



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:39 AM UTC

PDB ID : 2KUL / pdb_00002kul
BMRB ID : 16738
Title : Solution structure of human vaccinia related kinase 1(VRK1)
Authors : Shin, J.; Yoon, H.
Deposited on : 2010-02-19

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

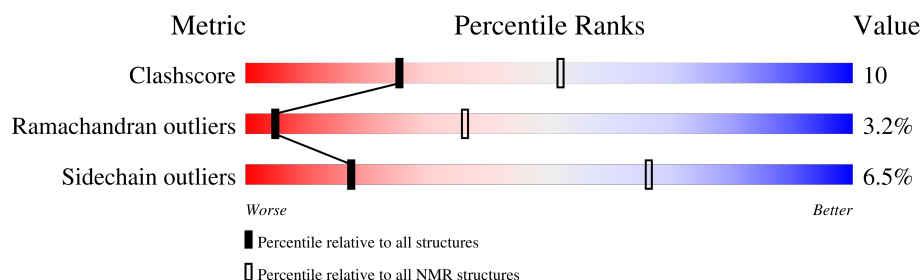
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 73%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	368	 66% 18% 14% .

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:25-A:59, A:66-A:217, A:222-A:338, A:352-A:356 (309)	1.69	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 3 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5844 atoms, of which 2943 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Serine/threonine-protein kinase VRK1.

Mol	Chain	Residues	Atoms						Trace
1	A	360	Total	C	H	N	O	S	0
			5844	1848	2943	508	531	14	

There are 8 discrepancies between the modelled and reference sequences:

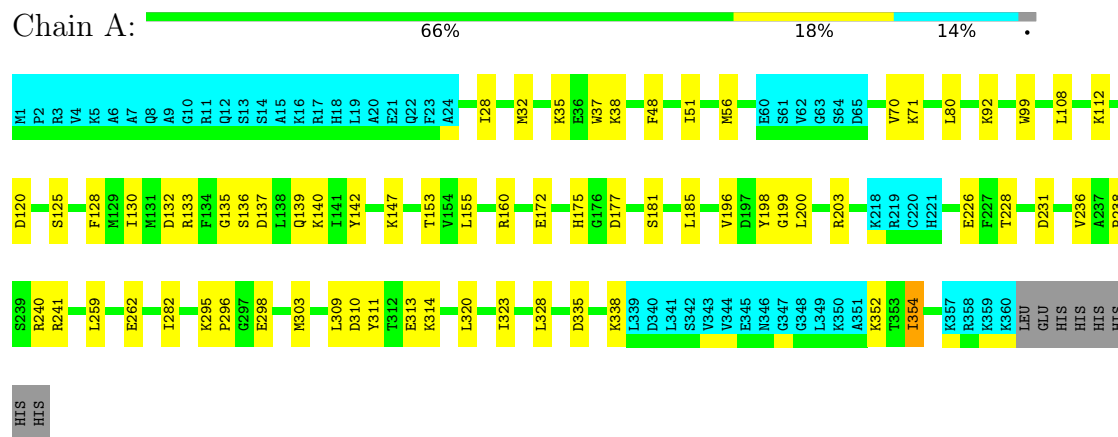
Chain	Residue	Modelled	Actual	Comment	Reference
A	361	LEU	-	expression tag	UNP Q99986
A	362	GLU	-	expression tag	UNP Q99986
A	363	HIS	-	expression tag	UNP Q99986
A	364	HIS	-	expression tag	UNP Q99986
A	365	HIS	-	expression tag	UNP Q99986
A	366	HIS	-	expression tag	UNP Q99986
A	367	HIS	-	expression tag	UNP Q99986
A	368	HIS	-	expression tag	UNP Q99986

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: Serine/threonine-protein kinase VRK1

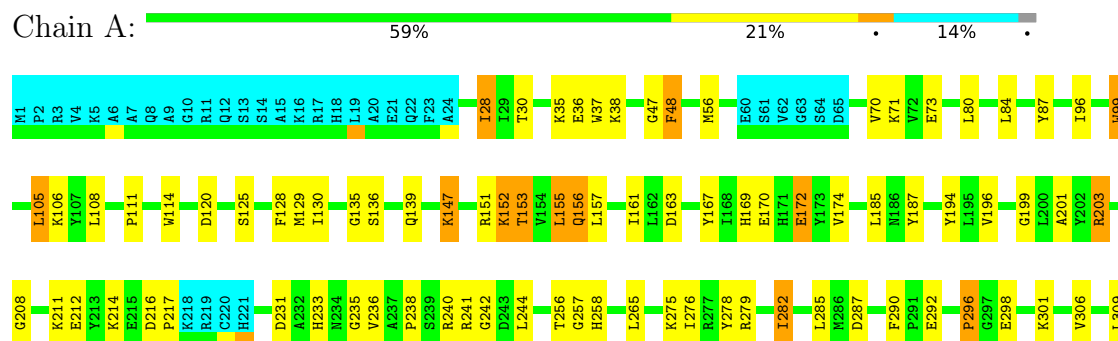


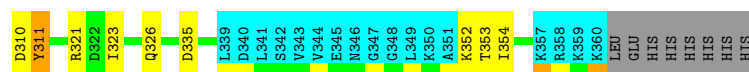
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

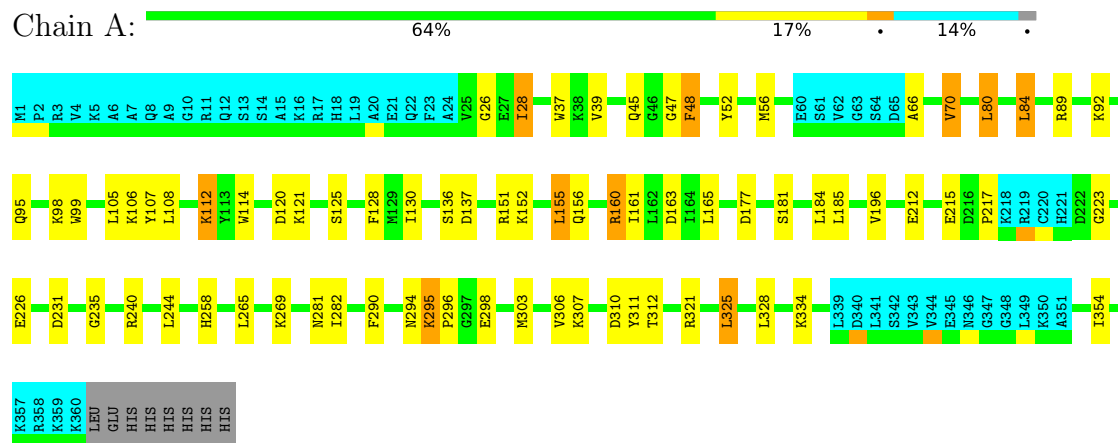
- Molecule 1: Serine/threonine-protein kinase VRK1





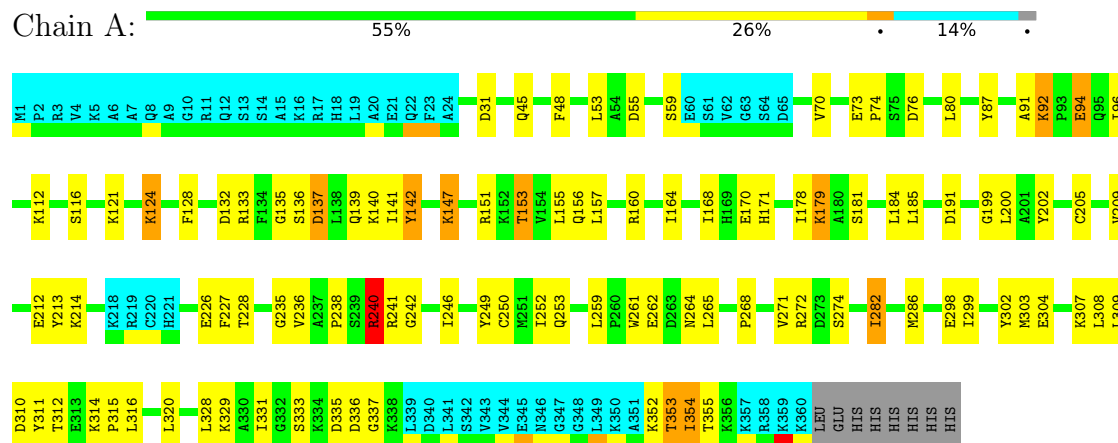
4.2.2 Score per residue for model 2

- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.3 Score per residue for model 3

- Molecule 1: Serine/threonine-protein kinase VRK1



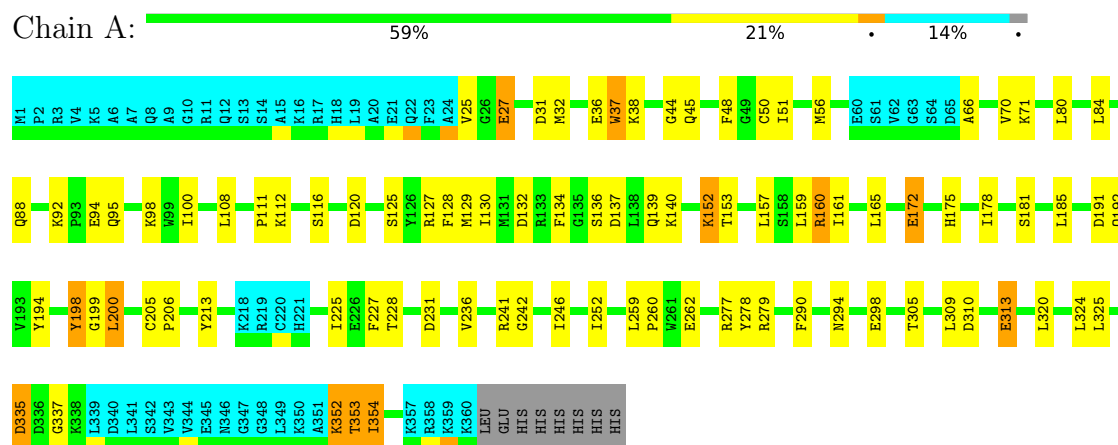
4.2.4 Score per residue for model 4

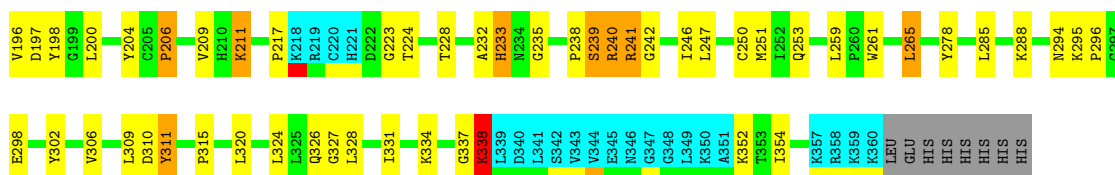
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.7 Score per residue for model 7

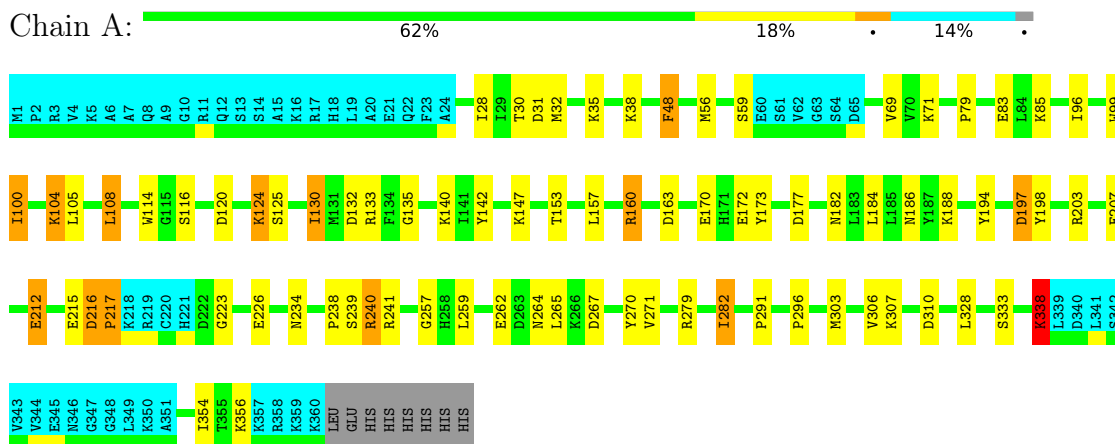
- Molecule 1: Serine/threonine-protein kinase VRK1





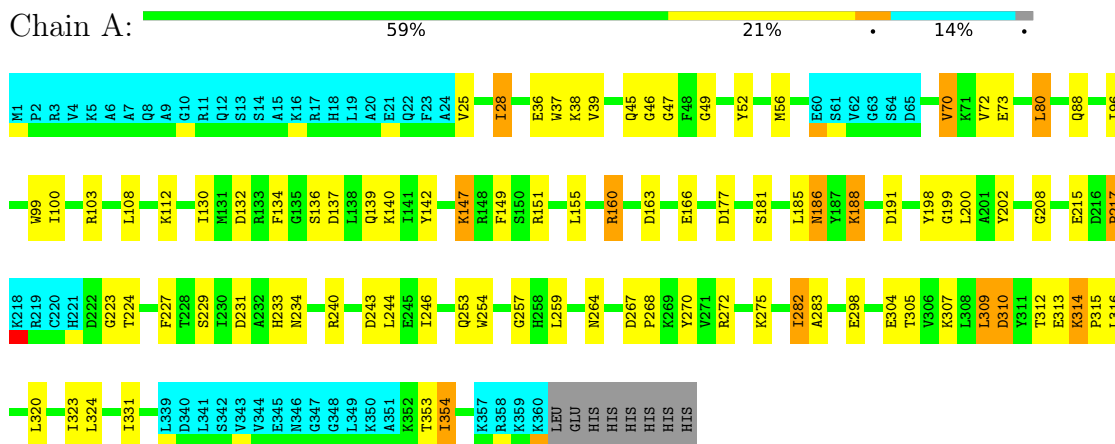
4.2.10 Score per residue for model 10

- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.11 Score per residue for model 11

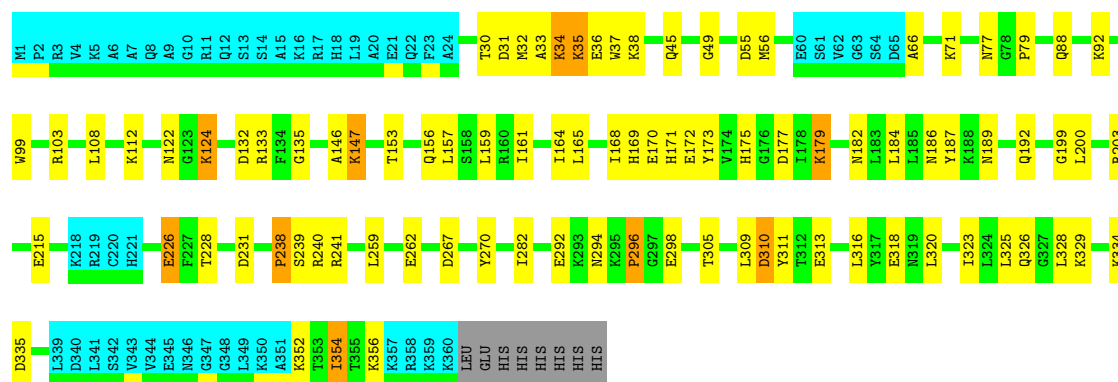
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.12 Score per residue for model 12

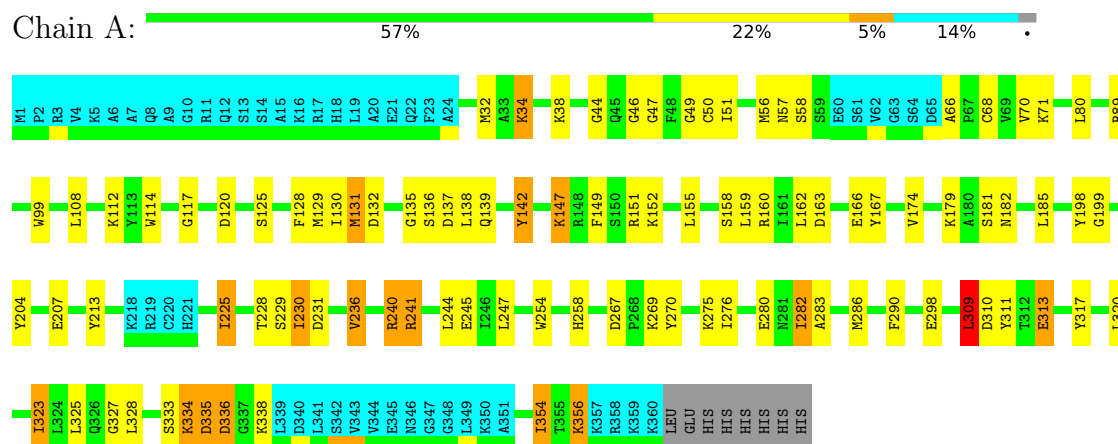
- Molecule 1: Serine/threonine-protein kinase VRK1





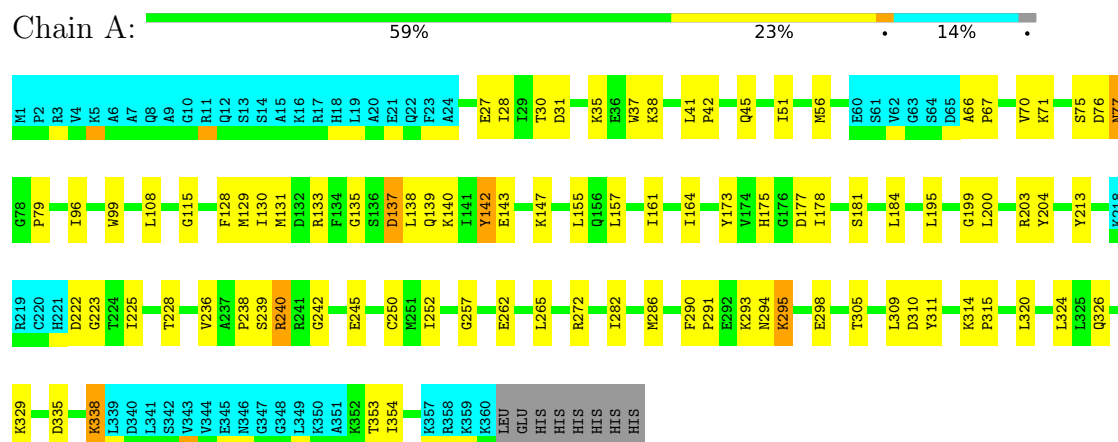
4.2.13 Score per residue for model 13

- Molecule 1: Serine/threonine-protein kinase VRK1



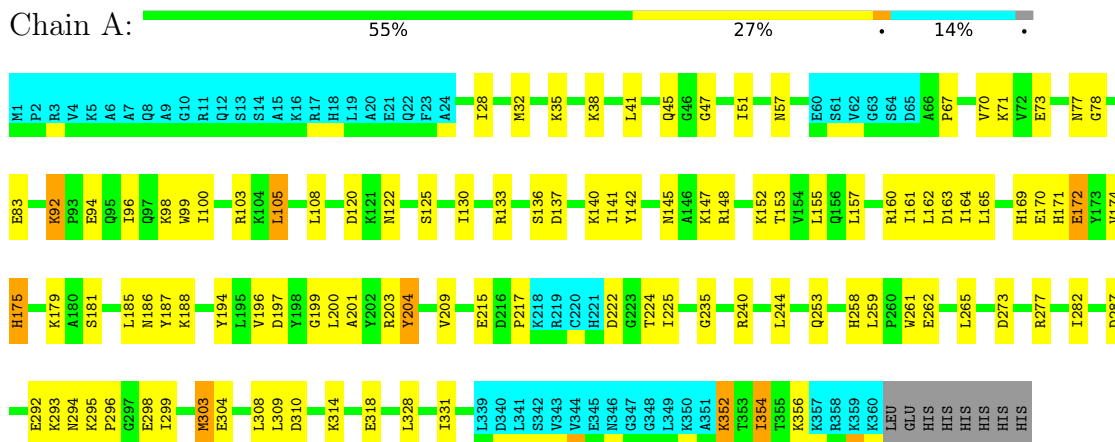
4.2.14 Score per residue for model 14

- Molecule 1: Serine/threonine-protein kinase VRK1



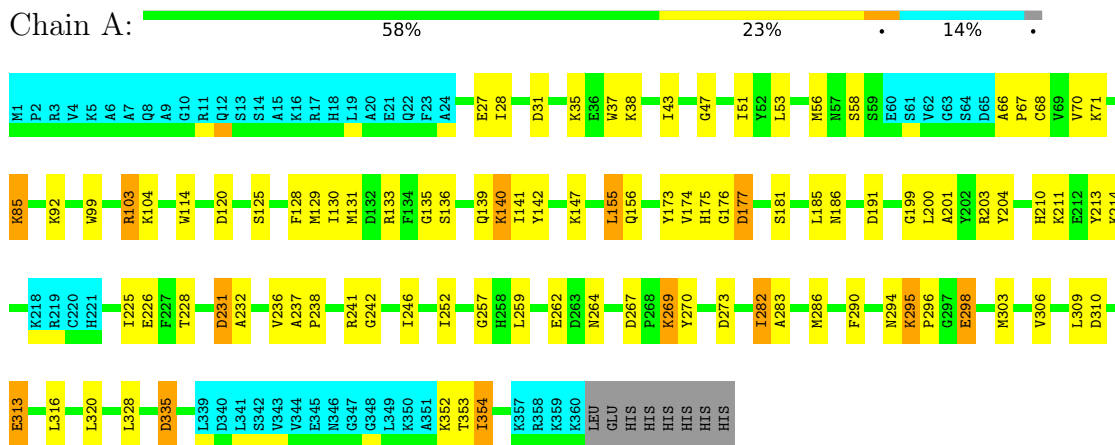
4.2.15 Score per residue for model 15

- Molecule 1: Serine/threonine-protein kinase VRK1



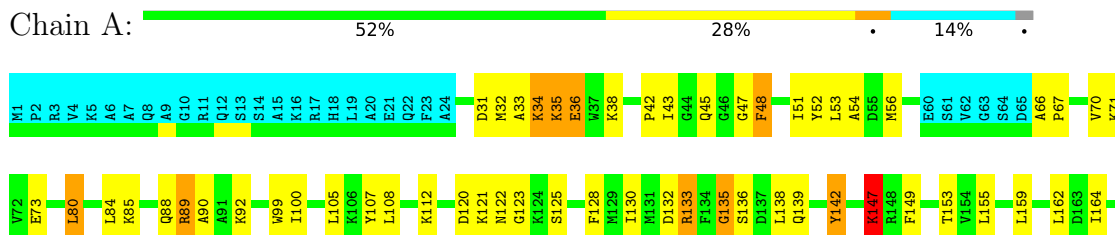
4.2.16 Score per residue for model 16

- Molecule 1: Serine/threonine-protein kinase VRK1



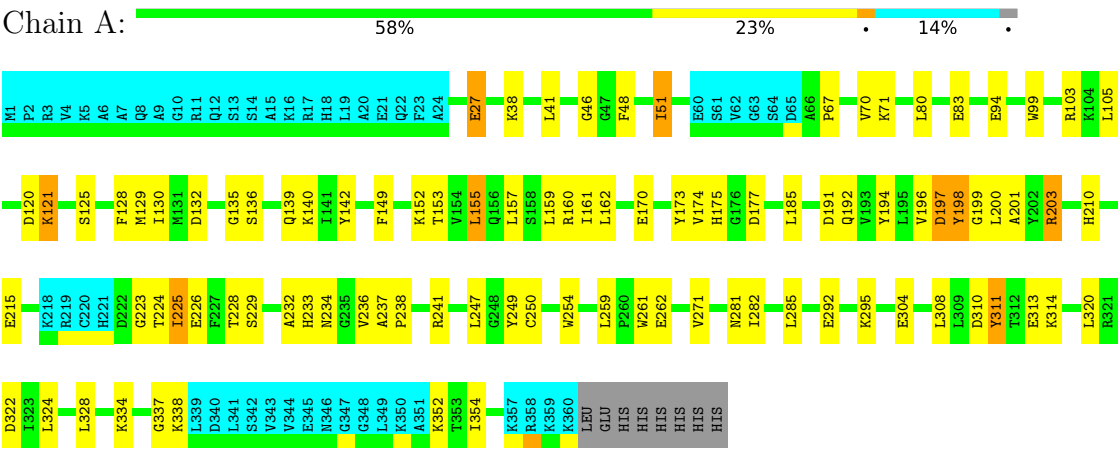
4.2.17 Score per residue for model 17

- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.20 Score per residue for model 20

● Molecule 1: Serine/threonine-protein kinase VRK1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS, simulated annealing, TORSION ANGLE DYNAMICS*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	1.1

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	3551
Number of shifts mapped to atoms	3551
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	73%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.37±0.01	0±0/2572 (0.0± 0.0%)	0.70±0.01	0±0/3468 (0.0± 0.0%)
All	All	0.37	0/51440 (0.0%)	0.70	1/69360 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	240	ARG	N-CA-C	-5.49	108.36	114.62	9	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2512	2531	2524	52±7
All	All	50240	50620	50480	1044

