Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 01:30 AM EDT

PDB ID	:	2KZH
BMRB ID	:	17005
Title	:	Three-dimensional structure of a truncated phosphoribosylanthranilate isomerase (residues 255-384) from Escherichia coli
Authors	:	Setiyaputra, S.; Mackay, J.P.; Patrick, W.M.
Deposited on	:	2010-06-17

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 (i) 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 (1)) were used in the production of this report:

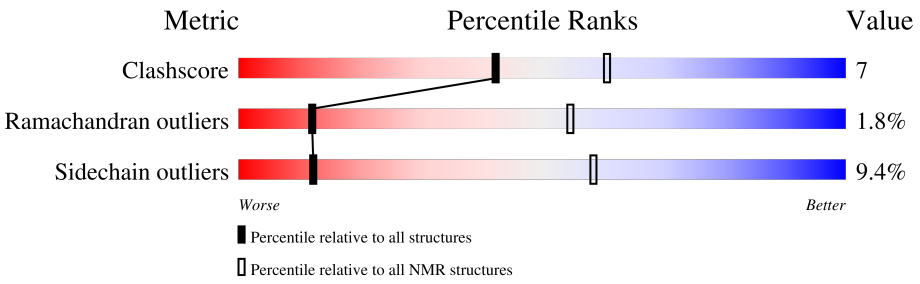
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	140	64% 16% 16% ·

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:4-A:106, A:117-A:125 (112)	0.75	13

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1999 atoms, of which 994 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tryptophan biosynthesis protein trpCF.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	134	1999	632	994	177	192	4	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P00909
A	132	ALA	-	SEE REMARK 999	UNP P00909
A	133	GLY	-	SEE REMARK 999	UNP P00909
A	134	SER	-	SEE REMARK 999	UNP P00909
A	135	HIS	-	expression tag	UNP P00909
A	136	HIS	-	expression tag	UNP P00909
A	137	HIS	-	expression tag	UNP P00909
A	138	HIS	-	expression tag	UNP P00909
A	139	HIS	-	expression tag	UNP P00909
A	140	HIS	-	expression tag	UNP P00909

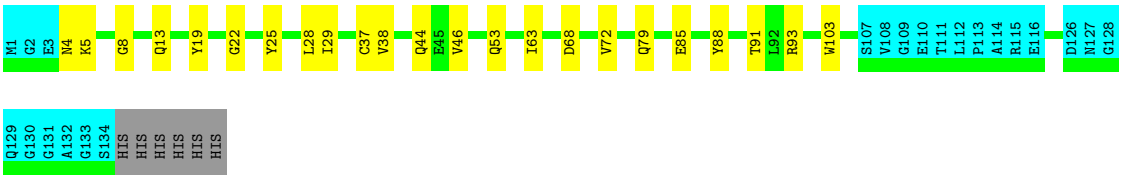
4 Residue-property plots (i)

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: Tryptophan biosynthesis protein trpCF

Chain A:



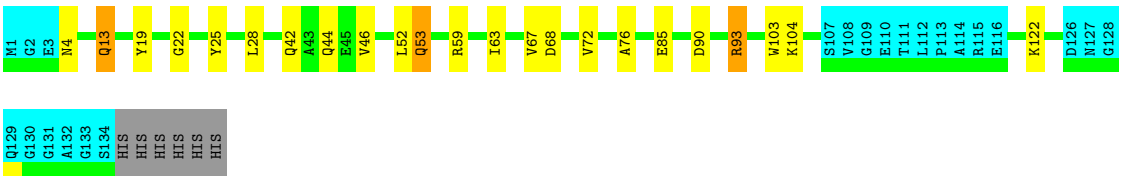
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Tryptophan biosynthesis protein trpCF

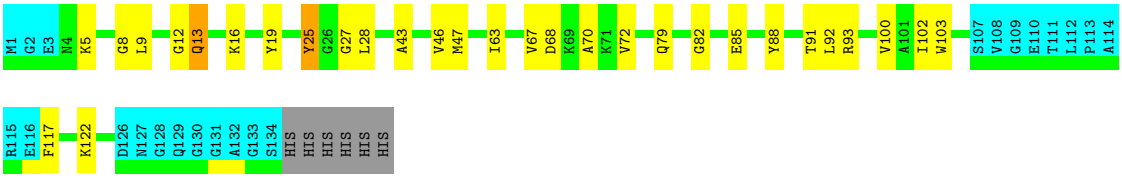
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A:



4.2.3 Score per residue for model 3

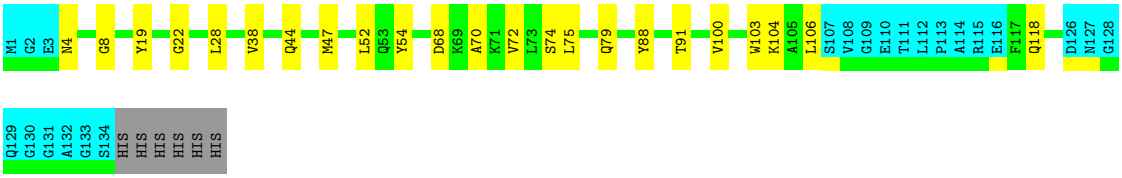
- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A:

4.2.4 Score per residue for model 4

- Molecule 1: Tryptophan biosynthesis protein trpCF

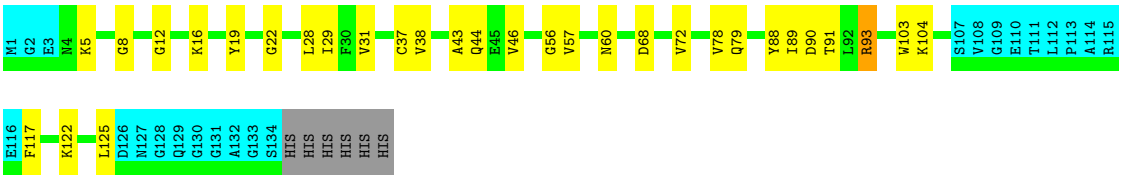
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 59% 19% • 16% •

M1 G2 E3 N4 K5 V6 C7 G8 Q13 Y19 G22 Y25 L28 I29 F30 V31 A32 C37 V38 N39 V40 Q44 L52 Q53 G56 V57 I63 D68 K69 V72 L73 Q86 L87 Y88 T91 L92 K104 S107 V108 G109 E110 T111 L112 P113 A114 R115 E116 F117 D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS HIS

4.2.7 Score per residue for model 7

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 59% 20% • 16% •

M1 G2 E3 G8 L9 Q13 Y19 Y25 L28 I29 R36 C37 V38 N39 V40 E41 Q44 L52 I63 V67 D68 K69 A70 K71 V72 L73 S74 Q79 G82 E85 D90 R93 W103 S107 V108 G109 E110 T111 L112 P113 A114 R115 E116 F117 K122 D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS HIS

4.2.8 Score per residue for model 8

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 59% 19% • 16% •

M1 G2 E3 N4 K5 G8 L9 Q13 Y19 G22 Y25 L28 I29 F30 C37 V38 N39 Q42 A43 Q44 E45 V46 Q53 G56 V57 F58 R59 D68 V72 L73 Q79 G82 N83 E84 I89 R93 W103 S107 V108 G109 E110 T111 L112 P113 A114 R115 E116 H119 D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS HIS

4.2.9 Score per residue for model 9

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 61% 18% • 16% •

M1 G2 E3 N4 K5 G8 Y19 Y25 L28 I29 F30 C37 V38 A43 Q44 E45 V46 M47 G56 D68 V72 L73 V78 Q79 E84 Y88 T91 L92 R93 W103 S107 V108 G109 E110 T111 L112 P113 A114 R115 E116 K122 D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS HIS

4.2.10 Score per residue for model 10

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 61% 19% 16% •

M1 G2 E3 N4 K5 L9 Q13 Y25 L28 A32 V38 Q42 A43 Q44 E45 V46 Q53 I63 D68 V72 Q79 G82 E85 Y88 I89 D90 T91 L92 W103 K104 S107 V108 G109 E110 T111 L112 P113 A114 R115 E116 F117 Q118 H119

K122 D126 N127 G128 G129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS HIS

4.2.11 Score per residue for model 11

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 56% 23% • 16% •

M1 G2 E3 N4 C7 G8 L9 Y19 G22 A23 I24 L28 I29 R36 C37 A43 V46 M47 L52 Q53 Y54 V57 F58 I63 V67 D68 K69 A70 K71 V72 Q79 L80 Y88 I89 D90 T91 L92 R93 V100 A101 I102 W103 S107 V108 G109

E110 T111 L112 P113 A114 R115 E116 V120 D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS HIS

4.2.12 Score per residue for model 12

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 67% 13% 16% •

M1 G2 E3 N4 K5 R11 D14 A15 K16 Y19 Y25 L28 A32 I63 V67 D68 V72 Q79 E85 Y88 T91 L92 W103 S107 V108 G109 E110 T111 L112 P113 A114 R115 E116 D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS

HIS HIS HIS HIS

4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 57% 21% • 16% •

M1 G2 E3 N4 K5 G8 L9 G12 Q13 K16 Y19 Y25 L28 S34 C37 V38 Q42 E45 I63 A64 D65 V66 V67 D68 K69 A70 K71 V72 Q79 G82 Y88 I89 D90 T91 L92 R93 V100 W103 S107 V108 G109 E110 T111

L112 P113 A114 R115 E116 F117 Q118 H119 K122 D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS HIS

4.2.14 Score per residue for model 14

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 58% 19% • 16% •

M1 G2 E3 N4 K5 L9 Q13 K16 Y19 Y25 G26 I29 F30 C37 V38 N39 V40 Q44 M47 Y54 V55 G56 V57 D65 D68 V72 L73 Q79 L80 E84 Y88 I89 D90 T91 L92 R93 I102 W103 S107 V108 G109 E110
T111 L112 P113 A114 R115 E116 D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS

4.2.15 Score per residue for model 15

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 56% 21% •• 16% •

M1 G2 E3 N4 Y19 G22 A23 I24 L28 I29 R36 C37 V38 N39 V40 E41 Q42 E45 V46 L52 Q53 V57 I63 D68 V72 L73 Q79 L80 H81 E85 Q86 L87 Y88 I89 D90 T91 L92 R93 I102 W103 S107 V108 G109 E110 T111 L112
P113 A114 R115 E116 D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS HIS

4.2.16 Score per residue for model 16

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 60% 20% 16% •

M1 G2 E3 N4 G8 Y19 G22 A23 I24 Y25 L28 I29 F30 Y31 A32 C37 V38 N39 V40 Q44 G56 V57 A70 L73 S74 Q79 L80 H81 G82 E85 Y88 T91 I102 W103 S107 V108 G109 E110 T111 L112 P113 A114 R115 E116 F117
D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS

4.2.17 Score per residue for model 17

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 59% 21% 16% •

M1 G2 E3 N4 K5 Q13 Y19 G22 L28 I29 C37 V38 Q44 Q53 V57 D68 K69 A70 K71 V72 L73 S74 L75 A76 Q79 G82 E85 Y88 T91 L92 R93 V100 W103 K104 S107 V108 G109 E110 T111 L112 P113 A114 R115
E116 F117 K122 L125 D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS HIS

4.2.18 Score per residue for model 18

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 58% 22% 16% •

M1 G2 E3 N4 K5 G8 Q13 Y19 G22 Y25 L28 I29 A32 R36 C37 A43 Q44 E45 V46 L52 Q53 Y54 V57 I63 D68 V72 Q79 E85 Q86 L87 Y88 I89 D90 T91 L92 R93 I102 W103 S107 V108 G109 E110

T111 L112 P113 A114 R115 E116 D126 N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS

4.2.19 Score per residue for model 19

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 63% 17% 16% •

M1 G2 E3 N4 K5 G8 Y19 Y25 L28 I29 Q44 Q53 V57 N60 I63 V67 D68 K69 A70 K71 V72 L73 S74 Q79 Y88 T91 L92 R93 I102 W103 S107 V108 G109 E110 T111 L112 P113 A114 R115 E116 D126 N127 G128 Q129

G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS HIS

4.2.20 Score per residue for model 20

- Molecule 1: Tryptophan biosynthesis protein trpCF

Chain A: 63% 14% • 16% •

M1 G2 E3 V6 C7 G8 Q13 Y19 L28 I29 V38 N39 V40 E41 Q42 A43 Q44 E45 V46 M47 Y54 D68 V72 L73 Q79 L80 H81 E85 Q86 D90 R93 W103 S107 V108 G109 E110 T111 L112 P113 A114 R115 E116 K122 D126

N127 G128 Q129 G130 G131 A132 G133 S134 HIS HIS HIS HIS HIS HIS

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CNS	structure solution	1.21
CNS	refinement	1.21

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	1482
Number of shifts mapped to atoms	1482
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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	0.91±0.02	0±0/876 (0.0± 0.0%)	0.74±0.03	0±0/1193 (0.0± 0.0%)
All	All	0.91	1/17520 (0.0%)	0.74	0/23860 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.4
All	All	0	3

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	39	ASN	CG-ND2	-5.18	1.20	1.32	8	1

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	93	ARG	Sidechain	2
1	A	59	ARG	Sidechain	1

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	859	862	862	12±4
All	All	17180	17240	17240	247

