Full wwPDB NMR Structure Validation Report

Dec 25, 2024 – 02:21 AM EST

PDB ID	:	2RNG
BMRB ID	:	11022
Title	:	Solution structure of big defensin
Authors	:	Kouno, T.; Fujitani, N.; Osaki, T.; Kawabata, S.; Nishimura, S.; Mizuguchi, M.; Aizawa, T.; Demura, M.; Nitta, K.; Kawano, K.
Deposited on	:	2007-12-27

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

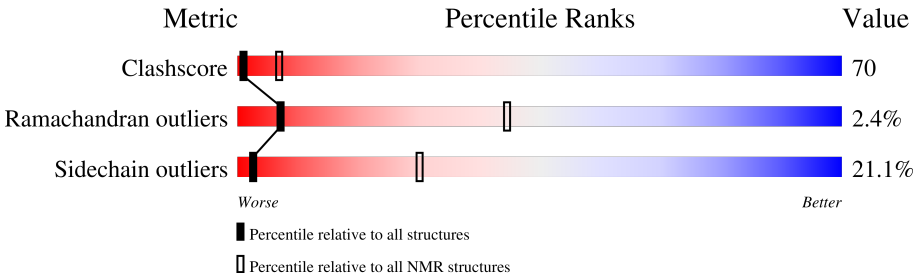
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 49%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	79	24% 57% 14% 5%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:5-A:79 (75)	0.40	18

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

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

The models can be grouped into 5 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 5, 9, 13, 14, 15, 16, 17, 22, 24, 25
2	6, 10, 11, 18, 19, 20, 21
3	8, 23
4	4, 7
5	3, 12

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1188 atoms, of which 582 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Big defensin.

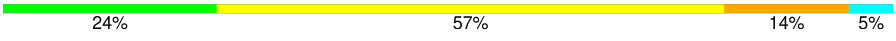
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	79	1188	380	582	114	106	6	0

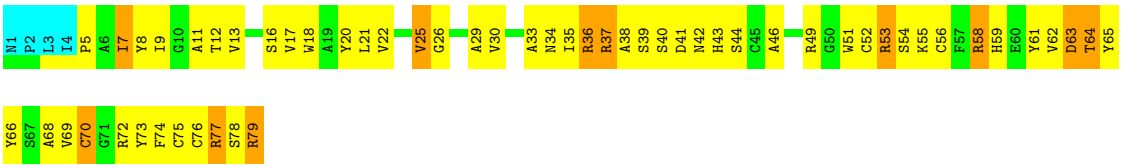
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Big defensin

Chain A: 



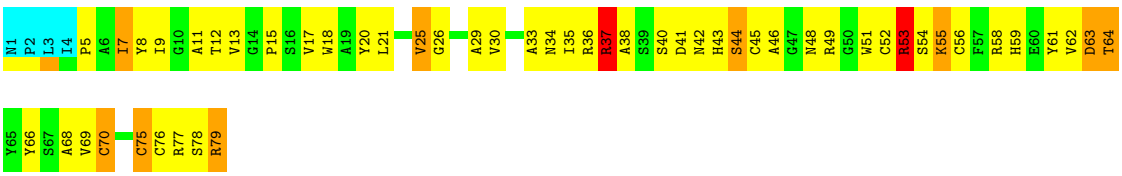
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

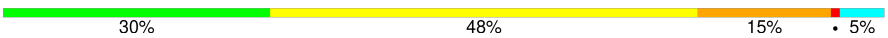
• Molecule 1: Big defensin

Chain A: 



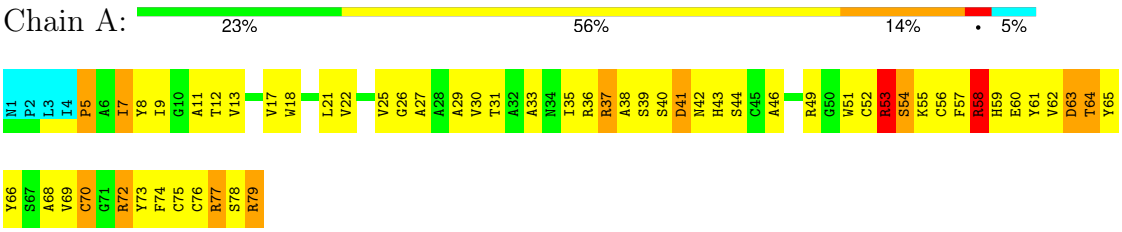
4.2.2 Score per residue for model 2

• Molecule 1: Big defensin

Chain A: 

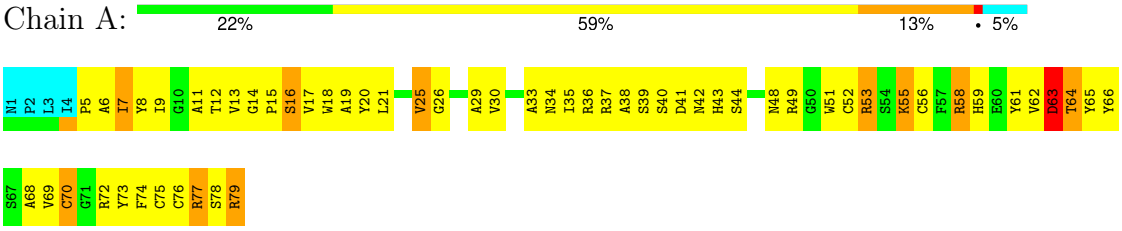
4.2.3 Score per residue for model 3

• Molecule 1: Big defensin



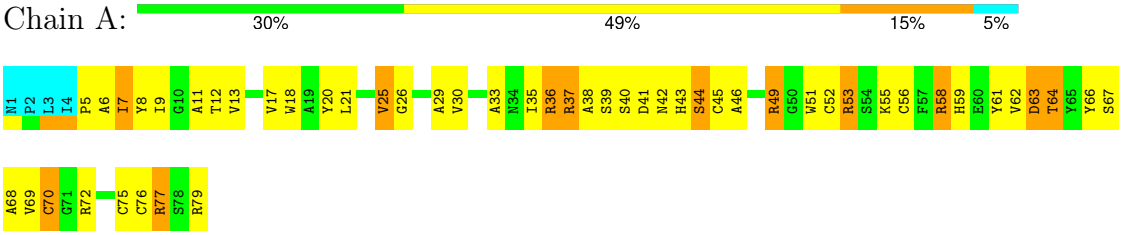
4.2.4 Score per residue for model 4

• Molecule 1: Big defensin



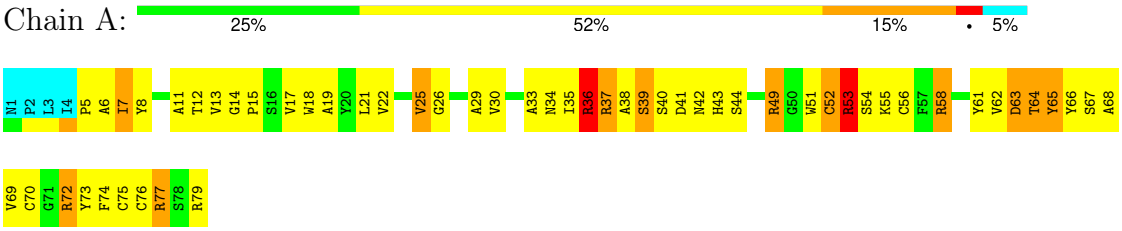
4.2.5 Score per residue for model 5

• Molecule 1: Big defensin



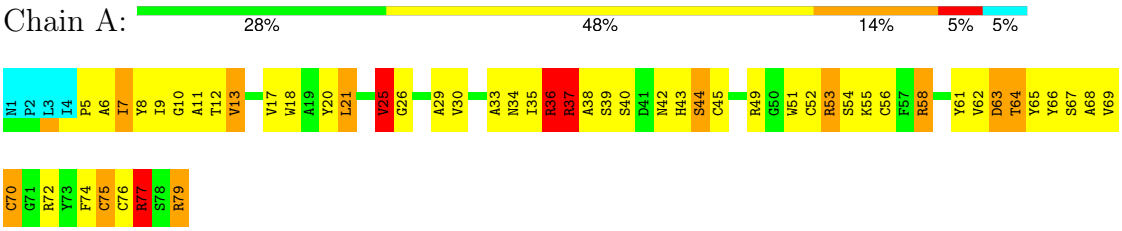
4.2.6 Score per residue for model 6

• Molecule 1: Big defensin



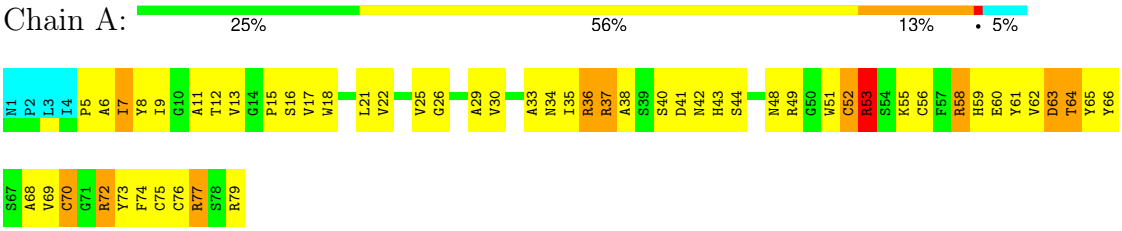
4.2.7 Score per residue for model 7

- Molecule 1: Big defensin



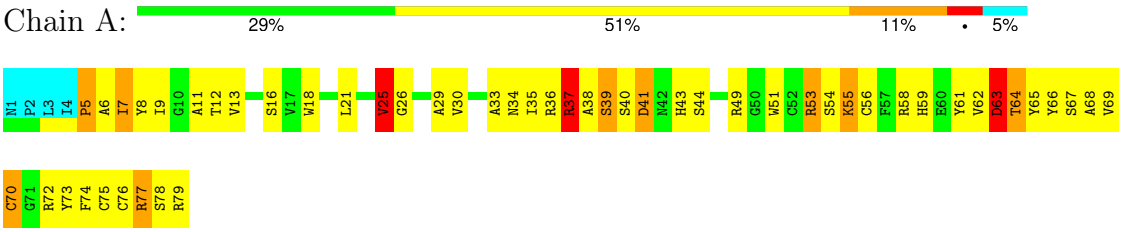
4.2.8 Score per residue for model 8

- Molecule 1: Big defensin



4.2.9 Score per residue for model 9

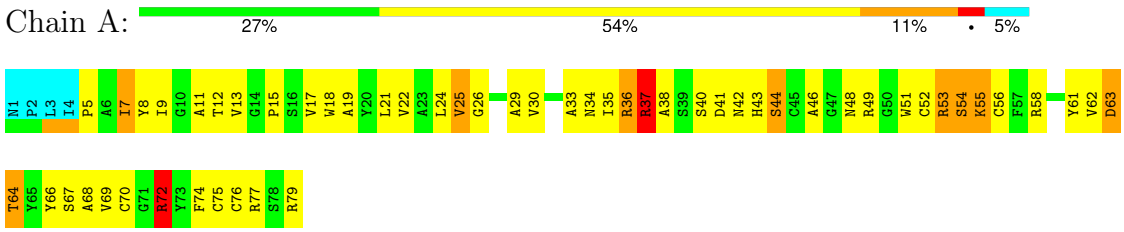
- Molecule 1: Big defensin



4.2.10 Score per residue for model 10

• Molecule 1: Big defensin

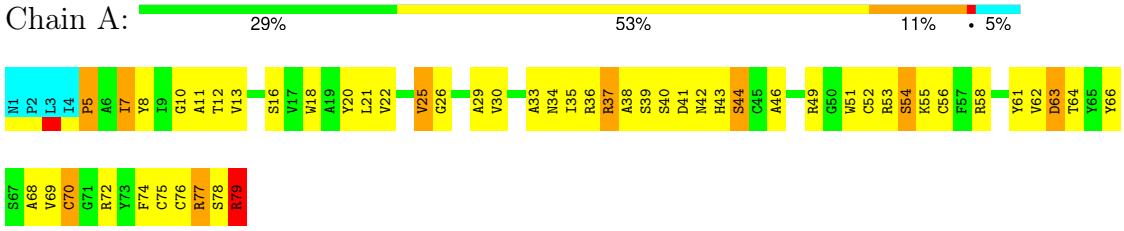
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Big defensin

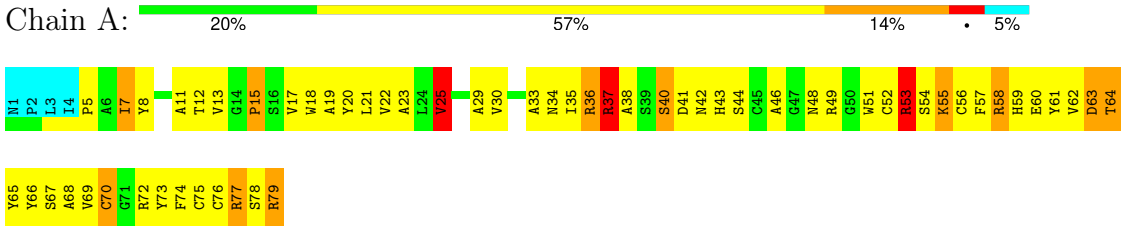
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Big defensin

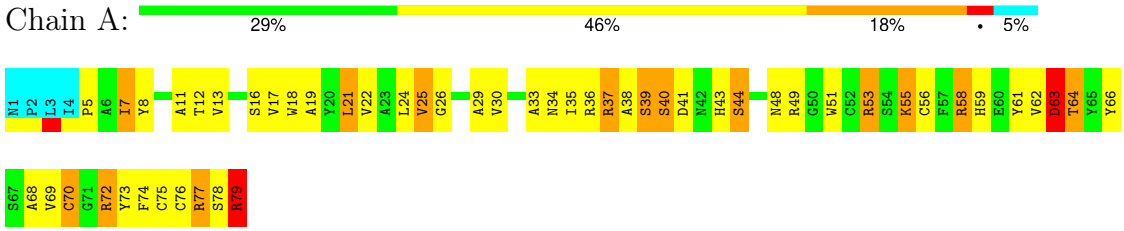
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Big defensin

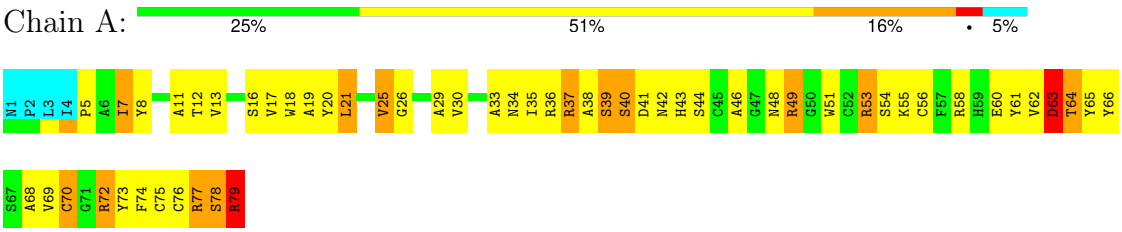
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Big defensin

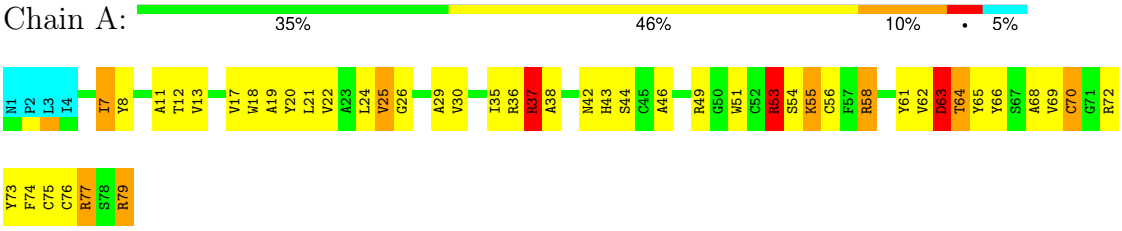
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Big defensin

