinement protocol and experimental data overview

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

Of the 120 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
CNS	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	832
Number of shifts mapped to atoms	832
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	42%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	557	541	540	13±2
1	B	558	541	540	12±3
All	All	22300	21640	21600	477

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ASP:HB3	1:A:40:LYS:HG3	0.89	1.41	8	1
1:A:69:GLN:HA	1:A:72:ILE:HG12	0.86	1.47	1	9
1:A:20:ASP:HB3	1:A:40:LYS:HD3	0.82	1.49	1	6
1:B:156:ASN:HD21	1:B:166:LEU:HD22	0.79	1.37	11	4
1:A:59:ARG:HG3	1:A:67:ILE:HG13	0.77	1.56	1	5
1:B:156:ASN:HD21	1:B:166:LEU:HB3	0.76	1.40	1	1
1:A:32:LEU:HD11	1:A:35:ILE:HG13	0.76	1.58	1	13
1:B:121:LYS:HE3	1:B:175:TRP:HB3	0.76	1.55	10	2
1:B:159:ARG:HG3	1:B:167:ILE:HG13	0.75	1.59	4	2
1:B:111:PRO:HA	1:B:128:VAL:HA	0.73	1.58	7	13
1:B:158:ILE:HD11	1:B:166:LEU:HD23	0.72	1.60	5	6
1:B:167:ILE:HG23	1:B:171:GLU:HB3	0.71	1.61	12	4
1:A:58:ILE:HD11	1:A:66:LEU:HD23	0.70	1.64	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:PRO:HA	1:A:28:VAL:HA	0.69	1.64	4	10
1:A:28:VAL:HG11	1:B:128:VAL:HG11	0.69	1.64	4	2
1:B:138:VAL:HG22	1:B:144:PRO:HB3	0.69	1.63	13	7
1:B:132:LEU:HD11	1:B:135:ILE:HG13	0.68	1.65	2	12
1:B:114:THR:HB	1:B:125:GLU:HB2	0.68	1.66	8	4
1:A:70:TRP:HA	1:A:73:PHE:CZ	0.67	2.25	14	2
1:B:122:THR:HB	1:B:138:VAL:HB	0.67	1.65	20	4
1:A:56:ASN:HD21	1:A:66:LEU:HD22	0.66	1.49	15	2
1:A:28:VAL:HG13	1:A:29:ASN:H	0.66	1.51	1	7
1:B:137:VAL:O	1:B:144:PRO:HA	0.66	1.91	8	12
1:B:120:ASP:HB3	1:B:140:LYS:HD3	0.65	1.68	7	6
1:B:169:GLN:O	1:B:172:ILE:HG12	0.65	1.91	16	5
1:B:169:GLN:HA	1:B:172:ILE:HG12	0.64	1.69	4	4
1:A:37:VAL:O	1:A:44:PRO:HA	0.64	1.91	19	11
1:A:38:VAL:HG22	1:A:44:PRO:HB3	0.64	1.69	16	9
1:B:162:GLN:HG3	1:B:165:LYS:HB2	0.64	1.69	9	1
1:A:21:LYS:HA	1:A:39:PRO:HA	0.63	1.70	4	4
1:B:159:ARG:HD2	1:B:167:ILE:HD11	0.62	1.70	17	1
1:A:21:LYS:HE3	1:A:75:TRP:HB2	0.62	1.71	19	2
1:A:59:ARG:HG3	1:A:67:ILE:HD11	0.62	1.71	3	1
1:A:67:ILE:HG23	1:A:71:GLU:HB3	0.61	1.73	20	6
1:A:51:ASP:OD1	1:B:111:PRO:HB2	0.60	1.97	16	3
1:A:56:ASN:HD21	1:A:66:LEU:HB3	0.60	1.57	1	1
1:A:38:VAL:HG13	1:A:44:PRO:HG3	0.59	1.75	10	2
1:A:60:SER:HB2	1:B:163:PRO:HB3	0.58	1.74	7	2
1:B:124:GLN:HB2	1:B:136:LYS:HB3	0.58	1.75	10	4
1:B:113:VAL:HG21	1:B:124:GLN:HB3	0.57	1.75	10	9
1:B:113:VAL:CG2	1:B:124:GLN:HB3	0.56	2.30	20	10
1:A:37:VAL:O	1:A:39:PRO:HD3	0.56	2.01	13	6
1:A:69:GLN:O	1:A:72:ILE:HG12	0.55	2.02	10	4
1:A:23:ILE:HG12	1:A:37:VAL:HG23	0.55	1.77	7	1
1:B:128:VAL:HG13	1:B:129:ASN:H	0.55	1.62	15	4
1:B:120:ASP:HB3	1:B:140:LYS:HD2	0.55	1.79	4	1
1:A:20:ASP:O	1:A:40:LYS:HG3	0.55	2.01	14	3
1:B:111:PRO:HB3	1:B:128:VAL:HB	0.55	1.78	16	1
1:A:9:GLY:O	1:A:11:PRO:HD3	0.55	2.02	11	1
1:A:13:VAL:HG21	1:A:24:GLN:HB3	0.55	1.79	15	9
1:A:13:VAL:CG2	1:A:24:GLN:HB3	0.54	2.31	2	13
1:A:59:ARG:HB2	1:A:67:ILE:HG13	0.54	1.79	18	3
1:A:24:GLN:HB2	1:A:36:LYS:HB3	0.54	1.80	15	4
1:A:20:ASP:CB	1:A:40:LYS:HD3	0.54	2.32	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ASP:HB2	1:B:112:ASP:HA	0.54	1.79	17	1
1:A:46:PHE:HB2	1:A:60:SER:HB3	0.53	1.80	12	3
1:A:51:ASP:HB2	1:B:126:TYR:CD2	0.53	2.37	16	2
1:A:31:PHE:CZ	1:B:111:PRO:HG3	0.53	2.38	18	4
1:B:116:ARG:HB2	1:B:123:ILE:HB	0.53	1.79	15	1
1:B:121:LYS:HE3	1:B:175:TRP:HB2	0.53	1.81	17	2
1:A:18:GLU:O	1:A:21:LYS:HG2	0.52	2.04	14	3
1:B:162:GLN:HE21	1:B:162:GLN:HA	0.52	1.65	20	1
1:B:137:VAL:HG12	1:B:139:PRO:HD3	0.52	1.80	15	9
1:A:22:THR:HB	1:A:38:VAL:HB	0.52	1.80	3	5
1:A:37:VAL:HG12	1:A:39:PRO:HD3	0.52	1.81	18	5
1:A:21:LYS:HD2	1:A:23:ILE:HD11	0.52	1.81	13	1
1:A:46:PHE:O	1:A:59:ARG:HA	0.52	2.05	8	2
1:B:117:GLN:HG2	1:B:122:THR:HA	0.51	1.81	4	1
1:A:59:ARG:HG2	1:A:61:ASP:HB3	0.51	1.82	18	2
1:A:59:ARG:HD2	1:A:61:ASP:HB3	0.51	1.83	7	1
1:A:11:PRO:HG3	1:B:131:PHE:CZ	0.50	2.41	3	1
1:B:113:VAL:HA	1:B:125:GLU:O	0.50	2.06	18	1
1:A:62:GLN:HG2	1:A:65:LYS:HB3	0.50	1.82	12	1
1:B:121:LYS:HA	1:B:139:PRO:HA	0.50	1.84	2	2
1:B:121:LYS:HE3	1:B:175:TRP:HE3	0.50	1.65	9	1
1:B:111:PRO:HB3	1:B:128:VAL:HA	0.50	1.82	12	1
1:B:156:ASN:OD1	1:B:168:PRO:HA	0.50	2.07	2	1
1:B:171:GLU:O	1:B:174:SER:HB2	0.50	2.06	20	4
1:B:159:ARG:HE	1:B:161:ASP:HB3	0.50	1.67	8	1
1:A:28:VAL:HG21	1:B:131:PHE:CD2	0.50	2.41	10	1
1:A:16:ARG:HB2	1:A:23:ILE:HB	0.50	1.82	15	1
1:B:121:LYS:HD2	1:B:175:TRP:HB2	0.49	1.83	15	1
1:B:123:ILE:HG12	1:B:137:VAL:HG13	0.49	1.83	6	1
1:B:118:GLU:HG3	1:B:123:ILE:HD12	0.49	1.83	12	2
1:B:118:GLU:O	1:B:121:LYS:HG2	0.49	2.07	3	2
1:A:51:ASP:HB3	1:B:126:TYR:CE2	0.49	2.43	20	2
1:A:11:PRO:HA	1:A:27:ARG:O	0.49	2.08	20	1
1:A:21:LYS:HB3	1:A:39:PRO:HB3	0.49	1.84	18	3
1:B:162:GLN:HB3	1:B:165:LYS:HB3	0.48	1.85	13	2
1:B:168:PRO:O	1:B:172:ILE:HG23	0.48	2.08	11	8
1:B:120:ASP:HB3	1:B:140:LYS:HB2	0.48	1.86	12	2
1:B:146:PHE:HB2	1:B:160:SER:HB3	0.48	1.86	12	5
1:A:51:ASP:OD2	1:B:126:TYR:HA	0.48	2.09	8	1
1:A:70:TRP:HA	1:A:73:PHE:CE2	0.48	2.44	11	1
1:A:37:VAL:HG13	1:A:45:TYR:CE1	0.48	2.44	17	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LYS:HE3	1:A:75:TRP:HB3	0.48	1.85	10	1
1:B:128:VAL:HG22	1:B:129:ASN:H	0.47	1.68	8	1
1:A:20:ASP:CB	1:A:40:LYS:HG3	0.47	2.28	8	1
1:B:149:ARG:NH1	1:B:153:SER:HA	0.47	2.23	16	1
1:B:120:ASP:CB	1:B:140:LYS:HD3	0.47	2.40	7	3
1:B:128:VAL:HG13	1:B:129:ASN:N	0.47	2.25	8	1
1:A:47:LEU:HG	1:A:57:PHE:CD2	0.47	2.45	15	2
1:A:26:TYR:HA	1:B:151:ASP:OD2	0.47	2.09	12	1
1:B:118:GLU:HB2	1:B:121:LYS:HE3	0.47	1.85	8	1
1:A:20:ASP:HB3	1:A:40:LYS:CG	0.47	2.28	8	1
1:B:146:PHE:HB2	1:B:160:SER:HB2	0.47	1.85	8	1
1:A:31:PHE:CD2	1:B:128:VAL:HG21	0.46	2.45	2	2
1:B:134:ALA:HA	1:B:147:LEU:O	0.46	2.10	4	2
1:A:31:PHE:CG	1:B:128:VAL:HG21	0.46	2.45	3	1
1:A:49:ARG:HG2	1:A:57:PHE:CE2	0.46	2.46	3	1
1:A:28:VAL:HG13	1:A:29:ASN:N	0.46	2.26	16	3
1:B:127:ARG:HG2	1:B:132:LEU:HA	0.46	1.87	12	2
1:B:137:VAL:O	1:B:139:PRO:HD3	0.46	2.10	17	2
1:A:26:TYR:HB3	1:A:33:TYR:CZ	0.46	2.46	6	2
1:A:26:TYR:CE2	1:B:151:ASP:HB3	0.46	2.47	11	5
1:A:11:PRO:CA	1:A:28:VAL:HA	0.45	2.38	4	2
1:A:49:ARG:HD2	1:A:53:SER:HA	0.45	1.87	18	1
1:A:18:GLU:HG3	1:A:23:ILE:HD12	0.45	1.87	5	3
1:B:121:LYS:HE2	1:B:123:ILE:HD11	0.45	1.86	17	1
1:A:68:PRO:O	1:A:72:ILE:HG23	0.45	2.12	6	5
1:A:69:GLN:HA	1:A:72:ILE:CG1	0.45	2.32	1	2
1:A:20:ASP:HB3	1:A:40:LYS:HB2	0.45	1.88	2	4
1:B:147:LEU:HG	1:B:157:PHE:CD1	0.45	2.47	1	1
1:A:71:GLU:O	1:A:74:SER:HB2	0.45	2.11	15	2
1:A:34:ALA:HA	1:A:47:LEU:O	0.44	2.12	8	2
1:B:132:LEU:HD21	1:B:135:ILE:CG1	0.44	2.42	4	1
1:B:137:VAL:HG13	1:B:145:TYR:CE1	0.44	2.47	16	4
1:B:157:PHE:HB2	1:B:167:ILE:HB	0.44	1.88	6	1
1:B:167:ILE:CG2	1:B:171:GLU:HB3	0.44	2.43	18	1
1:B:126:TYR:HB3	1:B:133:TYR:CZ	0.44	2.47	14	1
1:A:26:TYR:CD2	1:B:151:ASP:HB2	0.44	2.47	16	1
1:B:121:LYS:HE2	1:B:175:TRP:HB2	0.43	1.88	5	1
1:B:128:VAL:HG22	1:B:129:ASN:N	0.43	2.27	8	1
1:B:170:TRP:CD1	1:B:171:GLU:HG2	0.43	2.49	1	1
1:B:146:PHE:O	1:B:159:ARG:HA	0.43	2.14	4	2
1:B:158:ILE:CD1	1:B:166:LEU:HD23	0.43	2.44	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:VAL:HG13	1:A:44:PRO:HB3	0.43	1.90	20	2
1:A:49:ARG:HH21	1:A:53:SER:HA	0.43	1.74	7	1
1:B:121:LYS:CB	1:B:139:PRO:HA	0.43	2.44	18	1
1:A:32:LEU:HD11	1:A:35:ILE:CG1	0.42	2.41	3	1
1:A:25:GLU:HB3	1:A:32:LEU:HD13	0.42	1.91	10	1
1:B:121:LYS:HB3	1:B:139:PRO:HA	0.42	1.90	18	1
1:A:14:THR:O	1:A:24:GLN:HA	0.42	2.14	20	1
1:B:149:ARG:HH11	1:B:149:ARG:HG3	0.42	1.74	6	1
1:A:14:THR:HB	1:A:25:GLU:HB2	0.42	1.90	11	2
1:B:142:GLY:O	1:B:143:LYS:HB2	0.42	2.14	1	2
1:B:120:ASP:HB3	1:B:140:LYS:CD	0.42	2.44	19	1
1:A:22:THR:O	1:A:37:VAL:HA	0.42	2.15	12	1
1:A:21:LYS:HB2	1:A:37:VAL:HG23	0.42	1.92	12	1
1:B:156:ASN:ND2	1:B:166:LEU:HD23	0.42	2.30	15	1
1:A:54:ASP:OD2	1:A:56:ASN:HB3	0.42	2.14	6	1
1:A:66:LEU:N	1:A:66:LEU:HD12	0.41	2.30	18	1
1:B:172:ILE:HG13	1:B:173:PHE:CD2	0.41	2.50	6	1
1:A:67:ILE:CG2	1:A:71:GLU:HB3	0.41	2.45	4	1
1:A:26:TYR:HD2	1:B:151:ASP:HB2	0.41	1.76	9	1
1:A:19:GLY:C	1:A:21:LYS:H	0.41	2.19	6	1
1:B:166:LEU:HD12	1:B:166:LEU:N	0.41	2.31	6	1
1:A:49:ARG:HH11	1:A:49:ARG:HG3	0.41	1.76	9	1
1:B:120:ASP:O	1:B:140:LYS:HG3	0.41	2.15	20	3
1:B:147:LEU:HG	1:B:157:PHE:CD2	0.41	2.50	11	1
1:A:35:ILE:HB	1:A:47:LEU:HB2	0.41	1.93	4	1
1:B:159:ARG:HB3	1:B:161:ASP:OD1	0.41	2.15	15	1
1:B:134:ALA:HB1	1:B:146:PHE:CE2	0.41	2.51	7	1
1:B:123:ILE:HD13	1:B:175:TRP:CE3	0.41	2.51	13	1
1:A:58:ILE:CD1	1:A:66:LEU:HD23	0.41	2.45	9	1
1:B:116:ARG:NE	1:B:116:ARG:HA	0.41	2.30	11	1
1:A:39:PRO:HD2	1:A:43:LYS:C	0.41	2.37	12	1
1:A:59:ARG:HE	1:A:61:ASP:HB3	0.41	1.75	18	1
1:A:28:VAL:HB	1:A:33:TYR:CE1	0.41	2.51	20	1
1:A:21:LYS:HE3	1:A:75:TRP:O	0.40	2.16	5	1
1:A:67:ILE:HD12	1:A:71:GLU:OE2	0.40	2.16	3	1
1:A:59:ARG:HG3	1:A:67:ILE:CD1	0.40	2.45	3	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	67/75 (89%)	60±2 (90±3%)	6±2 (9±3%)	1±1 (1±1%)	13	60
1	B	67/75 (89%)	60±2 (90±3%)	6±2 (10±3%)	0±1 (1±1%)	24	72
All	All	2680/3000 (89%)	2407 (90%)	248 (9%)	25 (1%)	17	67