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:ALA:HA	1:A:46:VAL:HG12	0.75	1.57	2	5
1:A:93:ARG:NH2	1:A:102:ILE:HB	0.69	2.02	11	1
1:A:76:ALA:O	1:A:100:VAL:HA	0.66	1.91	17	1
1:A:47:MET:HA	1:A:54:TYR:OH	0.63	1.93	11	3
1:A:90:ASP:HA	1:A:93:ARG:NE	0.62	2.09	5	3
1:A:93:ARG:HD2	1:A:102:ILE:HD12	0.62	1.72	3	2
1:A:13:GLN:H	1:A:13:GLN:NE2	0.61	1.94	2	10
1:A:47:MET:SD	1:A:73:LEU:HA	0.59	2.37	9	1
1:A:90:ASP:HA	1:A:93:ARG:NH1	0.57	2.15	15	2
1:A:90:ASP:HA	1:A:93:ARG:CZ	0.57	2.29	14	5
1:A:79:GLN:NE2	1:A:103:TRP:HB2	0.56	2.15	14	18
1:A:42:GLN:O	1:A:45:GLU:HG2	0.55	2.01	13	2
1:A:82:GLY:HA3	1:A:117:PHE:CZ	0.55	2.37	7	4
1:A:42:GLN:O	1:A:46:VAL:HG23	0.54	2.02	1	6
1:A:53:GLN:NE2	1:A:76:ALA:HB2	0.54	2.16	1	1
1:A:29:ILE:O	1:A:37:CYS:HB3	0.54	2.03	16	10
1:A:79:GLN:HE22	1:A:103:TRP:HB2	0.53	1.63	20	3
1:A:93:ARG:NH2	1:A:120:VAL:HA	0.53	2.18	11	1
1:A:93:ARG:HD2	1:A:102:ILE:HD13	0.53	1.79	18	2
1:A:63:ILE:HG13	1:A:92:LEU:HD13	0.53	1.81	3	7
1:A:70:ALA:O	1:A:74:SER:HA	0.53	2.03	7	5
1:A:40:VAL:HG23	1:A:73:LEU:HB2	0.52	1.81	7	4
1:A:70:ALA:HB1	1:A:100:VAL:HG21	0.52	1.79	13	5
1:A:4:ASN:HD21	1:A:24:ILE:HB	0.52	1.65	15	1
1:A:29:ILE:HG23	1:A:57:VAL:HB	0.52	1.82	6	2
1:A:30:PHE:CE2	1:A:56:GLY:HA3	0.51	2.40	16	5
1:A:4:ASN:OD1	1:A:24:ILE:HB	0.51	2.06	16	2
1:A:4:ASN:HD22	1:A:4:ASN:N	0.50	2.04	15	2
1:A:40:VAL:HG21	1:A:69:LYS:HD2	0.50	1.83	6	1
1:A:29:ILE:HG22	1:A:57:VAL:O	0.50	2.05	8	4
1:A:88:TYR:O	1:A:91:THR:HB	0.50	2.07	10	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:ASP:O	1:A:72:VAL:HG23	0.50	2.06	12	19
1:A:12:GLY:O	1:A:16:LYS:HG3	0.49	2.07	13	3
1:A:29:ILE:CG2	1:A:57:VAL:HB	0.49	2.38	14	6
1:A:103:TRP:CD1	1:A:122:LYS:HB2	0.48	2.43	13	5
1:A:82:GLY:HA3	1:A:117:PHE:CE1	0.47	2.45	2	1
1:A:28:LEU:HD11	1:A:54:TYR:CD2	0.47	2.45	20	1
1:A:88:TYR:CZ	1:A:92:LEU:HD21	0.47	2.45	15	2
1:A:103:TRP:CD1	1:A:122:LYS:HB3	0.46	2.45	5	4
1:A:25:TYR:HA	1:A:53:GLN:HB3	0.46	1.87	8	1
1:A:63:ILE:CD1	1:A:91:THR:HG22	0.46	2.41	3	2
1:A:34:SER:OG	1:A:37:CYS:HB2	0.46	2.10	13	1
1:A:6:VAL:O	1:A:28:LEU:HB3	0.46	2.11	20	2
1:A:82:GLY:HA3	1:A:117:PHE:CE2	0.46	2.46	13	1
1:A:8:GLY:HA2	1:A:38:VAL:HG23	0.46	1.88	6	2
1:A:36:ARG:HA	1:A:36:ARG:HE	0.46	1.70	18	1
1:A:36:ARG:HG3	1:A:37:CYS:SG	0.45	2.51	15	2
1:A:93:ARG:CZ	1:A:119:HIS:HB2	0.45	2.42	13	1
1:A:82:GLY:HA2	1:A:89:ILE:HD11	0.45	1.87	13	3
1:A:118:GLN:HG3	1:A:119:HIS:CD2	0.45	2.47	10	1
1:A:63:ILE:O	1:A:67:VAL:HG23	0.45	2.11	7	7
1:A:65:ASP:O	1:A:68:ASP:HB3	0.45	2.12	13	2
1:A:79:GLN:HA	1:A:103:TRP:O	0.44	2.12	4	2
1:A:44:GLN:O	1:A:47:MET:HG2	0.44	2.12	14	1
1:A:80:LEU:HD13	1:A:92:LEU:HG	0.44	1.88	14	2
1:A:39:ASN:ND2	1:A:41:GLU:HB2	0.44	2.27	7	2
1:A:40:VAL:HG23	1:A:73:LEU:HD23	0.44	1.89	14	1
1:A:5:LYS:HG3	1:A:27:GLY:HA3	0.44	1.90	2	1
1:A:11:ARG:HB2	1:A:14:ASP:HB3	0.44	1.90	12	2
1:A:43:ALA:HA	1:A:46:VAL:CG1	0.43	2.38	2	2
1:A:8:GLY:HA3	1:A:37:CYS:N	0.43	2.28	18	1
1:A:85:GLU:CD	1:A:86:GLN:H	0.43	2.16	15	2
1:A:93:ARG:HG3	1:A:102:ILE:HD12	0.43	1.89	15	1
1:A:93:ARG:NH2	1:A:119:HIS:HB2	0.43	2.28	13	1
1:A:26:GLY:O	1:A:55:VAL:HG12	0.43	2.13	14	1
1:A:93:ARG:CD	1:A:102:ILE:HD12	0.43	2.42	2	2
1:A:9:LEU:HD11	1:A:14:ASP:HB3	0.43	1.90	3	1
1:A:29:ILE:HG13	1:A:37:CYS:SG	0.43	2.53	17	2
1:A:80:LEU:CD1	1:A:92:LEU:HG	0.43	2.44	15	1
1:A:4:ASN:ND2	1:A:24:ILE:HB	0.42	2.27	15	1
1:A:85:GLU:HB3	1:A:88:TYR:HB2	0.42	1.92	16	1
1:A:56:GLY:O	1:A:78:VAL:HA	0.42	2.15	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ARG:NH1	1:A:119:HIS:HB2	0.42	2.30	8	1
1:A:87:LEU:O	1:A:90:ASP:HB3	0.42	2.15	18	1
1:A:59:ARG:HD3	1:A:84:GLU:OE1	0.41	2.15	8	1
1:A:11:ARG:HB2	1:A:14:ASP:CB	0.41	2.46	3	1
1:A:80:LEU:HD12	1:A:102:ILE:HG12	0.41	1.92	14	1
1:A:93:ARG:CZ	1:A:102:ILE:HB	0.41	2.45	11	1
1:A:93:ARG:H	1:A:93:ARG:HD3	0.41	1.75	9	1
1:A:40:VAL:CG2	1:A:69:LYS:HD2	0.41	2.46	6	1
1:A:86:GLN:HA	1:A:117:PHE:CD1	0.41	2.50	6	1
1:A:7:CYS:HB2	1:A:36:ARG:O	0.41	2.15	11	1
1:A:80:LEU:CD2	1:A:89:ILE:HG13	0.41	2.46	11	1
1:A:5:LYS:HD3	1:A:25:TYR:OH	0.40	2.16	2	1
1:A:44:GLN:HE21	1:A:44:GLN:HB3	0.40	1.60	14	1
1:A:80:LEU:HD23	1:A:102:ILE:HG23	0.40	1.93	16	1
1:A:89:ILE:HD13	1:A:117:PHE:CD1	0.40	2.52	5	1
1:A:8:GLY:O	1:A:9:LEU:HB3	0.40	2.15	13	1
1:A:79:GLN:OE1	1:A:103:TRP:HB2	0.40	2.16	15	1
1:A:31:VAL:CG1	1:A:37:CYS:HB2	0.40	2.47	5	1
1:A:93:ARG:HG3	1:A:119:HIS:CE1	0.40	2.51	3	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	112/140 (80%)	100±2 (89±1%)	10±2 (9±1%)	2±1 (2±1%)	12	54
All	All	2240/2800 (80%)	1990 (89%)	210 (9%)	40 (2%)	12	54

All 6 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	22	GLY	11
1	A	8	GLY	11
1	A	5	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	32	ALA	5
1	A	81	HIS	2
1	A	83	ASN	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	87/107 (81%)	79±2 (91±2%)	8±2 (9±2%)	12 58
All	All	1740/2140 (81%)	1577 (91%)	163 (9%)	12 58

All 25 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	19	TYR	19
1	A	28	LEU	19
1	A	44	GLN	15
1	A	25	TYR	13
1	A	38	VAL	11
1	A	13	GLN	9
1	A	53	GLN	9
1	A	85	GLU	9
1	A	93	ARG	9
1	A	52	LEU	8
1	A	4	ASN	7
1	A	9	LEU	7
1	A	104	LYS	6
1	A	73	LEU	4
1	A	16	LYS	3
1	A	47	MET	2
1	A	75	LEU	2
1	A	60	ASN	2
1	A	125	LEU	2
1	A	84	GLU	2
1	A	106	LEU	1
1	A	118	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	58	PHE	1
1	A	54	TYR	1
1	A	29	ILE	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 monosaccharides 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 85% for the well-defined parts and 85% 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	1482
Number of shifts mapped to atoms	1482
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	132	-0.27 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	119	0.06 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	134	-0.08 ± 0.13	None needed (< 0.5 ppm)
^{15}N	125	-0.05 ± 0.38	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 85%, i.e. 1289 atoms were assigned a chemical shift out of a possible 1513. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	552/561 (98%)	224/228 (98%)	223/224 (100%)	105/109 (96%)
Sidechain	699/837 (84%)	476/551 (86%)	214/257 (83%)	9/29 (31%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	38/115 (33%)	37/57 (65%)	0/53 (0%)	1/5 (20%)
Overall	1289/1513 (85%)	737/836 (88%)	437/534 (82%)	115/143 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1482 atoms were assigned a chemical shift out of a possible 1749. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	661/675 (98%)	270/277 (97%)	266/268 (99%)	125/130 (96%)
Sidechain	783/959 (82%)	535/629 (85%)	237/296 (80%)	11/34 (32%)
Aromatic	38/115 (33%)	37/57 (65%)	0/53 (0%)	1/5 (20%)
Overall	1482/1749 (85%)	842/963 (87%)	503/617 (82%)	137/169 (81%)

7.1.4 Statistically unusual chemical shifts (i)

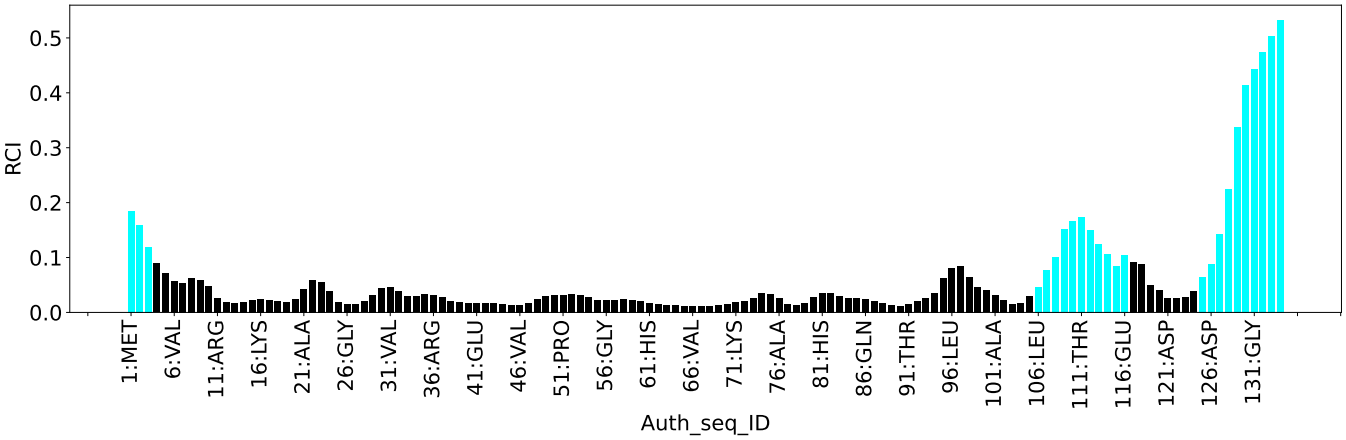
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	122	LYS	HB2	0.39	0.58 – 2.97	-5.8
1	A	77	ALA	HB1	0.04	0.14 – 2.58	-5.4
1	A	77	ALA	HB2	0.04	0.14 – 2.58	-5.4
1	A	77	ALA	HB3	0.04	0.14 – 2.58	-5.4
1	A	122	LYS	HD2	0.55	0.58 – 2.64	-5.1
1	A	115	ARG	HG2	0.23	0.26 – 2.87	-5.1

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
1:MET
6:VAL
11:ARG
16:LYS
21:ALA
26:GLY
31:VAL
36:ARG
41:GLU
46:VAL
51:PRO
56:GLY
61:HIS
66:VAL
71:LYS
76:ALA
81:HIS
86:GLN
91:THR
96:LEU
101:ALA
106:LEU
111:THR
116:GLU
121:ASP
126:ASP
131:GLY
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	2297
Intra-residue (|i-j|=0)	515
Sequential (|i-j|=1)	595
Medium range (|i-j|>1 and |i-j|<5)	507
Long range (|i-j|≥5)	621
Inter-chain	0
Hydrogen bond restraints	59
Disulfide bond restraints	0
Total dihedral-angle restraints	208
Number of unmapped restraints	0
Number of restraints per residue	17.9
Number of long range restraints per residue[1]	4.6

[1]Long 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 (i)

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 (i)