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:ASP:HB2	1:A:223:GLY:HA3	0.92	1.38	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:HIS:HB2	1:A:201:ALA:HA	0.88	1.41	15	1
1:A:136:SER:HB2	1:A:185:LEU:HB2	0.87	1.46	6	14
1:A:215:GLU:HB2	1:A:236:VAL:HA	0.87	1.46	20	1
1:A:112:LYS:HB3	1:A:132:ASP:HB2	0.84	1.47	12	8
1:A:104:LYS:HE3	1:A:104:LYS:HA	0.83	1.49	10	1
1:A:177:ASP:HB2	1:A:223:GLY:HA2	0.82	1.51	14	3
1:A:241:ARG:HG3	1:A:311:TYR:HA	0.81	1.53	1	4
1:A:205:CYS:HB2	1:A:209:VAL:HA	0.81	1.50	17	2
1:A:73:GLU:HG2	1:A:80:LEU:HB2	0.81	1.50	1	1
1:A:37:TRP:HB3	1:A:56:MET:HG2	0.80	1.51	14	1
1:A:139:GLN:HB3	1:A:181:SER:HA	0.79	1.55	13	4
1:A:310:ASP:HB3	1:A:313:GLU:HB2	0.79	1.53	13	2
1:A:124:LYS:HE3	1:A:124:LYS:HA	0.78	1.53	10	2
1:A:133:ARG:HD2	1:A:188:LYS:HB2	0.78	1.55	15	1
1:A:35:LYS:HG3	1:A:36:GLU:HG3	0.78	1.56	17	2
1:A:176:GLY:HA2	1:A:243:ASP:HB3	0.78	1.55	18	1
1:A:309:LEU:HG	1:A:310:ASP:H	0.77	1.36	4	1
1:A:227:PHE:HB3	1:A:246:ILE:HG23	0.77	1.57	4	3
1:A:56:MET:HE2	1:A:56:MET:HA	0.76	1.58	17	1
1:A:328:LEU:HD11	1:A:334:LYS:HA	0.75	1.59	12	1
1:A:253:GLN:HE21	1:A:259:LEU:HG	0.75	1.40	17	1
1:A:32:MET:HA	1:A:32:MET:HE2	0.75	1.58	18	8
1:A:120:ASP:HA	1:A:125:SER:HA	0.74	1.58	13	10
1:A:137:ASP:HB3	1:A:139:GLN:HG2	0.73	1.60	7	1
1:A:259:LEU:HB2	1:A:262:GLU:HB2	0.72	1.59	10	5
1:A:213:TYR:HB2	1:A:236:VAL:HG21	0.72	1.60	17	1
1:A:290:PHE:HB3	1:A:296:PRO:HB3	0.72	1.60	2	1
1:A:200:LEU:HD11	1:A:352:LYS:HD2	0.72	1.60	9	1
1:A:200:LEU:HA	1:A:354:ILE:HB	0.71	1.62	3	2
1:A:298:GLU:HG3	1:A:327:GLY:HA3	0.71	1.61	9	4
1:A:278:TYR:HA	1:A:285:LEU:HG	0.71	1.60	9	2
1:A:37:TRP:HA	1:A:56:MET:SD	0.71	2.24	7	3
1:A:241:ARG:HD3	1:A:311:TYR:HD1	0.71	1.46	3	1
1:A:79:PRO:HB3	1:A:199:GLY:HA2	0.71	1.60	14	1
1:A:31:ASP:HB3	1:A:37:TRP:CZ2	0.71	2.21	7	2
1:A:213:TYR:HA	1:A:236:VAL:HG21	0.70	1.63	4	2
1:A:87:TYR:HE1	1:A:111:PRO:HG2	0.70	1.45	1	1
1:A:138:LEU:HA	1:A:141:ILE:HB	0.70	1.62	6	1
1:A:45:GLN:H	1:A:49:GLY:HA2	0.70	1.47	11	2
1:A:28:ILE:HB	1:A:36:GLU:HG2	0.69	1.62	1	1
1:A:121:LYS:HA	1:A:121:LYS:HE2	0.69	1.64	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:GLN:HB2	1:A:181:SER:HA	0.69	1.62	4	1
1:A:179:LYS:HE3	1:A:224:THR:HG21	0.69	1.64	15	1
1:A:248:GLY:HA3	1:A:303:MET:SD	0.69	2.28	4	1
1:A:104:LYS:HA	1:A:104:LYS:HE2	0.69	1.63	8	1
1:A:259:LEU:HB2	1:A:262:GLU:HG3	0.68	1.64	16	1
1:A:200:LEU:HD11	1:A:352:LYS:HA	0.68	1.65	3	1
1:A:156:GLN:HE21	1:A:335:ASP:HB2	0.68	1.48	12	1
1:A:240:ARG:HG2	1:A:315:PRO:HB3	0.68	1.65	11	1
1:A:142:TYR:HD1	1:A:147:LYS:HB3	0.67	1.48	8	2
1:A:38:LYS:HG2	1:A:56:MET:HA	0.67	1.66	16	2
1:A:42:PRO:HA	1:A:52:TYR:HD1	0.67	1.48	8	2
1:A:186:ASN:HB3	1:A:189:ASN:HB3	0.67	1.65	12	2
1:A:152:LYS:HG2	1:A:335:ASP:HA	0.67	1.67	7	1
1:A:217:PRO:HA	1:A:235:GLY:HA3	0.67	1.67	17	1
1:A:215:GLU:HA	1:A:234:ASN:HB3	0.67	1.67	10	1
1:A:139:GLN:HA	1:A:142:TYR:HD2	0.66	1.49	14	1
1:A:264:ASN:HB3	1:A:270:TYR:HB3	0.65	1.67	19	5
1:A:38:LYS:HG2	1:A:57:ASN:HB2	0.65	1.67	15	1
1:A:70:VAL:HB	1:A:130:ILE:HD13	0.65	1.69	1	9
1:A:160:ARG:HA	1:A:160:ARG:HE	0.65	1.51	10	3
1:A:301:LYS:HA	1:A:301:LYS:HE2	0.65	1.68	1	1
1:A:309:LEU:O	1:A:313:GLU:HB2	0.65	1.92	5	2
1:A:51:ILE:HD12	1:A:71:LYS:HA	0.65	1.68	13	3
1:A:173:TYR:HA	1:A:203:ARG:HA	0.64	1.68	10	1
1:A:47:GLY:HA3	1:A:51:ILE:HD11	0.64	1.67	13	1
1:A:47:GLY:HA3	1:A:196:VAL:HG11	0.64	1.68	1	1
1:A:142:TYR:CE1	1:A:147:LYS:HD3	0.64	2.28	16	1
1:A:137:ASP:HB3	1:A:184:LEU:HD13	0.64	1.69	19	1
1:A:137:ASP:HB3	1:A:139:GLN:HG3	0.64	1.69	11	2
1:A:124:LYS:HE2	1:A:124:LYS:HA	0.64	1.70	3	1
1:A:165:LEU:O	1:A:169:HIS:HB3	0.63	1.94	12	1
1:A:51:ILE:HG23	1:A:71:LYS:HB3	0.63	1.69	15	1
1:A:37:TRP:HA	1:A:56:MET:HA	0.63	1.70	11	2
1:A:67:PRO:HA	1:A:133:ARG:HG2	0.63	1.68	16	1
1:A:201:ALA:H	1:A:354:ILE:HG22	0.62	1.54	5	1
1:A:142:TYR:HB2	1:A:147:LYS:HA	0.62	1.69	15	1
1:A:41:LEU:HB3	1:A:53:LEU:HD12	0.62	1.70	4	1
1:A:35:LYS:HA	1:A:35:LYS:HE2	0.62	1.71	6	1
1:A:73:GLU:HB3	1:A:74:PRO:HD2	0.62	1.71	5	2
1:A:138:LEU:HB3	1:A:180:ALA:O	0.62	1.95	4	2
1:A:267:ASP:HB2	1:A:270:TYR:CD1	0.62	2.30	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:ASP:HB3	1:A:200:LEU:HB2	0.62	1.72	12	1
1:A:186:ASN:HB2	1:A:194:TYR:HE1	0.61	1.55	15	4
1:A:287:ASP:HA	1:A:296:PRO:HB2	0.61	1.72	15	1
1:A:169:HIS:CE1	1:A:174:VAL:HG12	0.61	2.30	1	1
1:A:240:ARG:HD3	1:A:315:PRO:HG3	0.61	1.69	14	1
1:A:178:ILE:HB	1:A:250:CYS:SG	0.61	2.35	8	1
1:A:73:GLU:OE1	1:A:77:ASN:HA	0.61	1.96	15	1
1:A:35:LYS:H	1:A:37:TRP:HZ3	0.61	1.37	18	1
1:A:110:VAL:HG22	1:A:111:PRO:HD2	0.61	1.72	9	1
1:A:200:LEU:HD21	1:A:352:LYS:HB3	0.60	1.72	6	1
1:A:83:GLU:HG3	1:A:198:TYR:HB2	0.60	1.73	4	2
1:A:271:VAL:O	1:A:275:LYS:HG2	0.60	1.96	6	2
1:A:31:ASP:HB3	1:A:37:TRP:HZ2	0.60	1.56	7	1
1:A:172:GLU:HB3	1:A:203:ARG:HB2	0.60	1.72	10	1
1:A:140:LYS:HE3	1:A:140:LYS:HA	0.60	1.71	16	1
1:A:106:LYS:HA	1:A:106:LYS:HE2	0.60	1.71	6	1
1:A:229:SER:HA	1:A:275:LYS:HE2	0.60	1.73	11	1
1:A:200:LEU:HD21	1:A:352:LYS:HE3	0.60	1.73	8	1
1:A:92:LYS:HB3	1:A:94:GLU:HG2	0.60	1.72	15	1
1:A:155:LEU:HD22	1:A:328:LEU:HG	0.60	1.72	15	1
1:A:242:GLY:O	1:A:246:ILE:HG13	0.60	1.97	7	8
1:A:159:LEU:HG	1:A:321:ARG:HD2	0.59	1.73	6	1
1:A:48:PHE:HZ	1:A:199:GLY:HA3	0.59	1.55	3	1
1:A:267:ASP:OD1	1:A:269:LYS:HG2	0.59	1.97	13	3
1:A:33:ALA:HB3	1:A:35:LYS:HE2	0.59	1.74	9	1
1:A:226:GLU:HG3	1:A:265:LEU:HG	0.59	1.72	3	1
1:A:85:LYS:HE2	1:A:85:LYS:HA	0.59	1.72	18	2
1:A:198:TYR:HB2	1:A:201:ALA:HB2	0.59	1.75	17	1
1:A:329:LYS:HA	1:A:333:SER:O	0.59	1.97	3	2
1:A:165:LEU:O	1:A:169:HIS:HB2	0.59	1.97	19	2
1:A:204:TYR:HB2	1:A:209:VAL:HG12	0.59	1.74	15	1
1:A:71:LYS:HE3	1:A:129:MET:HB3	0.58	1.75	5	1
1:A:155:LEU:HB3	1:A:328:LEU:HD22	0.58	1.75	16	1
1:A:45:GLN:HB2	1:A:51:ILE:HG12	0.58	1.76	7	2
1:A:138:LEU:O	1:A:142:TYR:HB3	0.58	1.98	13	3
1:A:156:GLN:O	1:A:160:ARG:HG2	0.58	1.99	18	4
1:A:240:ARG:HD2	1:A:315:PRO:HG3	0.58	1.75	3	1
1:A:320:LEU:O	1:A:323:ILE:HG13	0.58	1.99	6	1
1:A:211:LYS:HA	1:A:211:LYS:HE2	0.58	1.75	9	1
1:A:43:ILE:HG22	1:A:45:GLN:HG2	0.58	1.74	17	1
1:A:142:TYR:HA	1:A:149:PHE:CZ	0.58	2.34	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:LYS:HA	1:A:85:LYS:HE3	0.58	1.76	16	1
1:A:309:LEU:HG	1:A:310:ASP:N	0.57	2.13	4	1
1:A:160:ARG:HA	1:A:160:ARG:NH1	0.57	2.13	5	1
1:A:265:LEU:HA	1:A:271:VAL:CG1	0.57	2.29	5	1
1:A:133:ARG:HG3	1:A:187:TYR:HB3	0.57	1.75	15	1
1:A:335:ASP:HB3	1:A:338:LYS:HB2	0.57	1.75	4	1
1:A:142:TYR:CE1	1:A:147:LYS:HB3	0.57	2.34	17	3
1:A:295:LYS:HD3	1:A:331:ILE:HD12	0.57	1.76	18	1
1:A:338:LYS:NZ	1:A:338:LYS:HB3	0.57	2.15	10	2
1:A:48:PHE:HB2	1:A:71:LYS:HE3	0.57	1.75	18	1
1:A:140:LYS:HA	1:A:140:LYS:HE2	0.57	1.75	20	1
1:A:155:LEU:HG	1:A:328:LEU:HB2	0.57	1.76	20	3
1:A:175:HIS:CE1	1:A:200:LEU:HB2	0.57	2.35	20	2
1:A:334:LYS:HD2	1:A:336:ASP:HB2	0.57	1.75	13	1
1:A:172:GLU:HB2	1:A:206:PRO:HA	0.57	1.76	19	1
1:A:111:PRO:HD3	1:A:194:TYR:HB3	0.57	1.75	1	1
1:A:153:THR:O	1:A:157:LEU:HG	0.57	1.99	12	4
1:A:48:PHE:CE2	1:A:198:TYR:HA	0.57	2.33	7	1
1:A:191:ASP:CB	1:A:338:LYS:HB3	0.57	2.30	8	1
1:A:92:LYS:HB3	1:A:95:GLN:HE21	0.57	1.59	4	1
1:A:169:HIS:CD2	1:A:170:GLU:HG3	0.57	2.35	12	1
1:A:328:LEU:HG	1:A:333:SER:O	0.57	2.00	13	3
1:A:191:ASP:HB3	1:A:338:LYS:HB2	0.56	1.77	9	1
1:A:200:LEU:HA	1:A:354:ILE:HG23	0.56	1.77	9	2
1:A:295:LYS:HE3	1:A:295:LYS:HA	0.56	1.76	5	3
1:A:139:GLN:HA	1:A:142:TYR:HD1	0.56	1.60	19	1
1:A:304:GLU:O	1:A:308:LEU:HG	0.56	2.01	3	3
1:A:156:GLN:NE2	1:A:335:ASP:HB2	0.56	2.15	12	1
1:A:261:TRP:HB2	1:A:271:VAL:HA	0.56	1.78	3	2
1:A:199:GLY:HA3	1:A:352:LYS:O	0.56	2.01	19	3
1:A:155:LEU:HG	1:A:328:LEU:HD22	0.56	1.76	6	2
1:A:112:LYS:HE3	1:A:112:LYS:HA	0.56	1.77	8	1
1:A:281:ASN:HD22	1:A:285:LEU:HD23	0.56	1.60	20	1
1:A:89:ARG:NE	1:A:89:ARG:HA	0.56	2.16	2	1
1:A:229:SER:HA	1:A:275:LYS:CD	0.56	2.31	13	1
1:A:142:TYR:HE1	1:A:147:LYS:HD3	0.56	1.60	16	2
1:A:160:ARG:NE	1:A:160:ARG:HA	0.56	2.16	15	1
1:A:99:TRP:HH2	1:A:163:ASP:HB2	0.56	1.61	13	2
1:A:152:LYS:HD2	1:A:335:ASP:HB2	0.56	1.76	13	1
1:A:99:TRP:HZ2	1:A:108:LEU:HD22	0.56	1.59	6	4
1:A:142:TYR:HA	1:A:149:PHE:HZ	0.56	1.61	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:199:GLY:HA3	1:A:354:ILE:CG2	0.55	2.31	15	1
1:A:200:LEU:HA	1:A:354:ILE:HA	0.55	1.77	17	1
1:A:179:LYS:HG3	1:A:227:PHE:CE2	0.55	2.37	3	1
1:A:212:GLU:H	1:A:212:GLU:CD	0.55	2.09	10	2
1:A:83:GLU:HB2	1:A:198:TYR:HD2	0.55	1.60	8	1
1:A:179:LYS:HD2	1:A:224:THR:OG1	0.55	2.01	8	1
1:A:252:ILE:HD12	1:A:286:MET:SD	0.55	2.41	14	2
1:A:199:GLY:HA3	1:A:352:LYS:HB2	0.55	1.78	12	1
1:A:32:MET:HG2	1:A:116:SER:O	0.55	2.01	10	3
1:A:147:LYS:HD3	1:A:257:GLY:O	0.55	2.01	10	2
1:A:118:LEU:HB3	1:A:127:ARG:HG3	0.55	1.79	19	1
1:A:213:TYR:HD1	1:A:236:VAL:HB	0.55	1.60	16	2
1:A:31:ASP:HB3	1:A:37:TRP:CH2	0.55	2.37	18	1
1:A:237:ALA:HB3	1:A:238:PRO:HD3	0.55	1.79	20	1
1:A:172:GLU:HG2	1:A:207:GLU:H	0.55	1.62	17	1
1:A:227:PHE:HZ	1:A:253:GLN:HG3	0.55	1.61	5	1
1:A:84:LEU:HD23	1:A:129:MET:HE3	0.55	1.76	1	1
1:A:187:TYR:CE2	1:A:188:LYS:HE2	0.55	2.36	4	1
1:A:52:TYR:HE1	1:A:72:VAL:HB	0.55	1.62	11	1
1:A:38:LYS:HE3	1:A:56:MET:HB3	0.55	1.77	17	1
1:A:94:GLU:HG2	1:A:98:LYS:HE3	0.55	1.79	4	1
1:A:192:GLN:HB3	1:A:194:TYR:CE2	0.55	2.37	5	3
1:A:169:HIS:HD2	1:A:240:ARG:HD3	0.54	1.61	1	1
1:A:135:GLY:HA3	1:A:187:TYR:HD1	0.54	1.62	9	3
1:A:241:ARG:HD3	1:A:310:ASP:O	0.54	2.03	19	2
1:A:268:PRO:O	1:A:272:ARG:HG3	0.54	2.02	11	2
1:A:255:LEU:HD11	1:A:294:ASN:HD21	0.54	1.62	8	1
1:A:151:ARG:NH2	1:A:295:LYS:HB3	0.54	2.17	2	1
1:A:121:LYS:HG2	1:A:122:ASN:HD22	0.54	1.62	17	1
1:A:199:GLY:O	1:A:354:ILE:HB	0.54	2.02	13	1
1:A:352:LYS:HE3	1:A:353:THR:O	0.54	2.03	16	1
1:A:309:LEU:HD22	1:A:314:LYS:O	0.54	2.02	15	1
1:A:71:LYS:HE2	1:A:129:MET:SD	0.54	2.42	1	1
1:A:159:LEU:HD21	1:A:325:LEU:HD11	0.54	1.79	6	1
1:A:40:GLY:HA3	1:A:55:ASP:HB2	0.54	1.79	8	1
1:A:282:ILE:HG13	1:A:303:MET:HB2	0.54	1.80	10	1
1:A:188:LYS:HE3	1:A:188:LYS:HA	0.54	1.78	11	1
1:A:103:ARG:HG3	1:A:105:LEU:HD13	0.54	1.79	20	1
1:A:259:LEU:HB2	1:A:262:GLU:HB3	0.54	1.79	20	1
1:A:99:TRP:CH2	1:A:108:LEU:HD22	0.53	2.38	1	1
1:A:166:GLU:HA	1:A:169:HIS:HB2	0.53	1.77	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:325:LEU:O	1:A:329:LYS:HG3	0.53	2.03	19	1
1:A:305:THR:O	1:A:309:LEU:HG	0.53	2.02	5	4
1:A:133:ARG:HD3	1:A:133:ARG:H	0.53	1.63	10	1
1:A:105:LEU:HG	1:A:163:ASP:OD1	0.53	2.03	1	1
1:A:216:ASP:HB3	1:A:236:VAL:HB	0.53	1.78	1	1
1:A:32:MET:HB2	1:A:117:GLY:HA2	0.53	1.81	13	1
1:A:28:ILE:H	1:A:28:ILE:HD13	0.53	1.62	1	3
1:A:38:LYS:HB3	1:A:56:MET:HA	0.53	1.79	1	1
1:A:151:ARG:NH1	1:A:331:ILE:HB	0.53	2.18	3	1
1:A:231:ASP:O	1:A:236:VAL:HG12	0.53	2.04	6	1
1:A:197:ASP:HB2	1:A:198:TYR:CD2	0.53	2.38	10	1
1:A:198:TYR:HD2	1:A:200:LEU:H	0.53	1.45	6	2
1:A:173:TYR:CD1	1:A:203:ARG:HA	0.53	2.39	12	1
1:A:156:GLN:NE2	1:A:335:ASP:HA	0.53	2.18	1	1
1:A:281:ASN:ND2	1:A:284:SER:HB2	0.53	2.19	5	1
1:A:295:LYS:HE3	1:A:331:ILE:HG21	0.53	1.81	17	1
1:A:95:GLN:HA	1:A:98:LYS:HE3	0.53	1.80	19	1
1:A:316:LEU:O	1:A:320:LEU:HG	0.53	2.04	12	6
1:A:182:ASN:ND2	1:A:195:LEU:HD22	0.53	2.19	6	1
1:A:320:LEU:O	1:A:324:LEU:HG	0.53	2.03	9	6
1:A:147:LYS:HG3	1:A:257:GLY:HA2	0.53	1.79	16	1
1:A:105:LEU:HG	1:A:163:ASP:HB2	0.52	1.79	15	1
1:A:147:LYS:HD3	1:A:253:GLN:HG2	0.52	1.79	15	1
1:A:47:GLY:O	1:A:48:PHE:HB2	0.52	2.05	17	2
1:A:48:PHE:HA	1:A:352:LYS:HD2	0.52	1.80	3	1
1:A:204:TYR:CE1	1:A:239:SER:HA	0.52	2.39	14	1
1:A:37:TRP:CE3	1:A:56:MET:HB2	0.52	2.40	5	1
1:A:286:MET:HE3	1:A:303:MET:SD	0.52	2.45	16	2
1:A:172:GLU:HB2	1:A:205:CYS:O	0.52	2.04	7	1
1:A:47:GLY:HA2	1:A:181:SER:O	0.52	2.04	15	1
1:A:241:ARG:HG3	1:A:311:TYR:HD1	0.52	1.65	6	1
1:A:67:PRO:O	1:A:133:ARG:HB3	0.52	2.05	14	1
1:A:96:ILE:HA	1:A:99:TRP:CZ3	0.52	2.40	1	2
1:A:169:HIS:HE1	1:A:174:VAL:HG12	0.52	1.65	17	2
1:A:97:GLN:HE21	1:A:97:GLN:HA	0.52	1.65	18	1
1:A:352:LYS:O	1:A:353:THR:HG22	0.52	2.05	7	1
1:A:172:GLU:O	1:A:203:ARG:HA	0.52	2.05	15	1
1:A:354:ILE:HG13	1:A:356:LYS:HD3	0.52	1.82	12	1
1:A:147:LYS:HE3	1:A:253:GLN:HB3	0.52	1.82	9	1
1:A:46:GLY:O	1:A:71:LYS:HE2	0.52	2.05	13	1
1:A:89:ARG:HG3	1:A:173:TYR:CE2	0.51	2.40	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:THR:O	1:A:232:ALA:HB3	0.51	2.05	20	2
1:A:186:ASN:HB2	1:A:194:TYR:CE1	0.51	2.40	15	1
1:A:114:TRP:CD1	1:A:130:ILE:HG22	0.51	2.40	1	3
1:A:352:LYS:O	1:A:353:THR:HB	0.51	2.05	4	2
1:A:171:HIS:C	1:A:172:GLU:HG3	0.51	2.30	4	1
1:A:47:GLY:HA2	1:A:71:LYS:HE3	0.51	1.82	16	1
1:A:178:ILE:HB	1:A:246:ILE:HG22	0.51	1.81	7	2
1:A:69:VAL:HG22	1:A:132:ASP:O	0.51	2.06	10	1
1:A:56:MET:HA	1:A:56:MET:CE	0.51	2.35	17	1
1:A:94:GLU:HG2	1:A:98:LYS:HE2	0.51	1.82	19	1
1:A:273:ASP:O	1:A:277:ARG:HB2	0.51	2.05	15	1
1:A:160:ARG:HA	1:A:160:ARG:NE	0.51	2.21	13	2
1:A:39:VAL:HG23	1:A:52:TYR:CD2	0.51	2.40	11	1
1:A:157:LEU:O	1:A:161:ILE:HG12	0.51	2.06	7	5
1:A:147:LYS:O	1:A:257:GLY:HA2	0.51	2.05	11	1
1:A:99:TRP:CZ3	1:A:108:LEU:HD13	0.51	2.40	12	1
1:A:38:LYS:HG2	1:A:56:MET:O	0.51	2.06	14	1
1:A:108:LEU:H	1:A:108:LEU:HD23	0.51	1.66	5	2
1:A:231:ASP:OD2	1:A:238:PRO:HA	0.51	2.06	12	2
1:A:147:LYS:HG3	1:A:253:GLN:HE22	0.51	1.66	11	1
1:A:290:PHE:HB3	1:A:294:ASN:O	0.51	2.06	14	1
1:A:47:GLY:HA3	1:A:196:VAL:CG1	0.51	2.34	1	1
1:A:161:ILE:O	1:A:165:LEU:HB2	0.51	2.05	12	3
1:A:167:TYR:O	1:A:171:HIS:HB2	0.51	2.06	9	1
1:A:310:ASP:CG	1:A:311:TYR:H	0.51	2.12	14	2
1:A:107:TYR:HE2	1:A:160:ARG:HD3	0.51	1.66	18	1
1:A:179:LYS:HG3	1:A:227:PHE:HE2	0.51	1.65	3	1
1:A:175:HIS:HB3	1:A:198:TYR:HD2	0.51	1.66	17	1
1:A:302:TYR:CD1	1:A:320:LEU:HD12	0.51	2.41	9	2
1:A:306:VAL:HA	1:A:309:LEU:HB2	0.51	1.82	16	1
1:A:200:LEU:HB3	1:A:222:ASP:HB3	0.50	1.84	14	1
1:A:215:GLU:O	1:A:216:ASP:HB2	0.50	2.07	10	1
1:A:174:VAL:O	1:A:201:ALA:HA	0.50	2.05	20	3
1:A:142:TYR:CD1	1:A:147:LYS:HB3	0.50	2.42	3	5
1:A:267:ASP:HB3	1:A:270:TYR:HD2	0.50	1.67	12	2
1:A:67:PRO:O	1:A:132:ASP:HA	0.50	2.07	20	2
1:A:90:ALA:HA	1:A:99:TRP:CH2	0.50	2.41	19	1
1:A:286:MET:HE1	1:A:299:ILE:HG22	0.50	1.81	4	1
1:A:244:LEU:HG	1:A:320:LEU:HD21	0.50	1.83	11	1
1:A:238:PRO:HG2	1:A:242:GLY:HA3	0.50	1.84	14	1
1:A:240:ARG:HG2	1:A:312:THR:HG23	0.50	1.83	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:GLY:HA2	1:A:50:CYS:HA	0.50	1.83	7	2
1:A:155:LEU:HG	1:A:328:LEU:HG	0.50	1.82	8	2
1:A:259:LEU:HB2	1:A:262:GLU:CG	0.50	2.36	16	1
1:A:205:CYS:CB	1:A:209:VAL:HA	0.50	2.31	17	1
1:A:196:VAL:HG13	1:A:197:ASP:N	0.50	2.21	20	1
1:A:202:TYR:HD1	1:A:354:ILE:HD11	0.50	1.66	3	1
1:A:314:LYS:HD2	1:A:314:LYS:H	0.50	1.66	5	1
1:A:314:LYS:HD2	1:A:314:LYS:N	0.50	2.21	5	2
1:A:104:LYS:HB2	1:A:104:LYS:NZ	0.50	2.22	9	1
1:A:169:HIS:HA	1:A:174:VAL:HG12	0.50	1.84	15	1
1:A:222:ASP:OD1	1:A:228:THR:HG21	0.50	2.06	19	1
1:A:106:LYS:HZ2	1:A:106:LYS:HB3	0.49	1.67	4	1
1:A:31:ASP:OD1	1:A:35:LYS:HE3	0.49	2.07	9	1
1:A:105:LEU:HG	1:A:163:ASP:OD2	0.49	2.08	2	1
1:A:27:GLU:O	1:A:38:LYS:HA	0.49	2.06	20	2
1:A:238:PRO:HB2	1:A:242:GLY:HA3	0.49	1.84	1	1
1:A:26:GLY:HA2	1:A:56:MET:SD	0.49	2.48	2	1
1:A:94:GLU:O	1:A:98:LYS:HG2	0.49	2.08	7	1
1:A:111:PRO:HB3	1:A:134:PHE:HE2	0.49	1.67	7	1
1:A:111:PRO:HG3	1:A:196:VAL:HG12	0.49	1.83	9	1
1:A:267:ASP:O	1:A:271:VAL:HG23	0.49	2.08	10	1
1:A:169:HIS:HD2	1:A:170:GLU:HG3	0.49	1.66	12	1
1:A:142:TYR:CE2	1:A:143:GLU:HG3	0.49	2.42	14	1
1:A:30:THR:HA	1:A:35:LYS:O	0.49	2.08	9	5
1:A:106:LYS:HG3	1:A:107:TYR:CD1	0.49	2.42	2	1
1:A:259:LEU:O	1:A:262:GLU:HG3	0.49	2.07	7	2
1:A:196:VAL:HG22	1:A:197:ASP:H	0.49	1.68	4	1
1:A:200:LEU:HG	1:A:353:THR:HA	0.49	1.84	7	1
1:A:48:PHE:HZ	1:A:79:PRO:HB2	0.49	1.68	8	1
1:A:155:LEU:HD22	1:A:328:LEU:HD22	0.49	1.83	13	2
1:A:70:VAL:CG2	1:A:128:PHE:HB2	0.49	2.37	18	12
1:A:164:ILE:O	1:A:168:ILE:HG12	0.49	2.08	3	4
1:A:83:GLU:O	1:A:87:TYR:HB2	0.49	2.08	5	2
1:A:106:LYS:HD2	1:A:107:TYR:CD1	0.49	2.43	5	1
1:A:253:GLN:HG2	1:A:259:LEU:HG	0.49	1.85	11	1
1:A:197:ASP:O	1:A:200:LEU:HG	0.49	2.07	4	1
1:A:133:ARG:HD2	1:A:187:TYR:CD1	0.49	2.42	12	1
1:A:287:ASP:HA	1:A:296:PRO:CB	0.49	2.37	15	1
1:A:107:TYR:CE2	1:A:160:ARG:HD3	0.49	2.43	18	1
1:A:328:LEU:O	1:A:331:ILE:HG22	0.49	2.08	6	4
1:A:151:ARG:HD2	1:A:298:GLU:OE2	0.49	2.07	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:354:ILE:HD13	1:A:354:ILE:H	0.49	1.68	7	3
1:A:328:LEU:HB3	1:A:333:SER:O	0.49	2.08	8	1
1:A:240:ARG:CZ	1:A:241:ARG:HA	0.49	2.38	13	1
1:A:192:GLN:HA	1:A:192:GLN:OE1	0.49	2.08	19	1
1:A:259:LEU:HB2	1:A:262:GLU:CB	0.49	2.37	20	1
1:A:286:MET:HE2	1:A:303:MET:HG3	0.49	1.83	18	2
1:A:261:TRP:O	1:A:265:LEU:HB3	0.49	2.08	15	2
1:A:241:ARG:HG2	1:A:311:TYR:O	0.49	2.08	12	1
1:A:51:ILE:HD12	1:A:71:LYS:HB3	0.49	1.85	17	2
1:A:287:ASP:HA	1:A:296:PRO:HG2	0.49	1.84	1	1
1:A:53:LEU:HD13	1:A:54:ALA:N	0.49	2.23	8	1
1:A:239:SER:O	1:A:240:ARG:HB2	0.49	2.07	12	1
1:A:47:GLY:HA3	1:A:196:VAL:CG2	0.49	2.37	17	1
1:A:34:LYS:O	1:A:35:LYS:HE2	0.49	2.08	18	1
1:A:241:ARG:HB2	1:A:310:ASP:O	0.48	2.08	5	2
1:A:114:TRP:HB2	1:A:130:ILE:CG2	0.48	2.37	10	1
1:A:203:ARG:HD2	1:A:215:GLU:OE2	0.48	2.08	12	1
1:A:162:LEU:HB3	1:A:317:TYR:CE1	0.48	2.43	13	1
1:A:79:PRO:HG3	1:A:353:THR:HA	0.48	1.85	14	1
1:A:282:ILE:H	1:A:282:ILE:HD13	0.48	1.68	8	8
1:A:38:LYS:O	1:A:55:ASP:HB3	0.48	2.08	12	1
1:A:28:ILE:HG22	1:A:38:LYS:HG2	0.48	1.85	11	1
1:A:38:LYS:HG2	1:A:56:MET:SD	0.48	2.48	8	1
1:A:337:GLY:C	1:A:338:LYS:HD2	0.48	2.33	9	1
1:A:160:ARG:HA	1:A:163:ASP:OD2	0.48	2.07	11	1
1:A:34:LYS:O	1:A:35:LYS:HB3	0.48	2.09	12	2
1:A:37:TRP:HB2	1:A:56:MET:O	0.48	2.07	19	1
1:A:228:THR:CG2	1:A:232:ALA:HB3	0.48	2.39	6	1
1:A:273:ASP:O	1:A:277:ARG:HG2	0.48	2.07	6	1
1:A:182:ASN:CG	1:A:198:TYR:HB3	0.48	2.34	13	1
1:A:299:ILE:H	1:A:299:ILE:HD12	0.48	1.69	15	1
1:A:290:PHE:HE2	1:A:294:ASN:HB3	0.48	1.67	16	3
1:A:282:ILE:HG12	1:A:283:ALA:N	0.48	2.23	5	4
1:A:158:SER:O	1:A:162:LEU:HG	0.48	2.09	13	1
1:A:309:LEU:O	1:A:310:ASP:HB2	0.48	2.09	12	3
1:A:269:LYS:HB2	1:A:269:LYS:NZ	0.48	2.23	6	1
1:A:149:PHE:HD2	1:A:254:TRP:HB3	0.48	1.69	13	2
1:A:99:TRP:O	1:A:103:ARG:HB2	0.48	2.08	16	1
1:A:47:GLY:N	1:A:184:LEU:HD11	0.48	2.23	17	1
1:A:31:ASP:HA	1:A:117:GLY:HA3	0.48	1.86	18	2
1:A:53:LEU:HD23	1:A:69:VAL:HG12	0.48	1.86	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:LEU:HD21	1:A:325:LEU:HD21	0.48	1.85	13	2
1:A:200:LEU:HG	1:A:353:THR:O	0.48	2.08	11	1
1:A:83:GLU:HB3	1:A:197:ASP:O	0.48	2.09	15	1
1:A:87:TYR:CE1	1:A:111:PRO:HG2	0.48	2.35	1	2
1:A:90:ALA:HA	1:A:99:TRP:HH2	0.48	1.69	17	1
1:A:290:PHE:CE2	1:A:292:GLU:HB2	0.48	2.44	18	1
1:A:294:ASN:O	1:A:295:LYS:HB2	0.47	2.09	2	4
1:A:177:ASP:CB	1:A:223:GLY:HA3	0.47	2.27	10	1
1:A:241:ARG:NH2	1:A:279:ARG:HD2	0.47	2.24	10	1
1:A:326:GLN:HA	1:A:329:LYS:HE2	0.47	1.84	12	1
1:A:70:VAL:HA	1:A:129:MET:O	0.47	2.09	14	4
1:A:204:TYR:CE1	1:A:237:ALA:HB3	0.47	2.44	17	1
1:A:186:ASN:ND2	1:A:194:TYR:HE1	0.47	2.06	10	1
1:A:178:ILE:HG12	1:A:178:ILE:O	0.47	2.09	14	1
1:A:262:GLU:O	1:A:265:LEU:HD22	0.47	2.08	15	1
1:A:42:PRO:HA	1:A:52:TYR:CD1	0.47	2.44	17	1
1:A:28:ILE:HA	1:A:37:TRP:O	0.47	2.10	2	1
1:A:89:ARG:HA	1:A:89:ARG:HE	0.47	1.66	2	2
1:A:87:TYR:O	1:A:91:ALA:HB3	0.47	2.09	6	2
1:A:310:ASP:HB3	1:A:313:GLU:OE1	0.47	2.09	4	1
1:A:298:GLU:CD	1:A:298:GLU:H	0.47	2.17	12	6
1:A:121:LYS:O	1:A:121:LYS:HD3	0.47	2.09	3	1
1:A:114:TRP:HB2	1:A:130:ILE:HG22	0.47	1.86	6	5
1:A:184:LEU:CD1	1:A:194:TYR:HB2	0.47	2.40	10	1
1:A:310:ASP:HB3	1:A:313:GLU:HB3	0.47	1.87	11	1
1:A:265:LEU:HA	1:A:271:VAL:CG2	0.47	2.39	6	1
1:A:47:GLY:CA	1:A:71:LYS:HE3	0.47	2.40	16	1
1:A:152:LYS:HD3	1:A:153:THR:N	0.47	2.24	1	1
1:A:335:ASP:CG	1:A:336:ASP:H	0.47	2.18	3	1
1:A:70:VAL:HB	1:A:130:ILE:CD1	0.47	2.39	16	10
1:A:145:ASN:OD1	1:A:148:ARG:HB2	0.47	2.10	5	1
1:A:137:ASP:O	1:A:141:ILE:HG13	0.47	2.10	9	1
1:A:96:ILE:O	1:A:100:ILE:HD13	0.47	2.09	10	1
1:A:51:ILE:HD12	1:A:71:LYS:HG3	0.47	1.86	14	1
1:A:259:LEU:O	1:A:262:GLU:HB2	0.47	2.10	17	1
1:A:111:PRO:HB3	1:A:134:PHE:HZ	0.47	1.70	4	1
1:A:106:LYS:HD2	1:A:107:TYR:HD1	0.47	1.70	5	1
1:A:224:THR:HB	1:A:226:GLU:OE1	0.47	2.09	6	1
1:A:146:ALA:C	1:A:147:LYS:HD3	0.47	2.35	12	1
1:A:100:ILE:HG13	1:A:105:LEU:HB2	0.47	1.86	17	1
1:A:137:ASP:HB2	1:A:140:LYS:HG3	0.47	1.86	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:ASP:HB2	1:A:198:TYR:CE2	0.47	2.45	10	1
1:A:175:HIS:HE1	1:A:200:LEU:HB2	0.47	1.70	20	1
1:A:204:TYR:HB2	1:A:237:ALA:HB1	0.46	1.87	4	1
1:A:241:ARG:HB2	1:A:311:TYR:O	0.46	2.11	4	1
1:A:165:LEU:HD13	1:A:175:HIS:CD2	0.46	2.45	7	1
1:A:196:VAL:HG23	1:A:198:TYR:CE2	0.46	2.46	19	1
1:A:205:CYS:SG	1:A:211:LYS:HB2	0.46	2.50	19	1
1:A:173:TYR:HB3	1:A:201:ALA:HB1	0.46	1.86	20	1
1:A:256:THR:HG22	1:A:290:PHE:HB2	0.46	1.86	1	1
1:A:276:ILE:HG12	1:A:279:ARG:HH21	0.46	1.70	1	1
1:A:309:LEU:HA	1:A:313:GLU:HB3	0.46	1.87	8	1
1:A:240:ARG:O	1:A:244:LEU:HD23	0.46	2.10	15	1
1:A:303:MET:HA	1:A:303:MET:HE2	0.46	1.87	15	1
1:A:232:ALA:HB2	1:A:238:PRO:HG3	0.46	1.87	16	2
1:A:152:LYS:HD2	1:A:152:LYS:N	0.46	2.25	15	1
1:A:263:ASP:O	1:A:266:LYS:HD2	0.46	2.09	19	1
1:A:240:ARG:O	1:A:244:LEU:HG	0.46	2.10	1	3
1:A:241:ARG:HD3	1:A:306:VAL:O	0.46	2.10	1	1
1:A:303:MET:HA	1:A:306:VAL:HG22	0.46	1.87	2	5
1:A:67:PRO:HB3	1:A:187:TYR:OH	0.46	2.11	4	1
1:A:41:LEU:HD22	1:A:42:PRO:HD2	0.46	1.86	14	1
1:A:151:ARG:O	1:A:155:LEU:HB2	0.46	2.11	1	1
1:A:137:ASP:OD1	1:A:181:SER:HA	0.46	2.11	2	1
1:A:176:GLY:O	1:A:246:ILE:HD13	0.46	2.11	5	1
1:A:288:LYS:NZ	1:A:288:LYS:HB3	0.46	2.25	6	1
1:A:227:PHE:O	1:A:246:ILE:HG12	0.46	2.10	11	3
1:A:66:ALA:N	1:A:67:PRO:HD2	0.46	2.25	14	2
1:A:112:LYS:HD2	1:A:114:TRP:CE2	0.46	2.46	2	1
1:A:264:ASN:CB	1:A:270:TYR:HB3	0.46	2.41	11	1
1:A:230:ILE:H	1:A:230:ILE:HD13	0.46	1.69	13	1
1:A:173:TYR:HB3	1:A:203:ARG:HA	0.46	1.86	14	1
1:A:313:GLU:O	1:A:314:LYS:HD3	0.46	2.11	20	1
1:A:99:TRP:HH2	1:A:108:LEU:HD22	0.46	1.70	1	1
1:A:110:VAL:CG2	1:A:111:PRO:HD2	0.46	2.40	9	1
1:A:139:GLN:HA	1:A:142:TYR:HB3	0.46	1.87	11	1
1:A:31:ASP:HA	1:A:128:PHE:HZ	0.46	1.71	16	1
1:A:173:TYR:HB3	1:A:203:ARG:HD2	0.46	1.87	16	1
1:A:174:VAL:HG13	1:A:204:TYR:HE2	0.46	1.69	19	1
1:A:259:LEU:HD13	1:A:261:TRP:CZ2	0.46	2.46	15	2
1:A:133:ARG:O	1:A:133:ARG:HG2	0.46	2.10	9	2
1:A:175:HIS:HB3	1:A:177:ASP:OD1	0.46	2.11	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:302:TYR:CD1	1:A:320:LEU:HD22	0.45	2.47	18	2
1:A:100:ILE:HD11	1:A:108:LEU:HG	0.45	1.86	7	2
1:A:48:PHE:CZ	1:A:79:PRO:HG2	0.45	2.46	10	1
1:A:186:ASN:HD21	1:A:194:TYR:HE1	0.45	1.52	10	1
1:A:38:LYS:HB2	1:A:56:MET:HA	0.45	1.88	13	1
1:A:267:ASP:OD1	1:A:269:LYS:HE3	0.45	2.11	16	1
1:A:321:ARG:O	1:A:325:LEU:HB2	0.45	2.11	2	1
1:A:104:LYS:HE3	1:A:104:LYS:CA	0.45	2.33	10	1
1:A:320:LEU:O	1:A:323:ILE:HG22	0.45	2.11	13	1
1:A:231:ASP:HB3	1:A:238:PRO:HA	0.45	1.86	16	1
1:A:85:LYS:O	1:A:89:ARG:HG2	0.45	2.11	6	1
1:A:139:GLN:HA	1:A:142:TYR:CD2	0.45	2.47	20	2
1:A:225:ILE:HA	1:A:228:THR:OG1	0.45	2.10	14	1
1:A:66:ALA:HB3	1:A:67:PRO:HD3	0.45	1.87	17	1
1:A:173:TYR:CD2	1:A:201:ALA:HB1	0.45	2.47	19	1
1:A:199:GLY:O	1:A:354:ILE:HA	0.45	2.11	19	1
1:A:290:PHE:CE2	1:A:294:ASN:HB3	0.45	2.47	2	2
1:A:92:LYS:HG2	1:A:94:GLU:OE2	0.45	2.11	3	1
1:A:295:LYS:HA	1:A:295:LYS:CE	0.45	2.41	14	1
1:A:35:LYS:HB2	1:A:37:TRP:CZ3	0.45	2.47	18	1
1:A:269:LYS:NZ	1:A:269:LYS:HB3	0.45	2.26	2	1
1:A:252:ILE:HB	1:A:299:ILE:HG21	0.45	1.87	3	1
1:A:106:LYS:HG2	1:A:321:ARG:NH2	0.45	2.27	4	1
1:A:152:LYS:HG3	1:A:153:THR:N	0.45	2.26	20	1
1:A:174:VAL:HG11	1:A:203:ARG:NH1	0.45	2.27	20	1
1:A:184:LEU:HD23	1:A:196:VAL:HG22	0.45	1.87	2	1
1:A:205:CYS:HB2	1:A:209:VAL:O	0.45	2.12	3	1
1:A:175:HIS:CE1	1:A:200:LEU:HB3	0.45	2.47	18	1
1:A:135:GLY:HA3	1:A:187:TYR:CD1	0.45	2.44	9	2
1:A:83:GLU:HA	1:A:198:TYR:HB2	0.45	1.88	10	1
1:A:175:HIS:CB	1:A:201:ALA:HA	0.45	2.28	15	1
1:A:152:LYS:CG	1:A:335:ASP:HA	0.45	2.38	7	1
1:A:43:ILE:HD11	1:A:53:LEU:HD12	0.45	1.88	9	1
1:A:99:TRP:CE2	1:A:103:ARG:HG3	0.45	2.46	11	1
1:A:304:GLU:O	1:A:307:LYS:HG3	0.45	2.11	18	1
1:A:147:LYS:O	1:A:147:LYS:HG2	0.45	2.12	12	1
1:A:103:ARG:O	1:A:103:ARG:HD3	0.44	2.12	9	1
1:A:92:LYS:O	1:A:96:ILE:HG13	0.44	2.11	3	1
1:A:199:GLY:O	1:A:354:ILE:HG23	0.44	2.12	7	2
1:A:48:PHE:CZ	1:A:79:PRO:HB2	0.44	2.46	8	1
1:A:137:ASP:HA	1:A:184:LEU:HA	0.44	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:206:PRO:HG2	1:A:209:VAL:HG23	0.44	1.89	9	1
1:A:147:LYS:HG3	1:A:253:GLN:OE1	0.44	2.12	3	1
1:A:249:TYR:O	1:A:253:GLN:HB2	0.44	2.12	3	1
1:A:157:LEU:O	1:A:160:ARG:HG3	0.44	2.13	7	1
1:A:66:ALA:O	1:A:133:ARG:HG3	0.44	2.13	12	1
1:A:178:ILE:HG23	1:A:250:CYS:SG	0.44	2.52	14	1
1:A:175:HIS:CE1	1:A:177:ASP:HB3	0.44	2.47	16	1
1:A:303:MET:O	1:A:306:VAL:HG22	0.44	2.12	16	1
1:A:191:ASP:CB	1:A:338:LYS:HA	0.44	2.42	20	1
1:A:51:ILE:CD1	1:A:71:LYS:HB3	0.44	2.43	5	1
1:A:191:ASP:HB2	1:A:338:LYS:HD3	0.44	1.89	5	1
1:A:84:LEU:HD22	1:A:127:ARG:HD3	0.44	1.89	7	1
1:A:142:TYR:HD1	1:A:147:LYS:HB2	0.44	1.72	9	1
1:A:103:ARG:HG2	1:A:105:LEU:HD13	0.44	1.90	15	1
1:A:84:LEU:O	1:A:88:GLN:HG2	0.44	2.12	17	1
1:A:149:PHE:HD2	1:A:153:THR:HG21	0.44	1.71	17	1
1:A:139:GLN:HG2	1:A:181:SER:HA	0.44	1.87	11	1
1:A:71:LYS:HB2	1:A:131:MET:HE1	0.44	1.89	14	1
1:A:149:PHE:HB2	1:A:254:TRP:HB3	0.44	1.90	20	1
1:A:197:ASP:C	1:A:199:GLY:H	0.44	2.21	20	1
1:A:246:ILE:O	1:A:249:TYR:HB2	0.44	2.13	5	1
1:A:89:ARG:HG3	1:A:173:TYR:HE2	0.44	1.73	6	1
1:A:68:CYS:HA	1:A:131:MET:O	0.44	2.12	16	2
1:A:67:PRO:CA	1:A:133:ARG:HG2	0.44	2.42	16	1
1:A:191:ASP:HB2	1:A:338:LYS:HA	0.44	1.89	20	1
1:A:241:ARG:CG	1:A:311:TYR:HA	0.44	2.36	1	1
1:A:265:LEU:O	1:A:265:LEU:HD13	0.44	2.12	10	1
1:A:133:ARG:HE	1:A:187:TYR:HE1	0.44	1.55	5	1
1:A:213:TYR:HA	1:A:236:VAL:HG23	0.44	1.90	14	1
1:A:213:TYR:CD1	1:A:236:VAL:HB	0.44	2.45	16	1
1:A:32:MET:HA	1:A:32:MET:CE	0.44	2.37	18	1
1:A:195:LEU:HD23	1:A:196:VAL:N	0.44	2.28	5	1
1:A:231:ASP:HB3	1:A:238:PRO:HB3	0.44	1.90	5	1
1:A:240:ARG:HD2	1:A:311:TYR:O	0.44	2.13	8	1
1:A:298:GLU:HA	1:A:323:ILE:CD1	0.44	2.42	8	1
1:A:225:ILE:HD13	1:A:225:ILE:O	0.44	2.13	13	2
1:A:99:TRP:CZ2	1:A:108:LEU:HD22	0.44	2.47	14	2
1:A:210:HIS:HB2	1:A:238:PRO:HB2	0.44	1.90	20	1
1:A:275:LYS:O	1:A:279:ARG:HG3	0.43	2.12	1	1
1:A:80:LEU:HD12	1:A:127:ARG:HE	0.43	1.73	5	1
1:A:247:LEU:O	1:A:251:MET:HG3	0.43	2.13	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:GLU:H	1:A:226:GLU:HG3	0.43	1.41	12	1
1:A:328:LEU:HD21	1:A:334:LYS:HA	0.43	1.90	13	1
1:A:177:ASP:HB3	1:A:199:GLY:HA3	0.43	1.89	17	1
1:A:321:ARG:HG3	1:A:322:ASP:N	0.43	2.28	17	1
1:A:171:HIS:CD2	1:A:172:GLU:HG2	0.43	2.48	19	1
1:A:178:ILE:O	1:A:178:ILE:HG22	0.43	2.13	19	1
1:A:189:ASN:HB3	1:A:191:ASP:OD1	0.43	2.13	5	1
1:A:226:GLU:HA	1:A:265:LEU:HD21	0.43	1.89	10	1
1:A:137:ASP:HA	1:A:184:LEU:HD13	0.43	1.90	14	1
1:A:252:ILE:HD12	1:A:286:MET:HE1	0.43	1.89	17	1
1:A:281:ASN:HB3	1:A:285:LEU:HD23	0.43	1.90	18	1
1:A:137:ASP:HB3	1:A:184:LEU:HB3	0.43	1.90	9	1
1:A:224:THR:O	1:A:228:THR:HB	0.43	2.13	20	1
1:A:106:LYS:HB2	1:A:321:ARG:HH22	0.43	1.74	1	1
1:A:39:VAL:HG12	1:A:52:TYR:CE1	0.43	2.48	2	1
1:A:29:ILE:HB	1:A:128:PHE:CZ	0.43	2.47	4	1
1:A:94:GLU:O	1:A:98:LYS:HG3	0.43	2.13	4	1
1:A:124:LYS:HA	1:A:124:LYS:CE	0.43	2.35	10	1
1:A:137:ASP:OD1	1:A:140:LYS:HG2	0.43	2.14	18	1
1:A:306:VAL:O	1:A:309:LEU:HG	0.43	2.13	1	1
1:A:80:LEU:O	1:A:84:LEU:HB2	0.43	2.14	2	2
1:A:247:LEU:HD12	1:A:250:CYS:SG	0.43	2.54	5	2
1:A:157:LEU:O	1:A:161:ILE:HB	0.43	2.14	12	1
1:A:309:LEU:HD13	1:A:315:PRO:HA	0.43	1.91	14	1
1:A:178:ILE:HB	1:A:246:ILE:CG2	0.43	2.44	3	1
1:A:196:VAL:C	1:A:198:TYR:H	0.43	2.21	5	1
1:A:30:THR:HG23	1:A:35:LYS:HB2	0.43	1.89	4	1
1:A:179:LYS:HZ3	1:A:226:GLU:CD	0.43	2.21	4	1
1:A:31:ASP:HB2	1:A:116:SER:O	0.43	2.14	10	1
1:A:316:LEU:O	1:A:320:LEU:HD13	0.43	2.14	11	1
1:A:309:LEU:HD22	1:A:315:PRO:HA	0.43	1.90	14	1
1:A:155:LEU:O	1:A:159:LEU:HG	0.43	2.14	20	2
1:A:314:LYS:C	1:A:314:LYS:HD3	0.43	2.39	19	1
1:A:142:TYR:CD1	1:A:142:TYR:C	0.43	2.96	20	1
1:A:203:ARG:NH2	1:A:207:GLU:H	0.43	2.12	5	1
1:A:31:ASP:OD2	1:A:115:GLY:HA3	0.43	2.13	14	1
1:A:132:ASP:HB2	1:A:134:PHE:CE1	0.43	2.48	19	1
1:A:138:LEU:C	1:A:180:ALA:HB1	0.43	2.38	19	1
1:A:229:SER:HA	1:A:249:TYR:CE2	0.43	2.49	20	1
1:A:147:LYS:HG3	1:A:257:GLY:O	0.43	2.14	1	2
1:A:167:TYR:HA	1:A:170:GLU:OE2	0.43	2.14	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:GLU:HG2	1:A:203:ARG:HB2	0.43	1.90	1	1
1:A:177:ASP:HB2	1:A:223:GLY:CA	0.43	2.44	11	2
1:A:200:LEU:HG	1:A:353:THR:CA	0.43	2.44	7	1
1:A:77:ASN:OD1	1:A:79:PRO:HD2	0.43	2.13	12	1
1:A:45:GLN:HB2	1:A:137:ASP:OD2	0.43	2.13	15	1
1:A:51:ILE:HD11	1:A:71:LYS:HD2	0.43	1.91	18	1
1:A:95:GLN:O	1:A:98:LYS:HB3	0.42	2.14	2	1
1:A:178:ILE:HG22	1:A:250:CYS:SG	0.42	2.54	3	1
1:A:160:ARG:HH21	1:A:164:ILE:HG21	0.42	1.74	9	1
1:A:31:ASP:CG	1:A:33:ALA:H	0.42	2.22	12	2
1:A:262:GLU:O	1:A:265:LEU:HG	0.42	2.14	14	1
1:A:145:ASN:O	1:A:148:ARG:HG2	0.42	2.14	15	1
1:A:39:VAL:HG22	1:A:52:TYR:CE1	0.42	2.49	5	1
1:A:37:TRP:CZ3	1:A:56:MET:HG2	0.42	2.49	12	1
1:A:177:ASP:HB2	1:A:182:ASN:ND2	0.42	2.29	12	1
1:A:298:GLU:CD	1:A:298:GLU:N	0.42	2.77	17	1
1:A:191:ASP:HB2	1:A:338:LYS:HB3	0.42	1.91	8	1
1:A:43:ILE:HB	1:A:51:ILE:O	0.42	2.14	17	1
1:A:41:LEU:HD12	1:A:42:PRO:HD2	0.42	1.90	4	1
1:A:281:ASN:ND2	1:A:284:SER:HB3	0.42	2.29	8	1
1:A:152:LYS:HE2	1:A:152:LYS:O	0.42	2.15	9	1
1:A:153:THR:O	1:A:157:LEU:HD13	0.42	2.15	10	1
1:A:174:VAL:HG13	1:A:204:TYR:CD1	0.42	2.48	13	1
1:A:33:ALA:HB3	1:A:37:TRP:CH2	0.42	2.49	18	1
1:A:175:HIS:CE1	1:A:178:ILE:HD13	0.42	2.49	5	1
1:A:294:ASN:O	1:A:295:LYS:HB3	0.42	2.15	8	1
1:A:160:ARG:O	1:A:160:ARG:HD2	0.42	2.15	11	1
1:A:164:ILE:HD13	1:A:195:LEU:HB3	0.42	1.91	14	1
1:A:138:LEU:HB3	1:A:180:ALA:HB1	0.42	1.92	19	2
1:A:202:TYR:HB2	1:A:222:ASP:HB3	0.42	1.91	6	1
1:A:225:ILE:HG12	1:A:271:VAL:HG11	0.42	1.92	8	1
1:A:302:TYR:O	1:A:306:VAL:HG13	0.42	2.15	9	1
1:A:276:ILE:O	1:A:280:GLU:HG3	0.42	2.15	13	1
1:A:43:ILE:HD11	1:A:53:LEU:HB2	0.42	1.91	16	1
1:A:53:LEU:HD23	1:A:54:ALA:N	0.42	2.30	17	2
1:A:240:ARG:HG2	1:A:315:PRO:HG3	0.42	1.91	9	1
1:A:170:GLU:O	1:A:207:GLU:HA	0.42	2.14	10	1
1:A:96:ILE:O	1:A:100:ILE:HG13	0.42	2.15	11	2
1:A:199:GLY:HA3	1:A:352:LYS:CB	0.42	2.44	12	1
1:A:38:LYS:CB	1:A:56:MET:HA	0.42	2.45	13	1
1:A:200:LEU:HD13	1:A:352:LYS:NZ	0.42	2.30	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:LEU:CB	1:A:328:LEU:HD22	0.42	2.43	16	1
1:A:224:THR:OG1	1:A:226:GLU:HG2	0.42	2.14	17	1
1:A:103:ARG:O	1:A:103:ARG:HG3	0.42	2.13	18	1
1:A:240:ARG:HG3	1:A:315:PRO:HG3	0.42	1.91	19	1
1:A:213:TYR:HA	1:A:236:VAL:CG2	0.42	2.45	3	3
1:A:182:ASN:O	1:A:195:LEU:HA	0.42	2.15	6	2
1:A:226:GLU:HG2	1:A:265:LEU:HD13	0.42	1.91	2	1
1:A:261:TRP:HB3	1:A:274:SER:CB	0.42	2.44	4	1
1:A:298:GLU:H	1:A:298:GLU:CD	0.42	2.23	14	2
1:A:67:PRO:HA	1:A:133:ARG:CZ	0.42	2.44	15	1
1:A:282:ILE:HB	1:A:304:GLU:HG2	0.42	1.91	15	1
1:A:93:PRO:O	1:A:97:GLN:HG3	0.42	2.14	19	1
1:A:354:ILE:HD13	1:A:355:THR:N	0.41	2.30	3	2
1:A:200:LEU:HD21	1:A:352:LYS:HB2	0.41	1.92	5	1
1:A:196:VAL:O	1:A:197:ASP:HB3	0.41	2.15	8	2
1:A:99:TRP:CE3	1:A:108:LEU:HG	0.41	2.50	10	1
1:A:325:LEU:O	1:A:329:LYS:HG2	0.41	2.15	12	1
1:A:240:ARG:HH21	1:A:244:LEU:HB2	0.41	1.75	13	1
1:A:293:LYS:HD3	1:A:293:LYS:O	0.41	2.15	15	1
1:A:177:ASP:CB	1:A:199:GLY:HA3	0.41	2.45	17	1
1:A:70:VAL:HB	1:A:130:ILE:HG12	0.41	1.91	5	1
1:A:96:ILE:HD12	1:A:112:LYS:NZ	0.41	2.30	8	1
1:A:73:GLU:HB2	1:A:80:LEU:HG	0.41	1.91	9	1
1:A:56:MET:HE3	1:A:59:SER:HA	0.41	1.90	10	1
1:A:46:GLY:HA3	1:A:137:ASP:OD2	0.41	2.15	11	1
1:A:30:THR:HA	1:A:35:LYS:HA	0.41	1.90	12	1
1:A:34:LYS:O	1:A:34:LYS:HD3	0.41	2.15	13	1
1:A:47:GLY:HA2	1:A:71:LYS:CE	0.41	2.43	16	1
1:A:73:GLU:OE1	1:A:80:LEU:HB2	0.41	2.16	3	2
1:A:176:GLY:O	1:A:228:THR:HA	0.41	2.15	16	2
1:A:111:PRO:HG3	1:A:134:PHE:HZ	0.41	1.74	8	1
1:A:83:GLU:HG2	1:A:87:TYR:CE2	0.41	2.50	18	1
1:A:121:LYS:HE2	1:A:121:LYS:CA	0.41	2.43	20	1
1:A:261:TRP:HB3	1:A:274:SER:HB2	0.41	1.92	3	1
1:A:204:TYR:OH	1:A:239:SER:HA	0.41	2.14	9	1
1:A:151:ARG:HG2	1:A:331:ILE:HD13	0.41	1.92	11	1
1:A:305:THR:O	1:A:309:LEU:HB2	0.41	2.14	12	1
1:A:51:ILE:CD1	1:A:71:LYS:HG3	0.41	2.46	14	1
1:A:241:ARG:HD2	1:A:310:ASP:O	0.41	2.15	16	1
1:A:229:SER:HA	1:A:249:TYR:HE2	0.41	1.75	20	1
1:A:151:ARG:HH11	1:A:331:ILE:HB	0.41	1.74	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LYS:O	1:A:128:PHE:HA	0.41	2.15	6	1
1:A:80:LEU:O	1:A:80:LEU:HD13	0.41	2.14	6	1
1:A:239:SER:C	1:A:240:ARG:HD2	0.41	2.41	9	1
1:A:173:TYR:CB	1:A:203:ARG:HA	0.41	2.46	14	1
1:A:293:LYS:NZ	1:A:293:LYS:HB3	0.41	2.30	17	1
1:A:249:TYR:CZ	1:A:275:LYS:HD2	0.41	2.50	6	1
1:A:51:ILE:CD1	1:A:71:LYS:HD3	0.41	2.45	7	1
1:A:295:LYS:HE2	1:A:331:ILE:HA	0.41	1.92	9	1
1:A:79:PRO:O	1:A:83:GLU:HG2	0.41	2.15	10	1
1:A:73:GLU:HB2	1:A:80:LEU:HB2	0.41	1.92	11	1
1:A:259:LEU:O	1:A:262:GLU:HG2	0.41	2.16	15	1
1:A:29:ILE:HG12	1:A:37:TRP:O	0.41	2.14	18	1
1:A:142:TYR:CZ	1:A:147:LYS:HE3	0.41	2.50	5	1
1:A:155:LEU:HD21	1:A:324:LEU:HB3	0.41	1.93	5	1
1:A:103:ARG:NE	1:A:103:ARG:HA	0.41	2.30	12	1
1:A:161:ILE:HA	1:A:164:ILE:HG22	0.41	1.91	15	1
1:A:104:LYS:HD2	1:A:104:LYS:N	0.41	2.31	16	1
1:A:122:ASN:HD22	1:A:122:ASN:N	0.41	2.14	18	1
1:A:169:HIS:CD2	1:A:240:ARG:HD3	0.41	2.47	1	1
1:A:53:LEU:HD12	1:A:133:ARG:HH21	0.41	1.74	3	1
1:A:95:GLN:HA	1:A:95:GLN:OE1	0.41	2.16	7	1
1:A:77:ASN:CG	1:A:78:GLY:H	0.41	2.24	4	1
1:A:151:ARG:HD3	1:A:294:ASN:HD21	0.41	1.76	5	1
1:A:261:TRP:HB2	1:A:271:VAL:HG12	0.41	1.93	5	1
1:A:169:HIS:HE1	1:A:240:ARG:HA	0.41	1.76	8	1
1:A:247:LEU:HA	1:A:250:CYS:SG	0.41	2.55	18	2
1:A:253:GLN:HG3	1:A:259:LEU:CD1	0.41	2.46	9	1
1:A:100:ILE:HG22	1:A:105:LEU:HB2	0.41	1.92	10	1
1:A:313:GLU:OE1	1:A:314:LYS:HG2	0.41	2.16	11	1
1:A:179:LYS:HB3	1:A:179:LYS:NZ	0.41	2.30	12	1
1:A:286:MET:HA	1:A:286:MET:HE2	0.41	1.93	13	1
1:A:204:TYR:HA	1:A:237:ALA:HB1	0.41	1.92	16	1
1:A:251:MET:HE2	1:A:299:ILE:HG13	0.41	1.93	4	1
1:A:174:VAL:HG22	1:A:202:TYR:O	0.41	2.16	5	1
1:A:116:SER:HB3	1:A:129:MET:HG3	0.41	1.93	7	1
1:A:260:PRO:HG2	1:A:278:TYR:HE1	0.41	1.76	7	1
1:A:282:ILE:HD13	1:A:282:ILE:N	0.41	2.31	11	1
1:A:166:GLU:HG3	1:A:167:TYR:N	0.41	2.30	13	1
1:A:283:ALA:HA	1:A:300:ALA:HB1	0.41	1.93	17	1
1:A:172:GLU:OE2	1:A:203:ARG:HD3	0.41	2.16	18	1
1:A:238:PRO:HB3	1:A:242:GLY:HA3	0.40	1.93	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:ILE:HG22	1:A:178:ILE:O	0.40	2.17	4	1
1:A:352:LYS:HG3	1:A:353:THR:H	0.40	1.76	6	1
1:A:134:PHE:HD1	1:A:186:ASN:HA	0.40	1.75	11	1
1:A:132:ASP:C	1:A:133:ARG:HG2	0.40	2.41	17	1
1:A:189:ASN:HB3	1:A:192:GLN:HG3	0.40	1.92	18	1
1:A:99:TRP:HZ2	1:A:108:LEU:HD11	0.40	1.75	2	1
1:A:301:LYS:HB3	1:A:323:ILE:HD11	0.40	1.93	4	1
1:A:199:GLY:O	1:A:354:ILE:HG22	0.40	2.16	11	1
1:A:310:ASP:HB3	1:A:313:GLU:HG2	0.40	1.92	17	1
1:A:67:PRO:C	1:A:133:ARG:HB2	0.40	2.41	19	1
1:A:118:LEU:HD23	1:A:119:HIS:N	0.40	2.31	6	1
1:A:267:ASP:HB3	1:A:270:TYR:CD1	0.40	2.51	13	1
1:A:161:ILE:O	1:A:165:LEU:HG	0.40	2.17	15	1
1:A:225:ILE:HB	1:A:265:LEU:HD12	0.40	1.93	15	1
1:A:352:LYS:HG2	1:A:353:THR:N	0.40	2.31	16	1
1:A:119:HIS:HB2	1:A:128:PHE:HE2	0.40	1.76	4	1
1:A:186:ASN:HB3	1:A:189:ASN:O	0.40	2.16	9	1
1:A:294:ASN:O	1:A:296:PRO:HD3	0.40	2.17	12	1
1:A:31:ASP:HB2	1:A:116:SER:C	0.40	2.42	3	1
1:A:71:LYS:NZ	1:A:129:MET:SD	0.40	2.95	4	1
1:A:202:TYR:HB2	1:A:354:ILE:HG13	0.40	1.92	4	1
1:A:171:HIS:O	1:A:172:GLU:HB2	0.40	2.16	6	1
1:A:177:ASP:CG	1:A:224:THR:H	0.40	2.24	8	1
1:A:217:PRO:HD3	1:A:234:ASN:O	0.40	2.16	10	1
1:A:36:GLU:O	1:A:56:MET:HG2	0.40	2.17	11	1
1:A:240:ARG:HH11	1:A:309:LEU:HD11	0.40	1.75	13	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	309/368 (84%)	264±5 (85±2%)	36±4 (12±1%)	10±2 (3±1%)	5	36
All	All	6180/7360 (84%)	5270 (85%)	712 (12%)	198 (3%)	5	36