All 12 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	55	GLY	4
1	A	29	ASN	4
1	A	43	LYS	3
1	A	10	GLU	3
1	B	142	GLY	2
1	A	9	GLY	2
1	B	109	GLY	2
1	B	153	SER	1
1	B	128	VAL	1
1	A	28	VAL	1
1	B	163	PRO	1
1	B	155	GLY	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	60/64 (94%)	58±1 (97±2%)	2±1 (3±2%)	41	89
1	B	60/64 (94%)	59±1 (98±2%)	1±1 (2±2%)	47	91
All	All	2400/2560 (94%)	2342 (98%)	58 (2%)	45	90

All 27 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	B	149	ARG	8
1	A	49	ARG	6
1	A	61	ASP	4
1	A	65	LYS	4
1	B	118	GLU	3
1	A	10	GLU	3
1	A	21	LYS	3
1	A	37	VAL	3
1	B	171	GLU	2
1	B	175	TRP	2
1	B	161	ASP	2
1	B	137	VAL	2
1	B	165	LYS	2
1	A	12	ASP	1
1	A	17	GLN	1
1	A	69	GLN	1
1	B	146	PHE	1
1	A	40	LYS	1
1	A	18	GLU	1
1	B	174	SER	1
1	A	29	ASN	1
1	B	110	GLU	1
1	A	75	TRP	1
1	A	51	ASP	1
1	A	73	PHE	1
1	B	129	ASN	1
1	B	162	GLN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 42% for the well-defined parts and 41% 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	832
Number of shifts mapped to atoms	832
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 3 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	LEU	HD11	0.740	.	2
1	A	32	LEU	HD12	0.740	.	2
1	A	32	LEU	HD13	0.740	.	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	71	-0.16 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	66	-0.15 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	65	0.51 ± 0.38	None needed (imprecise)

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 42%, i.e. 794 atoms were assigned a chemical shift out of a possible 1904. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	266/672 (40%)	137/274 (50%)	66/272 (24%)	63/126 (50%)
Sidechain	467/1034 (45%)	320/664 (48%)	141/324 (44%)	6/46 (13%)
Aromatic	61/198 (31%)	36/96 (38%)	23/94 (24%)	2/8 (25%)
Overall	794/1904 (42%)	493/1034 (48%)	230/690 (33%)	71/180 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 829 atoms were assigned a chemical shift out of a possible 2030. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	281/740 (38%)	145/302 (48%)	71/300 (24%)	65/138 (47%)
Sidechain	487/1092 (45%)	334/700 (48%)	147/346 (42%)	6/46 (13%)
Aromatic	61/198 (31%)	36/96 (38%)	23/94 (24%)	2/8 (25%)
Overall	829/2030 (41%)	515/1098 (47%)	241/740 (33%)	73/192 (38%)

7.1.4 Statistically unusual chemical shifts [i](#)

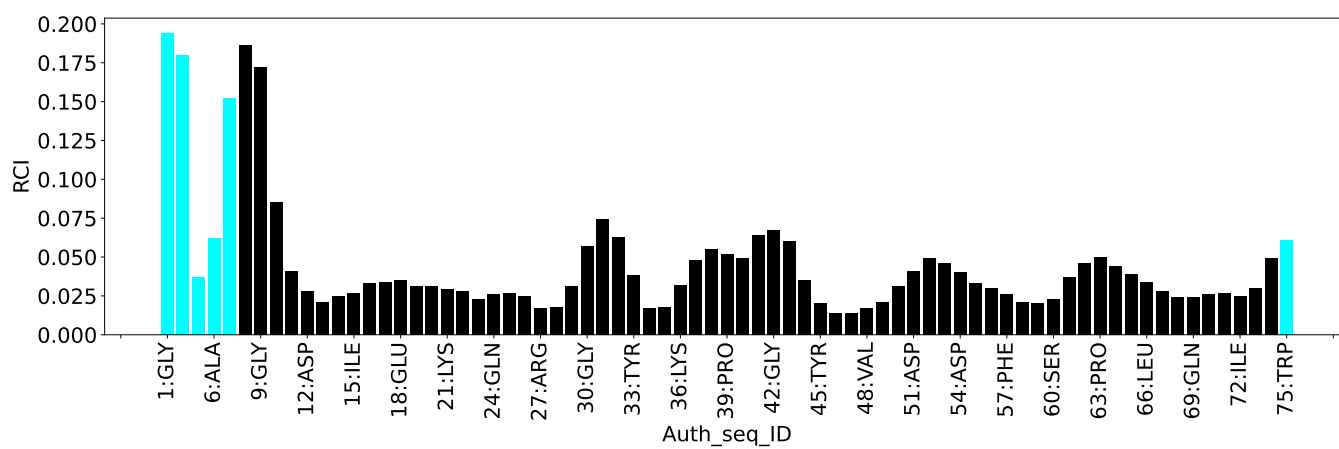
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	36	LYS	HG2	0.03	0.13 – 2.61	-5.4
1	A	59	ARG	HH12	8.69	5.04 – 8.65	5.1

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	2701
Intra-residue ($ i-j =0$)	674
Sequential ($ i-j =1$)	782
Medium range ($ i-j >1$ and $ i-j <5$)	321
Long range ($ i-j \geq 5$)	826
Inter-chain	98
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	18.0
Number of long range restraints per residue ¹	5.5

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)	16.5	0.2
0.2-0.5 (Medium)	2.0	0.45
>0.5 (Large)	None	None

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

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

9 Distance violation analysis ⓘ

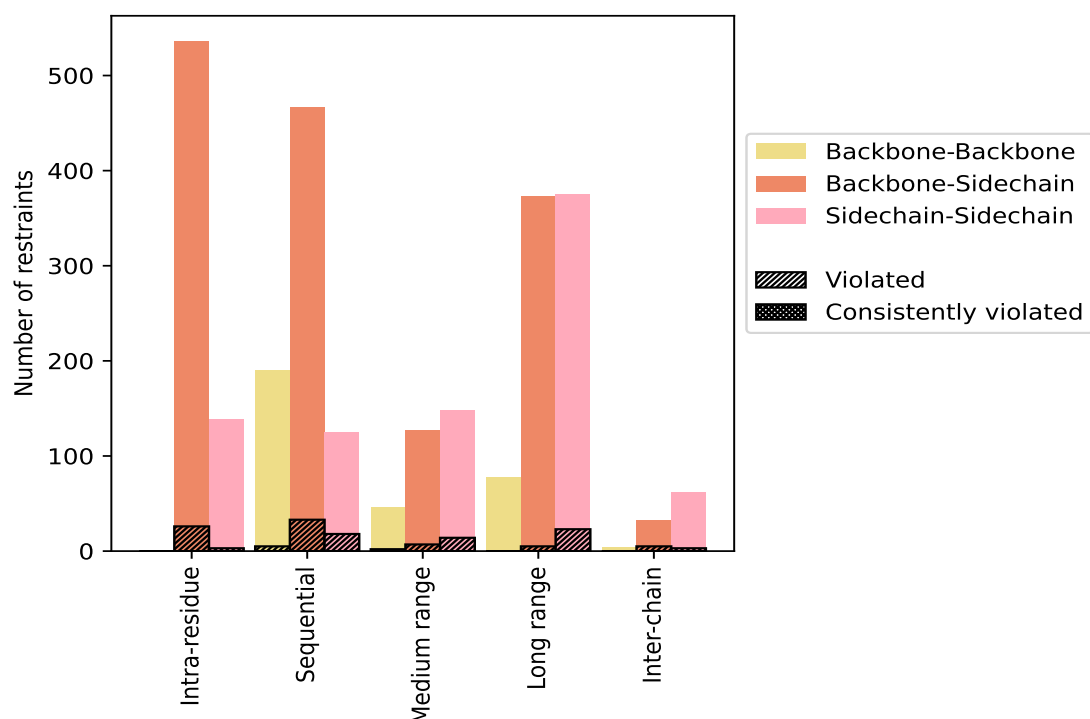
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	674	25.0	29	4.3	1.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	536	19.8	26	4.9	1.0	0	0.0	0.0
Sidechain-Sidechain	138	5.1	3	2.2	0.1	0	0.0	0.0
Sequential ($i-j =1$)	782	29.0	56	7.2	2.1	0	0.0	0.0
Backbone-Backbone	190	7.0	5	2.6	0.2	0	0.0	0.0
Backbone-Sidechain	467	17.3	33	7.1	1.2	0	0.0	0.0
Sidechain-Sidechain	125	4.6	18	14.4	0.7	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	321	11.9	23	7.2	0.9	0	0.0	0.0
Backbone-Backbone	46	1.7	2	4.3	0.1	0	0.0	0.0
Backbone-Sidechain	127	4.7	7	5.5	0.3	0	0.0	0.0
Sidechain-Sidechain	148	5.5	14	9.5	0.5	0	0.0	0.0
Long range ($i-j \geq 5$)	826	30.6	28	3.4	1.0	0	0.0	0.0
Backbone-Backbone	78	2.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	373	13.8	5	1.3	0.2	0	0.0	0.0
Sidechain-Sidechain	375	13.9	23	6.1	0.9	0	0.0	0.0
Inter-chain	98	3.6	8	8.2	0.3	0	0.0	0.0
Backbone-Backbone	4	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	32	1.2	5	15.6	0.2	0	0.0	0.0
Sidechain-Sidechain	62	2.3	3	4.8	0.1	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2701	100.0	144	5.3	5.3	0	0.0	0.0
Backbone-Backbone	318	11.8	7	2.2	0.3	0	0.0	0.0
Backbone-Sidechain	1535	56.8	76	5.0	2.8	0	0.0	0.0
Sidechain-Sidechain	848	31.4	61	7.2	2.3	0	0.0	0.0

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid 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	5	12	3	6	0	26	0.15	0.28	0.05	0.13
2	6	7	3	2	2	20	0.17	0.4	0.07	0.16
3	3	9	3	5	1	21	0.14	0.25	0.04	0.14
4	3	9	5	1	0	18	0.16	0.45	0.08	0.14
5	5	4	6	1	0	16	0.13	0.22	0.03	0.12
6	5	7	4	5	0	21	0.14	0.21	0.03	0.13
7	6	8	2	8	0	24	0.15	0.36	0.06	0.14
8	2	6	4	5	0	17	0.15	0.34	0.06	0.13
9	6	14	5	4	2	31	0.15	0.34	0.05	0.14
10	3	5	4	1	0	13	0.15	0.3	0.05	0.14

