Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 12:51 PM EDT

PDB ID	:	2LKH
BMRB ID	:	17992
Title	:	WSA minor conformation
Authors	:	Xu, Y.; Mowrey, D.; Cui, T.; Perez-Aguilar, J.; Saven, J.G.; Eckenhoff, R.; Tang, P.
Deposited on	:	2011-10-11

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:

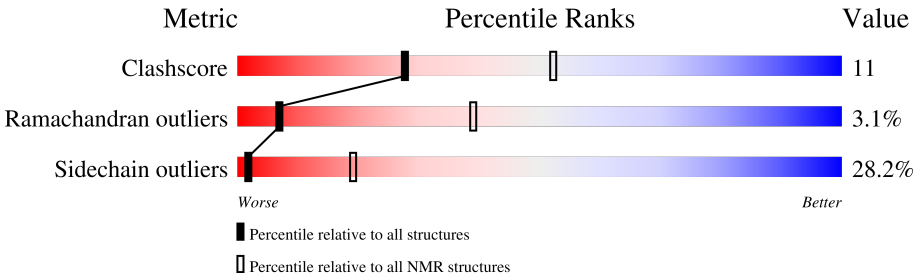
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 73%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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	54% 39% • 5%

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:8-A:140 (133)	1.42	15

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 5, 7, 8, 10, 11, 13, 14, 15
2	3, 6, 9, 12

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2207 atoms, of which 1118 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Acetylcholine receptor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	140	2207	699	1118	181	202	7	0

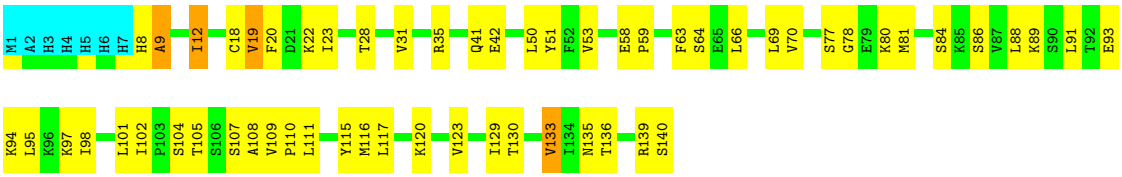
4 Residue-property plots

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: Acetylcholine receptor

Chain A: 



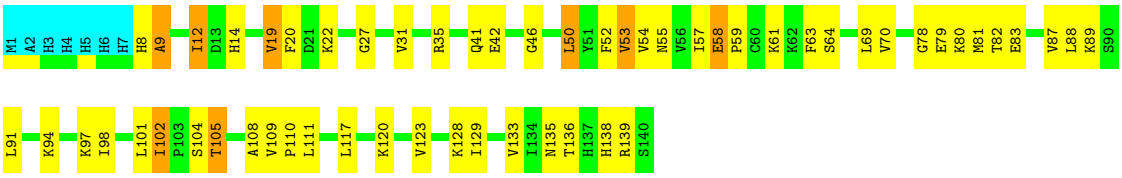
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Acetylcholine receptor

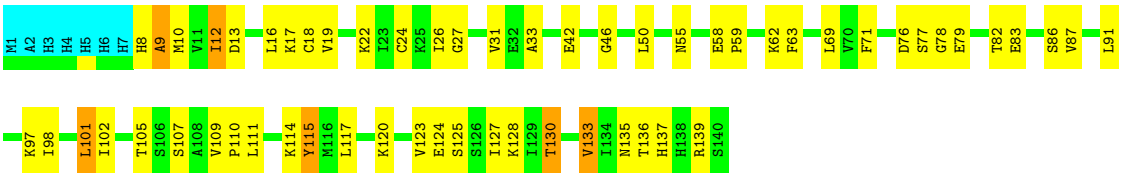
Chain A: 



4.2.2 Score per residue for model 2

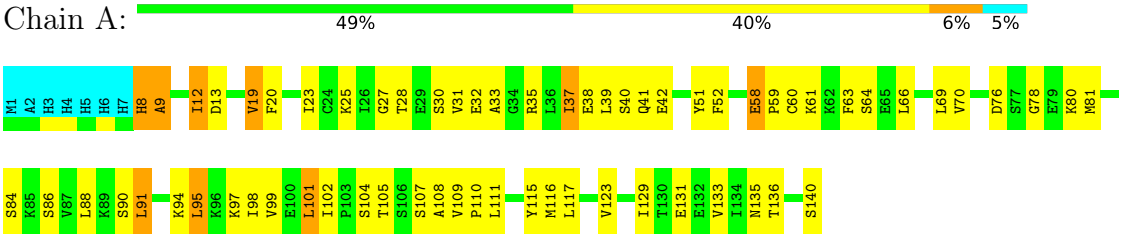
• Molecule 1: Acetylcholine receptor

Chain A: 



