Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 12:01 AM EDT

PDB ID	:	2LRV
BMRB ID	:	18283
Title	:	Assignment of E coli periplasmic protein YmgD
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Deposited on	:	2012-04-13

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

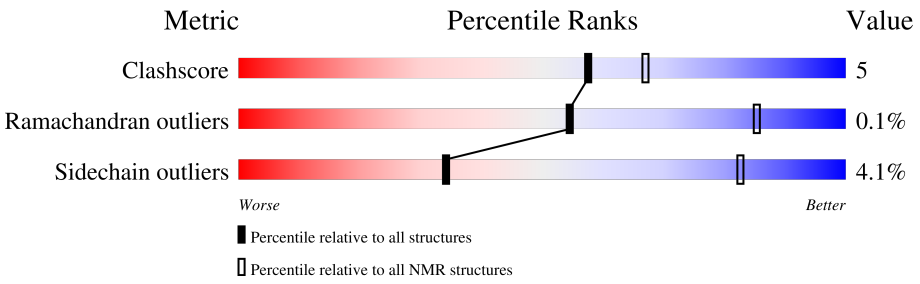
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 88%.

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	90	78% 9% 7% 7%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:11-A:88 (78)	0.95	3

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

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

The models can be grouped into 2 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1260 atoms, of which 638 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein ymgD.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	84	1260	382	638	105	129	6	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Uncharacterized protein ymgD

Chain A:

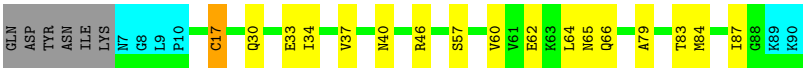
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Uncharacterized protein ymgD

Chain A:



4.2.2 Score per residue for model 2

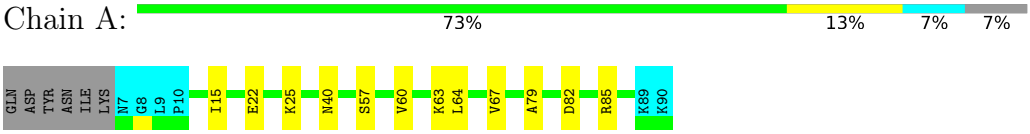
• Molecule 1: Uncharacterized protein ymgD

Chain A:

4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Uncharacterized protein ymgD

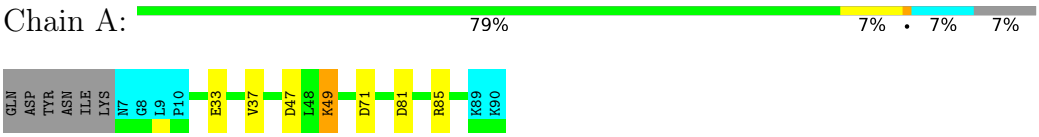
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein ymgD

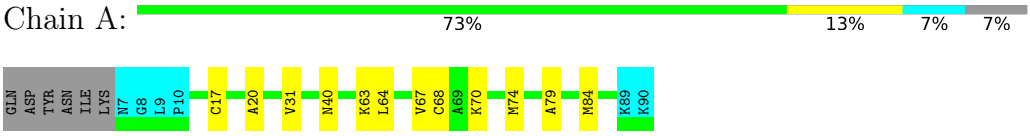
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein ymgD

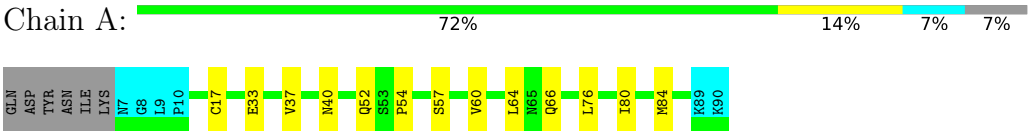
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein ymgD

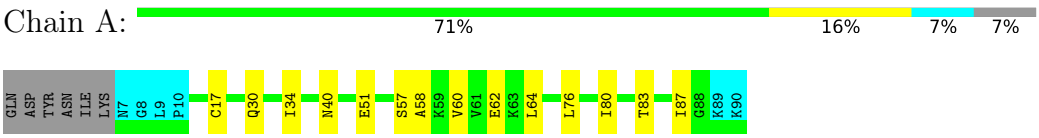
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein ymgD

Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein ymgD

Chain A: 79% 7% • 7% 7%

GLN ASP TYR ASN ILE LYS N7 G8 L9 P10 C17 N40 L64 D81 D82 T83 M84 I87 G88 K89 K90

4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein ymgD

Chain A: 69% 18% 7% 7%

GLN ASP TYR ASN ILE LYS N7 G8 L9 P10 T16 C17 Q30 E33 I34 V37 M38 G39 N40 V43 R46 I50 V60 L64 N65 Q66 A79 T83 K89 K90

4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein ymgD

Chain A: 74% 12% 7% 7%

GLN ASP TYR ASN ILE LYS N7 G8 L9 P10 A20 N21 E22 V31 N40 V60 K63 L64 N65 Q66 A79 I80 D81 M84 K89 K90

4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein ymgD

Chain A: 76% 11% 7% 7%

GLN ASP TYR ASN ILE LYS N7 G8 L9 P10 E33 V37 N40 R46 L56 V60 L64 D81 D82 T83 M84 K89 K90

4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein ymgD

Chain A: 69% 17% • 7% 7%

GLN ASP TYR ASN ILE LYS N7 G8 L9 P10 C17 A18 E19 E33 V37 M38 G39 N40 S57 V60 L64 N65 Q66 L76 I80 D81 D82 T83 I M84 I87 G88 K89 K90

4.2.13 Score per residue for model 13

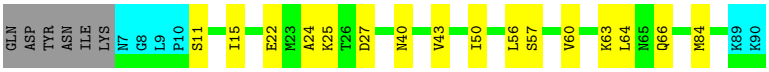
• Molecule 1: Uncharacterized protein ymgD

Chain A: 72% 13% • 7% 7%

4.2.14 Score per residue for model 14

• Molecule 1: Uncharacterized protein ymgD

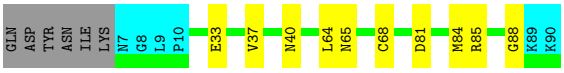
Chain A: 69% 18% 7% 7%



4.2.15 Score per residue for model 15

• Molecule 1: Uncharacterized protein ymgD

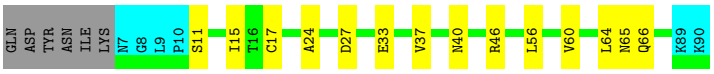
Chain A: 76% 11% 7% 7%



4.2.16 Score per residue for model 16

• Molecule 1: Uncharacterized protein ymgD

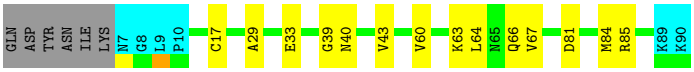
Chain A: 71% 16% 7% 7%



4.2.17 Score per residue for model 17

• Molecule 1: Uncharacterized protein ymgD

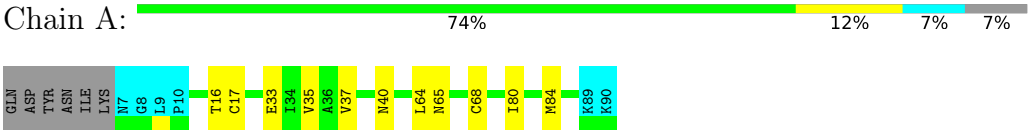
Chain A: 71% 16% 7% 7%



4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein ymgD

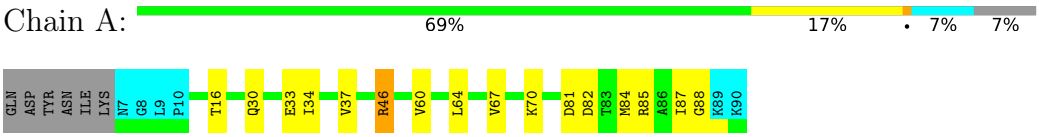
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein ymgD

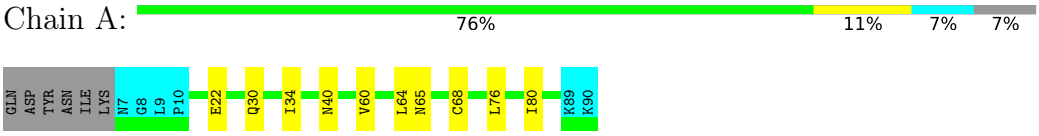
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein ymgD

Chain A:



5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	Classification	Version
Xplor-NIH	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	1034
Number of shifts mapped to atoms	959
Number of unparsed shifts	0
Number of shifts with mapping errors	75
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	576	585	585	6±2
All	All	11520	11700	11700	117