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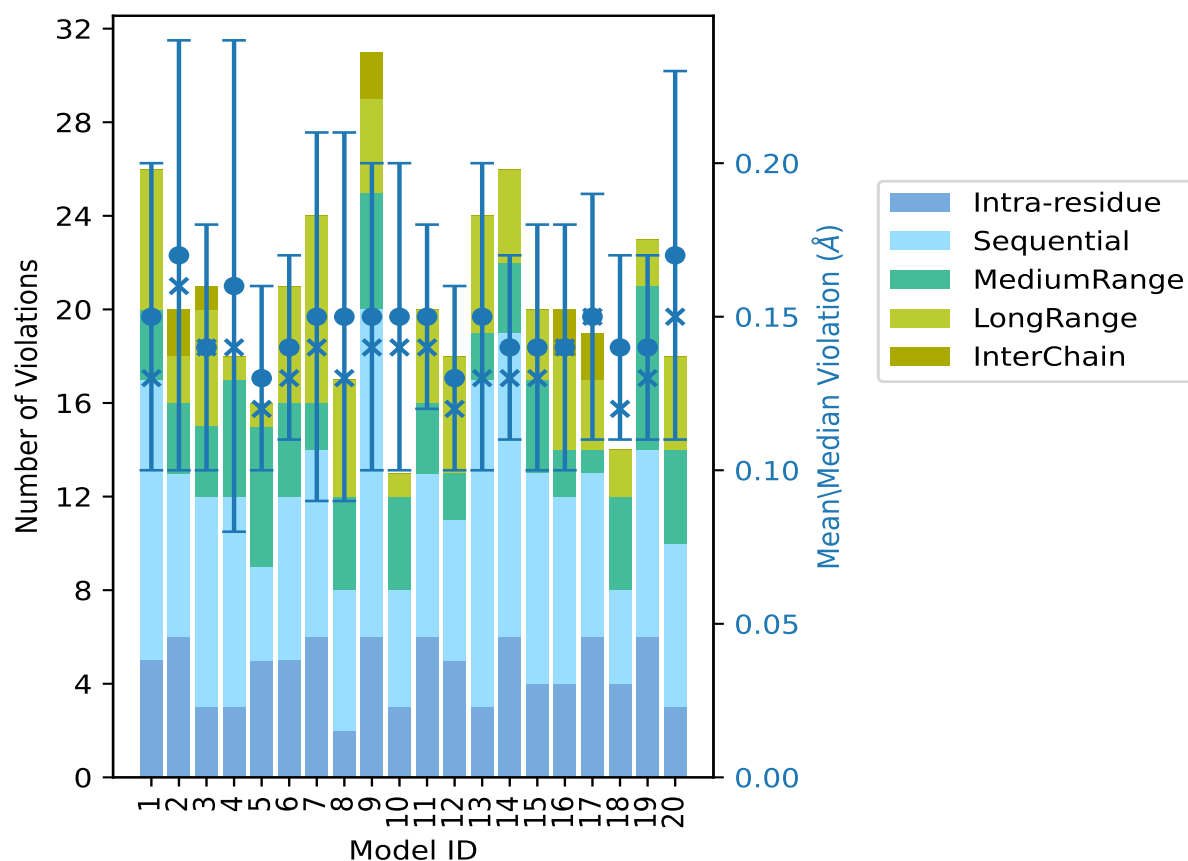
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	6	7	3	4	0	20	0.15	0.21	0.03	0.14
12	5	6	2	5	0	18	0.13	0.19	0.03	0.12
13	3	14	2	5	0	24	0.15	0.33	0.05	0.13
14	6	13	3	4	0	26	0.14	0.21	0.03	0.13
15	4	9	4	3	0	20	0.14	0.26	0.04	0.13
16	4	8	2	4	2	20	0.14	0.28	0.04	0.14
17	6	7	1	3	2	19	0.15	0.24	0.04	0.15
18	4	4	4	2	0	14	0.14	0.22	0.03	0.12
19	6	8	7	2	0	23	0.14	0.24	0.03	0.13
20	3	7	4	4	0	18	0.17	0.32	0.06	0.15

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

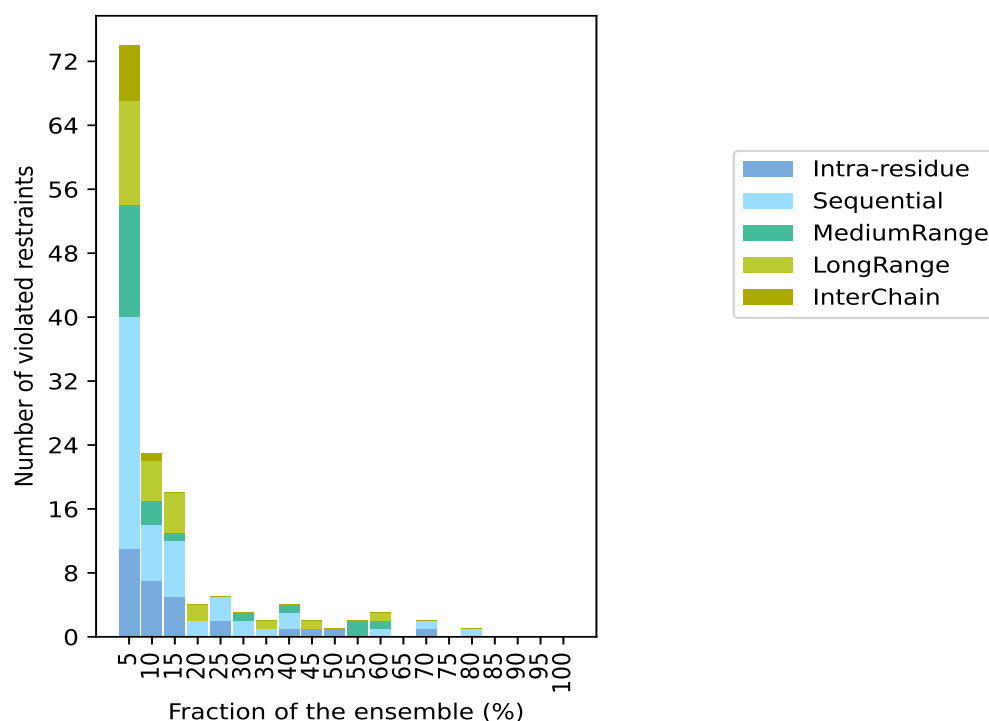
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2557(IR:645, SQ:726, MR:298, LR:798, IC:90) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
11	29	14	13	7	74	1	5.0
7	7	3	5	1	23	2	10.0
5	7	1	5	0	18	3	15.0
0	2	0	2	0	4	4	20.0
2	3	0	0	0	5	5	25.0
0	2	1	0	0	3	6	30.0
0	1	0	1	0	2	7	35.0
1	2	1	0	0	4	8	40.0
1	0	0	1	0	2	9	45.0
1	0	0	0	0	1	10	50.0
0	0	2	0	0	2	11	55.0
0	1	1	1	0	3	12	60.0
0	0	0	0	0	0	13	65.0
1	1	0	0	0	2	14	70.0
0	0	0	0	0	0	15	75.0
0	1	0	0	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

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

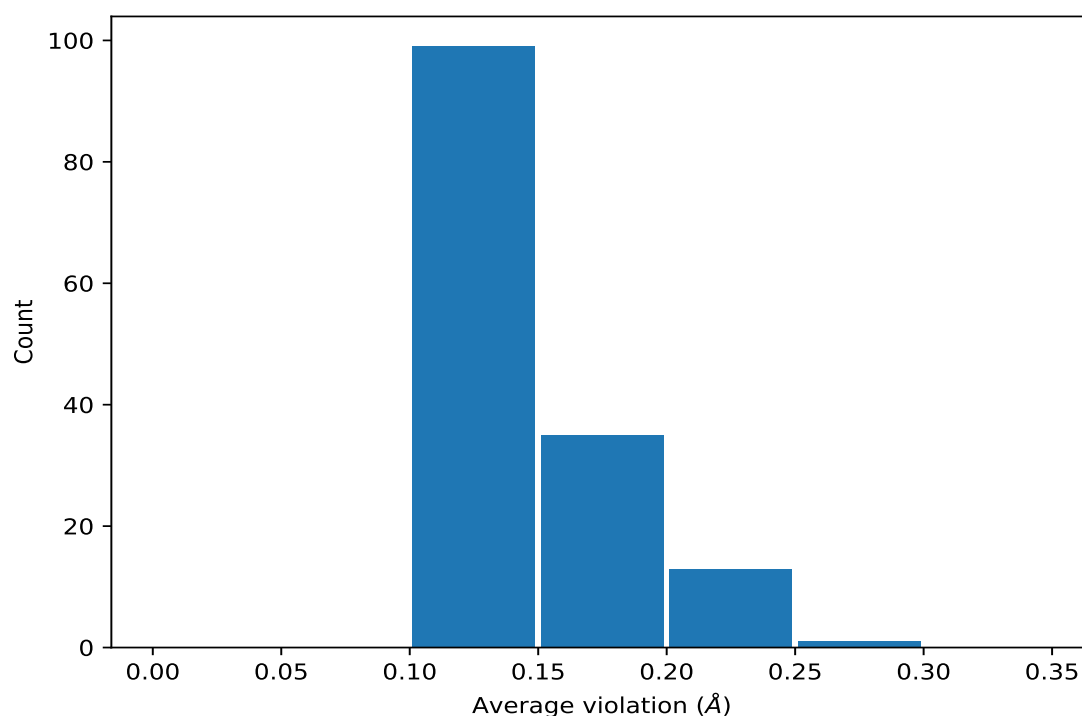
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	16	0.16	0.03	0.16
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	14	0.14	0.03	0.14
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	14	0.14	0.04	0.12
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	14	0.14	0.04	0.12
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	12	0.18	0.05	0.16
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	12	0.18	0.05	0.16
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	12	0.15	0.03	0.14
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	12	0.13	0.02	0.13
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	11	0.14	0.01	0.14
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	11	0.14	0.01	0.14
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	11	0.14	0.01	0.14
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	11	0.13	0.02	0.14
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD2	10	0.16	0.04	0.14
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD3	10	0.16	0.04	0.14
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	9	0.18	0.06	0.22
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	9	0.18	0.06	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE1	9	0.15	0.02	0.16
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE2	9	0.15	0.02	0.16
(1,1159)	1:10:A:GLU:H	1:11:A:PRO:HB3	8	0.2	0.05	0.19
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH11	8	0.14	0.04	0.12
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH12	8	0.14	0.04	0.12
(1,1669)	1:37:A:VAL:HG21	1:39:A:PRO:HD2	8	0.14	0.01	0.14
(1,1669)	1:37:A:VAL:HG22	1:39:A:PRO:HD2	8	0.14	0.01	0.14
(1,1669)	1:37:A:VAL:HG23	1:39:A:PRO:HD2	8	0.14	0.01	0.14
(1,315)	1:113:B:VAL:HG11	1:114:B:THR:H	8	0.11	0.01	0.11
(1,315)	1:113:B:VAL:HG12	1:114:B:THR:H	8	0.11	0.01	0.11
(1,315)	1:113:B:VAL:HG13	1:114:B:THR:H	8	0.11	0.01	0.11
(1,1542)	1:171:B:GLU:HB3	1:172:B:ILE:HG12	7	0.13	0.02	0.12
(1,64)	1:123:B:ILE:HD11	1:175:B:TRP:HE1	7	0.12	0.02	0.11
(1,64)	1:123:B:ILE:HD12	1:175:B:TRP:HE1	7	0.12	0.02	0.11
(1,64)	1:123:B:ILE:HD13	1:175:B:TRP:HE1	7	0.12	0.02	0.11
(1,693)	1:152:B:GLY:H	1:153:B:SER:H	6	0.22	0.11	0.18
(1,2040)	1:70:A:TRP:HZ2	1:71:A:GLU:HB2	6	0.14	0.02	0.14
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG2	6	0.12	0.01	0.12
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG3	6	0.12	0.01	0.12
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG2	6	0.12	0.01	0.12
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG3	6	0.12	0.01	0.12
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG2	6	0.12	0.01	0.12
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG3	6	0.12	0.01	0.12
(1,692)	1:52:A:GLY:H	1:53:A:SER:H	5	0.23	0.07	0.21
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB2	5	0.17	0.05	0.14
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB3	5	0.17	0.05	0.14
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB2	5	0.17	0.05	0.14
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB3	5	0.17	0.05	0.14
(1,314)	1:13:A:VAL:HG11	1:14:A:THR:H	5	0.13	0.01	0.13
(1,314)	1:13:A:VAL:HG12	1:14:A:THR:H	5	0.13	0.01	0.13
(1,314)	1:13:A:VAL:HG13	1:14:A:THR:H	5	0.13	0.01	0.13
(1,362)	1:117:B:GLN:H	1:117:B:GLN:HB3	5	0.12	0.02	0.11
(1,361)	1:17:A:GLN:H	1:17:A:GLN:HB3	5	0.11	0.01	0.11
(1,1568)	1:120:B:ASP:HB2	1:140:B:LYS:HG2	4	0.12	0.02	0.12
(1,63)	1:23:A:ILE:HD11	1:75:A:TRP:HE1	4	0.12	0.02	0.12
(1,63)	1:23:A:ILE:HD12	1:75:A:TRP:HE1	4	0.12	0.02	0.12
(1,63)	1:23:A:ILE:HD13	1:75:A:TRP:HE1	4	0.12	0.02	0.12
(1,1310)	1:40:A:LYS:HB2	1:41:A:HIS:HB3	4	0.12	0.01	0.12
(1,2041)	1:170:B:TRP:HZ2	1:171:B:GLU:HB2	4	0.12	0.02	0.12
(1,2072)	1:12:A:ASP:HB2	1:13:A:VAL:H	3	0.24	0.07	0.2
(1,2072)	1:12:A:ASP:HB3	1:13:A:VAL:H	3	0.24	0.07	0.2
(1,2355)	1:62:A:GLN:H	1:62:A:GLN:HE21	3	0.23	0.12	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2355)	1:62:A:GLN:H	1:62:A:GLN:HE22	3	0.23	0.12	0.15