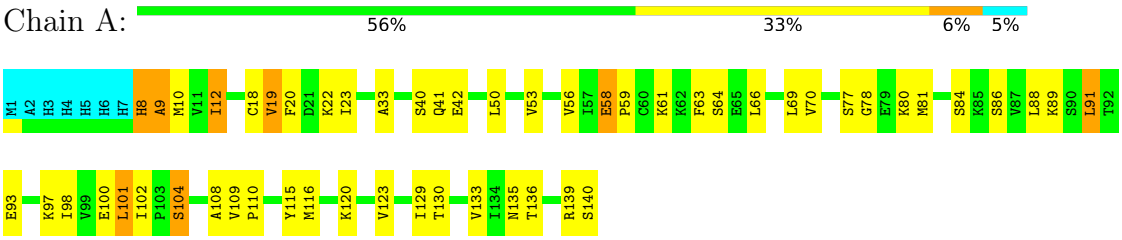
4.2.3 Score per residue for model 3

• Molecule 1: Acetylcholine receptor



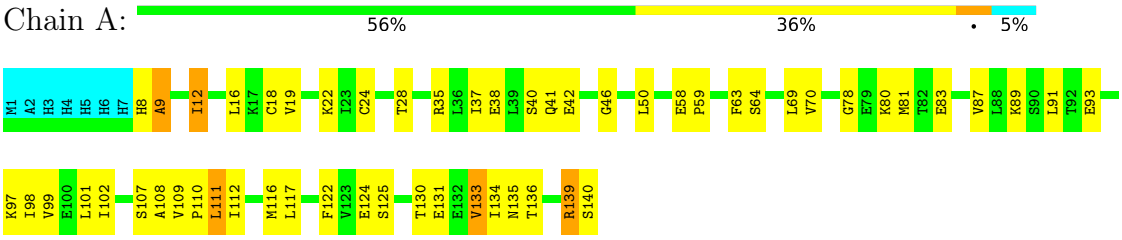
4.2.4 Score per residue for model 4

• Molecule 1: Acetylcholine receptor



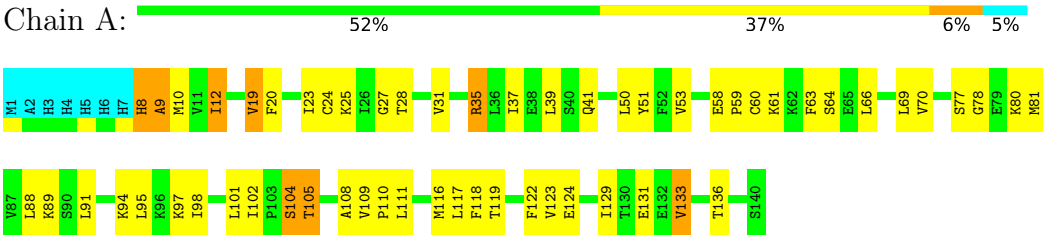
4.2.5 Score per residue for model 5

• Molecule 1: Acetylcholine receptor



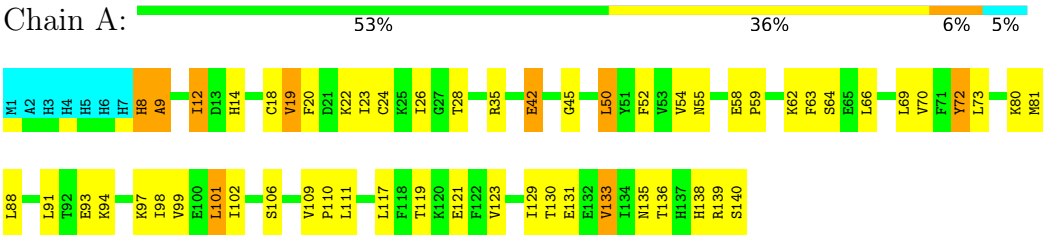
4.2.6 Score per residue for model 6

• Molecule 1: Acetylcholine receptor



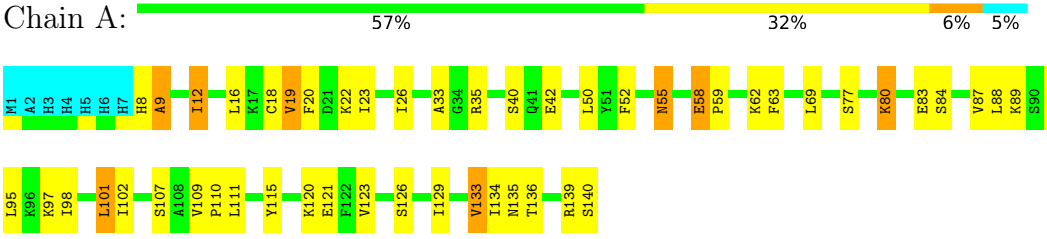
4.2.7 Score per residue for model 7

• Molecule 1: Acetylcholine receptor



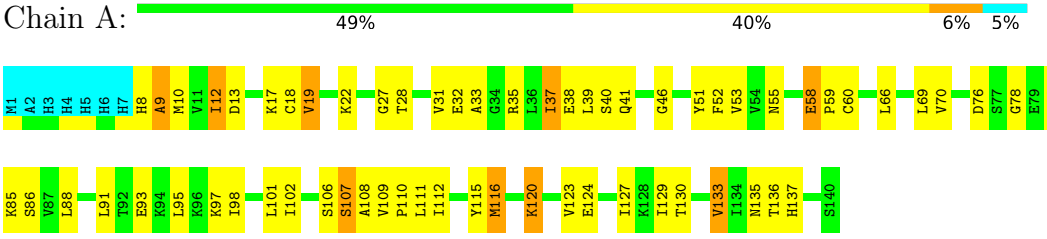
4.2.8 Score per residue for model 8

• Molecule 1: Acetylcholine receptor



4.2.9 Score per residue for model 9

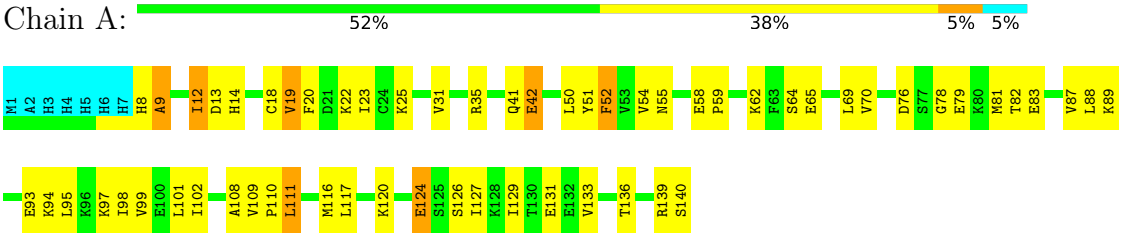
• Molecule 1: Acetylcholine receptor



4.2.10 Score per residue for model 10

• Molecule 1: Acetylcholine receptor

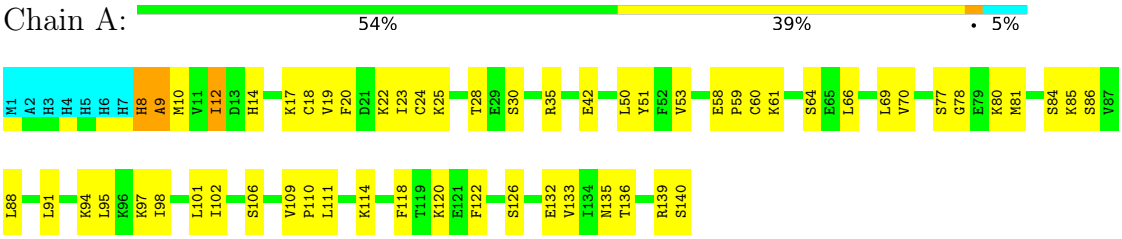
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Acetylcholine receptor

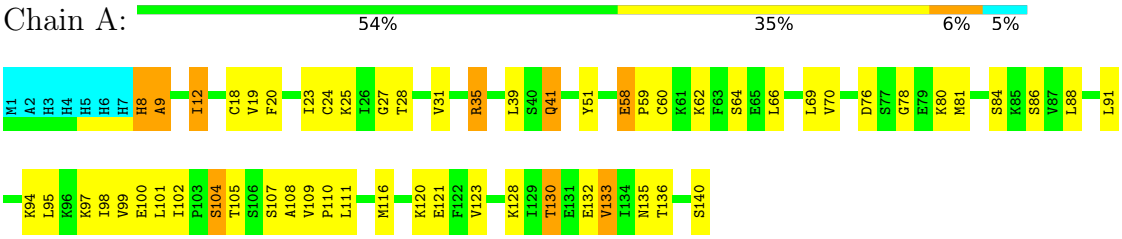
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Acetylcholine receptor

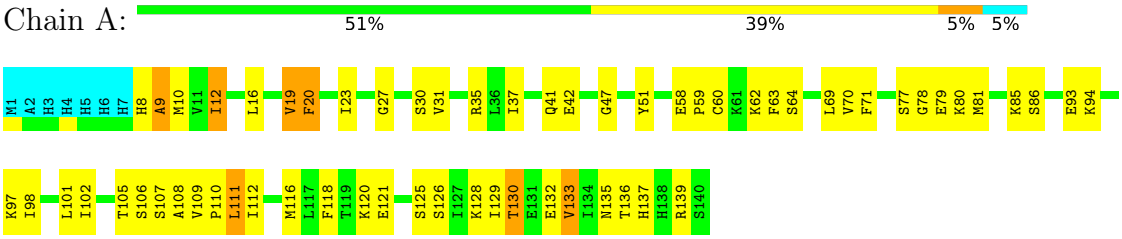
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Acetylcholine receptor

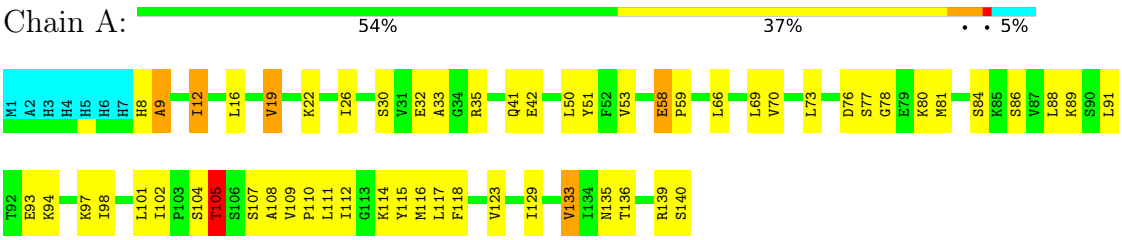
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Acetylcholine receptor

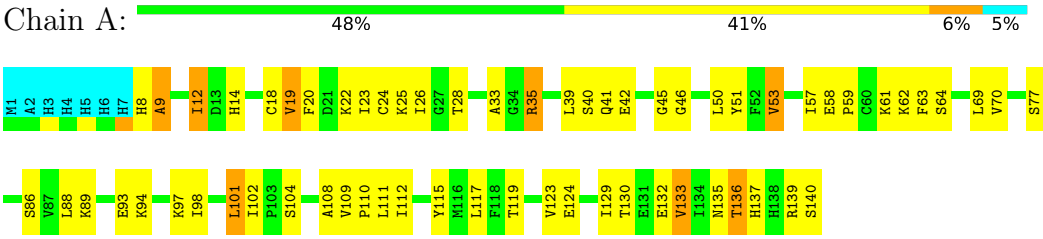
Chain A:



4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: Acetylcholine receptor

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	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	1312
Number of shifts mapped to atoms	1312
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	73%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1026	1069	1069	22±5
All	All	15390	16035	16035	336