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:CYS:SG	1:A:65:ASN:HA	0.75	2.21	16	3
1:A:46:ARG:HD2	1:A:84:MET:SD	0.65	2.31	11	1
1:A:22:GLU:O	1:A:25:LYS:HG2	0.63	1.94	14	2
1:A:67:VAL:O	1:A:70:LYS:HG2	0.61	1.95	19	1
1:A:60:VAL:O	1:A:64:LEU:HB2	0.60	1.97	10	12
1:A:46:ARG:HG3	1:A:84:MET:SD	0.59	2.38	1	1
1:A:65:ASN:HA	1:A:68:CYS:SG	0.58	2.38	18	3
1:A:82:ASP:O	1:A:85:ARG:HG2	0.56	2.01	3	1
1:A:47:ASP:OD2	1:A:49:LYS:HE2	0.55	2.02	4	1
1:A:64:LEU:HD11	1:A:79:ALA:HB1	0.54	1.79	1	5
1:A:17:CYS:SG	1:A:64:LEU:HG	0.54	2.42	1	3
1:A:67:VAL:HG12	1:A:74:MET:SD	0.54	2.43	5	1
1:A:46:ARG:NE	1:A:46:ARG:HA	0.54	2.18	19	2
1:A:43:VAL:HG23	1:A:84:MET:HG3	0.54	1.79	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:SER:O	1:A:15:ILE:HG13	0.52	2.04	14	2
1:A:43:VAL:HB	1:A:84:MET:SD	0.52	2.45	17	1
1:A:52:GLN:O	1:A:54:PRO:HD3	0.52	2.05	6	1
1:A:64:LEU:HG	1:A:83:THR:OG1	0.51	2.06	11	1
1:A:80:ILE:O	1:A:84:MET:HG3	0.51	2.05	18	1
1:A:20:ALA:O	1:A:31:VAL:HG11	0.50	2.05	10	2
1:A:57:SER:O	1:A:60:VAL:HG12	0.50	2.07	7	5
1:A:29:ALA:O	1:A:33:GLU:HG2	0.50	2.06	17	2
1:A:33:GLU:O	1:A:37:VAL:HG23	0.49	2.07	12	12
1:A:68:CYS:SG	1:A:79:ALA:HB2	0.49	2.47	5	1
1:A:81:ASP:O	1:A:85:ARG:HG3	0.49	2.07	17	3
1:A:63:LYS:O	1:A:66:GLN:HG2	0.49	2.07	14	2
1:A:58:ALA:O	1:A:62:GLU:HG3	0.49	2.07	7	1
1:A:82:ASP:HA	1:A:85:ARG:HD2	0.49	1.83	19	1
1:A:43:VAL:HG22	1:A:50:ILE:HG13	0.49	1.84	14	1
1:A:63:LYS:O	1:A:67:VAL:HG23	0.48	2.08	5	4
1:A:39:GLY:HA2	1:A:80:ILE:HG21	0.48	1.85	12	1
1:A:81:ASP:O	1:A:84:MET:HG2	0.48	2.09	15	2
1:A:76:LEU:O	1:A:80:ILE:HG12	0.48	2.09	12	1
1:A:56:LEU:O	1:A:60:VAL:HG13	0.48	2.09	14	1
1:A:80:ILE:O	1:A:84:MET:HG2	0.47	2.09	6	1
1:A:81:ASP:O	1:A:84:MET:HB3	0.47	2.10	19	2
1:A:60:VAL:O	1:A:64:LEU:HB3	0.46	2.11	14	1
1:A:56:LEU:O	1:A:60:VAL:HG23	0.46	2.11	16	2
1:A:24:ALA:HA	1:A:27:ASP:O	0.46	2.10	16	3
1:A:81:ASP:O	1:A:84:MET:HG3	0.45	2.10	10	2
1:A:66:GLN:CA	1:A:66:GLN:HE21	0.45	2.24	13	1
1:A:30:GLN:O	1:A:34:ILE:HG12	0.45	2.10	20	3
1:A:82:ASP:HA	1:A:85:ARG:CD	0.45	2.41	19	1
1:A:83:THR:O	1:A:87:ILE:HG13	0.44	2.13	1	3
1:A:39:GLY:O	1:A:43:VAL:HG12	0.44	2.12	17	1
1:A:17:CYS:HB3	1:A:64:LEU:CD2	0.43	2.44	5	1
1:A:82:ASP:HA	1:A:85:ARG:NE	0.43	2.29	19	1
1:A:57:SER:O	1:A:60:VAL:HG22	0.42	2.14	14	1
1:A:67:VAL:HA	1:A:70:LYS:NZ	0.42	2.30	5	1
1:A:30:GLN:O	1:A:34:ILE:HG13	0.42	2.14	9	2
1:A:76:LEU:O	1:A:80:ILE:HG13	0.42	2.14	20	3
1:A:39:GLY:O	1:A:43:VAL:HG22	0.42	2.14	9	1
1:A:50:ILE:O	1:A:50:ILE:HG23	0.41	2.15	9	1
1:A:35:VAL:HA	1:A:80:ILE:HD11	0.41	1.93	18	1
1:A:83:THR:O	1:A:87:ILE:HG12	0.41	2.15	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:GLU:HA	1:A:22:GLU:OE1	0.41	2.16	10	1
1:A:66:GLN:HE21	1:A:66:GLN:HA	0.40	1.76	13	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	78/90 (87%)	73±2 (94±2%)	5±2 (6±2%)	0±0 (0±0%)	54	85
All	All	1560/1800 (87%)	1461 (94%)	97 (6%)	2 (0%)	54	85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	88	GLY	2

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	64/75 (85%)	61±1 (96±2%)	3±1 (4±2%)	34	82
All	All	1280/1500 (85%)	1227 (96%)	53 (4%)	34	82

All 16 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	40	ASN	18
1	A	66	GLN	8
1	A	17	CYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	16	THR	3
1	A	46	ARG	3
1	A	15	ILE	2
1	A	84	MET	2
1	A	64	LEU	2
1	A	62	GLU	1
1	A	73	GLN	1
1	A	49	LYS	1
1	A	71	ASP	1
1	A	51	GLU	1
1	A	83	THR	1
1	A	19	GLU	1
1	A	22	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	1034
Number of shifts mapped to atoms	959
Number of unparsed shifts	0
Number of shifts with mapping errors	75
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 75 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	GLN	HA	4.267	0.005	1
1	A	1	GLN	HB3	1.947	0.005	2
1	A	1	GLN	HB2	1.947	0.005	2
1	A	1	GLN	HG3	2.347	0.005	2
1	A	1	GLN	HG2	2.347	0.005	2
1	A	1	GLN	HE21	6.787	0.005	2
1	A	1	GLN	C	177.162	0.05	1
1	A	1	GLN	CA	59.52	0.108	1
1	A	1	GLN	CB	27.8	0.053	1
1	A	1	GLN	CG	31.936	0.05	1
1	A	1	GLN	NE2	109.976	0.05	1
1	A	2	ASP	H	8.324	0.004	1
1	A	2	ASP	HA	4.574	0.013	1
1	A	2	ASP	HB3	2.544	0.026	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ASP	HB2	2.544	0.026	2
1	A	2	ASP	C	175.354	0.059	1
1	A	2	ASP	CA	54.102	0.074	1
1	A	2	ASP	CB	41.053	0.056	1
1	A	2	ASP	N	120.838	0.116	1
1	A	3	TYR	H	8.14	0.003	1
1	A	3	TYR	HA	4.473	0.023	1
1	A	3	TYR	HB3	2.894	0.004	2
1	A	3	TYR	HB2	2.894	0.004	2
1	A	3	TYR	HD1	6.931	0.018	3
1	A	3	TYR	HD2	6.931	0.018	3
1	A	3	TYR	HE1	6.661	0.012	3
1	A	3	TYR	HE2	6.661	0.012	3
1	A	3	TYR	C	174.769	0.055	1
1	A	3	TYR	CA	57.671	0.039	1
1	A	3	TYR	CB	39.006	0.105	1
1	A	3	TYR	N	120.96	0.033	1
1	A	4	ASN	H	8.216	0.003	1
1	A	4	ASN	HA	4.706	0.024	1
1	A	4	ASN	HB3	2.747	0.019	2
1	A	4	ASN	HB2	2.747	0.019	2
1	A	4	ASN	HD22	7.634	0.013	2
1	A	4	ASN	HD21	6.797	0.005	2
1	A	4	ASN	C	175.662	0.05	1
1	A	4	ASN	CA	52.742	0.099	1
1	A	4	ASN	CB	39.74	0.076	1
1	A	4	ASN	N	122.518	0.030	1
1	A	4	ASN	ND2	112.626	0.003	1
1	A	5	ILE	H	8.598	0.011	1
1	A	5	ILE	HA	4.103	0.012	1
1	A	5	ILE	HB	1.865	0.028	1
1	A	5	ILE	HG13	1.473	0.017	2
1	A	5	ILE	HG12	1.473	0.017	2
1	A	5	ILE	HG21	0.86	0.005	1
1	A	5	ILE	HG22	0.86	0.005	1
1	A	5	ILE	HG23	0.86	0.005	1
1	A	5	ILE	HD11	0.838	0.003	1
1	A	5	ILE	HD12	0.838	0.003	1
1	A	5	ILE	HD13	0.838	0.003	1
1	A	5	ILE	C	175.763	0.037	1
1	A	5	ILE	CA	62.056	0.090	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	ILE	CB	38.547	0.031	1
1	A	5	ILE	CG1	28.524	0.145	1
1	A	5	ILE	CG2	17.875	0.127	1
1	A	5	ILE	CD1	14.403	0.128	1
1	A	5	ILE	N	123.297	0.019	1
1	A	6	LYS	H	8.053	0.008	1
1	A	6	LYS	HA	3.99	0.028	1
1	A	6	LYS	HB3	1.685	0.034	2
1	A	6	LYS	HB2	1.685	0.034	2
1	A	6	LYS	HG3	1.341	0.022	2
1	A	6	LYS	HG2	1.341	0.022	2
1	A	6	LYS	HE3	2.904	0.003	2
1	A	6	LYS	HE2	2.904	0.003	2
1	A	6	LYS	C	177.324	0.055	1
1	A	6	LYS	CA	58.282	0.042	1
1	A	6	LYS	CB	31.707	0.109	1
1	A	6	LYS	CG	25.003	0.05	1
1	A	6	LYS	CD	29.125	0.05	1
1	A	6	LYS	CE	41.801	0.05	1
1	A	6	LYS	N	121.049	0.049	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	85	-0.31 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	84	0.30 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	84	-0.30 ± 0.12	None needed (< 0.5 ppm)
^{15}N	86	0.48 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 886 atoms were assigned a chemical shift out of a possible 1004. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	377/388 (97%)	156/156 (100%)	145/156 (93%)	76/76 (100%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	505/607 (83%)	352/398 (88%)	146/191 (76%)	7/18 (39%)
Aromatic	4/9 (44%)	4/4 (100%)	0/5 (0%)	0/0 (—%)
Overall	886/1004 (88%)	512/558 (92%)	291/352 (83%)	83/94 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 955 atoms were assigned a chemical shift out of a possible 1088. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	406/417 (97%)	168/168 (100%)	157/168 (93%)	81/81 (100%)
Sidechain	545/662 (82%)	377/433 (87%)	160/208 (77%)	8/21 (38%)
Aromatic	4/9 (44%)	4/4 (100%)	0/5 (0%)	0/0 (—%)
Overall	955/1088 (88%)	549/605 (91%)	317/381 (83%)	89/102 (87%)