All 73 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	310	ASP	14
1	A	135	GLY	11
1	A	231	ASP	9
1	A	296	PRO	9
1	A	92	LYS	9
1	A	172	GLU	8
1	A	295	LYS	7
1	A	48	PHE	6
1	A	314	LYS	6
1	A	217	PRO	5
1	A	335	ASP	5
1	A	66	ALA	4
1	A	240	ARG	4
1	A	238	PRO	4
1	A	338	LYS	4
1	A	356	LYS	4
1	A	215	GLU	3
1	A	311	TYR	3
1	A	337	GLY	3
1	A	47	GLY	3
1	A	197	ASP	3
1	A	239	SER	3
1	A	147	LYS	3
1	A	313	GLU	3
1	A	208	GLY	2
1	A	292	GLU	2
1	A	36	GLU	2
1	A	78	GLY	2
1	A	207	GLU	2
1	A	336	ASP	2
1	A	206	PRO	2
1	A	294	ASN	2
1	A	291	PRO	2
1	A	198	TYR	2
1	A	309	LEU	2
1	A	34	LYS	2
1	A	35	LYS	2
1	A	122	ASN	2
1	A	334	LYS	2
1	A	214	LYS	2
1	A	212	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	312	THR	1
1	A	55	ASP	1
1	A	179	LYS	1
1	A	228	THR	1
1	A	353	THR	1
1	A	56	MET	1
1	A	107	TYR	1
1	A	196	VAL	1
1	A	352	LYS	1
1	A	50	CYS	1
1	A	216	ASP	1
1	A	171	HIS	1
1	A	49	GLY	1
1	A	57	ASN	1
1	A	75	SER	1
1	A	76	ASP	1
1	A	293	LYS	1
1	A	175	HIS	1
1	A	204	TYR	1
1	A	120	ASP	1
1	A	177	ASP	1
1	A	210	HIS	1
1	A	211	LYS	1
1	A	123	GLY	1
1	A	133	ARG	1
1	A	201	ALA	1
1	A	200	LEU	1
1	A	178	ILE	1
1	A	199	GLY	1
1	A	222	ASP	1
1	A	46	GLY	1
1	A	203	ARG	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	271/319 (85%)	254±3 (94±1%)	18±3 (6±1%)	17 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5420/6380 (85%)	5070 (94%)	350 (6%)	17 66

All 135 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	354	ILE	18
1	A	282	ILE	14
1	A	28	ILE	11
1	A	155	LEU	10
1	A	142	TYR	10
1	A	80	LEU	8
1	A	323	ILE	7
1	A	147	LYS	6
1	A	160	ARG	6
1	A	307	LYS	6
1	A	170	GLU	6
1	A	258	HIS	5
1	A	212	GLU	5
1	A	27	GLU	5
1	A	35	LYS	5
1	A	228	THR	5
1	A	99	TRP	4
1	A	311	TYR	4
1	A	70	VAL	4
1	A	171	HIS	4
1	A	309	LEU	4
1	A	352	LYS	4
1	A	89	ARG	4
1	A	224	THR	4
1	A	226	GLU	4
1	A	318	GLU	4
1	A	225	ILE	4
1	A	108	LEU	4
1	A	152	LYS	3
1	A	153	THR	3
1	A	326	GLN	3
1	A	298	GLU	3
1	A	124	LYS	3
1	A	181	SER	3
1	A	240	ARG	3
1	A	106	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	71	LYS	3
1	A	85	LYS	3
1	A	295	LYS	3
1	A	179	LYS	3
1	A	88	GLN	3
1	A	233	HIS	3
1	A	338	LYS	3
1	A	92	LYS	3
1	A	356	LYS	3
1	A	162	LEU	3
1	A	105	LEU	2
1	A	211	LYS	2
1	A	214	LYS	2
1	A	265	LEU	2
1	A	353	THR	2
1	A	84	LEU	2
1	A	112	LYS	2
1	A	121	LYS	2
1	A	325	LEU	2
1	A	334	LYS	2
1	A	94	GLU	2
1	A	137	ASP	2
1	A	312	THR	2
1	A	51	ILE	2
1	A	118	LEU	2
1	A	292	GLU	2
1	A	252	ILE	2
1	A	269	LYS	2
1	A	200	LEU	2
1	A	140	LYS	2
1	A	197	ASP	2
1	A	38	LYS	2
1	A	166	GLU	2
1	A	241	ARG	2
1	A	188	LYS	2
1	A	186	ASN	2
1	A	243	ASP	2
1	A	230	ILE	2
1	A	245	GLU	2
1	A	98	LYS	2
1	A	222	ASP	2
1	A	103	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	156	GLN	1
1	A	203	ARG	1
1	A	281	ASN	1
1	A	59	SER	1
1	A	76	ASP	1
1	A	264	ASN	1
1	A	132	ASP	1
1	A	213	TYR	1
1	A	314	LYS	1
1	A	29	ILE	1
1	A	82	THR	1
1	A	119	HIS	1
1	A	37	TRP	1
1	A	198	TYR	1
1	A	277	ARG	1
1	A	279	ARG	1
1	A	313	GLU	1
1	A	336	ASP	1
1	A	58	SER	1
1	A	133	ARG	1
1	A	172	GLU	1
1	A	288	LYS	1
1	A	100	ILE	1
1	A	104	LYS	1
1	A	130	ILE	1
1	A	182	ASN	1
1	A	202	TYR	1
1	A	215	GLU	1
1	A	234	ASN	1
1	A	304	GLU	1
1	A	159	LEU	1
1	A	184	LEU	1
1	A	192	GLN	1
1	A	34	LYS	1
1	A	131	MET	1
1	A	236	VAL	1
1	A	247	LEU	1
1	A	290	PHE	1
1	A	77	ASN	1
1	A	175	HIS	1
1	A	272	ARG	1
1	A	329	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	303	MET	1
1	A	125	SER	1
1	A	273	ASP	1
1	A	107	TYR	1
1	A	293	LYS	1
1	A	328	LEU	1
1	A	56	MET	1
1	A	97	GLN	1
1	A	122	ASN	1
1	A	231	ASP	1
1	A	262	GLU	1
1	A	266	LYS	1
1	A	151	ARG	1
1	A	41	LEU	1
1	A	322	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 73% for the well-defined parts and 70% 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 [i](#)

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	3551
Number of shifts mapped to atoms	3551
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	354	0.09 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	317	0.61 ± 0.06	Should be checked
$^{13}\text{C}'$	343	0.18 ± 0.09	None needed (< 0.5 ppm)
^{15}N	327	-0.41 ± 0.13	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 73%, i.e. 3170 atoms were assigned a chemical shift out of a possible 4356. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1501/1539 (98%)	601/627 (96%)	612/618 (99%)	288/294 (98%)
Sidechain	1553/2441 (64%)	1132/1577 (72%)	416/765 (54%)	5/99 (5%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	116/376 (31%)	111/178 (62%)	0/179 (0%)	5/19 (26%)
Overall	3170/4356 (73%)	1844/2382 (77%)	1028/1562 (66%)	298/412 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 3551 atoms were assigned a chemical shift out of a possible 5052. 0 out of 53 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	1702/1796 (95%)	678/732 (93%)	697/720 (97%)	327/344 (95%)
Sidechain	1729/2854 (61%)	1251/1842 (68%)	473/887 (53%)	5/125 (4%)
Aromatic	120/402 (30%)	115/191 (60%)	0/188 (0%)	5/23 (22%)
Overall	3551/5052 (70%)	2044/2765 (74%)	1170/1795 (65%)	337/492 (68%)

7.1.4 Statistically unusual chemical shifts [i](#)

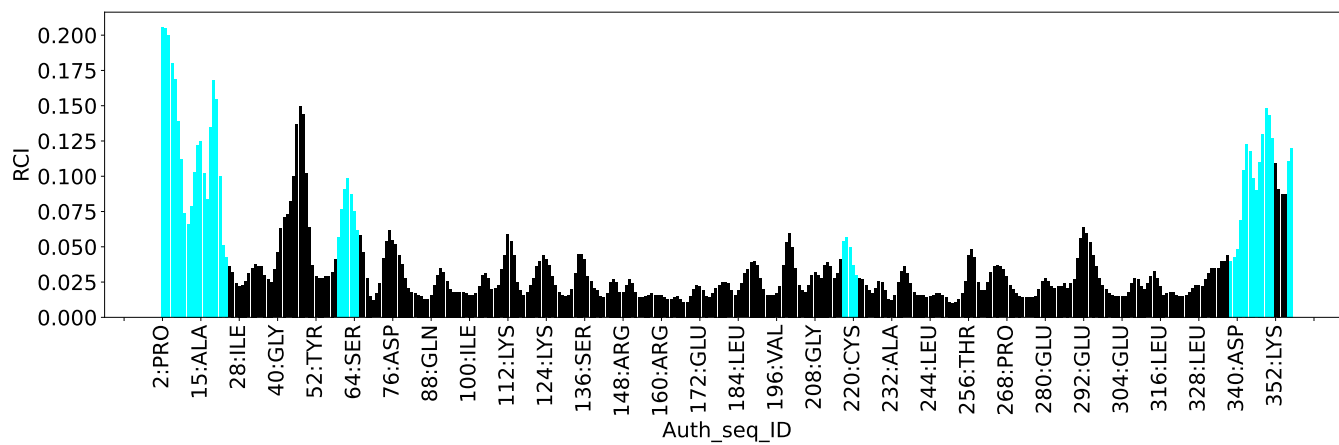
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	29	ILE	HG21	-0.80	-0.56 – 2.11	-5.9
1	A	29	ILE	HG22	-0.80	-0.56 – 2.11	-5.9
1	A	29	ILE	HG23	-0.80	-0.56 – 2.11	-5.9
1	A	29	ILE	HD11	-0.94	-0.72 – 2.09	-5.8
1	A	29	ILE	HD12	-0.94	-0.72 – 2.09	-5.8
1	A	29	ILE	HD13	-0.94	-0.72 – 2.09	-5.8
1	A	130	ILE	HG21	-0.62	-0.56 – 2.11	-5.2
1	A	130	ILE	HG22	-0.62	-0.56 – 2.11	-5.2
1	A	130	ILE	HG23	-0.62	-0.56 – 2.11	-5.2

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	5406
Intra-residue ($ i-j =0$)	969
Sequential ($ i-j =1$)	1387
Medium range ($ i-j >1$ and $ i-j <5$)	1135
Long range ($ i-j \geq 5$)	1693
Inter-chain	0
Hydrogen bond restraints	222
Disulfide bond restraints	0
Total dihedral-angle restraints	370
Number of unmapped restraints	0
Number of restraints per residue	15.7
Number of long range restraints per residue ¹	4.7

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)	16.3	0.2
0.2-0.5 (Medium)	1.4	0.36
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	25.6	4.69
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

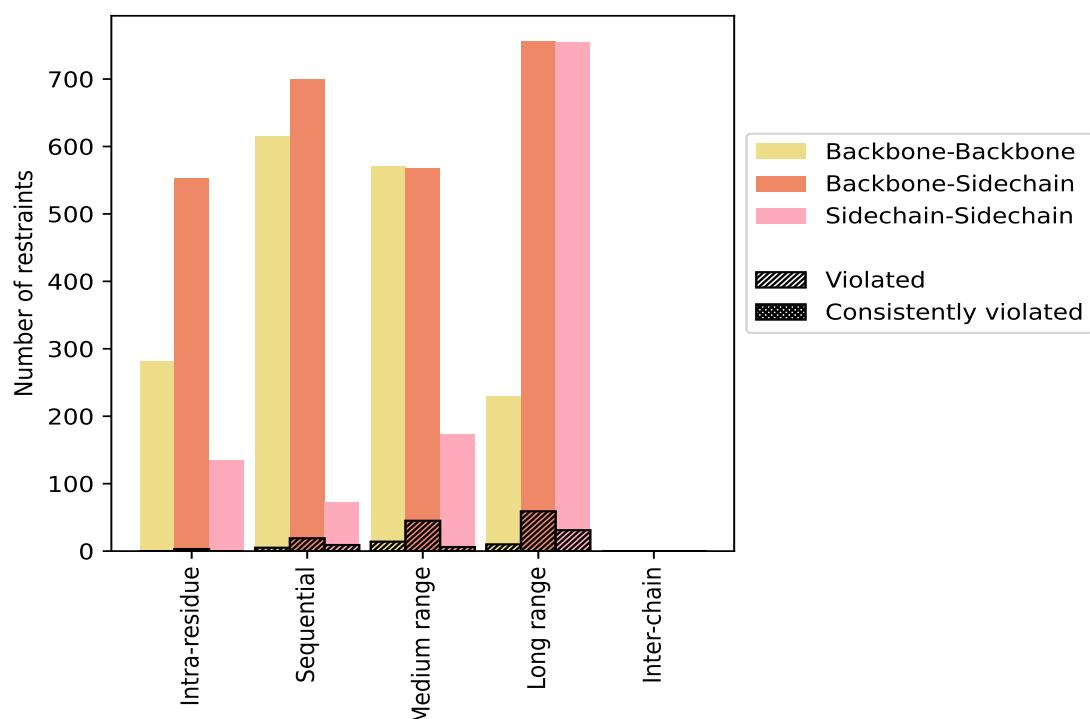
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	969	17.9	3	0.3	0.1	0	0.0	0.0
Backbone-Backbone	282	5.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	552	10.2	3	0.5	0.1	0	0.0	0.0
Sidechain-Sidechain	135	2.5	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	1387	25.7	33	2.4	0.6	0	0.0	0.0
Backbone-Backbone	615	11.4	5	0.8	0.1	0	0.0	0.0
Backbone-Sidechain	700	12.9	19	2.7	0.4	0	0.0	0.0
Sidechain-Sidechain	72	1.3	9	12.5	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	1135	21.0	52	4.6	1.0	0	0.0	0.0
Backbone-Backbone	570	10.5	14	2.5	0.3	0	0.0	0.0
Backbone-Sidechain	392	7.3	32	8.2	0.6	0	0.0	0.0
Sidechain-Sidechain	173	3.2	6	3.5	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	1693	31.3	94	5.6	1.7	0	0.0	0.0
Backbone-Backbone	229	4.2	10	4.4	0.2	0	0.0	0.0
Backbone-Sidechain	710	13.1	53	7.5	1.0	0	0.0	0.0
Sidechain-Sidechain	754	13.9	31	4.1	0.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	222	4.1	19	8.6	0.4	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	5406	100.0	201	3.7	3.7	0	0.0	0.0
Backbone-Backbone	1696	31.4	29	1.7	0.5	0	0.0	0.0
Backbone-Sidechain	2576	47.7	126	4.9	2.3	0	0.0	0.0
Sidechain-Sidechain	1134	21.0	46	4.1	0.9	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	1	2	9	0	13	0.13	0.2	0.03	0.12
2	1	4	5	12	0	22	0.15	0.19	0.02	0.14
3	0	5	9	9	0	23	0.16	0.27	0.04	0.14
4	0	2	3	7	0	12	0.16	0.33	0.06	0.13
5	0	2	6	11	0	19	0.14	0.26	0.04	0.13
6	0	2	11	6	0	19	0.14	0.35	0.07	0.11
7	0	3	4	9	0	16	0.13	0.21	0.03	0.12
8	1	2	6	9	0	18	0.15	0.29	0.05	0.13
9	1	2	6	12	0	21	0.14	0.2	0.03	0.13
10	1	7	5	7	0	20	0.15	0.24	0.04	0.16