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:VAL:HG23	1:A:129:ILE:HD12	0.98	1.36	3	10
1:A:66:LEU:HD13	1:A:84:SER:OG	0.64	1.93	6	7
1:A:27:GLY:O	1:A:31:VAL:HG23	0.64	1.93	9	7
1:A:70:VAL:HG21	1:A:81:MET:HG2	0.63	1.70	10	13
1:A:83:GLU:O	1:A:87:VAL:HG23	0.63	1.94	10	5
1:A:41:GLN:NE2	1:A:108:ALA:HB2	0.62	2.09	9	4
1:A:72:TYR:O	1:A:73:LEU:HD22	0.62	1.94	7	1
1:A:69:LEU:HD23	1:A:80:LYS:HD2	0.61	1.73	6	13
1:A:88:LEU:HD11	1:A:123:VAL:HG21	0.61	1.71	14	7
1:A:12:ILE:HD12	1:A:133:VAL:HG21	0.60	1.72	6	3
1:A:46:GLY:HA3	1:A:102:ILE:HD13	0.60	1.72	2	1
1:A:46:GLY:HA3	1:A:102:ILE:HG21	0.60	1.74	1	1
1:A:37:ILE:CG2	1:A:111:LEU:HD13	0.60	2.26	5	1
1:A:37:ILE:HG13	1:A:111:LEU:HD13	0.60	1.72	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:VAL:HG22	1:A:57:ILE:CD1	0.60	2.26	1	2
1:A:19:VAL:CG2	1:A:129:ILE:HD12	0.60	2.22	3	2
1:A:16:LEU:HD12	1:A:71:PHE:HB2	0.59	1.73	2	1
1:A:101:LEU:HB3	1:A:102:ILE:HD12	0.59	1.74	5	9
1:A:124:GLU:CD	1:A:127:ILE:HD11	0.59	2.18	10	1
1:A:107:SER:O	1:A:111:LEU:HD23	0.59	1.96	12	1
1:A:41:GLN:HG3	1:A:108:ALA:HB2	0.58	1.75	15	5
1:A:41:GLN:CB	1:A:105:THR:HG21	0.57	2.30	13	1
1:A:41:GLN:CD	1:A:108:ALA:HB2	0.56	2.21	12	4
1:A:20:PHE:HA	1:A:23:ILE:HD12	0.56	1.77	3	10
1:A:33:ALA:HB1	1:A:115:TYR:CZ	0.55	2.37	2	7
1:A:12:ILE:CD1	1:A:133:VAL:HG21	0.55	2.32	3	5
1:A:26:ILE:HG13	1:A:119:THR:HG22	0.55	1.78	7	1
1:A:37:ILE:HG23	1:A:111:LEU:HD13	0.55	1.78	5	1
1:A:19:VAL:HG23	1:A:129:ILE:CD1	0.54	2.32	14	9
1:A:101:LEU:C	1:A:102:ILE:HD13	0.54	2.23	11	2
1:A:66:LEU:HD13	1:A:84:SER:CB	0.54	2.32	3	6
1:A:88:LEU:HD13	1:A:120:LYS:HG2	0.53	1.80	9	1
1:A:8:HIS:HB3	1:A:12:ILE:HD13	0.53	1.80	10	11
1:A:55:ASN:OD1	1:A:95:LEU:HD13	0.52	2.04	8	1
1:A:88:LEU:CD1	1:A:123:VAL:HG21	0.52	2.34	1	4
1:A:124:GLU:O	1:A:127:ILE:HD12	0.52	2.04	2	1
1:A:101:LEU:C	1:A:102:ILE:HD12	0.52	2.25	9	1
1:A:108:ALA:HA	1:A:111:LEU:HD12	0.52	1.80	6	1
1:A:107:SER:O	1:A:111:LEU:HD12	0.52	2.04	3	2
1:A:37:ILE:HD11	1:A:111:LEU:HD22	0.51	1.82	3	2
1:A:69:LEU:HD23	1:A:80:LYS:CD	0.51	2.36	5	7
1:A:70:VAL:HG21	1:A:81:MET:CG	0.51	2.35	7	4
1:A:59:PRO:HB3	1:A:91:LEU:HD21	0.51	1.82	3	2
1:A:59:PRO:HB2	1:A:91:LEU:HD22	0.51	1.81	14	2
1:A:26:ILE:CG1	1:A:119:THR:HG22	0.50	2.37	7	1
1:A:8:HIS:CG	1:A:12:ILE:HD13	0.50	2.42	8	4
1:A:63:PHE:CD2	1:A:88:LEU:HD21	0.50	2.42	4	1
1:A:95:LEU:HD23	1:A:116:MET:SD	0.50	2.46	9	1
1:A:41:GLN:HB2	1:A:105:THR:HG21	0.50	1.84	13	1
1:A:63:PHE:CG	1:A:66:LEU:HD12	0.49	2.43	4	2
1:A:66:LEU:HD12	1:A:84:SER:CB	0.49	2.38	7	1
1:A:124:GLU:HG3	1:A:127:ILE:HD11	0.49	1.85	9	1
1:A:8:HIS:CB	1:A:12:ILE:HD13	0.49	2.38	12	2
1:A:35:ARG:O	1:A:39:LEU:HD22	0.49	2.08	6	3
1:A:105:THR:O	1:A:109:VAL:HG23	0.49	2.06	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:GLU:O	1:A:69:LEU:HD23	0.49	2.07	10	1
1:A:109:VAL:N	1:A:110:PRO:HD2	0.49	2.23	5	15
1:A:59:PRO:CG	1:A:91:LEU:HD22	0.48	2.39	2	2
1:A:63:PHE:CD2	1:A:66:LEU:HD12	0.48	2.44	4	2
1:A:53:VAL:HG22	1:A:57:ILE:HD11	0.47	1.85	1	2
1:A:119:THR:O	1:A:123:VAL:HG23	0.47	2.10	6	2
1:A:85:LYS:HA	1:A:88:LEU:HD12	0.47	1.85	9	2
1:A:59:PRO:CB	1:A:91:LEU:HD21	0.46	2.40	3	1
1:A:63:PHE:CE2	1:A:88:LEU:HD21	0.46	2.46	6	1
1:A:58:GLU:CB	1:A:59:PRO:CD	0.46	2.94	12	15
1:A:59:PRO:HG2	1:A:91:LEU:HD22	0.46	1.87	5	1
1:A:101:LEU:O	1:A:102:ILE:HD13	0.46	2.11	11	2
1:A:41:GLN:OE1	1:A:108:ALA:HB2	0.46	2.10	12	2
1:A:59:PRO:HB3	1:A:91:LEU:HD11	0.45	1.87	3	2
1:A:130:THR:O	1:A:133:VAL:HG12	0.45	2.12	12	6
1:A:88:LEU:HD13	1:A:120:LYS:HB3	0.45	1.86	4	2
1:A:88:LEU:HD13	1:A:120:LYS:CG	0.45	2.40	9	1
1:A:71:PHE:CE2	1:A:130:THR:HG23	0.45	2.47	13	1
1:A:8:HIS:HB2	1:A:12:ILE:HD13	0.45	1.88	12	1
1:A:50:LEU:O	1:A:54:VAL:HG23	0.45	2.12	7	3
1:A:8:HIS:CE1	1:A:133:VAL:HG22	0.44	2.47	13	1
1:A:95:LEU:HD13	1:A:116:MET:SD	0.44	2.52	3	1
1:A:120:LYS:O	1:A:123:VAL:HG12	0.44	2.11	4	1
1:A:88:LEU:HD13	1:A:123:VAL:HG21	0.44	1.89	8	1
1:A:19:VAL:HG21	1:A:126:SER:HA	0.44	1.89	13	1
1:A:108:ALA:O	1:A:112:ILE:HG22	0.44	2.11	13	1
1:A:58:GLU:N	1:A:59:PRO:HD2	0.44	2.28	7	15
1:A:31:VAL:HG22	1:A:52:PHE:CZ	0.43	2.48	10	1
1:A:79:GLU:O	1:A:82:THR:HG22	0.43	2.13	2	3
1:A:124:GLU:CG	1:A:127:ILE:HD11	0.43	2.42	9	1
1:A:59:PRO:HG3	1:A:91:LEU:HD13	0.43	1.91	5	1
1:A:9:ALA:CA	1:A:12:ILE:HG22	0.43	2.44	12	15
1:A:45:GLY:CA	1:A:102:ILE:HG21	0.42	2.44	15	1
1:A:8:HIS:NE2	1:A:133:VAL:HG22	0.42	2.29	15	1
1:A:91:LEU:HD12	1:A:91:LEU:O	0.42	2.15	6	4
1:A:104:SER:O	1:A:105:THR:HG23	0.42	2.15	6	1
1:A:66:LEU:HD13	1:A:84:SER:HB3	0.41	1.91	4	3
1:A:12:ILE:HD13	1:A:133:VAL:HG21	0.41	1.92	5	1
1:A:109:VAL:HG12	1:A:110:PRO:N	0.41	2.31	2	9
1:A:35:ARG:O	1:A:39:LEU:HD13	0.41	2.16	9	2
1:A:41:GLN:NE2	1:A:111:LEU:HD12	0.41	2.30	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ILE:HG12	1:A:111:LEU:HD22	0.41	1.92	13	1
1:A:45:GLY:O	1:A:102:ILE:HG21	0.41	2.16	7	1
1:A:45:GLY:HA2	1:A:102:ILE:HG21	0.41	1.93	15	1
1:A:91:LEU:O	1:A:91:LEU:HD12	0.41	2.15	11	1
1:A:16:LEU:HD12	1:A:71:PHE:CB	0.40	2.45	2	1
1:A:109:VAL:CB	1:A:110:PRO:CD	0.40	3.00	14	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	132/140 (94%)	120±2 (91±2%)	8±2 (6±2%)	4±1 (3±1%)	7	39
All	All	1980/2100 (94%)	1804 (91%)	114 (6%)	62 (3%)	7	39

All 10 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	9	ALA	15
1	A	78	GLY	13
1	A	42	GLU	11
1	A	139	ARG	8
1	A	104	SER	5
1	A	105	THR	3
1	A	46	GLY	3
1	A	8	HIS	2
1	A	41	GLN	1
1	A	47	GLY	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	119/125 (95%)	85±3 (72±2%)	34±3 (28±2%)	2 19
All	All	1785/1875 (95%)	1281 (72%)	504 (28%)	2 19

All 86 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	12	ILE	15
1	A	19	VAL	15
1	A	97	LYS	15
1	A	98	ILE	15
1	A	136	THR	15
1	A	133	VAL	14
1	A	135	ASN	13
1	A	22	LYS	11
1	A	35	ARG	11
1	A	64	SER	11
1	A	94	LYS	11
1	A	50	LEU	10
1	A	111	LEU	10
1	A	18	CYS	10
1	A	86	SER	10
1	A	140	SER	10
1	A	101	LEU	9
1	A	117	LEU	9
1	A	51	TYR	9
1	A	93	GLU	9
1	A	89	LYS	8
1	A	77	SER	8
1	A	28	THR	8
1	A	116	MET	8
1	A	53	VAL	7
1	A	58	GLU	7
1	A	63	PHE	7
1	A	120	LYS	7
1	A	24	CYS	7
1	A	62	LYS	7
1	A	52	PHE	6
1	A	55	ASN	6
1	A	61	LYS	6
1	A	8	HIS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	10	MET	6
1	A	76	ASP	6
1	A	107	SER	6
1	A	25	LYS	6
1	A	40	SER	6
1	A	60	CYS	6
1	A	14	HIS	5
1	A	105	THR	5
1	A	130	THR	5
1	A	95	LEU	5
1	A	99	VAL	5
1	A	131	GLU	5
1	A	104	SER	4
1	A	128	LYS	4
1	A	139	ARG	4
1	A	13	ASP	4
1	A	26	ILE	4
1	A	137	HIS	4
1	A	30	SER	4
1	A	16	LEU	4
1	A	112	ILE	4
1	A	124	GLU	4
1	A	118	PHE	4
1	A	106	SER	4
1	A	121	GLU	4
1	A	132	GLU	4
1	A	102	ILE	3
1	A	17	LYS	3
1	A	114	LYS	3
1	A	125	SER	3
1	A	32	GLU	3
1	A	38	GLU	3
1	A	42	GLU	3
1	A	91	LEU	3
1	A	122	PHE	3
1	A	126	SER	3
1	A	20	PHE	2
1	A	138	HIS	2
1	A	37	ILE	2
1	A	100	GLU	2
1	A	134	ILE	2
1	A	85	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	69	LEU	1
1	A	115	TYR	1
1	A	123	VAL	1
1	A	90	SER	1
1	A	56	VAL	1
1	A	72	TYR	1
1	A	80	LYS	1
1	A	84	SER	1
1	A	79	GLU	1
1	A	73	LEU	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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 73% for the well-defined parts and 69% 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	1312
Number of shifts mapped to atoms	1312
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	129	-0.92 ± 0.13	Should be checked
$^{13}C_{\beta}$	104	0.33 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	122	0.93 ± 0.22	Should be applied

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 73%, i.e. 1311 atoms were assigned a chemical shift out of a possible 1806. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	507/666 (76%)	256/272 (94%)	129/266 (48%)	122/128 (95%)
Sidechain	776/1025 (76%)	567/673 (84%)	204/329 (62%)	5/23 (22%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	28/115 (24%)	27/58 (47%)	1/53 (2%)	0/4 (0%)
Overall	1311/1806 (73%)	850/1003 (85%)	334/648 (52%)	127/155 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 1311 atoms were assigned a chemical shift out of a possible 1905. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	507/701 (72%)	256/286 (90%)	129/280 (46%)	122/135 (90%)
Sidechain	776/1054 (74%)	567/693 (82%)	204/338 (60%)	5/23 (22%)
Aromatic	28/150 (19%)	27/78 (35%)	1/63 (2%)	0/9 (0%)
Overall	1311/1905 (69%)	850/1057 (80%)	334/681 (49%)	127/167 (76%)