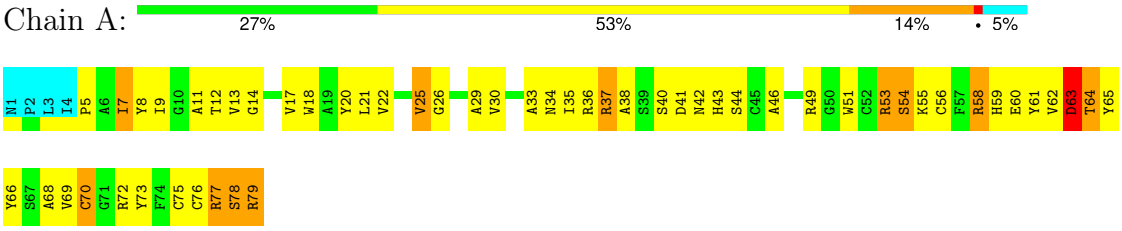
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Big defensin

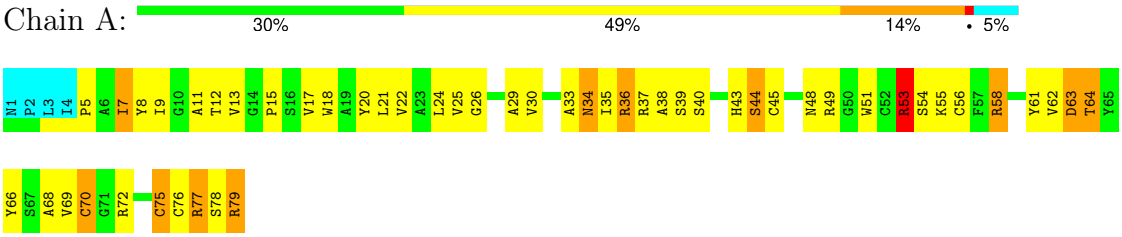
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Big defensin

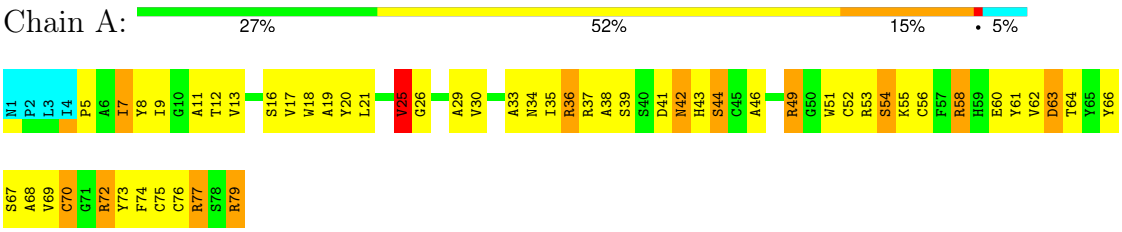
Chain A:



4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: Big defensin

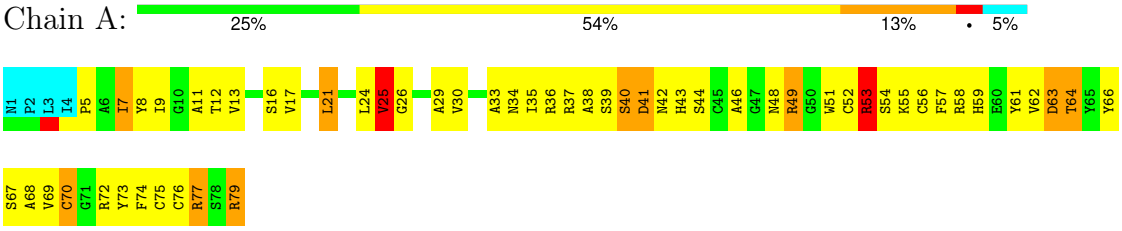
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Big defensin

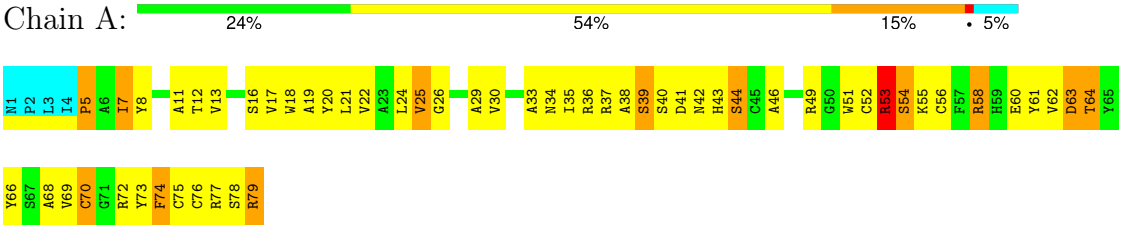
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Big defensin

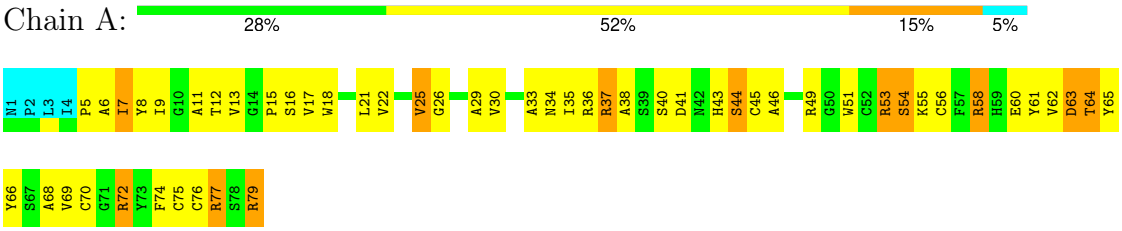
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Big defensin

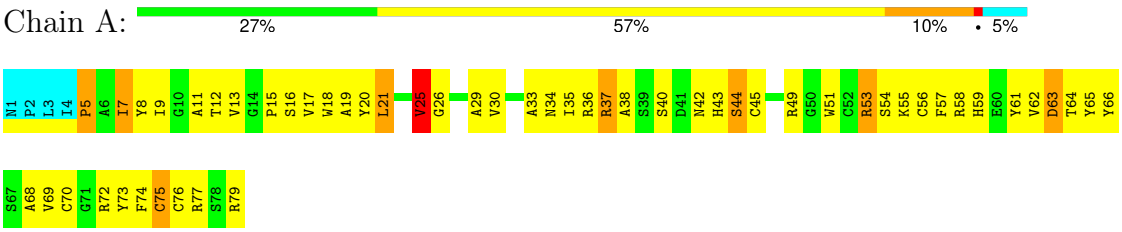
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Big defensin

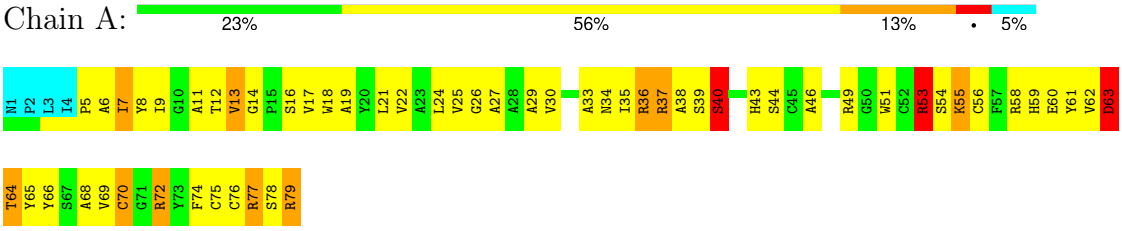
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: Big defensin

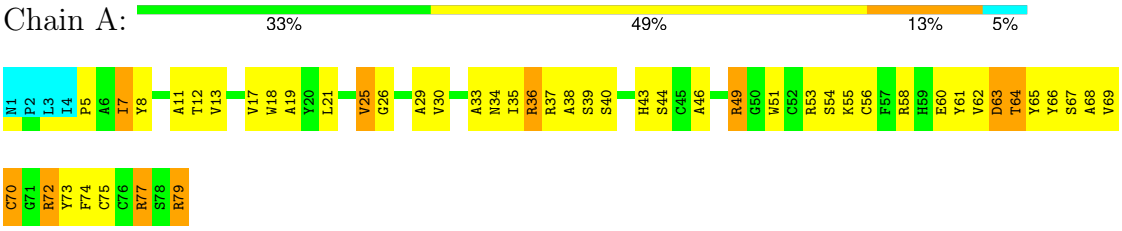
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: Big defensin

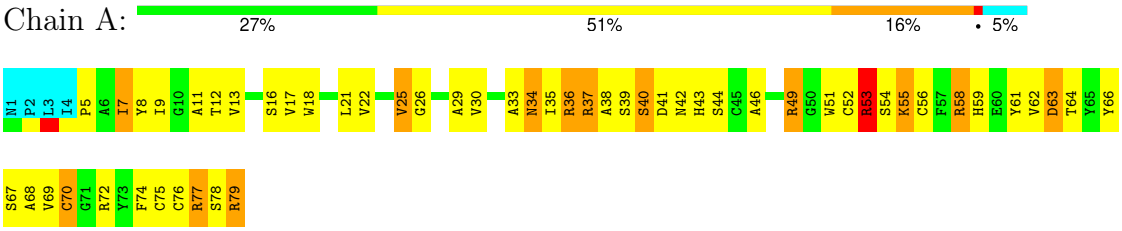
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: Big defensin

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
X-PLOR	structure solution	
X-PLOR	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	511
Number of shifts mapped to atoms	511
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	49%

6 Model quality

6.1 Standard geometry

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

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	7.6±0.7
All	All	0	190

There are no bond-length outliers.

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	37	ARG	Sidechain	25
1	A	49	ARG	Sidechain	25
1	A	58	ARG	Sidechain	25
1	A	79	ARG	Sidechain	25
1	A	53	ARG	Sidechain	24
1	A	36	ARG	Sidechain	24
1	A	72	ARG	Sidechain	23
1	A	77	ARG	Sidechain	19

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	575	545	545	78±7
All	All	14375	13625	13625	1952

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 70.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:VAL:HG21	1:A:29:ALA:HB3	1.01	1.33	13	20
1:A:13:VAL:HG12	1:A:69:VAL:HG23	0.96	1.35	24	25
1:A:25:VAL:HG22	1:A:29:ALA:HB1	0.93	1.40	23	1
1:A:8:TYR:CE1	1:A:68:ALA:HB1	0.92	1.99	2	9
1:A:7:ILE:HD13	1:A:68:ALA:HB3	0.92	1.38	3	6
1:A:25:VAL:HG22	1:A:29:ALA:CB	0.91	1.94	23	1
1:A:25:VAL:CG2	1:A:29:ALA:HB3	0.90	1.96	25	23
1:A:21:LEU:HD22	1:A:30:VAL:HG22	0.89	1.39	5	21
1:A:7:ILE:O	1:A:11:ALA:HB2	0.88	1.69	6	25
1:A:25:VAL:HG21	1:A:29:ALA:CB	0.85	2.02	20	20
1:A:7:ILE:CD1	1:A:68:ALA:HB3	0.84	2.03	3	6
1:A:25:VAL:CG2	1:A:29:ALA:HB1	0.82	2.03	23	1
1:A:13:VAL:CG1	1:A:69:VAL:HG23	0.82	2.05	16	24
1:A:43:HIS:CE1	1:A:69:VAL:HG22	0.81	2.11	1	25
1:A:46:ALA:HB1	1:A:77:ARG:NH2	0.81	1.89	5	1
1:A:56:CYS:SG	1:A:62:VAL:HG22	0.78	2.17	24	15
1:A:18:TRP:CZ3	1:A:35:ILE:HG22	0.78	2.13	2	11
1:A:25:VAL:HG22	1:A:26:GLY:N	0.77	1.95	10	19
1:A:33:ALA:HB3	1:A:35:ILE:CD1	0.76	2.10	19	7
1:A:21:LEU:CD1	1:A:35:ILE:HD13	0.76	2.10	13	8
1:A:25:VAL:CG2	1:A:30:VAL:HG23	0.75	2.11	3	2
1:A:33:ALA:HB3	1:A:35:ILE:HD11	0.74	1.59	19	2
1:A:21:LEU:HD23	1:A:21:LEU:O	0.74	1.80	17	21
1:A:7:ILE:HD11	1:A:66:TYR:CD1	0.72	2.20	5	9
1:A:5:PRO:HB2	1:A:7:ILE:HG22	0.71	1.62	17	15
1:A:7:ILE:HD11	1:A:66:TYR:CD2	0.71	2.19	7	8
1:A:21:LEU:HD13	1:A:35:ILE:HD13	0.71	1.62	5	15
1:A:25:VAL:HG23	1:A:29:ALA:HB3	0.70	1.61	8	3
1:A:26:GLY:O	1:A:30:VAL:HG23	0.67	1.89	24	21
1:A:7:ILE:CD1	1:A:66:TYR:CD2	0.66	2.79	17	8
1:A:21:LEU:C	1:A:21:LEU:HD23	0.66	2.10	11	6
1:A:18:TRP:O	1:A:22:VAL:HG23	0.66	1.91	20	3
1:A:7:ILE:CD1	1:A:66:TYR:CD1	0.65	2.79	11	11
1:A:8:TYR:HE1	1:A:68:ALA:HB1	0.65	1.47	5	1
1:A:5:PRO:CG	1:A:8:TYR:CD1	0.64	2.81	2	4
1:A:62:VAL:HG13	1:A:74:PHE:HB3	0.64	1.68	2	14
1:A:61:TYR:CE1	1:A:77:ARG:CB	0.64	2.81	24	17
1:A:18:TRP:CE3	1:A:37:ARG:CG	0.63	2.81	15	6
1:A:74:PHE:CD1	1:A:74:PHE:N	0.63	2.67	13	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:SER:N	1:A:51:TRP:CZ3	0.63	2.66	10	22
1:A:6:ALA:HA	1:A:9:ILE:HD12	0.63	1.71	23	2
1:A:12:THR:O	1:A:43:HIS:CE1	0.63	2.52	14	25
1:A:18:TRP:CE3	1:A:37:ARG:NE	0.63	2.67	3	3
1:A:18:TRP:CE3	1:A:37:ARG:CD	0.62	2.81	8	3
1:A:7:ILE:HD12	1:A:7:ILE:O	0.62	1.94	2	2
1:A:12:THR:H	1:A:69:VAL:HG21	0.61	1.53	13	25
1:A:25:VAL:HG22	1:A:30:VAL:HG23	0.61	1.71	3	1
1:A:33:ALA:HB3	1:A:35:ILE:HD12	0.61	1.71	23	3
1:A:13:VAL:HG23	1:A:14:GLY:N	0.61	2.08	23	1
1:A:21:LEU:CD2	1:A:30:VAL:HG22	0.61	2.25	11	2
1:A:5:PRO:HG2	1:A:8:TYR:CD1	0.61	2.30	2	4
1:A:18:TRP:CZ3	1:A:37:ARG:NH2	0.60	2.69	1	1
1:A:66:TYR:O	1:A:69:VAL:HG12	0.60	1.96	10	19
1:A:7:ILE:O	1:A:7:ILE:HD12	0.60	1.96	5	10
1:A:13:VAL:HG12	1:A:69:VAL:CG2	0.60	2.20	16	11
1:A:30:VAL:O	1:A:35:ILE:HD12	0.60	1.96	4	7
1:A:38:ALA:HB1	1:A:43:HIS:HB3	0.60	1.74	6	9
1:A:21:LEU:O	1:A:25:VAL:HG22	0.60	1.97	12	1
1:A:5:PRO:CG	1:A:8:TYR:CE2	0.60	2.85	7	10
1:A:51:TRP:CB	1:A:53:ARG:CZ	0.59	2.80	6	6
1:A:18:TRP:CD2	1:A:37:ARG:CG	0.59	2.85	15	2
1:A:8:TYR:O	1:A:35:ILE:HD13	0.59	1.98	12	1
1:A:6:ALA:HB3	1:A:65:TYR:OH	0.59	1.96	21	2
1:A:7:ILE:HG21	1:A:68:ALA:CB	0.59	2.28	8	8
1:A:18:TRP:CZ3	1:A:35:ILE:CG2	0.58	2.86	2	2
1:A:21:LEU:HD22	1:A:30:VAL:CG2	0.58	2.26	11	8
1:A:21:LEU:CD2	1:A:25:VAL:HG21	0.58	2.28	12	1
1:A:21:LEU:CD1	1:A:35:ILE:CD1	0.58	2.81	7	3
1:A:41:ASP:O	1:A:43:HIS:CD2	0.58	2.57	6	13
1:A:18:TRP:CE3	1:A:37:ARG:HD3	0.58	2.34	8	4
1:A:62:VAL:O	1:A:64:THR:N	0.58	2.37	3	25
1:A:21:LEU:CD2	1:A:25:VAL:CG2	0.58	2.82	12	1
1:A:61:TYR:CZ	1:A:77:ARG:HB2	0.57	2.33	24	14
1:A:42:ASN:OD1	1:A:73:TYR:CD2	0.57	2.57	20	4
1:A:54:SER:O	1:A:74:PHE:CE2	0.57	2.57	3	4
1:A:12:THR:O	1:A:43:HIS:ND1	0.57	2.38	13	25
1:A:25:VAL:CG2	1:A:26:GLY:N	0.57	2.68	15	21
1:A:18:TRP:CH2	1:A:30:VAL:HG12	0.57	2.34	13	3
1:A:18:TRP:CE3	1:A:37:ARG:HG2	0.56	2.35	15	3
1:A:25:VAL:CG2	1:A:29:ALA:CB	0.56	2.78	2	22