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB1	3	0.2	0.1	0.18
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB2	3	0.2	0.1	0.18
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB3	3	0.2	0.1	0.18
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB1	3	0.2	0.1	0.18
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB2	3	0.2	0.1	0.18
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB3	3	0.2	0.1	0.18
(1,2418)	1:112:B:ASP:HB2	1:113:B:VAL:H	3	0.19	0.06	0.16
(1,2418)	1:112:B:ASP:HB3	1:113:B:VAL:H	3	0.19	0.06	0.16
(1,2389)	1:71:A:GLU:H	1:71:A:GLU:HG2	3	0.18	0.04	0.18
(1,2389)	1:71:A:GLU:H	1:71:A:GLU:HG3	3	0.18	0.04	0.18
(1,1486)	1:158:B:ILE:HD11	1:166:B:LEU:HG	3	0.16	0.02	0.17
(1,1486)	1:158:B:ILE:HD12	1:166:B:LEU:HG	3	0.16	0.02	0.17
(1,1486)	1:158:B:ILE:HD13	1:166:B:LEU:HG	3	0.16	0.02	0.17
(1,1095)	1:17:A:GLN:HA	1:18:A:GLU:HG2	3	0.16	0.04	0.15
(1,1095)	1:17:A:GLN:HA	1:18:A:GLU:HG3	3	0.16	0.04	0.15
(1,1096)	1:117:B:GLN:HA	1:118:B:GLU:HG2	3	0.16	0.04	0.16
(1,1096)	1:117:B:GLN:HA	1:118:B:GLU:HG3	3	0.16	0.04	0.16
(1,696)	1:53:A:SER:H	1:53:A:SER:HB3	3	0.15	0.01	0.15
(1,697)	1:153:B:SER:H	1:153:B:SER:HB3	3	0.14	0.02	0.16
(1,1577)	1:65:A:LYS:HA	1:65:A:LYS:HG2	3	0.14	0.0	0.14
(1,1240)	1:20:A:ASP:HB2	1:40:A:LYS:HB3	3	0.14	0.04	0.12
(1,903)	1:116:B:ARG:HD3	1:117:B:GLN:H	3	0.13	0.01	0.14
(1,1508)	1:137:B:VAL:HG21	1:139:B:PRO:HG2	3	0.12	0.02	0.11
(1,1508)	1:137:B:VAL:HG21	1:139:B:PRO:HG3	3	0.12	0.02	0.11
(1,1508)	1:137:B:VAL:HG22	1:139:B:PRO:HG2	3	0.12	0.02	0.11
(1,1508)	1:137:B:VAL:HG22	1:139:B:PRO:HG3	3	0.12	0.02	0.11
(1,1508)	1:137:B:VAL:HG23	1:139:B:PRO:HG2	3	0.12	0.02	0.11
(1,1508)	1:137:B:VAL:HG23	1:139:B:PRO:HG3	3	0.12	0.02	0.11
(1,1567)	1:20:A:ASP:HB2	1:40:A:LYS:HG2	3	0.12	0.01	0.12
(1,2440)	1:116:B:ARG:HG2	1:117:B:GLN:H	3	0.12	0.01	0.12
(1,2440)	1:116:B:ARG:HG3	1:117:B:GLN:H	3	0.12	0.01	0.12
(1,896)	1:58:A:ILE:HD11	1:66:A:LEU:HB2	3	0.12	0.01	0.12
(1,896)	1:58:A:ILE:HD12	1:66:A:LEU:HB2	3	0.12	0.01	0.12
(1,896)	1:58:A:ILE:HD13	1:66:A:LEU:HB2	3	0.12	0.01	0.12
(1,1988)	1:23:A:ILE:HG21	1:75:A:TRP:HZ3	3	0.11	0.01	0.11
(1,1988)	1:23:A:ILE:HG22	1:75:A:TRP:HZ3	3	0.11	0.01	0.11
(1,1988)	1:23:A:ILE:HG23	1:75:A:TRP:HZ3	3	0.11	0.01	0.11
(1,732)	1:156:B:ASN:HB3	1:156:B:ASN:HD22	2	0.29	0.01	0.29
(1,833)	1:52:A:GLY:H	1:111:B:PRO:HB3	2	0.17	0.02	0.17
(1,1376)	1:165:B:LYS:HA	1:165:B:LYS:HD2	2	0.16	0.04	0.16
(1,1376)	1:165:B:LYS:HA	1:165:B:LYS:HD3	2	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1541)	1:71:A:GLU:HB3	1:72:A:ILE:HG12	2	0.16	0.01	0.16
(1,910)	1:116:B:ARG:HD2	1:117:B:GLN:H	2	0.15	0.01	0.15
(1,694)	1:53:A:SER:H	1:53:A:SER:HB2	2	0.15	0.0	0.15
(1,951)	1:140:B:LYS:HE2	1:141:B:HIS:HE1	2	0.15	0.0	0.15
(1,951)	1:140:B:LYS:HE3	1:141:B:HIS:HE1	2	0.15	0.0	0.15
(1,1994)	1:75:A:TRP:HA	1:75:A:TRP:HE3	2	0.15	0.02	0.15
(1,435)	1:65:A:LYS:H	1:65:A:LYS:HB2	2	0.14	0.02	0.14
(1,1233)	1:20:A:ASP:HB3	1:40:A:LYS:HB3	2	0.14	0.03	0.14
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG11	2	0.14	0.01	0.14
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG12	2	0.14	0.01	0.14
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG13	2	0.14	0.01	0.14
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG21	2	0.14	0.01	0.14
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG22	2	0.14	0.01	0.14
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG23	2	0.14	0.01	0.14
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG11	2	0.14	0.01	0.14
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG12	2	0.14	0.01	0.14
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG13	2	0.14	0.01	0.14
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG21	2	0.14	0.01	0.14
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG22	2	0.14	0.01	0.14
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG23	2	0.14	0.01	0.14
(1,2387)	1:70:A:TRP:HD1	1:71:A:GLU:HG2	2	0.14	0.04	0.14
(1,2387)	1:70:A:TRP:HD1	1:71:A:GLU:HG3	2	0.14	0.04	0.14
(1,1485)	1:58:A:ILE:HD11	1:66:A:LEU:HG	2	0.14	0.01	0.14
(1,1485)	1:58:A:ILE:HD12	1:66:A:LEU:HG	2	0.14	0.01	0.14
(1,1485)	1:58:A:ILE:HD13	1:66:A:LEU:HG	2	0.14	0.01	0.14
(1,1131)	1:65:A:LYS:HB3	1:67:A:ILE:HD11	2	0.13	0.0	0.13
(1,1131)	1:65:A:LYS:HB3	1:67:A:ILE:HD12	2	0.13	0.0	0.13
(1,1131)	1:65:A:LYS:HB3	1:67:A:ILE:HD13	2	0.13	0.0	0.13
(1,1588)	1:132:B:LEU:HD21	1:134:B:ALA:H	2	0.13	0.02	0.13
(1,1588)	1:132:B:LEU:HD22	1:134:B:ALA:H	2	0.13	0.02	0.13
(1,1588)	1:132:B:LEU:HD23	1:134:B:ALA:H	2	0.13	0.02	0.13
(1,2306)	1:50:A:ALA:HB1	1:56:A:ASN:HB2	2	0.13	0.01	0.13
(1,2306)	1:50:A:ALA:HB1	1:56:A:ASN:HB3	2	0.13	0.01	0.13
(1,2306)	1:50:A:ALA:HB2	1:56:A:ASN:HB2	2	0.13	0.01	0.13
(1,2306)	1:50:A:ALA:HB2	1:56:A:ASN:HB3	2	0.13	0.01	0.13
(1,2306)	1:50:A:ALA:HB3	1:56:A:ASN:HB2	2	0.13	0.01	0.13
(1,2306)	1:50:A:ALA:HB3	1:56:A:ASN:HB3	2	0.13	0.01	0.13
(1,2372)	1:65:A:LYS:HG2	1:66:A:LEU:H	2	0.13	0.0	0.13
(1,2372)	1:65:A:LYS:HG3	1:66:A:LEU:H	2	0.13	0.0	0.13
(1,2695)	1:171:B:GLU:H	1:171:B:GLU:HG2	2	0.13	0.0	0.13
(1,2695)	1:171:B:GLU:H	1:171:B:GLU:HG3	2	0.13	0.0	0.13
(1,1587)	1:32:A:LEU:HD21	1:34:A:ALA:H	2	0.12	0.01	0.12