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)	9.6	0.2
0.2-0.5 (Medium)	9.1	0.5
>0.5 (Large)	11.8	3.64

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)	9.6	4.4
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

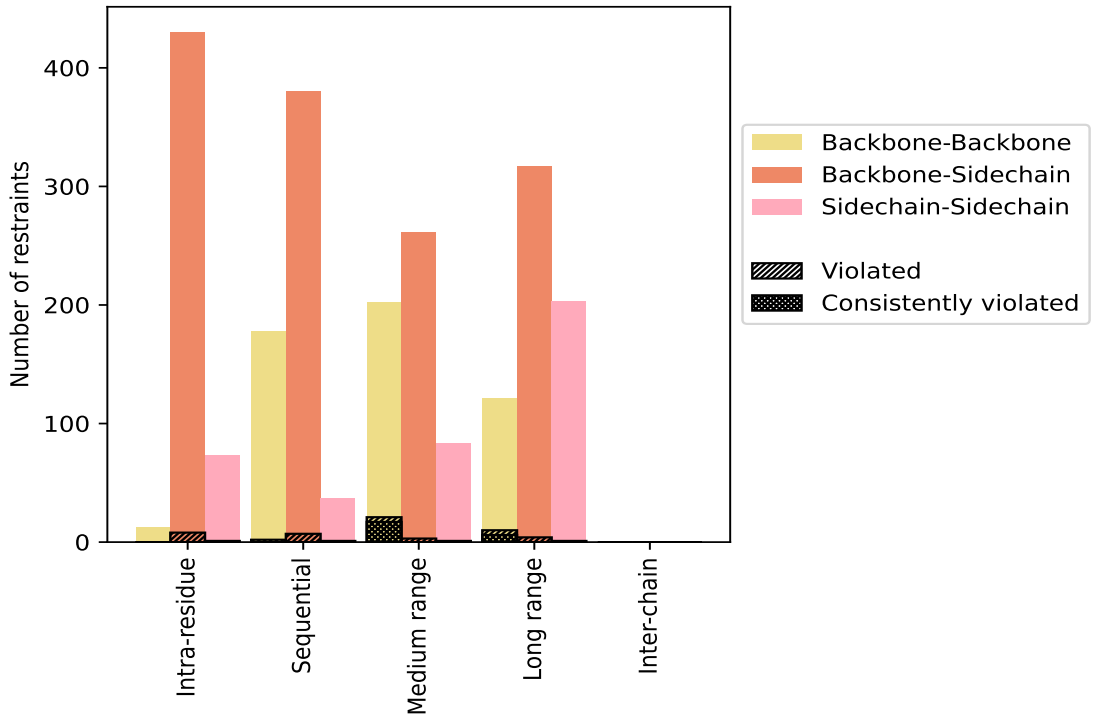
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	515	22.4	9	1.7	0.4	0	0.0	0.0
Backbone-Backbone	12	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	430	18.7	8	1.9	0.3	0	0.0	0.0
Sidechain-Sidechain	73	3.2	1	1.4	0.0	0	0.0	0.0
Sequential (|i-j|=1)	595	25.9	10	1.7	0.4	0	0.0	0.0
Backbone-Backbone	178	7.7	2	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	380	16.5	7	1.8	0.3	0	0.0	0.0
Sidechain-Sidechain	37	1.6	1	2.7	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	507	22.1	6	1.2	0.3	0	0.0	0.0
Backbone-Backbone	163	7.1	2	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	261	11.4	3	1.1	0.1	0	0.0	0.0
Sidechain-Sidechain	83	3.6	1	1.2	0.0	0	0.0	0.0
Long range (|i-j|≥5)	621	27.0	6	1.0	0.3	0	0.0	0.0
Backbone-Backbone	101	4.4	1	1.0	0.0	0	0.0	0.0
Backbone-Sidechain	317	13.8	4	1.3	0.2	0	0.0	0.0
Sidechain-Sidechain	203	8.8	1	0.5	0.0	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	59	2.6	28	47.5	1.2	23	39.0	1.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2297	100.0	59	2.6	2.6	23	1.0	1.0
Backbone-Backbone	513	22.3	33	6.4	1.4	23	4.5	1.0
Backbone-Sidechain	1388	60.4	22	1.6	1.0	0	0.0	0.0
Sidechain-Sidechain	396	17.2	4	1.0	0.2	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	2	1	19	7	0	29	0.52	1.62	0.43	0.39
2	3	2	19	7	0	31	0.53	2.19	0.49	0.35
3	2	3	18	8	0	31	0.54	1.77	0.5	0.39
4	4	2	18	7	0	31	0.52	1.79	0.41	0.39
5	3	3	19	6	0	31	0.47	1.59	0.4	0.29
6	2	4	19	8	0	33	0.46	1.75	0.43	0.26
7	2	2	17	6	0	27	0.55	1.62	0.42	0.43
8	4	2	19	7	0	32	0.47	1.45	0.37	0.29
9	1	0	18	6	0	25	0.68	1.95	0.49	0.6
10	3	3	18	10	0	34	0.5	1.85	0.48	0.29
11	4	0	19	9	0	32	0.49	1.45	0.41	0.32

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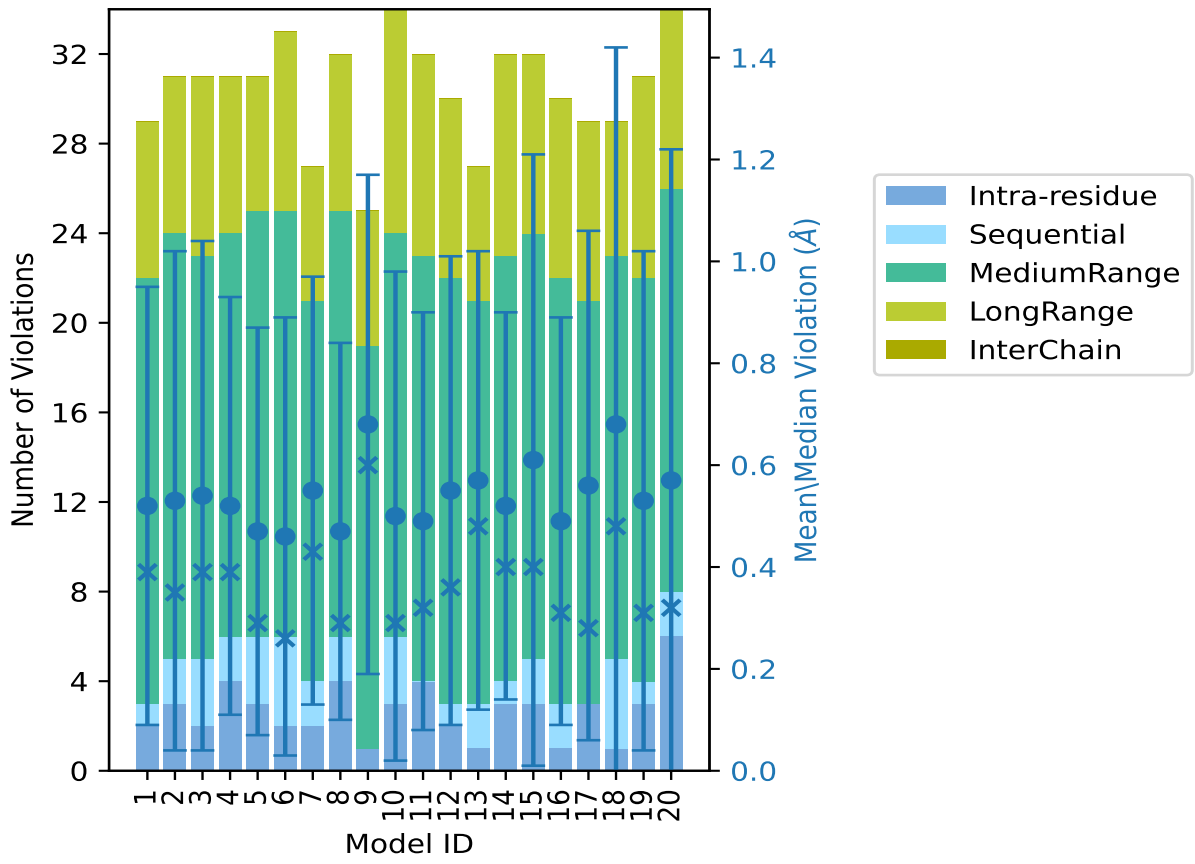
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	1	19	8	0	30	0.55	2.02	0.46	0.36
13	1	2	18	6	0	27	0.57	2.01	0.45	0.48
14	3	1	19	9	0	32	0.52	1.3	0.38	0.4
15	3	2	19	8	0	32	0.61	2.79	0.6	0.4
16	1	2	19	8	0	30	0.49	1.66	0.4	0.31
17	3	0	18	8	0	29	0.56	1.87	0.5	0.28
18	1	4	18	6	0	29	0.68	3.64	0.74	0.48
19	3	1	18	9	0	31	0.53	1.82	0.49	0.31
20	6	2	18	8	0	34	0.57	3.36	0.65	0.32

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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

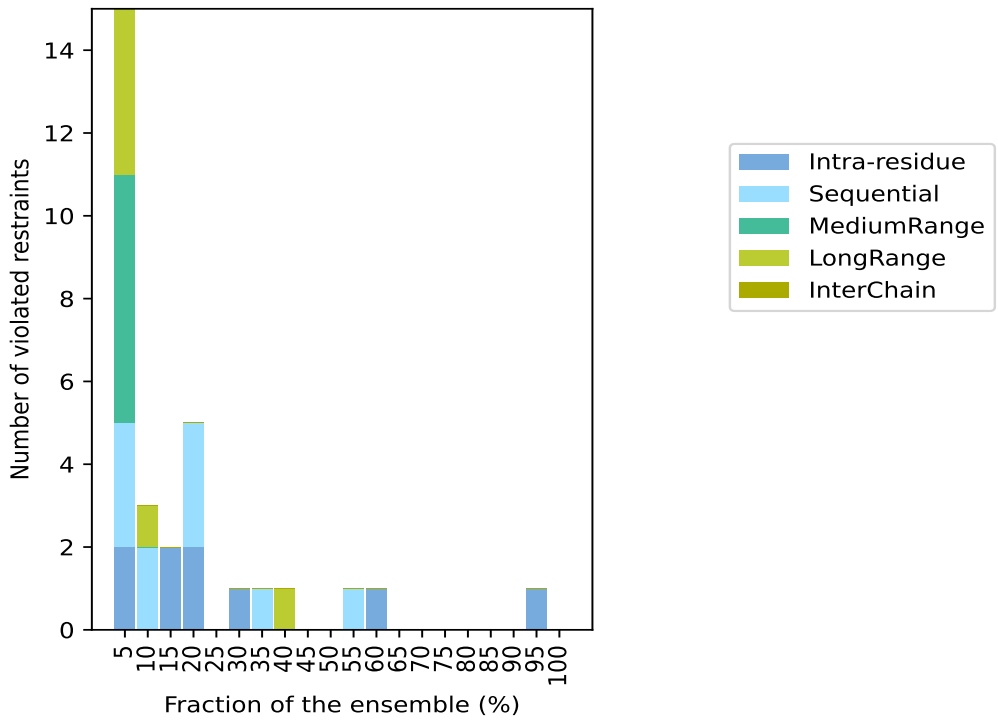
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2207(IR:506, SQ:585, MR:501, LR:615, 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	3	6	4	0	15	1	5.0
0	2	0	1	0	3	2	10.0
2	0	0	0	0	2	3	15.0
2	3	0	0	0	5	4	20.0
0	0	0	0	0	0	5	25.0
1	0	0	0	0	1	6	30.0
0	1	0	0	0	1	7	35.0
0	0	0	1	0	1	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	1	0	0	0	1	11	55.0
1	0	0	0	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	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
1	0	0	0	0	1	19	95.0
0	0	0	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

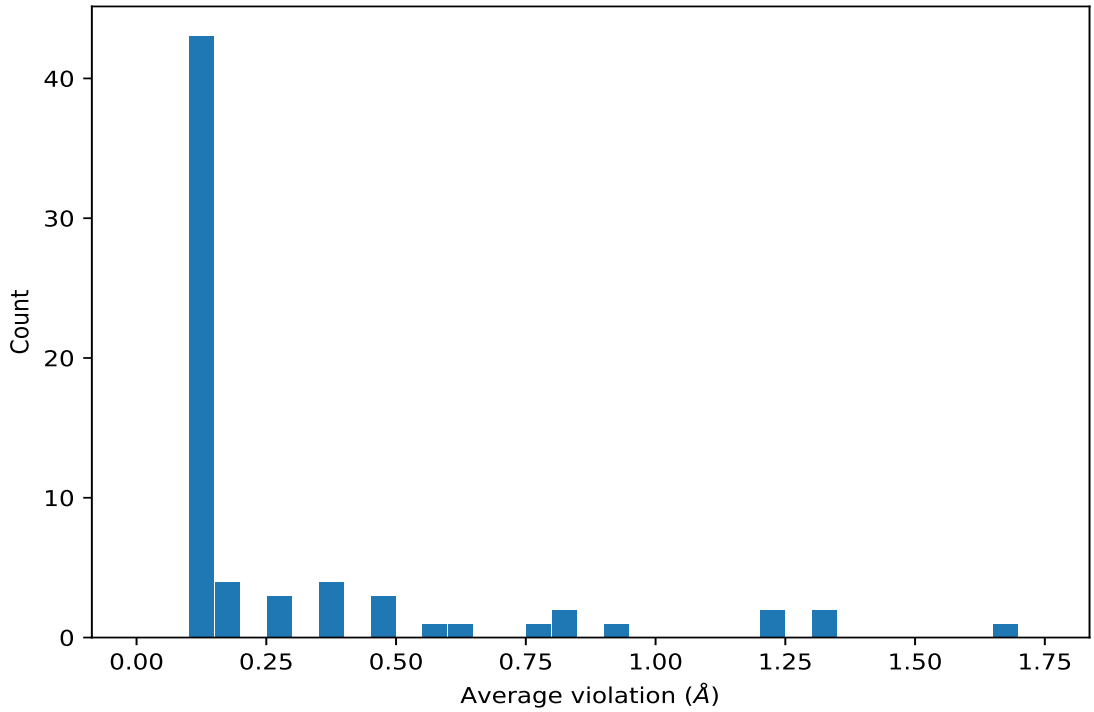
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	20	1.68	0.28	1.66
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	20	1.32	0.15	1.33
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	20	1.31	0.23	1.31
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	20	1.22	0.35	1.07
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	20	1.22	0.93	0.95
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	20	0.91	0.23	0.93
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	20	0.84	0.08	0.84
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	20	0.84	0.24	0.84
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	20	0.75	0.11	0.74
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	20	0.62	0.36	0.63
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	20	0.6	0.12	0.6
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	20	0.49	0.16	0.52
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	20	0.49	0.18	0.44
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	20	0.46	0.17	0.52
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	20	0.39	0.21	0.3
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	20	0.39	0.09	0.38