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:PRO:HG2	1:A:8:TYR:CE2	0.56	2.36	7	6
1:A:46:ALA:HB1	1:A:77:ARG:CZ	0.56	2.31	5	1
1:A:61:TYR:CE1	1:A:77:ARG:HB3	0.56	2.34	24	6
1:A:5:PRO:HG2	1:A:8:TYR:CD2	0.56	2.36	22	11
1:A:18:TRP:CE3	1:A:37:ARG:HG3	0.56	2.36	7	9
1:A:43:HIS:NE2	1:A:69:VAL:O	0.55	2.39	21	25
1:A:61:TYR:CZ	1:A:77:ARG:CB	0.55	2.89	24	6
1:A:21:LEU:O	1:A:25:VAL:HG12	0.55	2.00	23	1
1:A:18:TRP:CE3	1:A:37:ARG:CZ	0.55	2.90	1	1
1:A:21:LEU:O	1:A:21:LEU:HD23	0.55	2.02	23	2
1:A:43:HIS:HE1	1:A:69:VAL:HG22	0.55	1.62	22	20
1:A:63:ASP:CB	1:A:75:CYS:O	0.55	2.55	3	14
1:A:63:ASP:OD2	1:A:77:ARG:CG	0.55	2.55	5	1
1:A:8:TYR:CD2	1:A:21:LEU:HD12	0.54	2.38	3	1
1:A:7:ILE:HD13	1:A:66:TYR:CD1	0.54	2.37	6	5
1:A:12:THR:O	1:A:69:VAL:HG22	0.54	2.02	15	9
1:A:18:TRP:CD2	1:A:37:ARG:HG3	0.54	2.37	10	2
1:A:7:ILE:CD1	1:A:66:TYR:HA	0.54	2.32	3	11
1:A:18:TRP:HZ3	1:A:35:ILE:HG22	0.54	1.58	2	3
1:A:54:SER:O	1:A:74:PHE:CD1	0.54	2.61	11	7
1:A:70:CYS:SG	1:A:75:CYS:N	0.54	2.81	9	22
1:A:18:TRP:CD2	1:A:37:ARG:HD2	0.54	2.37	21	5
1:A:55:LYS:CG	1:A:56:CYS:N	0.54	2.71	1	9
1:A:44:SER:CA	1:A:51:TRP:CE3	0.54	2.91	21	11
1:A:7:ILE:HG21	1:A:68:ALA:HB3	0.54	1.78	21	7
1:A:17:VAL:HG23	1:A:41:ASP:OD1	0.54	2.03	1	5
1:A:21:LEU:HD23	1:A:21:LEU:C	0.54	2.24	20	10
1:A:18:TRP:CH2	1:A:30:VAL:CG1	0.54	2.90	4	3
1:A:22:VAL:O	1:A:26:GLY:N	0.53	2.41	8	5
1:A:73:TYR:N	1:A:73:TYR:CD1	0.53	2.76	8	7
1:A:18:TRP:CD2	1:A:37:ARG:CD	0.53	2.92	21	3
1:A:46:ALA:HB2	1:A:66:TYR:CD2	0.53	2.38	3	1
1:A:51:TRP:HB2	1:A:53:ARG:CZ	0.53	2.34	20	16
1:A:66:TYR:CB	1:A:75:CYS:SG	0.53	2.97	21	14
1:A:12:THR:O	1:A:12:THR:HG22	0.53	2.04	4	16
1:A:17:VAL:CG2	1:A:41:ASP:OD1	0.53	2.57	1	2
1:A:22:VAL:CG2	1:A:30:VAL:HG21	0.53	2.34	12	1
1:A:26:GLY:O	1:A:30:VAL:CG2	0.53	2.57	13	13
1:A:56:CYS:SG	1:A:62:VAL:CG2	0.53	2.97	22	14
1:A:8:TYR:O	1:A:35:ILE:CG1	0.53	2.57	8	2
1:A:12:THR:O	1:A:69:VAL:CG2	0.52	2.58	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:O	1:A:21:LEU:CD2	0.52	2.57	17	3
1:A:76:CYS:O	1:A:77:ARG:CG	0.52	2.56	21	2
1:A:44:SER:OG	1:A:51:TRP:CH2	0.52	2.57	21	2
1:A:18:TRP:CE3	1:A:37:ARG:HD2	0.52	2.40	3	3
1:A:44:SER:OG	1:A:51:TRP:CE2	0.52	2.57	7	3
1:A:25:VAL:HG23	1:A:29:ALA:CB	0.52	2.34	17	1
1:A:61:TYR:CD1	1:A:61:TYR:N	0.52	2.78	11	19
1:A:63:ASP:OD2	1:A:77:ARG:CD	0.52	2.57	5	5
1:A:21:LEU:O	1:A:25:VAL:CG2	0.52	2.57	12	1
1:A:42:ASN:ND2	1:A:52:CYS:O	0.52	2.43	2	6
1:A:45:CYS:HB2	1:A:66:TYR:CD1	0.52	2.40	22	2
1:A:70:CYS:SG	1:A:75:CYS:CB	0.52	2.98	17	4
1:A:44:SER:HB3	1:A:51:TRP:CH2	0.52	2.40	10	17
1:A:54:SER:O	1:A:74:PHE:CE1	0.52	2.63	25	6
1:A:51:TRP:HB3	1:A:53:ARG:CZ	0.51	2.34	6	5
1:A:25:VAL:HG23	1:A:26:GLY:N	0.51	2.20	8	2
1:A:22:VAL:HG13	1:A:27:ALA:CA	0.51	2.36	23	1
1:A:22:VAL:O	1:A:26:GLY:CA	0.51	2.59	23	1
1:A:12:THR:C	1:A:69:VAL:CG2	0.51	2.79	15	25
1:A:45:CYS:HB2	1:A:66:TYR:CD2	0.51	2.41	1	3
1:A:60:GLU:CG	1:A:77:ARG:O	0.51	2.58	24	5
1:A:62:VAL:O	1:A:62:VAL:HG12	0.51	2.04	10	7
1:A:21:LEU:CD2	1:A:25:VAL:CG1	0.51	2.89	15	5
1:A:57:PHE:N	1:A:57:PHE:CD1	0.51	2.74	19	3
1:A:18:TRP:CZ3	1:A:35:ILE:O	0.51	2.63	9	2
1:A:48:ASN:N	1:A:48:ASN:OD1	0.50	2.44	14	1
1:A:25:VAL:HG22	1:A:26:GLY:H	0.50	1.67	20	18
1:A:44:SER:HB2	1:A:51:TRP:CZ3	0.50	2.42	1	2
1:A:53:ARG:CD	1:A:56:CYS:SG	0.50	2.99	15	3
1:A:44:SER:HB3	1:A:51:TRP:CZ3	0.50	2.41	17	1
1:A:44:SER:HB3	1:A:51:TRP:CZ2	0.50	2.42	21	13
1:A:61:TYR:CE1	1:A:77:ARG:HB2	0.50	2.41	21	6
1:A:63:ASP:CG	1:A:77:ARG:CD	0.50	2.80	13	1
1:A:76:CYS:SG	1:A:77:ARG:N	0.50	2.84	2	2
1:A:43:HIS:CE1	1:A:69:VAL:O	0.50	2.64	13	10
1:A:21:LEU:CD2	1:A:21:LEU:C	0.50	2.80	14	9
1:A:70:CYS:SG	1:A:75:CYS:CA	0.50	3.00	21	4
1:A:5:PRO:HD2	1:A:8:TYR:CD2	0.50	2.42	6	1
1:A:33:ALA:CB	1:A:35:ILE:HD11	0.50	2.34	19	1
1:A:44:SER:HB2	1:A:51:TRP:CH2	0.49	2.42	1	5
1:A:44:SER:CB	1:A:51:TRP:CZ3	0.49	2.95	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:ILE:O	1:A:11:ALA:CB	0.49	2.59	8	10
1:A:8:TYR:N	1:A:8:TYR:CD1	0.49	2.76	1	6
1:A:7:ILE:HG23	1:A:8:TYR:CD1	0.49	2.41	11	2
1:A:63:ASP:O	1:A:63:ASP:OD1	0.49	2.31	8	3
1:A:54:SER:O	1:A:74:PHE:CD2	0.49	2.66	3	4
1:A:8:TYR:CZ	1:A:68:ALA:HB1	0.49	2.42	7	3
1:A:13:VAL:HG12	1:A:69:VAL:HA	0.49	1.83	22	4
1:A:7:ILE:HG23	1:A:8:TYR:H	0.49	1.67	17	11
1:A:46:ALA:HB2	1:A:66:TYR:CE2	0.49	2.42	3	1
1:A:60:GLU:CB	1:A:77:ARG:O	0.49	2.61	24	1
1:A:63:ASP:OD1	1:A:75:CYS:O	0.49	2.31	8	6
1:A:42:ASN:HB2	1:A:73:TYR:CD2	0.49	2.43	6	3
1:A:18:TRP:CH2	1:A:35:ILE:O	0.49	2.65	9	2
1:A:5:PRO:HG3	1:A:8:TYR:CD1	0.48	2.43	3	3
1:A:7:ILE:HG23	1:A:8:TYR:N	0.48	2.23	12	6
1:A:15:PRO:CD	1:A:40:SER:HA	0.48	2.39	17	8
1:A:21:LEU:C	1:A:21:LEU:CD2	0.48	2.81	15	5
1:A:63:ASP:OD2	1:A:75:CYS:SG	0.48	2.72	8	7
1:A:51:TRP:HB2	1:A:53:ARG:NH2	0.48	2.24	15	3
1:A:8:TYR:O	1:A:35:ILE:CD1	0.48	2.61	12	1
1:A:43:HIS:C	1:A:51:TRP:CE3	0.48	2.86	21	2
1:A:44:SER:HA	1:A:51:TRP:CE3	0.48	2.44	21	6
1:A:46:ALA:HA	1:A:66:TYR:CZ	0.48	2.44	24	4
1:A:66:TYR:HB3	1:A:75:CYS:SG	0.47	2.49	3	15
1:A:30:VAL:O	1:A:35:ILE:CG1	0.47	2.62	12	1
1:A:55:LYS:O	1:A:56:CYS:SG	0.47	2.72	13	6
1:A:59:HIS:CD2	1:A:60:GLU:HG3	0.47	2.44	8	1
1:A:55:LYS:CD	1:A:55:LYS:N	0.47	2.77	13	2
1:A:38:ALA:CB	1:A:43:HIS:HB3	0.47	2.40	10	23
1:A:42:ASN:OD1	1:A:73:TYR:CG	0.47	2.68	22	1
1:A:44:SER:OG	1:A:51:TRP:CD2	0.47	2.61	1	1
1:A:63:ASP:OD2	1:A:76:CYS:C	0.47	2.53	5	2
1:A:61:TYR:O	1:A:76:CYS:CB	0.47	2.63	13	1
1:A:63:ASP:OD2	1:A:75:CYS:O	0.47	2.32	23	3
1:A:39:SER:O	1:A:40:SER:CB	0.47	2.61	23	1
1:A:39:SER:O	1:A:40:SER:OG	0.47	2.33	20	6
1:A:73:TYR:C	1:A:74:PHE:CD1	0.47	2.88	3	2
1:A:6:ALA:CB	1:A:65:TYR:OH	0.47	2.62	6	1
1:A:25:VAL:HB	1:A:29:ALA:CB	0.47	2.40	8	2
1:A:20:TYR:O	1:A:23:ALA:HB3	0.47	2.08	12	1
1:A:44:SER:HB3	1:A:51:TRP:CE2	0.47	2.45	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:TRP:HB3	1:A:53:ARG:NH1	0.47	2.25	6	4
1:A:42:ASN:OD1	1:A:52:CYS:O	0.47	2.33	3	8
1:A:63:ASP:OD1	1:A:63:ASP:O	0.47	2.32	7	2
1:A:62:VAL:CG1	1:A:74:PHE:HB3	0.47	2.40	3	9
1:A:46:ALA:HA	1:A:66:TYR:CE2	0.47	2.45	16	5
1:A:18:TRP:CE2	1:A:37:ARG:HD2	0.47	2.44	14	1
1:A:63:ASP:CG	1:A:75:CYS:O	0.46	2.54	5	11
1:A:66:TYR:HB3	1:A:75:CYS:CB	0.46	2.41	10	1
1:A:51:TRP:HB3	1:A:53:ARG:NH2	0.46	2.25	1	1
1:A:63:ASP:OD1	1:A:63:ASP:N	0.46	2.48	5	1
1:A:37:ARG:CZ	1:A:37:ARG:CB	0.46	2.94	10	1
1:A:62:VAL:HG13	1:A:74:PHE:CB	0.46	2.40	3	1
1:A:55:LYS:O	1:A:76:CYS:SG	0.46	2.74	23	1
1:A:7:ILE:HD12	1:A:65:TYR:O	0.46	2.11	16	5
1:A:63:ASP:HB3	1:A:75:CYS:O	0.45	2.11	3	8
1:A:30:VAL:O	1:A:35:ILE:CD1	0.45	2.64	22	1
1:A:8:TYR:O	1:A:35:ILE:HG13	0.45	2.12	23	2
1:A:41:ASP:O	1:A:52:CYS:SG	0.45	2.74	25	1
1:A:51:TRP:O	1:A:75:CYS:HA	0.45	2.11	8	6
1:A:8:TYR:HD2	1:A:21:LEU:HD12	0.45	1.69	3	1
1:A:63:ASP:OD1	1:A:75:CYS:SG	0.45	2.74	14	5
1:A:63:ASP:OD2	1:A:77:ARG:HG3	0.45	2.12	5	2
1:A:63:ASP:OD1	1:A:77:ARG:HB2	0.45	2.12	5	2
1:A:7:ILE:HD12	1:A:68:ALA:HB3	0.45	1.87	9	1
1:A:53:ARG:HD3	1:A:56:CYS:SG	0.45	2.52	9	2
1:A:62:VAL:O	1:A:63:ASP:C	0.45	2.55	24	12
1:A:63:ASP:O	1:A:65:TYR:N	0.45	2.50	4	8
1:A:53:ARG:NH1	1:A:53:ARG:CG	0.45	2.80	17	1
1:A:61:TYR:O	1:A:76:CYS:HA	0.45	2.12	8	22
1:A:54:SER:OG	1:A:55:LYS:N	0.45	2.49	12	3
1:A:18:TRP:CD2	1:A:37:ARG:HD3	0.45	2.47	1	1
1:A:63:ASP:N	1:A:75:CYS:O	0.45	2.49	3	3
1:A:16:SER:HB2	1:A:41:ASP:OD1	0.45	2.12	4	1
1:A:51:TRP:HB2	1:A:53:ARG:NE	0.45	2.26	21	1
1:A:22:VAL:HA	1:A:30:VAL:HG21	0.45	1.88	10	2
1:A:12:THR:HA	1:A:36:ARG:O	0.45	2.12	6	7
1:A:70:CYS:SG	1:A:75:CYS:SG	0.45	3.14	1	4
1:A:70:CYS:SG	1:A:75:CYS:HB2	0.45	2.52	10	6
1:A:16:SER:CB	1:A:41:ASP:OD1	0.45	2.64	4	1
1:A:5:PRO:CG	1:A:8:TYR:CD2	0.45	3.00	20	1
1:A:46:ALA:HB2	1:A:77:ARG:HD2	0.45	1.88	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:TRP:HB3	1:A:53:ARG:NE	0.44	2.27	6	1
1:A:46:ALA:HB1	1:A:77:ARG:HH11	0.44	1.72	18	1
1:A:13:VAL:HA	1:A:43:HIS:NE2	0.44	2.27	10	1
1:A:13:VAL:HB	1:A:17:VAL:CG1	0.44	2.43	24	18
1:A:18:TRP:CZ3	1:A:37:ARG:CZ	0.44	2.99	1	1
1:A:7:ILE:HG23	1:A:8:TYR:HD1	0.44	1.73	5	2
1:A:7:ILE:HD12	1:A:7:ILE:C	0.44	2.31	6	3
1:A:13:VAL:HB	1:A:17:VAL:HG11	0.44	1.88	2	1
1:A:63:ASP:OD2	1:A:77:ARG:HD3	0.44	2.12	2	5
1:A:54:SER:N	1:A:73:TYR:CD2	0.44	2.86	9	1
1:A:9:ILE:HA	1:A:33:ALA:O	0.44	2.13	7	17
1:A:66:TYR:HB2	1:A:75:CYS:SG	0.44	2.52	13	4
1:A:33:ALA:O	1:A:34:ASN:C	0.44	2.56	2	7
1:A:15:PRO:HD2	1:A:40:SER:HA	0.44	1.90	4	4
1:A:25:VAL:HG13	1:A:26:GLY:H	0.44	1.73	9	16
1:A:53:ARG:O	1:A:54:SER:C	0.44	2.55	23	5
1:A:43:HIS:C	1:A:51:TRP:CZ3	0.44	2.91	12	2
1:A:54:SER:OG	1:A:73:TYR:CE1	0.44	2.69	14	1
1:A:27:ALA:O	1:A:31:THR:OG1	0.43	2.33	3	1
1:A:5:PRO:HG2	1:A:8:TYR:CG	0.43	2.48	6	1
1:A:25:VAL:HG13	1:A:29:ALA:HB3	0.43	1.89	23	1
1:A:42:ASN:OD1	1:A:42:ASN:C	0.43	2.57	8	5
1:A:21:LEU:HD13	1:A:35:ILE:CD1	0.43	2.43	14	2
1:A:39:SER:C	1:A:40:SER:OG	0.43	2.57	3	5
1:A:48:ASN:OD1	1:A:48:ASN:O	0.43	2.37	19	2
1:A:44:SER:N	1:A:51:TRP:CE3	0.43	2.86	21	1
1:A:20:TYR:O	1:A:21:LEU:C	0.43	2.57	5	12
1:A:61:TYR:CD1	1:A:79:ARG:HB2	0.43	2.49	11	1
1:A:38:ALA:O	1:A:40:SER:N	0.43	2.52	5	7
1:A:13:VAL:O	1:A:38:ALA:N	0.43	2.52	6	1
1:A:78:SER:O	1:A:78:SER:OG	0.43	2.36	9	1
1:A:68:ALA:O	1:A:70:CYS:N	0.43	2.51	8	1
1:A:46:ALA:CB	1:A:77:ARG:HD2	0.43	2.44	19	9
1:A:61:TYR:O	1:A:76:CYS:SG	0.43	2.76	13	2
1:A:7:ILE:HD13	1:A:66:TYR:CD2	0.43	2.47	17	2
1:A:51:TRP:CB	1:A:53:ARG:NE	0.43	2.81	3	4
1:A:43:HIS:HE1	1:A:69:VAL:HG13	0.43	1.72	24	6
1:A:13:VAL:O	1:A:37:ARG:HA	0.43	2.14	11	3
1:A:30:VAL:HG13	1:A:35:ILE:CD1	0.43	2.44	17	1
1:A:38:ALA:O	1:A:39:SER:C	0.43	2.57	17	7
1:A:46:ALA:HB1	1:A:77:ARG:HH21	0.43	1.70	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:PRO:HB2	1:A:7:ILE:CG2	0.43	2.44	25	2
1:A:76:CYS:O	1:A:77:ARG:HG2	0.43	2.14	21	1
1:A:8:TYR:O	1:A:11:ALA:HB3	0.42	2.14	7	2
1:A:53:ARG:HD2	1:A:56:CYS:SG	0.42	2.54	25	1
1:A:33:ALA:O	1:A:34:ASN:HB3	0.42	2.15	7	15
1:A:18:TRP:CE3	1:A:35:ILE:HG22	0.42	2.49	2	1
1:A:18:TRP:O	1:A:19:ALA:C	0.42	2.58	12	12
1:A:60:GLU:OE2	1:A:77:ARG:C	0.42	2.57	14	2
1:A:58:ARG:O	1:A:59:HIS:C	0.42	2.58	12	2
1:A:14:GLY:O	1:A:18:TRP:HB2	0.42	2.15	23	3
1:A:48:ASN:OD1	1:A:48:ASN:C	0.42	2.57	12	2
1:A:14:GLY:HA2	1:A:38:ALA:HB3	0.42	1.92	6	1
1:A:21:LEU:HD23	1:A:25:VAL:CG2	0.42	2.44	12	1
1:A:22:VAL:O	1:A:26:GLY:HA2	0.42	2.13	23	1
1:A:42:ASN:C	1:A:42:ASN:OD1	0.42	2.58	10	2
1:A:43:HIS:NE2	1:A:70:CYS:HA	0.42	2.28	22	2
1:A:63:ASP:CG	1:A:77:ARG:HD3	0.42	2.34	13	2
1:A:18:TRP:NE1	1:A:30:VAL:HG11	0.42	2.29	12	1
1:A:17:VAL:O	1:A:18:TRP:C	0.42	2.58	20	5
1:A:63:ASP:OD1	1:A:75:CYS:HB3	0.42	2.15	14	4
1:A:60:GLU:CD	1:A:77:ARG:O	0.42	2.58	16	2
1:A:6:ALA:HA	1:A:9:ILE:CD1	0.42	2.43	23	1
1:A:8:TYR:O	1:A:35:ILE:HG12	0.42	2.15	1	5
1:A:21:LEU:O	1:A:22:VAL:C	0.42	2.57	11	3
1:A:12:THR:OG1	1:A:36:ARG:HB2	0.42	2.15	12	3
1:A:48:ASN:O	1:A:48:ASN:CG	0.42	2.57	10	1
1:A:60:GLU:HG2	1:A:77:ARG:O	0.42	2.14	14	2
1:A:70:CYS:SG	1:A:74:PHE:C	0.42	2.98	14	2
1:A:16:SER:OG	1:A:17:VAL:N	0.42	2.52	18	2
1:A:21:LEU:CD2	1:A:21:LEU:O	0.42	2.65	18	1
1:A:76:CYS:C	1:A:77:ARG:CG	0.42	2.88	21	1
1:A:45:CYS:O	1:A:46:ALA:C	0.42	2.57	21	2
1:A:68:ALA:O	1:A:69:VAL:C	0.42	2.55	8	9
1:A:70:CYS:SG	1:A:73:TYR:C	0.42	2.98	8	1
1:A:66:TYR:CB	1:A:75:CYS:CB	0.42	2.98	10	1
1:A:25:VAL:HB	1:A:29:ALA:HB3	0.42	1.91	12	1
1:A:76:CYS:O	1:A:77:ARG:HG3	0.42	2.15	2	2
1:A:60:GLU:HB3	1:A:76:CYS:SG	0.42	2.55	12	1
1:A:51:TRP:CB	1:A:53:ARG:NH2	0.42	2.83	15	1
1:A:7:ILE:HD13	1:A:66:TYR:HA	0.42	1.91	18	1
1:A:18:TRP:CZ2	1:A:30:VAL:CG1	0.42	3.03	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ILE:O	1:A:10:GLY:C	0.41	2.57	7	1
1:A:78:SER:O	1:A:79:ARG:C	0.41	2.57	13	4
1:A:18:TRP:CG	1:A:37:ARG:NE	0.41	2.88	14	1
1:A:41:ASP:N	1:A:41:ASP:OD1	0.41	2.53	21	1
1:A:60:GLU:HB3	1:A:77:ARG:O	0.41	2.16	24	1
1:A:63:ASP:O	1:A:64:THR:C	0.41	2.58	7	5
1:A:55:LYS:C	1:A:56:CYS:SG	0.41	2.98	23	1
1:A:18:TRP:CE3	1:A:37:ARG:NH1	0.41	2.87	1	1
1:A:41:ASP:OD2	1:A:72:ARG:HD3	0.41	2.16	12	1
1:A:53:ARG:HB2	1:A:55:LYS:O	0.41	2.16	23	1
1:A:53:ARG:HD2	1:A:76:CYS:SG	0.41	2.56	19	1
1:A:13:VAL:CG2	1:A:14:GLY:N	0.41	2.78	23	1
1:A:17:VAL:O	1:A:20:TYR:HB3	0.41	2.16	1	4
1:A:18:TRP:CG	1:A:37:ARG:HD3	0.41	2.50	1	1
1:A:7:ILE:HG12	1:A:68:ALA:HB3	0.41	1.91	6	1
1:A:18:TRP:CG	1:A:37:ARG:HD2	0.41	2.51	11	1
1:A:8:TYR:HB3	1:A:21:LEU:HD11	0.41	1.92	23	1
1:A:20:TYR:C	1:A:20:TYR:CD1	0.41	2.94	4	1
1:A:7:ILE:CD1	1:A:66:TYR:CE1	0.41	3.03	5	1
1:A:6:ALA:O	1:A:9:ILE:HB	0.41	2.16	9	3
1:A:44:SER:CB	1:A:51:TRP:CH2	0.41	3.04	21	1
1:A:49:ARG:HB3	1:A:77:ARG:NH1	0.41	2.30	6	1
1:A:61:TYR:CE1	1:A:79:ARG:HB2	0.41	2.51	7	1
1:A:61:TYR:CZ	1:A:77:ARG:HB3	0.41	2.51	7	1
1:A:25:VAL:CB	1:A:29:ALA:HB3	0.41	2.45	8	1
1:A:7:ILE:HD12	1:A:66:TYR:HA	0.41	1.92	14	1
1:A:7:ILE:C	1:A:7:ILE:HD12	0.41	2.37	8	2
1:A:58:ARG:O	1:A:60:GLU:N	0.40	2.53	3	1
1:A:41:ASP:OD2	1:A:72:ARG:HD2	0.40	2.17	10	1
1:A:10:GLY:HA2	1:A:34:ASN:OD1	0.40	2.17	11	1
1:A:57:PHE:CD1	1:A:57:PHE:N	0.40	2.89	22	1
1:A:63:ASP:OD1	1:A:66:TYR:HB2	0.40	2.16	4	1
1:A:58:ARG:C	1:A:60:GLU:N	0.40	2.72	3	1
1:A:61:TYR:CD1	1:A:77:ARG:O	0.40	2.75	4	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	74/79 (94%)	58±1 (78±2%)	14±1 (19±2%)	2±1 (2±1%)	7 44
All	All	1850/1975 (94%)	1447 (78%)	359 (19%)	44 (2%)	7 44