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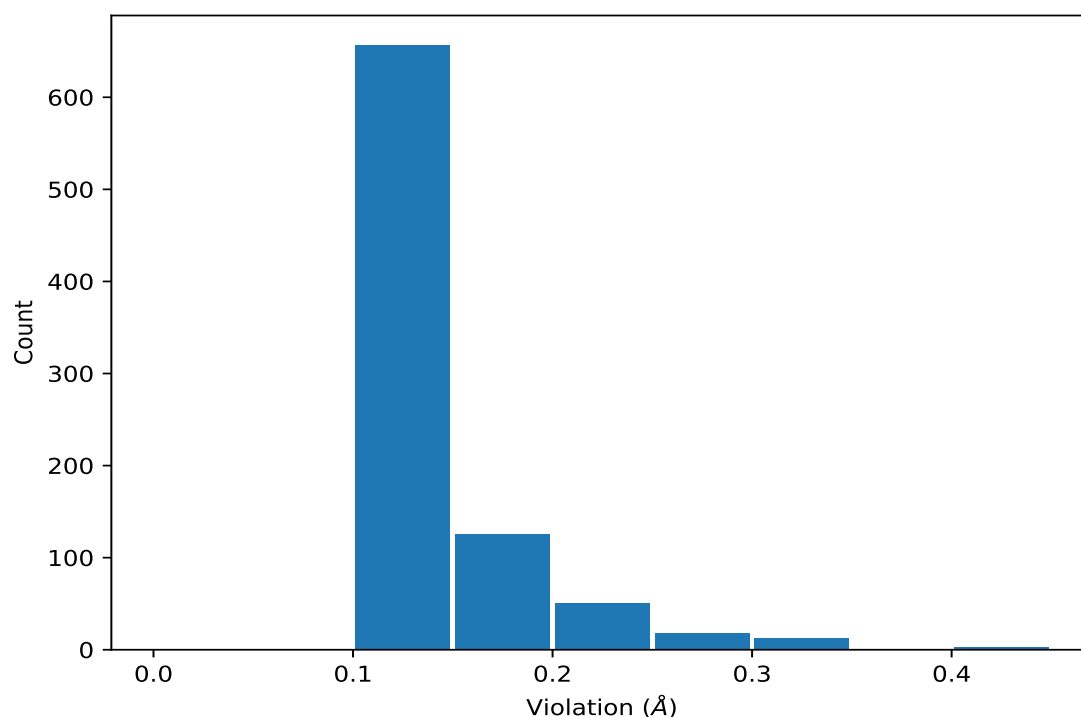
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1587)	1:32:A:LEU:HD22	1:34:A:ALA:H	2	0.12	0.01	0.12
(1,1587)	1:32:A:LEU:HD23	1:34:A:ALA:H	2	0.12	0.01	0.12
(1,1995)	1:175:B:TRP:HA	1:175:B:TRP:HE3	2	0.12	0.01	0.12
(1,1067)	1:24:A:GLN:HA	1:25:A:GLU:HG2	2	0.12	0.0	0.12
(1,1137)	1:24:A:GLN:HG2	1:36:A:LYS:H	2	0.11	0.0	0.11
(1,1311)	1:140:B:LYS:HB2	1:141:B:HIS:HB3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,693)	1:152:B:GLY:H	1:153:B:SER:H	4	0.45
(1,2355)	1:62:A:GLN:H	1:62:A:GLN:HE21	2	0.4
(1,2355)	1:62:A:GLN:H	1:62:A:GLN:HE22	2	0.4
(1,692)	1:52:A:GLY:H	1:53:A:SER:H	7	0.36
(1,2072)	1:12:A:ASP:HB2	1:13:A:VAL:H	9	0.34
(1,2072)	1:12:A:ASP:HB3	1:13:A:VAL:H	9	0.34
(1,736)	1:117:B:GLN:HB3	1:119:B:GLY:H	8	0.34
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB1	13	0.33
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB2	13	0.33
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB3	13	0.33
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB1	13	0.33
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB2	13	0.33
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB3	13	0.33
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	7	0.33
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	7	0.33
(1,221)	1:105:B:ASP:HA	1:106:B:ALA:H	20	0.32
(1,1159)	1:10:A:GLU:H	1:11:A:PRO:HB3	10	0.3
(1,732)	1:156:B:ASN:HB3	1:156:B:ASN:HD22	9	0.3
(1,2418)	1:112:B:ASP:HB2	1:113:B:VAL:H	16	0.28
(1,2418)	1:112:B:ASP:HB3	1:113:B:VAL:H	16	0.28
(1,732)	1:156:B:ASN:HB3	1:156:B:ASN:HD22	1	0.28
(1,220)	1:5:A:ASP:HA	1:6:A:ALA:H	20	0.28
(1,2656)	1:161:B:ASP:HB2	1:162:B:GLN:HB2	15	0.26
(1,2656)	1:161:B:ASP:HB2	1:162:B:GLN:HB3	15	0.26
(1,2656)	1:161:B:ASP:HB3	1:162:B:GLN:HB2	15	0.26
(1,2656)	1:161:B:ASP:HB3	1:162:B:GLN:HB3	15	0.26
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	2	0.26
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	2	0.26
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB2	13	0.25
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB3	13	0.25
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB2	13	0.25
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB3	13	0.25
(1,1159)	1:10:A:GLU:H	1:11:A:PRO:HB3	3	0.25
(1,487)	1:69:A:GLN:H	1:69:A:GLN:HB3	1	0.25
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	17	0.24
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	17	0.24
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	19	0.24
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	19	0.24
(1,693)	1:152:B:GLY:H	1:153:B:SER:H	17	0.24
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH11	4	0.24
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH12	4	0.24
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD2	7	0.23
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD3	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	1	0.23
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	1	0.23
(1,1159)	1:10:A:GLU:H	1:11:A:PRO:HB3	2	0.23
(1,692)	1:52:A:GLY:H	1:53:A:SER:H	20	0.23
(1,2389)	1:71:A:GLU:H	1:71:A:GLU:HG2	5	0.22
(1,2389)	1:71:A:GLU:H	1:71:A:GLU:HG3	5	0.22
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB2	9	0.22
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB3	9	0.22
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB2	9	0.22
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB3	9	0.22
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	4	0.22
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	4	0.22
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	18	0.22
(1,693)	1:152:B:GLY:H	1:153:B:SER:H	8	0.22
(1,1375)	1:65:A:LYS:HA	1:65:A:LYS:HD2	10	0.21
(1,1375)	1:65:A:LYS:HA	1:65:A:LYS:HD3	10	0.21
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD2	1	0.21
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD3	1	0.21
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD2	11	0.21
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD3	11	0.21
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD2	14	0.21
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD3	14	0.21
(1,1096)	1:117:B:GLN:HA	1:118:B:GLU:HG2	3	0.21
(1,1096)	1:117:B:GLN:HA	1:118:B:GLU:HG3	3	0.21
(1,1095)	1:17:A:GLN:HA	1:18:A:GLU:HG2	6	0.21
(1,1095)	1:17:A:GLN:HA	1:18:A:GLU:HG3	6	0.21
(1,949)	1:149:B:ARG:HA	1:149:B:ARG:HD3	13	0.21
(1,692)	1:52:A:GLY:H	1:53:A:SER:H	4	0.21
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	6	0.21
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	6	0.21
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	14	0.21
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	14	0.21
(1,2072)	1:12:A:ASP:HB2	1:13:A:VAL:H	14	0.2
(1,2072)	1:12:A:ASP:HB3	1:13:A:VAL:H	14	0.2
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	11	0.2
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	11	0.2
(1,1376)	1:165:B:LYS:HA	1:165:B:LYS:HD2	20	0.2
(1,1376)	1:165:B:LYS:HA	1:165:B:LYS:HD3	20	0.2
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	2	0.2
(1,1159)	1:10:A:GLU:H	1:11:A:PRO:HB3	17	0.2
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	19	0.2
(1,2072)	1:12:A:ASP:HB2	1:13:A:VAL:H	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2072)	1:12:A:ASP:HB3	1:13:A:VAL:H	12	0.19
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	12	0.19
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	12	0.19
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	20	0.19
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	20	0.19
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	1	0.19
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	5	0.19
(1,1486)	1:158:B:ILE:HD11	1:166:B:LEU:HG	11	0.19
(1,1486)	1:158:B:ILE:HD12	1:166:B:LEU:HG	11	0.19
(1,1486)	1:158:B:ILE:HD13	1:166:B:LEU:HG	11	0.19
(1,1240)	1:20:A:ASP:HB2	1:40:A:LYS:HB3	8	0.19
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	11	0.19
(1,833)	1:52:A:GLY:H	1:111:B:PRO:HB3	2	0.19
(1,692)	1:52:A:GLY:H	1:53:A:SER:H	3	0.19
(1,472)	1:154:B:ASP:H	1:154:B:ASP:HB2	9	0.19
(1,2652)	1:159:B:ARG:HG2	1:161:B:ASP:HB2	1	0.18
(1,2652)	1:159:B:ARG:HG2	1:161:B:ASP:HB3	1	0.18
(1,2652)	1:159:B:ARG:HG3	1:161:B:ASP:HB2	1	0.18
(1,2652)	1:159:B:ARG:HG3	1:161:B:ASP:HB3	1	0.18
(1,2628)	1:152:B:GLY:HA2	1:154:B:ASP:HB2	6	0.18
(1,2628)	1:152:B:GLY:HA3	1:154:B:ASP:HB2	6	0.18
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB1	15	0.18
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB2	15	0.18
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB3	15	0.18
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB1	15	0.18
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB2	15	0.18
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB3	15	0.18
(1,2389)	1:71:A:GLU:H	1:71:A:GLU:HG2	9	0.18
(1,2389)	1:71:A:GLU:H	1:71:A:GLU:HG3	9	0.18
(1,2387)	1:70:A:TRP:HD1	1:71:A:GLU:HG2	9	0.18
(1,2387)	1:70:A:TRP:HD1	1:71:A:GLU:HG3	9	0.18
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE1	7	0.18
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE2	7	0.18
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE1	11	0.18
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE2	11	0.18
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	2	0.18
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	2	0.18
(1,1579)	1:36:A:LYS:HG3	1:37:A:VAL:H	17	0.18
(1,1578)	1:165:B:LYS:HA	1:165:B:LYS:HG2	11	0.18
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	3	0.18
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	9	0.18
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	14	0.18
(1,1159)	1:10:A:GLU:H	1:11:A:PRO:HB3	13	0.18
(1,2058)	1:9:A:GLY:HA2	1:10:A:GLU:HG2	12	0.17
(1,2058)	1:9:A:GLY:HA2	1:10:A:GLU:HG3	12	0.17
(1,2058)	1:9:A:GLY:HA3	1:10:A:GLU:HG2	12	0.17
(1,2058)	1:9:A:GLY:HA3	1:10:A:GLU:HG3	12	0.17
(1,2040)	1:70:A:TRP:HZ2	1:71:A:GLU:HB2	10	0.17
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE1	16	0.17
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE2	16	0.17
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	17	0.17
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	17	0.17
(1,1542)	1:171:B:GLU:HB3	1:172:B:ILE:HG12	1	0.17
(1,1541)	1:71:A:GLU:HB3	1:72:A:ILE:HG12	2	0.17
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	7	0.17
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	13	0.17
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	2	0.17
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	11	0.17
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	15	0.17
(1,1486)	1:158:B:ILE:HD11	1:166:B:LEU:HG	18	0.17
(1,1486)	1:158:B:ILE:HD12	1:166:B:LEU:HG	18	0.17
(1,1486)	1:158:B:ILE:HD13	1:166:B:LEU:HG	18	0.17
(1,1233)	1:20:A:ASP:HB3	1:40:A:LYS:HB3	16	0.17
(1,832)	1:11:A:PRO:HB3	1:152:B:GLY:H	2	0.17
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	11	0.17
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	11	0.17
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	12	0.17
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	12	0.17
(1,2467)	1:121:B:LYS:HD2	1:137:B:VAL:HG11	20	0.16
(1,2467)	1:121:B:LYS:HD2	1:137:B:VAL:HG12	20	0.16
(1,2467)	1:121:B:LYS:HD2	1:137:B:VAL:HG13	20	0.16
(1,2467)	1:121:B:LYS:HD2	1:137:B:VAL:HG21	20	0.16
(1,2467)	1:121:B:LYS:HD2	1:137:B:VAL:HG22	20	0.16
(1,2467)	1:121:B:LYS:HD2	1:137:B:VAL:HG23	20	0.16
(1,2467)	1:121:B:LYS:HD3	1:137:B:VAL:HG11	20	0.16
(1,2467)	1:121:B:LYS:HD3	1:137:B:VAL:HG12	20	0.16
(1,2467)	1:121:B:LYS:HD3	1:137:B:VAL:HG13	20	0.16
(1,2467)	1:121:B:LYS:HD3	1:137:B:VAL:HG21	20	0.16
(1,2467)	1:121:B:LYS:HD3	1:137:B:VAL:HG22	20	0.16
(1,2467)	1:121:B:LYS:HD3	1:137:B:VAL:HG23	20	0.16
(1,2418)	1:112:B:ASP:HB2	1:113:B:VAL:H	13	0.16
(1,2418)	1:112:B:ASP:HB3	1:113:B:VAL:H	13	0.16
(1,2334)	1:56:A:ASN:HD21	1:58:A:ILE:HD11	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2334)	1:56:A:ASN:HD21	1:58:A:ILE:HD12	9	0.16
(1,2334)	1:56:A:ASN:HD21	1:58:A:ILE:HD13	9	0.16
(1,2334)	1:56:A:ASN:HD22	1:58:A:ILE:HD11	9	0.16
(1,2334)	1:56:A:ASN:HD22	1:58:A:ILE:HD12	9	0.16
(1,2334)	1:56:A:ASN:HD22	1:58:A:ILE:HD13	9	0.16
(1,2040)	1:70:A:TRP:HZ2	1:71:A:GLU:HB2	14	0.16
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE1	12	0.16
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE2	12	0.16
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE1	17	0.16
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE2	17	0.16
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	1	0.16
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	1	0.16
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	13	0.16
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	13	0.16
(1,1994)	1:75:A:TRP:HA	1:75:A:TRP:HE3	10	0.16
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	4	0.16
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	4	0.16
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	4	0.16
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	6	0.16
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	6	0.16
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	6	0.16
(1,1568)	1:120:B:ASP:HB2	1:140:B:LYS:HG2	1	0.16
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	4	0.16
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	11	0.16
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	19	0.16
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	3	0.16
(1,1096)	1:117:B:GLN:HA	1:118:B:GLU:HG2	15	0.16
(1,1096)	1:117:B:GLN:HA	1:118:B:GLU:HG3	15	0.16
(1,950)	1:40:A:LYS:HE2	1:41:A:HIS:HE1	20	0.16
(1,950)	1:40:A:LYS:HE3	1:41:A:HIS:HE1	20	0.16
(1,910)	1:116:B:ARG:HD2	1:117:B:GLN:H	9	0.16
(1,697)	1:153:B:SER:H	1:153:B:SER:HB3	2	0.16
(1,697)	1:153:B:SER:H	1:153:B:SER:HB3	19	0.16
(1,696)	1:53:A:SER:H	1:53:A:SER:HB3	2	0.16
(1,435)	1:65:A:LYS:H	1:65:A:LYS:HB2	5	0.16