7.1.4 Statistically unusual chemical shifts (i)

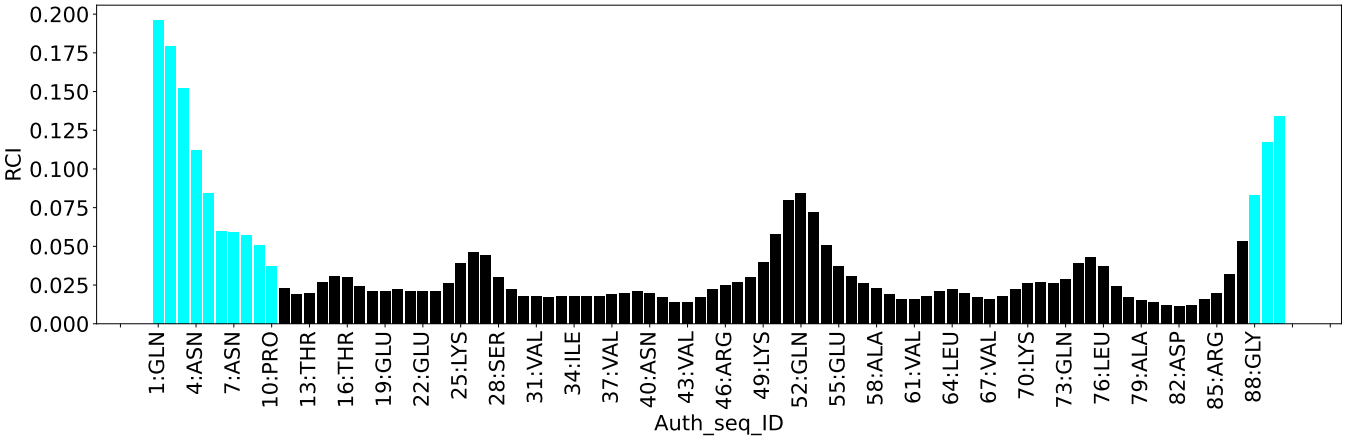
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	52	GLN	NE2	125.33	103.38 – 120.35	7.9
1	A	73	GLN	CB	39.29	20.34 – 37.98	5.7

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
1:GLN
4:ASN
7:ASN
10:PRO
13:THR
16:THR
19:GLU
22:GLU
25:LYS
28:SER
31:VAL
34:ILE
37:VAL
40:ASN
43:VAL
46:ARG
49:LYS
52:GLN
55:GLU
58:ALA
61:VAL
64:LEU
67:VAL
70:LYS
73:GLN
76:LEU
79:ALA
82:ASP
85:ARG
88:GLY
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	1045
Intra-residue (|i-j|=0)	260
Sequential (|i-j|=1)	376
Medium range (|i-j|>1 and |i-j|<5)	316
Long range (|i-j|≥5)	93
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	154
Number of unmapped restraints	60
Number of restraints per residue	13.3
Number of long range restraints per residue[1]	1.0

[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 (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	12.8	0.2
0.2-0.5 (Medium)	4.8	0.48
>0.5 (Large)	0.1	0.52

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)	5.5	7.7
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

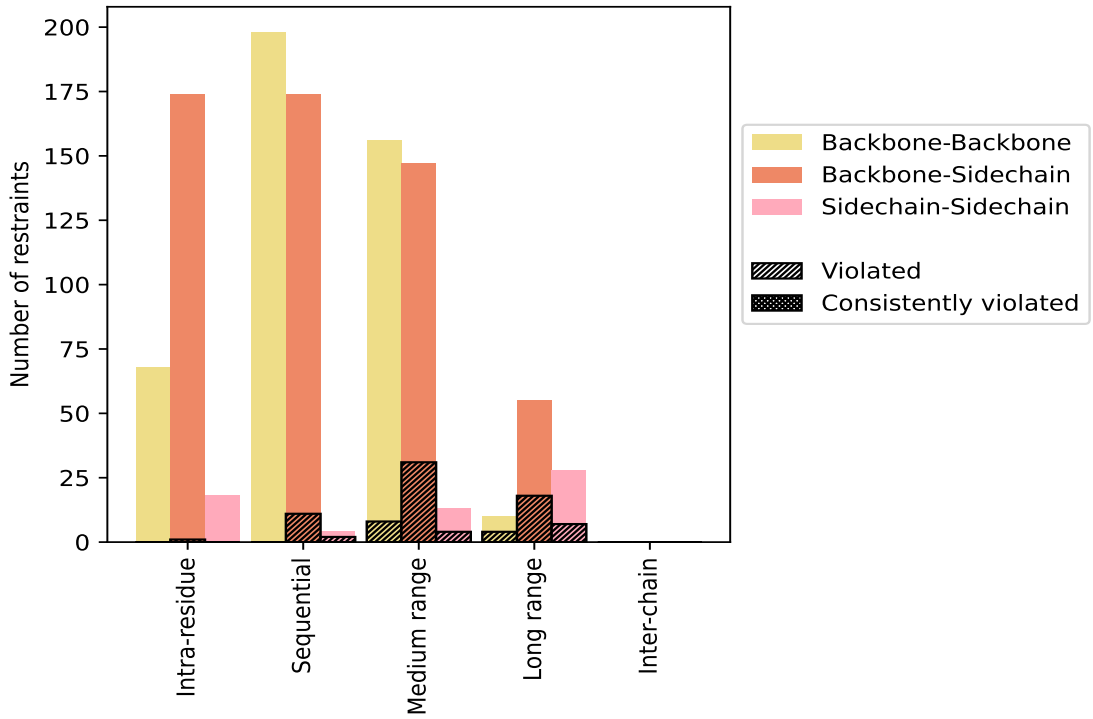
9.1 Summary of distance violations (i)

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)	260	24.9	1	0.4	0.1	0	0.0	0.0
Backbone-Backbone	68	6.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	174	16.7	1	0.6	0.1	0	0.0	0.0
Sidechain-Sidechain	18	1.7	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	376	36.0	13	3.5	1.2	0	0.0	0.0
Backbone-Backbone	198	18.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	174	16.7	11	6.3	1.1	0	0.0	0.0
Sidechain-Sidechain	4	0.4	2	50.0	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	316	30.2	43	13.6	4.1	0	0.0	0.0
Backbone-Backbone	156	14.9	8	5.1	0.8	0	0.0	0.0
Backbone-Sidechain	147	14.1	31	21.1	3.0	0	0.0	0.0
Sidechain-Sidechain	13	1.2	4	30.8	0.4	0	0.0	0.0
Long range (|i-j|≥5)	93	8.9	29	31.2	2.8	0	0.0	0.0
Backbone-Backbone	10	1.0	4	40.0	0.4	0	0.0	0.0
Backbone-Sidechain	55	5.3	18	32.7	1.7	0	0.0	0.0
Sidechain-Sidechain	28	2.7	7	25.0	0.7	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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1045	100.0	86	8.2	8.2	0	0.0	0.0
Backbone-Backbone	432	41.3	12	2.8	1.1	0	0.0	0.0
Backbone-Sidechain	550	52.6	61	11.1	5.8	0	0.0	0.0
Sidechain-Sidechain	63	6.0	13	20.6	1.2	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	1	5	10	6	0	22	0.19	0.47	0.08	0.16
2	1	3	9	4	0	17	0.21	0.46	0.09	0.2
3	1	1	11	4	0	17	0.19	0.46	0.08	0.17
4	1	5	10	7	0	23	0.21	0.33	0.07	0.18
5	1	3	15	2	0	21	0.2	0.3	0.06	0.19
6	1	2	8	3	0	14	0.15	0.27	0.04	0.14
7	0	1	7	4	0	12	0.2	0.41	0.1	0.16
8	1	3	9	2	0	15	0.16	0.26	0.05	0.14
9	0	4	8	8	0	20	0.17	0.36	0.06	0.16
10	1	3	9	8	0	21	0.19	0.43	0.08	0.17
11	1	4	12	5	0	22	0.16	0.22	0.03	0.16

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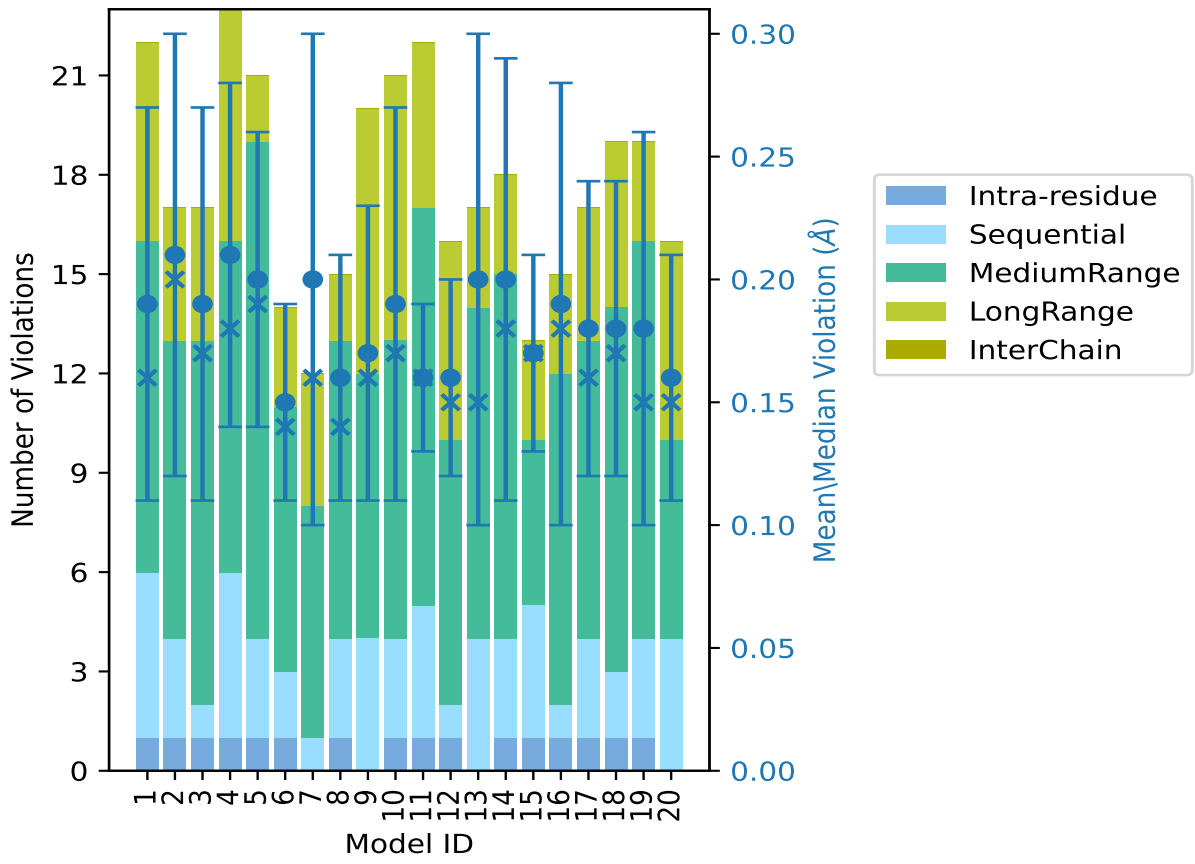
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	1	8	6	0	16	0.16	0.27	0.04	0.15
13	0	4	10	3	0	17	0.2	0.52	0.1	0.15
14	1	3	11	3	0	18	0.2	0.52	0.09	0.18
15	1	4	5	3	0	13	0.17	0.25	0.04	0.17
16	1	1	10	3	0	15	0.19	0.48	0.09	0.18
17	1	3	9	4	0	17	0.18	0.32	0.06	0.16
18	1	2	11	5	0	19	0.18	0.38	0.06	0.17
19	1	3	12	3	0	19	0.18	0.42	0.08	0.15
20	0	4	6	6	0	16	0.16	0.3	0.05	0.15