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	63	ASP	25
1	A	5	PRO	7
1	A	25	VAL	6
1	A	13	VAL	3
1	A	40	SER	2
1	A	15	PRO	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	57/61 (93%)	45±2 (79±3%)	12±2 (21±3%)	2 30
All	All	1425/1525 (93%)	1125 (79%)	300 (21%)	2 30

All 33 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	7	ILE	25
1	A	70	CYS	22
1	A	25	VAL	21
1	A	64	THR	21
1	A	55	LYS	19
1	A	79	ARG	15
1	A	58	ARG	15
1	A	53	ARG	14
1	A	44	SER	12
1	A	54	SER	12

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Mol	Chain	Res	Type	Models (Total)
1	A	59	HIS	11
1	A	67	SER	11
1	A	72	ARG	11
1	A	16	SER	11
1	A	78	SER	10
1	A	39	SER	8
1	A	63	ASP	7
1	A	40	SER	7
1	A	37	ARG	6
1	A	49	ARG	6
1	A	36	ARG	5
1	A	21	LEU	5
1	A	48	ASN	4
1	A	75	CYS	4
1	A	41	ASP	3
1	A	77	ARG	3
1	A	42	ASN	3
1	A	52	CYS	2
1	A	65	TYR	2
1	A	34	ASN	2
1	A	56	CYS	1
1	A	57	PHE	1
1	A	74	PHE	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 49% for the well-defined parts and 49% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	511
Number of shifts mapped to atoms	511
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 49%, i.e. 482 atoms were assigned a chemical shift out of a possible 976. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	154/377 (41%)	154/154 (100%)	0/150 (0%)	0/73 (0%)
Sidechain	281/487 (58%)	281/320 (88%)	0/139 (0%)	0/28 (0%)
Aromatic	47/112 (42%)	47/54 (87%)	0/54 (0%)	0/4 (0%)
Overall	482/976 (49%)	482/528 (91%)	0/343 (0%)	0/105 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 49%, i.e. 511 atoms were assigned a chemical shift out of a possible 1036. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	159/395 (40%)	159/161 (99%)	0/158 (0%)	0/76 (0%)
Sidechain	305/529 (58%)	305/348 (88%)	0/152 (0%)	0/29 (0%)
Aromatic	47/112 (42%)	47/54 (87%)	0/54 (0%)	0/4 (0%)
Overall	511/1036 (49%)	511/563 (91%)	0/364 (0%)	0/109 (0%)

7.1.4 Statistically unusual chemical shifts (i)

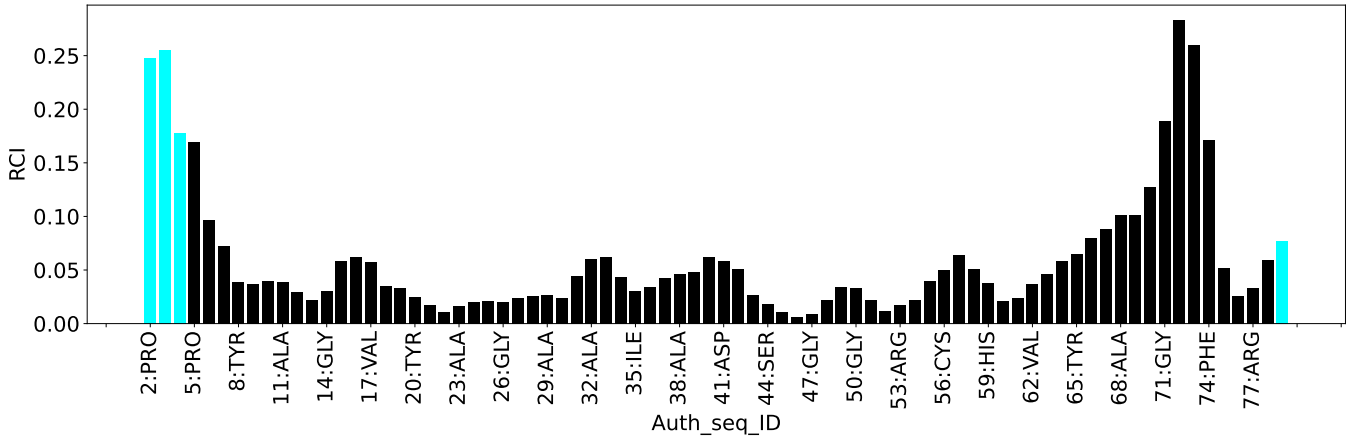
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	37	ARG	HD2	1.38	1.97 – 4.26	-7.6
1	A	37	ARG	HG3	-0.01	0.15 – 2.94	-5.6
1	A	41	ASP	HB2	1.27	1.41 – 4.01	-5.5