(1,362)	1:117:B:GLN:H	1:117:B:GLN:HB3	3	0.16
(1,163)	1:117:B:GLN:HB3	1:118:B:GLU:H	14	0.16
(1,64)	1:123:B:ILE:HD11	1:175:B:TRP:HE1	7	0.16
(1,64)	1:123:B:ILE:HD12	1:175:B:TRP:HE1	7	0.16
(1,64)	1:123:B:ILE:HD13	1:175:B:TRP:HE1	7	0.16
(1,2355)	1:62:A:GLN:H	1:62:A:GLN:HE21	17	0.15
(1,2355)	1:62:A:GLN:H	1:62:A:GLN:HE22	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG11	14	0.15
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG12	14	0.15
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG13	14	0.15
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG21	14	0.15
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG22	14	0.15
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG23	14	0.15
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG11	14	0.15
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG12	14	0.15
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG13	14	0.15
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG21	14	0.15
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG22	14	0.15
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG23	14	0.15
(1,2041)	1:170:B:TRP:HZ2	1:171:B:GLU:HB2	6	0.15
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE1	13	0.15
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE2	13	0.15
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	14	0.15
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	14	0.15
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	16	0.15
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	16	0.15
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	8	0.15
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	8	0.15
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	8	0.15
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	15	0.15
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	15	0.15
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	15	0.15
(1,1669)	1:37:A:VAL:HG21	1:39:A:PRO:HD2	18	0.15
(1,1669)	1:37:A:VAL:HG22	1:39:A:PRO:HD2	18	0.15
(1,1669)	1:37:A:VAL:HG23	1:39:A:PRO:HD2	18	0.15
(1,1588)	1:132:B:LEU:HD21	1:134:B:ALA:H	19	0.15
(1,1588)	1:132:B:LEU:HD22	1:134:B:ALA:H	19	0.15
(1,1588)	1:132:B:LEU:HD23	1:134:B:ALA:H	19	0.15
(1,1577)	1:65:A:LYS:HA	1:65:A:LYS:HG2	5	0.15
(1,1541)	1:71:A:GLU:HB3	1:72:A:ILE:HG12	16	0.15
(1,1508)	1:137:B:VAL:HG21	1:139:B:PRO:HG2	20	0.15
(1,1508)	1:137:B:VAL:HG21	1:139:B:PRO:HG3	20	0.15
(1,1508)	1:137:B:VAL:HG22	1:139:B:PRO:HG2	20	0.15
(1,1508)	1:137:B:VAL:HG22	1:139:B:PRO:HG3	20	0.15
(1,1508)	1:137:B:VAL:HG23	1:139:B:PRO:HG2	20	0.15
(1,1508)	1:137:B:VAL:HG23	1:139:B:PRO:HG3	20	0.15
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	6	0.15
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	16	0.15
(1,1372)	1:165:B:LYS:HD2	1:166:B:LEU:H	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:165:B:LYS:HD3	1:166:B:LEU:H	18	0.15
(1,1305)	1:110:B:GLU:HB2	1:111:B:PRO:HD2	9	0.15
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	17	0.15
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	19	0.15
(1,1159)	1:10:A:GLU:H	1:11:A:PRO:HB3	14	0.15
(1,1159)	1:10:A:GLU:H	1:11:A:PRO:HB3	19	0.15
(1,1095)	1:17:A:GLN:HA	1:18:A:GLU:HG2	9	0.15
(1,1095)	1:17:A:GLN:HA	1:18:A:GLU:HG3	9	0.15
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	8	0.15
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	17	0.15
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	19	0.15
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	10	0.15
(1,966)	1:36:A:LYS:HE2	1:44:A:PRO:HG2	13	0.15
(1,966)	1:36:A:LYS:HE2	1:44:A:PRO:HG3	13	0.15
(1,966)	1:36:A:LYS:HE3	1:44:A:PRO:HG2	13	0.15
(1,966)	1:36:A:LYS:HE3	1:44:A:PRO:HG3	13	0.15
(1,951)	1:140:B:LYS:HE2	1:141:B:HIS:HE1	4	0.15
(1,951)	1:140:B:LYS:HE3	1:141:B:HIS:HE1	4	0.15
(1,833)	1:52:A:GLY:H	1:111:B:PRO:HB3	17	0.15
(1,696)	1:53:A:SER:H	1:53:A:SER:HB3	9	0.15
(1,694)	1:53:A:SER:H	1:53:A:SER:HB2	19	0.15
(1,693)	1:152:B:GLY:H	1:153:B:SER:H	1	0.15
(1,187)	1:165:B:LYS:HG3	1:166:B:LEU:H	9	0.15
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	15	0.15
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	15	0.15
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH11	7	0.15
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH12	7	0.15
(1,2625)	1:151:B:ASP:HB2	1:152:B:GLY:H	9	0.14
(1,2625)	1:151:B:ASP:HB3	1:152:B:GLY:H	9	0.14
(1,2410)	1:109:B:GLY:HA2	1:110:B:GLU:HG2	1	0.14
(1,2410)	1:109:B:GLY:HA2	1:110:B:GLU:HG3	1	0.14
(1,2410)	1:109:B:GLY:HA3	1:110:B:GLU:HG2	1	0.14
(1,2410)	1:109:B:GLY:HA3	1:110:B:GLU:HG3	1	0.14
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB2	3	0.14
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB3	3	0.14
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB2	3	0.14
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB3	3	0.14
(1,2306)	1:50:A:ALA:HB1	1:56:A:ASN:HB2	7	0.14
(1,2306)	1:50:A:ALA:HB1	1:56:A:ASN:HB3	7	0.14
(1,2306)	1:50:A:ALA:HB2	1:56:A:ASN:HB2	7	0.14
(1,2306)	1:50:A:ALA:HB2	1:56:A:ASN:HB3	7	0.14
(1,2306)	1:50:A:ALA:HB3	1:56:A:ASN:HB2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2306)	1:50:A:ALA:HB3	1:56:A:ASN:HB3	7	0.14
(1,2212)	1:35:A:ILE:HG21	1:37:A:VAL:HG11	7	0.14
(1,2212)	1:35:A:ILE:HG21	1:37:A:VAL:HG12	7	0.14
(1,2212)	1:35:A:ILE:HG21	1:37:A:VAL:HG13	7	0.14
(1,2212)	1:35:A:ILE:HG21	1:37:A:VAL:HG21	7	0.14
(1,2212)	1:35:A:ILE:HG21	1:37:A:VAL:HG22	7	0.14
(1,2212)	1:35:A:ILE:HG21	1:37:A:VAL:HG23	7	0.14
(1,2212)	1:35:A:ILE:HG22	1:37:A:VAL:HG11	7	0.14
(1,2212)	1:35:A:ILE:HG22	1:37:A:VAL:HG12	7	0.14
(1,2212)	1:35:A:ILE:HG22	1:37:A:VAL:HG13	7	0.14
(1,2212)	1:35:A:ILE:HG22	1:37:A:VAL:HG21	7	0.14
(1,2212)	1:35:A:ILE:HG22	1:37:A:VAL:HG22	7	0.14
(1,2212)	1:35:A:ILE:HG22	1:37:A:VAL:HG23	7	0.14
(1,2212)	1:35:A:ILE:HG23	1:37:A:VAL:HG11	7	0.14
(1,2212)	1:35:A:ILE:HG23	1:37:A:VAL:HG12	7	0.14
(1,2212)	1:35:A:ILE:HG23	1:37:A:VAL:HG13	7	0.14
(1,2212)	1:35:A:ILE:HG23	1:37:A:VAL:HG21	7	0.14
(1,2212)	1:35:A:ILE:HG23	1:37:A:VAL:HG22	7	0.14
(1,2212)	1:35:A:ILE:HG23	1:37:A:VAL:HG23	7	0.14
(1,2040)	1:70:A:TRP:HZ2	1:71:A:GLU:HB2	13	0.14
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE1	3	0.14
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE2	3	0.14
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	8	0.14
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	8	0.14
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE1	9	0.14
(1,2026)	1:37:A:VAL:HA	1:45:A:TYR:HE2	9	0.14
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	2	0.14
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	2	0.14
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	2	0.14
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	5	0.14
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	5	0.14
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	5	0.14
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	19	0.14
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	19	0.14
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	19	0.14
(1,1669)	1:37:A:VAL:HG21	1:39:A:PRO:HD2	3	0.14
(1,1669)	1:37:A:VAL:HG22	1:39:A:PRO:HD2	3	0.14
(1,1669)	1:37:A:VAL:HG23	1:39:A:PRO:HD2	3	0.14
(1,1669)	1:37:A:VAL:HG21	1:39:A:PRO:HD2	4	0.14
(1,1669)	1:37:A:VAL:HG22	1:39:A:PRO:HD2	4	0.14
(1,1669)	1:37:A:VAL:HG23	1:39:A:PRO:HD2	4	0.14
(1,1669)	1:37:A:VAL:HG21	1:39:A:PRO:HD2	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1669)	1:37:A:VAL:HG22	1:39:A:PRO:HD2	19	0.14
(1,1669)	1:37:A:VAL:HG23	1:39:A:PRO:HD2	19	0.14
(1,1577)	1:65:A:LYS:HA	1:65:A:LYS:HG2	11	0.14
(1,1577)	1:65:A:LYS:HA	1:65:A:LYS:HG2	14	0.14
(1,1542)	1:171:B:GLU:HB3	1:172:B:ILE:HG12	5	0.14
(1,1542)	1:171:B:GLU:HB3	1:172:B:ILE:HG12	13	0.14
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	2	0.14
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	17	0.14
(1,1485)	1:58:A:ILE:HD11	1:66:A:LEU:HG	4	0.14
(1,1485)	1:58:A:ILE:HD12	1:66:A:LEU:HG	4	0.14
(1,1485)	1:58:A:ILE:HD13	1:66:A:LEU:HG	4	0.14
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD2	16	0.14
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD3	16	0.14
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD2	20	0.14
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD3	20	0.14
(1,1310)	1:40:A:LYS:HB2	1:41:A:HIS:HB3	16	0.14
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	10	0.14
(1,1159)	1:10:A:GLU:H	1:11:A:PRO:HB3	15	0.14
(1,1138)	1:124:B:GLN:HG2	1:136:B:LYS:H	6	0.14
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	5	0.14
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	9	0.14
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	12	0.14
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	18	0.14
(1,951)	1:140:B:LYS:HE2	1:141:B:HIS:HE1	3	0.14
(1,951)	1:140:B:LYS:HE3	1:141:B:HIS:HE1	3	0.14
(1,910)	1:116:B:ARG:HD2	1:117:B:GLN:H	3	0.14
(1,909)	1:16:A:ARG:HD2	1:17:A:GLN:H	12	0.14
(1,903)	1:116:B:ARG:HD3	1:117:B:GLN:H	4	0.14
(1,903)	1:116:B:ARG:HD3	1:117:B:GLN:H	7	0.14
(1,831)	1:52:A:GLY:H	1:111:B:PRO:HD3	16	0.14
(1,716)	1:73:A:PHE:HD1	1:74:A:SER:H	12	0.14
(1,716)	1:73:A:PHE:HD2	1:74:A:SER:H	12	0.14
(1,696)	1:53:A:SER:H	1:53:A:SER:HB3	16	0.14
(1,694)	1:53:A:SER:H	1:53:A:SER:HB2	15	0.14
(1,693)	1:152:B:GLY:H	1:153:B:SER:H	7	0.14
(1,693)	1:152:B:GLY:H	1:153:B:SER:H	20	0.14
(1,692)	1:52:A:GLY:H	1:53:A:SER:H	17	0.14
(1,314)	1:13:A:VAL:HG11	1:14:A:THR:H	10	0.14
(1,314)	1:13:A:VAL:HG12	1:14:A:THR:H	10	0.14
(1,314)	1:13:A:VAL:HG13	1:14:A:THR:H	10	0.14
(1,314)	1:13:A:VAL:HG11	1:14:A:THR:H	11	0.14
(1,314)	1:13:A:VAL:HG12	1:14:A:THR:H	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:13:A:VAL:HG13	1:14:A:THR:H	11	0.14
(1,63)	1:23:A:ILE:HD11	1:75:A:TRP:HE1	1	0.14
(1,63)	1:23:A:ILE:HD12	1:75:A:TRP:HE1	1	0.14
(1,63)	1:23:A:ILE:HD13	1:75:A:TRP:HE1	1	0.14
(1,63)	1:23:A:ILE:HD11	1:75:A:TRP:HE1	3	0.14
(1,63)	1:23:A:ILE:HD12	1:75:A:TRP:HE1	3	0.14
(1,63)	1:23:A:ILE:HD13	1:75:A:TRP:HE1	3	0.14
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	7	0.14
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	7	0.14
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH11	8	0.14
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH12	8	0.14
(1,2695)	1:171:B:GLU:H	1:171:B:GLU:HG2	3	0.13
(1,2695)	1:171:B:GLU:H	1:171:B:GLU:HG3	3	0.13
(1,2695)	1:171:B:GLU:H	1:171:B:GLU:HG2	7	0.13
(1,2695)	1:171:B:GLU:H	1:171:B:GLU:HG3	7	0.13
(1,2440)	1:116:B:ARG:HG2	1:117:B:GLN:H	14	0.13
(1,2440)	1:116:B:ARG:HG3	1:117:B:GLN:H	14	0.13
(1,2418)	1:112:B:ASP:HB2	1:113:B:VAL:H	1	0.13
(1,2418)	1:112:B:ASP:HB3	1:113:B:VAL:H	1	0.13
(1,2389)	1:71:A:GLU:H	1:71:A:GLU:HG2	17	0.13
(1,2389)	1:71:A:GLU:H	1:71:A:GLU:HG3	17	0.13
(1,2372)	1:65:A:LYS:HG2	1:66:A:LEU:H	11	0.13
(1,2372)	1:65:A:LYS:HG3	1:66:A:LEU:H	11	0.13
(1,2372)	1:65:A:LYS:HG2	1:66:A:LEU:H	14	0.13
(1,2372)	1:65:A:LYS:HG3	1:66:A:LEU:H	14	0.13
(1,2355)	1:62:A:GLN:H	1:62:A:GLN:HE21	9	0.13
(1,2355)	1:62:A:GLN:H	1:62:A:GLN:HE22	9	0.13
(1,2350)	1:59:A:ARG:HG2	1:61:A:ASP:HB2	15	0.13
(1,2350)	1:59:A:ARG:HG2	1:61:A:ASP:HB3	15	0.13
(1,2350)	1:59:A:ARG:HG3	1:61:A:ASP:HB2	15	0.13
(1,2350)	1:59:A:ARG:HG3	1:61:A:ASP:HB3	15	0.13
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB2	8	0.13
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB3	8	0.13
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB2	8	0.13
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB3	8	0.13
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG11	20	0.13
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG12	20	0.13
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG13	20	0.13
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG21	20	0.13
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG22	20	0.13
(1,2123)	1:21:A:LYS:HD2	1:37:A:VAL:HG23	20	0.13
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG11	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG12	20	0.13