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

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



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

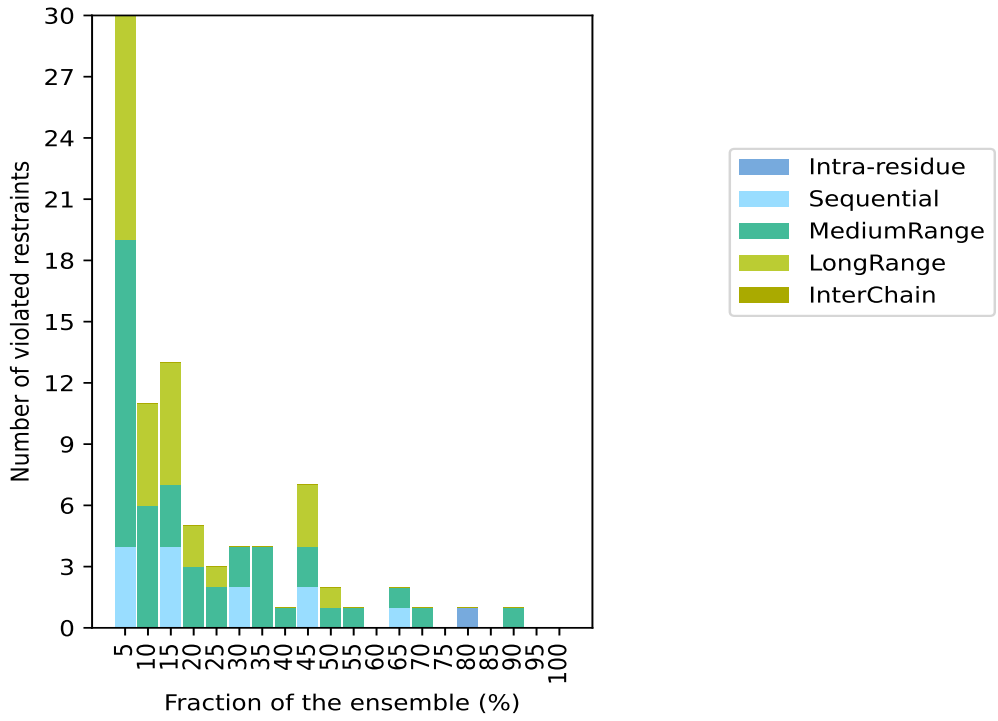
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 959(IR:259, SQ:363, MR:273, LR:64, 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]	%
0	4	15	11	0	30	1	5.0
0	0	6	5	0	11	2	10.0
0	4	3	6	0	13	3	15.0
0	0	3	2	0	5	4	20.0
0	0	2	1	0	3	5	25.0
0	2	2	0	0	4	6	30.0
0	0	4	0	0	4	7	35.0
0	0	1	0	0	1	8	40.0
0	2	2	3	0	7	9	45.0
0	0	1	1	0	2	10	50.0
0	0	1	0	0	1	11	55.0
0	0	0	0	0	0	12	60.0
0	1	1	0	0	2	13	65.0
0	0	1	0	0	1	14	70.0
0	0	0	0	0	0	15	75.0
1	0	0	0	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	1	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

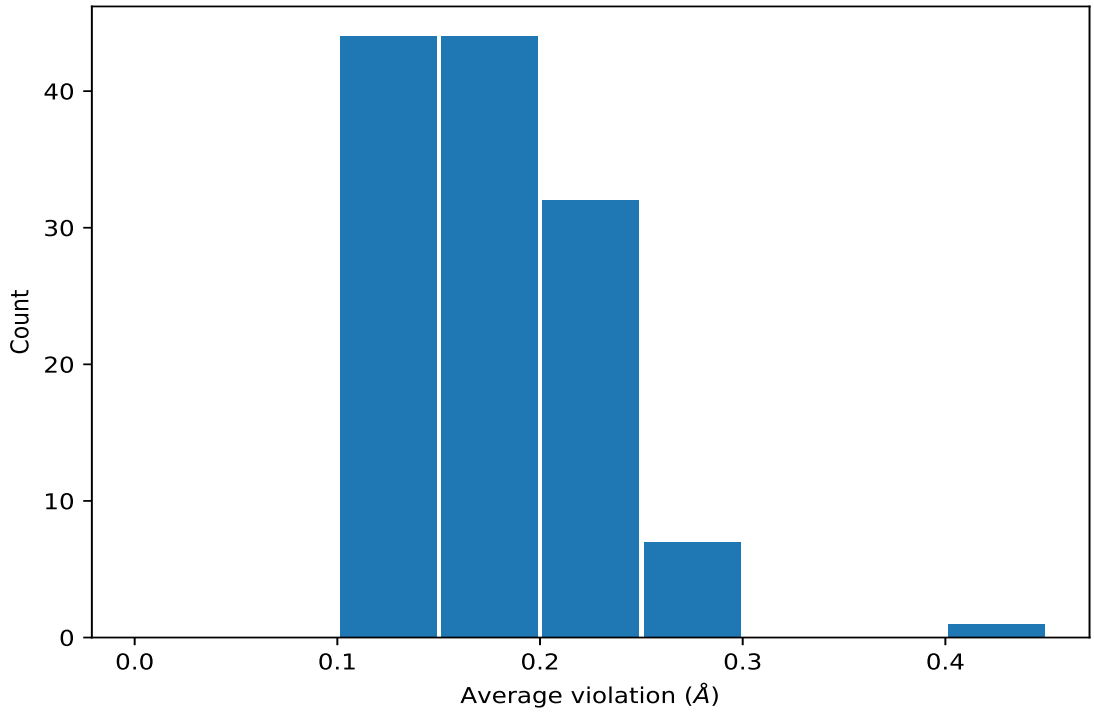
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	18	0.18	0.04	0.18
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	16	0.17	0.03	0.17
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	16	0.17	0.03	0.17
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	14	0.14	0.03	0.12
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	14	0.14	0.03	0.12
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	14	0.14	0.03	0.12
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	13	0.22	0.05	0.21
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	13	0.2	0.07	0.17
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	13	0.2	0.07	0.17
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	11	0.2	0.05	0.22
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG21	10	0.21	0.06	0.2
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG22	10	0.21	0.06	0.2
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG23	10	0.21	0.06	0.2
(1,120)	1:A:16:THR:H	1:A:20:ALA:HA	10	0.15	0.03	0.15
(1,597)	1:A:65:ASN:H	1:A:66:GLN:HE22	9	0.25	0.12	0.22
(1,425)	1:A:45:SER:H	1:A:84:MET:HB2	9	0.19	0.07	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,425)	1:A:45:SER:H	1:A:84:MET:HB3	9	0.19	0.07	0.2
(1,882)	1:A:15:ILE:HD11	1:A:75:LEU:HA	9	0.19	0.05	0.17
(1,882)	1:A:15:ILE:HD12	1:A:75:LEU:HA	9	0.19	0.05	0.17
(1,882)	1:A:15:ILE:HD13	1:A:75:LEU:HA	9	0.19	0.05	0.17
(1,701)	1:A:74:MET:H	1:A:73:GLN:HE21	9	0.18	0.06	0.17
(1,776)	1:A:83:THR:H	1:A:64:LEU:HB2	9	0.18	0.06	0.16
(1,439)	1:A:46:ARG:H	1:A:50:ILE:HB	9	0.17	0.06	0.14
(1,789)	1:A:83:THR:H	1:A:87:ILE:H	9	0.17	0.05	0.15
(1,648)	1:A:69:ALA:H	1:A:65:ASN:H	8	0.15	0.02	0.15
(1,215)	1:A:25:LYS:H	1:A:27:ASP:HB2	7	0.4	0.14	0.46
(1,1022)	1:A:84:MET:HE1	1:A:88:GLY:HA2	7	0.2	0.06	0.22
(1,1022)	1:A:84:MET:HE2	1:A:88:GLY:HA2	7	0.2	0.06	0.22
(1,1022)	1:A:84:MET:HE3	1:A:88:GLY:HA2	7	0.2	0.06	0.22
(1,865)	1:A:9:LEU:HD11	1:A:7:ASN:HD22	7	0.19	0.05	0.2
(1,865)	1:A:9:LEU:HD12	1:A:7:ASN:HD22	7	0.19	0.05	0.2
(1,865)	1:A:9:LEU:HD13	1:A:7:ASN:HD22	7	0.19	0.05	0.2
(1,304)	1:A:35:VAL:H	1:A:31:VAL:H	7	0.15	0.04	0.13
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG21	6	0.26	0.1	0.24
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG22	6	0.26	0.1	0.24
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG23	6	0.26	0.1	0.24
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE1	6	0.2	0.07	0.17
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE2	6	0.2	0.07	0.17
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE1	6	0.2	0.07	0.17
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE2	6	0.2	0.07	0.17
(1,875)	1:A:13:THR:HG21	1:A:9:LEU:H	6	0.18	0.03	0.17
(1,875)	1:A:13:THR:HG22	1:A:9:LEU:H	6	0.18	0.03	0.17
(1,875)	1:A:13:THR:HG23	1:A:9:LEU:H	6	0.18	0.03	0.17
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE1	6	0.13	0.03	0.12
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE2	6	0.13	0.03	0.12
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE3	6	0.13	0.03	0.12
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD11	5	0.23	0.1	0.22
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD12	5	0.23	0.1	0.22
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD13	5	0.23	0.1	0.22
(1,422)	1:A:45:SER:H	1:A:47:ASP:HB2	5	0.2	0.05	0.2
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD11	5	0.14	0.03	0.13
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD12	5	0.14	0.03	0.13
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD13	5	0.14	0.03	0.13
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE1	4	0.19	0.04	0.2
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE2	4	0.19	0.04	0.2
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE3	4	0.19	0.04	0.2
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE1	4	0.19	0.04	0.2
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE2	4	0.19	0.04	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE3	4	0.19	0.04	0.2
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE1	4	0.19	0.04	0.2
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE2	4	0.19	0.04	0.2
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE3	4	0.19	0.04	0.2
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE1	4	0.18	0.06	0.16
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE2	4	0.18	0.06	0.16
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE3	4	0.18	0.06	0.16
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG11	4	0.17	0.05	0.16
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG12	4	0.17	0.05	0.16
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG13	4	0.17	0.05	0.16
(1,620)	1:A:67:VAL:H	1:A:65:ASN:HB2	4	0.15	0.01	0.15
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG21	4	0.14	0.0	0.14
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG22	4	0.14	0.0	0.14
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG23	4	0.14	0.0	0.14
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE1	3	0.24	0.11	0.23
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE2	3	0.24	0.11	0.23
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE3	3	0.24	0.11	0.23
(1,292)	1:A:33:GLU:H	1:A:34:ILE:HG12	3	0.24	0.04	0.25
(1,292)	1:A:33:GLU:H	1:A:34:ILE:HG13	3	0.24	0.04	0.25
(1,896)	1:A:23:MET:HE1	1:A:30:GLN:H	3	0.2	0.04	0.2
(1,896)	1:A:23:MET:HE2	1:A:30:GLN:H	3	0.2	0.04	0.2
(1,896)	1:A:23:MET:HE3	1:A:30:GLN:H	3	0.2	0.04	0.2
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH11	3	0.2	0.07	0.17
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH12	3	0.2	0.07	0.17
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH21	3	0.2	0.07	0.17
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH22	3	0.2	0.07	0.17
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG21	3	0.19	0.02	0.18
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG22	3	0.19	0.02	0.18
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG23	3	0.19	0.02	0.18
(1,565)	1:A:62:GLU:H	1:A:63:LYS:HG2	3	0.19	0.05	0.17
(1,565)	1:A:62:GLU:H	1:A:63:LYS:HG3	3	0.19	0.05	0.17
(1,853)	1:A:90:LYS:H	1:A:88:GLY:HA3	3	0.17	0.06	0.13
(1,675)	1:A:71:ASP:H	1:A:67:VAL:HB	3	0.16	0.05	0.14
(1,136)	1:A:18:ALA:H	1:A:65:ASN:HB2	3	0.15	0.04	0.13
(1,684)	1:A:71:ASP:H	1:A:70:LYS:HE2	3	0.15	0.02	0.14
(1,684)	1:A:71:ASP:H	1:A:70:LYS:HE3	3	0.15	0.02	0.14
(1,924)	1:A:38:MET:HE1	1:A:81:ASP:HB2	3	0.15	0.02	0.14
(1,924)	1:A:38:MET:HE2	1:A:81:ASP:HB2	3	0.15	0.02	0.14
(1,924)	1:A:38:MET:HE3	1:A:81:ASP:HB2	3	0.15	0.02	0.14
(1,645)	1:A:69:ALA:H	1:A:18:ALA:H	3	0.14	0.03	0.12
(1,887)	1:A:16:THR:HG21	1:A:68:CYS:HA	3	0.13	0.02	0.11
(1,887)	1:A:16:THR:HG22	1:A:68:CYS:HA	3	0.13	0.02	0.11