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1158
Intra-residue (|i-j|=0)	434
Sequential (|i-j|=1)	246
Medium range (|i-j|>1 and |i-j|<5)	133
Long range (|i-j|≥5)	283
Inter-chain	0
Hydrogen bond restraints	62
Disulfide bond restraints	0
Total dihedral-angle restraints	37
Number of unmapped restraints	0
Number of restraints per residue	15.1
Number of long range restraints per residue[1]	4.0

[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

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å
are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	8.3	0.2
0.2-0.5 (Medium)	1.4	0.27
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.4	2.22
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

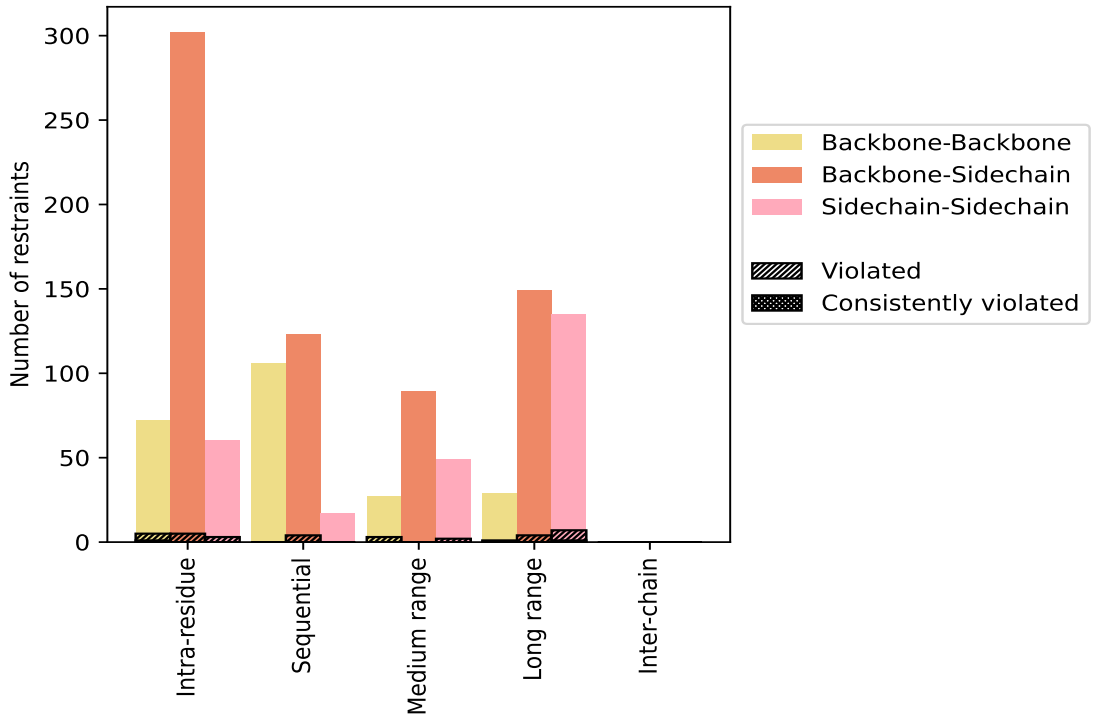
9.1 Summary of distance violations (i)

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)	434	37.5	13	3.0	1.1	1	0.2	0.1
Backbone-Backbone	72	6.2	5	6.9	0.4	1	1.4	0.1
Backbone-Sidechain	302	26.1	5	1.7	0.4	0	0.0	0.0
Sidechain-Sidechain	60	5.2	3	5.0	0.3	0	0.0	0.0
Sequential (|i-j|=1)	246	21.2	4	1.6	0.3	0	0.0	0.0
Backbone-Backbone	106	9.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	123	10.6	4	3.3	0.3	0	0.0	0.0
Sidechain-Sidechain	17	1.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	133	11.5	5	3.8	0.4	0	0.0	0.0
Backbone-Backbone	27	2.3	3	11.1	0.3	0	0.0	0.0
Backbone-Sidechain	57	4.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	49	4.2	2	4.1	0.2	0	0.0	0.0
Long range (|i-j|≥5)	283	24.4	10	3.5	0.9	1	0.4	0.1
Backbone-Backbone	29	2.5	1	3.4	0.1	0	0.0	0.0
Backbone-Sidechain	119	10.3	2	1.7	0.2	0	0.0	0.0
Sidechain-Sidechain	135	11.7	7	5.2	0.6	1	0.7	0.1
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	62	5.4	2	3.2	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1158	100.0	34	2.9	2.9	2	0.2	0.2
Backbone-Backbone	234	20.2	9	3.8	0.8	1	0.4	0.1
Backbone-Sidechain	663	57.3	13	2.0	1.1	0	0.0	0.0
Sidechain-Sidechain	261	22.5	12	4.6	1.0	1	0.4	0.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

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	3	0	1	4	0	8	0.15	0.25	0.05	0.12
2	4	2	1	3	0	10	0.17	0.25	0.05	0.16
3	4	0	3	6	0	13	0.14	0.24	0.04	0.13
4	5	1	1	5	0	12	0.14	0.24	0.04	0.14
5	2	2	1	5	0	10	0.15	0.25	0.04	0.13
6	4	2	1	2	0	9	0.17	0.25	0.05	0.15
7	4	1	1	6	0	12	0.14	0.24	0.04	0.12
8	6	0	1	5	0	12	0.13	0.18	0.03	0.12
9	3	1	2	5	0	11	0.14	0.24	0.04	0.13
10	4	2	2	4	0	12	0.13	0.24	0.04	0.12

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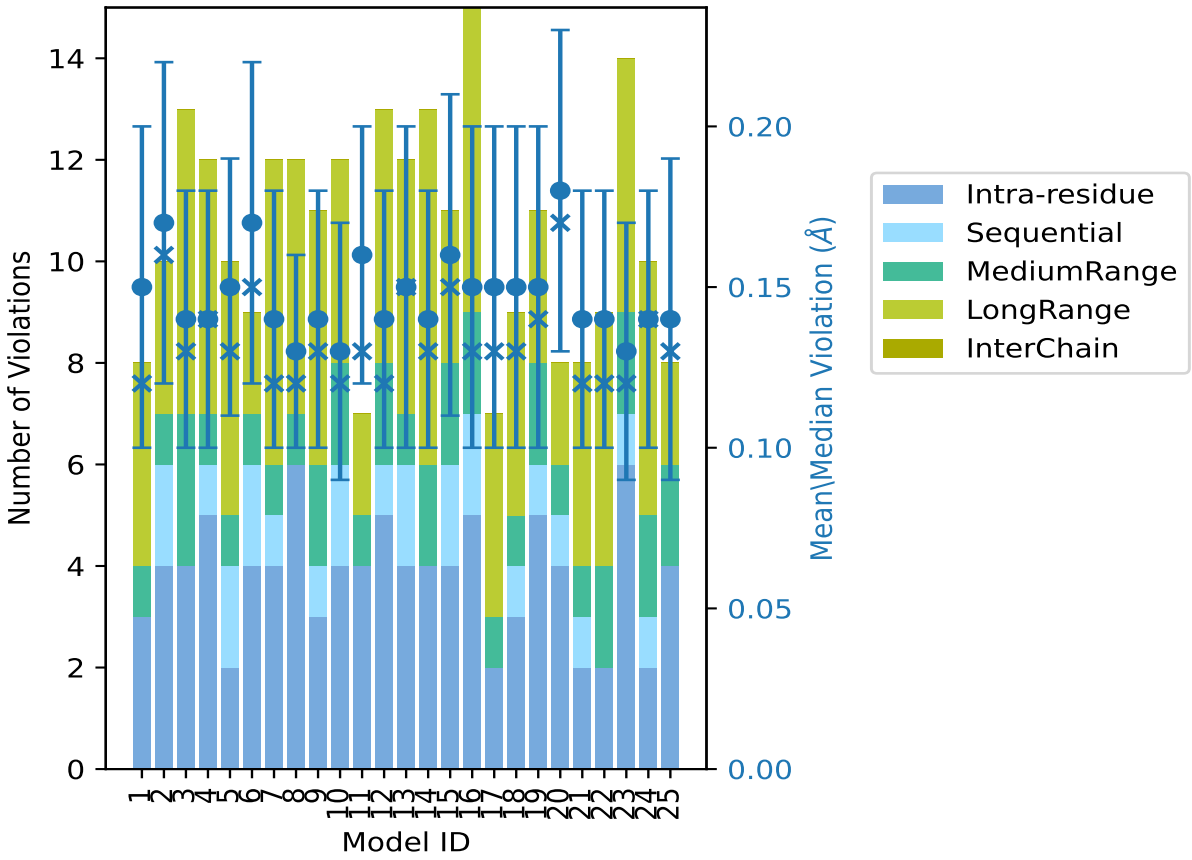
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	4	0	1	2	0	7	0.16	0.25	0.04	0.13
12	5	1	2	5	0	13	0.14	0.22	0.04	0.12
13	4	2	1	5	0	12	0.15	0.26	0.05	0.15
14	4	0	2	7	0	13	0.14	0.25	0.04	0.13
15	4	2	2	3	0	11	0.16	0.25	0.05	0.15
16	5	2	2	6	0	15	0.15	0.27	0.05	0.13
17	2	0	1	4	0	7	0.15	0.25	0.05	0.13
18	3	1	1	4	0	9	0.15	0.25	0.05	0.13
19	5	1	2	3	0	11	0.15	0.25	0.05	0.14
20	4	1	1	2	0	8	0.18	0.25	0.05	0.17
21	2	1	1	4	0	8	0.14	0.25	0.04	0.12
22	2	0	2	5	0	9	0.14	0.24	0.04	0.12
23	6	1	2	5	0	14	0.13	0.26	0.04	0.12
24	2	1	2	5	0	10	0.14	0.25	0.04	0.14
25	4	0	2	2	0	8	0.14	0.25	0.05	0.13

[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



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

9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1064(IR:421, SQ:242, MR:128, LR:273, 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]	%
5	0	1	4	0	10	1	4.0
1	1	1	1	0	4	2	8.0
0	0	0	1	0	1	3	12.0
0	0	1	0	0	1	4	16.0
2	1	0	0	0	3	5	20.0
0	0	0	1	0	1	6	24.0

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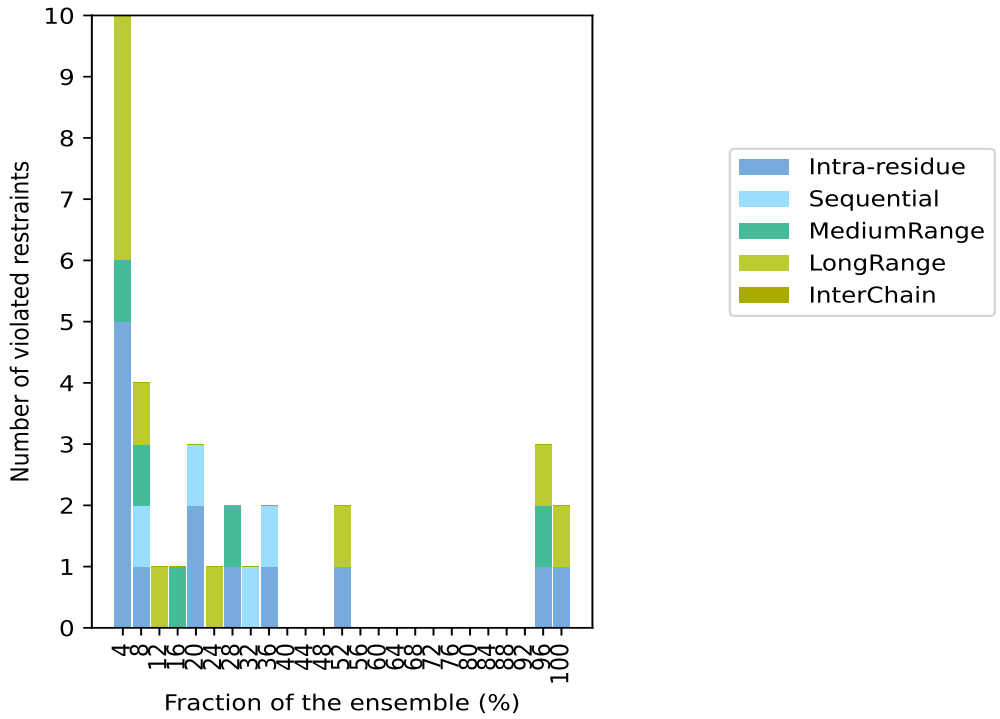
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	0	1	0	0	2	7	28.0
0	1	0	0	0	1	8	32.0
1	1	0	0	0	2	9	36.0
0	0	0	0	0	0	10	40.0
0	0	0	0	0	0	11	44.0
0	0	0	0	0	0	12	48.0
1	0	0	1	0	2	13	52.0
0	0	0	0	0	0	14	56.0
0	0	0	0	0	0	15	60.0
0	0	0	0	0	0	16	64.0
0	0	0	0	0	0	17	68.0
0	0	0	0	0	0	18	72.0
0	0	0	0	0	0	19	76.0
0	0	0	0	0	0	20	80.0
0	0	0	0	0	0	21	84.0
0	0	0	0	0	0	22	88.0
0	0	0	0	0	0	23	92.0
1	0	1	1	0	3	24	96.0
1	0	0	1	0	2	25	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