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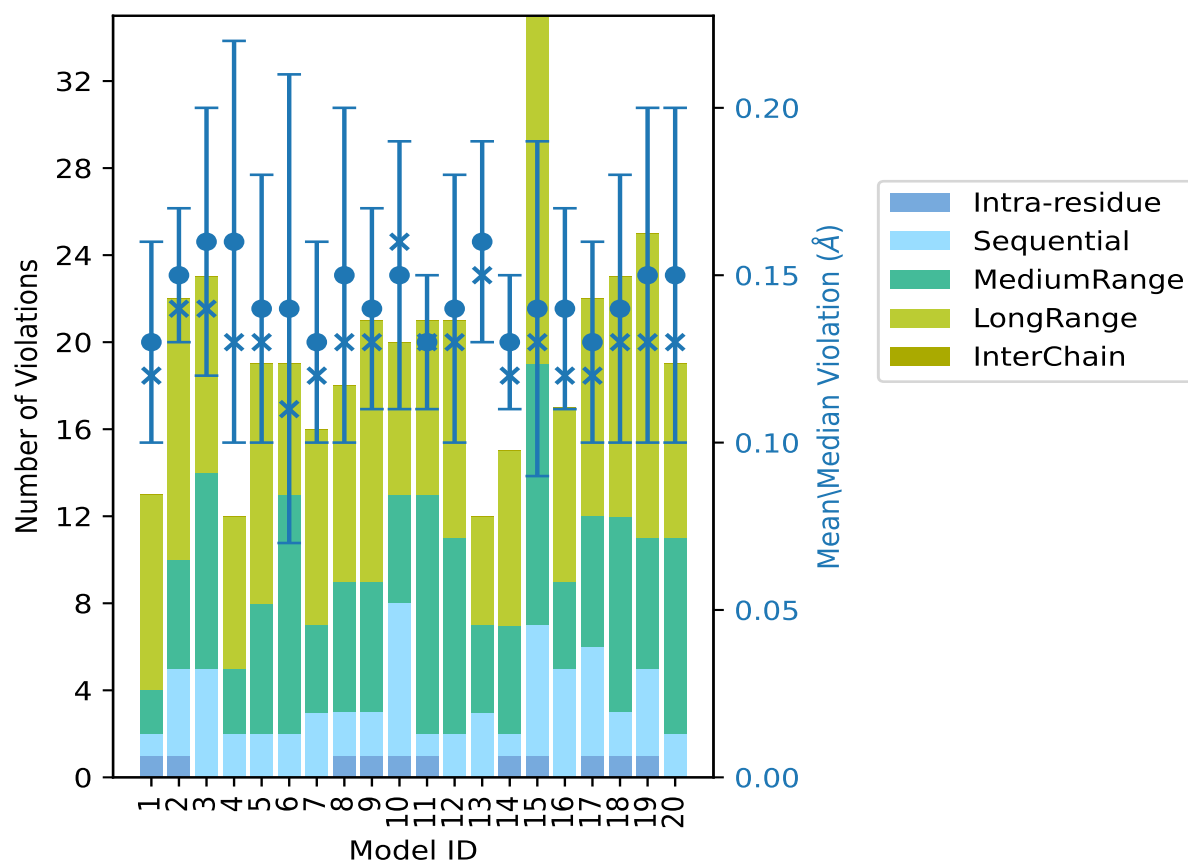
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	1	11	8	0	21	0.13	0.19	0.02	0.13
12	0	2	9	10	0	21	0.14	0.24	0.04	0.13
13	0	3	4	5	0	12	0.16	0.22	0.03	0.15
14	1	1	5	8	0	15	0.13	0.16	0.02	0.12
15	1	6	12	16	0	35	0.14	0.36	0.05	0.13
16	0	5	4	8	0	17	0.14	0.2	0.03	0.12
17	1	5	6	10	0	22	0.13	0.22	0.03	0.12
18	1	2	9	11	0	23	0.14	0.24	0.04	0.13
19	1	4	6	14	0	25	0.15	0.29	0.05	0.13
20	0	2	9	8	0	19	0.15	0.29	0.05	0.13

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

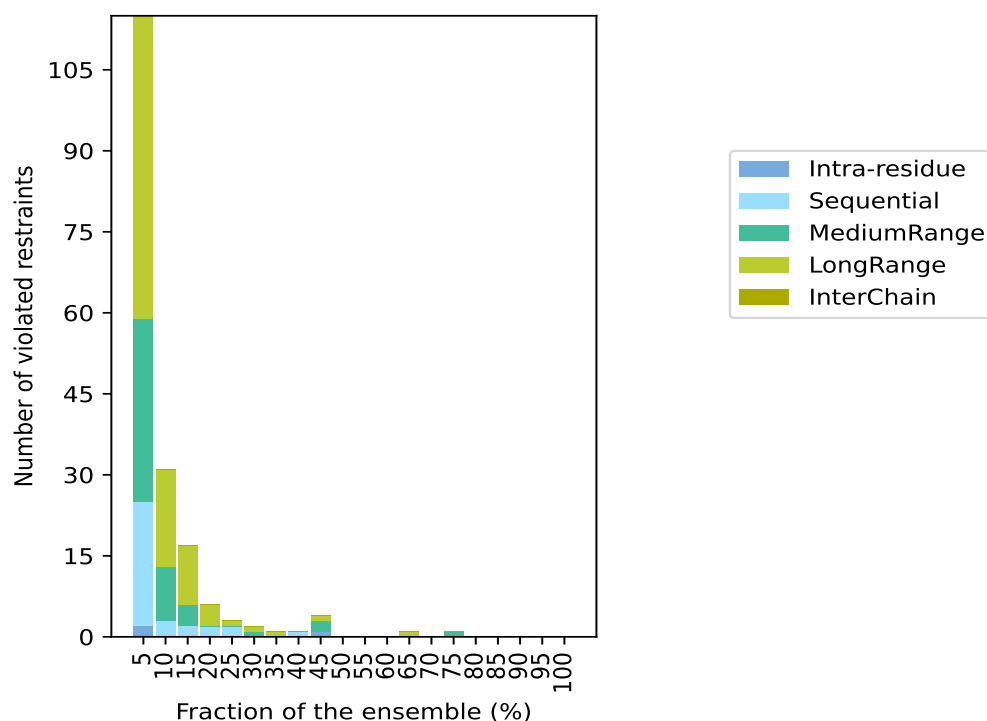
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 5002(IR:966, SQ:1354, MR:1083, LR:1599, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	23	34	56	0	115	1	5.0
0	3	10	18	0	31	2	10.0
0	2	4	11	0	17	3	15.0
0	2	0	4	0	6	4	20.0
0	2	0	1	0	3	5	25.0
0	0	1	1	0	2	6	30.0
0	0	0	1	0	1	7	35.0
0	1	0	0	0	1	8	40.0
1	0	2	1	0	4	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	1	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	1	0	0	1	15	75.0
0	0	0	0	0	0	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

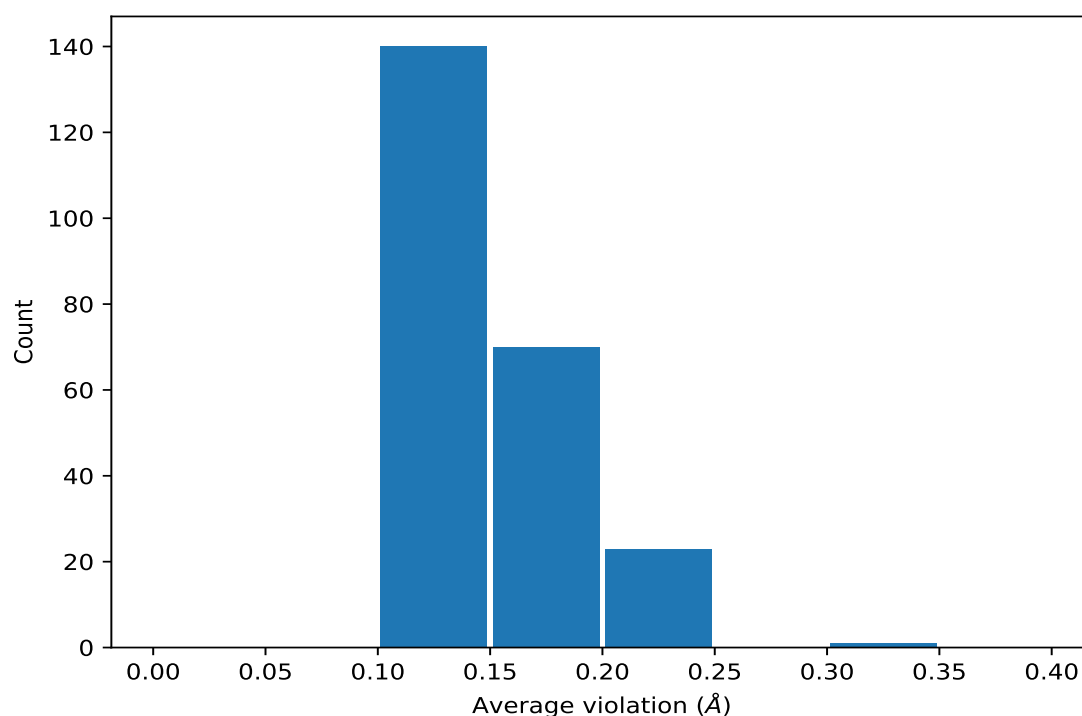
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	15	0.16	0.03	0.16
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	15	0.16	0.03	0.16
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	15	0.16	0.03	0.16
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	13	0.15	0.03	0.14
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	13	0.15	0.03	0.14
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	13	0.15	0.03	0.14
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE1	9	0.17	0.02	0.18
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE2	9	0.17	0.02	0.18
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD11	9	0.15	0.03	0.15
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD12	9	0.15	0.03	0.15
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD13	9	0.15	0.03	0.15
(1,2718)	1:262:A:GLU:HA	1:266:A:LYS:H	9	0.13	0.01	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB1	9	0.12	0.01	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB2	9	0.12	0.01	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB3	9	0.12	0.01	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB1	9	0.12	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB2	9	0.12	0.01	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB3	9	0.12	0.01	0.13
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG21	8	0.11	0.01	0.11
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG22	8	0.11	0.01	0.11
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG23	8	0.11	0.01	0.11
(1,4387)	1:48:A:PHE:HD1	1:198:A:TYR:H	7	0.13	0.04	0.11
(1,4387)	1:48:A:PHE:HD2	1:198:A:TYR:H	7	0.13	0.04	0.11
(1,4588)	1:65:A:ASP:HB2	1:68:A:CYS:H	6	0.2	0.09	0.16
(1,4588)	1:65:A:ASP:HB3	1:68:A:CYS:H	6	0.2	0.09	0.16
(1,2292)	1:241:A:ARG:HD2	1:313:A:GLU:H	6	0.16	0.06	0.14
(1,2292)	1:241:A:ARG:HD3	1:313:A:GLU:H	6	0.16	0.06	0.14
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG21	5	0.19	0.03	0.18
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG22	5	0.19	0.03	0.18
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG23	5	0.19	0.03	0.18
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG21	5	0.19	0.03	0.18
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG22	5	0.19	0.03	0.18
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG23	5	0.19	0.03	0.18
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG21	5	0.19	0.03	0.18
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG22	5	0.19	0.03	0.18
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG23	5	0.19	0.03	0.18
(1,5179)	1:82:A:THR:HB	1:354:A:ILE:H	5	0.15	0.03	0.13
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB2	5	0.14	0.03	0.14
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB3	5	0.14	0.03	0.14
(2,111)	1:163:A:ASP:O	1:167:A:TYR:H	5	0.12	0.03	0.11
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG11	4	0.16	0.05	0.15
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG12	4	0.16	0.05	0.15
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG13	4	0.16	0.05	0.15
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG11	4	0.16	0.05	0.15
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG12	4	0.16	0.05	0.15
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG13	4	0.16	0.05	0.15
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG11	4	0.16	0.05	0.15
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG12	4	0.16	0.05	0.15
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG13	4	0.16	0.05	0.15
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD11	4	0.16	0.0	0.16
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD12	4	0.16	0.0	0.16
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD13	4	0.16	0.0	0.16
(1,870)	1:151:A:ARG:HD2	1:295:A:LYS:H	4	0.16	0.03	0.16
(1,870)	1:151:A:ARG:HD3	1:295:A:LYS:H	4	0.16	0.03	0.16
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD11	4	0.15	0.02	0.15
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD12	4	0.15	0.02	0.15
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD13	4	0.15	0.02	0.15
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD21	4	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD22	4	0.15	0.02	0.15
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD23	4	0.15	0.02	0.15
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD11	4	0.14	0.02	0.15
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD12	4	0.14	0.02	0.15
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD13	4	0.14	0.02	0.15
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD21	4	0.14	0.02	0.15
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD22	4	0.14	0.02	0.15
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD23	4	0.14	0.02	0.15
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG11	4	0.14	0.02	0.14
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG12	4	0.14	0.02	0.14
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG13	4	0.14	0.02	0.14
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG21	4	0.14	0.02	0.14
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG22	4	0.14	0.02	0.14
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG23	4	0.14	0.02	0.14
(2,105)	1:166:A:GLU:O	1:170:A:GLU:H	4	0.13	0.03	0.13
(1,4012)	1:340:A:ASP:H	1:342:A:SER:H	3	0.19	0.06	0.16
(1,3302)	1:299:A:ILE:HD11	1:301:A:LYS:H	3	0.16	0.02	0.15
(1,3302)	1:299:A:ILE:HD12	1:301:A:LYS:H	3	0.16	0.02	0.15
(1,3302)	1:299:A:ILE:HD13	1:301:A:LYS:H	3	0.16	0.02	0.15
(1,4031)	1:341:A:LEU:HD21	1:344:A:VAL:H	3	0.16	0.05	0.16
(1,4031)	1:341:A:LEU:HD22	1:344:A:VAL:H	3	0.16	0.05	0.16
(1,4031)	1:341:A:LEU:HD23	1:344:A:VAL:H	3	0.16	0.05	0.16
(1,1393)	1:175:A:HIS:HB2	1:201:A:ALA:H	3	0.15	0.04	0.12
(1,1393)	1:175:A:HIS:HB3	1:201:A:ALA:H	3	0.15	0.04	0.12
(1,2289)	1:241:A:ARG:HG2	1:313:A:GLU:H	3	0.15	0.02	0.15
(1,2289)	1:241:A:ARG:HG3	1:313:A:GLU:H	3	0.15	0.02	0.15
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG21	3	0.14	0.05	0.11
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG22	3	0.14	0.05	0.11
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG23	3	0.14	0.05	0.11
(1,1446)	1:178:A:ILE:HD11	1:254:A:TRP:HZ2	3	0.14	0.04	0.12
(1,1446)	1:178:A:ILE:HD12	1:254:A:TRP:HZ2	3	0.14	0.04	0.12
(1,1446)	1:178:A:ILE:HD13	1:254:A:TRP:HZ2	3	0.14	0.04	0.12
(1,1689)	1:190:A:PRO:HB2	1:340:A:ASP:H	3	0.14	0.02	0.13
(1,1689)	1:190:A:PRO:HB3	1:340:A:ASP:H	3	0.14	0.02	0.13
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD11	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD12	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD13	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD21	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD22	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD23	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD11	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD12	3	0.13	0.01	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD13	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD21	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD22	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD23	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD11	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD12	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD13	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD21	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD22	3	0.13	0.01	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD23	3	0.13	0.01	0.14
(1,1760)	1:196:A:VAL:HG21	1:197:A:ASP:H	3	0.13	0.0	0.13
(1,1760)	1:196:A:VAL:HG22	1:197:A:ASP:H	3	0.13	0.0	0.13
(1,1760)	1:196:A:VAL:HG23	1:197:A:ASP:H	3	0.13	0.0	0.13
(1,4351)	1:45:A:GLN:H	1:51:A:ILE:HA	3	0.13	0.01	0.14
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG21	3	0.13	0.01	0.13
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG22	3	0.13	0.01	0.13
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG23	3	0.13	0.01	0.13
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG21	3	0.13	0.01	0.13
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG22	3	0.13	0.01	0.13
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG23	3	0.13	0.01	0.13
(1,1754)	1:196:A:VAL:HB	1:198:A:TYR:H	3	0.13	0.02	0.12
(2,139)	1:240:A:ARG:O	1:244:A:LEU:H	3	0.13	0.01	0.12
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE1	3	0.12	0.01	0.13
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE2	3	0.12	0.01	0.13
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE3	3	0.12	0.01	0.13
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE1	3	0.12	0.01	0.13
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE2	3	0.12	0.01	0.13
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE3	3	0.12	0.01	0.13
(2,85)	1:82:A:THR:O	1:86:A:PHE:H	3	0.12	0.01	0.12
(1,1991)	1:221:A:HIS:H	1:233:A:HIS:HB2	3	0.12	0.01	0.12
(1,1991)	1:221:A:HIS:H	1:233:A:HIS:HB3	3	0.12	0.01	0.12
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG21	3	0.12	0.02	0.1
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG22	3	0.12	0.02	0.1
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG23	3	0.12	0.02	0.1
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG21	3	0.12	0.02	0.1
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG22	3	0.12	0.02	0.1
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG23	3	0.12	0.02	0.1
(1,4698)	1:70:A:VAL:HG11	1:130:A:ILE:H	3	0.11	0.01	0.11
(1,4698)	1:70:A:VAL:HG12	1:130:A:ILE:H	3	0.11	0.01	0.11
(1,4698)	1:70:A:VAL:HG13	1:130:A:ILE:H	3	0.11	0.01	0.11
(1,1971)	1:21:A:GLU:H	1:23:A:PHE:H	2	0.32	0.04	0.32
(1,4126)	1:352:A:LYS:HG2	1:353:A:THR:HG21	2	0.24	0.09	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4126)	1:352:A:LYS:HG2	1:353:A:THR:HG22	2	0.24	0.09	0.24
(1,4126)	1:352:A:LYS:HG2	1:353:A:THR:HG23	2	0.24	0.09	0.24
(1,4126)	1:352:A:LYS:HG3	1:353:A:THR:HG21	2	0.24	0.09	0.24
(1,4126)	1:352:A:LYS:HG3	1:353:A:THR:HG22	2	0.24	0.09	0.24
(1,4126)	1:352:A:LYS:HG3	1:353:A:THR:HG23	2	0.24	0.09	0.24
(1,3562)	1:30:A:THR:HB	1:35:A:LYS:H	2	0.22	0.0	0.22
(1,1329)	1:173:A:TYR:H	1:204:A:TYR:HB2	2	0.21	0.03	0.21
(1,1329)	1:173:A:TYR:H	1:204:A:TYR:HB3	2	0.21	0.03	0.21
(1,1439)	1:178:A:ILE:HD11	1:243:A:ASP:HB2	2	0.2	0.02	0.2
(1,1439)	1:178:A:ILE:HD11	1:243:A:ASP:HB3	2	0.2	0.02	0.2
(1,1439)	1:178:A:ILE:HD12	1:243:A:ASP:HB2	2	0.2	0.02	0.2
(1,1439)	1:178:A:ILE:HD12	1:243:A:ASP:HB3	2	0.2	0.02	0.2
(1,1439)	1:178:A:ILE:HD13	1:243:A:ASP:HB2	2	0.2	0.02	0.2
(1,1439)	1:178:A:ILE:HD13	1:243:A:ASP:HB3	2	0.2	0.02	0.2
(1,4896)	1:81:A:PHE:HD1	1:82:A:THR:HG21	2	0.2	0.04	0.2
(1,4896)	1:81:A:PHE:HD1	1:82:A:THR:HG22	2	0.2	0.04	0.2
(1,4896)	1:81:A:PHE:HD1	1:82:A:THR:HG23	2	0.2	0.04	0.2
(1,4896)	1:81:A:PHE:HD2	1:82:A:THR:HG21	2	0.2	0.04	0.2
(1,4896)	1:81:A:PHE:HD2	1:82:A:THR:HG22	2	0.2	0.04	0.2
(1,4896)	1:81:A:PHE:HD2	1:82:A:THR:HG23	2	0.2	0.04	0.2
(1,3691)	1:31:A:ASP:H	1:36:A:GLU:HG2	2	0.19	0.01	0.19
(1,3691)	1:31:A:ASP:H	1:36:A:GLU:HG3	2	0.19	0.01	0.19
(1,5045)	1:92:A:LYS:H	1:112:A:LYS:HA	2	0.19	0.08	0.19
(1,295)	1:118:A:LEU:HD21	1:126:A:TYR:HB2	2	0.18	0.02	0.18
(1,295)	1:118:A:LEU:HD21	1:126:A:TYR:HB3	2	0.18	0.02	0.18
(1,295)	1:118:A:LEU:HD22	1:126:A:TYR:HB2	2	0.18	0.02	0.18
(1,295)	1:118:A:LEU:HD22	1:126:A:TYR:HB3	2	0.18	0.02	0.18
(1,295)	1:118:A:LEU:HD23	1:126:A:TYR:HB2	2	0.18	0.02	0.18
(1,295)	1:118:A:LEU:HD23	1:126:A:TYR:HB3	2	0.18	0.02	0.18
(1,2755)	1:265:A:LEU:HD11	1:271:A:VAL:H	2	0.18	0.08	0.18
(1,2755)	1:265:A:LEU:HD12	1:271:A:VAL:H	2	0.18	0.08	0.18
(1,2755)	1:265:A:LEU:HD13	1:271:A:VAL:H	2	0.18	0.08	0.18
(1,2755)	1:265:A:LEU:HD21	1:271:A:VAL:H	2	0.18	0.08	0.18
(1,2755)	1:265:A:LEU:HD22	1:271:A:VAL:H	2	0.18	0.08	0.18
(1,2755)	1:265:A:LEU:HD23	1:271:A:VAL:H	2	0.18	0.08	0.18
(1,4086)	1:347:A:GLY:H	1:349:A:LEU:H	2	0.18	0.01	0.18
(1,4161)	1:354:A:ILE:HG21	1:355:A:THR:HG21	2	0.17	0.03	0.17
(1,4161)	1:354:A:ILE:HG21	1:355:A:THR:HG22	2	0.17	0.03	0.17
(1,4161)	1:354:A:ILE:HG21	1:355:A:THR:HG23	2	0.17	0.03	0.17
(1,4161)	1:354:A:ILE:HG22	1:355:A:THR:HG21	2	0.17	0.03	0.17
(1,4161)	1:354:A:ILE:HG22	1:355:A:THR:HG22	2	0.17	0.03	0.17
(1,4161)	1:354:A:ILE:HG22	1:355:A:THR:HG23	2	0.17	0.03	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4161)	1:354:A:ILE:HG23	1:355:A:THR:HG21	2	0.17	0.03	0.17
(1,4161)	1:354:A:ILE:HG23	1:355:A:THR:HG22	2	0.17	0.03	0.17
(1,4161)	1:354:A:ILE:HG23	1:355:A:THR:HG23	2	0.17	0.03	0.17
(1,425)	1:131:A:MET:HE1	1:133:A:ARG:HA	2	0.16	0.01	0.16
(1,425)	1:131:A:MET:HE2	1:133:A:ARG:HA	2	0.16	0.01	0.16
(1,425)	1:131:A:MET:HE3	1:133:A:ARG:HA	2	0.16	0.01	0.16
(1,4775)	1:73:A:GLU:H	1:126:A:TYR:HE1	2	0.16	0.03	0.16
(1,4775)	1:73:A:GLU:H	1:126:A:TYR:HE2	2	0.16	0.03	0.16
(1,5184)	1:222:A:ASP:H	1:355:A:THR:H	2	0.16	0.04	0.16
(1,4017)	1:340:A:ASP:HB2	1:342:A:SER:H	2	0.16	0.02	0.16
(1,4017)	1:340:A:ASP:HB3	1:342:A:SER:H	2	0.16	0.02	0.16
(1,1988)	1:221:A:HIS:H	1:232:A:ALA:HA	2	0.14	0.03	0.14
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD11	2	0.14	0.02	0.14
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD12	2	0.14	0.02	0.14
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD13	2	0.14	0.02	0.14
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD21	2	0.14	0.02	0.14
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD22	2	0.14	0.02	0.14
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD23	2	0.14	0.02	0.14
(1,4227)	1:38:A:LYS:H	1:57:A:ASN:HB2	2	0.14	0.02	0.14
(1,4227)	1:38:A:LYS:H	1:57:A:ASN:HB3	2	0.14	0.02	0.14
(1,4240)	1:39:A:VAL:HA	1:56:A:MET:H	2	0.13	0.03	0.13
(2,201)	1:304:A:GLU:O	1:308:A:LEU:H	2	0.13	0.02	0.13
(1,1984)	1:220:A:CYS:HA	1:235:A:GLY:H	2	0.12	0.01	0.12
(1,3180)	1:28:A:ILE:HG12	1:36:A:GLU:H	2	0.12	0.01	0.12
(1,3180)	1:28:A:ILE:HG13	1:36:A:GLU:H	2	0.12	0.01	0.12
(1,3385)	1:302:A:TYR:H	1:323:A:ILE:HB	2	0.12	0.02	0.12
(1,2084)	1:226:A:GLU:H	1:228:A:THR:HG21	2	0.12	0.01	0.12
(1,2084)	1:226:A:GLU:H	1:228:A:THR:HG22	2	0.12	0.01	0.12
(1,2084)	1:226:A:GLU:H	1:228:A:THR:HG23	2	0.12	0.01	0.12
(1,4047)	1:343:A:VAL:H	1:345:A:GLU:H	2	0.12	0.01	0.12
(1,4558)	1:62:A:VAL:HG11	1:64:A:SER:HA	2	0.12	0.0	0.12
(1,4558)	1:62:A:VAL:HG12	1:64:A:SER:HA	2	0.12	0.0	0.12
(1,4558)	1:62:A:VAL:HG13	1:64:A:SER:HA	2	0.12	0.0	0.12
(2,75)	1:182:A:ASN:O	1:196:A:VAL:H	2	0.12	0.0	0.12
(1,1907)	1:213:A:TYR:HA	1:236:A:VAL:HG21	2	0.12	0.02	0.12
(1,1907)	1:213:A:TYR:HA	1:236:A:VAL:HG22	2	0.12	0.02	0.12
(1,1907)	1:213:A:TYR:HA	1:236:A:VAL:HG23	2	0.12	0.02	0.12
(1,3581)	1:310:A:ASP:HA	1:313:A:GLU:H	2	0.11	0.01	0.11
(2,161)	1:251:A:MET:O	1:255:A:LEU:H	2	0.11	0.0	0.11
(1,3382)	1:302:A:TYR:H	1:305:A:THR:HG21	2	0.11	0.0	0.11
(1,3382)	1:302:A:TYR:H	1:305:A:THR:HG22	2	0.11	0.0	0.11
(1,3382)	1:302:A:TYR:H	1:305:A:THR:HG23	2	0.11	0.0	0.11