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	20	0.36	0.06	0.36
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	20	0.36	0.06	0.36
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	20	0.3	0.07	0.29
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	20	0.27	0.09	0.24
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	20	0.25	0.08	0.25
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	20	0.18	0.06	0.17
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	20	0.18	0.04	0.18
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	19	0.12	0.01	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	19	0.12	0.01	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	19	0.12	0.01	0.12
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	16	0.18	0.05	0.16
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	12	0.14	0.03	0.13
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	12	0.14	0.03	0.13
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	11	0.13	0.01	0.13
(3,2)	1:A:78:VAL:N	1:A:101:ALA:O	8	0.15	0.02	0.14
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG21	8	0.12	0.01	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG22	8	0.12	0.01	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG23	8	0.12	0.01	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG21	8	0.12	0.01	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG22	8	0.12	0.01	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG23	8	0.12	0.01	0.12
(3,20)	1:A:72:VAL:N	1:A:68:ASP:O	7	0.16	0.04	0.17
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD2	7	0.13	0.01	0.14
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD3	7	0.13	0.01	0.14
(2,5)	1:A:79:GLN:H	1:A:56:GLY:O	6	0.13	0.01	0.13
(1,982)	1:A:42:GLN:H	1:A:42:GLN:HE22	6	0.12	0.01	0.12
(1,496)	1:A:44:GLN:HA	1:A:44:GLN:HE22	4	0.12	0.01	0.13
(1,594)	1:A:53:GLN:H	1:A:53:GLN:HG2	4	0.12	0.01	0.12
(1,594)	1:A:53:GLN:H	1:A:53:GLN:HG3	4	0.12	0.01	0.12
(1,839)	1:A:91:THR:HG21	1:A:92:LEU:H	4	0.12	0.0	0.12
(1,839)	1:A:91:THR:HG22	1:A:92:LEU:H	4	0.12	0.0	0.12
(1,839)	1:A:91:THR:HG23	1:A:92:LEU:H	4	0.12	0.0	0.12
(1,566)	1:A:93:ARG:HD3	1:A:94:GLU:H	4	0.11	0.0	0.11
(1,1213)	1:A:29:ILE:HG21	1:A:30:PHE:H	4	0.11	0.0	0.11
(1,1213)	1:A:29:ILE:HG22	1:A:30:PHE:H	4	0.11	0.0	0.11
(1,1213)	1:A:29:ILE:HG23	1:A:30:PHE:H	4	0.11	0.0	0.11
(2,4)	1:A:101:ALA:H	1:A:76:ALA:O	3	0.13	0.02	0.14
(1,1556)	1:A:79:GLN:H	1:A:79:GLN:HB3	3	0.12	0.0	0.12
(1,384)	1:A:6:VAL:HA	1:A:6:VAL:HB	3	0.11	0.0	0.11
(1,384)	1:A:116:GLU:HA	1:A:116:GLU:HB2	3	0.11	0.0	0.11
(1,1877)	1:A:13:GLN:HE21	1:A:14:ASP:HB2	2	0.14	0.02	0.14
(1,1877)	1:A:13:GLN:HE21	1:A:14:ASP:HB3	2	0.14	0.02	0.14

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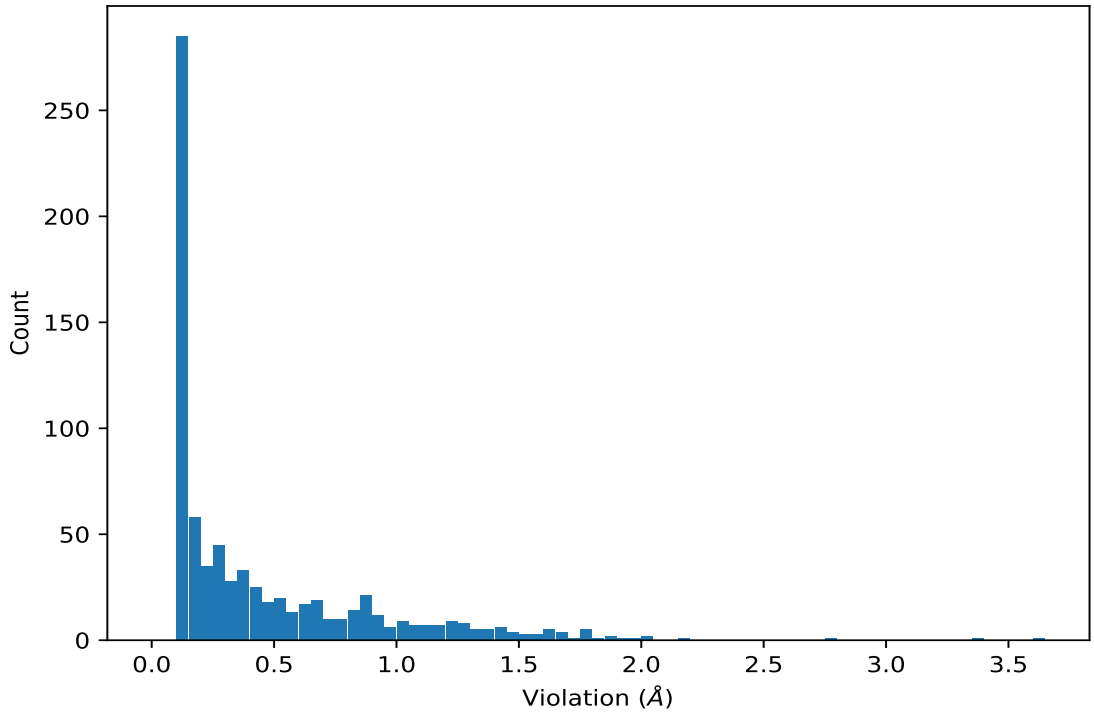
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1877)	1:A:13:GLN:HE22	1:A:14:ASP:HB2	2	0.14	0.02	0.14
(1,1877)	1:A:13:GLN:HE22	1:A:14:ASP:HB3	2	0.14	0.02	0.14
(1,2000)	1:A:45:GLU:HB2	1:A:46:VAL:H	2	0.12	0.0	0.12
(1,2000)	1:A:45:GLU:HB3	1:A:46:VAL:H	2	0.12	0.0	0.12
(1,2106)	1:A:78:VAL:HG11	1:A:103:TRP:H	2	0.12	0.0	0.12
(1,2106)	1:A:78:VAL:HG12	1:A:103:TRP:H	2	0.12	0.0	0.12
(1,2106)	1:A:78:VAL:HG13	1:A:103:TRP:H	2	0.12	0.0	0.12
(1,2106)	1:A:78:VAL:HG21	1:A:103:TRP:H	2	0.12	0.0	0.12
(1,2106)	1:A:78:VAL:HG22	1:A:103:TRP:H	2	0.12	0.0	0.12
(1,2106)	1:A:78:VAL:HG23	1:A:103:TRP:H	2	0.12	0.0	0.12