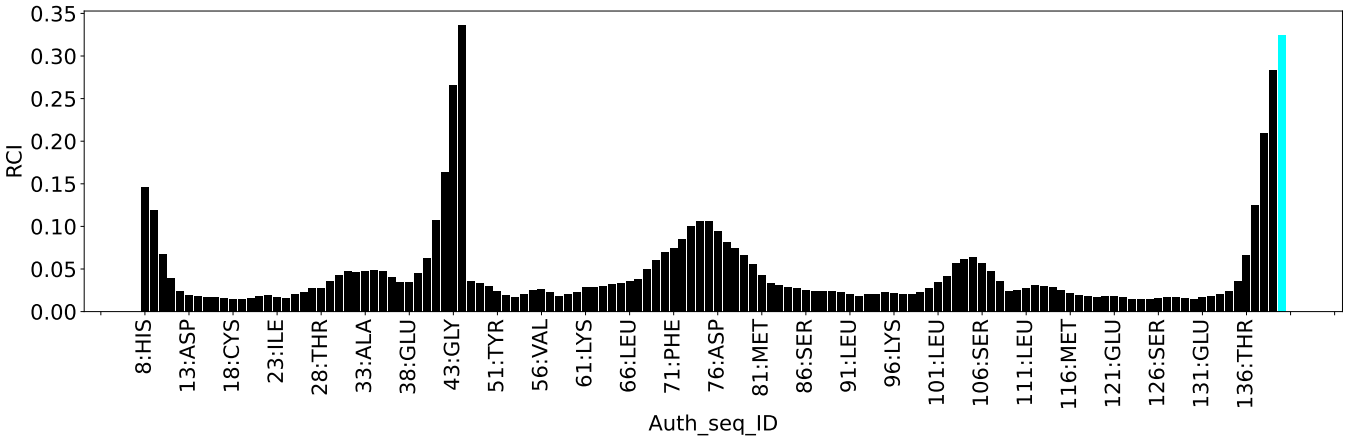
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1109
Intra-residue (|i-j|=0)	362
Sequential (|i-j|=1)	376
Medium range (|i-j|>1 and |i-j|<5)	265
Long range (|i-j|≥5)	42
Inter-chain	0
Hydrogen bond restraints	64
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	7.9
Number of long range restraints per residue[1]	0.3

[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)	8.9	0.2
0.2-0.5 (Medium)	4.6	0.5
>0.5 (Large)	25.8	2.88

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

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

9 Distance violation analysis (i)

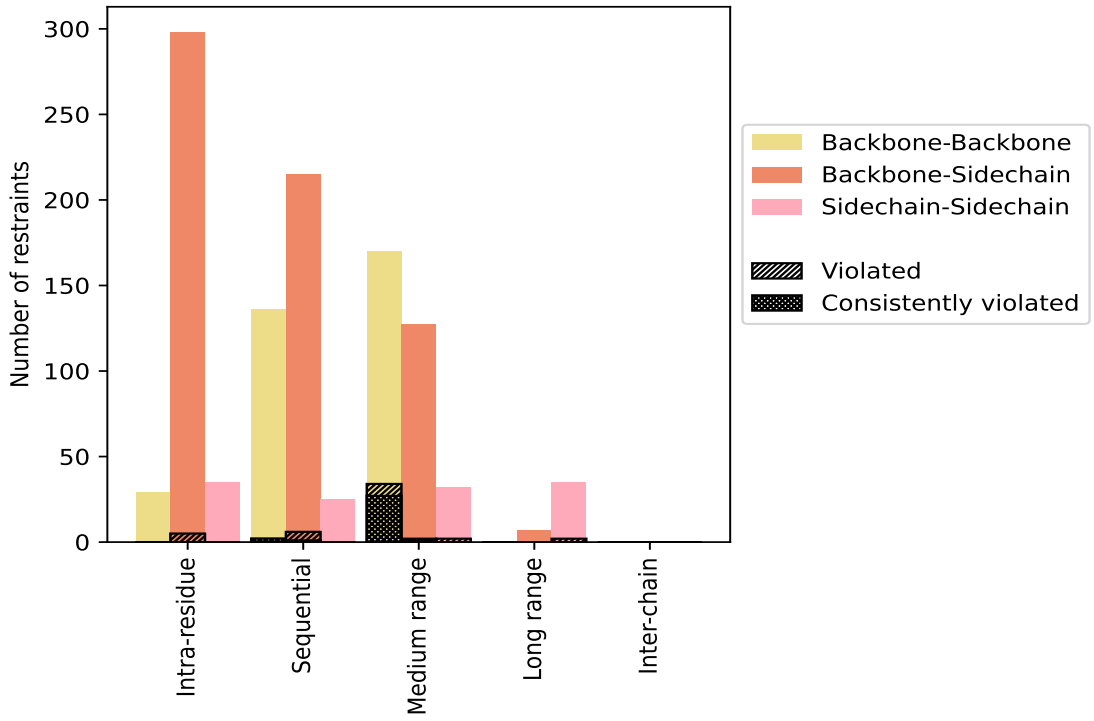
9.1 Summary of distance violations (i)

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)	362	32.6	5	1.4	0.5	0	0.0	0.0
Backbone-Backbone	29	2.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	298	26.9	5	1.7	0.5	0	0.0	0.0
Sidechain-Sidechain	35	3.2	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	376	33.9	8	2.1	0.7	3	0.8	0.3
Backbone-Backbone	136	12.3	2	1.5	0.2	2	1.5	0.2
Backbone-Sidechain	215	19.4	6	2.8	0.5	1	0.5	0.1
Sidechain-Sidechain	25	2.3	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	265	23.9	6	2.3	0.5	2	0.8	0.2
Backbone-Backbone	106	9.6	2	1.9	0.2	1	0.9	0.1
Backbone-Sidechain	127	11.5	2	1.6	0.2	1	0.8	0.1
Sidechain-Sidechain	32	2.9	2	6.2	0.2	0	0.0	0.0
Long range (|i-j|≥5)	42	3.8	2	4.8	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	7	0.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	35	3.2	2	5.7	0.2	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	64	5.8	32	50.0	2.9	26	40.6	2.3
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1109	100.0	53	4.8	4.8	31	2.8	2.8
Backbone-Backbone	335	30.2	36	10.7	3.2	29	8.7	2.6
Backbone-Sidechain	647	58.3	13	2.0	1.2	2	0.3	0.2
Sidechain-Sidechain	127	11.5	4	3.1	0.4	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



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	1	4	34	0	0	39	0.74	2.59	0.55	0.66
2	1	4	33	0	0	38	0.78	2.65	0.61	0.66
3	0	3	35	1	0	39	0.84	2.59	0.64	0.74
4	0	3	35	0	0	38	0.78	2.56	0.62	0.64
5	0	3	36	0	0	39	0.8	2.65	0.53	0.77
6	0	4	33	0	0	37	0.85	2.61	0.62	0.87
7	1	4	35	0	0	40	0.81	2.59	0.6	0.64
8	0	4	37	0	0	41	0.76	2.57	0.58	0.62
9	2	3	35	2	0	42	0.79	2.6	0.62	0.68
10	1	4	34	0	0	39	0.68	2.68	0.53	0.66
11	0	4	34	0	0	38	0.79	2.88	0.57	0.74

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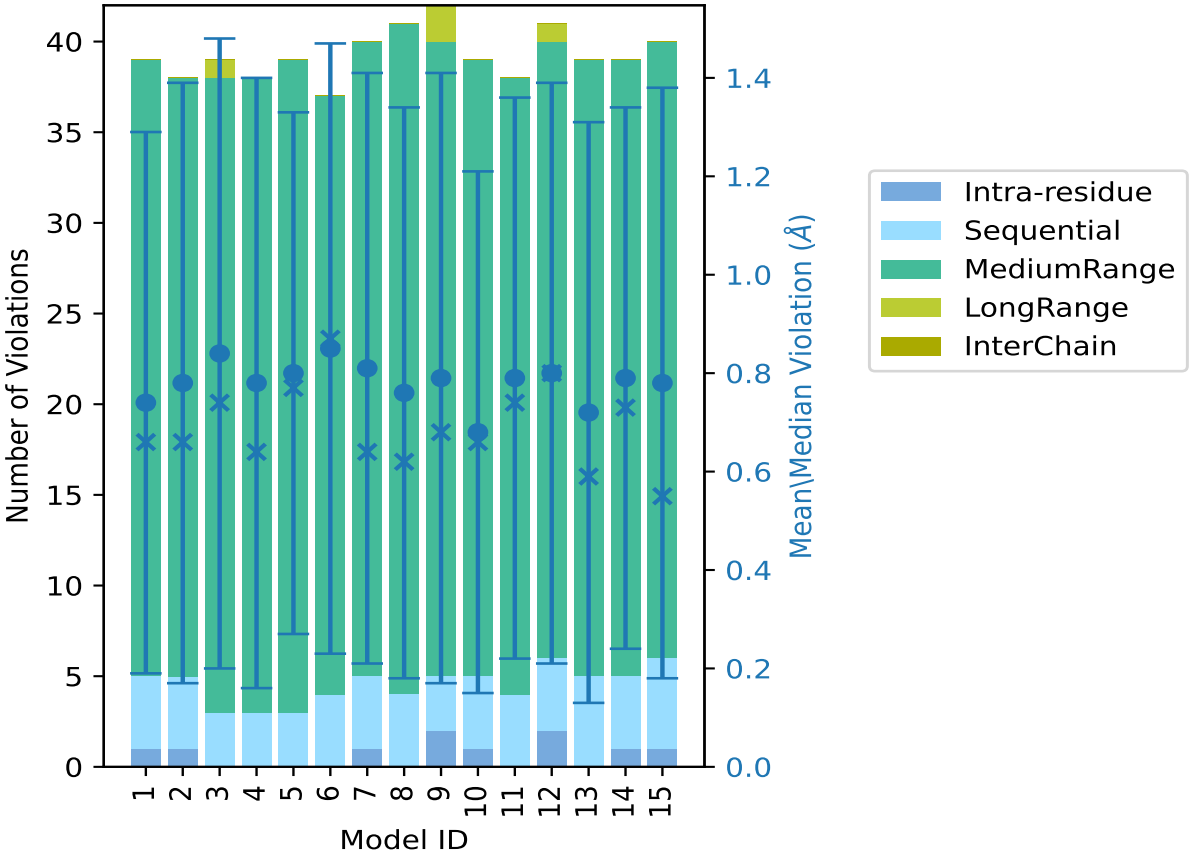
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	4	34	1	0	41	0.8	2.64	0.59	0.8
13	0	5	34	0	0	39	0.72	2.57	0.59	0.59
14	1	4	34	0	0	39	0.79	2.64	0.55	0.73
15	1	5	34	0	0	40	0.78	2.59	0.6	0.55