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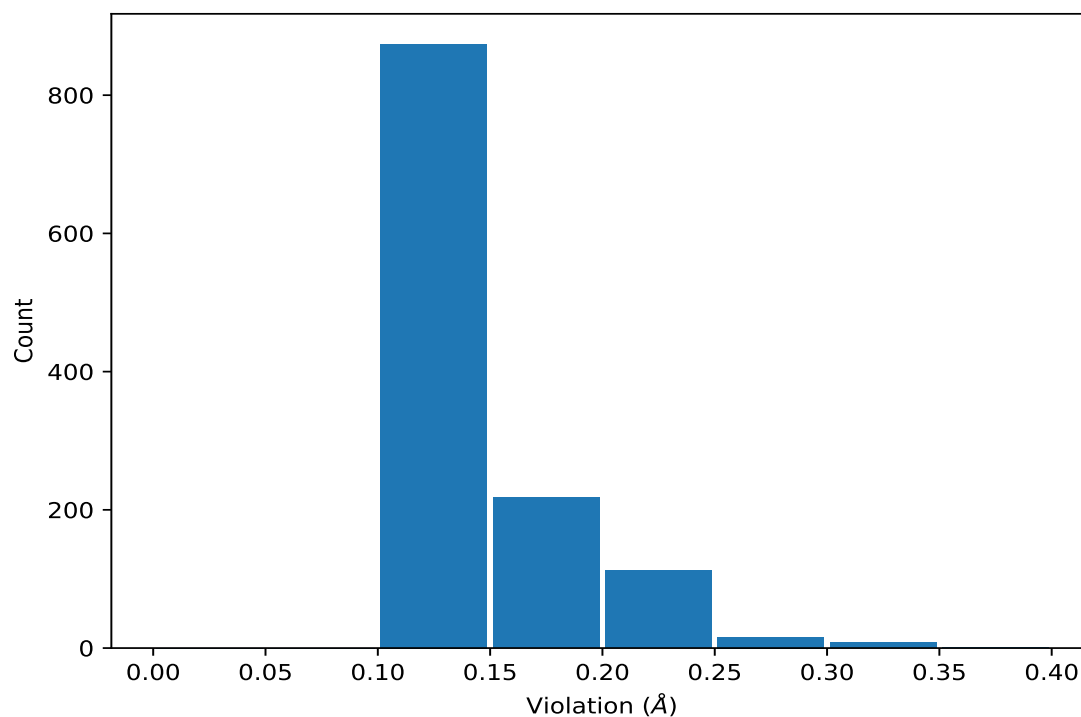
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4692)	1:70:A:VAL:HB	1:130:A:ILE:HD11	2	0.11	0.0	0.11
(1,4692)	1:70:A:VAL:HB	1:130:A:ILE:HD12	2	0.11	0.0	0.11
(1,4692)	1:70:A:VAL:HB	1:130:A:ILE:HD13	2	0.11	0.0	0.11
(2,17)	1:54:A:ALA:H	1:68:A:CYS:O	2	0.11	0.0	0.11
(2,117)	1:160:A:ARG:O	1:164:A:ILE:H	2	0.11	0.0	0.11
(1,3185)	1:28:A:ILE:HG21	1:36:A:GLU:H	2	0.1	0.0	0.1
(1,3185)	1:28:A:ILE:HG22	1:36:A:GLU:H	2	0.1	0.0	0.1
(1,3185)	1:28:A:ILE:HG23	1:36:A:GLU:H	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:21:A:GLU:H	1:23:A:PHE:H	15	0.36
(1,4588)	1:65:A:ASP:HB2	1:68:A:CYS:H	6	0.35
(1,4588)	1:65:A:ASP:HB3	1:68:A:CYS:H	6	0.35
(1,4126)	1:352:A:LYS:HG2	1:353:A:THR:HG21	4	0.33
(1,4126)	1:352:A:LYS:HG2	1:353:A:THR:HG22	4	0.33
(1,4126)	1:352:A:LYS:HG2	1:353:A:THR:HG23	4	0.33
(1,4126)	1:352:A:LYS:HG3	1:353:A:THR:HG21	4	0.33
(1,4126)	1:352:A:LYS:HG3	1:353:A:THR:HG22	4	0.33
(1,4126)	1:352:A:LYS:HG3	1:353:A:THR:HG23	4	0.33
(1,4588)	1:65:A:ASP:HB2	1:68:A:CYS:H	19	0.29
(1,4588)	1:65:A:ASP:HB3	1:68:A:CYS:H	19	0.29
(1,4417)	1:51:A:ILE:HD11	1:72:A:VAL:HA	8	0.29
(1,4417)	1:51:A:ILE:HD12	1:72:A:VAL:HA	8	0.29
(1,4417)	1:51:A:ILE:HD13	1:72:A:VAL:HA	8	0.29
(1,2292)	1:241:A:ARG:HD2	1:313:A:GLU:H	20	0.29
(1,2292)	1:241:A:ARG:HD3	1:313:A:GLU:H	20	0.29
(1,4012)	1:340:A:ASP:H	1:342:A:SER:H	6	0.28
(1,5045)	1:92:A:LYS:H	1:112:A:LYS:HA	8	0.27
(1,1971)	1:21:A:GLU:H	1:23:A:PHE:H	3	0.27
(1,2755)	1:265:A:LEU:HD11	1:271:A:VAL:H	5	0.26
(1,2755)	1:265:A:LEU:HD12	1:271:A:VAL:H	5	0.26
(1,2755)	1:265:A:LEU:HD13	1:271:A:VAL:H	5	0.26
(1,2755)	1:265:A:LEU:HD21	1:271:A:VAL:H	5	0.26
(1,2755)	1:265:A:LEU:HD22	1:271:A:VAL:H	5	0.26
(1,2755)	1:265:A:LEU:HD23	1:271:A:VAL:H	5	0.26
(1,4896)	1:81:A:PHE:HD1	1:82:A:THR:HG21	12	0.24
(1,4896)	1:81:A:PHE:HD1	1:82:A:THR:HG22	12	0.24
(1,4896)	1:81:A:PHE:HD1	1:82:A:THR:HG23	12	0.24
(1,4896)	1:81:A:PHE:HD2	1:82:A:THR:HG21	12	0.24
(1,4896)	1:81:A:PHE:HD2	1:82:A:THR:HG22	12	0.24
(1,4896)	1:81:A:PHE:HD2	1:82:A:THR:HG23	12	0.24
(1,1768)	1:196:A:VAL:HG21	1:198:A:TYR:HE1	10	0.24
(1,1768)	1:196:A:VAL:HG21	1:198:A:TYR:HE2	10	0.24
(1,1768)	1:196:A:VAL:HG22	1:198:A:TYR:HE1	10	0.24
(1,1768)	1:196:A:VAL:HG22	1:198:A:TYR:HE2	10	0.24
(1,1768)	1:196:A:VAL:HG23	1:198:A:TYR:HE1	10	0.24
(1,1768)	1:196:A:VAL:HG23	1:198:A:TYR:HE2	10	0.24
(1,1329)	1:173:A:TYR:H	1:204:A:TYR:HB2	19	0.24
(1,1329)	1:173:A:TYR:H	1:204:A:TYR:HB3	19	0.24
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG11	18	0.24
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG12	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG13	18	0.24
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG11	18	0.24
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG12	18	0.24
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG13	18	0.24
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG11	18	0.24
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG12	18	0.24
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG13	18	0.24
(1,1967)	1:219:A:ARG:HA	1:221:A:HIS:H	20	0.23
(1,4387)	1:48:A:PHE:HD1	1:198:A:TYR:H	15	0.22
(1,4387)	1:48:A:PHE:HD2	1:198:A:TYR:H	15	0.22
(1,4031)	1:341:A:LEU:HD21	1:344:A:VAL:H	3	0.22
(1,4031)	1:341:A:LEU:HD22	1:344:A:VAL:H	3	0.22
(1,4031)	1:341:A:LEU:HD23	1:344:A:VAL:H	3	0.22
(1,3886)	1:32:A:MET:H	1:37:A:TRP:HE1	18	0.22
(1,3562)	1:30:A:THR:HB	1:35:A:LYS:H	12	0.22
(1,3562)	1:30:A:THR:HB	1:35:A:LYS:H	17	0.22
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG21	6	0.22
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG22	6	0.22
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG23	6	0.22
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG21	6	0.22
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG22	6	0.22
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG23	6	0.22
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG21	6	0.22
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG22	6	0.22
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG23	6	0.22
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG21	19	0.22
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG22	19	0.22
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG23	19	0.22
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG21	19	0.22
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG22	19	0.22
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG23	19	0.22
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG21	19	0.22
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG22	19	0.22
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG23	19	0.22
(1,1915)	1:213:A:TYR:HD1	1:215:A:GLU:H	13	0.22
(1,1915)	1:213:A:TYR:HD2	1:215:A:GLU:H	13	0.22
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG21	3	0.22
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG22	3	0.22
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG23	3	0.22
(1,5179)	1:82:A:THR:HB	1:354:A:ILE:H	3	0.21
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	5	0.21
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	5	0.21
(1,4034)	1:342:A:SER:H	1:343:A:VAL:HG21	13	0.21
(1,4034)	1:342:A:SER:H	1:343:A:VAL:HG22	13	0.21
(1,4034)	1:342:A:SER:H	1:343:A:VAL:HG23	13	0.21
(1,1439)	1:178:A:ILE:HD11	1:243:A:ASP:HB2	7	0.21
(1,1439)	1:178:A:ILE:HD11	1:243:A:ASP:HB3	7	0.21
(1,1439)	1:178:A:ILE:HD12	1:243:A:ASP:HB2	7	0.21
(1,1439)	1:178:A:ILE:HD12	1:243:A:ASP:HB3	7	0.21
(1,1439)	1:178:A:ILE:HD13	1:243:A:ASP:HB2	7	0.21
(1,1439)	1:178:A:ILE:HD13	1:243:A:ASP:HB3	7	0.21
(1,1393)	1:175:A:HIS:HB2	1:201:A:ALA:H	10	0.21
(1,1393)	1:175:A:HIS:HB3	1:201:A:ALA:H	10	0.21
(1,5184)	1:222:A:ASP:H	1:355:A:THR:H	19	0.2
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	10	0.2
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	10	0.2
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	10	0.2
(1,4161)	1:354:A:ILE:HG21	1:355:A:THR:HG21	16	0.2
(1,4161)	1:354:A:ILE:HG21	1:355:A:THR:HG22	16	0.2
(1,4161)	1:354:A:ILE:HG21	1:355:A:THR:HG23	16	0.2
(1,4161)	1:354:A:ILE:HG22	1:355:A:THR:HG21	16	0.2
(1,4161)	1:354:A:ILE:HG22	1:355:A:THR:HG22	16	0.2
(1,4161)	1:354:A:ILE:HG22	1:355:A:THR:HG23	16	0.2
(1,4161)	1:354:A:ILE:HG23	1:355:A:THR:HG21	16	0.2
(1,4161)	1:354:A:ILE:HG23	1:355:A:THR:HG22	16	0.2
(1,4161)	1:354:A:ILE:HG23	1:355:A:THR:HG23	16	0.2
(1,3691)	1:31:A:ASP:H	1:36:A:GLU:HG2	17	0.2
(1,3691)	1:31:A:ASP:H	1:36:A:GLU:HG3	17	0.2
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	1	0.2
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	1	0.2
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	1	0.2
(1,1919)	1:213:A:TYR:HE1	1:236:A:VAL:HG21	4	0.2
(1,1919)	1:213:A:TYR:HE1	1:236:A:VAL:HG22	4	0.2
(1,1919)	1:213:A:TYR:HE1	1:236:A:VAL:HG23	4	0.2
(1,1919)	1:213:A:TYR:HE2	1:236:A:VAL:HG21	4	0.2
(1,1919)	1:213:A:TYR:HE2	1:236:A:VAL:HG22	4	0.2
(1,1919)	1:213:A:TYR:HE2	1:236:A:VAL:HG23	4	0.2
(1,1813)	1:200:A:LEU:HD21	1:224:A:THR:HG21	9	0.2
(1,1813)	1:200:A:LEU:HD21	1:224:A:THR:HG22	9	0.2
(1,1813)	1:200:A:LEU:HD21	1:224:A:THR:HG23	9	0.2
(1,1813)	1:200:A:LEU:HD22	1:224:A:THR:HG21	9	0.2
(1,1813)	1:200:A:LEU:HD22	1:224:A:THR:HG22	9	0.2
(1,1813)	1:200:A:LEU:HD22	1:224:A:THR:HG23	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1813)	1:200:A:LEU:HD23	1:224:A:THR:HG21	9	0.2
(1,1813)	1:200:A:LEU:HD23	1:224:A:THR:HG22	9	0.2
(1,1813)	1:200:A:LEU:HD23	1:224:A:THR:HG23	9	0.2
(1,1446)	1:178:A:ILE:HD11	1:254:A:TRP:HZ2	10	0.2
(1,1446)	1:178:A:ILE:HD12	1:254:A:TRP:HZ2	10	0.2
(1,1446)	1:178:A:ILE:HD13	1:254:A:TRP:HZ2	10	0.2
(1,295)	1:118:A:LEU:HD21	1:126:A:TYR:HB2	16	0.2
(1,295)	1:118:A:LEU:HD21	1:126:A:TYR:HB3	16	0.2
(1,295)	1:118:A:LEU:HD22	1:126:A:TYR:HB2	16	0.2
(1,295)	1:118:A:LEU:HD22	1:126:A:TYR:HB3	16	0.2
(1,295)	1:118:A:LEU:HD23	1:126:A:TYR:HB2	16	0.2
(1,295)	1:118:A:LEU:HD23	1:126:A:TYR:HB3	16	0.2
(1,4775)	1:73:A:GLU:H	1:126:A:TYR:HE1	6	0.19
(1,4775)	1:73:A:GLU:H	1:126:A:TYR:HE2	6	0.19
(1,4563)	1:62:A:VAL:HG21	1:64:A:SER:HA	2	0.19
(1,4563)	1:62:A:VAL:HG22	1:64:A:SER:HA	2	0.19
(1,4563)	1:62:A:VAL:HG23	1:64:A:SER:HA	2	0.19
(1,4086)	1:347:A:GLY:H	1:349:A:LEU:H	4	0.19
(1,4041)	1:342:A:SER:HB2	1:344:A:VAL:H	7	0.19
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	15	0.19
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	15	0.19
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	15	0.19
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	18	0.19
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	18	0.19
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	18	0.19
(1,3302)	1:299:A:ILE:HD11	1:301:A:LYS:H	11	0.19
(1,3302)	1:299:A:ILE:HD12	1:301:A:LYS:H	11	0.19
(1,3302)	1:299:A:ILE:HD13	1:301:A:LYS:H	11	0.19
(1,870)	1:151:A:ARG:HD2	1:295:A:LYS:H	8	0.19
(1,870)	1:151:A:ARG:HD3	1:295:A:LYS:H	8	0.19
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD11	8	0.19
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD12	8	0.19
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD13	8	0.19
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD11	9	0.18
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD12	9	0.18
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD13	9	0.18
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD21	9	0.18
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD22	9	0.18
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD23	9	0.18
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	9	0.18
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	9	0.18
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	20	0.18
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	20	0.18
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	20	0.18
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG11	19	0.18
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG12	19	0.18
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG13	19	0.18
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG21	19	0.18
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG22	19	0.18
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG23	19	0.18
(1,4017)	1:340:A:ASP:HB2	1:342:A:SER:H	16	0.18
(1,4017)	1:340:A:ASP:HB3	1:342:A:SER:H	16	0.18
(1,3997)	1:339:A:LEU:HD21	1:341:A:LEU:H	3	0.18
(1,3997)	1:339:A:LEU:HD22	1:341:A:LEU:H	3	0.18
(1,3997)	1:339:A:LEU:HD23	1:341:A:LEU:H	3	0.18
(1,3691)	1:31:A:ASP:H	1:36:A:GLU:HG2	12	0.18
(1,3691)	1:31:A:ASP:H	1:36:A:GLU:HG3	12	0.18
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	8	0.18
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	8	0.18
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	8	0.18
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB2	3	0.18
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB3	3	0.18
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG21	10	0.18
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG22	10	0.18
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG23	10	0.18
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG21	10	0.18
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG22	10	0.18
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG23	10	0.18
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG21	10	0.18
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG22	10	0.18
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG23	10	0.18
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE1	1	0.18
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE2	1	0.18
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE1	2	0.18
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE2	2	0.18
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE1	11	0.18
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE2	11	0.18
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE1	17	0.18
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE2	17	0.18
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE1	18	0.18
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE2	18	0.18
(1,1439)	1:178:A:ILE:HD11	1:243:A:ASP:HB2	5	0.18
(1,1439)	1:178:A:ILE:HD11	1:243:A:ASP:HB3	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1439)	1:178:A:ILE:HD12	1:243:A:ASP:HB2	5	0.18
(1,1439)	1:178:A:ILE:HD12	1:243:A:ASP:HB3	5	0.18
(1,1439)	1:178:A:ILE:HD13	1:243:A:ASP:HB2	5	0.18
(1,1439)	1:178:A:ILE:HD13	1:243:A:ASP:HB3	5	0.18
(1,1329)	1:173:A:TYR:H	1:204:A:TYR:HB2	10	0.18
(1,1329)	1:173:A:TYR:H	1:204:A:TYR:HB3	10	0.18
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD11	9	0.18
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD12	9	0.18
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD13	9	0.18
(2,111)	1:163:A:ASP:O	1:167:A:TYR:H	12	0.17
(2,105)	1:166:A:GLU:O	1:170:A:GLU:H	12	0.17
(1,5179)	1:82:A:THR:HB	1:354:A:ILE:H	4	0.17
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD11	2	0.17
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD12	2	0.17
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD13	2	0.17
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD21	2	0.17
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD22	2	0.17
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD23	2	0.17
(1,4355)	1:45:A:GLN:HA	1:48:A:PHE:H	3	0.17
(1,4086)	1:347:A:GLY:H	1:349:A:LEU:H	19	0.17
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	3	0.17
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	3	0.17
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	3	0.17
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	7	0.17
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	7	0.17
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	7	0.17
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	13	0.17
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	13	0.17
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	13	0.17
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB2	19	0.17
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB3	19	0.17
(1,2289)	1:241:A:ARG:HG2	1:313:A:GLU:H	2	0.17
(1,2289)	1:241:A:ARG:HG3	1:313:A:GLU:H	2	0.17
(1,1988)	1:221:A:HIS:H	1:232:A:ALA:HA	5	0.17
(1,1689)	1:190:A:PRO:HB2	1:340:A:ASP:H	11	0.17
(1,1689)	1:190:A:PRO:HB3	1:340:A:ASP:H	11	0.17
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE1	10	0.17
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE2	10	0.17
(1,1415)	1:177:A:ASP:HB2	1:200:A:LEU:H	1	0.17
(1,1415)	1:177:A:ASP:HB3	1:200:A:LEU:H	1	0.17
(1,1405)	1:177:A:ASP:H	1:200:A:LEU:HD11	15	0.17
(1,1405)	1:177:A:ASP:H	1:200:A:LEU:HD12	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1405)	1:177:A:ASP:H	1:200:A:LEU:HD13	15	0.17
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD11	12	0.17
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD12	12	0.17
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD13	12	0.17
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD21	12	0.17
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD22	12	0.17
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD23	12	0.17
(1,1322)	1:172:A:GLU:HB2	1:207:A:GLU:H	20	0.17
(1,1322)	1:172:A:GLU:HB3	1:207:A:GLU:H	20	0.17
(1,1312)	1:171:A:HIS:HA	1:173:A:TYR:H	20	0.17
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD11	10	0.17
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD12	10	0.17
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD13	10	0.17
(1,870)	1:151:A:ARG:HD2	1:295:A:LYS:H	2	0.17
(1,870)	1:151:A:ARG:HD3	1:295:A:LYS:H	2	0.17
(1,425)	1:131:A:MET:HE1	1:133:A:ARG:HA	2	0.17
(1,425)	1:131:A:MET:HE2	1:133:A:ARG:HA	2	0.17
(1,425)	1:131:A:MET:HE3	1:133:A:ARG:HA	2	0.17
(1,295)	1:118:A:LEU:HD21	1:126:A:TYR:HB2	13	0.17
(1,295)	1:118:A:LEU:HD21	1:126:A:TYR:HB3	13	0.17
(1,295)	1:118:A:LEU:HD22	1:126:A:TYR:HB2	13	0.17
(1,295)	1:118:A:LEU:HD22	1:126:A:TYR:HB3	13	0.17
(1,295)	1:118:A:LEU:HD23	1:126:A:TYR:HB2	13	0.17
(1,295)	1:118:A:LEU:HD23	1:126:A:TYR:HB3	13	0.17
(1,5159)	1:99:A:TRP:HD1	1:100:A:ILE:HD11	10	0.16
(1,5159)	1:99:A:TRP:HD1	1:100:A:ILE:HD12	10	0.16
(1,5159)	1:99:A:TRP:HD1	1:100:A:ILE:HD13	10	0.16
(1,4588)	1:65:A:ASP:HB2	1:68:A:CYS:H	15	0.16
(1,4588)	1:65:A:ASP:HB3	1:68:A:CYS:H	15	0.16
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	19	0.16
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	19	0.16
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	19	0.16
(1,4362)	1:46:A:GLY:H	1:49:A:GLY:H	11	0.16
(1,4240)	1:39:A:VAL:HA	1:56:A:MET:H	12	0.16
(1,4125)	1:352:A:LYS:HB2	1:353:A:THR:H	10	0.16
(1,4125)	1:352:A:LYS:HB3	1:353:A:THR:H	10	0.16
(1,4031)	1:341:A:LEU:HD21	1:344:A:VAL:H	8	0.16
(1,4031)	1:341:A:LEU:HD22	1:344:A:VAL:H	8	0.16
(1,4031)	1:341:A:LEU:HD23	1:344:A:VAL:H	8	0.16
(1,4012)	1:340:A:ASP:H	1:342:A:SER:H	14	0.16
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	9	0.16
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	9	0.16
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG21	15	0.16
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG22	15	0.16
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG23	15	0.16
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG21	15	0.16
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG22	15	0.16
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG23	15	0.16
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG21	15	0.16
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG22	15	0.16
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG23	15	0.16
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG21	16	0.16
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG22	16	0.16
(1,3173)	1:28:A:ILE:HD11	1:29:A:ILE:HG23	16	0.16
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG21	16	0.16
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG22	16	0.16
(1,3173)	1:28:A:ILE:HD12	1:29:A:ILE:HG23	16	0.16
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG21	16	0.16
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG22	16	0.16
(1,3173)	1:28:A:ILE:HD13	1:29:A:ILE:HG23	16	0.16
(1,2292)	1:241:A:ARG:HD2	1:313:A:GLU:H	3	0.16
(1,2292)	1:241:A:ARG:HD3	1:313:A:GLU:H	3	0.16
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE1	14	0.16
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE2	14	0.16
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD11	15	0.16
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD12	15	0.16
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD13	15	0.16
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD21	15	0.16
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD22	15	0.16
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD23	15	0.16
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD11	2	0.16
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD12	2	0.16
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD13	2	0.16
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD11	3	0.16
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD12	3	0.16
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD13	3	0.16
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD11	11	0.16
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD12	11	0.16
(1,1095)	1:160:A:ARG:HA	1:161:A:ILE:HD13	11	0.16
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG11	14	0.16
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG12	14	0.16
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG13	14	0.16
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG11	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG12	14	0.16
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG13	14	0.16
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG11	14	0.16
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG12	14	0.16
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG13	14	0.16
(1,705)	1:141:A:ILE:HG12	1:185:A:LEU:HD21	17	0.16
(1,705)	1:141:A:ILE:HG12	1:185:A:LEU:HD22	17	0.16
(1,705)	1:141:A:ILE:HG12	1:185:A:LEU:HD23	17	0.16
(1,705)	1:141:A:ILE:HG13	1:185:A:LEU:HD21	17	0.16
(1,705)	1:141:A:ILE:HG13	1:185:A:LEU:HD22	17	0.16
(1,705)	1:141:A:ILE:HG13	1:185:A:LEU:HD23	17	0.16
(1,425)	1:131:A:MET:HE1	1:133:A:ARG:HA	13	0.16
(1,425)	1:131:A:MET:HE2	1:133:A:ARG:HA	13	0.16
(1,425)	1:131:A:MET:HE3	1:133:A:ARG:HA	13	0.16
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD11	3	0.16
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD12	3	0.16
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD13	3	0.16
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD11	12	0.16
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD12	12	0.16
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD13	12	0.16
(2,201)	1:304:A:GLU:O	1:308:A:LEU:H	18	0.15
(2,145)	1:243:A:ASP:O	1:247:A:LEU:H	9	0.15
(2,105)	1:166:A:GLU:O	1:170:A:GLU:H	20	0.15
(1,4896)	1:81:A:PHE:HD1	1:82:A:THR:HG21	5	0.15
(1,4896)	1:81:A:PHE:HD1	1:82:A:THR:HG22	5	0.15
(1,4896)	1:81:A:PHE:HD1	1:82:A:THR:HG23	5	0.15
(1,4896)	1:81:A:PHE:HD2	1:82:A:THR:HG21	5	0.15
(1,4896)	1:81:A:PHE:HD2	1:82:A:THR:HG22	5	0.15
(1,4896)	1:81:A:PHE:HD2	1:82:A:THR:HG23	5	0.15
(1,4588)	1:65:A:ASP:HB2	1:68:A:CYS:H	18	0.15
(1,4588)	1:65:A:ASP:HB3	1:68:A:CYS:H	18	0.15
(1,4560)	1:62:A:VAL:HG11	1:65:A:ASP:HA	15	0.15
(1,4560)	1:62:A:VAL:HG12	1:65:A:ASP:HA	15	0.15
(1,4560)	1:62:A:VAL:HG13	1:65:A:ASP:HA	15	0.15
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	15	0.15
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	15	0.15
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	15	0.15
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG11	17	0.15
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG12	17	0.15
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG13	17	0.15
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG21	17	0.15
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG22	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG23	17	0.15
(1,4256)	1:39:A:VAL:HG11	1:52:A:TYR:HA	2	0.15
(1,4256)	1:39:A:VAL:HG12	1:52:A:TYR:HA	2	0.15
(1,4256)	1:39:A:VAL:HG13	1:52:A:TYR:HA	2	0.15
(1,4256)	1:39:A:VAL:HG21	1:52:A:TYR:HA	2	0.15
(1,4256)	1:39:A:VAL:HG22	1:52:A:TYR:HA	2	0.15
(1,4256)	1:39:A:VAL:HG23	1:52:A:TYR:HA	2	0.15
(1,4227)	1:38:A:LYS:H	1:57:A:ASN:HB2	16	0.15
(1,4227)	1:38:A:LYS:H	1:57:A:ASN:HB3	16	0.15
(1,4126)	1:352:A:LYS:HG2	1:353:A:THR:HG21	13	0.15
(1,4126)	1:352:A:LYS:HG2	1:353:A:THR:HG22	13	0.15
(1,4126)	1:352:A:LYS:HG2	1:353:A:THR:HG23	13	0.15
(1,4126)	1:352:A:LYS:HG3	1:353:A:THR:HG21	13	0.15
(1,4126)	1:352:A:LYS:HG3	1:353:A:THR:HG22	13	0.15
(1,4126)	1:352:A:LYS:HG3	1:353:A:THR:HG23	13	0.15
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	10	0.15
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	10	0.15
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	10	0.15
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	11	0.15
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	11	0.15
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	11	0.15
(1,3302)	1:299:A:ILE:HD11	1:301:A:LYS:H	10	0.15
(1,3302)	1:299:A:ILE:HD12	1:301:A:LYS:H	10	0.15
(1,3302)	1:299:A:ILE:HD13	1:301:A:LYS:H	10	0.15
(1,3302)	1:299:A:ILE:HD11	1:301:A:LYS:H	12	0.15
(1,3302)	1:299:A:ILE:HD12	1:301:A:LYS:H	12	0.15
(1,3302)	1:299:A:ILE:HD13	1:301:A:LYS:H	12	0.15
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD11	19	0.15
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD12	19	0.15
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD13	19	0.15
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD21	19	0.15
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD22	19	0.15
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD23	19	0.15
(1,3012)	1:281:A:ASN:HB2	1:282:A:ILE:HD11	19	0.15
(1,3012)	1:281:A:ASN:HB2	1:282:A:ILE:HD12	19	0.15
(1,3012)	1:281:A:ASN:HB2	1:282:A:ILE:HD13	19	0.15
(1,3012)	1:281:A:ASN:HB3	1:282:A:ILE:HD11	19	0.15
(1,3012)	1:281:A:ASN:HB3	1:282:A:ILE:HD12	19	0.15
(1,3012)	1:281:A:ASN:HB3	1:282:A:ILE:HD13	19	0.15
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG21	13	0.15
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG22	13	0.15
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG23	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG21	13	0.15
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG22	13	0.15
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG23	13	0.15
(1,2292)	1:241:A:ARG:HD2	1:313:A:GLU:H	9	0.15
(1,2292)	1:241:A:ARG:HD3	1:313:A:GLU:H	9	0.15
(1,2289)	1:241:A:ARG:HG2	1:313:A:GLU:H	5	0.15
(1,2289)	1:241:A:ARG:HG3	1:313:A:GLU:H	5	0.15
(1,2152)	1:230:A:ILE:H	1:245:A:GLU:HB2	2	0.15
(1,2152)	1:230:A:ILE:H	1:245:A:GLU:HB3	2	0.15
(1,2104)	1:227:A:PHE:H	1:229:A:SER:H	18	0.15
(1,1754)	1:196:A:VAL:HB	1:198:A:TYR:H	20	0.15
(1,1666)	1:187:A:TYR:HE1	1:188:A:LYS:H	15	0.15
(1,1666)	1:187:A:TYR:HE2	1:188:A:LYS:H	15	0.15
(1,1478)	1:179:A:LYS:HG2	1:180:A:ALA:H	17	0.15
(1,1478)	1:179:A:LYS:HG3	1:180:A:ALA:H	17	0.15
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB1	15	0.15
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB2	15	0.15
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB3	15	0.15
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB1	15	0.15
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB2	15	0.15
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB3	15	0.15
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD11	5	0.15
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD12	5	0.15
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD13	5	0.15
(2,139)	1:240:A:ARG:O	1:244:A:LEU:H	3	0.14
(2,112)	1:163:A:ASP:O	1:167:A:TYR:N	12	0.14
(2,111)	1:163:A:ASP:O	1:167:A:TYR:H	14	0.14
(2,85)	1:82:A:THR:O	1:86:A:PHE:H	15	0.14
(2,71)	1:133:A:ARG:O	1:187:A:TYR:H	5	0.14
(1,5168)	1:99:A:TRP:HE1	1:163:A:ASP:HB2	3	0.14
(1,5168)	1:99:A:TRP:HE1	1:163:A:ASP:HB3	3	0.14
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	3	0.14
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	3	0.14
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	3	0.14
(1,4387)	1:48:A:PHE:HD1	1:198:A:TYR:H	7	0.14
(1,4387)	1:48:A:PHE:HD2	1:198:A:TYR:H	7	0.14
(1,4351)	1:45:A:GLN:H	1:51:A:ILE:HA	8	0.14
(1,4351)	1:45:A:GLN:H	1:51:A:ILE:HA	13	0.14
(1,4180)	1:356:A:LYS:HB2	1:357:A:LYS:H	3	0.14
(1,4180)	1:356:A:LYS:HB3	1:357:A:LYS:H	3	0.14
(1,4161)	1:354:A:ILE:HG21	1:355:A:THR:HG21	8	0.14
(1,4161)	1:354:A:ILE:HG21	1:355:A:THR:HG22	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4161)	1:354:A:ILE:HG21	1:355:A:THR:HG23	8	0.14
(1,4161)	1:354:A:ILE:HG22	1:355:A:THR:HG21	8	0.14
(1,4161)	1:354:A:ILE:HG22	1:355:A:THR:HG22	8	0.14
(1,4161)	1:354:A:ILE:HG22	1:355:A:THR:HG23	8	0.14
(1,4161)	1:354:A:ILE:HG23	1:355:A:THR:HG21	8	0.14
(1,4161)	1:354:A:ILE:HG23	1:355:A:THR:HG22	8	0.14
(1,4161)	1:354:A:ILE:HG23	1:355:A:THR:HG23	8	0.14
(1,4027)	1:341:A:LEU:HD11	1:343:A:VAL:H	15	0.14
(1,4027)	1:341:A:LEU:HD12	1:343:A:VAL:H	15	0.14
(1,4027)	1:341:A:LEU:HD13	1:343:A:VAL:H	15	0.14
(1,3615)	1:315:A:PRO:HG2	1:320:A:LEU:HD11	11	0.14
(1,3615)	1:315:A:PRO:HG2	1:320:A:LEU:HD12	11	0.14
(1,3615)	1:315:A:PRO:HG2	1:320:A:LEU:HD13	11	0.14
(1,3615)	1:315:A:PRO:HG2	1:320:A:LEU:HD21	11	0.14
(1,3615)	1:315:A:PRO:HG2	1:320:A:LEU:HD22	11	0.14
(1,3615)	1:315:A:PRO:HG2	1:320:A:LEU:HD23	11	0.14
(1,3615)	1:315:A:PRO:HG3	1:320:A:LEU:HD11	11	0.14
(1,3615)	1:315:A:PRO:HG3	1:320:A:LEU:HD12	11	0.14
(1,3615)	1:315:A:PRO:HG3	1:320:A:LEU:HD13	11	0.14
(1,3615)	1:315:A:PRO:HG3	1:320:A:LEU:HD21	11	0.14
(1,3615)	1:315:A:PRO:HG3	1:320:A:LEU:HD22	11	0.14
(1,3615)	1:315:A:PRO:HG3	1:320:A:LEU:HD23	11	0.14
(1,3385)	1:302:A:TYR:H	1:323:A:ILE:HB	16	0.14
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB2	2	0.14
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB3	2	0.14
(1,2718)	1:262:A:GLU:HA	1:266:A:LYS:H	6	0.14
(1,2718)	1:262:A:GLU:HA	1:266:A:LYS:H	16	0.14
(1,2718)	1:262:A:GLU:HA	1:266:A:LYS:H	18	0.14
(1,1844)	1:204:A:TYR:HD1	1:211:A:LYS:H	2	0.14
(1,1844)	1:204:A:TYR:HD2	1:211:A:LYS:H	2	0.14
(1,1760)	1:196:A:VAL:HG21	1:197:A:ASP:H	20	0.14
(1,1760)	1:196:A:VAL:HG22	1:197:A:ASP:H	20	0.14
(1,1760)	1:196:A:VAL:HG23	1:197:A:ASP:H	20	0.14
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE1	9	0.14
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE2	9	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD11	2	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD12	2	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD13	2	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD21	2	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD22	2	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD23	2	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD11	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD12	2	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD13	2	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD21	2	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD22	2	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD23	2	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD11	2	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD12	2	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD13	2	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD21	2	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD22	2	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD23	2	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD11	11	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD12	11	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD13	11	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD21	11	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD22	11	0.14
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD23	11	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD11	11	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD12	11	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD13	11	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD21	11	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD22	11	0.14
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD23	11	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD11	11	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD12	11	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD13	11	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD21	11	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD22	11	0.14
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD23	11	0.14
(1,1536)	1:183:A:LEU:HD21	1:193:A:VAL:H	5	0.14
(1,1536)	1:183:A:LEU:HD22	1:193:A:VAL:H	5	0.14
(1,1536)	1:183:A:LEU:HD23	1:193:A:VAL:H	5	0.14
(1,1370)	1:174:A:VAL:HG11	1:204:A:TYR:HB2	20	0.14
(1,1370)	1:174:A:VAL:HG11	1:204:A:TYR:HB3	20	0.14
(1,1370)	1:174:A:VAL:HG12	1:204:A:TYR:HB2	20	0.14
(1,1370)	1:174:A:VAL:HG12	1:204:A:TYR:HB3	20	0.14
(1,1370)	1:174:A:VAL:HG13	1:204:A:TYR:HB2	20	0.14
(1,1370)	1:174:A:VAL:HG13	1:204:A:TYR:HB3	20	0.14
(1,989)	1:155:A:LEU:HD11	1:299:A:ILE:H	17	0.14
(1,989)	1:155:A:LEU:HD12	1:299:A:ILE:H	17	0.14
(1,989)	1:155:A:LEU:HD13	1:299:A:ILE:H	17	0.14
(1,989)	1:155:A:LEU:HD21	1:299:A:ILE:H	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:155:A:LEU:HD22	1:299:A:ILE:H	17	0.14
(1,989)	1:155:A:LEU:HD23	1:299:A:ILE:H	17	0.14
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG21	19	0.14
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG22	19	0.14
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG23	19	0.14
(1,870)	1:151:A:ARG:HD2	1:295:A:LYS:H	9	0.14
(1,870)	1:151:A:ARG:HD3	1:295:A:LYS:H	9	0.14
(1,742)	1:142:A:TYR:HE1	1:254:A:TRP:HE1	9	0.14
(1,742)	1:142:A:TYR:HE2	1:254:A:TRP:HE1	9	0.14
(1,532)	1:137:A:ASP:HB2	1:183:A:LEU:H	3	0.14
(1,532)	1:137:A:ASP:HB3	1:183:A:LEU:H	3	0.14
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD11	2	0.14
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD12	2	0.14
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD13	2	0.14
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG21	13	0.14
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG22	13	0.14
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG23	13	0.14
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG21	13	0.14
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG22	13	0.14
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG23	13	0.14
(2,183)	1:283:A:ALA:O	1:287:A:ASP:H	12	0.13
(2,23)	1:71:A:LYS:H	1:129:A:MET:O	15	0.13
(1,5179)	1:82:A:THR:HB	1:354:A:ILE:H	15	0.13
(1,5179)	1:82:A:THR:HB	1:354:A:ILE:H	19	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD11	7	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD12	7	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD13	7	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD21	7	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD22	7	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD23	7	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD11	15	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD12	15	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD13	15	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD21	15	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD22	15	0.13
(1,5026)	1:91:A:ALA:H	1:108:A:LEU:HD23	15	0.13
(1,4988)	1:87:A:TYR:HD1	1:113:A:TYR:H	11	0.13
(1,4988)	1:87:A:TYR:HD2	1:113:A:TYR:H	11	0.13
(1,4775)	1:73:A:GLU:H	1:126:A:TYR:HE1	9	0.13
(1,4775)	1:73:A:GLU:H	1:126:A:TYR:HE2	9	0.13
(1,4699)	1:70:A:VAL:HG11	1:130:A:ILE:HB	18	0.13
(1,4699)	1:70:A:VAL:HG12	1:130:A:ILE:HB	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4699)	1:70:A:VAL:HG13	1:130:A:ILE:HB	18	0.13
(1,4698)	1:70:A:VAL:HG11	1:130:A:ILE:H	18	0.13
(1,4698)	1:70:A:VAL:HG12	1:130:A:ILE:H	18	0.13
(1,4698)	1:70:A:VAL:HG13	1:130:A:ILE:H	18	0.13
(1,4561)	1:62:A:VAL:HG11	1:65:A:ASP:HB2	13	0.13
(1,4561)	1:62:A:VAL:HG11	1:65:A:ASP:HB3	13	0.13
(1,4561)	1:62:A:VAL:HG12	1:65:A:ASP:HB2	13	0.13
(1,4561)	1:62:A:VAL:HG12	1:65:A:ASP:HB3	13	0.13
(1,4561)	1:62:A:VAL:HG13	1:65:A:ASP:HB2	13	0.13
(1,4561)	1:62:A:VAL:HG13	1:65:A:ASP:HB3	13	0.13
(1,4548)	1:62:A:VAL:HB	1:65:A:ASP:H	20	0.13
(1,4538)	1:60:A:GLU:HG2	1:61:A:SER:H	2	0.13
(1,4538)	1:60:A:GLU:HG3	1:61:A:SER:H	2	0.13
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	11	0.13
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	11	0.13
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	11	0.13
(1,4349)	1:44:A:GLY:HA2	1:51:A:ILE:HD11	8	0.13
(1,4349)	1:44:A:GLY:HA2	1:51:A:ILE:HD12	8	0.13
(1,4349)	1:44:A:GLY:HA2	1:51:A:ILE:HD13	8	0.13
(1,4349)	1:44:A:GLY:HA3	1:51:A:ILE:HD11	8	0.13
(1,4349)	1:44:A:GLY:HA3	1:51:A:ILE:HD12	8	0.13
(1,4349)	1:44:A:GLY:HA3	1:51:A:ILE:HD13	8	0.13
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE1	7	0.13
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE2	7	0.13
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE3	7	0.13
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE1	7	0.13
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE2	7	0.13
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE3	7	0.13
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE1	20	0.13
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE2	20	0.13
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE3	20	0.13
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE1	20	0.13
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE2	20	0.13
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE3	20	0.13
(1,4196)	1:35:A:LYS:HG2	1:37:A:TRP:HE1	18	0.13
(1,4196)	1:35:A:LYS:HG3	1:37:A:TRP:HE1	18	0.13
(1,4047)	1:343:A:VAL:H	1:345:A:GLU:H	11	0.13
(1,4017)	1:340:A:ASP:HB2	1:342:A:SER:H	15	0.13
(1,4017)	1:340:A:ASP:HB3	1:342:A:SER:H	15	0.13
(1,4012)	1:340:A:ASP:H	1:342:A:SER:H	9	0.13
(1,3981)	1:338:A:LYS:HG2	1:339:A:LEU:H	9	0.13
(1,3981)	1:338:A:LYS:HG3	1:339:A:LEU:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	2	0.13
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	2	0.13
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	2	0.13
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	5	0.13
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	5	0.13
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	5	0.13
(1,3180)	1:28:A:ILE:HG12	1:36:A:GLU:H	1	0.13
(1,3180)	1:28:A:ILE:HG13	1:36:A:GLU:H	1	0.13
(1,2718)	1:262:A:GLU:HA	1:266:A:LYS:H	5	0.13
(1,2718)	1:262:A:GLU:HA	1:266:A:LYS:H	7	0.13
(1,2718)	1:262:A:GLU:HA	1:266:A:LYS:H	9	0.13
(1,2461)	1:24:A:ALA:H	1:27:A:GLU:HB2	7	0.13
(1,2461)	1:24:A:ALA:H	1:27:A:GLU:HB3	7	0.13
(1,2292)	1:241:A:ARG:HD2	1:313:A:GLU:H	4	0.13
(1,2292)	1:241:A:ARG:HD3	1:313:A:GLU:H	4	0.13
(1,2084)	1:226:A:GLU:H	1:228:A:THR:HG21	8	0.13
(1,2084)	1:226:A:GLU:H	1:228:A:THR:HG22	8	0.13
(1,2084)	1:226:A:GLU:H	1:228:A:THR:HG23	8	0.13
(1,1991)	1:221:A:HIS:H	1:233:A:HIS:HB2	14	0.13
(1,1991)	1:221:A:HIS:H	1:233:A:HIS:HB3	14	0.13
(1,1984)	1:220:A:CYS:HA	1:235:A:GLY:H	18	0.13
(1,1939)	1:215:A:GLU:HB2	1:216:A:ASP:H	17	0.13
(1,1939)	1:215:A:GLU:HB3	1:216:A:ASP:H	17	0.13
(1,1907)	1:213:A:TYR:HA	1:236:A:VAL:HG21	4	0.13
(1,1907)	1:213:A:TYR:HA	1:236:A:VAL:HG22	4	0.13
(1,1907)	1:213:A:TYR:HA	1:236:A:VAL:HG23	4	0.13
(1,1892)	1:211:A:LYS:HG2	1:237:A:ALA:HB1	17	0.13
(1,1892)	1:211:A:LYS:HG2	1:237:A:ALA:HB2	17	0.13
(1,1892)	1:211:A:LYS:HG2	1:237:A:ALA:HB3	17	0.13
(1,1892)	1:211:A:LYS:HG3	1:237:A:ALA:HB1	17	0.13
(1,1892)	1:211:A:LYS:HG3	1:237:A:ALA:HB2	17	0.13
(1,1892)	1:211:A:LYS:HG3	1:237:A:ALA:HB3	17	0.13
(1,1788)	1:199:A:GLY:H	1:200:A:LEU:HD11	16	0.13
(1,1788)	1:199:A:GLY:H	1:200:A:LEU:HD12	16	0.13
(1,1788)	1:199:A:GLY:H	1:200:A:LEU:HD13	16	0.13
(1,1760)	1:196:A:VAL:HG21	1:197:A:ASP:H	1	0.13
(1,1760)	1:196:A:VAL:HG22	1:197:A:ASP:H	1	0.13
(1,1760)	1:196:A:VAL:HG23	1:197:A:ASP:H	1	0.13
(1,1760)	1:196:A:VAL:HG21	1:197:A:ASP:H	4	0.13
(1,1760)	1:196:A:VAL:HG22	1:197:A:ASP:H	4	0.13
(1,1760)	1:196:A:VAL:HG23	1:197:A:ASP:H	4	0.13
(1,1689)	1:190:A:PRO:HB2	1:340:A:ASP:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1689)	1:190:A:PRO:HB3	1:340:A:ASP:H	8	0.13
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE1	15	0.13
(1,1665)	1:187:A:TYR:H	1:187:A:TYR:HE2	15	0.13
(1,1390)	1:175:A:HIS:HB2	1:178:A:ILE:H	18	0.13
(1,1390)	1:175:A:HIS:HB3	1:178:A:ILE:H	18	0.13
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD11	2	0.13
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD12	2	0.13
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD13	2	0.13
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD21	2	0.13
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD22	2	0.13
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD23	2	0.13
(1,1323)	1:172:A:GLU:HG2	1:208:A:GLY:H	19	0.13
(1,1323)	1:172:A:GLU:HG3	1:208:A:GLY:H	19	0.13
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG11	3	0.13
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG12	3	0.13
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG13	3	0.13
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG11	3	0.13
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG12	3	0.13
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG13	3	0.13
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG11	3	0.13
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG12	3	0.13
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG13	3	0.13
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG21	5	0.13
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG22	5	0.13
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG23	5	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB1	2	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB2	2	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB3	2	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB1	2	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB2	2	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB3	2	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB1	5	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB2	5	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB3	5	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB1	5	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB2	5	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB3	5	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB1	9	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB2	9	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB3	9	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB1	9	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB3	9	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB1	10	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB2	10	0.13
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB3	10	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB1	10	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB2	10	0.13
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB3	10	0.13
(1,703)	1:141:A:ILE:HG12	1:145:A:ASN:H	15	0.13
(1,703)	1:141:A:ILE:HG13	1:145:A:ASN:H	15	0.13
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG21	9	0.13
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG22	9	0.13
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG23	9	0.13
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG21	9	0.13
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG22	9	0.13
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG23	9	0.13
(2,181)	1:276:A:ILE:O	1:280:A:GLU:H	11	0.12
(2,139)	1:240:A:ARG:O	1:244:A:LEU:H	5	0.12
(2,139)	1:240:A:ARG:O	1:244:A:LEU:H	8	0.12
(2,85)	1:82:A:THR:O	1:86:A:PHE:H	10	0.12
(2,75)	1:182:A:ASN:O	1:196:A:VAL:H	2	0.12
(2,75)	1:182:A:ASN:O	1:196:A:VAL:H	19	0.12
(1,5184)	1:222:A:ASP:H	1:355:A:THR:H	15	0.12
(1,5181)	1:202:A:TYR:HB2	1:355:A:THR:HB	4	0.12
(1,5181)	1:202:A:TYR:HB3	1:355:A:THR:HB	4	0.12
(1,5179)	1:82:A:THR:HB	1:354:A:ILE:H	14	0.12
(1,4887)	1:81:A:PHE:HA	1:129:A:MET:HE1	1	0.12
(1,4887)	1:81:A:PHE:HA	1:129:A:MET:HE2	1	0.12
(1,4887)	1:81:A:PHE:HA	1:129:A:MET:HE3	1	0.12
(1,4588)	1:65:A:ASP:HB2	1:68:A:CYS:H	12	0.12
(1,4588)	1:65:A:ASP:HB3	1:68:A:CYS:H	12	0.12
(1,4558)	1:62:A:VAL:HG11	1:64:A:SER:HA	8	0.12
(1,4558)	1:62:A:VAL:HG12	1:64:A:SER:HA	8	0.12
(1,4558)	1:62:A:VAL:HG13	1:64:A:SER:HA	8	0.12
(1,4558)	1:62:A:VAL:HG11	1:64:A:SER:HA	11	0.12
(1,4558)	1:62:A:VAL:HG12	1:64:A:SER:HA	11	0.12
(1,4558)	1:62:A:VAL:HG13	1:64:A:SER:HA	11	0.12
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	1	0.12
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	1	0.12
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	1	0.12
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	17	0.12
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	17	0.12
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4387)	1:48:A:PHE:HD1	1:198:A:TYR:H	14	0.12
(1,4387)	1:48:A:PHE:HD2	1:198:A:TYR:H	14	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG11	1	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG12	1	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG13	1	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG21	1	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG22	1	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG23	1	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG11	6	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG12	6	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG13	6	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG21	6	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG22	6	0.12
(1,4363)	1:46:A:GLY:H	1:196:A:VAL:HG23	6	0.12
(1,4351)	1:45:A:GLN:H	1:51:A:ILE:HA	2	0.12
(1,4227)	1:38:A:LYS:H	1:57:A:ASN:HB2	8	0.12
(1,4227)	1:38:A:LYS:H	1:57:A:ASN:HB3	8	0.12
(1,3961)	1:336:A:ASP:H	1:339:A:LEU:HD11	6	0.12
(1,3961)	1:336:A:ASP:H	1:339:A:LEU:HD12	6	0.12
(1,3961)	1:336:A:ASP:H	1:339:A:LEU:HD13	6	0.12
(1,3961)	1:336:A:ASP:H	1:339:A:LEU:HD21	6	0.12
(1,3961)	1:336:A:ASP:H	1:339:A:LEU:HD22	6	0.12
(1,3961)	1:336:A:ASP:H	1:339:A:LEU:HD23	6	0.12
(1,3958)	1:335:A:ASP:HB2	1:338:A:LYS:H	5	0.12
(1,3958)	1:335:A:ASP:HB3	1:338:A:LYS:H	5	0.12
(1,3953)	1:335:A:ASP:HA	1:337:A:GLY:H	17	0.12
(1,3950)	1:335:A:ASP:H	1:336:A:ASP:H	3	0.12
(1,3775)	1:323:A:ILE:HD11	1:325:A:LEU:H	16	0.12
(1,3775)	1:323:A:ILE:HD12	1:325:A:LEU:H	16	0.12
(1,3775)	1:323:A:ILE:HD13	1:325:A:LEU:H	16	0.12
(1,3581)	1:310:A:ASP:HA	1:313:A:GLU:H	4	0.12
(1,3535)	1:309:A:LEU:HD11	1:313:A:GLU:H	14	0.12
(1,3535)	1:309:A:LEU:HD12	1:313:A:GLU:H	14	0.12
(1,3535)	1:309:A:LEU:HD13	1:313:A:GLU:H	14	0.12
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	19	0.12
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	19	0.12
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	19	0.12
(1,3180)	1:28:A:ILE:HG12	1:36:A:GLU:H	5	0.12
(1,3180)	1:28:A:ILE:HG13	1:36:A:GLU:H	5	0.12
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD11	12	0.12
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD12	12	0.12
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD13	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD21	12	0.12
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD22	12	0.12
(1,3072)	1:283:A:ALA:HA	1:285:A:LEU:HD23	12	0.12
(1,2817)	1:26:A:GLY:HA2	1:40:A:GLY:H	16	0.12
(1,2817)	1:26:A:GLY:HA3	1:40:A:GLY:H	16	0.12
(1,2718)	1:262:A:GLU:HA	1:266:A:LYS:H	11	0.12
(1,2718)	1:262:A:GLU:HA	1:266:A:LYS:H	12	0.12
(1,2718)	1:262:A:GLU:HA	1:266:A:LYS:H	17	0.12
(1,2610)	1:256:A:THR:H	1:290:A:PHE:HD1	10	0.12
(1,2610)	1:256:A:THR:H	1:290:A:PHE:HD2	10	0.12
(1,2349)	1:244:A:LEU:HD11	1:317:A:TYR:HE1	20	0.12
(1,2349)	1:244:A:LEU:HD11	1:317:A:TYR:HE2	20	0.12
(1,2349)	1:244:A:LEU:HD12	1:317:A:TYR:HE1	20	0.12
(1,2349)	1:244:A:LEU:HD12	1:317:A:TYR:HE2	20	0.12
(1,2349)	1:244:A:LEU:HD13	1:317:A:TYR:HE1	20	0.12
(1,2349)	1:244:A:LEU:HD13	1:317:A:TYR:HE2	20	0.12
(1,2343)	1:244:A:LEU:HD11	1:315:A:PRO:HD2	12	0.12
(1,2343)	1:244:A:LEU:HD11	1:315:A:PRO:HD3	12	0.12
(1,2343)	1:244:A:LEU:HD12	1:315:A:PRO:HD2	12	0.12
(1,2343)	1:244:A:LEU:HD12	1:315:A:PRO:HD3	12	0.12
(1,2343)	1:244:A:LEU:HD13	1:315:A:PRO:HD2	12	0.12
(1,2343)	1:244:A:LEU:HD13	1:315:A:PRO:HD3	12	0.12
(1,2292)	1:241:A:ARG:HD2	1:313:A:GLU:H	13	0.12
(1,2292)	1:241:A:ARG:HD3	1:313:A:GLU:H	13	0.12
(1,2289)	1:241:A:ARG:HG2	1:313:A:GLU:H	14	0.12
(1,2289)	1:241:A:ARG:HG3	1:313:A:GLU:H	14	0.12
(1,2071)	1:225:A:ILE:HG21	1:265:A:LEU:H	3	0.12
(1,2071)	1:225:A:ILE:HG22	1:265:A:LEU:H	3	0.12
(1,2071)	1:225:A:ILE:HG23	1:265:A:LEU:H	3	0.12
(1,2009)	1:222:A:ASP:H	1:235:A:GLY:HA2	20	0.12
(1,2009)	1:222:A:ASP:H	1:235:A:GLY:HA3	20	0.12
(1,1991)	1:221:A:HIS:H	1:233:A:HIS:HB2	9	0.12
(1,1991)	1:221:A:HIS:H	1:233:A:HIS:HB3	9	0.12
(1,1984)	1:220:A:CYS:HA	1:235:A:GLY:H	12	0.12
(1,1754)	1:196:A:VAL:HB	1:198:A:TYR:H	18	0.12
(1,1578)	1:184:A:LEU:HD21	1:196:A:VAL:HG21	2	0.12
(1,1578)	1:184:A:LEU:HD21	1:196:A:VAL:HG22	2	0.12
(1,1578)	1:184:A:LEU:HD21	1:196:A:VAL:HG23	2	0.12
(1,1578)	1:184:A:LEU:HD22	1:196:A:VAL:HG21	2	0.12
(1,1578)	1:184:A:LEU:HD22	1:196:A:VAL:HG22	2	0.12
(1,1578)	1:184:A:LEU:HD22	1:196:A:VAL:HG23	2	0.12
(1,1578)	1:184:A:LEU:HD23	1:196:A:VAL:HG21	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1578)	1:184:A:LEU:HD23	1:196:A:VAL:HG22	2	0.12
(1,1578)	1:184:A:LEU:HD23	1:196:A:VAL:HG23	2	0.12
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD11	19	0.12
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD12	19	0.12
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD13	19	0.12
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD21	19	0.12
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD22	19	0.12
(1,1572)	1:184:A:LEU:HD11	1:195:A:LEU:HD23	19	0.12
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD11	19	0.12
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD12	19	0.12
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD13	19	0.12
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD21	19	0.12
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD22	19	0.12
(1,1572)	1:184:A:LEU:HD12	1:195:A:LEU:HD23	19	0.12
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD11	19	0.12
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD12	19	0.12
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD13	19	0.12
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD21	19	0.12
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD22	19	0.12
(1,1572)	1:184:A:LEU:HD13	1:195:A:LEU:HD23	19	0.12
(1,1446)	1:178:A:ILE:HD11	1:254:A:TRP:HZ2	1	0.12
(1,1446)	1:178:A:ILE:HD12	1:254:A:TRP:HZ2	1	0.12
(1,1446)	1:178:A:ILE:HD13	1:254:A:TRP:HZ2	1	0.12
(1,1393)	1:175:A:HIS:HB2	1:201:A:ALA:H	16	0.12
(1,1393)	1:175:A:HIS:HB3	1:201:A:ALA:H	16	0.12
(1,1372)	1:174:A:VAL:HG11	1:238:A:PRO:HA	9	0.12
(1,1372)	1:174:A:VAL:HG12	1:238:A:PRO:HA	9	0.12
(1,1372)	1:174:A:VAL:HG13	1:238:A:PRO:HA	9	0.12
(1,1372)	1:174:A:VAL:HG21	1:238:A:PRO:HA	9	0.12
(1,1372)	1:174:A:VAL:HG22	1:238:A:PRO:HA	9	0.12
(1,1372)	1:174:A:VAL:HG23	1:238:A:PRO:HA	9	0.12
(1,1315)	1:172:A:GLU:H	1:173:A:TYR:H	7	0.12
(1,1299)	1:169:A:HIS:HA	1:174:A:VAL:HG11	15	0.12
(1,1299)	1:169:A:HIS:HA	1:174:A:VAL:HG12	15	0.12
(1,1299)	1:169:A:HIS:HA	1:174:A:VAL:HG13	15	0.12
(1,1299)	1:169:A:HIS:HA	1:174:A:VAL:HG21	15	0.12
(1,1299)	1:169:A:HIS:HA	1:174:A:VAL:HG22	15	0.12
(1,1299)	1:169:A:HIS:HA	1:174:A:VAL:HG23	15	0.12
(1,1290)	1:168:A:ILE:HG21	1:175:A:HIS:HB2	15	0.12
(1,1290)	1:168:A:ILE:HG21	1:175:A:HIS:HB3	15	0.12
(1,1290)	1:168:A:ILE:HG22	1:175:A:HIS:HB2	15	0.12
(1,1290)	1:168:A:ILE:HG22	1:175:A:HIS:HB3	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1290)	1:168:A:ILE:HG23	1:175:A:HIS:HB2	15	0.12
(1,1290)	1:168:A:ILE:HG23	1:175:A:HIS:HB3	15	0.12
(1,1262)	1:166:A:GLU:H	1:317:A:TYR:HD1	14	0.12
(1,1262)	1:166:A:GLU:H	1:317:A:TYR:HD2	14	0.12
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG11	15	0.12
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG12	15	0.12
(1,900)	1:153:A:THR:HG21	1:154:A:VAL:HG13	15	0.12
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG11	15	0.12
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG12	15	0.12
(1,900)	1:153:A:THR:HG22	1:154:A:VAL:HG13	15	0.12
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG11	15	0.12
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG12	15	0.12
(1,900)	1:153:A:THR:HG23	1:154:A:VAL:HG13	15	0.12
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG21	2	0.12
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG22	2	0.12
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG23	2	0.12
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG21	9	0.12
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG22	9	0.12
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG23	9	0.12
(1,870)	1:151:A:ARG:HD2	1:295:A:LYS:H	4	0.12
(1,870)	1:151:A:ARG:HD3	1:295:A:LYS:H	4	0.12
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB1	11	0.12
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB2	11	0.12
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB3	11	0.12
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB1	11	0.12
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB2	11	0.12
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB3	11	0.12
(1,232)	1:114:A:TRP:HB2	1:130:A:ILE:HG21	10	0.12
(1,232)	1:114:A:TRP:HB2	1:130:A:ILE:HG22	10	0.12
(1,232)	1:114:A:TRP:HB2	1:130:A:ILE:HG23	10	0.12
(1,232)	1:114:A:TRP:HB3	1:130:A:ILE:HG21	10	0.12
(1,232)	1:114:A:TRP:HB3	1:130:A:ILE:HG22	10	0.12
(1,232)	1:114:A:TRP:HB3	1:130:A:ILE:HG23	10	0.12
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD11	1	0.12
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD12	1	0.12
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD13	1	0.12
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG21	16	0.12
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG22	16	0.12
(1,214)	1:113:A:TYR:HE1	1:130:A:ILE:HG23	16	0.12
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG21	16	0.12
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG22	16	0.12
(1,214)	1:113:A:TYR:HE2	1:130:A:ILE:HG23	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,199)	1:112:A:LYS:HE2	1:114:A:TRP:H	2	0.12
(1,199)	1:112:A:LYS:HE3	1:114:A:TRP:H	2	0.12
(1,46)	1:100:A:ILE:HG21	1:108:A:LEU:HD21	3	0.12
(1,46)	1:100:A:ILE:HG21	1:108:A:LEU:HD22	3	0.12
(1,46)	1:100:A:ILE:HG21	1:108:A:LEU:HD23	3	0.12
(1,46)	1:100:A:ILE:HG22	1:108:A:LEU:HD21	3	0.12
(1,46)	1:100:A:ILE:HG22	1:108:A:LEU:HD22	3	0.12
(1,46)	1:100:A:ILE:HG22	1:108:A:LEU:HD23	3	0.12
(1,46)	1:100:A:ILE:HG23	1:108:A:LEU:HD21	3	0.12
(1,46)	1:100:A:ILE:HG23	1:108:A:LEU:HD22	3	0.12
(1,46)	1:100:A:ILE:HG23	1:108:A:LEU:HD23	3	0.12
(2,201)	1:304:A:GLU:O	1:308:A:LEU:H	17	0.11
(2,171)	1:271:A:VAL:O	1:275:A:LYS:H	15	0.11
(2,161)	1:251:A:MET:O	1:255:A:LEU:H	8	0.11
(2,161)	1:251:A:MET:O	1:255:A:LEU:H	20	0.11
(2,151)	1:246:A:ILE:O	1:250:A:CYS:H	20	0.11
(2,117)	1:160:A:ARG:O	1:164:A:ILE:H	18	0.11
(2,111)	1:163:A:ASP:O	1:167:A:TYR:H	11	0.11
(2,105)	1:166:A:GLU:O	1:170:A:GLU:H	17	0.11
(2,85)	1:82:A:THR:O	1:86:A:PHE:H	3	0.11
(2,63)	1:71:A:LYS:O	1:129:A:MET:H	15	0.11
(2,17)	1:54:A:ALA:H	1:68:A:CYS:O	19	0.11
(2,13)	1:52:A:TYR:H	1:70:A:VAL:O	18	0.11
(1,5045)	1:92:A:LYS:H	1:112:A:LYS:HA	7	0.11
(1,4804)	1:75:A:SER:H	1:127:A:ARG:HB2	18	0.11
(1,4804)	1:75:A:SER:H	1:127:A:ARG:HB3	18	0.11
(1,4698)	1:70:A:VAL:HG11	1:130:A:ILE:H	8	0.11
(1,4698)	1:70:A:VAL:HG12	1:130:A:ILE:H	8	0.11
(1,4698)	1:70:A:VAL:HG13	1:130:A:ILE:H	8	0.11
(1,4692)	1:70:A:VAL:HB	1:130:A:ILE:HD11	1	0.11
(1,4692)	1:70:A:VAL:HB	1:130:A:ILE:HD12	1	0.11
(1,4692)	1:70:A:VAL:HB	1:130:A:ILE:HD13	1	0.11
(1,4588)	1:65:A:ASP:HB2	1:68:A:CYS:H	5	0.11
(1,4588)	1:65:A:ASP:HB3	1:68:A:CYS:H	5	0.11
(1,4571)	1:63:A:GLY:H	1:66:A:ALA:HB1	20	0.11
(1,4571)	1:63:A:GLY:H	1:66:A:ALA:HB2	20	0.11
(1,4571)	1:63:A:GLY:H	1:66:A:ALA:HB3	20	0.11
(1,4539)	1:61:A:SER:H	1:62:A:VAL:H	12	0.11
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	7	0.11
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	7	0.11
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	7	0.11
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	14	0.11
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	14	0.11
(1,4387)	1:48:A:PHE:HD1	1:198:A:TYR:H	16	0.11
(1,4387)	1:48:A:PHE:HD2	1:198:A:TYR:H	16	0.11
(1,4357)	1:45:A:GLN:HA	1:50:A:CYS:H	6	0.11
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE1	6	0.11
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE2	6	0.11
(1,4236)	1:38:A:LYS:HG2	1:56:A:MET:HE3	6	0.11
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE1	6	0.11
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE2	6	0.11
(1,4236)	1:38:A:LYS:HG3	1:56:A:MET:HE3	6	0.11
(1,4075)	1:344:A:VAL:HG11	1:345:A:GLU:H	18	0.11
(1,4075)	1:344:A:VAL:HG12	1:345:A:GLU:H	18	0.11
(1,4075)	1:344:A:VAL:HG13	1:345:A:GLU:H	18	0.11
(1,4047)	1:343:A:VAL:H	1:345:A:GLU:H	6	0.11
(1,4046)	1:343:A:VAL:H	1:344:A:VAL:H	15	0.11
(1,3837)	1:326:A:GLN:HE21	1:328:A:LEU:H	6	0.11
(1,3837)	1:326:A:GLN:HE22	1:328:A:LEU:H	6	0.11
(1,3605)	1:313:A:GLU:HB2	1:314:A:LYS:H	20	0.11
(1,3605)	1:313:A:GLU:HB3	1:314:A:LYS:H	20	0.11
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	6	0.11
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	6	0.11
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	6	0.11
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG21	14	0.11
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG22	14	0.11
(1,3423)	1:303:A:MET:H	1:305:A:THR:HG23	14	0.11
(1,3385)	1:302:A:TYR:H	1:323:A:ILE:HB	19	0.11
(1,3382)	1:302:A:TYR:H	1:305:A:THR:HG21	9	0.11
(1,3382)	1:302:A:TYR:H	1:305:A:THR:HG22	9	0.11
(1,3382)	1:302:A:TYR:H	1:305:A:THR:HG23	9	0.11
(1,3234)	1:294:A:ASN:HB3	1:295:A:LYS:H	15	0.11
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB2	7	0.11
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB3	7	0.11
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB2	8	0.11
(1,3212)	1:292:A:GLU:H	1:293:A:LYS:HB3	8	0.11
(1,3063)	1:282:A:ILE:HG21	1:304:A:GLU:HG2	14	0.11
(1,3063)	1:282:A:ILE:HG21	1:304:A:GLU:HG3	14	0.11
(1,3063)	1:282:A:ILE:HG22	1:304:A:GLU:HG2	14	0.11
(1,3063)	1:282:A:ILE:HG22	1:304:A:GLU:HG3	14	0.11
(1,3063)	1:282:A:ILE:HG23	1:304:A:GLU:HG2	14	0.11
(1,3063)	1:282:A:ILE:HG23	1:304:A:GLU:HG3	14	0.11
(1,2854)	1:271:A:VAL:HG11	1:275:A:LYS:HG2	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2854)	1:271:A:VAL:HG11	1:275:A:LYS:HG3	16	0.11
(1,2854)	1:271:A:VAL:HG12	1:275:A:LYS:HG2	16	0.11
(1,2854)	1:271:A:VAL:HG12	1:275:A:LYS:HG3	16	0.11
(1,2854)	1:271:A:VAL:HG13	1:275:A:LYS:HG2	16	0.11
(1,2854)	1:271:A:VAL:HG13	1:275:A:LYS:HG3	16	0.11
(1,2755)	1:265:A:LEU:HD11	1:271:A:VAL:H	6	0.11
(1,2755)	1:265:A:LEU:HD12	1:271:A:VAL:H	6	0.11
(1,2755)	1:265:A:LEU:HD13	1:271:A:VAL:H	6	0.11
(1,2755)	1:265:A:LEU:HD21	1:271:A:VAL:H	6	0.11
(1,2755)	1:265:A:LEU:HD22	1:271:A:VAL:H	6	0.11
(1,2755)	1:265:A:LEU:HD23	1:271:A:VAL:H	6	0.11
(1,2413)	1:247:A:LEU:HD21	1:324:A:LEU:HD21	13	0.11
(1,2413)	1:247:A:LEU:HD21	1:324:A:LEU:HD22	13	0.11
(1,2413)	1:247:A:LEU:HD21	1:324:A:LEU:HD23	13	0.11
(1,2413)	1:247:A:LEU:HD22	1:324:A:LEU:HD21	13	0.11
(1,2413)	1:247:A:LEU:HD22	1:324:A:LEU:HD22	13	0.11
(1,2413)	1:247:A:LEU:HD22	1:324:A:LEU:HD23	13	0.11
(1,2413)	1:247:A:LEU:HD23	1:324:A:LEU:HD21	13	0.11
(1,2413)	1:247:A:LEU:HD23	1:324:A:LEU:HD22	13	0.11
(1,2413)	1:247:A:LEU:HD23	1:324:A:LEU:HD23	13	0.11
(1,2270)	1:240:A:ARG:HB2	1:241:A:ARG:H	17	0.11
(1,2270)	1:240:A:ARG:HB3	1:241:A:ARG:H	17	0.11
(1,2161)	1:230:A:ILE:H	1:230:A:ILE:HD11	19	0.11
(1,2161)	1:230:A:ILE:H	1:230:A:ILE:HD12	19	0.11
(1,2161)	1:230:A:ILE:H	1:230:A:ILE:HD13	19	0.11
(1,2153)	1:230:A:ILE:H	1:245:A:GLU:HG2	11	0.11
(1,2153)	1:230:A:ILE:H	1:245:A:GLU:HG3	11	0.11
(1,2084)	1:226:A:GLU:H	1:228:A:THR:HG21	14	0.11
(1,2084)	1:226:A:GLU:H	1:228:A:THR:HG22	14	0.11
(1,2084)	1:226:A:GLU:H	1:228:A:THR:HG23	14	0.11
(1,2006)	1:222:A:ASP:H	1:232:A:ALA:HA	19	0.11
(1,1991)	1:221:A:HIS:H	1:233:A:HIS:HB2	15	0.11
(1,1991)	1:221:A:HIS:H	1:233:A:HIS:HB3	15	0.11
(1,1988)	1:221:A:HIS:H	1:232:A:ALA:HA	19	0.11
(1,1942)	1:215:A:GLU:HG2	1:236:A:VAL:H	11	0.11
(1,1942)	1:215:A:GLU:HG3	1:236:A:VAL:H	11	0.11
(1,1912)	1:213:A:TYR:HB2	1:215:A:GLU:H	11	0.11
(1,1912)	1:213:A:TYR:HB3	1:215:A:GLU:H	11	0.11
(1,1846)	1:205:A:CYS:HA	1:209:A:VAL:H	15	0.11
(1,1754)	1:196:A:VAL:HB	1:198:A:TYR:H	4	0.11
(1,1689)	1:190:A:PRO:HB2	1:340:A:ASP:H	7	0.11
(1,1689)	1:190:A:PRO:HB3	1:340:A:ASP:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1677)	1:189:A:ASN:H	1:194:A:TYR:HE1	19	0.11
(1,1677)	1:189:A:ASN:H	1:194:A:TYR:HE2	19	0.11
(1,1482)	1:179:A:LYS:HD2	1:182:A:ASN:H	17	0.11
(1,1482)	1:179:A:LYS:HD3	1:182:A:ASN:H	17	0.11
(1,1466)	1:179:A:LYS:H	1:195:A:LEU:HD11	6	0.11
(1,1466)	1:179:A:LYS:H	1:195:A:LEU:HD12	6	0.11
(1,1466)	1:179:A:LYS:H	1:195:A:LEU:HD13	6	0.11
(1,1466)	1:179:A:LYS:H	1:195:A:LEU:HD21	6	0.11
(1,1466)	1:179:A:LYS:H	1:195:A:LEU:HD22	6	0.11
(1,1466)	1:179:A:LYS:H	1:195:A:LEU:HD23	6	0.11
(1,1395)	1:176:A:GLY:H	1:200:A:LEU:HD11	5	0.11
(1,1395)	1:176:A:GLY:H	1:200:A:LEU:HD12	5	0.11
(1,1395)	1:176:A:GLY:H	1:200:A:LEU:HD13	5	0.11
(1,1395)	1:176:A:GLY:H	1:200:A:LEU:HD21	5	0.11
(1,1395)	1:176:A:GLY:H	1:200:A:LEU:HD22	5	0.11
(1,1395)	1:176:A:GLY:H	1:200:A:LEU:HD23	5	0.11
(1,1393)	1:175:A:HIS:HB2	1:201:A:ALA:H	12	0.11
(1,1393)	1:175:A:HIS:HB3	1:201:A:ALA:H	12	0.11
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD11	1	0.11
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD12	1	0.11
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD13	1	0.11
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD21	1	0.11
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD22	1	0.11
(1,1380)	1:175:A:HIS:H	1:195:A:LEU:HD23	1	0.11
(1,1292)	1:168:A:ILE:HG21	1:198:A:TYR:HE1	7	0.11
(1,1292)	1:168:A:ILE:HG21	1:198:A:TYR:HE2	7	0.11
(1,1292)	1:168:A:ILE:HG22	1:198:A:TYR:HE1	7	0.11
(1,1292)	1:168:A:ILE:HG22	1:198:A:TYR:HE2	7	0.11
(1,1292)	1:168:A:ILE:HG23	1:198:A:TYR:HE1	7	0.11
(1,1292)	1:168:A:ILE:HG23	1:198:A:TYR:HE2	7	0.11
(1,1272)	1:167:A:TYR:HE1	1:168:A:ILE:HD11	10	0.11
(1,1272)	1:167:A:TYR:HE1	1:168:A:ILE:HD12	10	0.11
(1,1272)	1:167:A:TYR:HE1	1:168:A:ILE:HD13	10	0.11
(1,1272)	1:167:A:TYR:HE2	1:168:A:ILE:HD11	10	0.11
(1,1272)	1:167:A:TYR:HE2	1:168:A:ILE:HD12	10	0.11
(1,1272)	1:167:A:TYR:HE2	1:168:A:ILE:HD13	10	0.11
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB1	3	0.11
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB2	3	0.11
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB3	3	0.11
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB1	3	0.11
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB2	3	0.11
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB1	6	0.11
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB2	6	0.11
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB3	6	0.11
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB1	6	0.11
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB2	6	0.11
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB3	6	0.11
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB1	17	0.11
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB2	17	0.11
(1,738)	1:142:A:TYR:HE1	1:146:A:ALA:HB3	17	0.11
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB1	17	0.11
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB2	17	0.11
(1,738)	1:142:A:TYR:HE2	1:146:A:ALA:HB3	17	0.11
(1,715)	1:141:A:ILE:HG21	1:185:A:LEU:HD21	12	0.11
(1,715)	1:141:A:ILE:HG21	1:185:A:LEU:HD22	12	0.11
(1,715)	1:141:A:ILE:HG21	1:185:A:LEU:HD23	12	0.11
(1,715)	1:141:A:ILE:HG22	1:185:A:LEU:HD21	12	0.11
(1,715)	1:141:A:ILE:HG22	1:185:A:LEU:HD22	12	0.11
(1,715)	1:141:A:ILE:HG22	1:185:A:LEU:HD23	12	0.11
(1,715)	1:141:A:ILE:HG23	1:185:A:LEU:HD21	12	0.11
(1,715)	1:141:A:ILE:HG23	1:185:A:LEU:HD22	12	0.11
(1,715)	1:141:A:ILE:HG23	1:185:A:LEU:HD23	12	0.11
(1,571)	1:138:A:LEU:HB2	1:254:A:TRP:HE1	18	0.11
(1,571)	1:138:A:LEU:HB3	1:254:A:TRP:HE1	18	0.11
(1,503)	1:136:A:SER:HB2	1:187:A:TYR:H	20	0.11
(1,503)	1:136:A:SER:HB3	1:187:A:TYR:H	20	0.11
(1,358)	1:124:A:LYS:H	1:126:A:TYR:HE1	6	0.11
(1,358)	1:124:A:LYS:H	1:126:A:TYR:HE2	6	0.11
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG21	12	0.11
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG22	12	0.11
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG23	12	0.11
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD11	4	0.11
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD12	4	0.11
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD13	4	0.11
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD11	11	0.11
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD12	11	0.11
(1,223)	1:114:A:TRP:HE1	1:130:A:ILE:HD13	11	0.11
(2,117)	1:160:A:ARG:O	1:164:A:ILE:H	3	0.1
(2,111)	1:163:A:ASP:O	1:167:A:TYR:H	1	0.1
(2,111)	1:163:A:ASP:O	1:167:A:TYR:H	20	0.1
(2,105)	1:166:A:GLU:O	1:170:A:GLU:H	11	0.1
(2,17)	1:54:A:ALA:H	1:68:A:CYS:O	15	0.1
(1,4698)	1:70:A:VAL:HG11	1:130:A:ILE:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4698)	1:70:A:VAL:HG12	1:130:A:ILE:H	9	0.1
(1,4698)	1:70:A:VAL:HG13	1:130:A:ILE:H	9	0.1
(1,4692)	1:70:A:VAL:HB	1:130:A:ILE:HD11	18	0.1
(1,4692)	1:70:A:VAL:HB	1:130:A:ILE:HD12	18	0.1
(1,4692)	1:70:A:VAL:HB	1:130:A:ILE:HD13	18	0.1
(1,4576)	1:64:A:SER:H	1:66:A:ALA:H	19	0.1
(1,4559)	1:62:A:VAL:HG11	1:64:A:SER:HB2	6	0.1
(1,4559)	1:62:A:VAL:HG11	1:64:A:SER:HB3	6	0.1
(1,4559)	1:62:A:VAL:HG12	1:64:A:SER:HB2	6	0.1
(1,4559)	1:62:A:VAL:HG12	1:64:A:SER:HB3	6	0.1
(1,4559)	1:62:A:VAL:HG13	1:64:A:SER:HB2	6	0.1
(1,4559)	1:62:A:VAL:HG13	1:64:A:SER:HB3	6	0.1
(1,4423)	1:51:A:ILE:HG21	1:72:A:VAL:HA	18	0.1
(1,4423)	1:51:A:ILE:HG22	1:72:A:VAL:HA	18	0.1
(1,4423)	1:51:A:ILE:HG23	1:72:A:VAL:HA	18	0.1
(1,4387)	1:48:A:PHE:HD1	1:198:A:TYR:H	10	0.1
(1,4387)	1:48:A:PHE:HD2	1:198:A:TYR:H	10	0.1
(1,4387)	1:48:A:PHE:HD1	1:198:A:TYR:H	17	0.1
(1,4387)	1:48:A:PHE:HD2	1:198:A:TYR:H	17	0.1
(1,4387)	1:48:A:PHE:HD1	1:198:A:TYR:H	18	0.1
(1,4387)	1:48:A:PHE:HD2	1:198:A:TYR:H	18	0.1
(1,4240)	1:39:A:VAL:HA	1:56:A:MET:H	15	0.1
(1,4151)	1:354:A:ILE:H	1:354:A:ILE:HD11	8	0.1
(1,4151)	1:354:A:ILE:H	1:354:A:ILE:HD12	8	0.1
(1,4151)	1:354:A:ILE:H	1:354:A:ILE:HD13	8	0.1
(1,4033)	1:342:A:SER:H	1:343:A:VAL:HG11	7	0.1
(1,4033)	1:342:A:SER:H	1:343:A:VAL:HG12	7	0.1
(1,4033)	1:342:A:SER:H	1:343:A:VAL:HG13	7	0.1
(1,4031)	1:341:A:LEU:HD21	1:344:A:VAL:H	15	0.1
(1,4031)	1:341:A:LEU:HD22	1:344:A:VAL:H	15	0.1
(1,4031)	1:341:A:LEU:HD23	1:344:A:VAL:H	15	0.1
(1,4018)	1:341:A:LEU:H	1:342:A:SER:H	10	0.1
(1,3581)	1:310:A:ASP:HA	1:313:A:GLU:H	19	0.1
(1,3382)	1:302:A:TYR:H	1:305:A:THR:HG21	6	0.1
(1,3382)	1:302:A:TYR:H	1:305:A:THR:HG22	6	0.1
(1,3382)	1:302:A:TYR:H	1:305:A:THR:HG23	6	0.1
(1,3220)	1:292:A:GLU:HG2	1:294:A:ASN:H	12	0.1
(1,3220)	1:292:A:GLU:HG3	1:294:A:ASN:H	12	0.1
(1,3185)	1:28:A:ILE:HG21	1:36:A:GLU:H	14	0.1
(1,3185)	1:28:A:ILE:HG22	1:36:A:GLU:H	14	0.1
(1,3185)	1:28:A:ILE:HG23	1:36:A:GLU:H	14	0.1
(1,3185)	1:28:A:ILE:HG21	1:36:A:GLU:H	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3185)	1:28:A:ILE:HG22	1:36:A:GLU:H	15	0.1
(1,3185)	1:28:A:ILE:HG23	1:36:A:GLU:H	15	0.1
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG21	15	0.1
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG22	15	0.1
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG23	15	0.1
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG21	15	0.1
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG22	15	0.1
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG23	15	0.1
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG21	17	0.1
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG22	17	0.1
(1,2985)	1:27:A:GLU:HG2	1:28:A:ILE:HG23	17	0.1
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG21	17	0.1
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG22	17	0.1
(1,2985)	1:27:A:GLU:HG3	1:28:A:ILE:HG23	17	0.1
(1,2292)	1:241:A:ARG:HD2	1:313:A:GLU:H	17	0.1
(1,2292)	1:241:A:ARG:HD3	1:313:A:GLU:H	17	0.1
(1,2163)	1:230:A:ILE:HD11	1:245:A:GLU:HG2	17	0.1
(1,2163)	1:230:A:ILE:HD11	1:245:A:GLU:HG3	17	0.1
(1,2163)	1:230:A:ILE:HD12	1:245:A:GLU:HG2	17	0.1
(1,2163)	1:230:A:ILE:HD12	1:245:A:GLU:HG3	17	0.1
(1,2163)	1:230:A:ILE:HD13	1:245:A:GLU:HG2	17	0.1
(1,2163)	1:230:A:ILE:HD13	1:245:A:GLU:HG3	17	0.1
(1,1907)	1:213:A:TYR:HA	1:236:A:VAL:HG21	5	0.1
(1,1907)	1:213:A:TYR:HA	1:236:A:VAL:HG22	5	0.1
(1,1907)	1:213:A:TYR:HA	1:236:A:VAL:HG23	5	0.1
(1,1587)	1:185:A:LEU:H	1:193:A:VAL:HG21	15	0.1
(1,1587)	1:185:A:LEU:H	1:193:A:VAL:HG22	15	0.1
(1,1587)	1:185:A:LEU:H	1:193:A:VAL:HG23	15	0.1
(1,1526)	1:183:A:LEU:HA	1:196:A:VAL:HG11	16	0.1
(1,1526)	1:183:A:LEU:HA	1:196:A:VAL:HG12	16	0.1
(1,1526)	1:183:A:LEU:HA	1:196:A:VAL:HG13	16	0.1
(1,1446)	1:178:A:ILE:HD11	1:254:A:TRP:HZ2	18	0.1
(1,1446)	1:178:A:ILE:HD12	1:254:A:TRP:HZ2	18	0.1
(1,1446)	1:178:A:ILE:HD13	1:254:A:TRP:HZ2	18	0.1
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG21	6	0.1
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG22	6	0.1
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG23	6	0.1
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG21	10	0.1
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG22	10	0.1
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG23	10	0.1
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG21	16	0.1
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG22	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG23	16	0.1
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG21	17	0.1
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG22	17	0.1
(1,878)	1:152:A:LYS:HA	1:153:A:THR:HG23	17	0.1
(1,525)	1:137:A:ASP:HB3	1:184:A:LEU:HD11	19	0.1
(1,525)	1:137:A:ASP:HB3	1:184:A:LEU:HD12	19	0.1
(1,525)	1:137:A:ASP:HB3	1:184:A:LEU:HD13	19	0.1
(1,367)	1:124:A:LYS:HG2	1:125:A:SER:H	16	0.1
(1,367)	1:124:A:LYS:HG3	1:125:A:SER:H	16	0.1
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG21	7	0.1
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG22	7	0.1
(1,253)	1:116:A:SER:H	1:130:A:ILE:HG23	7	0.1