[1]Number of violated models, [2]Standard 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)
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	18	3.64
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	20	3.36
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	15	2.79
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	2	2.19
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	12	2.02
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	13	2.01
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	9	1.95
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	9	1.93
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	17	1.87
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	10	1.85
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	19	1.82
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	4	1.79
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	18	1.77
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	3	1.77
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	6	1.75
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	19	1.75
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	3	1.72
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	15	1.67
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	6	1.66
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	16	1.66
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	18	1.65
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	20	1.64
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	1	1.62
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	7	1.62
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	3	1.6
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	18	1.6
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	10	1.59
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	5	1.59
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	18	1.57
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	1	1.54
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	20	1.53
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	13	1.5
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	15	1.49
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	2	1.49
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	8	1.45
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	11	1.45
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	2	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	17	1.42
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	10	1.41
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	7	1.4
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	17	1.4
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	5	1.4
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	11	1.39
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	3	1.36
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	19	1.36
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	15	1.35
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	20	1.35
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	3	1.33
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	9	1.32
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	4	1.32
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	13	1.31
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	14	1.3
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	14	1.29
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	16	1.29
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	10	1.29
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	17	1.28
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	5	1.27
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	10	1.26
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	15	1.26
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	8	1.26
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	2	1.24
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	14	1.24
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	7	1.24
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	15	1.24
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	12	1.23
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	17	1.21
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	19	1.21
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	17	1.2
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	6	1.2
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	7	1.19
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	11	1.19
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	12	1.19
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	12	1.18
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	11	1.17
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	16	1.17
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	14	1.16
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	1	1.14
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	11	1.14
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	1	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,10)	1:A:57:VAL:N	1:A:28:LEU:O	8	1.12
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	9	1.11
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	20	1.11
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	17	1.1
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	12	1.08
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	12	1.07
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	5	1.07
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	14	1.07
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	16	1.05
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	16	1.05
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	19	1.05
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	12	1.04
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	4	1.04
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	11	1.04
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	19	1.04
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	19	1.03
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	2	1.02
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	10	1.02
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	6	1.01
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	9	1.0
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	9	0.99
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	7	0.98
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	9	0.98
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	17	0.98
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	7	0.97
(3,25)	1:A:89:ILE:N	1:A:85:GLU:O	4	0.95
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	1	0.94
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	13	0.93
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	14	0.93
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	8	0.93
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	20	0.92
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	15	0.91
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	8	0.91
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	5	0.9
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	13	0.9
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	1	0.9
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	4	0.9
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	1	0.9
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	13	0.89
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	20	0.89
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	6	0.89
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	20	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	11	0.89
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	4	0.89
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	4	0.88
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	4	0.88
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	3	0.88
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	14	0.88
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	14	0.87
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	8	0.87
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	15	0.87
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	20	0.87
(3,24)	1:A:90:ASP:N	1:A:86:GLN:O	6	0.86
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	6	0.86
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	4	0.85
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	8	0.85
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	1	0.85
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	3	0.85
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	10	0.85
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	18	0.84
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	10	0.84
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	19	0.84
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	2	0.83
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	14	0.83
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	15	0.83
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	4	0.82
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	8	0.82
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	15	0.82
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	13	0.82
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	2	0.82
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	5	0.81
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	16	0.81
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	19	0.8
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	18	0.79
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	12	0.79
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	9	0.77
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	13	0.77
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	9	0.77
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	5	0.77
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	7	0.77
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	12	0.76
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	7	0.75
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	20	0.75
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	8	0.74
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	6	0.74
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	11	0.73
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	18	0.73
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	8	0.72
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	18	0.71
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	12	0.71
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	3	0.7
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	10	0.7
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	16	0.69
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	18	0.69
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	16	0.69
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	6	0.68
(3,21)	1:A:93:ARG:N	1:A:89:ILE:O	12	0.68
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	9	0.68
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	9	0.68
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	15	0.67
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	3	0.67
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	16	0.67
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	14	0.67
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	15	0.67
(3,8)	1:A:77:ALA:N	1:A:54:TYR:O	11	0.66
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	5	0.66
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	19	0.66
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	9	0.65
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	20	0.65
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	1	0.65
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	7	0.65
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	17	0.64
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	10	0.63
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	13	0.63
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	17	0.62
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	18	0.61
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	5	0.61
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	7	0.61
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	10	0.61
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	13	0.61
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	16	0.61
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	9	0.6
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	12	0.6
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	2	0.6
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	17	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	9	0.6
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	4	0.6
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	11	0.6
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	4	0.59
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	10	0.59
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	18	0.59
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	2	0.58
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	5	0.58
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	7	0.57
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	19	0.57
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	6	0.57
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	7	0.56
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	16	0.56
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	18	0.55
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	10	0.55
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	18	0.55
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	11	0.54
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	2	0.54
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	6	0.54
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	15	0.54
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	2	0.54
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	2	0.54
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	14	0.54
(3,12)	1:A:95:ALA:N	1:A:91:THR:O	17	0.54
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	13	0.53
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	5	0.53
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	19	0.52
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	14	0.52
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	14	0.52
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	14	0.51
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	20	0.51
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	7	0.51
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	10	0.5
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	1	0.5
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	8	0.5
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	13	0.5
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	1	0.49
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	3	0.49
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	13	0.49
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	11	0.49
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	14	0.48
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	18	0.48
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	3	0.48
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	13	0.48
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	18	0.48
(3,9)	1:A:55:VAL:N	1:A:26:GLY:O	8	0.47
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	3	0.47
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	3	0.47
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	20	0.46
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	5	0.46
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	14	0.46
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	18	0.45
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	2	0.45
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	2	0.43
(3,28)	1:A:115:ARG:N	1:A:113:PRO:O	5	0.43
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	9	0.43
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	16	0.43
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	7	0.43
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	9	0.43
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	4	0.42
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	3	0.42
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	4	0.42
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	15	0.42
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	2	0.42
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	1	0.41
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	8	0.41
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	12	0.41
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	1	0.41
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	11	0.41
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	13	0.41
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	4	0.41
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	12	0.41
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	20	0.4
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	6	0.4
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	15	0.4
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	19	0.4
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	6	0.4
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	15	0.4
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	16	0.39
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	1	0.39
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	5	0.39
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	15	0.39
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	4	0.39
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	20	0.39
(3,13)	1:A:66:VAL:N	1:A:62:ASP:O	3	0.39
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	8	0.38
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	12	0.38
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	17	0.38
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	4	0.38
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	17	0.38
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	16	0.37
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	11	0.37
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	20	0.37
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	15	0.37
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	9	0.36
(3,29)	1:A:84:GLU:N	1:A:81:HIS:O	7	0.36
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	10	0.36
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	11	0.36
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	13	0.36
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	10	0.36
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	11	0.36
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	13	0.36
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	2	0.35
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	14	0.35
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	2	0.35
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	14	0.35
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	12	0.35
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	19	0.35
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	2	0.35
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	14	0.35
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	12	0.34
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	7	0.33
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	1	0.33
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	4	0.33
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	4	0.33
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	9	0.32
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	7	0.32
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	20	0.32
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	8	0.32
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	9	0.32
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	3	0.32
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	19	0.32
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	7	0.32
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	4	0.31
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	15	0.31
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	16	0.31
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	1	0.31
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	16	0.31
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	19	0.31
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	20	0.31
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	13	0.31
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	1	0.31
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	16	0.31
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	9	0.3
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	6	0.3
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	6	0.3
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	8	0.3
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	5	0.29
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	11	0.29
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	20	0.29
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	5	0.29
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	10	0.29
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	16	0.29
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	10	0.28
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	17	0.28
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	13	0.28
(3,22)	1:A:91:THR:N	1:A:87:LEU:O	8	0.28
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	2	0.28
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	12	0.28
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	11	0.28
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	17	0.28
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	6	0.28
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	17	0.28
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	8	0.27
(3,6)	1:A:56:GLY:N	1:A:77:ALA:O	13	0.27
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	4	0.27
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	8	0.27
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	19	0.27
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	7	0.27
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	14	0.27
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	11	0.27
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	18	0.27
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	8	0.27
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	19	0.27
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	6	0.26
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	2	0.26
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	5	0.26
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	6	0.26
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	12	0.26
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	15	0.25
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	8	0.25
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	14	0.25
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	5	0.25
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	8	0.25
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	4	0.25
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	17	0.25
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	14	0.25
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	15	0.25
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	12	0.25
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	14	0.25
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	16	0.25
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	3	0.24
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	11	0.24
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	12	0.24
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	3	0.24
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	18	0.24
(3,16)	1:A:69:LYS:N	1:A:65:ASP:O	6	0.24
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	11	0.24
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	1	0.24
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	16	0.24
(3,20)	1:A:72:VAL:N	1:A:68:ASP:O	16	0.23
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	2	0.23
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	7	0.23
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	20	0.23
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	5	0.22
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	16	0.22
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	11	0.22
(3,23)	1:A:92:LEU:N	1:A:88:TYR:O	5	0.22
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	17	0.22
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	20	0.22
(3,11)	1:A:92:LEU:N	1:A:88:TYR:O	5	0.22
(1,1338)	1:A:39:ASN:HB2	1:A:39:ASN:HD21	8	0.22
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	6	0.21
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	13	0.21
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	6	0.21
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	17	0.21
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	5	0.21
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	18	0.21
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	8	0.21
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	8	0.21
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	11	0.2
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	3	0.2
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	1	0.2
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	5	0.2
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	5	0.2
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	9	0.19
(3,20)	1:A:72:VAL:N	1:A:68:ASP:O	18	0.19
(3,2)	1:A:78:VAL:N	1:A:101:ALA:O	14	0.19
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	4	0.19
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	13	0.19
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	9	0.19
(1,491)	1:A:80:LEU:H	1:A:82:GLY:H	14	0.19
(3,3)	1:A:80:LEU:N	1:A:103:TRP:O	17	0.18
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	7	0.18
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	19	0.18
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	5	0.18
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	18	0.18
(3,2)	1:A:78:VAL:N	1:A:101:ALA:O	3	0.18
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	10	0.18
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	12	0.18
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	16	0.18
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	18	0.18
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	2	0.18
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	12	0.17
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	15	0.17
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	16	0.17
(3,20)	1:A:72:VAL:N	1:A:68:ASP:O	2	0.17
(3,20)	1:A:72:VAL:N	1:A:68:ASP:O	12	0.17
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	1	0.17
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	14	0.17
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	15	0.17
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	6	0.17
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	3	0.17
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	8	0.17
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	6	0.16
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	11	0.16
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1877)	1:A:13:GLN:HE21	1:A:14:ASP:HB2	19	0.16
(1,1877)	1:A:13:GLN:HE21	1:A:14:ASP:HB3	19	0.16
(1,1877)	1:A:13:GLN:HE22	1:A:14:ASP:HB2	19	0.16
(1,1877)	1:A:13:GLN:HE22	1:A:14:ASP:HB3	19	0.16
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	15	0.16
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	10	0.15
(3,27)	1:A:100:VAL:N	1:A:97:PRO:O	17	0.15
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	20	0.15
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	20	0.15
(3,18)	1:A:73:LEU:N	1:A:69:LYS:O	10	0.15
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	9	0.15
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	10	0.15
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	12	0.15
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	16	0.15
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	10	0.15
(3,14)	1:A:68:ASP:N	1:A:64:ALA:O	15	0.15
(2,5)	1:A:79:GLN:H	1:A:56:GLY:O	2	0.15
(2,4)	1:A:101:ALA:H	1:A:76:ALA:O	17	0.15
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD2	2	0.15
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD3	2	0.15
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD2	10	0.15
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD3	10	0.15
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	2	0.15
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	2	0.15
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	20	0.15
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	20	0.15
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	1	0.14
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	1	0.14
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	13	0.14
(3,2)	1:A:78:VAL:N	1:A:101:ALA:O	8	0.14
(3,2)	1:A:78:VAL:N	1:A:101:ALA:O	10	0.14
(3,2)	1:A:78:VAL:N	1:A:101:ALA:O	19	0.14
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	17	0.14
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	19	0.14
(2,5)	1:A:79:GLN:H	1:A:56:GLY:O	12	0.14
(2,4)	1:A:101:ALA:H	1:A:76:ALA:O	11	0.14
(1,982)	1:A:42:GLN:H	1:A:42:GLN:HE22	20	0.14
(1,962)	1:A:39:ASN:HD21	1:A:41:GLU:HA	8	0.14
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	3	0.14
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	3	0.14
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	3	0.14
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	4	0.14
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	4	0.14
(1,594)	1:A:53:GLN:H	1:A:53:GLN:HG2	5	0.14
(1,594)	1:A:53:GLN:H	1:A:53:GLN:HG3	5	0.14
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD2	3	0.14
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD3	3	0.14
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD2	18	0.14
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD3	18	0.14
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	15	0.14
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	15	0.14
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	8	0.14
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	14	0.14
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	20	0.14
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	2	0.13
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	3	0.13
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	10	0.13
(3,20)	1:A:72:VAL:N	1:A:68:ASP:O	6	0.13
(3,2)	1:A:78:VAL:N	1:A:101:ALA:O	6	0.13
(3,2)	1:A:78:VAL:N	1:A:101:ALA:O	17	0.13
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	9	0.13
(3,19)	1:A:70:ALA:N	1:A:66:VAL:O	13	0.13
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	1	0.13
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	19	0.13
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	19	0.13
(2,5)	1:A:79:GLN:H	1:A:56:GLY:O	1	0.13
(2,5)	1:A:79:GLN:H	1:A:56:GLY:O	3	0.13
(2,5)	1:A:79:GLN:H	1:A:56:GLY:O	10	0.13
(1,982)	1:A:42:GLN:H	1:A:42:GLN:HE22	19	0.13
(1,88)	1:A:28:LEU:HD21	1:A:55:VAL:H	19	0.13
(1,88)	1:A:28:LEU:HD22	1:A:55:VAL:H	19	0.13
(1,88)	1:A:28:LEU:HD23	1:A:55:VAL:H	19	0.13
(1,88)	1:A:93:ARG:H	1:A:102:ILE:HD11	19	0.13
(1,88)	1:A:93:ARG:H	1:A:102:ILE:HD12	19	0.13
(1,88)	1:A:93:ARG:H	1:A:102:ILE:HD13	19	0.13
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	8	0.13
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	8	0.13
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	8	0.13
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	14	0.13
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	14	0.13
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	14	0.13
(1,496)	1:A:44:GLN:HA	1:A:44:GLN:HE22	1	0.13
(1,496)	1:A:44:GLN:HA	1:A:44:GLN:HE22	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:A:44:GLN:HA	1:A:44:GLN:HE22	20	0.13
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG21	12	0.13
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG22	12	0.13
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG23	12	0.13
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG21	12	0.13
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG22	12	0.13
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG23	12	0.13
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG21	15	0.13
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG22	15	0.13
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG23	15	0.13
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG21	15	0.13
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG22	15	0.13
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG23	15	0.13
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	4	0.13
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	4	0.13
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	11	0.13
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	11	0.13
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	12	0.13
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	12	0.13
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	19	0.13
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	19	0.13
(1,1298)	1:A:75:LEU:H	1:A:75:LEU:HG	17	0.13
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	1	0.13
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	4	0.13
(3,7)	1:A:58:PHE:N	1:A:79:GLN:O	19	0.12
(3,20)	1:A:72:VAL:N	1:A:68:ASP:O	3	0.12
(3,20)	1:A:72:VAL:N	1:A:68:ASP:O	15	0.12
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	2	0.12
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	7	0.12
(3,15)	1:A:67:VAL:N	1:A:63:ILE:O	17	0.12
(2,5)	1:A:79:GLN:H	1:A:56:GLY:O	4	0.12
(1,982)	1:A:42:GLN:H	1:A:42:GLN:HE22	4	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	5	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	5	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	5	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	6	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	6	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	6	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	13	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	13	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	13	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	16	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	16	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	19	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	19	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	19	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	20	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	20	0.12
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	20	0.12
(1,839)	1:A:91:THR:HG21	1:A:92:LEU:H	10	0.12
(1,839)	1:A:91:THR:HG22	1:A:92:LEU:H	10	0.12
(1,839)	1:A:91:THR:HG23	1:A:92:LEU:H	10	0.12
(1,839)	1:A:91:THR:HG21	1:A:92:LEU:H	18	0.12
(1,839)	1:A:91:THR:HG22	1:A:92:LEU:H	18	0.12
(1,839)	1:A:91:THR:HG23	1:A:92:LEU:H	18	0.12
(1,594)	1:A:53:GLN:H	1:A:53:GLN:HG2	20	0.12
(1,594)	1:A:53:GLN:H	1:A:53:GLN:HG3	20	0.12
(1,566)	1:A:93:ARG:HD3	1:A:94:GLU:H	16	0.12
(1,2149)	1:A:93:ARG:HB2	1:A:94:GLU:H	5	0.12
(1,2149)	1:A:93:ARG:HB3	1:A:94:GLU:H	5	0.12
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD2	6	0.12
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD3	6	0.12
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD2	12	0.12
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD3	12	0.12
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD2	16	0.12
(1,2143)	1:A:92:LEU:H	1:A:93:ARG:HD3	16	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG21	10	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG22	10	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG23	10	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG21	10	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG22	10	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG23	10	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG21	11	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG22	11	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG23	11	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG21	11	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG22	11	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG23	11	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG21	19	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG22	19	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG23	19	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG21	19	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG22	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG23	19	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG21	20	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG22	20	0.12
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG23	20	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG21	20	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG22	20	0.12
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG23	20	0.12
(1,2106)	1:A:78:VAL:HG11	1:A:103:TRP:H	14	0.12
(1,2106)	1:A:78:VAL:HG12	1:A:103:TRP:H	14	0.12
(1,2106)	1:A:78:VAL:HG13	1:A:103:TRP:H	14	0.12
(1,2106)	1:A:78:VAL:HG21	1:A:103:TRP:H	14	0.12
(1,2106)	1:A:78:VAL:HG22	1:A:103:TRP:H	14	0.12
(1,2106)	1:A:78:VAL:HG23	1:A:103:TRP:H	14	0.12
(1,2106)	1:A:78:VAL:HG11	1:A:103:TRP:H	20	0.12
(1,2106)	1:A:78:VAL:HG12	1:A:103:TRP:H	20	0.12
(1,2106)	1:A:78:VAL:HG13	1:A:103:TRP:H	20	0.12
(1,2106)	1:A:78:VAL:HG21	1:A:103:TRP:H	20	0.12
(1,2106)	1:A:78:VAL:HG22	1:A:103:TRP:H	20	0.12
(1,2106)	1:A:78:VAL:HG23	1:A:103:TRP:H	20	0.12
(1,2000)	1:A:45:GLU:HB2	1:A:46:VAL:H	13	0.12
(1,2000)	1:A:45:GLU:HB3	1:A:46:VAL:H	13	0.12
(1,2000)	1:A:45:GLU:HB2	1:A:46:VAL:H	15	0.12
(1,2000)	1:A:45:GLU:HB3	1:A:46:VAL:H	15	0.12
(1,1877)	1:A:13:GLN:HE21	1:A:14:ASP:HB2	5	0.12
(1,1877)	1:A:13:GLN:HE21	1:A:14:ASP:HB3	5	0.12
(1,1877)	1:A:13:GLN:HE22	1:A:14:ASP:HB2	5	0.12
(1,1877)	1:A:13:GLN:HE22	1:A:14:ASP:HB3	5	0.12
(1,1556)	1:A:79:GLN:H	1:A:79:GLN:HB3	15	0.12
(1,1556)	1:A:79:GLN:H	1:A:79:GLN:HB3	20	0.12
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	10	0.12
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	10	0.12
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	17	0.12
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	17	0.12
(1,1213)	1:A:29:ILE:HG21	1:A:30:PHE:H	2	0.12
(1,1213)	1:A:29:ILE:HG22	1:A:30:PHE:H	2	0.12
(1,1213)	1:A:29:ILE:HG23	1:A:30:PHE:H	2	0.12
(1,1194)	1:A:41:GLU:H	1:A:44:GLN:HE22	11	0.12
(1,1064)	1:A:34:SER:HA	1:A:37:CYS:H	5	0.12
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	5	0.12
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	6	0.12
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	13	0.12
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	7	0.11
(3,26)	1:A:96:LEU:N	1:A:92:LEU:O	19	0.11
(3,2)	1:A:78:VAL:N	1:A:101:ALA:O	15	0.11
(3,17)	1:A:71:LYS:N	1:A:67:VAL:O	8	0.11
(2,4)	1:A:101:ALA:H	1:A:76:ALA:O	16	0.11
(1,982)	1:A:42:GLN:H	1:A:42:GLN:HE22	1	0.11
(1,982)	1:A:42:GLN:H	1:A:42:GLN:HE22	2	0.11
(1,982)	1:A:42:GLN:H	1:A:42:GLN:HE22	14	0.11
(1,868)	1:A:102:ILE:HG21	1:A:121:ASP:H	11	0.11
(1,868)	1:A:102:ILE:HG22	1:A:121:ASP:H	11	0.11
(1,868)	1:A:102:ILE:HG23	1:A:121:ASP:H	11	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	2	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	2	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	2	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	7	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	7	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	7	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	9	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	9	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	9	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	10	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	10	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	10	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	11	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	11	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	11	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	12	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	12	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	12	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	15	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	15	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	15	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	17	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	17	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	17	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG11	18	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG12	18	0.11
(1,843)	1:A:100:VAL:H	1:A:100:VAL:HG13	18	0.11
(1,839)	1:A:91:THR:HG21	1:A:92:LEU:H	3	0.11
(1,839)	1:A:91:THR:HG22	1:A:92:LEU:H	3	0.11
(1,839)	1:A:91:THR:HG23	1:A:92:LEU:H	3	0.11
(1,839)	1:A:91:THR:HG21	1:A:92:LEU:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,839)	1:A:91:THR:HG22	1:A:92:LEU:H	6	0.11
(1,839)	1:A:91:THR:HG23	1:A:92:LEU:H	6	0.11
(1,722)	1:A:95:ALA:HA	1:A:96:LEU:H	7	0.11
(1,594)	1:A:53:GLN:H	1:A:53:GLN:HG2	4	0.11
(1,594)	1:A:53:GLN:H	1:A:53:GLN:HG3	4	0.11
(1,594)	1:A:53:GLN:H	1:A:53:GLN:HG2	8	0.11
(1,594)	1:A:53:GLN:H	1:A:53:GLN:HG3	8	0.11
(1,580)	1:A:31:VAL:HB	1:A:34:SER:H	5	0.11
(1,566)	1:A:93:ARG:HD3	1:A:94:GLU:H	3	0.11
(1,566)	1:A:93:ARG:HD3	1:A:94:GLU:H	6	0.11
(1,566)	1:A:93:ARG:HD3	1:A:94:GLU:H	10	0.11
(1,496)	1:A:44:GLN:HA	1:A:44:GLN:HE22	10	0.11
(1,411)	1:A:42:GLN:HB2	1:A:46:VAL:HG11	1	0.11
(1,411)	1:A:42:GLN:HB2	1:A:46:VAL:HG12	1	0.11
(1,411)	1:A:42:GLN:HB2	1:A:46:VAL:HG13	1	0.11
(1,411)	1:A:45:GLU:HB2	1:A:46:VAL:HG11	1	0.11
(1,411)	1:A:45:GLU:HB2	1:A:46:VAL:HG12	1	0.11
(1,411)	1:A:45:GLU:HB2	1:A:46:VAL:HG13	1	0.11
(1,384)	1:A:6:VAL:HA	1:A:6:VAL:HB	3	0.11
(1,384)	1:A:116:GLU:HA	1:A:116:GLU:HB2	3	0.11
(1,384)	1:A:6:VAL:HA	1:A:6:VAL:HB	6	0.11
(1,384)	1:A:116:GLU:HA	1:A:116:GLU:HB2	6	0.11
(1,384)	1:A:6:VAL:HA	1:A:6:VAL:HB	11	0.11
(1,384)	1:A:116:GLU:HA	1:A:116:GLU:HB2	11	0.11
(1,2130)	1:A:86:GLN:H	1:A:87:LEU:HD11	18	0.11
(1,2130)	1:A:86:GLN:H	1:A:87:LEU:HD12	18	0.11
(1,2130)	1:A:86:GLN:H	1:A:87:LEU:HD13	18	0.11
(1,2130)	1:A:86:GLN:H	1:A:87:LEU:HD21	18	0.11
(1,2130)	1:A:86:GLN:H	1:A:87:LEU:HD22	18	0.11
(1,2130)	1:A:86:GLN:H	1:A:87:LEU:HD23	18	0.11
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG21	6	0.11
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG22	6	0.11
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG23	6	0.11
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG21	6	0.11
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG22	6	0.11
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG23	6	0.11
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG21	14	0.11
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG22	14	0.11
(1,2109)	1:A:79:GLN:HE21	1:A:102:ILE:HG23	14	0.11
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG21	14	0.11
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG22	14	0.11
(1,2109)	1:A:79:GLN:HE22	1:A:102:ILE:HG23	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:A:79:GLN:H	1:A:79:GLN:HB3	11	0.11
(1,1476)	1:A:29:ILE:HG21	1:A:56:GLY:HA2	16	0.11
(1,1476)	1:A:29:ILE:HG22	1:A:56:GLY:HA2	16	0.11
(1,1476)	1:A:29:ILE:HG23	1:A:56:GLY:HA2	16	0.11
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE1	14	0.11
(1,1362)	1:A:25:TYR:HA	1:A:25:TYR:HE2	14	0.11
(1,1353)	1:A:8:GLY:H	1:A:37:CYS:H	10	0.11
(1,1213)	1:A:29:ILE:HG21	1:A:30:PHE:H	4	0.11
(1,1213)	1:A:29:ILE:HG22	1:A:30:PHE:H	4	0.11
(1,1213)	1:A:29:ILE:HG23	1:A:30:PHE:H	4	0.11
(1,1213)	1:A:29:ILE:HG21	1:A:30:PHE:H	8	0.11
(1,1213)	1:A:29:ILE:HG22	1:A:30:PHE:H	8	0.11
(1,1213)	1:A:29:ILE:HG23	1:A:30:PHE:H	8	0.11
(1,1213)	1:A:29:ILE:HG21	1:A:30:PHE:H	20	0.11
(1,1213)	1:A:29:ILE:HG22	1:A:30:PHE:H	20	0.11
(1,1213)	1:A:29:ILE:HG23	1:A:30:PHE:H	20	0.11
(1,1006)	1:A:60:ASN:H	1:A:61:HIS:H	7	0.11