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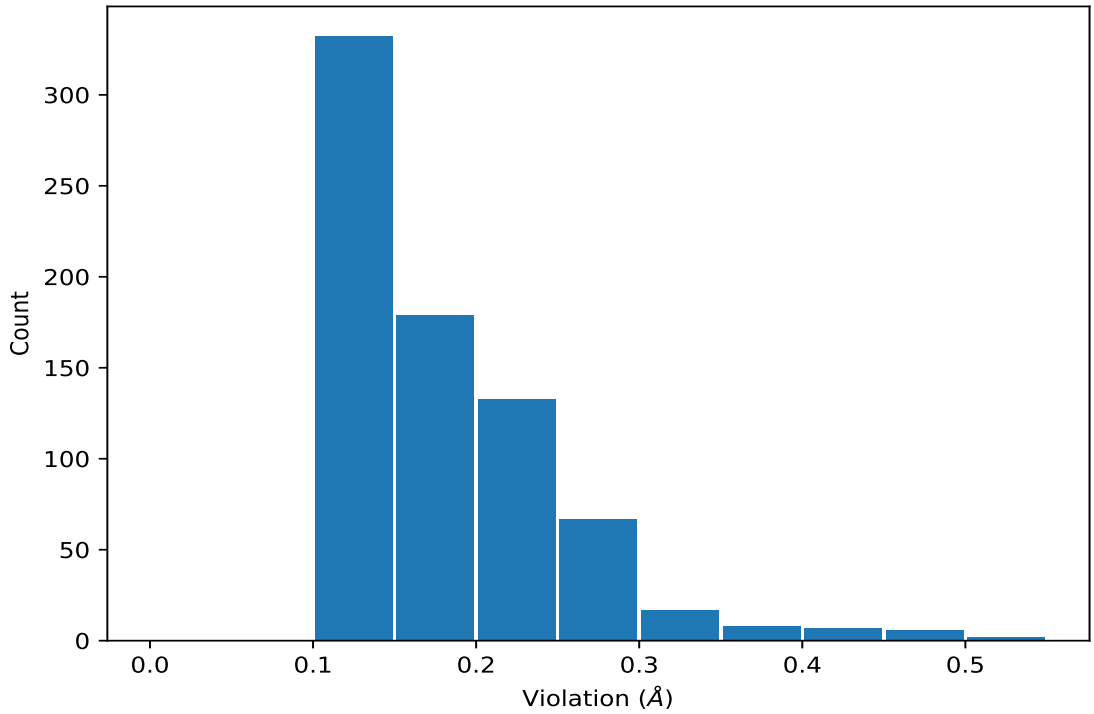
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,887)	1:A:16:THR:HG23	1:A:68:CYS:HA	3	0.13	0.02	0.11
(1,787)	1:A:83:THR:H	1:A:85:ARG:HD3	2	0.28	0.09	0.28
(1,495)	1:A:53:SER:H	1:A:51:GLU:HG2	2	0.26	0.15	0.26
(1,495)	1:A:53:SER:H	1:A:51:GLU:HG3	2	0.26	0.15	0.26
(1,662)	1:A:70:LYS:H	1:A:66:GLN:HG2	2	0.21	0.09	0.21
(1,662)	1:A:70:LYS:H	1:A:66:GLN:HG3	2	0.21	0.09	0.21
(1,721)	1:A:78:THR:H	1:A:16:THR:HA	2	0.17	0.02	0.17
(1,338)	1:A:37:VAL:H	1:A:80:ILE:HD11	2	0.16	0.02	0.16
(1,338)	1:A:37:VAL:H	1:A:80:ILE:HD12	2	0.16	0.02	0.16
(1,338)	1:A:37:VAL:H	1:A:80:ILE:HD13	2	0.16	0.02	0.16
(1,243)	1:A:27:ASP:H	1:A:30:GLN:HG2	2	0.15	0.03	0.15
(1,243)	1:A:27:ASP:H	1:A:30:GLN:HG3	2	0.15	0.03	0.15
(1,522)	1:A:57:SER:H	1:A:53:SER:HA	2	0.15	0.03	0.15
(1,943)	1:A:48:LEU:HD11	1:A:46:ARG:HA	2	0.15	0.02	0.15
(1,943)	1:A:48:LEU:HD12	1:A:46:ARG:HA	2	0.15	0.02	0.15
(1,943)	1:A:48:LEU:HD13	1:A:46:ARG:HA	2	0.15	0.02	0.15
(1,943)	1:A:48:LEU:HD21	1:A:46:ARG:HA	2	0.15	0.02	0.15
(1,943)	1:A:48:LEU:HD22	1:A:46:ARG:HA	2	0.15	0.02	0.15
(1,943)	1:A:48:LEU:HD23	1:A:46:ARG:HA	2	0.15	0.02	0.15
(1,575)	1:A:63:LYS:H	1:A:83:THR:HG21	2	0.14	0.02	0.14
(1,575)	1:A:63:LYS:H	1:A:83:THR:HG22	2	0.14	0.02	0.14
(1,575)	1:A:63:LYS:H	1:A:83:THR:HG23	2	0.14	0.02	0.14
(1,907)	1:A:32:ALA:HB1	1:A:58:ALA:H	2	0.12	0.02	0.12
(1,907)	1:A:32:ALA:HB2	1:A:58:ALA:H	2	0.12	0.02	0.12
(1,907)	1:A:32:ALA:HB3	1:A:58:ALA:H	2	0.12	0.02	0.12
(1,100)	1:A:14:TYR:H	1:A:77:ILE:HD11	2	0.12	0.0	0.12
(1,100)	1:A:14:TYR:H	1:A:77:ILE:HD12	2	0.12	0.0	0.12
(1,100)	1:A:14:TYR:H	1:A:77:ILE:HD13	2	0.12	0.0	0.12