[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

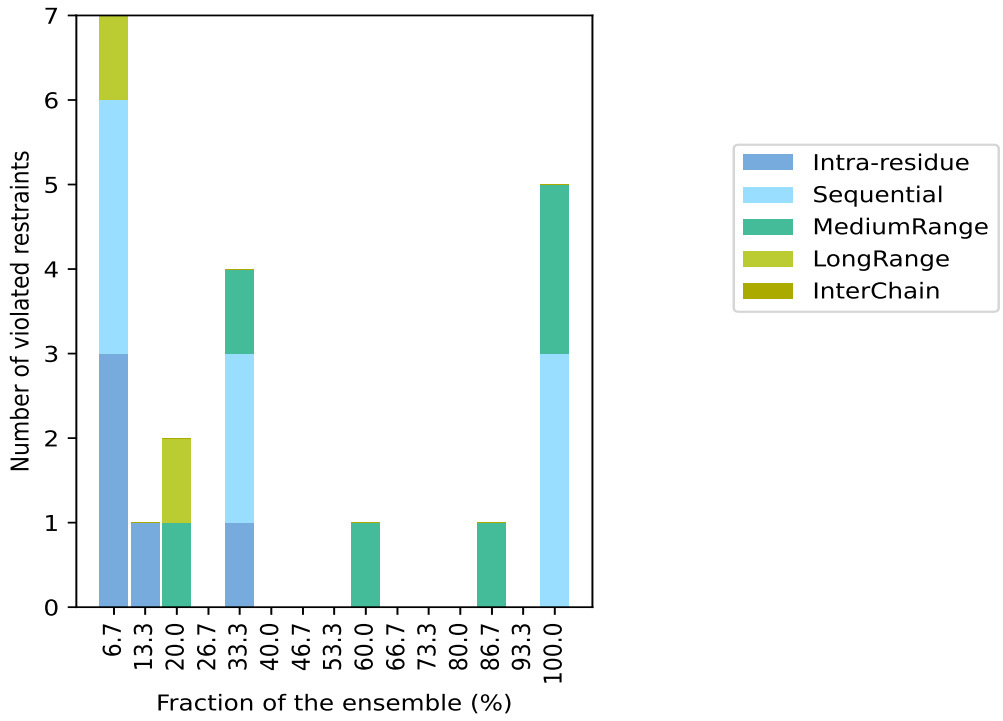
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for

a given fraction of the ensemble. In total, 1024(IR:357, SQ:368, MR:259, LR:40, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
3	3	0	1	0	7	1	6.7
1	0	0	0	0	1	2	13.3
0	0	1	1	0	2	3	20.0
0	0	0	0	0	0	4	26.7
1	2	1	0	0	4	5	33.3
0	0	0	0	0	0	6	40.0
0	0	0	0	0	0	7	46.7
0	0	0	0	0	0	8	53.3
0	0	1	0	0	1	9	60.0
0	0	0	0	0	0	10	66.7
0	0	0	0	0	0	11	73.3
0	0	0	0	0	0	12	80.0
0	0	1	0	0	1	13	86.7
0	0	0	0	0	0	14	93.3
0	3	2	0	0	5	15	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

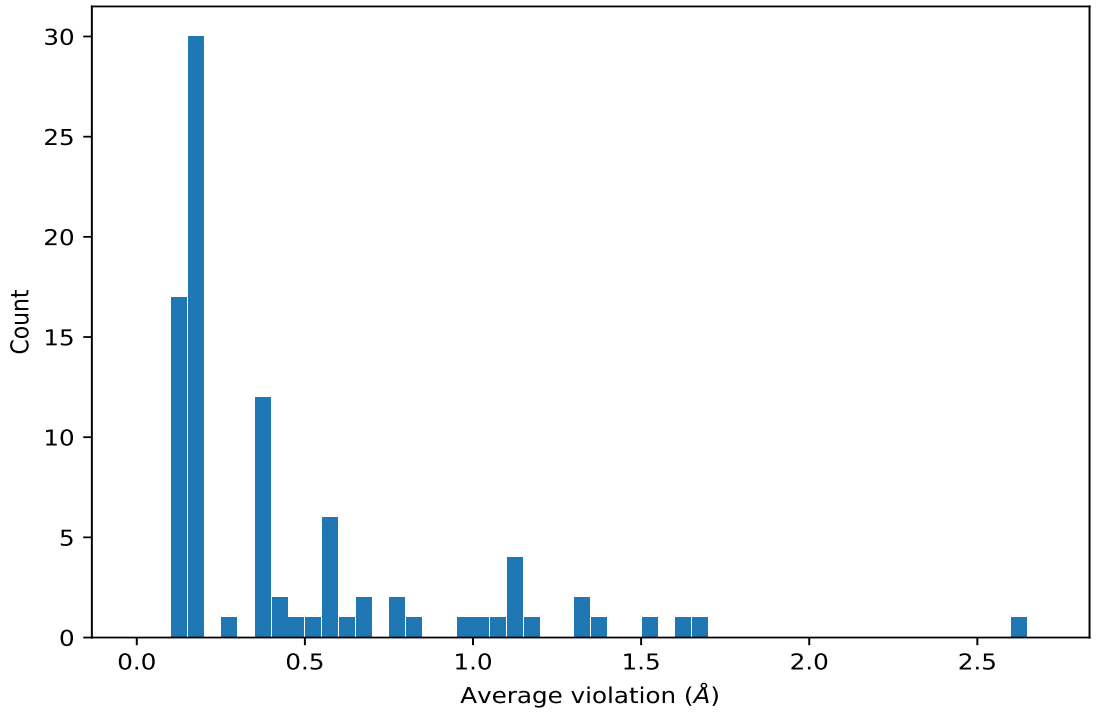
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (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)
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	15	2.63	0.08	2.6
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	15	1.68	0.26	1.65
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	15	1.6	0.49	1.89
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	15	1.51	0.36	1.48
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	15	1.36	0.1	1.4
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	15	1.34	0.28	1.35
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	15	1.31	0.03	1.31
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	15	1.16	0.16	1.13
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	15	1.13	0.19	1.08
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	15	1.12	0.19	1.17
(2,17)	1:A:82:THR:O	1:A:86:SER:N	15	1.11	0.23	1.08
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	15	1.1	0.25	1.08
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	15	1.09	0.14	1.09
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	15	1.03	0.24	1.06
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	15	0.8	0.17	0.81
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	15	0.78	0.09	0.75

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	15	0.75	0.13	0.72
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	15	0.68	0.24	0.6
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	15	0.62	0.19	0.58
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	15	0.6	0.26	0.62
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	15	0.6	0.1	0.61
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	15	0.58	0.04	0.6
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	15	0.55	0.02	0.55
(2,10)	1:A:86:SER:O	1:A:90:SER:N	15	0.55	0.21	0.55
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	15	0.54	0.32	0.73
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	15	0.42	0.12	0.38
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	15	0.18	0.04	0.18
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	15	0.18	0.03	0.17
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	15	0.13	0.0	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	15	0.13	0.0	0.13
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	15	0.13	0.03	0.12
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	15	0.13	0.03	0.12
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	15	0.11	0.0	0.11
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	13	0.69	0.06	0.68
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	13	0.55	0.31	0.48
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	13	0.47	0.26	0.51
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	13	0.42	0.16	0.44
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	13	0.12	0.01	0.12
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	13	0.12	0.01	0.12
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	12	0.96	1.03	0.2
(4,134)	1:A:33:ALA:H	1:A:35:ARG:H	9	0.12	0.01	0.12
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG21	5	0.39	0.14	0.48
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG22	5	0.39	0.14	0.48
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG23	5	0.39	0.14	0.48
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG21	5	0.39	0.14	0.48
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG22	5	0.39	0.14	0.48
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG23	5	0.39	0.14	0.48
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG21	5	0.39	0.14	0.48
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG22	5	0.39	0.14	0.48
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG23	5	0.39	0.14	0.48
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG21	5	0.39	0.14	0.48
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG22	5	0.39	0.14	0.48
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG23	5	0.39	0.14	0.48
(4,414)	1:A:35:ARG:HD2	1:A:36:LEU:H	5	0.18	0.03	0.17
(4,414)	1:A:35:ARG:HD3	1:A:36:LEU:H	5	0.18	0.03	0.17
(4,440)	1:A:38:GLU:HG2	1:A:39:LEU:H	5	0.16	0.03	0.17
(4,440)	1:A:38:GLU:HG3	1:A:39:LEU:H	5	0.16	0.03	0.17
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG2	5	0.11	0.0	0.11