10 Dihedral-angle violation analysis (i)

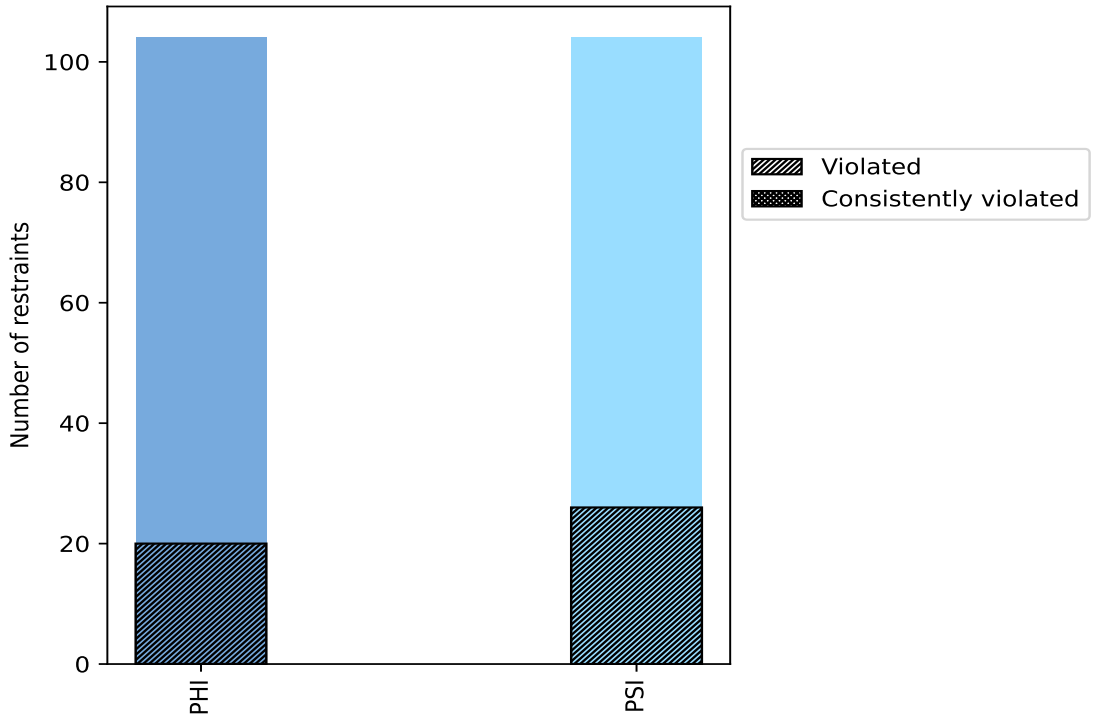
10.1 Summary of dihedral-angle violations (i)

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	104	50.0	20	19.2	9.6	0	0.0	0.0
PSI	104	50.0	26	25.0	12.5	0	0.0	0.0
Total	208	100.0	46	22.1	22.1	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)



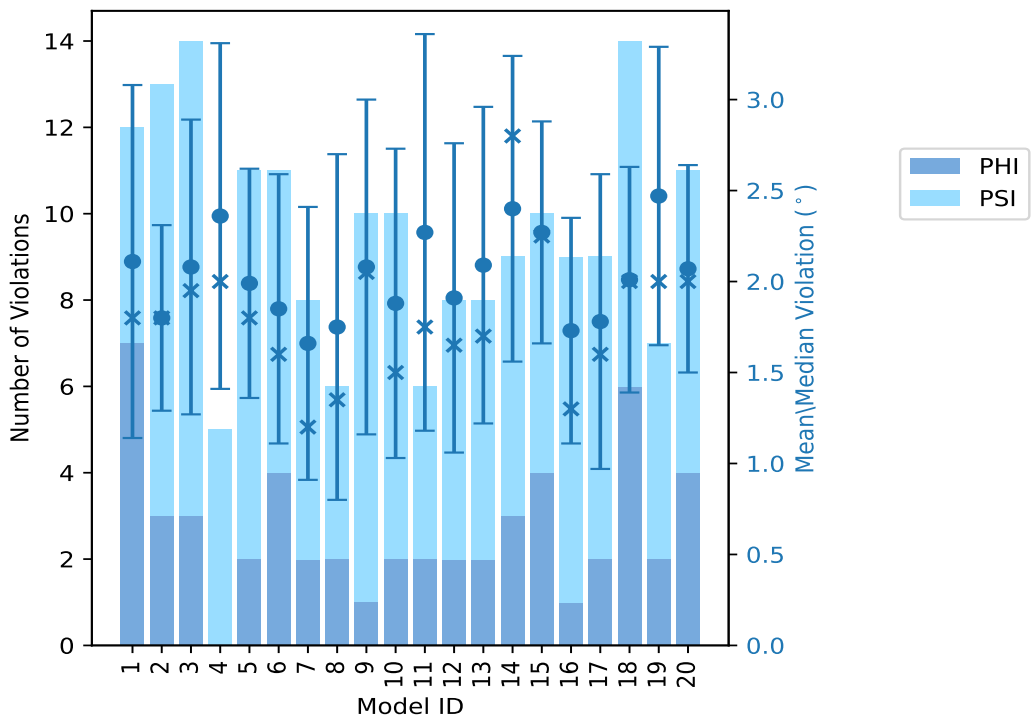
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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	7	5	12	2.11	4.4	0.97	1.8
2	3	10	13	1.8	2.9	0.51	1.8
3	3	11	14	2.08	4.2	0.81	1.95
4	0	5	5	2.36	4.2	0.95	2.0
5	2	9	11	1.99	3.5	0.63	1.8
6	4	7	11	1.85	3.4	0.74	1.6
7	2	6	8	1.66	3.2	0.75	1.2
8	2	4	6	1.75	3.8	0.95	1.35
9	1	9	10	2.08	4.4	0.92	2.05
10	2	8	10	1.88	4.0	0.85	1.5
11	2	4	6	2.27	4.3	1.09	1.75
12	2	6	8	1.91	3.7	0.85	1.65
13	2	6	8	2.09	4.0	0.87	1.7
14	3	6	9	2.4	3.8	0.84	2.8
15	4	6	10	2.27	3.3	0.61	2.25
16	1	8	9	1.73	2.6	0.62	1.3
17	2	7	9	1.78	4.0	0.81	1.6
18	6	8	14	2.01	3.2	0.62	2.0
19	2	5	7	2.47	3.8	0.82	2.0
20	4	7	11	2.07	3.1	0.57	2.0

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]	%
7	6	13	1	5.0
3	3	6	2	10.0
6	5	11	3	15.0
3	2	5	4	20.0
0	1	1	5	25.0
0	2	2	6	30.0
0	2	2	7	35.0
0	1	1	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
1	0	1	11	55.0