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:A:25:LYS:H	1:A:27:ASP:HB2	13	0.52
(1,215)	1:A:25:LYS:H	1:A:27:ASP:HB2	14	0.52
(1,215)	1:A:25:LYS:H	1:A:27:ASP:HB2	16	0.48
(1,597)	1:A:65:ASN:H	1:A:66:GLN:HE22	1	0.47
(1,215)	1:A:25:LYS:H	1:A:27:ASP:HB2	3	0.46
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG21	2	0.46
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG22	2	0.46
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG23	2	0.46
(1,597)	1:A:65:ASN:H	1:A:66:GLN:HE22	2	0.43
(1,215)	1:A:25:LYS:H	1:A:27:ASP:HB2	10	0.43
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD11	19	0.42
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD12	19	0.42
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD13	19	0.42
(1,495)	1:A:53:SER:H	1:A:51:GLU:HG2	7	0.41
(1,495)	1:A:53:SER:H	1:A:51:GLU:HG3	7	0.41
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE1	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE2	18	0.38
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE3	18	0.38
(1,787)	1:A:83:THR:H	1:A:85:ARG:HD3	19	0.37
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE1	9	0.36
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE2	9	0.36
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE1	9	0.36
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE2	9	0.36
(1,452)	1:A:48:LEU:H	1:A:43:VAL:HG21	4	0.33
(1,452)	1:A:48:LEU:H	1:A:43:VAL:HG22	4	0.33
(1,452)	1:A:48:LEU:H	1:A:43:VAL:HG23	4	0.33
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	7	0.33
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	7	0.33
(1,451)	1:A:48:LEU:H	1:A:43:VAL:HA	4	0.32
(1,425)	1:A:45:SER:H	1:A:84:MET:HB2	10	0.32
(1,425)	1:A:45:SER:H	1:A:84:MET:HB3	10	0.32
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	4	0.32
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG21	17	0.32
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG22	17	0.32
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG23	17	0.32
(1,701)	1:A:74:MET:H	1:A:73:GLN:HE21	4	0.31
(1,597)	1:A:65:ASN:H	1:A:66:GLN:HE22	14	0.31
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG21	1	0.31
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG22	1	0.31
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG23	1	0.31
(1,662)	1:A:70:LYS:H	1:A:66:GLN:HG2	5	0.3
(1,662)	1:A:70:LYS:H	1:A:66:GLN:HG3	5	0.3
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	4	0.3
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	4	0.3
(1,439)	1:A:46:ARG:H	1:A:50:ILE:HB	4	0.3
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH11	20	0.3
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH12	20	0.3
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH21	20	0.3
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH22	20	0.3
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	10	0.3
(1,882)	1:A:15:ILE:HD11	1:A:75:LEU:HA	1	0.29
(1,882)	1:A:15:ILE:HD12	1:A:75:LEU:HA	1	0.29
(1,882)	1:A:15:ILE:HD13	1:A:75:LEU:HA	1	0.29
(1,422)	1:A:45:SER:H	1:A:47:ASP:HB2	7	0.29
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG21	7	0.29
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG22	7	0.29
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG23	7	0.29
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE1	17	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE2	17	0.28
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE3	17	0.28
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	3	0.28
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	3	0.28
(1,425)	1:A:45:SER:H	1:A:84:MET:HB2	13	0.28
(1,425)	1:A:45:SER:H	1:A:84:MET:HB3	13	0.28
(1,292)	1:A:33:GLU:H	1:A:34:ILE:HG12	5	0.28
(1,292)	1:A:33:GLU:H	1:A:34:ILE:HG13	5	0.28
(1,1022)	1:A:84:MET:HE1	1:A:88:GLY:HA2	5	0.28
(1,1022)	1:A:84:MET:HE2	1:A:88:GLY:HA2	5	0.28
(1,1022)	1:A:84:MET:HE3	1:A:88:GLY:HA2	5	0.28
(1,789)	1:A:83:THR:H	1:A:87:ILE:H	5	0.27
(1,776)	1:A:83:THR:H	1:A:64:LEU:HB2	16	0.27
(1,701)	1:A:74:MET:H	1:A:73:GLN:HE21	13	0.27
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	5	0.27
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	6	0.27
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	14	0.27
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG21	12	0.27
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG22	12	0.27
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG23	12	0.27
(1,986)	1:A:77:ILE:HD11	1:A:42:SER:HB2	10	0.26
(1,986)	1:A:77:ILE:HD11	1:A:42:SER:HB3	10	0.26
(1,986)	1:A:77:ILE:HD12	1:A:42:SER:HB2	10	0.26
(1,986)	1:A:77:ILE:HD12	1:A:42:SER:HB3	10	0.26
(1,986)	1:A:77:ILE:HD13	1:A:42:SER:HB2	10	0.26
(1,986)	1:A:77:ILE:HD13	1:A:42:SER:HB3	10	0.26
(1,853)	1:A:90:LYS:H	1:A:88:GLY:HA3	17	0.26
(1,565)	1:A:62:GLU:H	1:A:63:LYS:HG2	8	0.26
(1,565)	1:A:62:GLU:H	1:A:63:LYS:HG3	8	0.26
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	13	0.26
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	3	0.26
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	10	0.26
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG21	19	0.26
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG22	19	0.26
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG23	19	0.26
(1,896)	1:A:23:MET:HE1	1:A:30:GLN:H	13	0.25
(1,896)	1:A:23:MET:HE2	1:A:30:GLN:H	13	0.25
(1,896)	1:A:23:MET:HE3	1:A:30:GLN:H	13	0.25
(1,865)	1:A:9:LEU:HD11	1:A:7:ASN:HD22	8	0.25
(1,865)	1:A:9:LEU:HD12	1:A:7:ASN:HD22	8	0.25
(1,865)	1:A:9:LEU:HD13	1:A:7:ASN:HD22	8	0.25
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	1	0.25
(1,439)	1:A:46:ARG:H	1:A:50:ILE:HB	5	0.25
(1,292)	1:A:33:GLU:H	1:A:34:ILE:HG12	4	0.25
(1,292)	1:A:33:GLU:H	1:A:34:ILE:HG13	4	0.25
(1,1022)	1:A:84:MET:HE1	1:A:88:GLY:HA2	15	0.25
(1,1022)	1:A:84:MET:HE2	1:A:88:GLY:HA2	15	0.25
(1,1022)	1:A:84:MET:HE3	1:A:88:GLY:HA2	15	0.25
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	1	0.24
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	1	0.24
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE1	9	0.24
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE2	9	0.24
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE3	9	0.24
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE1	9	0.24
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE2	9	0.24
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE3	9	0.24
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE1	9	0.24
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE2	9	0.24
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE3	9	0.24
(1,882)	1:A:15:ILE:HD11	1:A:75:LEU:HA	4	0.24
(1,882)	1:A:15:ILE:HD12	1:A:75:LEU:HA	4	0.24
(1,882)	1:A:15:ILE:HD13	1:A:75:LEU:HA	4	0.24
(1,776)	1:A:83:THR:H	1:A:64:LEU:HB2	20	0.24
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG11	18	0.24
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG12	18	0.24
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG13	18	0.24
(1,865)	1:A:9:LEU:HD11	1:A:7:ASN:HD22	16	0.23
(1,865)	1:A:9:LEU:HD12	1:A:7:ASN:HD22	16	0.23
(1,865)	1:A:9:LEU:HD13	1:A:7:ASN:HD22	16	0.23
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE1	4	0.23
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE2	4	0.23
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE3	4	0.23
(1,597)	1:A:65:ASN:H	1:A:66:GLN:HE22	5	0.23
(1,304)	1:A:35:VAL:H	1:A:31:VAL:H	17	0.23
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	1	0.23
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	5	0.23
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	14	0.23
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	16	0.23
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG21	2	0.23
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG22	2	0.23
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG23	2	0.23
(1,1022)	1:A:84:MET:HE1	1:A:88:GLY:HA2	13	0.23
(1,1022)	1:A:84:MET:HE2	1:A:88:GLY:HA2	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:A:84:MET:HE3	1:A:88:GLY:HA2	13	0.23
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	5	0.22
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	5	0.22
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	5	0.22
(1,882)	1:A:15:ILE:HD11	1:A:75:LEU:HA	18	0.22
(1,882)	1:A:15:ILE:HD12	1:A:75:LEU:HA	18	0.22
(1,882)	1:A:15:ILE:HD13	1:A:75:LEU:HA	18	0.22
(1,875)	1:A:13:THR:HG21	1:A:9:LEU:H	14	0.22
(1,875)	1:A:13:THR:HG22	1:A:9:LEU:H	14	0.22
(1,875)	1:A:13:THR:HG23	1:A:9:LEU:H	14	0.22
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD11	2	0.22
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD12	2	0.22
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD13	2	0.22
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD11	11	0.22
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD12	11	0.22
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD13	11	0.22
(1,789)	1:A:83:THR:H	1:A:87:ILE:H	11	0.22
(1,776)	1:A:83:THR:H	1:A:64:LEU:HB2	10	0.22
(1,776)	1:A:83:THR:H	1:A:64:LEU:HB2	19	0.22
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG21	8	0.22
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG22	8	0.22
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG23	8	0.22
(1,675)	1:A:71:ASP:H	1:A:67:VAL:HB	3	0.22
(1,597)	1:A:65:ASN:H	1:A:66:GLN:HE22	11	0.22
(1,574)	1:A:63:LYS:H	1:A:66:GLN:HB2	10	0.22
(1,574)	1:A:63:LYS:H	1:A:66:GLN:HB3	10	0.22
(1,422)	1:A:45:SER:H	1:A:47:ASP:HB2	16	0.22
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	20	0.22
(1,215)	1:A:25:LYS:H	1:A:27:ASP:HB2	18	0.22
(1,1022)	1:A:84:MET:HE1	1:A:88:GLY:HA2	19	0.22
(1,1022)	1:A:84:MET:HE2	1:A:88:GLY:HA2	19	0.22
(1,1022)	1:A:84:MET:HE3	1:A:88:GLY:HA2	19	0.22
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	2	0.21
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	2	0.21
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE1	14	0.21
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE2	14	0.21
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE3	14	0.21
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE1	14	0.21
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE2	14	0.21