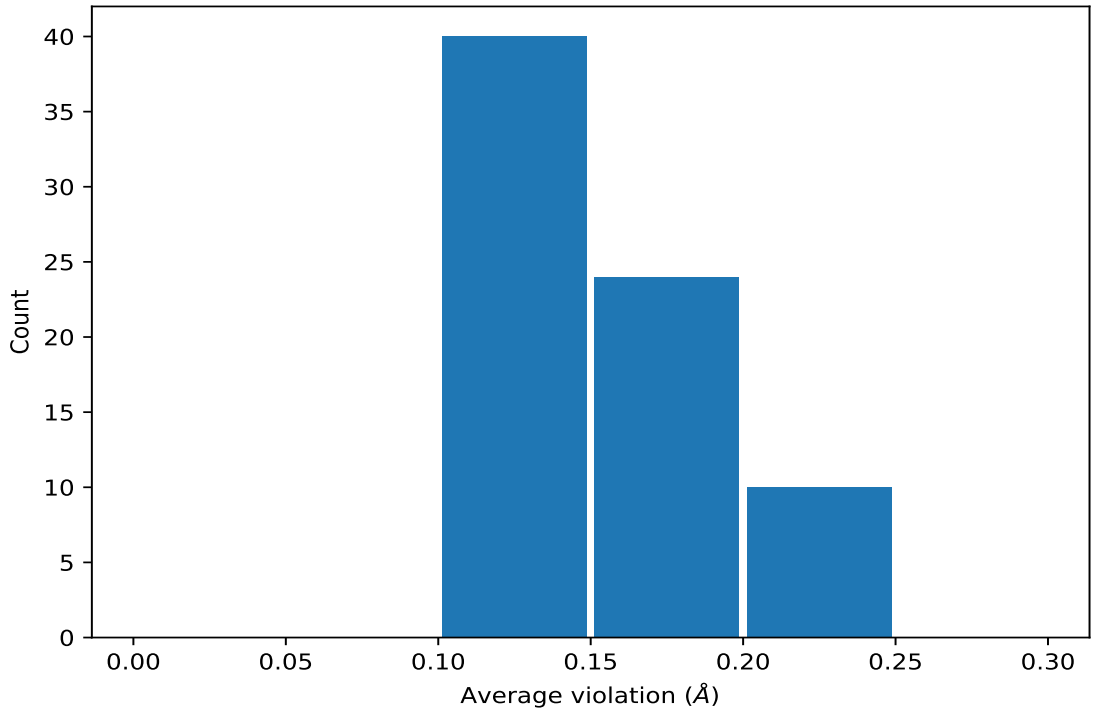
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	25	0.17	0.02	0.17
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	25	0.13	0.0	0.13
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	24	0.24	0.02	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	24	0.24	0.02	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	24	0.24	0.02	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	24	0.24	0.02	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	24	0.24	0.02	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	24	0.24	0.02	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	24	0.24	0.02	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	24	0.24	0.02	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	24	0.24	0.02	0.25
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	24	0.14	0.02	0.12
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	24	0.13	0.01	0.13
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	16	0.12	0.01	0.12
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	14	0.11	0.01	0.11
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	13	0.17	0.03	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	13	0.17	0.03	0.16
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	13	0.17	0.03	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	13	0.17	0.03	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	13	0.17	0.03	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	13	0.17	0.03	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	13	0.17	0.03	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	13	0.17	0.03	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	13	0.17	0.03	0.16
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	13	0.12	0.01	0.12
(2,1035)	1:76:A:CYS:HB2	1:77:A:ARG:H	9	0.15	0.04	0.13
(2,675)	1:53:A:ARG:HD2	1:53:A:ARG:HB3	9	0.12	0.02	0.11
(2,573)	1:45:A:CYS:HB3	1:46:A:ALA:H	8	0.11	0.01	0.11
(2,708)	1:55:A:LYS:HG2	1:55:A:LYS:H	7	0.21	0.06	0.24
(2,121)	1:9:A:ILE:HA	1:11:A:ALA:H	7	0.12	0.02	0.12
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD11	6	0.17	0.04	0.17
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD12	6	0.17	0.04	0.17
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD13	6	0.17	0.04	0.17
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD11	6	0.17	0.04	0.17
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD12	6	0.17	0.04	0.17
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD13	6	0.17	0.04	0.17
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD11	6	0.17	0.04	0.17
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD12	6	0.17	0.04	0.17
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD13	6	0.17	0.04	0.17
(2,709)	1:55:A:LYS:HG2	1:56:A:CYS:H	5	0.19	0.01	0.19
(2,777)	1:60:A:GLU:HB3	1:60:A:GLU:H	5	0.16	0.05	0.13
(2,704)	1:55:A:LYS:HB2	1:55:A:LYS:H	5	0.15	0.03	0.16
(2,746)	1:58:A:ARG:HA	1:60:A:GLU:H	4	0.11	0.0	0.11
(2,939)	1:69:A:VAL:HG21	1:12:A:THR:H	3	0.11	0.01	0.11
(2,939)	1:69:A:VAL:HG22	1:12:A:THR:H	3	0.11	0.01	0.11
(2,939)	1:69:A:VAL:HG23	1:12:A:THR:H	3	0.11	0.01	0.11
(2,798)	1:61:A:TYR:HB3	1:62:A:VAL:H	2	0.15	0.0	0.15
(2,24)	1:4:A:ILE:HG21	1:4:A:ILE:HD11	2	0.14	0.02	0.14
(2,24)	1:4:A:ILE:HG21	1:4:A:ILE:HD12	2	0.14	0.02	0.14
(2,24)	1:4:A:ILE:HG21	1:4:A:ILE:HD13	2	0.14	0.02	0.14
(2,24)	1:4:A:ILE:HG22	1:4:A:ILE:HD11	2	0.14	0.02	0.14
(2,24)	1:4:A:ILE:HG22	1:4:A:ILE:HD12	2	0.14	0.02	0.14
(2,24)	1:4:A:ILE:HG22	1:4:A:ILE:HD13	2	0.14	0.02	0.14
(2,24)	1:4:A:ILE:HG23	1:4:A:ILE:HD11	2	0.14	0.02	0.14
(2,24)	1:4:A:ILE:HG23	1:4:A:ILE:HD12	2	0.14	0.02	0.14
(2,24)	1:4:A:ILE:HG23	1:4:A:ILE:HD13	2	0.14	0.02	0.14
(2,426)	1:33:A:ALA:HB1	1:35:A:ILE:HD11	2	0.14	0.01	0.14
(2,426)	1:33:A:ALA:HB1	1:35:A:ILE:HD12	2	0.14	0.01	0.14

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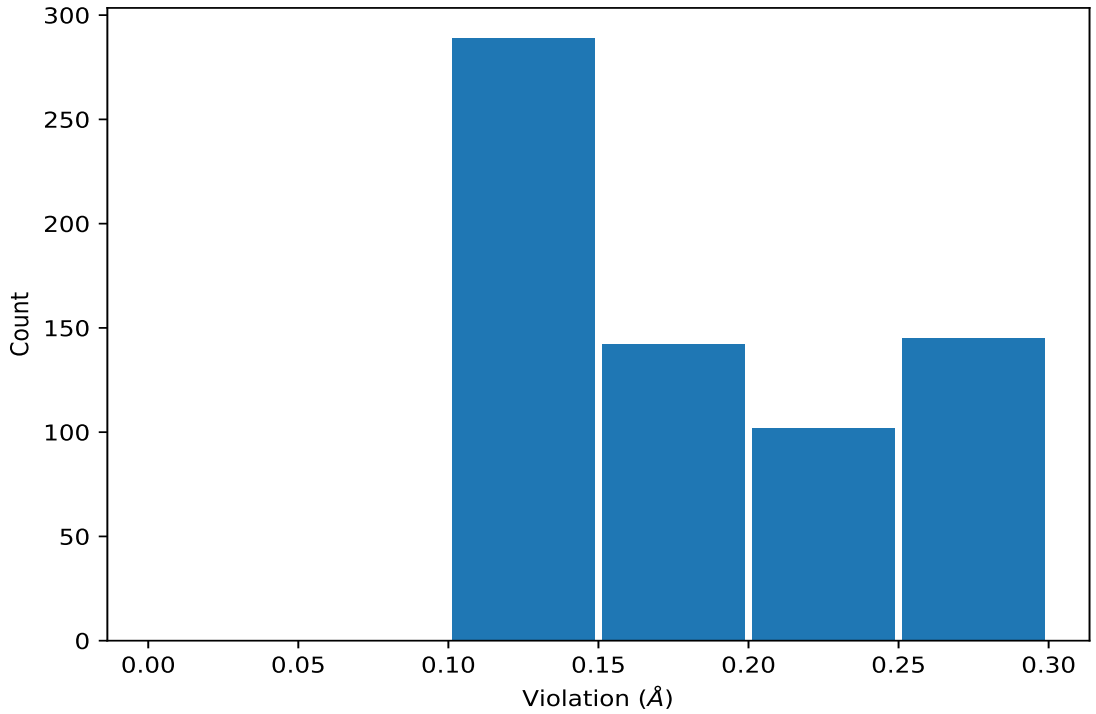
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,426)	1:33:A:ALA:HB1	1:35:A:ILE:HD13	2	0.14	0.01	0.14
(2,426)	1:33:A:ALA:HB2	1:35:A:ILE:HD11	2	0.14	0.01	0.14
(2,426)	1:33:A:ALA:HB2	1:35:A:ILE:HD12	2	0.14	0.01	0.14
(2,426)	1:33:A:ALA:HB2	1:35:A:ILE:HD13	2	0.14	0.01	0.14
(2,426)	1:33:A:ALA:HB3	1:35:A:ILE:HD11	2	0.14	0.01	0.14
(2,426)	1:33:A:ALA:HB3	1:35:A:ILE:HD12	2	0.14	0.01	0.14
(2,426)	1:33:A:ALA:HB3	1:35:A:ILE:HD13	2	0.14	0.01	0.14
(2,914)	1:68:A:ALA:HB1	1:7:A:ILE:HG21	2	0.1	0.0	0.1
(2,914)	1:68:A:ALA:HB1	1:7:A:ILE:HG22	2	0.1	0.0	0.1
(2,914)	1:68:A:ALA:HB1	1:7:A:ILE:HG23	2	0.1	0.0	0.1
(2,914)	1:68:A:ALA:HB2	1:7:A:ILE:HG21	2	0.1	0.0	0.1
(2,914)	1:68:A:ALA:HB2	1:7:A:ILE:HG22	2	0.1	0.0	0.1
(2,914)	1:68:A:ALA:HB2	1:7:A:ILE:HG23	2	0.1	0.0	0.1
(2,914)	1:68:A:ALA:HB3	1:7:A:ILE:HG21	2	0.1	0.0	0.1
(2,914)	1:68:A:ALA:HB3	1:7:A:ILE:HG22	2	0.1	0.0	0.1
(2,914)	1:68:A:ALA:HB3	1:7:A:ILE:HG23	2	0.1	0.0	0.1