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG13	20	0.13
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG21	20	0.13
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG22	20	0.13
(1,2123)	1:21:A:LYS:HD3	1:37:A:VAL:HG23	20	0.13
(1,2041)	1:170:B:TRP:HZ2	1:171:B:GLU:HB2	8	0.13
(1,2040)	1:70:A:TRP:HZ2	1:71:A:GLU:HB2	1	0.13
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE1	14	0.13
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE2	14	0.13
(1,1995)	1:175:B:TRP:HA	1:175:B:TRP:HE3	6	0.13
(1,1994)	1:75:A:TRP:HA	1:75:A:TRP:HE3	7	0.13
(1,1864)	1:72:A:ILE:HG21	1:73:A:PHE:HD1	14	0.13
(1,1864)	1:72:A:ILE:HG21	1:73:A:PHE:HD2	14	0.13
(1,1864)	1:72:A:ILE:HG22	1:73:A:PHE:HD1	14	0.13
(1,1864)	1:72:A:ILE:HG22	1:73:A:PHE:HD2	14	0.13
(1,1864)	1:72:A:ILE:HG23	1:73:A:PHE:HD1	14	0.13
(1,1864)	1:72:A:ILE:HG23	1:73:A:PHE:HD2	14	0.13
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	18	0.13
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	18	0.13
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	18	0.13
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	20	0.13
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	20	0.13
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	20	0.13
(1,1669)	1:37:A:VAL:HG21	1:39:A:PRO:HD2	5	0.13
(1,1669)	1:37:A:VAL:HG22	1:39:A:PRO:HD2	5	0.13
(1,1669)	1:37:A:VAL:HG23	1:39:A:PRO:HD2	5	0.13
(1,1669)	1:37:A:VAL:HG21	1:39:A:PRO:HD2	6	0.13
(1,1669)	1:37:A:VAL:HG22	1:39:A:PRO:HD2	6	0.13
(1,1669)	1:37:A:VAL:HG23	1:39:A:PRO:HD2	6	0.13
(1,1669)	1:37:A:VAL:HG21	1:39:A:PRO:HD2	10	0.13
(1,1669)	1:37:A:VAL:HG22	1:39:A:PRO:HD2	10	0.13
(1,1669)	1:37:A:VAL:HG23	1:39:A:PRO:HD2	10	0.13
(1,1587)	1:32:A:LEU:HD21	1:34:A:ALA:H	10	0.13
(1,1587)	1:32:A:LEU:HD22	1:34:A:ALA:H	10	0.13
(1,1587)	1:32:A:LEU:HD23	1:34:A:ALA:H	10	0.13
(1,1567)	1:20:A:ASP:HB2	1:40:A:LYS:HG2	19	0.13
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG2	15	0.13
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG3	15	0.13
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG2	15	0.13
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG3	15	0.13
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG2	15	0.13
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG3	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG2	18	0.13
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG3	18	0.13
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG2	18	0.13
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG3	18	0.13
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG2	18	0.13
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG3	18	0.13
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	10	0.13
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	12	0.13
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	19	0.13
(1,1486)	1:158:B:ILE:HD11	1:166:B:LEU:HG	7	0.13
(1,1486)	1:158:B:ILE:HD12	1:166:B:LEU:HG	7	0.13
(1,1486)	1:158:B:ILE:HD13	1:166:B:LEU:HG	7	0.13
(1,1485)	1:58:A:ILE:HD11	1:66:A:LEU:HG	15	0.13
(1,1485)	1:58:A:ILE:HD12	1:66:A:LEU:HG	15	0.13
(1,1485)	1:58:A:ILE:HD13	1:66:A:LEU:HG	15	0.13
(1,1388)	1:11:A:PRO:HG2	1:131:B:PHE:HD1	3	0.13
(1,1388)	1:11:A:PRO:HG2	1:131:B:PHE:HD2	3	0.13
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD2	2	0.13
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD3	2	0.13
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD2	13	0.13
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD3	13	0.13
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	11	0.13
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	11	0.13
(1,1241)	1:120:B:ASP:HB2	1:140:B:LYS:HB3	6	0.13
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	1	0.13
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	3	0.13
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	6	0.13
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	13	0.13
(1,1131)	1:65:A:LYS:HB3	1:67:A:ILE:HD11	11	0.13
(1,1131)	1:65:A:LYS:HB3	1:67:A:ILE:HD12	11	0.13
(1,1131)	1:65:A:LYS:HB3	1:67:A:ILE:HD13	11	0.13
(1,1131)	1:65:A:LYS:HB3	1:67:A:ILE:HD11	14	0.13
(1,1131)	1:65:A:LYS:HB3	1:67:A:ILE:HD12	14	0.13
(1,1131)	1:65:A:LYS:HB3	1:67:A:ILE:HD13	14	0.13
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	11	0.13
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	8	0.13
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	9	0.13
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	16	0.13
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	20	0.13
(1,896)	1:58:A:ILE:HD11	1:66:A:LEU:HB2	6	0.13
(1,896)	1:58:A:ILE:HD12	1:66:A:LEU:HB2	6	0.13
(1,896)	1:58:A:ILE:HD13	1:66:A:LEU:HB2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,695)	1:153:B:SER:H	1:153:B:SER:HB2	15	0.13
(1,593)	1:20:A:ASP:HB2	1:21:A:LYS:H	16	0.13
(1,362)	1:117:B:GLN:H	1:117:B:GLN:HB3	6	0.13
(1,361)	1:17:A:GLN:H	1:17:A:GLN:HB3	7	0.13
(1,314)	1:13:A:VAL:HG11	1:14:A:THR:H	1	0.13
(1,314)	1:13:A:VAL:HG12	1:14:A:THR:H	1	0.13
(1,314)	1:13:A:VAL:HG13	1:14:A:THR:H	1	0.13
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	13	0.13
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	13	0.13
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH11	16	0.13
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH12	16	0.13
(1,2592)	1:147:B:LEU:HD11	1:148:B:VAL:HB	12	0.12
(1,2592)	1:147:B:LEU:HD12	1:148:B:VAL:HB	12	0.12
(1,2592)	1:147:B:LEU:HD13	1:148:B:VAL:HB	12	0.12
(1,2592)	1:147:B:LEU:HD21	1:148:B:VAL:HB	12	0.12
(1,2592)	1:147:B:LEU:HD22	1:148:B:VAL:HB	12	0.12
(1,2592)	1:147:B:LEU:HD23	1:148:B:VAL:HB	12	0.12
(1,2470)	1:121:B:LYS:HE2	1:137:B:VAL:HG11	10	0.12
(1,2470)	1:121:B:LYS:HE2	1:137:B:VAL:HG12	10	0.12
(1,2470)	1:121:B:LYS:HE2	1:137:B:VAL:HG13	10	0.12
(1,2470)	1:121:B:LYS:HE2	1:137:B:VAL:HG21	10	0.12
(1,2470)	1:121:B:LYS:HE2	1:137:B:VAL:HG22	10	0.12
(1,2470)	1:121:B:LYS:HE2	1:137:B:VAL:HG23	10	0.12
(1,2470)	1:121:B:LYS:HE3	1:137:B:VAL:HG11	10	0.12
(1,2470)	1:121:B:LYS:HE3	1:137:B:VAL:HG12	10	0.12
(1,2470)	1:121:B:LYS:HE3	1:137:B:VAL:HG13	10	0.12
(1,2470)	1:121:B:LYS:HE3	1:137:B:VAL:HG21	10	0.12
(1,2470)	1:121:B:LYS:HE3	1:137:B:VAL:HG22	10	0.12
(1,2470)	1:121:B:LYS:HE3	1:137:B:VAL:HG23	10	0.12
(1,2444)	1:117:B:GLN:HB3	1:119:B:GLY:HA2	14	0.12
(1,2444)	1:117:B:GLN:HB3	1:119:B:GLY:HA3	14	0.12
(1,2440)	1:116:B:ARG:HG2	1:117:B:GLN:H	2	0.12
(1,2440)	1:116:B:ARG:HG3	1:117:B:GLN:H	2	0.12
(1,2306)	1:50:A:ALA:HB1	1:56:A:ASN:HB2	20	0.12
(1,2306)	1:50:A:ALA:HB1	1:56:A:ASN:HB3	20	0.12
(1,2306)	1:50:A:ALA:HB2	1:56:A:ASN:HB2	20	0.12
(1,2306)	1:50:A:ALA:HB2	1:56:A:ASN:HB3	20	0.12
(1,2306)	1:50:A:ALA:HB3	1:56:A:ASN:HB2	20	0.12
(1,2306)	1:50:A:ALA:HB3	1:56:A:ASN:HB3	20	0.12
(1,2303)	1:49:A:ARG:HD2	1:50:A:ALA:HB1	13	0.12
(1,2303)	1:49:A:ARG:HD2	1:50:A:ALA:HB2	13	0.12
(1,2303)	1:49:A:ARG:HD2	1:50:A:ALA:HB3	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2303)	1:49:A:ARG:HD3	1:50:A:ALA:HB1	13	0.12
(1,2303)	1:49:A:ARG:HD3	1:50:A:ALA:HB2	13	0.12
(1,2303)	1:49:A:ARG:HD3	1:50:A:ALA:HB3	13	0.12
(1,2071)	1:12:A:ASP:HA	1:151:B:ASP:HB2	16	0.12
(1,2071)	1:12:A:ASP:HA	1:151:B:ASP:HB3	16	0.12
(1,1995)	1:175:B:TRP:HA	1:175:B:TRP:HE3	14	0.12
(1,1988)	1:23:A:ILE:HG21	1:75:A:TRP:HZ3	5	0.12
(1,1988)	1:23:A:ILE:HG22	1:75:A:TRP:HZ3	5	0.12
(1,1988)	1:23:A:ILE:HG23	1:75:A:TRP:HZ3	5	0.12
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	1	0.12
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	1	0.12
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	1	0.12
(1,1670)	1:137:B:VAL:HG21	1:139:B:PRO:HD2	10	0.12
(1,1670)	1:137:B:VAL:HG22	1:139:B:PRO:HD2	10	0.12
(1,1670)	1:137:B:VAL:HG23	1:139:B:PRO:HD2	10	0.12
(1,1669)	1:37:A:VAL:HG21	1:39:A:PRO:HD2	15	0.12
(1,1669)	1:37:A:VAL:HG22	1:39:A:PRO:HD2	15	0.12
(1,1669)	1:37:A:VAL:HG23	1:39:A:PRO:HD2	15	0.12
(1,1587)	1:32:A:LEU:HD21	1:34:A:ALA:H	9	0.12
(1,1587)	1:32:A:LEU:HD22	1:34:A:ALA:H	9	0.12
(1,1587)	1:32:A:LEU:HD23	1:34:A:ALA:H	9	0.12
(1,1568)	1:120:B:ASP:HB2	1:140:B:LYS:HG2	7	0.12
(1,1567)	1:20:A:ASP:HB2	1:40:A:LYS:HG2	1	0.12
(1,1542)	1:171:B:GLU:HB3	1:172:B:ILE:HG12	19	0.12
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG2	4	0.12
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG3	4	0.12
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG2	4	0.12
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG3	4	0.12
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG2	4	0.12
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG3	4	0.12
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	14	0.12
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	15	0.12
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	8	0.12
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	17	0.12
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	18	0.12
(1,1376)	1:165:B:LYS:HA	1:165:B:LYS:HD2	18	0.12
(1,1376)	1:165:B:LYS:HA	1:165:B:LYS:HD3	18	0.12
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD2	19	0.12
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD3	19	0.12
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	12	0.12
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	12	0.12
(1,1310)	1:40:A:LYS:HB2	1:41:A:HIS:HB3	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1240)	1:20:A:ASP:HB2	1:40:A:LYS:HB3	9	0.12
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	7	0.12
(1,1095)	1:17:A:GLN:HA	1:18:A:GLU:HG2	13	0.12
(1,1095)	1:17:A:GLN:HA	1:18:A:GLU:HG3	13	0.12
(1,1067)	1:24:A:GLN:HA	1:25:A:GLU:HG2	2	0.12
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	7	0.12
(1,903)	1:116:B:ARG:HD3	1:117:B:GLN:H	16	0.12
(1,902)	1:16:A:ARG:HD3	1:17:A:GLN:H	8	0.12
(1,897)	1:158:B:ILE:HD11	1:166:B:LEU:HB2	6	0.12
(1,897)	1:158:B:ILE:HD12	1:166:B:LEU:HB2	6	0.12
(1,897)	1:158:B:ILE:HD13	1:166:B:LEU:HB2	6	0.12
(1,896)	1:58:A:ILE:HD11	1:66:A:LEU:HB2	18	0.12
(1,896)	1:58:A:ILE:HD12	1:66:A:LEU:HB2	18	0.12
(1,896)	1:58:A:ILE:HD13	1:66:A:LEU:HB2	18	0.12
(1,830)	1:11:A:PRO:HD3	1:152:B:GLY:H	9	0.12
(1,435)	1:65:A:LYS:H	1:65:A:LYS:HB2	11	0.12
(1,315)	1:113:B:VAL:HG11	1:114:B:THR:H	8	0.12
(1,315)	1:113:B:VAL:HG12	1:114:B:THR:H	8	0.12
(1,315)	1:113:B:VAL:HG13	1:114:B:THR:H	8	0.12
(1,314)	1:13:A:VAL:HG11	1:14:A:THR:H	13	0.12
(1,314)	1:13:A:VAL:HG12	1:14:A:THR:H	13	0.12
(1,314)	1:13:A:VAL:HG13	1:14:A:THR:H	13	0.12
(1,314)	1:13:A:VAL:HG11	1:14:A:THR:H	14	0.12
(1,314)	1:13:A:VAL:HG12	1:14:A:THR:H	14	0.12
(1,314)	1:13:A:VAL:HG13	1:14:A:THR:H	14	0.12
(1,230)	1:20:A:ASP:H	1:20:A:ASP:HB3	6	0.12
(1,94)	1:75:A:TRP:H	1:75:A:TRP:HB2	20	0.12
(1,93)	1:174:B:SER:HB3	1:175:B:TRP:H	6	0.12
(1,64)	1:123:B:ILE:HD11	1:175:B:TRP:HE1	1	0.12
(1,64)	1:123:B:ILE:HD12	1:175:B:TRP:HE1	1	0.12
(1,64)	1:123:B:ILE:HD13	1:175:B:TRP:HE1	1	0.12
(1,64)	1:123:B:ILE:HD11	1:175:B:TRP:HE1	13	0.12
(1,64)	1:123:B:ILE:HD12	1:175:B:TRP:HE1	13	0.12
(1,64)	1:123:B:ILE:HD13	1:175:B:TRP:HE1	13	0.12
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	3	0.12
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	3	0.12
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	9	0.12
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	9	0.12
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH11	2	0.12
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH12	2	0.12
(1,2605)	1:147:B:LEU:HD11	1:172:B:ILE:HG21	7	0.11
(1,2605)	1:147:B:LEU:HD11	1:172:B:ILE:HG22	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2605)	1:147:B:LEU:HD11	1:172:B:ILE:HG23	7	0.11
(1,2605)	1:147:B:LEU:HD12	1:172:B:ILE:HG21	7	0.11
(1,2605)	1:147:B:LEU:HD12	1:172:B:ILE:HG22	7	0.11
(1,2605)	1:147:B:LEU:HD12	1:172:B:ILE:HG23	7	0.11
(1,2605)	1:147:B:LEU:HD13	1:172:B:ILE:HG21	7	0.11
(1,2605)	1:147:B:LEU:HD13	1:172:B:ILE:HG22	7	0.11
(1,2605)	1:147:B:LEU:HD13	1:172:B:ILE:HG23	7	0.11
(1,2605)	1:147:B:LEU:HD21	1:172:B:ILE:HG21	7	0.11