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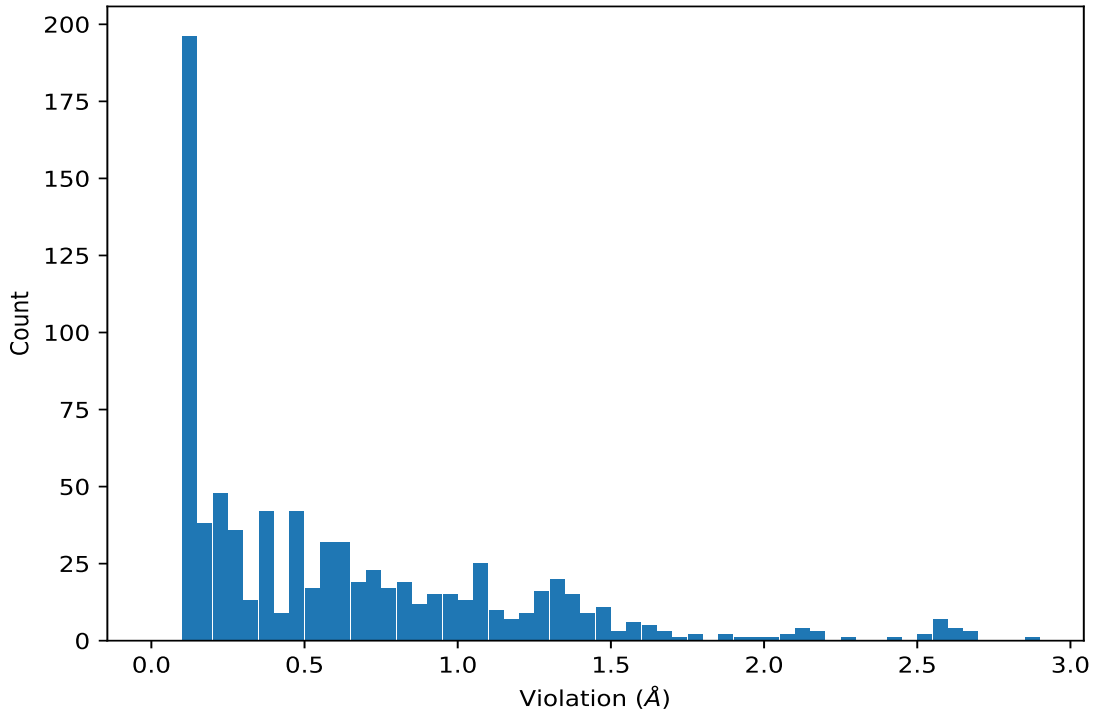
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG3	5	0.11	0.0	0.11
(2,7)	1:A:60:CYS:O	1:A:64:SER:N	3	0.29	0.07	0.29
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG11	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG12	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG13	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG21	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG22	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG23	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG11	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG12	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG13	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG21	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG22	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG23	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG11	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG12	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG13	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG21	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG22	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG23	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG11	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG12	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG13	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG21	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG22	3	0.19	0.05	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG23	3	0.19	0.05	0.2
(4,138)	1:A:35:ARG:HD2	1:A:38:GLU:HB2	3	0.15	0.02	0.14
(4,138)	1:A:35:ARG:HD2	1:A:38:GLU:HB3	3	0.15	0.02	0.14
(4,138)	1:A:35:ARG:HD3	1:A:38:GLU:HB2	3	0.15	0.02	0.14
(4,138)	1:A:35:ARG:HD3	1:A:38:GLU:HB3	3	0.15	0.02	0.14
(4,615)	1:A:67:THR:H	1:A:67:THR:HG21	2	0.11	0.0	0.11
(4,615)	1:A:67:THR:H	1:A:67:THR:HG22	2	0.11	0.0	0.11
(4,615)	1:A:67:THR:H	1:A:67:THR:HG23	2	0.11	0.0	0.11