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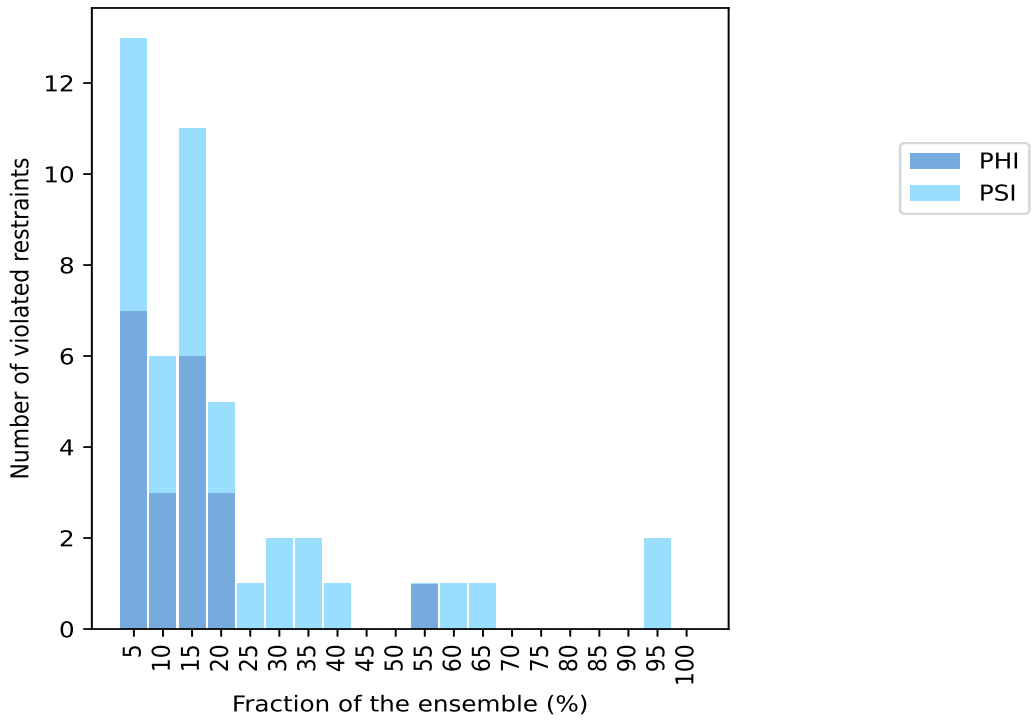
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	1	1	12	60.0
0	1	1	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	2	2	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

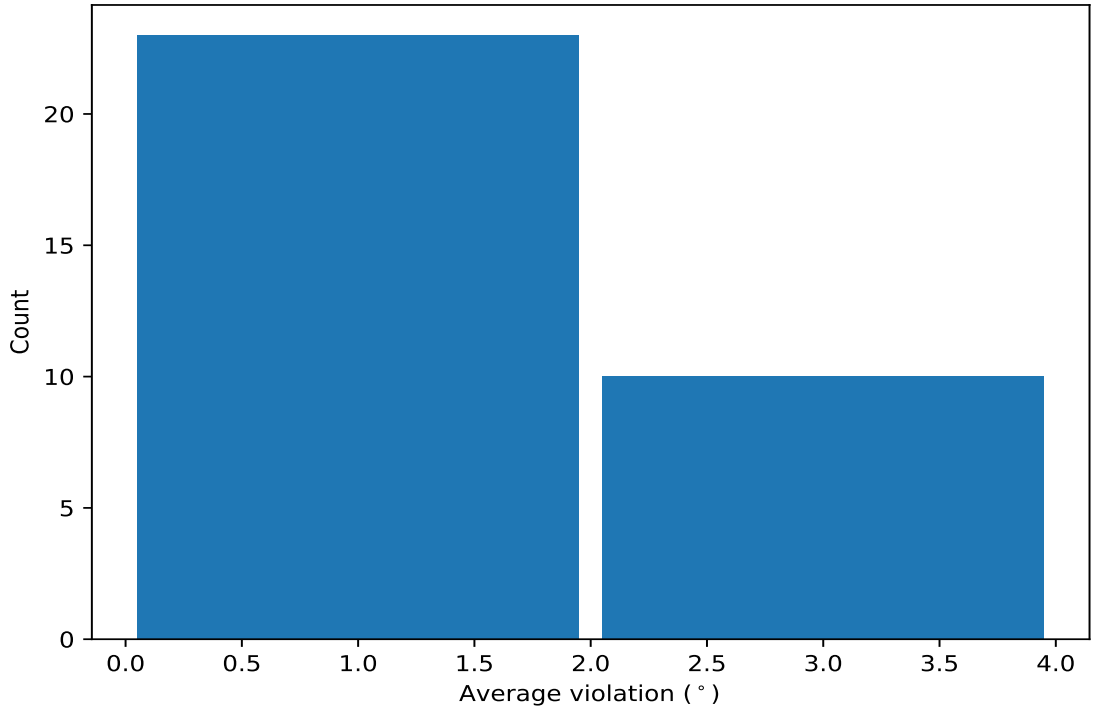


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	19	2.96	0.8	3.1
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	19	2.33	0.76	2.1
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	13	1.75	0.41	1.7
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	12	2.23	0.55	2.3
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	11	2.24	0.64	2.0
(1,134)	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	1:A:84:GLU:N	8	2.06	0.79	2.15
(1,96)	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	1:A:61:HIS:N	7	2.29	0.99	1.9
(1,22)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:ALA:N	7	1.64	0.33	1.7
(1,34)	1:A:24:ILE:N	1:A:24:ILE:CA	1:A:24:ILE:C	1:A:25:TYR:N	6	2.32	0.45	2.35
(1,132)	1:A:82:GLY:N	1:A:82:GLY:CA	1:A:82:GLY:C	1:A:83:ASN:N	6	2.08	1.09	1.55
(1,94)	1:A:59:ARG:N	1:A:59:ARG:CA	1:A:59:ARG:C	1:A:60:ASN:N	5	1.86	0.59	2.2
(1,129)	1:A:79:GLN:C	1:A:80:LEU:N	1:A:80:LEU:CA	1:A:80:LEU:C	4	2.68	0.59	2.85
(1,5)	1:A:6:VAL:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	4	2.1	1.34	1.45
(1,133)	1:A:82:GLY:C	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	4	1.72	0.47	1.65
(1,140)	1:A:87:LEU:N	1:A:87:LEU:CA	1:A:87:LEU:C	1:A:88:TYR:N	4	1.48	0.24	1.45
(1,160)	1:A:97:PRO:N	1:A:97:PRO:CA	1:A:97:PRO:C	1:A:98:ALA:N	4	1.2	0.07	1.2
(1,178)	1:A:106:LEU:N	1:A:106:LEU:CA	1:A:106:LEU:C	1:A:107:SER:N	3	1.8	0.08	1.8
(1,135)	1:A:83:ASN:C	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	3	1.77	0.33	1.7
(1,95)	1:A:59:ARG:C	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	3	1.7	0.65	1.4
(1,182)	1:A:108:VAL:N	1:A:108:VAL:CA	1:A:108:VAL:C	1:A:109:GLY:N	3	1.6	0.22	1.7

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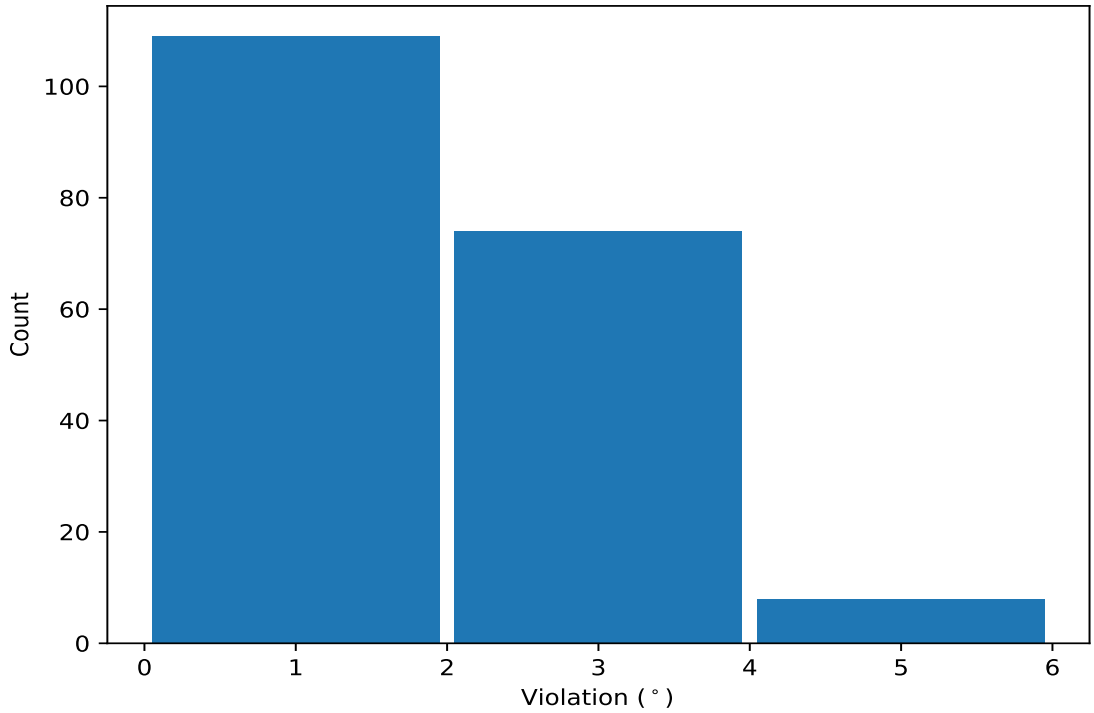
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,32)	1:A:21:ALA:N	1:A:21:ALA:CA	1:A:21:ALA:C	1:A:22:GLY:N	3	1.57	0.45	1.3
(1,186)	1:A:113:PRO:N	1:A:113:PRO:CA	1:A:113:PRO:C	1:A:114:ALA:N	3	1.43	0.25	1.5
(1,180)	1:A:107:SER:N	1:A:107:SER:CA	1:A:107:SER:C	1:A:108:VAL:N	3	1.4	0.22	1.3
(1,147)	1:A:90:ASP:C	1:A:91:THR:N	1:A:91:THR:CA	1:A:91:THR:C	3	1.37	0.17	1.3
(1,173)	1:A:103:TRP:C	1:A:104:LYS:N	1:A:104:LYS:CA	1:A:104:LYS:C	3	1.37	0.21	1.4
(1,43)	1:A:28:LEU:C	1:A:29:ILE:N	1:A:29:ILE:CA	1:A:29:ILE:C	3	1.23	0.19	1.1
(1,121)	1:A:75:LEU:C	1:A:76:ALA:N	1:A:76:ALA:CA	1:A:76:ALA:C	3	1.1	0.0	1.1
(1,8)	1:A:8:GLY:N	1:A:8:GLY:CA	1:A:8:GLY:C	1:A:9:LEU:N	2	1.65	0.55	1.65
(1,137)	1:A:85:GLU:C	1:A:86:GLN:N	1:A:86:GLN:CA	1:A:86:GLN:C	2	1.65	0.45	1.65
(1,16)	1:A:13:GLN:N	1:A:13:GLN:CA	1:A:13:GLN:C	1:A:14:ASP:N	2	1.6	0.5	1.6
(1,55)	1:A:37:CYS:C	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	2	1.5	0.2	1.5
(1,164)	1:A:99:HIS:N	1:A:99:HIS:CA	1:A:99:HIS:C	1:A:100:VAL:N	2	1.35	0.15	1.35
(1,93)	1:A:58:PHE:C	1:A:59:ARG:N	1:A:59:ARG:CA	1:A:59:ARG:C	2	1.2	0.1	1.2