(1,2605)	1:147:B:LEU:HD21	1:172:B:ILE:HG22	7	0.11
(1,2605)	1:147:B:LEU:HD21	1:172:B:ILE:HG23	7	0.11
(1,2605)	1:147:B:LEU:HD22	1:172:B:ILE:HG21	7	0.11
(1,2605)	1:147:B:LEU:HD22	1:172:B:ILE:HG22	7	0.11
(1,2605)	1:147:B:LEU:HD22	1:172:B:ILE:HG23	7	0.11
(1,2605)	1:147:B:LEU:HD23	1:172:B:ILE:HG21	7	0.11
(1,2605)	1:147:B:LEU:HD23	1:172:B:ILE:HG22	7	0.11
(1,2605)	1:147:B:LEU:HD23	1:172:B:ILE:HG23	7	0.11
(1,2512)	1:127:B:ARG:HD2	1:130:B:GLY:HA2	9	0.11
(1,2512)	1:127:B:ARG:HD2	1:130:B:GLY:HA3	9	0.11
(1,2512)	1:127:B:ARG:HD3	1:130:B:GLY:HA2	9	0.11
(1,2512)	1:127:B:ARG:HD3	1:130:B:GLY:HA3	9	0.11
(1,2440)	1:116:B:ARG:HG2	1:117:B:GLN:H	13	0.11
(1,2440)	1:116:B:ARG:HG3	1:117:B:GLN:H	13	0.11
(1,2365)	1:65:A:LYS:H	1:65:A:LYS:HB2	14	0.11
(1,2365)	1:65:A:LYS:H	1:65:A:LYS:HB3	14	0.11
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB2	14	0.11
(1,2327)	1:55:A:GLY:HA2	1:56:A:ASN:HB3	14	0.11
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB2	14	0.11
(1,2327)	1:55:A:GLY:HA3	1:56:A:ASN:HB3	14	0.11
(1,2174)	1:28:A:VAL:HA	1:29:A:ASN:HB2	14	0.11
(1,2174)	1:28:A:VAL:HA	1:29:A:ASN:HB3	14	0.11
(1,2169)	1:27:A:ARG:HD2	1:31:A:PHE:H	5	0.11
(1,2169)	1:27:A:ARG:HD3	1:31:A:PHE:H	5	0.11
(1,2040)	1:70:A:TRP:HZ2	1:71:A:GLU:HB2	11	0.11
(1,2031)	1:145:B:TYR:HE1	1:147:B:LEU:HG	20	0.11
(1,2031)	1:145:B:TYR:HE2	1:147:B:LEU:HG	20	0.11
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE1	9	0.11
(1,2027)	1:137:B:VAL:HA	1:145:B:TYR:HE2	9	0.11
(1,1988)	1:23:A:ILE:HG21	1:75:A:TRP:HZ3	1	0.11
(1,1988)	1:23:A:ILE:HG22	1:75:A:TRP:HZ3	1	0.11
(1,1988)	1:23:A:ILE:HG23	1:75:A:TRP:HZ3	1	0.11
(1,1951)	1:31:A:PHE:HA	1:31:A:PHE:HE1	5	0.11
(1,1951)	1:31:A:PHE:HA	1:31:A:PHE:HE2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1748)	1:26:A:TYR:HE1	1:150:B:ALA:HB1	9	0.11
(1,1748)	1:26:A:TYR:HE1	1:150:B:ALA:HB2	9	0.11
(1,1748)	1:26:A:TYR:HE1	1:150:B:ALA:HB3	9	0.11
(1,1748)	1:26:A:TYR:HE2	1:150:B:ALA:HB1	9	0.11
(1,1748)	1:26:A:TYR:HE2	1:150:B:ALA:HB2	9	0.11
(1,1748)	1:26:A:TYR:HE2	1:150:B:ALA:HB3	9	0.11
(1,1656)	1:121:B:LYS:HE2	1:137:B:VAL:HG11	12	0.11
(1,1656)	1:121:B:LYS:HE2	1:137:B:VAL:HG12	12	0.11
(1,1656)	1:121:B:LYS:HE2	1:137:B:VAL:HG13	12	0.11
(1,1656)	1:121:B:LYS:HE3	1:137:B:VAL:HG11	12	0.11
(1,1656)	1:121:B:LYS:HE3	1:137:B:VAL:HG12	12	0.11
(1,1656)	1:121:B:LYS:HE3	1:137:B:VAL:HG13	12	0.11
(1,1588)	1:132:B:LEU:HD21	1:134:B:ALA:H	16	0.11
(1,1588)	1:132:B:LEU:HD22	1:134:B:ALA:H	16	0.11
(1,1588)	1:132:B:LEU:HD23	1:134:B:ALA:H	16	0.11
(1,1568)	1:120:B:ASP:HB2	1:140:B:LYS:HG2	11	0.11
(1,1568)	1:120:B:ASP:HB2	1:140:B:LYS:HG2	14	0.11
(1,1567)	1:20:A:ASP:HB2	1:40:A:LYS:HG2	2	0.11
(1,1542)	1:171:B:GLU:HB3	1:172:B:ILE:HG12	15	0.11
(1,1542)	1:171:B:GLU:HB3	1:172:B:ILE:HG12	20	0.11
(1,1508)	1:137:B:VAL:HG21	1:139:B:PRO:HG2	2	0.11
(1,1508)	1:137:B:VAL:HG21	1:139:B:PRO:HG3	2	0.11
(1,1508)	1:137:B:VAL:HG22	1:139:B:PRO:HG2	2	0.11
(1,1508)	1:137:B:VAL:HG22	1:139:B:PRO:HG3	2	0.11
(1,1508)	1:137:B:VAL:HG23	1:139:B:PRO:HG2	2	0.11
(1,1508)	1:137:B:VAL:HG23	1:139:B:PRO:HG3	2	0.11
(1,1508)	1:137:B:VAL:HG21	1:139:B:PRO:HG2	19	0.11
(1,1508)	1:137:B:VAL:HG21	1:139:B:PRO:HG3	19	0.11
(1,1508)	1:137:B:VAL:HG22	1:139:B:PRO:HG2	19	0.11
(1,1508)	1:137:B:VAL:HG22	1:139:B:PRO:HG3	19	0.11
(1,1508)	1:137:B:VAL:HG23	1:139:B:PRO:HG2	19	0.11
(1,1508)	1:137:B:VAL:HG23	1:139:B:PRO:HG3	19	0.11
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG2	6	0.11
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG3	6	0.11
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG2	6	0.11
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG3	6	0.11
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG2	6	0.11
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG3	6	0.11
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG2	19	0.11
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG3	19	0.11
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG2	19	0.11
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG3	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG2	19	0.11
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG3	19	0.11
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	5	0.11
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	5	0.11
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	5	0.11
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	18	0.11
(1,1363)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	18	0.11
(1,1311)	1:140:B:LYS:HB2	1:141:B:HIS:HB3	7	0.11
(1,1310)	1:40:A:LYS:HB2	1:41:A:HIS:HB3	13	0.11
(1,1310)	1:40:A:LYS:HB2	1:41:A:HIS:HB3	19	0.11
(1,1240)	1:20:A:ASP:HB2	1:40:A:LYS:HB3	15	0.11
(1,1233)	1:20:A:ASP:HB3	1:40:A:LYS:HB3	7	0.11
(1,1223)	1:143:B:LYS:HB2	1:144:B:PRO:HD2	1	0.11
(1,1160)	1:110:B:GLU:H	1:111:B:PRO:HB3	4	0.11
(1,1137)	1:24:A:GLN:HG2	1:36:A:LYS:H	17	0.11
(1,1132)	1:165:B:LYS:HB3	1:167:B:ILE:HD11	11	0.11
(1,1132)	1:165:B:LYS:HB3	1:167:B:ILE:HD12	11	0.11
(1,1132)	1:165:B:LYS:HB3	1:167:B:ILE:HD13	11	0.11
(1,1096)	1:117:B:GLN:HA	1:118:B:GLU:HG2	4	0.11
(1,1096)	1:117:B:GLN:HA	1:118:B:GLU:HG3	4	0.11
(1,1067)	1:24:A:GLN:HA	1:25:A:GLU:HG2	1	0.11
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	2	0.11
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	4	0.11
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	5	0.11
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	13	0.11
(1,1053)	1:69:A:GLN:HG2	1:72:A:ILE:HB	14	0.11
(1,1021)	1:139:B:PRO:HG2	1:145:B:TYR:HB3	3	0.11
(1,1021)	1:139:B:PRO:HG3	1:145:B:TYR:HB3	3	0.11
(1,820)	1:154:B:ASP:HB3	1:155:B:GLY:H	15	0.11
(1,697)	1:153:B:SER:H	1:153:B:SER:HB3	4	0.11
(1,604)	1:154:B:ASP:HA	1:156:B:ASN:H	5	0.11
(1,518)	1:162:B:GLN:H	1:163:B:PRO:HD2	4	0.11
(1,467)	1:154:B:ASP:H	1:155:B:GLY:H	9	0.11
(1,362)	1:117:B:GLN:H	1:117:B:GLN:HB3	14	0.11
(1,362)	1:117:B:GLN:H	1:117:B:GLN:HB3	17	0.11
(1,361)	1:17:A:GLN:H	1:17:A:GLN:HB3	12	0.11
(1,361)	1:17:A:GLN:H	1:17:A:GLN:HB3	19	0.11
(1,315)	1:113:B:VAL:HG11	1:114:B:THR:H	14	0.11
(1,315)	1:113:B:VAL:HG12	1:114:B:THR:H	14	0.11
(1,315)	1:113:B:VAL:HG13	1:114:B:THR:H	14	0.11
(1,315)	1:113:B:VAL:HG11	1:114:B:THR:H	16	0.11
(1,315)	1:113:B:VAL:HG12	1:114:B:THR:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:113:B:VAL:HG13	1:114:B:THR:H	16	0.11
(1,315)	1:113:B:VAL:HG11	1:114:B:THR:H	18	0.11
(1,315)	1:113:B:VAL:HG12	1:114:B:THR:H	18	0.11
(1,315)	1:113:B:VAL:HG13	1:114:B:THR:H	18	0.11
(1,315)	1:113:B:VAL:HG11	1:114:B:THR:H	19	0.11
(1,315)	1:113:B:VAL:HG12	1:114:B:THR:H	19	0.11
(1,315)	1:113:B:VAL:HG13	1:114:B:THR:H	19	0.11
(1,186)	1:65:A:LYS:HG3	1:66:A:LEU:H	9	0.11
(1,64)	1:123:B:ILE:HD11	1:175:B:TRP:HE1	3	0.11
(1,64)	1:123:B:ILE:HD12	1:175:B:TRP:HE1	3	0.11
(1,64)	1:123:B:ILE:HD13	1:175:B:TRP:HE1	3	0.11
(1,64)	1:123:B:ILE:HD11	1:175:B:TRP:HE1	8	0.11
(1,64)	1:123:B:ILE:HD12	1:175:B:TRP:HE1	8	0.11
(1,64)	1:123:B:ILE:HD13	1:175:B:TRP:HE1	8	0.11
(1,64)	1:123:B:ILE:HD11	1:175:B:TRP:HE1	19	0.11
(1,64)	1:123:B:ILE:HD12	1:175:B:TRP:HE1	19	0.11
(1,64)	1:123:B:ILE:HD13	1:175:B:TRP:HE1	19	0.11
(1,63)	1:23:A:ILE:HD11	1:75:A:TRP:HE1	13	0.11
(1,63)	1:23:A:ILE:HD12	1:75:A:TRP:HE1	13	0.11
(1,63)	1:23:A:ILE:HD13	1:75:A:TRP:HE1	13	0.11
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	8	0.11
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	8	0.11
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	16	0.11
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	16	0.11
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	18	0.11
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	18	0.11
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	19	0.11
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	19	0.11
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH11	10	0.11
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH12	10	0.11
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH11	18	0.11
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH12	18	0.11
(1,2658)	1:162:B:GLN:H	1:162:B:GLN:HE21	6	0.1
(1,2658)	1:162:B:GLN:H	1:162:B:GLN:HE22	6	0.1
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB1	9	0.1
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB2	9	0.1
(1,2620)	1:149:B:ARG:HD2	1:150:B:ALA:HB3	9	0.1
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB1	9	0.1
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB2	9	0.1
(1,2620)	1:149:B:ARG:HD3	1:150:B:ALA:HB3	9	0.1
(1,2406)	1:108:B:SER:HB2	1:129:B:ASN:HD22	6	0.1
(1,2406)	1:108:B:SER:HB3	1:129:B:ASN:HD22	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2387)	1:70:A:TRP:HD1	1:71:A:GLU:HG2	5	0.1
(1,2387)	1:70:A:TRP:HD1	1:71:A:GLU:HG3	5	0.1
(1,2041)	1:170:B:TRP:HZ2	1:171:B:GLU:HB2	4	0.1
(1,2041)	1:170:B:TRP:HZ2	1:171:B:GLU:HB2	15	0.1
(1,2040)	1:70:A:TRP:HZ2	1:71:A:GLU:HB2	16	0.1
(1,1988)	1:23:A:ILE:HG21	1:75:A:TRP:HZ3	3	0.1
(1,1988)	1:23:A:ILE:HG22	1:75:A:TRP:HZ3	3	0.1
(1,1988)	1:23:A:ILE:HG23	1:75:A:TRP:HZ3	3	0.1
(1,1975)	1:174:B:SER:HB3	1:175:B:TRP:HD1	6	0.1
(1,1869)	1:171:B:GLU:HA	1:172:B:ILE:HG21	19	0.1
(1,1869)	1:171:B:GLU:HA	1:172:B:ILE:HG22	19	0.1
(1,1869)	1:171:B:GLU:HA	1:172:B:ILE:HG23	19	0.1
(1,1655)	1:21:A:LYS:HE2	1:37:A:VAL:HG11	8	0.1
(1,1655)	1:21:A:LYS:HE2	1:37:A:VAL:HG12	8	0.1
(1,1655)	1:21:A:LYS:HE2	1:37:A:VAL:HG13	8	0.1
(1,1655)	1:21:A:LYS:HE3	1:37:A:VAL:HG11	8	0.1
(1,1655)	1:21:A:LYS:HE3	1:37:A:VAL:HG12	8	0.1
(1,1655)	1:21:A:LYS:HE3	1:37:A:VAL:HG13	8	0.1
(1,1542)	1:171:B:GLU:HB3	1:172:B:ILE:HG12	9	0.1
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG2	3	0.1
(1,1507)	1:37:A:VAL:HG21	1:39:A:PRO:HG3	3	0.1
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG2	3	0.1
(1,1507)	1:37:A:VAL:HG22	1:39:A:PRO:HG3	3	0.1
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG2	3	0.1
(1,1507)	1:37:A:VAL:HG23	1:39:A:PRO:HG3	3	0.1
(1,1496)	1:168:B:PRO:HG3	1:169:B:GLN:H	6	0.1
(1,1495)	1:68:A:PRO:HG3	1:69:A:GLN:H	7	0.1
(1,1387)	1:31:A:PHE:HD1	1:111:B:PRO:HG2	17	0.1
(1,1387)	1:31:A:PHE:HD2	1:111:B:PRO:HG2	17	0.1
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD2	12	0.1
(1,1364)	1:140:B:LYS:HB3	1:140:B:LYS:HD3	12	0.1
(1,1311)	1:140:B:LYS:HB2	1:141:B:HIS:HB3	11	0.1
(1,1304)	1:10:A:GLU:HB2	1:11:A:PRO:HD2	9	0.1
(1,1137)	1:24:A:GLN:HG2	1:36:A:LYS:H	15	0.1
(1,1055)	1:69:A:GLN:HG3	1:72:A:ILE:HB	1	0.1
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	3	0.1
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	4	0.1
(1,1054)	1:169:B:GLN:HG2	1:172:B:ILE:HB	13	0.1
(1,991)	1:156:B:ASN:HB2	1:167:B:ILE:H	9	0.1
(1,896)	1:58:A:ILE:HD11	1:66:A:LEU:HB2	12	0.1
(1,896)	1:58:A:ILE:HD12	1:66:A:LEU:HB2	12	0.1
(1,896)	1:58:A:ILE:HD13	1:66:A:LEU:HB2	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:47:A:LEU:HG	1:57:A:PHE:HB3	16	0.1
(1,651)	1:128:B:VAL:H	1:131:B:PHE:H	12	0.1
(1,362)	1:117:B:GLN:H	1:117:B:GLN:HB3	12	0.1
(1,361)	1:17:A:GLN:H	1:17:A:GLN:HB3	15	0.1
(1,361)	1:17:A:GLN:H	1:17:A:GLN:HB3	17	0.1
(1,315)	1:113:B:VAL:HG11	1:114:B:THR:H	1	0.1
(1,315)	1:113:B:VAL:HG12	1:114:B:THR:H	1	0.1
(1,315)	1:113:B:VAL:HG13	1:114:B:THR:H	1	0.1
(1,315)	1:113:B:VAL:HG11	1:114:B:THR:H	7	0.1
(1,315)	1:113:B:VAL:HG12	1:114:B:THR:H	7	0.1
(1,315)	1:113:B:VAL:HG13	1:114:B:THR:H	7	0.1
(1,315)	1:113:B:VAL:HG11	1:114:B:THR:H	13	0.1
(1,315)	1:113:B:VAL:HG12	1:114:B:THR:H	13	0.1
(1,315)	1:113:B:VAL:HG13	1:114:B:THR:H	13	0.1
(1,64)	1:123:B:ILE:HD11	1:175:B:TRP:HE1	12	0.1
(1,64)	1:123:B:ILE:HD12	1:175:B:TRP:HE1	12	0.1
(1,64)	1:123:B:ILE:HD13	1:175:B:TRP:HE1	12	0.1
(1,63)	1:23:A:ILE:HD11	1:75:A:TRP:HE1	8	0.1
(1,63)	1:23:A:ILE:HD12	1:75:A:TRP:HE1	8	0.1
(1,63)	1:23:A:ILE:HD13	1:75:A:TRP:HE1	8	0.1
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH11	1	0.1
(1,38)	1:149:B:ARG:H	1:149:B:ARG:HH12	1	0.1
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH11	17	0.1
(1,37)	1:49:A:ARG:H	1:49:A:ARG:HH12	17	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found