[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)
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	11	2.88
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	10	2.68
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	2	2.65
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	5	2.65
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	12	2.64
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	14	2.64
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	6	2.61
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	9	2.6
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	1	2.59
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	3	2.59
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	7	2.59
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	15	2.59
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	8	2.57
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	13	2.57
(2,20)	1:A:96:LYS:O	1:A:100:GLU:N	4	2.56
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	3	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	9	2.53
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	4	2.44
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	12	2.26
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	6	2.18
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	6	2.17
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	2	2.15
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	8	2.14
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	7	2.11
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	9	2.1
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	13	2.1
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	15	2.06
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	2	2.05
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	15	2.02
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	12	1.96
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	7	1.91
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	3	1.89
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	1	1.88
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	5	1.79
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	7	1.78
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	3	1.74
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	3	1.67
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	6	1.67
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	13	1.65
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	4	1.64
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	4	1.62
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	8	1.61
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	7	1.61
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	8	1.6
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	3	1.59
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	8	1.58
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	9	1.58
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	13	1.56
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	13	1.55
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	14	1.55
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	11	1.53
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	15	1.53
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	13	1.5
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	6	1.49
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	12	1.49
(2,17)	1:A:82:THR:O	1:A:86:SER:N	2	1.49
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	1	1.48
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	15	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	11	1.48
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	3	1.48
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	10	1.46
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	7	1.46
(2,17)	1:A:82:THR:O	1:A:86:SER:N	14	1.46
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	9	1.45
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	9	1.42
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	14	1.42
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	6	1.42
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	7	1.42
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	12	1.42
(2,17)	1:A:82:THR:O	1:A:86:SER:N	4	1.41
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	9	1.4
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	10	1.4
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	11	1.4
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	11	1.39
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	10	1.37
(2,8)	1:A:62:LYS:O	1:A:66:LEU:N	11	1.37
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	5	1.37
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	10	1.36
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	2	1.36
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	4	1.36
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	14	1.35
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	3	1.35
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	3	1.35
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	4	1.35
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	7	1.35
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	9	1.35
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	14	1.35
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	6	1.35
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	10	1.34
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	11	1.34
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	12	1.34
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	2	1.33
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	11	1.33
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	8	1.32
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	15	1.32
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	13	1.32
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	5	1.32
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	15	1.32
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	1	1.32
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	1	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	4	1.31
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	14	1.31
(2,17)	1:A:82:THR:O	1:A:86:SER:N	3	1.31
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	1	1.31
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	8	1.3
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	5	1.3
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	7	1.3
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	1	1.3
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	8	1.29
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	15	1.29
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	10	1.29
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	14	1.29
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	4	1.29
(2,17)	1:A:82:THR:O	1:A:86:SER:N	5	1.29
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	6	1.28
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	1	1.27
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	15	1.27
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	5	1.27
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	4	1.26
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	14	1.25
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	5	1.25
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	5	1.25
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	14	1.25
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	11	1.25
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	12	1.23
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	8	1.23
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	1	1.23
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	2	1.23
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	8	1.22
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	15	1.22
(2,21)	1:A:97:LYS:O	1:A:101:LEU:N	9	1.21
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	13	1.2
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	14	1.2
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	5	1.19
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	3	1.18
(2,18)	1:A:89:LYS:O	1:A:93:GLU:N	13	1.18
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	8	1.17
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	9	1.17
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	5	1.15
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	4	1.15
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	14	1.13
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	1	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	6	1.13
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	7	1.12
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	2	1.11
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	12	1.11
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	7	1.11
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	13	1.1
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	6	1.1
(2,17)	1:A:82:THR:O	1:A:86:SER:N	11	1.1
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	6	1.09
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	14	1.09
(2,17)	1:A:82:THR:O	1:A:86:SER:N	15	1.09
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	6	1.09
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	15	1.09
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	2	1.09
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	4	1.08
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	15	1.08
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	2	1.08
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	11	1.08
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	12	1.08
(2,17)	1:A:82:THR:O	1:A:86:SER:N	1	1.08
(2,17)	1:A:82:THR:O	1:A:86:SER:N	9	1.08
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	2	1.08
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	9	1.08
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	5	1.07
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	7	1.07
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	12	1.07
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	10	1.06
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	11	1.06
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	3	1.06
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	6	1.06
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	11	1.06
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	12	1.05
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	8	1.05
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	1	1.04
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	4	1.04
(2,30)	1:A:132:GLU:O	1:A:136:THR:N	14	1.04
(2,17)	1:A:82:THR:O	1:A:86:SER:N	6	1.04
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	2	1.03
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	11	1.03
(2,17)	1:A:82:THR:O	1:A:86:SER:N	12	1.03
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	5	1.02
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	15	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	5	1.02
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	14	1.01
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	2	1.0
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	6	1.0
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	12	0.99
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	12	0.99
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	12	0.99
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	10	0.98
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	7	0.98
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	8	0.97
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	3	0.97
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	7	0.97
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	12	0.96
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	9	0.96
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	12	0.96
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	8	0.96
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	1	0.95
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	15	0.95
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	6	0.95
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	12	0.94
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	15	0.93
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	3	0.92
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	9	0.92
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	12	0.91
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	10	0.91
(2,17)	1:A:82:THR:O	1:A:86:SER:N	10	0.91
(2,17)	1:A:82:THR:O	1:A:86:SER:N	13	0.91
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	10	0.91
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	11	0.91
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	5	0.9
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	9	0.9
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	2	0.9
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	2	0.9
(2,19)	1:A:93:GLU:O	1:A:97:LYS:N	5	0.9
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	3	0.89
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	11	0.89
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	2	0.89
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	2	0.89
(2,10)	1:A:86:SER:O	1:A:90:SER:N	6	0.88
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	6	0.87
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	12	0.87
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	6	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	1	0.87
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	9	0.86
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	13	0.86
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	9	0.85
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	3	0.84
(2,23)	1:A:107:SER:O	1:A:111:LEU:N	3	0.84
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	14	0.84
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	15	0.82
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	8	0.82
(2,10)	1:A:86:SER:O	1:A:90:SER:N	3	0.82
(2,10)	1:A:86:SER:O	1:A:90:SER:N	11	0.82
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	5	0.81
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	9	0.81
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	10	0.81
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	1	0.81
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	14	0.81
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	4	0.8
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	14	0.8
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	5	0.8
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	4	0.8
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	12	0.8
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	13	0.8
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	10	0.8
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	13	0.79
(2,28)	1:A:120:LYS:O	1:A:124:GLU:N	5	0.79
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	14	0.79
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	10	0.78
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	5	0.77
(2,17)	1:A:82:THR:O	1:A:86:SER:N	7	0.77
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	5	0.77
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	1	0.76
(2,2)	1:A:29:GLU:O	1:A:33:ALA:N	1	0.76
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	8	0.76
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	11	0.75
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	2	0.75
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	12	0.75
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	1	0.75
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	4	0.75
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	3	0.75
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	15	0.75
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	4	0.74
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	10	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	11	0.74
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	3	0.74
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	6	0.74
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	11	0.74
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	13	0.74
(2,14)	1:A:64:SER:O	1:A:68:GLY:N	10	0.74
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	14	0.73
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	7	0.73
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	9	0.73
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	12	0.73
(2,16)	1:A:68:GLY:O	1:A:72:TYR:N	15	0.73
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	7	0.73
(2,10)	1:A:86:SER:O	1:A:90:SER:N	12	0.73
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	10	0.72
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	7	0.72
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	8	0.71
(2,25)	1:A:111:LEU:O	1:A:115:TYR:N	7	0.71
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	6	0.71
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	14	0.71
(2,17)	1:A:82:THR:O	1:A:86:SER:N	8	0.7
(2,10)	1:A:86:SER:O	1:A:90:SER:N	9	0.7
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	8	0.69
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	13	0.69
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	1	0.69
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	8	0.69
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	3	0.68
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	9	0.68
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	13	0.68
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	5	0.68
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	4	0.68
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	2	0.67
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	10	0.67
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	14	0.67
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	9	0.67
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	7	0.66
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	1	0.66
(2,12)	1:A:94:LYS:O	1:A:98:ILE:N	10	0.66
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	12	0.65
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	2	0.65
(2,10)	1:A:86:SER:O	1:A:90:SER:N	4	0.65
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	2	0.64
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	11	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	13	0.64
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	6	0.63
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	12	0.63
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	5	0.63
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	5	0.63
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	4	0.62
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	9	0.62
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	2	0.62
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	14	0.62
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	8	0.62
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	6	0.62
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	7	0.61
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	1	0.61
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	4	0.61
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	7	0.61
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	5	0.61
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	1	0.61
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	11	0.61
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	7	0.61
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	8	0.61
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	10	0.61
(2,10)	1:A:86:SER:O	1:A:90:SER:N	14	0.61
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	3	0.6
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	11	0.6
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	13	0.6
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	11	0.6
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	11	0.6
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	3	0.6
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	8	0.6
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	12	0.6
(2,26)	1:A:115:TYR:O	1:A:119:THR:N	13	0.59
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	2	0.59
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	3	0.59
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	4	0.59
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	9	0.59
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	10	0.58
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	10	0.58
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	13	0.57
(2,4)	1:A:36:LEU:O	1:A:40:SER:N	2	0.57
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	14	0.57
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	15	0.57
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	1	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	2	0.56
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	4	0.56
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	6	0.56
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	10	0.56
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	13	0.56
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	8	0.55
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	14	0.55
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	9	0.55
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	3	0.55
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	5	0.55
(2,10)	1:A:86:SER:O	1:A:90:SER:N	7	0.55
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	1	0.55
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	3	0.55
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	5	0.55
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	7	0.55
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	8	0.55
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	9	0.55
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	11	0.55
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	12	0.55
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	14	0.55
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	2	0.54
(2,5)	1:A:37:ILE:O	1:A:41:GLN:N	15	0.53
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	11	0.53
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	9	0.53
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	1	0.52
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	15	0.52
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	6	0.52
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	7	0.52
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	15	0.52
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	7	0.52
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	13	0.52
(2,9)	1:A:66:LEU:O	1:A:70:VAL:N	5	0.51
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	8	0.51
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	9	0.51
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	14	0.51
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	9	0.5
(2,11)	1:A:88:LEU:O	1:A:92:THR:N	4	0.5
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG21	7	0.49
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG22	7	0.49
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG23	7	0.49
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG21	7	0.49
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG22	7	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG23	7	0.49
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG21	7	0.49