[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)
(2,708)	1:55:A:LYS:HG2	1:55:A:LYS:H	16	0.27
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	13	0.26
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	13	0.26
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	13	0.26
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	13	0.26
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	13	0.26
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	13	0.26
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	13	0.26
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	13	0.26
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	13	0.26
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	23	0.26
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	23	0.26
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	23	0.26
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	23	0.26
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	23	0.26
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	23	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	23	0.26
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	23	0.26
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	23	0.26
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	1	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	1	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	1	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	1	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	1	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	1	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	1	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	1	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	1	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	2	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	2	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	2	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	2	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	2	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	2	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	2	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	2	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	2	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	5	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	5	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	5	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	5	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	5	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	5	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	5	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	5	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	5	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	6	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	6	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	6	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	6	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	6	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	6	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	6	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	6	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	6	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	11	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	11	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	11	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	11	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	11	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	11	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	11	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	11	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	14	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	14	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	14	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	14	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	14	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	14	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	14	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	14	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	14	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	15	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	15	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	15	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	15	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	15	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	15	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	15	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	15	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	15	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	17	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	17	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	17	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	17	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	17	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	17	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	17	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	17	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	17	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	18	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	18	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	18	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	18	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	18	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	18	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	18	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	18	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	19	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	19	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	19	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	19	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	19	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	19	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	19	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	19	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	19	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	20	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	20	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	20	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	20	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	20	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	20	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	20	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	20	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	20	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	21	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	21	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	21	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	21	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	21	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	21	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	21	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	21	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	21	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	24	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	24	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	24	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	24	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	24	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	24	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	24	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	24	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	24	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	25	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	25	0.25
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	25	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	25	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	25	0.25
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	25	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	25	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	25	0.25
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	25	0.25
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD11	3	0.24
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD12	3	0.24
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD13	3	0.24
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD11	3	0.24
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD12	3	0.24
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD13	3	0.24
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD11	3	0.24
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD12	3	0.24
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD13	3	0.24
(2,708)	1:55:A:LYS:HG2	1:55:A:LYS:H	6	0.24
(2,708)	1:55:A:LYS:HG2	1:55:A:LYS:H	15	0.24
(2,708)	1:55:A:LYS:HG2	1:55:A:LYS:H	20	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	4	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	4	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	4	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	4	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	4	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	4	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	4	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	4	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	4	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	7	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	7	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	7	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	7	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	7	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	7	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	7	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	7	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	7	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	9	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	9	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	9	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	9	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	9	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	9	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	9	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	9	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	10	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	10	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	10	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	10	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	10	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	10	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	10	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	10	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	10	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	16	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	16	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	16	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	16	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	16	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	16	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	16	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	16	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	16	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	22	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	22	0.24
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	22	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	22	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	22	0.24
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	22	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	22	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	22	0.24
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	22	0.24
(2,1035)	1:76:A:CYS:HB2	1:77:A:ARG:H	2	0.23
(2,708)	1:55:A:LYS:HG2	1:55:A:LYS:H	19	0.23
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	13	0.23
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	13	0.23
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	13	0.23
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	13	0.23
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	13	0.23
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	13	0.23
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	13	0.23
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	13	0.23
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	13	0.23
(2,1035)	1:76:A:CYS:HB2	1:77:A:ARG:H	12	0.22
(2,777)	1:60:A:GLU:HB3	1:60:A:GLU:H	12	0.22
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	18	0.21
(2,777)	1:60:A:GLU:HB3	1:60:A:GLU:H	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	5	0.21
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	5	0.21
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	5	0.21
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	5	0.21
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	5	0.21
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	5	0.21
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	5	0.21
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	5	0.21
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	5	0.21
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	1	0.2
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	20	0.2
(2,709)	1:55:A:LYS:HG2	1:56:A:CYS:H	16	0.2
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	7	0.2
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	7	0.2
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	7	0.2
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	7	0.2
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	7	0.2
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	7	0.2
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	7	0.2
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	7	0.2
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	7	0.2
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	3	0.19
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	4	0.19
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	6	0.19
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	17	0.19
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD11	9	0.19
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD12	9	0.19
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD13	9	0.19
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD11	9	0.19
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD12	9	0.19
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD13	9	0.19
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD11	9	0.19
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD12	9	0.19
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD13	9	0.19
(2,709)	1:55:A:LYS:HG2	1:56:A:CYS:H	15	0.19
(2,709)	1:55:A:LYS:HG2	1:56:A:CYS:H	19	0.19
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	3	0.19
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	3	0.19
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	3	0.19
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	3	0.19
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	3	0.19
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	3	0.19
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	3	0.19
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	3	0.19
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	10	0.19
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	10	0.19
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	10	0.19
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	10	0.19
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	10	0.19
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	10	0.19
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	10	0.19
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	10	0.19
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	10	0.19
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	8	0.18
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	11	0.18
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	22	0.18
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	25	0.18
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD11	16	0.18
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD12	16	0.18
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD13	16	0.18
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD11	16	0.18
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD12	16	0.18
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD13	16	0.18
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD11	16	0.18
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD12	16	0.18
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD13	16	0.18
(2,709)	1:55:A:LYS:HG2	1:56:A:CYS:H	6	0.18
(2,704)	1:55:A:LYS:HB2	1:55:A:LYS:H	4	0.18
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG21	8	0.18
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG22	8	0.18
(2,381)	1:29:A:ALA:HB1	1:25:A:VAL:HG23	8	0.18
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG21	8	0.18
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG22	8	0.18
(2,381)	1:29:A:ALA:HB2	1:25:A:VAL:HG23	8	0.18
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG21	8	0.18
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG22	8	0.18
(2,381)	1:29:A:ALA:HB3	1:25:A:VAL:HG23	8	0.18
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	14	0.18
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	14	0.18
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	14	0.18
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	14	0.18
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	14	0.18
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	14	0.18
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	14	0.18
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	14	0.18
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	2	0.17
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	13	0.17
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	15	0.17
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	19	0.17
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	23	0.17
(2,709)	1:55:A:LYS:HG2	1:56:A:CYS:H	20	0.17
(2,704)	1:55:A:LYS:HB2	1:55:A:LYS:H	13	0.17
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	2	0.17
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	3	0.17
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	9	0.17
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	11	0.17
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	16	0.17
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	20	0.17
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	22	0.17
(2,1035)	1:76:A:CYS:HB2	1:77:A:ARG:H	13	0.16
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	7	0.16
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	12	0.16
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	21	0.16
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	24	0.16
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD11	12	0.16
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD12	12	0.16
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD13	12	0.16
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD11	12	0.16
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD12	12	0.16
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD13	12	0.16
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD11	12	0.16
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD12	12	0.16
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD13	12	0.16
(2,704)	1:55:A:LYS:HB2	1:55:A:LYS:H	23	0.16
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	2	0.16
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	2	0.16
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	2	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	2	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	2	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	2	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	2	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	2	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	2	0.16
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	15	0.16
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	15	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	15	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	15	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	15	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	15	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	15	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	15	0.16
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	24	0.16
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	24	0.16
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	24	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	24	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	24	0.16
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	24	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	24	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	24	0.16
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	24	0.16
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	18	0.16
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	5	0.15
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	9	0.15
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	14	0.15
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	16	0.15
(2,798)	1:61:A:TYR:HB3	1:62:A:VAL:H	5	0.15
(2,798)	1:61:A:TYR:HB3	1:62:A:VAL:H	13	0.15
(2,675)	1:53:A:ARG:HD2	1:53:A:ARG:HB3	6	0.15
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	1	0.15
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	6	0.15
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	15	0.15
(2,24)	1:4:A:ILE:HG21	1:4:A:ILE:HD11	8	0.15
(2,24)	1:4:A:ILE:HG21	1:4:A:ILE:HD12	8	0.15
(2,24)	1:4:A:ILE:HG21	1:4:A:ILE:HD13	8	0.15
(2,24)	1:4:A:ILE:HG22	1:4:A:ILE:HD11	8	0.15
(2,24)	1:4:A:ILE:HG22	1:4:A:ILE:HD12	8	0.15
(2,24)	1:4:A:ILE:HG22	1:4:A:ILE:HD13	8	0.15
(2,24)	1:4:A:ILE:HG23	1:4:A:ILE:HD11	8	0.15
(2,24)	1:4:A:ILE:HG23	1:4:A:ILE:HD12	8	0.15
(2,24)	1:4:A:ILE:HG23	1:4:A:ILE:HD13	8	0.15
(2,927)	1:69:A:VAL:HB	1:43:A:HIS:HE1	10	0.14
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	2	0.14
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	4	0.14
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	8	0.14
(2,426)	1:33:A:ALA:HB1	1:35:A:ILE:HD11	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,426)	1:33:A:ALA:HB1	1:35:A:ILE:HD12	19	0.14
(2,426)	1:33:A:ALA:HB1	1:35:A:ILE:HD13	19	0.14
(2,426)	1:33:A:ALA:HB2	1:35:A:ILE:HD11	19	0.14
(2,426)	1:33:A:ALA:HB2	1:35:A:ILE:HD12	19	0.14
(2,426)	1:33:A:ALA:HB2	1:35:A:ILE:HD13	19	0.14
(2,426)	1:33:A:ALA:HB3	1:35:A:ILE:HD11	19	0.14
(2,426)	1:33:A:ALA:HB3	1:35:A:ILE:HD12	19	0.14
(2,426)	1:33:A:ALA:HB3	1:35:A:ILE:HD13	19	0.14
(2,397)	1:30:A:VAL:HG21	1:25:A:VAL:HG21	3	0.14
(2,397)	1:30:A:VAL:HG21	1:25:A:VAL:HG22	3	0.14
(2,397)	1:30:A:VAL:HG21	1:25:A:VAL:HG23	3	0.14
(2,397)	1:30:A:VAL:HG22	1:25:A:VAL:HG21	3	0.14
(2,397)	1:30:A:VAL:HG22	1:25:A:VAL:HG22	3	0.14
(2,397)	1:30:A:VAL:HG22	1:25:A:VAL:HG23	3	0.14
(2,397)	1:30:A:VAL:HG23	1:25:A:VAL:HG21	3	0.14
(2,397)	1:30:A:VAL:HG23	1:25:A:VAL:HG22	3	0.14
(2,397)	1:30:A:VAL:HG23	1:25:A:VAL:HG23	3	0.14
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	3	0.14
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	3	0.14
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	3	0.14
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	3	0.14
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	3	0.14
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	3	0.14
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	3	0.14
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	3	0.14
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	3	0.14
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	4	0.14
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	4	0.14
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	4	0.14
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	4	0.14
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	4	0.14
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	4	0.14
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	4	0.14
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	4	0.14
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	4	0.14
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	16	0.14
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	16	0.14
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	16	0.14
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	16	0.14
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	16	0.14
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	16	0.14
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	16	0.14
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	16	0.14
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	7	0.14
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	17	0.14
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	19	0.14
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	20	0.14
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	24	0.14
(2,121)	1:9:A:ILE:HA	1:11:A:ALA:H	14	0.14
(2,121)	1:9:A:ILE:HA	1:11:A:ALA:H	24	0.14
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	4	0.14
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	14	0.14
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	8	0.14
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	13	0.14
(2,1035)	1:76:A:CYS:HB2	1:77:A:ARG:H	4	0.13
(2,1035)	1:76:A:CYS:HB2	1:77:A:ARG:H	10	0.13
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD11	14	0.13
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD12	14	0.13
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD13	14	0.13
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD11	14	0.13
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD12	14	0.13
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD13	14	0.13
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD11	14	0.13
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD12	14	0.13
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD13	14	0.13
(2,777)	1:60:A:GLU:HB3	1:60:A:GLU:H	25	0.13
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	14	0.13
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	25	0.13
(2,675)	1:53:A:ARG:HD2	1:53:A:ARG:HB3	11	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	1	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	3	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	5	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	6	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	7	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	9	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	10	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	11	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	12	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	13	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	14	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	15	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	16	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	18	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	19	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	20	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	21	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	23	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	24	0.13
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	25	0.13
(2,451)	1:35:A:ILE:HG21	1:35:A:ILE:HD11	16	0.13
(2,451)	1:35:A:ILE:HG21	1:35:A:ILE:HD12	16	0.13
(2,451)	1:35:A:ILE:HG21	1:35:A:ILE:HD13	16	0.13
(2,451)	1:35:A:ILE:HG22	1:35:A:ILE:HD11	16	0.13
(2,451)	1:35:A:ILE:HG22	1:35:A:ILE:HD12	16	0.13
(2,451)	1:35:A:ILE:HG22	1:35:A:ILE:HD13	16	0.13
(2,451)	1:35:A:ILE:HG23	1:35:A:ILE:HD11	16	0.13
(2,451)	1:35:A:ILE:HG23	1:35:A:ILE:HD12	16	0.13
(2,451)	1:35:A:ILE:HG23	1:35:A:ILE:HD13	16	0.13
(2,426)	1:33:A:ALA:HB1	1:35:A:ILE:HD11	23	0.13
(2,426)	1:33:A:ALA:HB1	1:35:A:ILE:HD12	23	0.13
(2,426)	1:33:A:ALA:HB1	1:35:A:ILE:HD13	23	0.13
(2,426)	1:33:A:ALA:HB2	1:35:A:ILE:HD11	23	0.13
(2,426)	1:33:A:ALA:HB2	1:35:A:ILE:HD12	23	0.13
(2,426)	1:33:A:ALA:HB2	1:35:A:ILE:HD13	23	0.13
(2,426)	1:33:A:ALA:HB3	1:35:A:ILE:HD11	23	0.13
(2,426)	1:33:A:ALA:HB3	1:35:A:ILE:HD12	23	0.13
(2,426)	1:33:A:ALA:HB3	1:35:A:ILE:HD13	23	0.13
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	2	0.13
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	3	0.13
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	9	0.13
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	12	0.13
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	13	0.13
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	22	0.13
(2,121)	1:9:A:ILE:HA	1:11:A:ALA:H	16	0.13
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	5	0.13
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	18	0.13
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	7	0.13
(2,1069)	1:77:A:ARG:HG2	1:63:A:ASP:HB3	5	0.12
(2,1035)	1:76:A:CYS:HB2	1:77:A:ARG:H	15	0.12
(2,1035)	1:76:A:CYS:HB2	1:77:A:ARG:H	21	0.12
(2,939)	1:69:A:VAL:HG21	1:12:A:THR:H	22	0.12
(2,939)	1:69:A:VAL:HG22	1:12:A:THR:H	22	0.12
(2,939)	1:69:A:VAL:HG23	1:12:A:THR:H	22	0.12
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD11	24	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD12	24	0.12
(2,913)	1:68:A:ALA:HB1	1:7:A:ILE:HD13	24	0.12
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD11	24	0.12
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD12	24	0.12
(2,913)	1:68:A:ALA:HB2	1:7:A:ILE:HD13	24	0.12
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD11	24	0.12
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD12	24	0.12
(2,913)	1:68:A:ALA:HB3	1:7:A:ILE:HD13	24	0.12
(2,777)	1:60:A:GLU:HB3	1:60:A:GLU:H	3	0.12
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	4	0.12
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	6	0.12
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	7	0.12
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	8	0.12
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	11	0.12
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	23	0.12
(2,704)	1:55:A:LYS:HB2	1:55:A:LYS:H	1	0.12
(2,675)	1:53:A:ARG:HD2	1:53:A:ARG:HB3	14	0.12
(2,675)	1:53:A:ARG:HD2	1:53:A:ARG:HB3	19	0.12
(2,599)	1:48:A:ASN:HA	1:48:A:ASN:H	22	0.12
(2,573)	1:45:A:CYS:HB3	1:46:A:ALA:H	6	0.12
(2,573)	1:45:A:CYS:HB3	1:46:A:ALA:H	10	0.12
(2,573)	1:45:A:CYS:HB3	1:46:A:ALA:H	24	0.12
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	18	0.12
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	18	0.12
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	18	0.12
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	18	0.12
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	18	0.12
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	18	0.12
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	18	0.12
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	18	0.12
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	18	0.12
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD11	21	0.12
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD12	21	0.12
(2,295)	1:21:A:LEU:HD11	1:35:A:ILE:HD13	21	0.12
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD11	21	0.12
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD12	21	0.12
(2,295)	1:21:A:LEU:HD12	1:35:A:ILE:HD13	21	0.12
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD11	21	0.12
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD12	21	0.12
(2,295)	1:21:A:LEU:HD13	1:35:A:ILE:HD13	21	0.12
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	5	0.12
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	11	0.12
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	14	0.12
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	16	0.12
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	21	0.12
(2,121)	1:9:A:ILE:HA	1:11:A:ALA:H	12	0.12
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	1	0.12
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	7	0.12
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	10	0.12
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	15	0.12
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	17	0.12
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	19	0.12
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	24	0.12
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	25	0.12
(2,24)	1:4:A:ILE:HG21	1:4:A:ILE:HD11	23	0.12
(2,24)	1:4:A:ILE:HG21	1:4:A:ILE:HD12	23	0.12
(2,24)	1:4:A:ILE:HG21	1:4:A:ILE:HD13	23	0.12
(2,24)	1:4:A:ILE:HG22	1:4:A:ILE:HD11	23	0.12
(2,24)	1:4:A:ILE:HG22	1:4:A:ILE:HD12	23	0.12
(2,24)	1:4:A:ILE:HG22	1:4:A:ILE:HD13	23	0.12
(2,24)	1:4:A:ILE:HG23	1:4:A:ILE:HD11	23	0.12
(2,24)	1:4:A:ILE:HG23	1:4:A:ILE:HD12	23	0.12
(2,24)	1:4:A:ILE:HG23	1:4:A:ILE:HD13	23	0.12
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	5	0.12
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	1	0.12
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	4	0.12
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	10	0.12
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	12	0.12
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	14	0.12
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	17	0.12
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	21	0.12
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	22	0.12
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	23	0.12
(2,1035)	1:76:A:CYS:HB2	1:77:A:ARG:H	5	0.11
(2,1035)	1:76:A:CYS:HB2	1:77:A:ARG:H	9	0.11
(2,939)	1:69:A:VAL:HG21	1:12:A:THR:H	7	0.11
(2,939)	1:69:A:VAL:HG22	1:12:A:THR:H	7	0.11
(2,939)	1:69:A:VAL:HG23	1:12:A:THR:H	7	0.11
(2,777)	1:60:A:GLU:HB3	1:60:A:GLU:H	10	0.11
(2,746)	1:58:A:ARG:HA	1:60:A:GLU:H	3	0.11
(2,746)	1:58:A:ARG:HA	1:60:A:GLU:H	12	0.11
(2,746)	1:58:A:ARG:HA	1:60:A:GLU:H	15	0.11
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	9	0.11
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	12	0.11
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	15	0.11
(2,745)	1:58:A:ARG:HA	1:58:A:ARG:H	16	0.11
(2,708)	1:55:A:LYS:HG2	1:55:A:LYS:H	2	0.11
(2,708)	1:55:A:LYS:HG2	1:55:A:LYS:H	12	0.11
(2,675)	1:53:A:ARG:HD2	1:53:A:ARG:HB3	20	0.11
(2,675)	1:53:A:ARG:HD2	1:53:A:ARG:HB3	23	0.11
(2,628)	1:50:A:GLY:HA3	1:78:A:SER:H	10	0.11
(2,612)	1:49:A:ARG:HB3	1:49:A:ARG:H	19	0.11
(2,573)	1:45:A:CYS:HB3	1:46:A:ALA:H	7	0.11
(2,573)	1:45:A:CYS:HB3	1:46:A:ALA:H	16	0.11
(2,573)	1:45:A:CYS:HB3	1:46:A:ALA:H	18	0.11
(2,366)	1:27:A:ALA:HA	1:30:A:VAL:H	3	0.11
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	4	0.11
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	23	0.11
(2,173)	1:13:A:VAL:HA	1:43:A:HIS:HE1	25	0.11
(2,121)	1:9:A:ILE:HA	1:11:A:ALA:H	10	0.11
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	8	0.11
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	12	0.11
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	13	0.11
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	21	0.11
(2,51)	1:6:A:ALA:HA	1:6:A:ALA:H	23	0.11
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	1	0.11
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	4	0.11
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	7	0.11
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	9	0.11
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	12	0.11
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	14	0.11
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	16	0.11
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	17	0.11
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	23	0.11
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	9	0.11
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	16	0.11
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	24	0.11
(2,1033)	1:76:A:CYS:HB2	1:56:A:CYS:HB2	14	0.1
(2,939)	1:69:A:VAL:HG21	1:12:A:THR:H	13	0.1
(2,939)	1:69:A:VAL:HG22	1:12:A:THR:H	13	0.1
(2,939)	1:69:A:VAL:HG23	1:12:A:THR:H	13	0.1
(2,914)	1:68:A:ALA:HB1	1:7:A:ILE:HG21	8	0.1
(2,914)	1:68:A:ALA:HB1	1:7:A:ILE:HG22	8	0.1
(2,914)	1:68:A:ALA:HB1	1:7:A:ILE:HG23	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,914)	1:68:A:ALA:HB2	1:7:A:ILE:HG21	8	0.1
(2,914)	1:68:A:ALA:HB2	1:7:A:ILE:HG22	8	0.1
(2,914)	1:68:A:ALA:HB2	1:7:A:ILE:HG23	8	0.1
(2,914)	1:68:A:ALA:HB3	1:7:A:ILE:HG21	8	0.1
(2,914)	1:68:A:ALA:HB3	1:7:A:ILE:HG22	8	0.1
(2,914)	1:68:A:ALA:HB3	1:7:A:ILE:HG23	8	0.1
(2,914)	1:68:A:ALA:HB1	1:7:A:ILE:HG21	23	0.1
(2,914)	1:68:A:ALA:HB1	1:7:A:ILE:HG22	23	0.1
(2,914)	1:68:A:ALA:HB1	1:7:A:ILE:HG23	23	0.1
(2,914)	1:68:A:ALA:HB2	1:7:A:ILE:HG21	23	0.1
(2,914)	1:68:A:ALA:HB2	1:7:A:ILE:HG22	23	0.1
(2,914)	1:68:A:ALA:HB2	1:7:A:ILE:HG23	23	0.1
(2,914)	1:68:A:ALA:HB3	1:7:A:ILE:HG21	23	0.1
(2,914)	1:68:A:ALA:HB3	1:7:A:ILE:HG22	23	0.1
(2,914)	1:68:A:ALA:HB3	1:7:A:ILE:HG23	23	0.1
(2,746)	1:58:A:ARG:HA	1:60:A:GLU:H	25	0.1
(2,704)	1:55:A:LYS:HB2	1:55:A:LYS:H	7	0.1
(2,675)	1:53:A:ARG:HD2	1:53:A:ARG:HB3	4	0.1
(2,675)	1:53:A:ARG:HD2	1:53:A:ARG:HB3	8	0.1
(2,675)	1:53:A:ARG:HD2	1:53:A:ARG:HB3	18	0.1
(2,641)	1:51:A:TRP:HB3	1:51:A:TRP:H	10	0.1
(2,573)	1:45:A:CYS:HB3	1:46:A:ALA:H	2	0.1
(2,573)	1:45:A:CYS:HB3	1:46:A:ALA:H	23	0.1
(2,370)	1:28:A:ALA:HA	1:28:A:ALA:H	13	0.1
(2,325)	1:24:A:LEU:HA	1:24:A:LEU:H	8	0.1
(2,121)	1:9:A:ILE:HA	1:11:A:ALA:H	9	0.1
(2,121)	1:9:A:ILE:HA	1:11:A:ALA:H	22	0.1
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	3	0.1
(1,40)	1:50:A:GLY:H	1:45:A:CYS:O	22	0.1
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	8	0.1
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	18	0.1
(1,6)	1:11:A:ALA:H	1:34:A:ASN:O	19	0.1