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

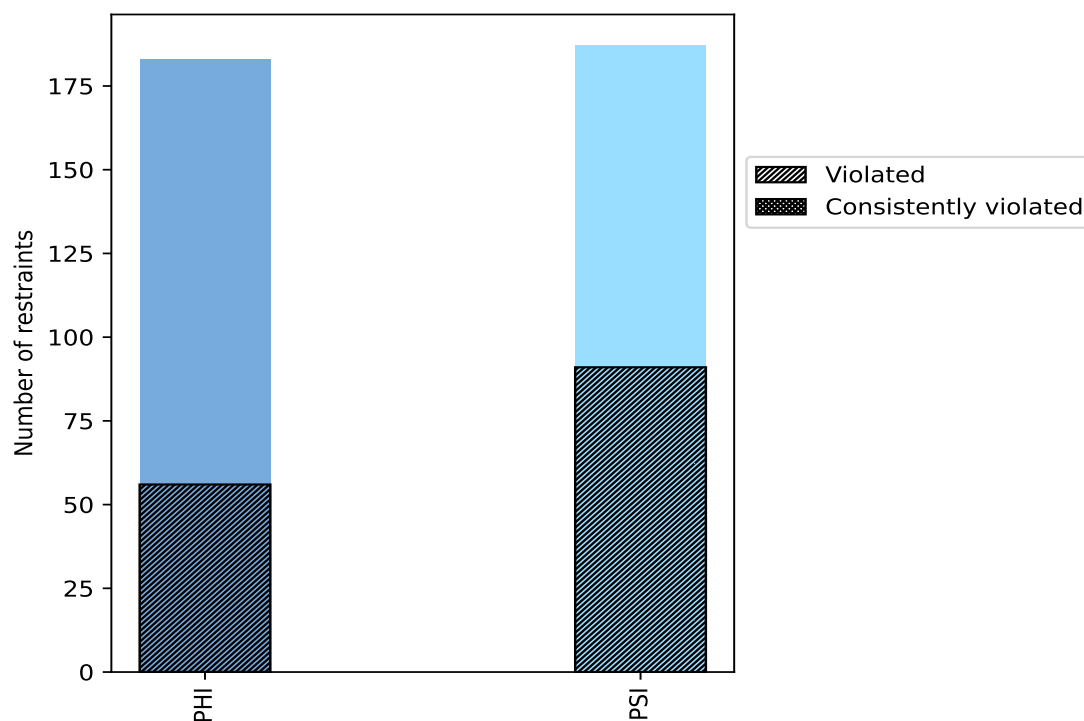
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	183	49.5	56	30.6	15.1	0	0.0	0.0
PSI	187	50.5	91	48.7	24.6	0	0.0	0.0
Total	370	100.0	147	39.7	39.7	0	0.0	0.0