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	1:A:61:HIS:N	9	4.4
(1,5)	1:A:6:VAL:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1	4.4
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	11	4.3
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	4	4.2
(1,132)	1:A:82:GLY:N	1:A:82:GLY:CA	1:A:82:GLY:C	1:A:83:ASN:N	3	4.2
(1,7)	1:A:7:CYS:C	1:A:8:GLY:N	1:A:8:GLY:CA	1:A:8:GLY:C	13	4.0
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	10	4.0
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	17	4.0
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	14	3.8
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	8	3.8
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	19	3.8
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	12	3.7
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	5	3.5
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	1	3.4
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	6	3.4
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	19	3.3
(1,129)	1:A:79:GLN:C	1:A:80:LEU:N	1:A:80:LEU:CA	1:A:80:LEU:C	15	3.3
(1,90)	1:A:57:VAL:N	1:A:57:VAL:CA	1:A:57:VAL:C	1:A:58:PHE:N	7	3.2
(1,4)	1:A:6:VAL:N	1:A:6:VAL:CA	1:A:6:VAL:C	1:A:7:CYS:N	1	3.2
(1,134)	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	1:A:84:GLU:N	18	3.2
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	15	3.1
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	11	3.1
(1,134)	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	1:A:84:GLU:N	20	3.1
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	14	3.0
(1,34)	1:A:24:ILE:N	1:A:24:ILE:CA	1:A:24:ILE:C	1:A:25:TYR:N	19	3.0
(1,96)	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	1:A:61:HIS:N	13	2.9
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	3	2.9
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	2	2.9
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	14	2.9
(1,129)	1:A:79:GLN:C	1:A:80:LEU:N	1:A:80:LEU:CA	1:A:80:LEU:C	14	2.9
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	15	2.8
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	12	2.8
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	20	2.8
(1,132)	1:A:82:GLY:N	1:A:82:GLY:CA	1:A:82:GLY:C	1:A:83:ASN:N	14	2.8
(1,129)	1:A:79:GLN:C	1:A:80:LEU:N	1:A:80:LEU:CA	1:A:80:LEU:C	18	2.8
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	9	2.7
(1,95)	1:A:59:ARG:C	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	3	2.6
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	16	2.6
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	10	2.6
(1,48)	1:A:32:ALA:N	1:A:32:ALA:CA	1:A:32:ALA:C	1:A:33:THR:N	5	2.6
(1,34)	1:A:24:ILE:N	1:A:24:ILE:CA	1:A:24:ILE:C	1:A:25:TYR:N	16	2.6
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	18	2.6
(1,94)	1:A:59:ARG:N	1:A:59:ARG:CA	1:A:59:ARG:C	1:A:60:ASN:N	20	2.5
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	3	2.5
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	7	2.5
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	16	2.5
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	10	2.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,34)	1:A:24:ILE:N	1:A:24:ILE:CA	1:A:24:ILE:C	1:A:25:TYR:N	20	2.5
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	2	2.5
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	6	2.5
(1,131)	1:A:81:HIS:C	1:A:82:GLY:N	1:A:82:GLY:CA	1:A:82:GLY:C	18	2.5
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	15	2.4
(1,134)	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	1:A:84:GLU:N	6	2.4
(1,134)	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	1:A:84:GLU:N	15	2.4
(1,133)	1:A:82:GLY:C	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	3	2.4
(1,96)	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	1:A:61:HIS:N	5	2.3
(1,94)	1:A:59:ARG:N	1:A:59:ARG:CA	1:A:59:ARG:C	1:A:60:ASN:N	3	2.3
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	18	2.3
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	6	2.3
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	6	2.3
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	9	2.3
(1,181)	1:A:107:SER:C	1:A:108:VAL:N	1:A:108:VAL:CA	1:A:108:VAL:C	5	2.3
(1,94)	1:A:59:ARG:N	1:A:59:ARG:CA	1:A:59:ARG:C	1:A:60:ASN:N	18	2.2
(1,8)	1:A:8:GLY:N	1:A:8:GLY:CA	1:A:8:GLY:C	1:A:9:LEU:N	13	2.2
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	2	2.2
(1,34)	1:A:24:ILE:N	1:A:24:ILE:CA	1:A:24:ILE:C	1:A:25:TYR:N	9	2.2
(1,32)	1:A:21:ALA:N	1:A:21:ALA:CA	1:A:21:ALA:C	1:A:22:GLY:N	4	2.2
(1,135)	1:A:83:ASN:C	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	20	2.2
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	18	2.1
(1,16)	1:A:13:GLN:N	1:A:13:GLN:CA	1:A:13:GLN:C	1:A:14:ASP:N	9	2.1
(1,137)	1:A:85:GLU:C	1:A:86:GLN:N	1:A:86:GLN:CA	1:A:86:GLN:C	2	2.1
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	15	2.1
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	20	2.0
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	4	2.0
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	5	2.0
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	12	2.0
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	19	2.0
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	1	2.0
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	9	2.0
(1,34)	1:A:24:ILE:N	1:A:24:ILE:CA	1:A:24:ILE:C	1:A:25:TYR:N	2	2.0
(1,22)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:ALA:N	3	2.0
(1,22)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:ALA:N	14	2.0
(1,96)	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	1:A:61:HIS:N	19	1.9
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	7	1.9
(1,22)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:ALA:N	15	1.9
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	19	1.9
(1,178)	1:A:106:LEU:N	1:A:106:LEU:CA	1:A:106:LEU:C	1:A:107:SER:N	4	1.9
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	3	1.9
(1,134)	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	1:A:84:GLU:N	3	1.9
(1,133)	1:A:82:GLY:C	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	18	1.9
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	2	1.8
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	8	1.8
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	1	1.8
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	16	1.8
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	20	1.8
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	2	1.8
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	5	1.8
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	11	1.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,182)	1:A:108:VAL:N	1:A:108:VAL:CA	1:A:108:VAL:C	1:A:109:GLY:N	1	1.8
(1,178)	1:A:106:LEU:N	1:A:106:LEU:CA	1:A:106:LEU:C	1:A:107:SER:N	18	1.8
(1,140)	1:A:87:LEU:N	1:A:87:LEU:CA	1:A:87:LEU:C	1:A:88:TYR:N	18	1.8
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	1	1.8
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	17	1.8
(1,96)	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	1:A:61:HIS:N	17	1.7
(1,6)	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	1:A:8:GLY:N	13	1.7
(1,55)	1:A:37:CYS:C	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1	1.7
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	17	1.7
(1,22)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:ALA:N	12	1.7
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	15	1.7
(1,186)	1:A:113:PRO:N	1:A:113:PRO:CA	1:A:113:PRO:C	1:A:114:ALA:N	5	1.7
(1,182)	1:A:108:VAL:N	1:A:108:VAL:CA	1:A:108:VAL:C	1:A:109:GLY:N	13	1.7
(1,180)	1:A:107:SER:N	1:A:107:SER:CA	1:A:107:SER:C	1:A:108:VAL:N	5	1.7
(1,178)	1:A:106:LEU:N	1:A:106:LEU:CA	1:A:106:LEU:C	1:A:107:SER:N	11	1.7
(1,135)	1:A:83:ASN:C	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	14	1.7
(1,129)	1:A:79:GLN:C	1:A:80:LEU:N	1:A:80:LEU:CA	1:A:80:LEU:C	20	1.7
(1,5)	1:A:6:VAL:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	10	1.6
(1,34)	1:A:24:ILE:N	1:A:24:ILE:CA	1:A:24:ILE:C	1:A:25:TYR:N	12	1.6
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	6	1.6
(1,173)	1:A:103:TRP:C	1:A:104:LYS:N	1:A:104:LYS:CA	1:A:104:LYS:C	11	1.6
(1,147)	1:A:90:ASP:C	1:A:91:THR:N	1:A:91:THR:CA	1:A:91:THR:C	15	1.6
(1,140)	1:A:87:LEU:N	1:A:87:LEU:CA	1:A:87:LEU:C	1:A:88:TYR:N	10	1.6
(1,132)	1:A:82:GLY:N	1:A:82:GLY:CA	1:A:82:GLY:C	1:A:83:ASN:N	17	1.6
(1,57)	1:A:38:VAL:C	1:A:39:ASN:N	1:A:39:ASN:CA	1:A:39:ASN:C	8	1.5
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	20	1.5
(1,46)	1:A:31:VAL:N	1:A:31:VAL:CA	1:A:31:VAL:C	1:A:32:ALA:N	5	1.5
(1,43)	1:A:28:LEU:C	1:A:29:ILE:N	1:A:29:ILE:CA	1:A:29:ILE:C	6	1.5
(1,22)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:ALA:N	9	1.5
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	3	1.5
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	13	1.5
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	20	1.5
(1,186)	1:A:113:PRO:N	1:A:113:PRO:CA	1:A:113:PRO:C	1:A:114:ALA:N	2	1.5
(1,165)	1:A:99:HIS:C	1:A:100:VAL:N	1:A:100:VAL:CA	1:A:100:VAL:C	1	1.5
(1,164)	1:A:99:HIS:N	1:A:99:HIS:CA	1:A:99:HIS:C	1:A:100:VAL:N	4	1.5
(1,132)	1:A:82:GLY:N	1:A:82:GLY:CA	1:A:82:GLY:C	1:A:83:ASN:N	2	1.5
(1,96)	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	1:A:61:HIS:N	2	1.4
(1,96)	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	1:A:61:HIS:N	10	1.4
(1,95)	1:A:59:ARG:C	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	1	1.4
(1,35)	1:A:24:ILE:C	1:A:25:TYR:N	1:A:25:TYR:CA	1:A:25:TYR:C	3	1.4
(1,192)	1:A:117:PHE:N	1:A:117:PHE:CA	1:A:117:PHE:C	1:A:118:GLN:N	14	1.4
(1,173)	1:A:103:TRP:C	1:A:104:LYS:N	1:A:104:LYS:CA	1:A:104:LYS:C	19	1.4
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	10	1.4
(1,136)	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	1:A:85:GLU:N	13	1.4
(1,135)	1:A:83:ASN:C	1:A:84:GLU:N	1:A:84:GLU:CA	1:A:84:GLU:C	18	1.4
(1,133)	1:A:82:GLY:C	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	15	1.4
(1,93)	1:A:58:PHE:C	1:A:59:ARG:N	1:A:59:ARG:CA	1:A:59:ARG:C	5	1.3
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	9	1.3
(1,56)	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	1:A:39:ASN:N	17	1.3
(1,55)	1:A:37:CYS:C	1:A:38:VAL:N	1:A:38:VAL:CA	1:A:38:VAL:C	13	1.3
(1,5)	1:A:6:VAL:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	12	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:A:21:ALA:N	1:A:21:ALA:CA	1:A:21:ALA:C	1:A:22:GLY:N	16	1.3
(1,22)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:ALA:N	10	1.3
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	17	1.3
(1,182)	1:A:108:VAL:N	1:A:108:VAL:CA	1:A:108:VAL:C	1:A:109:GLY:N	2	1.3
(1,180)	1:A:107:SER:N	1:A:107:SER:CA	1:A:107:SER:C	1:A:108:VAL:N	2	1.3
(1,160)	1:A:97:PRO:N	1:A:97:PRO:CA	1:A:97:PRO:C	1:A:98:ALA:N	17	1.3
(1,147)	1:A:90:ASP:C	1:A:91:THR:N	1:A:91:THR:CA	1:A:91:THR:C	17	1.3
(1,140)	1:A:87:LEU:N	1:A:87:LEU:CA	1:A:87:LEU:C	1:A:88:TYR:N	16	1.3
(1,132)	1:A:82:GLY:N	1:A:82:GLY:CA	1:A:82:GLY:C	1:A:83:ASN:N	18	1.3
(1,94)	1:A:59:ARG:N	1:A:59:ARG:CA	1:A:59:ARG:C	1:A:60:ASN:N	16	1.2
(1,32)	1:A:21:ALA:N	1:A:21:ALA:CA	1:A:21:ALA:C	1:A:22:GLY:N	3	1.2
(1,200)	1:A:122:LYS:N	1:A:122:LYS:CA	1:A:122:LYS:C	1:A:123:TYR:N	10	1.2
(1,180)	1:A:107:SER:N	1:A:107:SER:CA	1:A:107:SER:C	1:A:108:VAL:N	8	1.2
(1,164)	1:A:99:HIS:N	1:A:99:HIS:CA	1:A:99:HIS:C	1:A:100:VAL:N	3	1.2
(1,160)	1:A:97:PRO:N	1:A:97:PRO:CA	1:A:97:PRO:C	1:A:98:ALA:N	5	1.2
(1,160)	1:A:97:PRO:N	1:A:97:PRO:CA	1:A:97:PRO:C	1:A:98:ALA:N	16	1.2
(1,147)	1:A:90:ASP:C	1:A:91:THR:N	1:A:91:THR:CA	1:A:91:THR:C	1	1.2
(1,140)	1:A:87:LEU:N	1:A:87:LEU:CA	1:A:87:LEU:C	1:A:88:TYR:N	7	1.2
(1,137)	1:A:85:GLU:C	1:A:86:GLN:N	1:A:86:GLN:CA	1:A:86:GLN:C	7	1.2
(1,134)	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	1:A:84:GLU:N	9	1.2
(1,134)	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	1:A:84:GLU:N	10	1.2
(1,133)	1:A:82:GLY:C	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	20	1.2
(1,95)	1:A:59:ARG:C	1:A:60:ASN:N	1:A:60:ASN:CA	1:A:60:ASN:C	18	1.1
(1,94)	1:A:59:ARG:N	1:A:59:ARG:CA	1:A:59:ARG:C	1:A:60:ASN:N	12	1.1
(1,93)	1:A:58:PHE:C	1:A:59:ARG:N	1:A:59:ARG:CA	1:A:59:ARG:C	11	1.1
(1,9)	1:A:9:LEU:C	1:A:10:THR:N	1:A:10:THR:CA	1:A:10:THR:C	12	1.1
(1,8)	1:A:8:GLY:N	1:A:8:GLY:CA	1:A:8:GLY:C	1:A:9:LEU:N	16	1.1
(1,5)	1:A:6:VAL:C	1:A:7:CYS:N	1:A:7:CYS:CA	1:A:7:CYS:C	18	1.1
(1,43)	1:A:28:LEU:C	1:A:29:ILE:N	1:A:29:ILE:CA	1:A:29:ILE:C	1	1.1
(1,43)	1:A:28:LEU:C	1:A:29:ILE:N	1:A:29:ILE:CA	1:A:29:ILE:C	7	1.1
(1,22)	1:A:16:LYS:N	1:A:16:LYS:CA	1:A:16:LYS:C	1:A:17:ALA:N	6	1.1
(1,186)	1:A:113:PRO:N	1:A:113:PRO:CA	1:A:113:PRO:C	1:A:114:ALA:N	7	1.1
(1,173)	1:A:103:TRP:C	1:A:104:LYS:N	1:A:104:LYS:CA	1:A:104:LYS:C	6	1.1
(1,160)	1:A:97:PRO:N	1:A:97:PRO:CA	1:A:97:PRO:C	1:A:98:ALA:N	6	1.1
(1,16)	1:A:13:GLN:N	1:A:13:GLN:CA	1:A:13:GLN:C	1:A:14:ASP:N	3	1.1
(1,157)	1:A:95:ALA:C	1:A:96:LEU:N	1:A:96:LEU:CA	1:A:96:LEU:C	14	1.1
(1,134)	1:A:83:ASN:N	1:A:83:ASN:CA	1:A:83:ASN:C	1:A:84:GLU:N	8	1.1
(1,132)	1:A:82:GLY:N	1:A:82:GLY:CA	1:A:82:GLY:C	1:A:83:ASN:N	7	1.1
(1,121)	1:A:75:LEU:C	1:A:76:ALA:N	1:A:76:ALA:CA	1:A:76:ALA:C	2	1.1
(1,121)	1:A:75:LEU:C	1:A:76:ALA:N	1:A:76:ALA:CA	1:A:76:ALA:C	6	1.1
(1,121)	1:A:75:LEU:C	1:A:76:ALA:N	1:A:76:ALA:CA	1:A:76:ALA:C	8	1.1
(1,10)	1:A:10:THR:N	1:A:10:THR:CA	1:A:10:THR:C	1:A:11:ARG:N	9	1.1