10 Dihedral-angle violation analysis

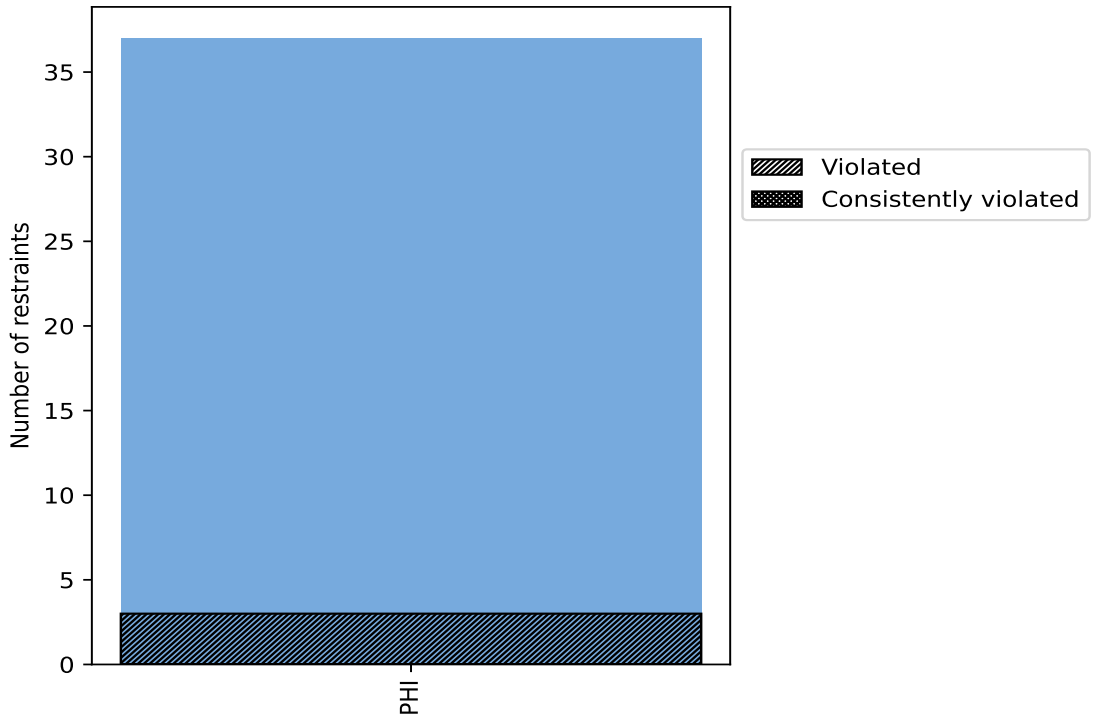
10.1 Summary of dihedral-angle violations

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	37	100.0	3	8.1	8.1	0	0.0	0.0
Total	37	100.0	3	8.1	8.1	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



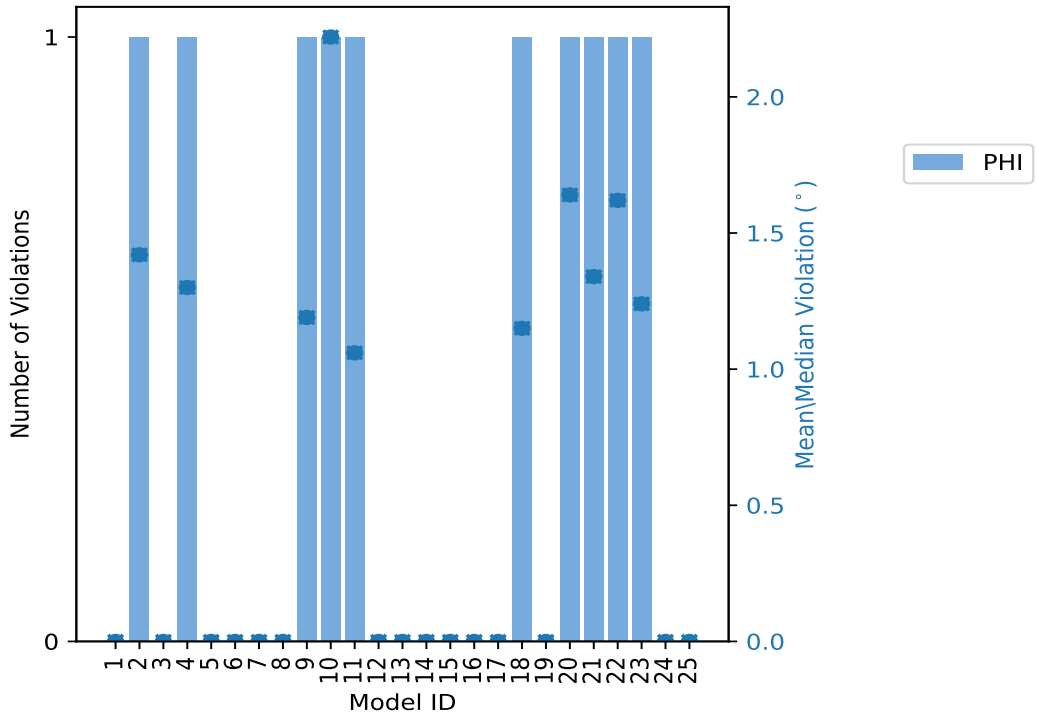
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	Total				
1	0	0	0.0	0.0	0.0	0.0
2	1	1	1.42	1.42	0.0	1.42
3	0	0	0.0	0.0	0.0	0.0
4	1	1	1.3	1.3	0.0	1.3
5	0	0	0.0	0.0	0.0	0.0
6	0	0	0.0	0.0	0.0	0.0
7	0	0	0.0	0.0	0.0	0.0
8	0	0	0.0	0.0	0.0	0.0
9	1	1	1.19	1.19	0.0	1.19
10	1	1	2.22	2.22	0.0	2.22
11	1	1	1.06	1.06	0.0	1.06
12	0	0	0.0	0.0	0.0	0.0
13	0	0	0.0	0.0	0.0	0.0
14	0	0	0.0	0.0	0.0	0.0
15	0	0	0.0	0.0	0.0	0.0
16	0	0	0.0	0.0	0.0	0.0
17	0	0	0.0	0.0	0.0	0.0
18	1	1	1.15	1.15	0.0	1.15
19	0	0	0.0	0.0	0.0	0.0
20	1	1	1.64	1.64	0.0	1.64
21	1	1	1.34	1.34	0.0	1.34
22	1	1	1.62	1.62	0.0	1.62
23	1	1	1.24	1.24	0.0	1.24
24	0	0	0.0	0.0	0.0	0.0
25	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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	Total	Count[1]	%
2	2	1	4.0
0	0	2	8.0
0	0	3	12.0
0	0	4	16.0
0	0	5	20.0
0	0	6	24.0
0	0	7	28.0
1	1	8	32.0
0	0	9	36.0
0	0	10	40.0
0	0	11	44.0

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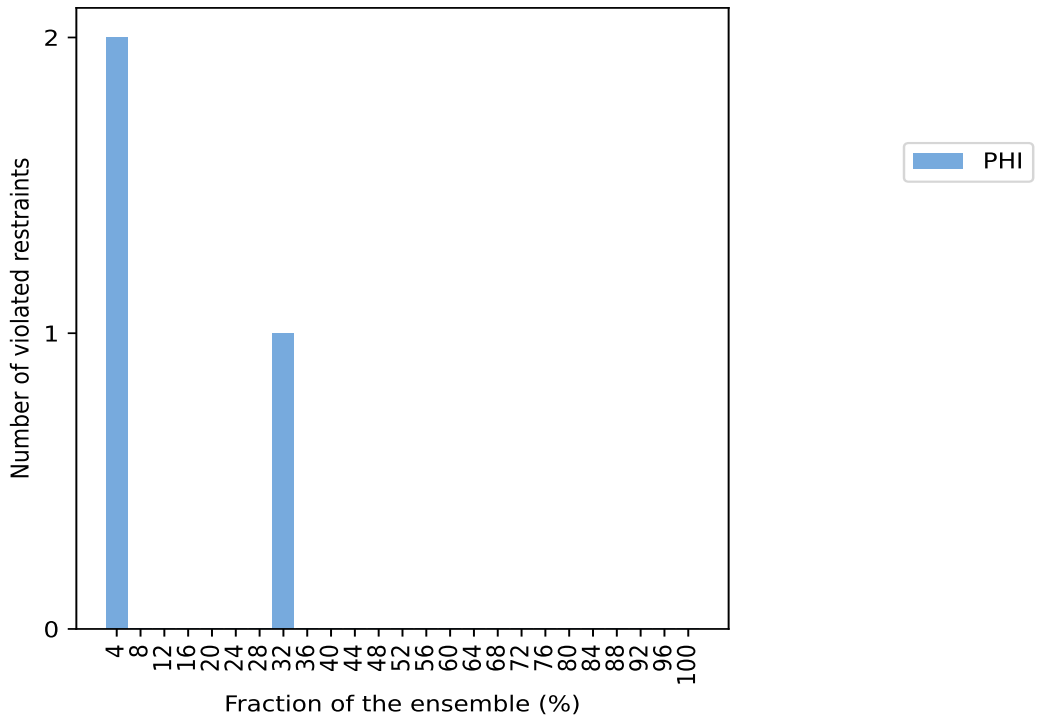
Number of violated restraints		Fraction of the ensemble	
PHI	Total	Count[1]	%
0	0	12	48.0
0	0	13	52.0
0	0	14	56.0
0	0	15	60.0
0	0	16	64.0
0	0	17	68.0
0	0	18	72.0
0	0	19	76.0
0	0	20	80.0
0	0	21	84.0
0	0	22	88.0
0	0	23	92.0
0	0	24	96.0
0	0	25	100.0

[1] Number of models with violations

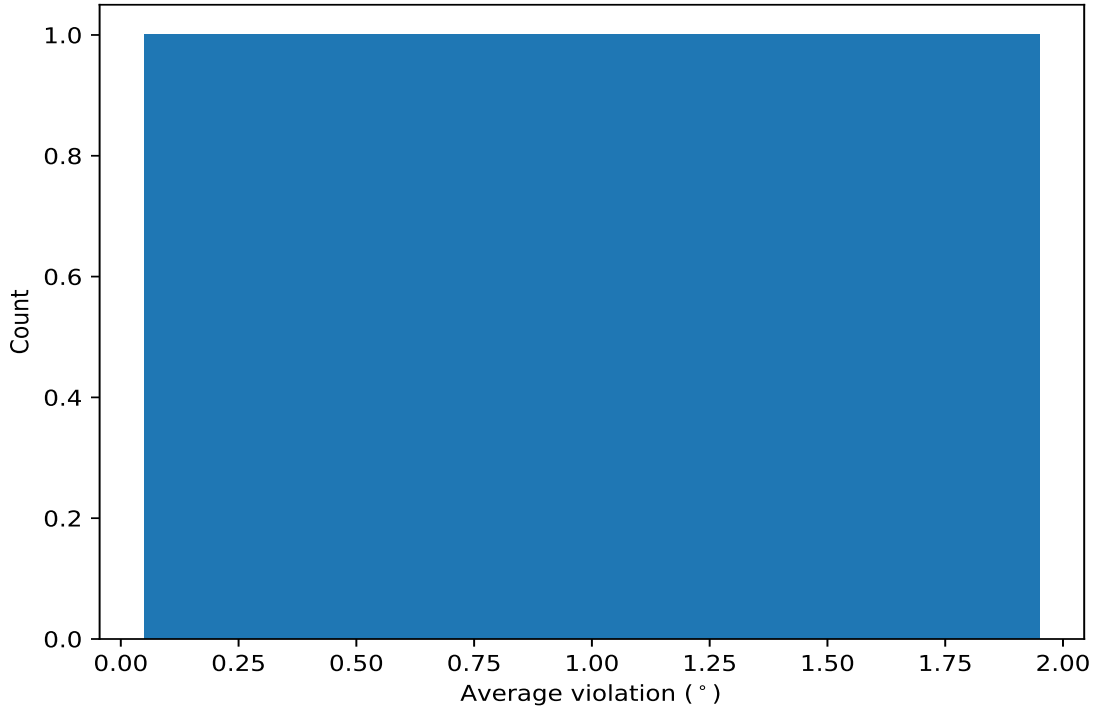
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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



10.4.2 Table: Most violated dihedral-angle restraints

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.

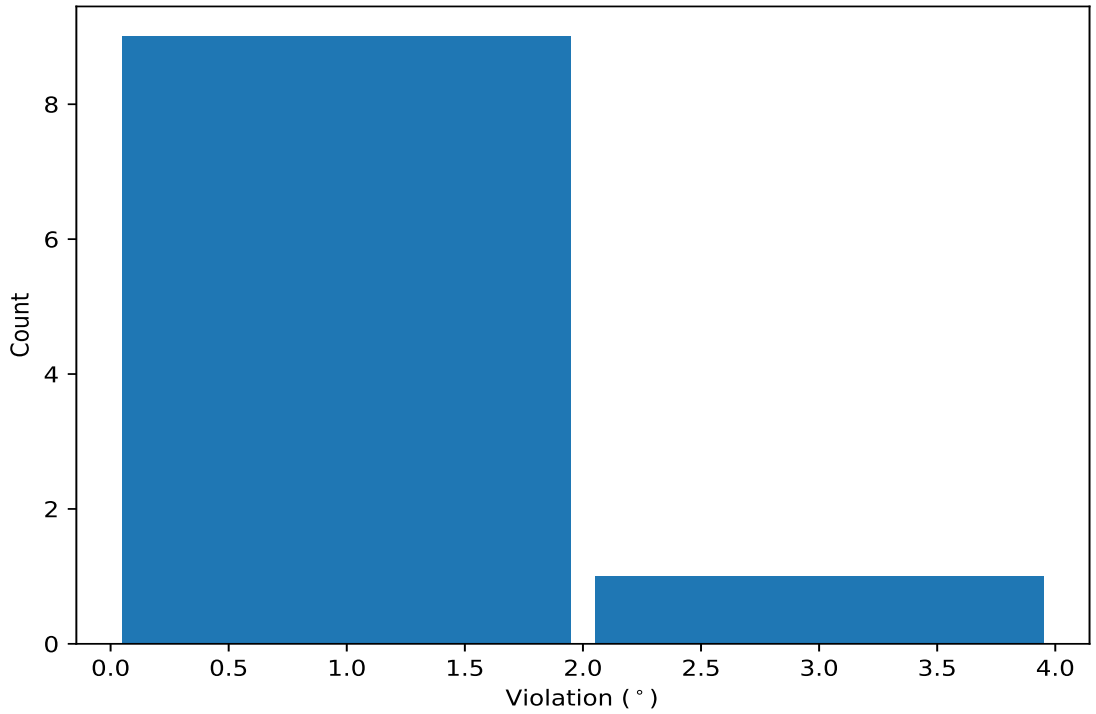
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,35)	1:75:A:CYS:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	8	1.47	0.34	1.38

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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 (°)
(1,35)	1:75:A:CYS:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	10	2.22
(1,35)	1:75:A:CYS:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	20	1.64
(1,35)	1:75:A:CYS:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	22	1.62
(1,35)	1:75:A:CYS:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	2	1.42
(1,35)	1:75:A:CYS:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	21	1.34
(1,35)	1:75:A:CYS:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	4	1.3
(1,34)	1:74:A:PHE:C	1:75:A:CYS:N	1:75:A:CYS:CA	1:75:A:CYS:C	23	1.24
(1,36)	1:76:A:CYS:C	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	9	1.19
(1,35)	1:75:A:CYS:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	18	1.15
(1,35)	1:75:A:CYS:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	11	1.06