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG22	7	0.49
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG23	7	0.49
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG21	7	0.49
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG22	7	0.49
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG23	7	0.49
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	13	0.49
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG21	8	0.48
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG22	8	0.48
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG23	8	0.48
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG21	8	0.48
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG22	8	0.48
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG23	8	0.48
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG21	8	0.48
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG22	8	0.48
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG23	8	0.48
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG21	8	0.48
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG22	8	0.48
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG23	8	0.48
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG21	15	0.48
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG22	15	0.48
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG23	15	0.48
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG21	15	0.48
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG22	15	0.48
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG23	15	0.48
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG21	15	0.48
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG22	15	0.48
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG23	15	0.48
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG21	15	0.48
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG22	15	0.48
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG23	15	0.48
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	7	0.48
(2,10)	1:A:86:SER:O	1:A:90:SER:N	5	0.48
(2,1)	1:A:9:ALA:O	1:A:13:ASP:N	15	0.48
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	7	0.47
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	15	0.45
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	3	0.44
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	4	0.44
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	8	0.43
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	8	0.42
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	15	0.41
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	1	0.41
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	15	0.41
(2,10)	1:A:86:SER:O	1:A:90:SER:N	15	0.41
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	6	0.39
(2,10)	1:A:86:SER:O	1:A:90:SER:N	1	0.39
(2,7)	1:A:60:CYS:O	1:A:64:SER:N	8	0.38
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	10	0.38
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	14	0.38
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG21	5	0.37
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG22	5	0.37
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG23	5	0.37
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG21	5	0.37
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG22	5	0.37
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG23	5	0.37
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG21	5	0.37
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG22	5	0.37
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG23	5	0.37
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG21	5	0.37
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG22	5	0.37
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG23	5	0.37
(4,38)	1:A:122:PHE:HD1	1:A:19:VAL:HG11	9	0.37
(4,38)	1:A:122:PHE:HD1	1:A:19:VAL:HG12	9	0.37
(4,38)	1:A:122:PHE:HD1	1:A:19:VAL:HG13	9	0.37
(4,38)	1:A:122:PHE:HD1	1:A:19:VAL:HG21	9	0.37
(4,38)	1:A:122:PHE:HD1	1:A:19:VAL:HG22	9	0.37
(4,38)	1:A:122:PHE:HD1	1:A:19:VAL:HG23	9	0.37
(4,38)	1:A:122:PHE:HD2	1:A:19:VAL:HG11	9	0.37
(4,38)	1:A:122:PHE:HD2	1:A:19:VAL:HG12	9	0.37
(4,38)	1:A:122:PHE:HD2	1:A:19:VAL:HG13	9	0.37
(4,38)	1:A:122:PHE:HD2	1:A:19:VAL:HG21	9	0.37
(4,38)	1:A:122:PHE:HD2	1:A:19:VAL:HG22	9	0.37
(4,38)	1:A:122:PHE:HD2	1:A:19:VAL:HG23	9	0.37
(4,38)	1:A:122:PHE:HE1	1:A:19:VAL:HG11	9	0.37
(4,38)	1:A:122:PHE:HE1	1:A:19:VAL:HG12	9	0.37
(4,38)	1:A:122:PHE:HE1	1:A:19:VAL:HG13	9	0.37
(4,38)	1:A:122:PHE:HE1	1:A:19:VAL:HG21	9	0.37
(4,38)	1:A:122:PHE:HE1	1:A:19:VAL:HG22	9	0.37
(4,38)	1:A:122:PHE:HE1	1:A:19:VAL:HG23	9	0.37
(4,38)	1:A:122:PHE:HE2	1:A:19:VAL:HG11	9	0.37
(4,38)	1:A:122:PHE:HE2	1:A:19:VAL:HG12	9	0.37
(4,38)	1:A:122:PHE:HE2	1:A:19:VAL:HG13	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,38)	1:A:122:PHE:HE2	1:A:19:VAL:HG21	9	0.37
(4,38)	1:A:122:PHE:HE2	1:A:19:VAL:HG22	9	0.37
(4,38)	1:A:122:PHE:HE2	1:A:19:VAL:HG23	9	0.37
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	3	0.37
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	4	0.34
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	4	0.34
(2,27)	1:A:118:PHE:O	1:A:122:PHE:N	4	0.32
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	6	0.32
(2,24)	1:A:109:VAL:O	1:A:113:GLY:N	13	0.32
(2,10)	1:A:86:SER:O	1:A:90:SER:N	13	0.32
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	3	0.31
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	5	0.31
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	9	0.31
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	13	0.31
(2,10)	1:A:86:SER:O	1:A:90:SER:N	8	0.31
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	11	0.3
(2,10)	1:A:86:SER:O	1:A:90:SER:N	2	0.3
(2,7)	1:A:60:CYS:O	1:A:64:SER:N	7	0.29
(2,3)	1:A:30:SER:O	1:A:34:GLY:N	1	0.29
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	10	0.28
(2,15)	1:A:65:GLU:O	1:A:69:LEU:N	10	0.28
(4,826)	1:A:99:VAL:H	1:A:99:VAL:HB	1	0.27
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	15	0.27
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG11	9	0.25
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG12	9	0.25
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG13	9	0.25
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG21	9	0.25
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG22	9	0.25
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG23	9	0.25
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG11	9	0.25
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG12	9	0.25
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG13	9	0.25
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG21	9	0.25
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG22	9	0.25
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG23	9	0.25
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG11	9	0.25
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG12	9	0.25
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG13	9	0.25
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG21	9	0.25
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG22	9	0.25
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG23	9	0.25
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG11	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG12	9	0.25
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG13	9	0.25
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG21	9	0.25
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG22	9	0.25
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG23	9	0.25
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	5	0.25
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	11	0.25
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	11	0.25
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	7	0.25
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	3	0.25
(2,10)	1:A:86:SER:O	1:A:90:SER:N	10	0.25
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	6	0.24
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	6	0.24
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	12	0.24
(4,414)	1:A:35:ARG:HD2	1:A:36:LEU:H	13	0.23
(4,414)	1:A:35:ARG:HD3	1:A:36:LEU:H	13	0.23
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	10	0.23
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	12	0.23
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	13	0.23
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	14	0.23
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	4	0.23
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	15	0.23
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	1	0.23
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	12	0.22
(2,13)	1:A:52:PHE:O	1:A:56:VAL:N	11	0.22
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	7	0.21
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	8	0.21
(2,7)	1:A:60:CYS:O	1:A:64:SER:N	5	0.21
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG11	3	0.2
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG12	3	0.2
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG13	3	0.2
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG21	3	0.2
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG22	3	0.2
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG23	3	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG11	3	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG12	3	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG13	3	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG21	3	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG22	3	0.2
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG23	3	0.2
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG11	3	0.2
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG12	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG13	3	0.2
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG21	3	0.2
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG22	3	0.2
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG23	3	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG11	3	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG12	3	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG13	3	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG21	3	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG22	3	0.2
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG23	3	0.2
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	1	0.2
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	15	0.2
(4,440)	1:A:38:GLU:HG2	1:A:39:LEU:H	15	0.2
(4,440)	1:A:38:GLU:HG3	1:A:39:LEU:H	15	0.2
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	2	0.2
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	3	0.2
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	1	0.2
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	11	0.19
(4,440)	1:A:38:GLU:HG2	1:A:39:LEU:H	7	0.19
(4,440)	1:A:38:GLU:HG3	1:A:39:LEU:H	7	0.19
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	4	0.19
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	8	0.19
(4,138)	1:A:35:ARG:HD2	1:A:38:GLU:HB2	15	0.18
(4,138)	1:A:35:ARG:HD2	1:A:38:GLU:HB3	15	0.18
(4,138)	1:A:35:ARG:HD3	1:A:38:GLU:HB2	15	0.18
(4,138)	1:A:35:ARG:HD3	1:A:38:GLU:HB3	15	0.18
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	3	0.18
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	9	0.18
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	12	0.17
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	13	0.17
(4,440)	1:A:38:GLU:HG2	1:A:39:LEU:H	8	0.17
(4,440)	1:A:38:GLU:HG3	1:A:39:LEU:H	8	0.17
(4,414)	1:A:35:ARG:HD2	1:A:36:LEU:H	10	0.17
(4,414)	1:A:35:ARG:HD3	1:A:36:LEU:H	10	0.17
(4,414)	1:A:35:ARG:HD2	1:A:36:LEU:H	12	0.17
(4,414)	1:A:35:ARG:HD3	1:A:36:LEU:H	12	0.17
(4,414)	1:A:35:ARG:HD2	1:A:36:LEU:H	14	0.17
(4,414)	1:A:35:ARG:HD3	1:A:36:LEU:H	14	0.17
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	1	0.17
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	13	0.17
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	3	0.16
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	6	0.16
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	9	0.16
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	10	0.16
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	14	0.16
(4,414)	1:A:35:ARG:HD2	1:A:36:LEU:H	6	0.16
(4,414)	1:A:35:ARG:HD3	1:A:36:LEU:H	6	0.16
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	13	0.16
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	14	0.16
(4,49)	1:A:37:ILE:HA	1:A:36:LEU:H	2	0.15
(4,134)	1:A:33:ALA:H	1:A:35:ARG:H	6	0.15
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	11	0.15
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	4	0.15
(2,22)	1:A:114:LYS:O	1:A:118:PHE:N	4	0.15
(4,439)	1:A:38:GLU:H	1:A:38:GLU:HG2	7	0.14
(4,439)	1:A:38:GLU:H	1:A:38:GLU:HG3	7	0.14
(4,426)	1:A:37:ILE:H	1:A:37:ILE:HD11	15	0.14
(4,426)	1:A:37:ILE:H	1:A:37:ILE:HD12	15	0.14
(4,426)	1:A:37:ILE:H	1:A:37:ILE:HD13	15	0.14
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	15	0.14
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	15	0.14
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	9	0.14
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	9	0.14
(4,138)	1:A:35:ARG:HD2	1:A:38:GLU:HB2	5	0.14
(4,138)	1:A:35:ARG:HD2	1:A:38:GLU:HB3	5	0.14
(4,138)	1:A:35:ARG:HD3	1:A:38:GLU:HB2	5	0.14
(4,138)	1:A:35:ARG:HD3	1:A:38:GLU:HB3	5	0.14
(4,138)	1:A:35:ARG:HD2	1:A:38:GLU:HB2	8	0.14
(4,138)	1:A:35:ARG:HD2	1:A:38:GLU:HB3	8	0.14
(4,138)	1:A:35:ARG:HD3	1:A:38:GLU:HB2	8	0.14
(4,138)	1:A:35:ARG:HD3	1:A:38:GLU:HB3	8	0.14
(4,134)	1:A:33:ALA:H	1:A:35:ARG:H	12	0.14
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	4	0.14
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	4	0.14
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	7	0.14
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	8	0.14
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	15	0.14
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	7	0.14
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	2	0.14
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	10	0.14
(2,31)	1:A:133:VAL:O	1:A:137:HIS:N	11	0.14
(2,29)	1:A:127:ILE:O	1:A:131:GLU:N	10	0.14
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG11	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG12	12	0.13
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG13	12	0.13
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG21	12	0.13
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG22	12	0.13
(4,5)	1:A:52:PHE:HD1	1:A:31:VAL:HG23	12	0.13
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG11	12	0.13
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG12	12	0.13
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG13	12	0.13
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG21	12	0.13
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG22	12	0.13
(4,5)	1:A:52:PHE:HD2	1:A:31:VAL:HG23	12	0.13
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG11	12	0.13
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG12	12	0.13
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG13	12	0.13
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG21	12	0.13
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG22	12	0.13
(4,5)	1:A:52:PHE:HE1	1:A:31:VAL:HG23	12	0.13
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG11	12	0.13
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG12	12	0.13
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG13	12	0.13
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG21	12	0.13
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG22	12	0.13
(4,5)	1:A:52:PHE:HE2	1:A:31:VAL:HG23	12	0.13
(4,440)	1:A:38:GLU:HG2	1:A:39:LEU:H	1	0.13
(4,440)	1:A:38:GLU:HG3	1:A:39:LEU:H	1	0.13
(4,440)	1:A:38:GLU:HG2	1:A:39:LEU:H	11	0.13
(4,440)	1:A:38:GLU:HG3	1:A:39:LEU:H	11	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	1	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	1	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	2	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	2	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	3	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	3	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	4	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	4	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	5	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	5	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	6	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	6	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	7	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	7	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	8	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	9	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	9	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	10	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	10	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	11	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	11	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	12	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	12	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	13	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	13	0.13
(4,268)	1:A:12:ILE:HG12	1:A:13:ASP:H	14	0.13
(4,268)	1:A:12:ILE:HG13	1:A:13:ASP:H	14	0.13
(4,134)	1:A:33:ALA:H	1:A:35:ARG:H	10	0.13
(4,134)	1:A:33:ALA:H	1:A:35:ARG:H	14	0.13
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	1	0.13
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	1	0.13
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	3	0.13
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	3	0.13
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	8	0.13
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	8	0.13
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	9	0.13
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	9	0.13
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	13	0.13
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	13	0.13
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	1	0.13
(4,130)	1:A:32:GLU:H	1:A:34:GLY:H	5	0.13
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	2	0.13
(2,32)	1:A:134:ILE:O	1:A:138:HIS:N	9	0.13
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG2	9	0.12
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG3	9	0.12
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG2	10	0.12
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG3	10	0.12
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG21	13	0.12
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG22	13	0.12
(4,587)	1:A:63:PHE:HD1	1:A:67:THR:HG23	13	0.12
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG21	13	0.12
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG22	13	0.12
(4,587)	1:A:63:PHE:HD2	1:A:67:THR:HG23	13	0.12
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG21	13	0.12
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG22	13	0.12
(4,587)	1:A:63:PHE:HE1	1:A:67:THR:HG23	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG21	13	0.12
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG22	13	0.12
(4,587)	1:A:63:PHE:HE2	1:A:67:THR:HG23	13	0.12
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	2	0.12
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	2	0.12
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	4	0.12
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	4	0.12
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	5	0.12
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	5	0.12
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	6	0.12
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	6	0.12
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	10	0.12
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	10	0.12
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	12	0.12
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	12	0.12
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	14	0.12
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	14	0.12
(4,157)	1:A:50:LEU:H	1:A:51:TYR:HB2	13	0.12
(4,157)	1:A:50:LEU:H	1:A:51:TYR:HB3	13	0.12
(4,134)	1:A:33:ALA:H	1:A:35:ARG:H	13	0.12
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	2	0.12
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	2	0.12
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	5	0.12
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	5	0.12
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	10	0.12
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	10	0.12
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	12	0.12
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	12	0.12
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	14	0.12
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	14	0.12
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	8	0.12
(2,6)	1:A:38:GLU:O	1:A:42:GLU:N	11	0.12
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG2	2	0.11
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG3	2	0.11
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG2	12	0.11
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG3	12	0.11
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG2	14	0.11
(4,803)	1:A:97:LYS:H	1:A:97:LYS:HG3	14	0.11
(4,615)	1:A:67:THR:H	1:A:67:THR:HG21	9	0.11
(4,615)	1:A:67:THR:H	1:A:67:THR:HG22	9	0.11
(4,615)	1:A:67:THR:H	1:A:67:THR:HG23	9	0.11
(4,615)	1:A:67:THR:H	1:A:67:THR:HG21	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,615)	1:A:67:THR:H	1:A:67:THR:HG22	12	0.11
(4,615)	1:A:67:THR:H	1:A:67:THR:HG23	12	0.11
(4,527)	1:A:53:VAL:HB	1:A:54:VAL:H	2	0.11
(4,432)	1:A:37:ILE:HG21	1:A:38:GLU:H	15	0.11
(4,432)	1:A:37:ILE:HG22	1:A:38:GLU:H	15	0.11
(4,432)	1:A:37:ILE:HG23	1:A:38:GLU:H	15	0.11
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	1	0.11
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	1	0.11
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	3	0.11
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	3	0.11
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	7	0.11
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	7	0.11
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	8	0.11
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	8	0.11
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	13	0.11
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	13	0.11
(4,208)	1:A:97:LYS:HE2	1:A:100:GLU:HA	15	0.11
(4,208)	1:A:97:LYS:HE3	1:A:100:GLU:HA	15	0.11
(4,134)	1:A:33:ALA:H	1:A:35:ARG:H	2	0.11
(4,134)	1:A:33:ALA:H	1:A:35:ARG:H	3	0.11
(4,134)	1:A:33:ALA:H	1:A:35:ARG:H	4	0.11
(4,134)	1:A:33:ALA:H	1:A:35:ARG:H	9	0.11
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	6	0.11
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	6	0.11
(4,131)	1:A:32:GLU:HB2	1:A:36:LEU:H	11	0.11
(4,131)	1:A:32:GLU:HB3	1:A:36:LEU:H	11	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	1	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	2	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	3	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	4	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	5	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	6	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	7	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	8	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	9	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	10	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	11	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	12	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	13	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	14	0.11
(4,127)	1:A:31:VAL:HA	1:A:32:GLU:H	15	0.11

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value