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE3	14	0.21
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE1	14	0.21
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE2	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE3	14	0.21
(1,882)	1:A:15:ILE:HD11	1:A:75:LEU:HA	5	0.21
(1,882)	1:A:15:ILE:HD12	1:A:75:LEU:HA	5	0.21
(1,882)	1:A:15:ILE:HD13	1:A:75:LEU:HA	5	0.21
(1,875)	1:A:13:THR:HG21	1:A:9:LEU:H	2	0.21
(1,875)	1:A:13:THR:HG22	1:A:9:LEU:H	2	0.21
(1,875)	1:A:13:THR:HG23	1:A:9:LEU:H	2	0.21
(1,865)	1:A:9:LEU:HD11	1:A:7:ASN:HD22	2	0.21
(1,865)	1:A:9:LEU:HD12	1:A:7:ASN:HD22	2	0.21
(1,865)	1:A:9:LEU:HD13	1:A:7:ASN:HD22	2	0.21
(1,425)	1:A:45:SER:H	1:A:84:MET:HB2	1	0.21
(1,425)	1:A:45:SER:H	1:A:84:MET:HB3	1	0.21
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	12	0.21
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	14	0.21
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	15	0.21
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG11	3	0.21
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG12	3	0.21
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG13	3	0.21
(1,120)	1:A:16:THR:H	1:A:20:ALA:HA	9	0.21
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG21	11	0.21
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG22	11	0.21
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG23	11	0.21
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	19	0.2
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	19	0.2
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE1	16	0.2
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE2	16	0.2
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE3	16	0.2
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE1	16	0.2
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE2	16	0.2
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE3	16	0.2
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE1	16	0.2
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE2	16	0.2
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE3	16	0.2
(1,896)	1:A:23:MET:HE1	1:A:30:GLN:H	15	0.2
(1,896)	1:A:23:MET:HE2	1:A:30:GLN:H	15	0.2
(1,896)	1:A:23:MET:HE3	1:A:30:GLN:H	15	0.2
(1,865)	1:A:9:LEU:HD11	1:A:7:ASN:HD22	4	0.2
(1,865)	1:A:9:LEU:HD12	1:A:7:ASN:HD22	4	0.2
(1,865)	1:A:9:LEU:HD13	1:A:7:ASN:HD22	4	0.2
(1,597)	1:A:65:ASN:H	1:A:66:GLN:HE22	15	0.2
(1,425)	1:A:45:SER:H	1:A:84:MET:HB2	2	0.2
(1,425)	1:A:45:SER:H	1:A:84:MET:HB3	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:A:45:SER:H	1:A:84:MET:HB2	7	0.2
(1,425)	1:A:45:SER:H	1:A:84:MET:HB3	7	0.2
(1,422)	1:A:45:SER:H	1:A:47:ASP:HB2	2	0.2
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD11	2	0.2
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD12	2	0.2
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD13	2	0.2
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	16	0.2
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	9	0.2
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	11	0.2
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG21	13	0.2
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG22	13	0.2
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG23	13	0.2
(1,136)	1:A:18:ALA:H	1:A:65:ASN:HB2	18	0.2
(1,120)	1:A:16:THR:H	1:A:20:ALA:HA	17	0.2
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	3	0.19
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	3	0.19
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	8	0.19
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	8	0.19
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	14	0.19
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	14	0.19
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE1	15	0.19
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE2	15	0.19
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE1	15	0.19
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE2	15	0.19
(1,787)	1:A:83:THR:H	1:A:85:ARG:HD3	18	0.19
(1,721)	1:A:78:THR:H	1:A:16:THR:HA	9	0.19
(1,701)	1:A:74:MET:H	1:A:73:GLN:HE21	18	0.19
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	12	0.19
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	12	0.19
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	1	0.19
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	4	0.19
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	5	0.19
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	9	0.19
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	20	0.19
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	12	0.19
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG21	6	0.19
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG22	6	0.19
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG23	6	0.19
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE1	9	0.19
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE2	9	0.19
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE3	9	0.19
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	16	0.18
(1,924)	1:A:38:MET:HE1	1:A:81:ASP:HB2	11	0.18
(1,924)	1:A:38:MET:HE2	1:A:81:ASP:HB2	11	0.18
(1,924)	1:A:38:MET:HE3	1:A:81:ASP:HB2	11	0.18
(1,917)	1:A:38:MET:HE1	1:A:35:VAL:HB	5	0.18
(1,917)	1:A:38:MET:HE2	1:A:35:VAL:HB	5	0.18
(1,917)	1:A:38:MET:HE3	1:A:35:VAL:HB	5	0.18
(1,865)	1:A:9:LEU:HD11	1:A:7:ASN:HD22	1	0.18
(1,865)	1:A:9:LEU:HD12	1:A:7:ASN:HD22	1	0.18
(1,865)	1:A:9:LEU:HD13	1:A:7:ASN:HD22	1	0.18
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG21	18	0.18
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG22	18	0.18
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG23	18	0.18
(1,701)	1:A:74:MET:H	1:A:73:GLN:HE21	14	0.18
(1,648)	1:A:69:ALA:H	1:A:65:ASN:H	19	0.18
(1,645)	1:A:69:ALA:H	1:A:18:ALA:H	11	0.18
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	2	0.18
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	2	0.18
(1,439)	1:A:46:ARG:H	1:A:50:ILE:HB	11	0.18
(1,423)	1:A:45:SER:H	1:A:50:ILE:HB	9	0.18
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	17	0.18
(1,338)	1:A:37:VAL:H	1:A:80:ILE:HD11	12	0.18
(1,338)	1:A:37:VAL:H	1:A:80:ILE:HD12	12	0.18
(1,338)	1:A:37:VAL:H	1:A:80:ILE:HD13	12	0.18
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	17	0.18
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	19	0.18
(1,292)	1:A:33:GLU:H	1:A:34:ILE:HG12	11	0.18
(1,292)	1:A:33:GLU:H	1:A:34:ILE:HG13	11	0.18
(1,243)	1:A:27:ASP:H	1:A:30:GLN:HG2	3	0.18
(1,243)	1:A:27:ASP:H	1:A:30:GLN:HG3	3	0.18
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG21	4	0.18
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG22	4	0.18
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG23	4	0.18
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	10	0.17
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	10	0.17
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	15	0.17
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	15	0.17
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	18	0.17
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	18	0.17
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	1	0.17
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	1	0.17
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	1:A:35:VAL:HG11	1:A:64:LEU:HG	18	0.17
(1,913)	1:A:35:VAL:HG12	1:A:64:LEU:HG	18	0.17
(1,913)	1:A:35:VAL:HG13	1:A:64:LEU:HG	18	0.17
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE1	6	0.17
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE2	6	0.17
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE1	6	0.17
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE2	6	0.17
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE1	17	0.17
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE2	17	0.17
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE1	17	0.17
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE2	17	0.17
(1,882)	1:A:15:ILE:HD11	1:A:75:LEU:HA	15	0.17
(1,882)	1:A:15:ILE:HD12	1:A:75:LEU:HA	15	0.17
(1,882)	1:A:15:ILE:HD13	1:A:75:LEU:HA	15	0.17
(1,882)	1:A:15:ILE:HD11	1:A:75:LEU:HA	19	0.17
(1,882)	1:A:15:ILE:HD12	1:A:75:LEU:HA	19	0.17
(1,882)	1:A:15:ILE:HD13	1:A:75:LEU:HA	19	0.17
(1,875)	1:A:13:THR:HG21	1:A:9:LEU:H	13	0.17
(1,875)	1:A:13:THR:HG22	1:A:9:LEU:H	13	0.17
(1,875)	1:A:13:THR:HG23	1:A:9:LEU:H	13	0.17
(1,875)	1:A:13:THR:HG21	1:A:9:LEU:H	18	0.17
(1,875)	1:A:13:THR:HG22	1:A:9:LEU:H	18	0.17
(1,875)	1:A:13:THR:HG23	1:A:9:LEU:H	18	0.17
(1,789)	1:A:83:THR:H	1:A:87:ILE:H	20	0.17
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG21	10	0.17
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG22	10	0.17
(1,747)	1:A:80:ILE:H	1:A:60:VAL:HG23	10	0.17
(1,701)	1:A:74:MET:H	1:A:73:GLN:HE21	7	0.17
(1,684)	1:A:71:ASP:H	1:A:70:LYS:HE2	10	0.17
(1,684)	1:A:71:ASP:H	1:A:70:LYS:HE3	10	0.17
(1,648)	1:A:69:ALA:H	1:A:65:ASN:H	10	0.17
(1,565)	1:A:62:GLU:H	1:A:63:LYS:HG2	11	0.17
(1,565)	1:A:62:GLU:H	1:A:63:LYS:HG3	11	0.17
(1,522)	1:A:57:SER:H	1:A:53:SER:HA	6	0.17
(1,488)	1:A:51:GLU:H	1:A:53:SER:H	9	0.17
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	11	0.17
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	11	0.17
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	14	0.17
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	14	0.17
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	16	0.17
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	16	0.17
(1,422)	1:A:45:SER:H	1:A:47:ASP:HB2	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH11	4	0.17
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH12	4	0.17
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH21	4	0.17
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH22	4	0.17
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	2	0.17
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG21	5	0.17
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG22	5	0.17
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG23	5	0.17
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE1	2	0.17