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

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



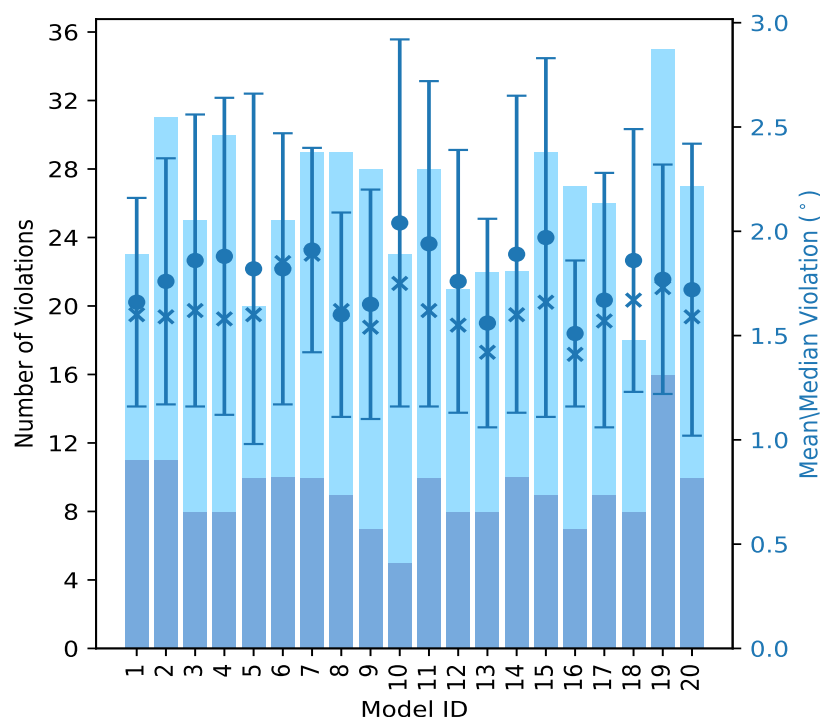
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	11	12	23	1.66	2.77	0.5	1.6
2	11	20	31	1.76	3.07	0.59	1.59
3	8	17	25	1.86	3.56	0.7	1.62
4	8	22	30	1.88	3.85	0.76	1.58
5	10	10	20	1.82	4.69	0.84	1.6
6	10	15	25	1.82	3.71	0.65	1.85
7	10	19	29	1.91	3.02	0.49	1.89
8	9	20	29	1.6	2.77	0.49	1.62
9	7	21	28	1.65	3.73	0.55	1.54
10	5	18	23	2.04	4.02	0.88	1.75
11	10	18	28	1.94	3.44	0.78	1.62
12	8	13	21	1.76	3.58	0.63	1.55
13	8	14	22	1.56	2.74	0.5	1.42
14	10	12	22	1.89	3.57	0.76	1.6
15	9	20	29	1.97	4.0	0.86	1.66
16	7	20	27	1.51	2.22	0.35	1.41
17	9	17	26	1.67	3.47	0.61	1.57
18	8	10	18	1.86	3.4	0.63	1.67
19	16	19	35	1.77	3.09	0.55	1.73
20	10	17	27	1.72	4.42	0.7	1.59

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
22	27	49	1	5.0
8	18	26	2	10.0
6	9	15	3	15.0
7	10	17	4	20.0
1	6	7	5	25.0
5	8	13	6	30.0
2	2	4	7	35.0
2	2	4	8	40.0
1	3	4	9	45.0
0	1	1	10	50.0
1	4	5	11	55.0

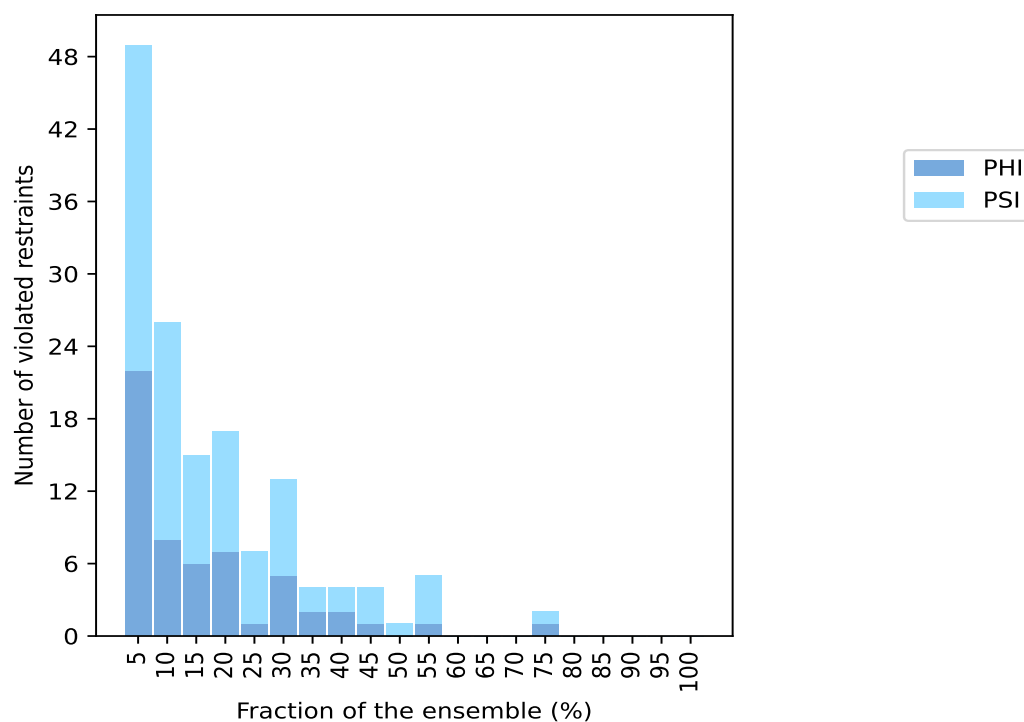
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
1	1	2	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

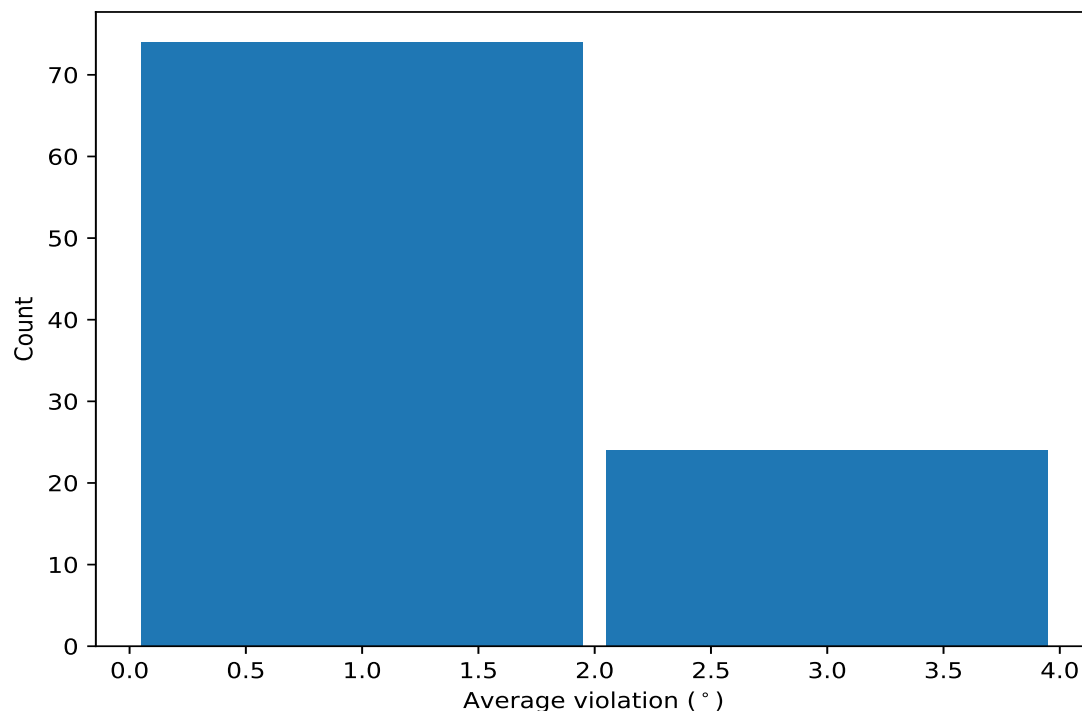


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	15	2.25	0.57	2.22
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	15	1.89	0.57	1.89
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	11	2.28	0.85	2.1
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	11	2.26	0.52	2.19
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	11	2.1	0.58	2.03
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	11	2.03	0.6	2.09
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	11	1.76	0.62	1.78
(1,69)	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	1:100:A:ILE:N	10	1.8	0.86	1.54
(1,35)	1:68:A:CYS:N	1:68:A:CYS:CA	1:68:A:CYS:C	1:69:A:VAL:N	9	2.46	0.78	2.43
(1,265)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:SER:N	9	1.63	0.41	1.58
(1,6)	1:25:A:VAL:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	9	1.61	0.61	1.42
(1,179)	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	1:237:A:ALA:N	9	1.54	0.72	1.09
(1,219)	1:283:A:ALA:N	1:283:A:ALA:CA	1:283:A:ALA:C	1:284:A:SER:N	8	2.35	0.99	1.89
(1,198)	1:255:A:LEU:C	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	8	2.34	0.75	2.3
(1,43)	1:79:A:PRO:N	1:79:A:PRO:CA	1:79:A:PRO:C	1:80:A:LEU:N	8	2.0	0.79	1.75
(1,204)	1:263:A:ASP:C	1:264:A:ASN:N	1:264:A:ASN:CA	1:264:A:ASN:C	8	1.48	0.39	1.41
(1,200)	1:257:A:GLY:C	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	7	2.05	0.64	1.71
(1,164)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:LYS:N	7	1.66	0.37	1.81
(1,24)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	7	1.57	0.39	1.58
(1,106)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ASN:N	7	1.41	0.37	1.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,201)	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	1:259:A:LEU:N	6	2.39	0.84	2.26
(1,108)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:ALA:N	6	2.1	0.94	1.87
(1,139)	1:177:A:ASP:C	1:178:A:ILE:N	1:178:A:ILE:CA	1:178:A:ILE:C	6	2.08	1.2	1.74
(1,97)	1:135:A:GLY:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	6	1.96	0.51	1.77
(1,59)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:ALA:N	6	1.81	0.39	1.76
(1,95)	1:133:A:ARG:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	6	1.72	0.4	1.82
(1,32)	1:61:A:SER:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	6	1.71	0.5	1.52
(1,268)	1:353:A:THR:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	6	1.63	0.4	1.5
(1,199)	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	1:257:A:GLY:N	6	1.61	0.38	1.67
(1,269)	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	1:355:A:THR:N	6	1.57	0.43	1.66
(1,96)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLY:N	6	1.46	0.29	1.31
(1,25)	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	1:52:A:TYR:N	6	1.41	0.45	1.22
(1,23)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:GLY:N	6	1.4	0.35	1.24
(1,3)	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	1:14:A:SER:N	5	2.36	0.77	1.92
(1,30)	1:57:A:ASN:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	5	1.74	0.28	1.71
(1,75)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:GLY:N	5	1.67	0.34	1.69
(1,243)	1:317:A:TYR:N	1:317:A:TYR:CA	1:317:A:TYR:C	1:318:A:GLU:N	5	1.61	0.47	1.66
(1,173)	1:232:A:ALA:N	1:232:A:ALA:CA	1:232:A:ALA:C	1:233:A:HIS:N	5	1.51	0.37	1.32
(1,110)	1:149:A:PHE:N	1:149:A:PHE:CA	1:149:A:PHE:C	1:150:A:SER:N	5	1.37	0.13	1.38
(1,163)	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	1:210:A:HIS:N	5	1.32	0.33	1.14
(1,279)	1:64:A:SER:N	1:64:A:SER:CA	1:64:A:SER:C	1:65:A:ASP:N	4	2.23	0.44	2.28
(1,13)	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	1:31:A:ASP:N	4	2.07	0.62	2.22
(1,1)	1:2:A:PRO:N	1:2:A:PRO:CA	1:2:A:PRO:C	1:3:A:ARG:N	4	2.01	0.58	2.13
(1,100)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:LYS:N	4	1.96	0.51	1.88
(1,33)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:GLY:N	4	1.8	0.46	1.9
(1,240)	1:306:A:VAL:N	1:306:A:VAL:CA	1:306:A:VAL:C	1:307:A:LYS:N	4	1.72	0.61	1.59
(1,255)	1:326:A:GLN:N	1:326:A:GLN:CA	1:326:A:GLN:C	1:327:A:GLY:N	4	1.64	0.29	1.76
(1,78)	1:111:A:PRO:N	1:111:A:PRO:CA	1:111:A:PRO:C	1:112:A:LYS:N	4	1.62	0.5	1.46
(1,44)	1:79:A:PRO:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	4	1.62	0.45	1.6
(1,4)	1:24:A:ALA:C	1:25:A:VAL:N	1:25:A:VAL:CA	1:25:A:VAL:C	4	1.6	0.14	1.56
(1,158)	1:201:A:ALA:C	1:202:A:TYR:N	1:202:A:TYR:CA	1:202:A:TYR:C	4	1.6	0.09	1.57
(1,157)	1:201:A:ALA:N	1:201:A:ALA:CA	1:201:A:ALA:C	1:202:A:TYR:N	4	1.58	0.53	1.55
(1,150)	1:190:A:PRO:N	1:190:A:PRO:CA	1:190:A:PRO:C	1:191:A:ASP:N	4	1.53	0.34	1.53
(1,165)	1:223:A:GLY:C	1:224:A:THR:N	1:224:A:THR:CA	1:224:A:THR:C	4	1.47	0.44	1.26
(1,74)	1:107:A:TYR:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	4	1.43	0.27	1.42
(1,151)	1:192:A:GLN:C	1:193:A:VAL:N	1:193:A:VAL:CA	1:193:A:VAL:C	4	1.33	0.33	1.28
(1,233)	1:301:A:LYS:C	1:302:A:TYR:N	1:302:A:TYR:CA	1:302:A:TYR:C	4	1.22	0.16	1.19
(1,29)	1:54:A:ALA:N	1:54:A:ALA:CA	1:54:A:ALA:C	1:55:A:ASP:N	3	2.71	0.4	2.9
(1,178)	1:235:A:GLY:C	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	3	2.67	0.55	2.41
(1,322)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:CYS:N	3	2.2	0.8	2.44
(1,136)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:HIS:N	3	1.93	0.82	1.4
(1,195)	1:254:A:TRP:N	1:254:A:TRP:CA	1:254:A:TRP:C	1:255:A:LEU:N	3	1.85	0.31	1.73
(1,263)	1:331:A:ILE:N	1:331:A:ILE:CA	1:331:A:ILE:C	1:332:A:GLY:N	3	1.82	0.88	1.37
(1,215)	1:278:A:TYR:N	1:278:A:TYR:CA	1:278:A:TYR:C	1:279:A:ARG:N	3	1.75	0.69	1.36
(1,104)	1:142:A:TYR:N	1:142:A:TYR:CA	1:142:A:TYR:C	1:143:A:GLU:N	3	1.71	0.49	1.51
(1,171)	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	1:231:A:ASP:N	3	1.63	0.6	1.35
(1,103)	1:141:A:ILE:C	1:142:A:TYR:N	1:142:A:TYR:CA	1:142:A:TYR:C	3	1.5	0.68	1.04
(1,101)	1:140:A:LYS:C	1:141:A:ILE:N	1:141:A:ILE:CA	1:141:A:ILE:C	3	1.49	0.49	1.22
(1,31)	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	1:59:A:SER:N	3	1.44	0.32	1.33
(1,202)	1:258:A:HIS:C	1:259:A:LEU:N	1:259:A:LEU:CA	1:259:A:LEU:C	3	1.41	0.08	1.41
(1,2)	1:12:A:GLN:C	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	3	1.34	0.14	1.34

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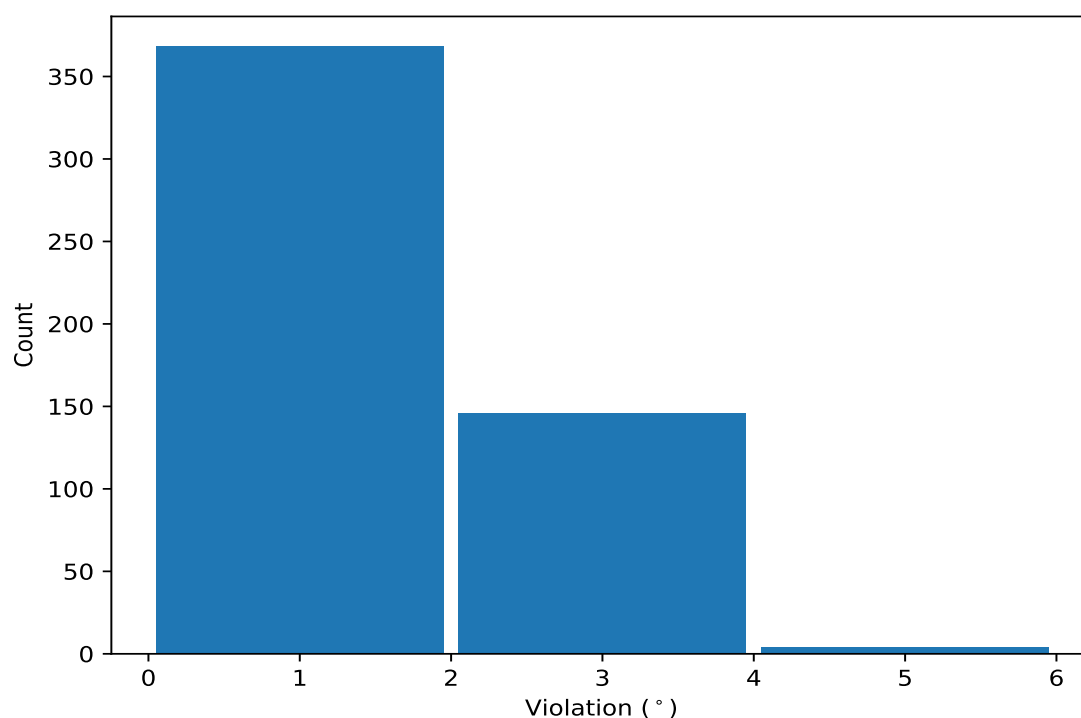
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,28)	1:53:A:LEU:C	1:54:A:ALA:N	1:54:A:ALA:CA	1:54:A:ALA:C	3	1.05	0.02	1.04
(1,327)	1:238:A:PRO:C	1:239:A:SER:N	1:239:A:SER:CA	1:239:A:SER:C	2	2.62	0.3	2.62
(1,227)	1:290:A:PHE:N	1:290:A:PHE:CA	1:290:A:PHE:C	1:291:A:PRO:N	2	2.58	1.14	2.58
(1,272)	1:22:A:GLN:C	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	2	2.52	1.24	2.52
(1,141)	1:181:A:SER:N	1:181:A:SER:CA	1:181:A:SER:C	1:182:A:ASN:N	2	2.06	0.17	2.06
(1,169)	1:226:A:GLU:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	2	1.98	0.0	1.98
(1,47)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	2	1.7	0.12	1.7
(1,203)	1:259:A:LEU:N	1:259:A:LEU:CA	1:259:A:LEU:C	1:260:A:PRO:N	2	1.66	0.6	1.66
(1,251)	1:324:A:LEU:N	1:324:A:LEU:CA	1:324:A:LEU:C	1:325:A:LEU:N	2	1.64	0.59	1.64
(1,84)	1:119:A:HIS:N	1:119:A:HIS:CA	1:119:A:HIS:C	1:120:A:ASP:N	2	1.64	0.26	1.64
(1,15)	1:32:A:MET:N	1:32:A:MET:CA	1:32:A:MET:C	1:33:A:ALA:N	2	1.63	0.25	1.63
(1,49)	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	1:83:A:GLU:N	2	1.56	0.19	1.56
(1,20)	1:38:A:LYS:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	2	1.55	0.41	1.55
(1,145)	1:184:A:LEU:N	1:184:A:LEU:CA	1:184:A:LEU:C	1:185:A:LEU:N	2	1.52	0.04	1.52
(1,58)	1:89:A:ARG:C	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	2	1.5	0.02	1.5
(1,207)	1:270:A:TYR:N	1:270:A:TYR:CA	1:270:A:TYR:C	1:271:A:VAL:N	2	1.48	0.05	1.48
(1,166)	1:224:A:THR:N	1:224:A:THR:CA	1:224:A:THR:C	1:225:A:ILE:N	2	1.47	0.12	1.47
(1,7)	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	1:27:A:GLU:N	2	1.46	0.05	1.46
(1,120)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:SER:N	2	1.42	0.05	1.42
(1,154)	1:194:A:TYR:N	1:194:A:TYR:CA	1:194:A:TYR:C	1:195:A:LEU:N	2	1.4	0.4	1.4
(1,138)	1:174:A:VAL:N	1:174:A:VAL:CA	1:174:A:VAL:C	1:175:A:HIS:N	2	1.38	0.03	1.38
(1,26)	1:51:A:ILE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	2	1.36	0.34	1.36
(1,90)	1:128:A:PHE:N	1:128:A:PHE:CA	1:128:A:PHE:C	1:129:A:MET:N	2	1.3	0.18	1.3
(1,187)	1:250:A:CYS:N	1:250:A:CYS:CA	1:250:A:CYS:C	1:251:A:MET:N	2	1.3	0.1	1.3
(1,320)	1:215:A:GLU:C	1:216:A:ASP:N	1:216:A:ASP:CA	1:216:A:ASP:C	2	1.3	0.1	1.3
(1,61)	1:93:A:PRO:N	1:93:A:PRO:CA	1:93:A:PRO:C	1:94:A:GLU:N	2	1.23	0.05	1.23
(1,140)	1:180:A:ALA:C	1:181:A:SER:N	1:181:A:SER:CA	1:181:A:SER:C	2	1.14	0.09	1.14

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,139)	1:177:A:ASP:C	1:178:A:ILE:N	1:178:A:ILE:CA	1:178:A:ILE:C	5	4.69
(1,219)	1:283:A:ALA:N	1:283:A:ALA:CA	1:283:A:ALA:C	1:284:A:SER:N	20	4.42
(1,198)	1:255:A:LEU:C	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	10	4.02
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	15	4.0
(1,69)	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	1:100:A:ILE:N	15	3.94
(1,35)	1:68:A:CYS:N	1:68:A:CYS:CA	1:68:A:CYS:C	1:69:A:VAL:N	4	3.85
(1,108)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:ALA:N	10	3.83
(1,272)	1:22:A:GLN:C	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	15	3.77
(1,201)	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	1:259:A:LEU:N	4	3.74
(1,227)	1:290:A:PHE:N	1:290:A:PHE:CA	1:290:A:PHE:C	1:291:A:PRO:N	9	3.73
(1,43)	1:79:A:PRO:N	1:79:A:PRO:CA	1:79:A:PRO:C	1:80:A:LEU:N	6	3.71
(1,219)	1:283:A:ALA:N	1:283:A:ALA:CA	1:283:A:ALA:C	1:284:A:SER:N	12	3.58
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	14	3.57
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	3	3.56
(1,3)	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	1:14:A:SER:N	17	3.47
(1,178)	1:235:A:GLY:C	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	11	3.44
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	18	3.4
(1,179)	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	1:237:A:ALA:N	11	3.38
(1,92)	1:129:A:MET:N	1:129:A:MET:CA	1:129:A:MET:C	1:130:A:ILE:N	15	3.34
(1,200)	1:257:A:GLY:C	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	10	3.31
(1,35)	1:68:A:CYS:N	1:68:A:CYS:CA	1:68:A:CYS:C	1:69:A:VAL:N	11	3.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	11	3.3
(1,277)	1:54:A:ALA:C	1:55:A:ASP:N	1:55:A:ASP:CA	1:55:A:ASP:C	6	3.24
(1,71)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:ARG:N	10	3.22
(1,6)	1:25:A:VAL:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	11	3.14
(1,136)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:HIS:N	19	3.09
(1,3)	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	1:14:A:SER:N	11	3.08
(1,29)	1:54:A:ALA:N	1:54:A:ALA:CA	1:54:A:ALA:C	1:55:A:ASP:N	2	3.07
(1,263)	1:331:A:ILE:N	1:331:A:ILE:CA	1:331:A:ILE:C	1:332:A:GLY:N	14	3.05
(1,322)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:CYS:N	14	3.04
(1,201)	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	1:259:A:LEU:N	10	3.02
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	7	3.02
(1,97)	1:135:A:GLY:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	2	2.98
(1,317)	1:179:A:LYS:N	1:179:A:LYS:CA	1:179:A:LYS:C	1:180:A:ALA:N	3	2.96
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	18	2.96
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	4	2.94
(1,35)	1:68:A:CYS:N	1:68:A:CYS:CA	1:68:A:CYS:C	1:69:A:VAL:N	3	2.94
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	3	2.92
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	19	2.92
(1,327)	1:238:A:PRO:C	1:239:A:SER:N	1:239:A:SER:CA	1:239:A:SER:C	14	2.91
(1,29)	1:54:A:ALA:N	1:54:A:ALA:CA	1:54:A:ALA:C	1:55:A:ASP:N	3	2.9
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	12	2.89
(1,69)	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	1:100:A:ILE:N	2	2.85
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	14	2.83
(1,264)	1:331:A:ILE:C	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	14	2.82
(1,32)	1:61:A:SER:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	5	2.8
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	19	2.78
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	11	2.78
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	1	2.77
(1,13)	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	1:31:A:ASP:N	8	2.77
(1,100)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:LYS:N	4	2.74
(1,35)	1:68:A:CYS:N	1:68:A:CYS:CA	1:68:A:CYS:C	1:69:A:VAL:N	13	2.74
(1,215)	1:278:A:TYR:N	1:278:A:TYR:CA	1:278:A:TYR:C	1:279:A:ARG:N	7	2.72
(1,108)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:ALA:N	8	2.72
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	17	2.71
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	15	2.71
(1,279)	1:64:A:SER:N	1:64:A:SER:CA	1:64:A:SER:C	1:65:A:ASP:N	4	2.69
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	4	2.69
(1,198)	1:255:A:LEU:C	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	15	2.69
(1,240)	1:306:A:VAL:N	1:306:A:VAL:CA	1:306:A:VAL:C	1:307:A:LYS:N	4	2.67
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	12	2.66
(1,1)	1:2:A:PRO:N	1:2:A:PRO:CA	1:2:A:PRO:C	1:3:A:ARG:N	10	2.66
(1,279)	1:64:A:SER:N	1:64:A:SER:CA	1:64:A:SER:C	1:65:A:ASP:N	18	2.63
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	19	2.62
(1,200)	1:257:A:GLY:C	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	5	2.62
(1,201)	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	1:259:A:LEU:N	15	2.57
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	17	2.55
(1,43)	1:79:A:PRO:N	1:79:A:PRO:CA	1:79:A:PRO:C	1:80:A:LEU:N	1	2.55
(1,214)	1:277:A:ARG:C	1:278:A:TYR:N	1:278:A:TYR:CA	1:278:A:TYR:C	17	2.54
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	20	2.54
(1,265)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:SER:N	2	2.49
(1,171)	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	1:231:A:ASP:N	5	2.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,103)	1:141:A:ILE:C	1:142:A:TYR:N	1:142:A:TYR:CA	1:142:A:TYR:C	2	2.47
(1,78)	1:111:A:PRO:N	1:111:A:PRO:CA	1:111:A:PRO:C	1:112:A:LYS:N	15	2.45
(1,24)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	8	2.45
(1,322)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:CYS:N	7	2.44
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	9	2.44
(1,198)	1:255:A:LEU:C	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	20	2.43
(1,35)	1:68:A:CYS:N	1:68:A:CYS:CA	1:68:A:CYS:C	1:69:A:VAL:N	20	2.43
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	10	2.42
(1,25)	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	1:52:A:TYR:N	9	2.42
(1,178)	1:235:A:GLY:C	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	7	2.41
(1,59)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:ALA:N	7	2.41
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	7	2.4
(1,268)	1:353:A:THR:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	7	2.39
(1,104)	1:142:A:TYR:N	1:142:A:TYR:CA	1:142:A:TYR:C	1:143:A:GLU:N	6	2.39
(1,243)	1:317:A:TYR:N	1:317:A:TYR:CA	1:317:A:TYR:C	1:318:A:GLU:N	10	2.38
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	13	2.38
(1,198)	1:255:A:LEU:C	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	4	2.36
(1,1)	1:2:A:PRO:N	1:2:A:PRO:CA	1:2:A:PRO:C	1:3:A:ARG:N	6	2.33
(1,327)	1:238:A:PRO:C	1:239:A:SER:N	1:239:A:SER:CA	1:239:A:SER:C	3	2.32
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	20	2.29
(1,43)	1:79:A:PRO:N	1:79:A:PRO:CA	1:79:A:PRO:C	1:80:A:LEU:N	18	2.29
(1,195)	1:254:A:TRP:N	1:254:A:TRP:CA	1:254:A:TRP:C	1:255:A:LEU:N	9	2.28
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	12	2.27
(1,204)	1:263:A:ASP:C	1:264:A:ASN:N	1:264:A:ASN:CA	1:264:A:ASN:C	4	2.26
(1,203)	1:259:A:LEU:N	1:259:A:LEU:CA	1:259:A:LEU:C	1:260:A:PRO:N	2	2.26
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	19	2.25
(1,33)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:GLY:N	20	2.25
(1,198)	1:255:A:LEU:C	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	18	2.24
(1,44)	1:79:A:PRO:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	6	2.24
(1,251)	1:324:A:LEU:N	1:324:A:LEU:CA	1:324:A:LEU:C	1:325:A:LEU:N	15	2.23
(1,165)	1:223:A:GLY:C	1:224:A:THR:N	1:224:A:THR:CA	1:224:A:THR:C	19	2.23
(1,141)	1:181:A:SER:N	1:181:A:SER:CA	1:181:A:SER:C	1:182:A:ASN:N	3	2.23
(1,33)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:GLY:N	13	2.23
(1,30)	1:57:A:ASN:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	6	2.23
(1,13)	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	1:31:A:ASP:N	18	2.23
(1,157)	1:201:A:ALA:N	1:201:A:ALA:CA	1:201:A:ALA:C	1:202:A:TYR:N	13	2.22
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	2	2.22
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	16	2.22
(1,13)	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	1:31:A:ASP:N	7	2.22
(1,147)	1:186:A:ASN:N	1:186:A:ASN:CA	1:186:A:ASN:C	1:187:A:TYR:N	16	2.2
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	8	2.2
(1,97)	1:135:A:GLY:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1	2.2
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	12	2.19
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	19	2.18
(1,95)	1:133:A:ARG:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	19	2.18
(1,178)	1:235:A:GLY:C	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	17	2.17
(1,101)	1:140:A:LYS:C	1:141:A:ILE:N	1:141:A:ILE:CA	1:141:A:ILE:C	19	2.17
(1,199)	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	1:257:A:GLY:N	19	2.16
(1,29)	1:54:A:ALA:N	1:54:A:ALA:CA	1:54:A:ALA:C	1:55:A:ASP:N	4	2.16
(1,59)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:ALA:N	2	2.13
(1,269)	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	1:355:A:THR:N	2	2.11

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,106)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ASN:N	5	2.11
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	1	2.1
(1,164)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:LYS:N	1	2.1
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	1	2.1
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	14	2.1
(1,95)	1:133:A:ARG:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	13	2.1
(1,41)	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	1:73:A:GLU:N	12	2.1
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	2	2.09
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	19	2.09
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	19	2.09
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	2	2.08
(1,200)	1:257:A:GLY:C	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	1	2.08
(1,35)	1:68:A:CYS:N	1:68:A:CYS:CA	1:68:A:CYS:C	1:69:A:VAL:N	5	2.08
(1,219)	1:283:A:ALA:N	1:283:A:ALA:CA	1:283:A:ALA:C	1:284:A:SER:N	6	2.07
(1,143)	1:183:A:LEU:N	1:183:A:LEU:CA	1:183:A:LEU:C	1:184:A:LEU:N	3	2.07
(1,75)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:GLY:N	6	2.07
(1,23)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:GLY:N	7	2.07
(1,148)	1:186:A:ASN:C	1:187:A:TYR:N	1:187:A:TYR:CA	1:187:A:TYR:C	16	2.06
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	8	2.06
(1,205)	1:264:A:ASN:N	1:264:A:ASN:CA	1:264:A:ASN:C	1:265:A:LEU:N	3	2.05
(1,198)	1:255:A:LEU:C	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	5	2.05
(1,173)	1:232:A:ALA:N	1:232:A:ALA:CA	1:232:A:ALA:C	1:233:A:HIS:N	7	2.05
(1,6)	1:25:A:VAL:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	16	2.05
(1,96)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLY:N	7	2.04
(1,274)	1:36:A:GLU:N	1:36:A:GLU:CA	1:36:A:GLU:C	1:37:A:TRP:N	4	2.03
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	1	2.03
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	7	2.02
(1,179)	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	1:237:A:ALA:N	4	1.99
(1,100)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:LYS:N	8	1.99
(1,265)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:SER:N	13	1.98
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	16	1.98
(1,169)	1:226:A:GLU:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	19	1.98
(1,169)	1:226:A:GLU:C	1:227:A:PHE:N	1:227:A:PHE:CA	1:227:A:PHE:C	20	1.98
(1,157)	1:201:A:ALA:N	1:201:A:ALA:CA	1:201:A:ALA:C	1:202:A:TYR:N	11	1.98
(1,150)	1:190:A:PRO:N	1:190:A:PRO:CA	1:190:A:PRO:C	1:191:A:ASP:N	15	1.98
(1,164)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:LYS:N	14	1.97
(1,20)	1:38:A:LYS:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	7	1.96
(1,197)	1:255:A:LEU:N	1:255:A:LEU:CA	1:255:A:LEU:C	1:256:A:THR:N	17	1.95
(1,163)	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	1:210:A:HIS:N	15	1.95
(1,279)	1:64:A:SER:N	1:64:A:SER:CA	1:64:A:SER:C	1:65:A:ASP:N	6	1.94
(1,269)	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	1:355:A:THR:N	7	1.94
(1,201)	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	1:259:A:LEU:N	17	1.94
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	9	1.94
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	17	1.94
(1,1)	1:2:A:PRO:N	1:2:A:PRO:CA	1:2:A:PRO:C	1:3:A:ARG:N	9	1.94
(1,265)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:SER:N	19	1.92
(1,219)	1:283:A:ALA:N	1:283:A:ALA:CA	1:283:A:ALA:C	1:284:A:SER:N	3	1.92
(1,201)	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	1:259:A:LEU:N	19	1.92
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	11	1.92
(1,95)	1:133:A:ARG:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	8	1.92
(1,3)	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	1:14:A:SER:N	2	1.92

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,255)	1:326:A:GLN:N	1:326:A:GLN:CA	1:326:A:GLN:C	1:327:A:GLY:N	2	1.91
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	4	1.91
(1,84)	1:119:A:HIS:N	1:119:A:HIS:CA	1:119:A:HIS:C	1:120:A:ASP:N	16	1.9
(1,141)	1:181:A:SER:N	1:181:A:SER:CA	1:181:A:SER:C	1:182:A:ASN:N	17	1.89
(1,108)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:ALA:N	7	1.89
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	1	1.89
(1,3)	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	1:14:A:SER:N	6	1.89
(1,139)	1:177:A:ASP:C	1:178:A:ILE:N	1:178:A:ILE:CA	1:178:A:ILE:C	7	1.88
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	9	1.88
(1,59)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:ALA:N	10	1.88
(1,31)	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	1:59:A:SER:N	14	1.88
(1,15)	1:32:A:MET:N	1:32:A:MET:CA	1:32:A:MET:C	1:33:A:ALA:N	7	1.88
(1,269)	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	1:355:A:THR:N	6	1.87
(1,204)	1:263:A:ASP:C	1:264:A:ASN:N	1:264:A:ASN:CA	1:264:A:ASN:C	6	1.87
(1,199)	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	1:257:A:GLY:N	7	1.87
(1,219)	1:283:A:ALA:N	1:283:A:ALA:CA	1:283:A:ALA:C	1:284:A:SER:N	15	1.86
(1,139)	1:177:A:ASP:C	1:178:A:ILE:N	1:178:A:ILE:CA	1:178:A:ILE:C	10	1.86
(1,173)	1:232:A:ALA:N	1:232:A:ALA:CA	1:232:A:ALA:C	1:233:A:HIS:N	6	1.85
(1,108)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:ALA:N	9	1.85
(1,75)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:GLY:N	13	1.85
(1,149)	1:187:A:TYR:N	1:187:A:TYR:CA	1:187:A:TYR:C	1:188:A:LYS:N	3	1.84
(1,268)	1:353:A:THR:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	20	1.83
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	11	1.83
(1,97)	1:135:A:GLY:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	6	1.83
(1,164)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:LYS:N	20	1.82
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	7	1.82
(1,35)	1:68:A:CYS:N	1:68:A:CYS:CA	1:68:A:CYS:C	1:69:A:VAL:N	18	1.82
(1,217)	1:282:A:ILE:N	1:282:A:ILE:CA	1:282:A:ILE:C	1:283:A:ALA:N	19	1.81
(1,164)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:LYS:N	11	1.81
(1,154)	1:194:A:TYR:N	1:194:A:TYR:CA	1:194:A:TYR:C	1:195:A:LEU:N	7	1.81
(1,47)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	11	1.81
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	20	1.8
(1,219)	1:283:A:ALA:N	1:283:A:ALA:CA	1:283:A:ALA:C	1:284:A:SER:N	8	1.8
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	17	1.79
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	18	1.79
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	8	1.79
(1,44)	1:79:A:PRO:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	10	1.79
(1,4)	1:24:A:ALA:C	1:25:A:VAL:N	1:25:A:VAL:CA	1:25:A:VAL:C	11	1.79
(1,255)	1:326:A:GLN:N	1:326:A:GLN:CA	1:326:A:GLN:C	1:327:A:GLY:N	3	1.78
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	2	1.78
(1,100)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:LYS:N	6	1.78
(1,74)	1:107:A:TYR:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	5	1.78
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	8	1.77
(1,240)	1:306:A:VAL:N	1:306:A:VAL:CA	1:306:A:VAL:C	1:307:A:LYS:N	20	1.76
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	9	1.76
(1,43)	1:79:A:PRO:N	1:79:A:PRO:CA	1:79:A:PRO:C	1:80:A:LEU:N	19	1.76
(1,30)	1:57:A:ASN:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	15	1.76
(1,243)	1:317:A:TYR:N	1:317:A:TYR:CA	1:317:A:TYR:C	1:318:A:GLU:N	14	1.75
(1,151)	1:192:A:GLN:C	1:193:A:VAL:N	1:193:A:VAL:CA	1:193:A:VAL:C	2	1.75
(1,49)	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	1:83:A:GLU:N	10	1.75
(1,43)	1:79:A:PRO:N	1:79:A:PRO:CA	1:79:A:PRO:C	1:80:A:LEU:N	15	1.74

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,255)	1:326:A:GLN:N	1:326:A:GLN:CA	1:326:A:GLN:C	1:327:A:GLY:N	12	1.73
(1,219)	1:283:A:ALA:N	1:283:A:ALA:CA	1:283:A:ALA:C	1:284:A:SER:N	19	1.73
(1,195)	1:254:A:TRP:N	1:254:A:TRP:CA	1:254:A:TRP:C	1:255:A:LEU:N	8	1.73
(1,158)	1:201:A:ALA:C	1:202:A:TYR:N	1:202:A:TYR:CA	1:202:A:TYR:C	7	1.73
(1,95)	1:133:A:ARG:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	12	1.73
(1,199)	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	1:257:A:GLY:N	9	1.72
(1,69)	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	1:100:A:ILE:N	17	1.72
(1,14)	1:31:A:ASP:C	1:32:A:MET:N	1:32:A:MET:CA	1:32:A:MET:C	18	1.72
(1,200)	1:257:A:GLY:C	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	13	1.71
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	17	1.71
(1,97)	1:135:A:GLY:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	4	1.71
(1,30)	1:57:A:ASN:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	20	1.71
(1,175)	1:233:A:HIS:N	1:233:A:HIS:CA	1:233:A:HIS:C	1:234:A:ASN:N	17	1.7
(1,150)	1:190:A:PRO:N	1:190:A:PRO:CA	1:190:A:PRO:C	1:191:A:ASP:N	7	1.7
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	16	1.7
(1,164)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:LYS:N	19	1.69
(1,75)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:GLY:N	10	1.69
(1,26)	1:51:A:ILE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	9	1.69
(1,35)	1:68:A:CYS:N	1:68:A:CYS:CA	1:68:A:CYS:C	1:69:A:VAL:N	8	1.68
(1,279)	1:64:A:SER:N	1:64:A:SER:CA	1:64:A:SER:C	1:65:A:ASP:N	5	1.67
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	5	1.67
(1,75)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:GLY:N	8	1.67
(1,243)	1:317:A:TYR:N	1:317:A:TYR:CA	1:317:A:TYR:C	1:318:A:GLU:N	19	1.66
(1,179)	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	1:237:A:ALA:N	12	1.66
(1,106)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ASN:N	7	1.66
(1,6)	1:25:A:VAL:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	15	1.66
(1,4)	1:24:A:ALA:C	1:25:A:VAL:N	1:25:A:VAL:CA	1:25:A:VAL:C	9	1.66
(1,59)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:ALA:N	1	1.65
(1,32)	1:61:A:SER:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	14	1.65
(1,30)	1:57:A:ASN:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	8	1.65
(1,216)	1:281:A:ASN:C	1:282:A:ILE:N	1:282:A:ILE:CA	1:282:A:ILE:C	20	1.64
(1,199)	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	1:257:A:GLY:N	1	1.63
(1,200)	1:257:A:GLY:C	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	3	1.62
(1,139)	1:177:A:ASP:C	1:178:A:ILE:N	1:178:A:ILE:CA	1:178:A:ILE:C	18	1.62
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	15	1.62
(1,96)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLY:N	11	1.62
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	8	1.62
(1,158)	1:201:A:ALA:C	1:202:A:TYR:N	1:202:A:TYR:CA	1:202:A:TYR:C	4	1.61
(1,89)	1:127:A:ARG:C	1:128:A:PHE:N	1:128:A:PHE:CA	1:128:A:PHE:C	12	1.61
(1,23)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:GLY:N	11	1.61
(1,24)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	1	1.6
(1,265)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:SER:N	20	1.59
(1,166)	1:224:A:THR:N	1:224:A:THR:CA	1:224:A:THR:C	1:225:A:ILE:N	16	1.59
(1,74)	1:107:A:TYR:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	2	1.59
(1,24)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	18	1.59
(1,265)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:SER:N	11	1.58
(1,69)	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	1:100:A:ILE:N	3	1.58
(1,59)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:ALA:N	9	1.58
(1,47)	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	1:82:A:THR:N	2	1.58
(1,24)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	16	1.58
(1,43)	1:79:A:PRO:N	1:79:A:PRO:CA	1:79:A:PRO:C	1:80:A:LEU:N	10	1.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,204)	1:263:A:ASP:C	1:264:A:ASN:N	1:264:A:ASN:CA	1:264:A:ASN:C	15	1.56
(1,110)	1:149:A:PHE:N	1:149:A:PHE:CA	1:149:A:PHE:C	1:150:A:SER:N	8	1.56
(1,69)	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	1:100:A:ILE:N	18	1.56
(1,33)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:GLY:N	4	1.56
(1,32)	1:61:A:SER:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	2	1.56
(1,145)	1:184:A:LEU:N	1:184:A:LEU:CA	1:184:A:LEU:C	1:185:A:LEU:N	9	1.55
(1,106)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ASN:N	11	1.55
(1,97)	1:135:A:GLY:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	12	1.55
(1,78)	1:111:A:PRO:N	1:111:A:PRO:CA	1:111:A:PRO:C	1:112:A:LYS:N	11	1.55
(1,55)	1:87:A:TYR:N	1:87:A:TYR:CA	1:87:A:TYR:C	1:88:A:GLN:N	2	1.55
(1,268)	1:353:A:THR:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	19	1.54
(1,204)	1:263:A:ASP:C	1:264:A:ASN:N	1:264:A:ASN:CA	1:264:A:ASN:C	14	1.54
(1,195)	1:254:A:TRP:N	1:254:A:TRP:CA	1:254:A:TRP:C	1:255:A:LEU:N	16	1.54
(1,151)	1:192:A:GLN:C	1:193:A:VAL:N	1:193:A:VAL:CA	1:193:A:VAL:C	9	1.54
(1,200)	1:257:A:GLY:C	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	14	1.53
(1,158)	1:201:A:ALA:C	1:202:A:TYR:N	1:202:A:TYR:CA	1:202:A:TYR:C	15	1.53
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	13	1.53
(1,207)	1:270:A:TYR:N	1:270:A:TYR:CA	1:270:A:TYR:C	1:271:A:VAL:N	16	1.52
(1,198)	1:255:A:LEU:C	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	13	1.52
(1,69)	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	1:100:A:ILE:N	4	1.52
(1,58)	1:89:A:ARG:C	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	5	1.52
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	16	1.51
(1,202)	1:258:A:HIS:C	1:259:A:LEU:N	1:259:A:LEU:CA	1:259:A:LEU:C	1	1.51
(1,158)	1:201:A:ALA:C	1:202:A:TYR:N	1:202:A:TYR:CA	1:202:A:TYR:C	19	1.51
(1,104)	1:142:A:TYR:N	1:142:A:TYR:CA	1:142:A:TYR:C	1:143:A:GLU:N	11	1.51
(1,2)	1:12:A:GLN:C	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	9	1.51
(1,7)	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	1:27:A:GLU:N	19	1.5
(1,6)	1:25:A:VAL:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	3	1.5
(1,265)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:SER:N	10	1.48
(1,233)	1:301:A:LYS:C	1:302:A:TYR:N	1:302:A:TYR:CA	1:302:A:TYR:C	16	1.48
(1,145)	1:184:A:LEU:N	1:184:A:LEU:CA	1:184:A:LEU:C	1:185:A:LEU:N	12	1.48
(1,97)	1:135:A:GLY:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	18	1.48
(1,90)	1:128:A:PHE:N	1:128:A:PHE:CA	1:128:A:PHE:C	1:129:A:MET:N	4	1.48
(1,58)	1:89:A:ARG:C	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	8	1.48
(1,120)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:SER:N	1	1.47
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	13	1.47
(1,32)	1:61:A:SER:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	11	1.47
(1,32)	1:61:A:SER:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	19	1.47
(1,4)	1:24:A:ALA:C	1:25:A:VAL:N	1:25:A:VAL:CA	1:25:A:VAL:C	15	1.47
(1,267)	1:333:A:SER:N	1:333:A:SER:CA	1:333:A:SER:C	1:334:A:LYS:N	2	1.46
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	11	1.46
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	9	1.46
(1,4)	1:24:A:ALA:C	1:25:A:VAL:N	1:25:A:VAL:CA	1:25:A:VAL:C	6	1.46
(1,269)	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	1:355:A:THR:N	5	1.45
(1,268)	1:353:A:THR:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	5	1.45
(1,200)	1:257:A:GLY:C	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	20	1.45
(1,198)	1:255:A:LEU:C	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	2	1.45
(1,132)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:GLU:N	12	1.45
(1,3)	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	1:14:A:SER:N	15	1.45
(1,227)	1:290:A:PHE:N	1:290:A:PHE:CA	1:290:A:PHE:C	1:291:A:PRO:N	17	1.44
(1,79)	1:112:A:LYS:C	1:113:A:TYR:N	1:113:A:TYR:CA	1:113:A:TYR:C	11	1.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,228)	1:296:A:PRO:N	1:296:A:PRO:CA	1:296:A:PRO:C	1:297:A:GLY:N	3	1.43
(1,219)	1:283:A:ALA:N	1:283:A:ALA:CA	1:283:A:ALA:C	1:284:A:SER:N	10	1.43
(1,207)	1:270:A:TYR:N	1:270:A:TYR:CA	1:270:A:TYR:C	1:271:A:VAL:N	20	1.43
(1,110)	1:149:A:PHE:N	1:149:A:PHE:CA	1:149:A:PHE:C	1:150:A:SER:N	9	1.43
(1,240)	1:306:A:VAL:N	1:306:A:VAL:CA	1:306:A:VAL:C	1:307:A:LYS:N	3	1.42
(1,44)	1:79:A:PRO:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	7	1.42
(1,6)	1:25:A:VAL:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	1	1.42
(1,202)	1:258:A:HIS:C	1:259:A:LEU:N	1:259:A:LEU:CA	1:259:A:LEU:C	14	1.41
(1,138)	1:174:A:VAL:N	1:174:A:VAL:CA	1:174:A:VAL:C	1:175:A:HIS:N	14	1.41
(1,7)	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	1:27:A:GLU:N	16	1.41
(1,320)	1:215:A:GLU:C	1:216:A:ASP:N	1:216:A:ASP:CA	1:216:A:ASP:C	18	1.4
(1,268)	1:353:A:THR:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	16	1.4
(1,187)	1:250:A:CYS:N	1:250:A:CYS:CA	1:250:A:CYS:C	1:251:A:MET:N	16	1.4
(1,136)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:HIS:N	9	1.4
(1,179)	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	1:237:A:ALA:N	16	1.39
(1,106)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ASN:N	20	1.39
(1,69)	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	1:100:A:ILE:N	6	1.39
(1,6)	1:25:A:VAL:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	6	1.39
(1,110)	1:149:A:PHE:N	1:149:A:PHE:CA	1:149:A:PHE:C	1:150:A:SER:N	5	1.38
(1,78)	1:111:A:PRO:N	1:111:A:PRO:CA	1:111:A:PRO:C	1:112:A:LYS:N	12	1.38
(1,15)	1:32:A:MET:N	1:32:A:MET:CA	1:32:A:MET:C	1:33:A:ALA:N	10	1.38
(1,263)	1:331:A:ILE:N	1:331:A:ILE:CA	1:331:A:ILE:C	1:332:A:GLY:N	3	1.37
(1,120)	1:157:A:LEU:N	1:157:A:LEU:CA	1:157:A:LEU:C	1:158:A:SER:N	14	1.37
(1,84)	1:119:A:HIS:N	1:119:A:HIS:CA	1:119:A:HIS:C	1:120:A:ASP:N	10	1.37
(1,215)	1:278:A:TYR:N	1:278:A:TYR:CA	1:278:A:TYR:C	1:279:A:ARG:N	15	1.36
(1,150)	1:190:A:PRO:N	1:190:A:PRO:CA	1:190:A:PRO:C	1:191:A:ASP:N	16	1.36
(1,96)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLY:N	4	1.36
(1,49)	1:82:A:THR:N	1:82:A:THR:CA	1:82:A:THR:C	1:83:A:GLU:N	15	1.36
(1,30)	1:57:A:ASN:C	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	13	1.36
(1,171)	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	1:231:A:ASP:N	19	1.35
(1,166)	1:224:A:THR:N	1:224:A:THR:CA	1:224:A:THR:C	1:225:A:ILE:N	1	1.35
(1,138)	1:174:A:VAL:N	1:174:A:VAL:CA	1:174:A:VAL:C	1:175:A:HIS:N	4	1.35
(1,57)	1:88:A:GLN:N	1:88:A:GLN:CA	1:88:A:GLN:C	1:89:A:ARG:N	12	1.35
(1,24)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	3	1.35
(1,100)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:LYS:N	10	1.34
(1,2)	1:12:A:GLN:C	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	19	1.34
(1,32)	1:61:A:SER:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	18	1.33
(1,31)	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	1:59:A:SER:N	12	1.33
(1,173)	1:232:A:ALA:N	1:232:A:ALA:CA	1:232:A:ALA:C	1:233:A:HIS:N	16	1.32
(1,110)	1:149:A:PHE:N	1:149:A:PHE:CA	1:149:A:PHE:C	1:150:A:SER:N	4	1.32
(1,35)	1:68:A:CYS:N	1:68:A:CYS:CA	1:68:A:CYS:C	1:69:A:VAL:N	16	1.32
(1,23)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:GLY:N	9	1.32
(1,202)	1:258:A:HIS:C	1:259:A:LEU:N	1:259:A:LEU:CA	1:259:A:LEU:C	19	1.31
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	8	1.31
(1,163)	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	1:210:A:HIS:N	7	1.31
(1,69)	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	1:100:A:ILE:N	9	1.31
(1,136)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:HIS:N	13	1.3
(1,165)	1:223:A:GLY:C	1:224:A:THR:N	1:224:A:THR:CA	1:224:A:THR:C	4	1.29
(1,272)	1:22:A:GLN:C	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	12	1.28
(1,204)	1:263:A:ASP:C	1:264:A:ASN:N	1:264:A:ASN:CA	1:264:A:ASN:C	19	1.28
(1,139)	1:177:A:ASP:C	1:178:A:ILE:N	1:178:A:ILE:CA	1:178:A:ILE:C	4	1.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,61)	1:93:A:PRO:N	1:93:A:PRO:CA	1:93:A:PRO:C	1:94:A:GLU:N	20	1.27
(1,6)	1:25:A:VAL:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	2	1.27
(1,173)	1:232:A:ALA:N	1:232:A:ALA:CA	1:232:A:ALA:C	1:233:A:HIS:N	20	1.26
(1,134)	1:167:A:TYR:N	1:167:A:TYR:CA	1:167:A:TYR:C	1:168:A:ILE:N	15	1.26
(1,96)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLY:N	10	1.26
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	20	1.26
(1,74)	1:107:A:TYR:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	11	1.26
(1,43)	1:79:A:PRO:N	1:79:A:PRO:CA	1:79:A:PRO:C	1:80:A:LEU:N	3	1.26
(1,275)	1:37:A:TRP:C	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	11	1.25
(1,249)	1:323:A:ILE:N	1:323:A:ILE:CA	1:323:A:ILE:C	1:324:A:LEU:N	9	1.25
(1,199)	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	1:257:A:GLY:N	4	1.25
(1,96)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLY:N	12	1.25
(1,95)	1:133:A:ARG:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	7	1.25
(1,319)	1:180:A:ALA:N	1:180:A:ALA:CA	1:180:A:ALA:C	1:181:A:SER:N	3	1.24
(1,140)	1:180:A:ALA:C	1:181:A:SER:N	1:181:A:SER:CA	1:181:A:SER:C	17	1.24
(1,104)	1:142:A:TYR:N	1:142:A:TYR:CA	1:142:A:TYR:C	1:143:A:GLU:N	4	1.24
(1,25)	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	1:52:A:TYR:N	15	1.24
(1,25)	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	1:52:A:TYR:N	18	1.24
(1,265)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:SER:N	5	1.23
(1,265)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:SER:N	16	1.23
(1,241)	1:315:A:PRO:N	1:315:A:PRO:CA	1:315:A:PRO:C	1:316:A:LEU:N	17	1.23
(1,165)	1:223:A:GLY:C	1:224:A:THR:N	1:224:A:THR:CA	1:224:A:THR:C	8	1.23
(1,235)	1:302:A:TYR:C	1:303:A:MET:N	1:303:A:MET:CA	1:303:A:MET:C	20	1.22
(1,101)	1:140:A:LYS:C	1:141:A:ILE:N	1:141:A:ILE:CA	1:141:A:ILE:C	17	1.22
(1,96)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLY:N	9	1.22
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	2	1.22
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	6	1.22
(1,72)	1:101:A:ARG:C	1:102:A:THR:N	1:102:A:THR:CA	1:102:A:THR:C	12	1.22
(1,233)	1:301:A:LYS:C	1:302:A:TYR:N	1:302:A:TYR:CA	1:302:A:TYR:C	13	1.21
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	4	1.21
(1,24)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	12	1.21
(1,24)	1:50:A:CYS:C	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	14	1.21
(1,320)	1:215:A:GLU:C	1:216:A:ASP:N	1:216:A:ASP:CA	1:216:A:ASP:C	6	1.2
(1,187)	1:250:A:CYS:N	1:250:A:CYS:CA	1:250:A:CYS:C	1:251:A:MET:N	17	1.2
(1,107)	1:144:A:ALA:C	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	5	1.2
(1,99)	1:138:A:LEU:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1	1.2
(1,59)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:ALA:N	8	1.2
(1,25)	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	1:52:A:TYR:N	17	1.2
(1,243)	1:317:A:TYR:N	1:317:A:TYR:CA	1:317:A:TYR:C	1:318:A:GLU:N	2	1.19
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	10	1.19
(1,170)	1:229:A:SER:C	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	14	1.19
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	15	1.19
(1,25)	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	1:52:A:TYR:N	16	1.19
(1,61)	1:93:A:PRO:N	1:93:A:PRO:CA	1:93:A:PRO:C	1:94:A:GLU:N	17	1.18
(1,233)	1:301:A:LYS:C	1:302:A:TYR:N	1:302:A:TYR:CA	1:302:A:TYR:C	19	1.17
(1,164)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:LYS:N	4	1.17
(1,110)	1:149:A:PHE:N	1:149:A:PHE:CA	1:149:A:PHE:C	1:150:A:SER:N	14	1.17
(1,2)	1:12:A:GLN:C	1:13:A:SER:N	1:13:A:SER:CA	1:13:A:SER:C	11	1.17
(1,215)	1:278:A:TYR:N	1:278:A:TYR:CA	1:278:A:TYR:C	1:279:A:ARG:N	19	1.16
(1,181)	1:244:A:LEU:N	1:244:A:LEU:CA	1:244:A:LEU:C	1:245:A:GLU:N	8	1.16
(1,139)	1:177:A:ASP:C	1:178:A:ILE:N	1:178:A:ILE:CA	1:178:A:ILE:C	16	1.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,108)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:ALA:N	5	1.16
(1,33)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:GLY:N	14	1.16
(1,23)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:GLY:N	20	1.16
(1,268)	1:353:A:THR:C	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	2	1.15
(1,255)	1:326:A:GLN:N	1:326:A:GLN:CA	1:326:A:GLN:C	1:327:A:GLY:N	17	1.15
(1,204)	1:263:A:ASP:C	1:264:A:ASN:N	1:264:A:ASN:CA	1:264:A:ASN:C	20	1.15
(1,25)	1:51:A:ILE:N	1:51:A:ILE:CA	1:51:A:ILE:C	1:52:A:TYR:N	1	1.15
(1,23)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:GLY:N	6	1.15
(1,265)	1:332:A:GLY:N	1:332:A:GLY:CA	1:332:A:GLY:C	1:333:A:SER:N	8	1.14
(1,163)	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	1:210:A:HIS:N	1	1.14
(1,163)	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	1:210:A:HIS:N	13	1.14
(1,106)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ASN:N	15	1.14
(1,98)	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1:137:A:ASP:N	6	1.14
(1,95)	1:133:A:ARG:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	20	1.14
(1,20)	1:38:A:LYS:C	1:39:A:VAL:N	1:39:A:VAL:CA	1:39:A:VAL:C	17	1.14
(1,322)	1:219:A:ARG:N	1:219:A:ARG:CA	1:219:A:ARG:C	1:220:A:CYS:N	9	1.13
(1,201)	1:258:A:HIS:N	1:258:A:HIS:CA	1:258:A:HIS:C	1:259:A:LEU:N	20	1.13
(1,165)	1:223:A:GLY:C	1:224:A:THR:N	1:224:A:THR:CA	1:224:A:THR:C	17	1.13
(1,108)	1:145:A:ASN:N	1:145:A:ASN:CA	1:145:A:ASN:C	1:146:A:ALA:N	13	1.13
(1,34)	1:67:A:PRO:C	1:68:A:CYS:N	1:68:A:CYS:CA	1:68:A:CYS:C	17	1.13
(1,157)	1:201:A:ALA:N	1:201:A:ALA:CA	1:201:A:ALA:C	1:202:A:TYR:N	1	1.12
(1,90)	1:128:A:PHE:N	1:128:A:PHE:CA	1:128:A:PHE:C	1:129:A:MET:N	9	1.12
(1,31)	1:58:A:SER:N	1:58:A:SER:CA	1:58:A:SER:C	1:59:A:SER:N	8	1.12
(1,16)	1:32:A:MET:C	1:33:A:ALA:N	1:33:A:ALA:CA	1:33:A:ALA:C	2	1.12
(1,152)	1:193:A:VAL:N	1:193:A:VAL:CA	1:193:A:VAL:C	1:194:A:TYR:N	15	1.11
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	13	1.11
(1,78)	1:111:A:PRO:N	1:111:A:PRO:CA	1:111:A:PRO:C	1:112:A:LYS:N	9	1.11
(1,204)	1:263:A:ASP:C	1:264:A:ASN:N	1:264:A:ASN:CA	1:264:A:ASN:C	13	1.1
(1,74)	1:107:A:TYR:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	3	1.1
(1,69)	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	1:100:A:ILE:N	20	1.1
(1,1)	1:2:A:PRO:N	1:2:A:PRO:CA	1:2:A:PRO:C	1:3:A:ARG:N	16	1.1
(1,204)	1:263:A:ASP:C	1:264:A:ASN:N	1:264:A:ASN:CA	1:264:A:ASN:C	3	1.09
(1,179)	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	1:237:A:ALA:N	6	1.09
(1,179)	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	1:237:A:ALA:N	8	1.09
(1,179)	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	1:237:A:ALA:N	10	1.09
(1,179)	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	1:237:A:ALA:N	18	1.09
(1,167)	1:224:A:THR:C	1:225:A:ILE:N	1:225:A:ILE:CA	1:225:A:ILE:C	8	1.09
(1,150)	1:190:A:PRO:N	1:190:A:PRO:CA	1:190:A:PRO:C	1:191:A:ASP:N	4	1.09
(1,65)	1:96:A:ILE:N	1:96:A:ILE:CA	1:96:A:ILE:C	1:97:A:GLN:N	15	1.09
(1,9)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:ILE:N	2	1.09
(1,194)	1:253:A:GLN:C	1:254:A:TRP:N	1:254:A:TRP:CA	1:254:A:TRP:C	16	1.08
(1,171)	1:230:A:ILE:N	1:230:A:ILE:CA	1:230:A:ILE:C	1:231:A:ASP:N	13	1.08
(1,93)	1:129:A:MET:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	11	1.08
(1,43)	1:79:A:PRO:N	1:79:A:PRO:CA	1:79:A:PRO:C	1:80:A:LEU:N	17	1.08
(1,28)	1:53:A:LEU:C	1:54:A:ALA:N	1:54:A:ALA:CA	1:54:A:ALA:C	19	1.08
(1,173)	1:232:A:ALA:N	1:232:A:ALA:CA	1:232:A:ALA:C	1:233:A:HIS:N	4	1.07
(1,101)	1:140:A:LYS:C	1:141:A:ILE:N	1:141:A:ILE:CA	1:141:A:ILE:C	15	1.07
(1,39)	1:70:A:VAL:N	1:70:A:VAL:CA	1:70:A:VAL:C	1:71:A:LYS:N	8	1.07
(1,23)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:GLY:N	13	1.07
(1,13)	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	1:31:A:ASP:N	11	1.07
(1,243)	1:317:A:TYR:N	1:317:A:TYR:CA	1:317:A:TYR:C	1:318:A:GLU:N	16	1.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,203)	1:259:A:LEU:N	1:259:A:LEU:CA	1:259:A:LEU:C	1:260:A:PRO:N	12	1.06
(1,164)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:LYS:N	7	1.06
(1,68)	1:98:A:LYS:C	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	14	1.06
(1,292)	1:104:A:LYS:C	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1	1.05
(1,251)	1:324:A:LEU:N	1:324:A:LEU:CA	1:324:A:LEU:C	1:325:A:LEU:N	19	1.05
(1,247)	1:320:A:LEU:N	1:320:A:LEU:CA	1:320:A:LEU:C	1:321:A:ARG:N	17	1.05
(1,179)	1:236:A:VAL:N	1:236:A:VAL:CA	1:236:A:VAL:C	1:237:A:ALA:N	5	1.05
(1,163)	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	1:210:A:HIS:N	2	1.05
(1,140)	1:180:A:ALA:C	1:181:A:SER:N	1:181:A:SER:CA	1:181:A:SER:C	3	1.05
(1,130)	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	1:165:A:LEU:N	18	1.05
(1,75)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:GLY:N	2	1.05
(1,103)	1:141:A:ILE:C	1:142:A:TYR:N	1:142:A:TYR:CA	1:142:A:TYR:C	5	1.04
(1,102)	1:141:A:ILE:N	1:141:A:ILE:CA	1:141:A:ILE:C	1:142:A:TYR:N	8	1.04
(1,69)	1:99:A:TRP:N	1:99:A:TRP:CA	1:99:A:TRP:C	1:100:A:ILE:N	19	1.04
(1,28)	1:53:A:LEU:C	1:54:A:ALA:N	1:54:A:ALA:CA	1:54:A:ALA:C	8	1.04
(1,6)	1:25:A:VAL:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	14	1.04
(1,6)	1:25:A:VAL:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	19	1.04
(1,269)	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	1:355:A:THR:N	9	1.03
(1,269)	1:354:A:ILE:N	1:354:A:ILE:CA	1:354:A:ILE:C	1:355:A:THR:N	16	1.03
(1,263)	1:331:A:ILE:N	1:331:A:ILE:CA	1:331:A:ILE:C	1:332:A:GLY:N	13	1.03
(1,240)	1:306:A:VAL:N	1:306:A:VAL:CA	1:306:A:VAL:C	1:307:A:LYS:N	6	1.03
(1,233)	1:301:A:LYS:C	1:302:A:TYR:N	1:302:A:TYR:CA	1:302:A:TYR:C	1	1.03
(1,199)	1:256:A:THR:N	1:256:A:THR:CA	1:256:A:THR:C	1:257:A:GLY:N	2	1.03
(1,191)	1:252:A:ILE:N	1:252:A:ILE:CA	1:252:A:ILE:C	1:253:A:GLN:N	8	1.03
(1,109)	1:148:A:ARG:C	1:149:A:PHE:N	1:149:A:PHE:CA	1:149:A:PHE:C	19	1.03
(1,278)	1:63:A:GLY:C	1:64:A:SER:N	1:64:A:SER:CA	1:64:A:SER:C	7	1.02
(1,153)	1:193:A:VAL:C	1:194:A:TYR:N	1:194:A:TYR:CA	1:194:A:TYR:C	9	1.02
(1,151)	1:192:A:GLN:C	1:193:A:VAL:N	1:193:A:VAL:CA	1:193:A:VAL:C	13	1.02
(1,106)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ASN:N	2	1.02
(1,44)	1:79:A:PRO:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	3	1.02
(1,28)	1:53:A:LEU:C	1:54:A:ALA:N	1:54:A:ALA:CA	1:54:A:ALA:C	1	1.02
(1,26)	1:51:A:ILE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	6	1.02
(1,45)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:PHE:N	11	1.01
(1,157)	1:201:A:ALA:N	1:201:A:ALA:CA	1:201:A:ALA:C	1:202:A:TYR:N	20	1.0
(1,154)	1:194:A:TYR:N	1:194:A:TYR:CA	1:194:A:TYR:C	1:195:A:LEU:N	10	1.0
(1,151)	1:192:A:GLN:C	1:193:A:VAL:N	1:193:A:VAL:CA	1:193:A:VAL:C	5	1.0
(1,106)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:ASN:N	4	1.0
(1,103)	1:141:A:ILE:C	1:142:A:TYR:N	1:142:A:TYR:CA	1:142:A:TYR:C	7	1.0