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE2	2	0.17
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE3	2	0.17
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG21	3	0.17
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG22	3	0.17
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG23	3	0.17
(1,1022)	1:A:84:MET:HE1	1:A:88:GLY:HA2	3	0.17
(1,1022)	1:A:84:MET:HE2	1:A:88:GLY:HA2	3	0.17
(1,1022)	1:A:84:MET:HE3	1:A:88:GLY:HA2	3	0.17
(1,943)	1:A:48:LEU:HD11	1:A:46:ARG:HA	8	0.16
(1,943)	1:A:48:LEU:HD12	1:A:46:ARG:HA	8	0.16
(1,943)	1:A:48:LEU:HD13	1:A:46:ARG:HA	8	0.16
(1,943)	1:A:48:LEU:HD21	1:A:46:ARG:HA	8	0.16
(1,943)	1:A:48:LEU:HD22	1:A:46:ARG:HA	8	0.16
(1,943)	1:A:48:LEU:HD23	1:A:46:ARG:HA	8	0.16
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	12	0.16
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	12	0.16
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	12	0.16
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	14	0.16
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	14	0.16
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	14	0.16
(1,896)	1:A:23:MET:HE1	1:A:30:GLN:H	3	0.16
(1,896)	1:A:23:MET:HE2	1:A:30:GLN:H	3	0.16
(1,896)	1:A:23:MET:HE3	1:A:30:GLN:H	3	0.16
(1,887)	1:A:16:THR:HG21	1:A:68:CYS:HA	6	0.16
(1,887)	1:A:16:THR:HG22	1:A:68:CYS:HA	6	0.16
(1,887)	1:A:16:THR:HG23	1:A:68:CYS:HA	6	0.16
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE1	8	0.16
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE2	8	0.16
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE1	8	0.16
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE2	8	0.16
(1,846)	1:A:89:LYS:H	1:A:87:ILE:HB	7	0.16
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE1	11	0.16
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE2	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE3	11	0.16
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE1	15	0.16
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE2	15	0.16
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE3	15	0.16
(1,790)	1:A:84:MET:H	1:A:43:VAL:HG11	17	0.16
(1,790)	1:A:84:MET:H	1:A:43:VAL:HG12	17	0.16
(1,790)	1:A:84:MET:H	1:A:43:VAL:HG13	17	0.16
(1,789)	1:A:83:THR:H	1:A:87:ILE:H	9	0.16
(1,776)	1:A:83:THR:H	1:A:64:LEU:HB2	9	0.16
(1,776)	1:A:83:THR:H	1:A:64:LEU:HB2	12	0.16
(1,701)	1:A:74:MET:H	1:A:73:GLN:HE21	12	0.16
(1,648)	1:A:69:ALA:H	1:A:65:ASN:H	11	0.16
(1,620)	1:A:67:VAL:H	1:A:65:ASN:HB2	5	0.16
(1,597)	1:A:65:ASN:H	1:A:66:GLN:HE22	4	0.16
(1,425)	1:A:45:SER:H	1:A:84:MET:HB2	20	0.16
(1,425)	1:A:45:SER:H	1:A:84:MET:HB3	20	0.16
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	18	0.16
(1,120)	1:A:16:THR:H	1:A:20:ALA:HA	4	0.16
(1,120)	1:A:16:THR:H	1:A:20:ALA:HA	20	0.16
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG21	9	0.16
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG22	9	0.16
(1,113)	1:A:15:ILE:H	1:A:16:THR:HG23	9	0.16
(1,1031)	1:A:87:ILE:HD11	1:A:50:ILE:HB	11	0.16
(1,1031)	1:A:87:ILE:HD12	1:A:50:ILE:HB	11	0.16
(1,1031)	1:A:87:ILE:HD13	1:A:50:ILE:HB	11	0.16
(1,980)	1:A:72:PRO:HD3	1:A:73:GLN:HE21	20	0.15
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	5	0.15
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	5	0.15
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	19	0.15
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	19	0.15
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	19	0.15
(1,882)	1:A:15:ILE:HD11	1:A:75:LEU:HA	9	0.15
(1,882)	1:A:15:ILE:HD12	1:A:75:LEU:HA	9	0.15
(1,882)	1:A:15:ILE:HD13	1:A:75:LEU:HA	9	0.15
(1,875)	1:A:13:THR:HG21	1:A:9:LEU:H	7	0.15
(1,875)	1:A:13:THR:HG22	1:A:9:LEU:H	7	0.15
(1,875)	1:A:13:THR:HG23	1:A:9:LEU:H	7	0.15
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD11	14	0.15
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD12	14	0.15
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD13	14	0.15
(1,789)	1:A:83:THR:H	1:A:87:ILE:H	8	0.15
(1,789)	1:A:83:THR:H	1:A:87:ILE:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:A:78:THR:H	1:A:16:THR:HA	3	0.15
(1,701)	1:A:74:MET:H	1:A:73:GLN:HE21	10	0.15
(1,65)	1:A:11:SER:H	1:A:12:GLU:HG2	15	0.15
(1,65)	1:A:11:SER:H	1:A:12:GLU:HG3	15	0.15
(1,648)	1:A:69:ALA:H	1:A:65:ASN:H	6	0.15
(1,620)	1:A:67:VAL:H	1:A:65:ASN:HB2	3	0.15
(1,575)	1:A:63:LYS:H	1:A:83:THR:HG21	14	0.15
(1,575)	1:A:63:LYS:H	1:A:83:THR:HG22	14	0.15
(1,575)	1:A:63:LYS:H	1:A:83:THR:HG23	14	0.15
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	13	0.15
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	13	0.15
(1,439)	1:A:46:ARG:H	1:A:50:ILE:HB	13	0.15
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	3	0.15
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	11	0.15
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG21	10	0.15
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG22	10	0.15
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG23	10	0.15
(1,304)	1:A:35:VAL:H	1:A:31:VAL:H	4	0.15
(1,304)	1:A:35:VAL:H	1:A:31:VAL:H	19	0.15
(1,215)	1:A:25:LYS:H	1:A:27:ASP:HB2	1	0.15
(1,120)	1:A:16:THR:H	1:A:20:ALA:HA	1	0.15
(1,1019)	1:A:84:MET:HE1	1:A:83:THR:H	13	0.15
(1,1019)	1:A:84:MET:HE2	1:A:83:THR:H	13	0.15
(1,1019)	1:A:84:MET:HE3	1:A:83:THR:H	13	0.15
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	4	0.14
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	4	0.14
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	11	0.14
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	11	0.14
(1,924)	1:A:38:MET:HE1	1:A:81:ASP:HB2	14	0.14
(1,924)	1:A:38:MET:HE2	1:A:81:ASP:HB2	14	0.14
(1,924)	1:A:38:MET:HE3	1:A:81:ASP:HB2	14	0.14
(1,907)	1:A:32:ALA:HB1	1:A:58:ALA:H	20	0.14
(1,907)	1:A:32:ALA:HB2	1:A:58:ALA:H	20	0.14
(1,907)	1:A:32:ALA:HB3	1:A:58:ALA:H	20	0.14
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE1	16	0.14
(1,884)	1:A:15:ILE:HG12	1:A:14:TYR:HE2	16	0.14
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE1	16	0.14
(1,884)	1:A:15:ILE:HG13	1:A:14:TYR:HE2	16	0.14
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD11	20	0.14
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD12	20	0.14
(1,847)	1:A:89:LYS:H	1:A:87:ILE:HD13	20	0.14
(1,684)	1:A:71:ASP:H	1:A:70:LYS:HE2	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:A:71:ASP:H	1:A:70:LYS:HE3	18	0.14
(1,675)	1:A:71:ASP:H	1:A:67:VAL:HB	14	0.14
(1,66)	1:A:11:SER:H	1:A:13:THR:HG1	11	0.14
(1,66)	1:A:11:SER:H	1:A:13:THR:HG21	11	0.14
(1,66)	1:A:11:SER:H	1:A:13:THR:HG22	11	0.14
(1,66)	1:A:11:SER:H	1:A:13:THR:HG23	11	0.14
(1,648)	1:A:69:ALA:H	1:A:65:ASN:H	4	0.14
(1,648)	1:A:69:ALA:H	1:A:65:ASN:H	12	0.14
(1,620)	1:A:67:VAL:H	1:A:65:ASN:HB2	12	0.14
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	6	0.14
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	6	0.14
(1,439)	1:A:46:ARG:H	1:A:50:ILE:HB	15	0.14
(1,425)	1:A:45:SER:H	1:A:84:MET:HB2	15	0.14
(1,425)	1:A:45:SER:H	1:A:84:MET:HB3	15	0.14
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	6	0.14
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	19	0.14
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG21	3	0.14
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG22	3	0.14
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG23	3	0.14
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG21	12	0.14
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG22	12	0.14
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG23	12	0.14
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG21	20	0.14
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG22	20	0.14
(1,325)	1:A:36:ALA:H	1:A:80:ILE:HG23	20	0.14
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	2	0.14
(1,302)	1:A:34:ILE:H	1:A:35:VAL:HB	8	0.14
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	4	0.14
(1,190)	1:A:23:MET:H	1:A:25:LYS:HD2	4	0.14
(1,190)	1:A:23:MET:H	1:A:25:LYS:HD3	4	0.14
(1,120)	1:A:16:THR:H	1:A:20:ALA:HA	11	0.14
(1,120)	1:A:16:THR:H	1:A:20:ALA:HA	18	0.14
(1,102)	1:A:15:ILE:H	1:A:11:SER:HB2	5	0.14
(1,996)	1:A:79:ALA:HB1	1:A:64:LEU:HD11	8	0.13
(1,996)	1:A:79:ALA:HB1	1:A:64:LEU:HD12	8	0.13
(1,996)	1:A:79:ALA:HB1	1:A:64:LEU:HD13	8	0.13
(1,996)	1:A:79:ALA:HB1	1:A:64:LEU:HD21	8	0.13
(1,996)	1:A:79:ALA:HB1	1:A:64:LEU:HD22	8	0.13
(1,996)	1:A:79:ALA:HB1	1:A:64:LEU:HD23	8	0.13
(1,996)	1:A:79:ALA:HB2	1:A:64:LEU:HD11	8	0.13
(1,996)	1:A:79:ALA:HB2	1:A:64:LEU:HD12	8	0.13
(1,996)	1:A:79:ALA:HB2	1:A:64:LEU:HD13	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,996)	1:A:79:ALA:HB2	1:A:64:LEU:HD21	8	0.13
(1,996)	1:A:79:ALA:HB2	1:A:64:LEU:HD22	8	0.13
(1,996)	1:A:79:ALA:HB2	1:A:64:LEU:HD23	8	0.13
(1,996)	1:A:79:ALA:HB3	1:A:64:LEU:HD11	8	0.13
(1,996)	1:A:79:ALA:HB3	1:A:64:LEU:HD12	8	0.13
(1,996)	1:A:79:ALA:HB3	1:A:64:LEU:HD13	8	0.13
(1,996)	1:A:79:ALA:HB3	1:A:64:LEU:HD21	8	0.13
(1,996)	1:A:79:ALA:HB3	1:A:64:LEU:HD22	8	0.13
(1,996)	1:A:79:ALA:HB3	1:A:64:LEU:HD23	8	0.13
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	6	0.13
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	6	0.13
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	12	0.13
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	12	0.13
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE1	17	0.13
(1,98)	1:A:14:TYR:H	1:A:14:TYR:HE2	17	0.13
(1,943)	1:A:48:LEU:HD11	1:A:46:ARG:HA	10	0.13
(1,943)	1:A:48:LEU:HD12	1:A:46:ARG:HA	10	0.13
(1,943)	1:A:48:LEU:HD13	1:A:46:ARG:HA	10	0.13
(1,943)	1:A:48:LEU:HD21	1:A:46:ARG:HA	10	0.13
(1,943)	1:A:48:LEU:HD22	1:A:46:ARG:HA	10	0.13
(1,943)	1:A:48:LEU:HD23	1:A:46:ARG:HA	10	0.13
(1,937)	1:A:44:ALA:HB1	1:A:49:LYS:H	4	0.13
(1,937)	1:A:44:ALA:HB2	1:A:49:LYS:H	4	0.13
(1,937)	1:A:44:ALA:HB3	1:A:49:LYS:H	4	0.13
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	9	0.13
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	9	0.13
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	9	0.13
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	15	0.13
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	15	0.13
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	15	0.13
(1,897)	1:A:23:MET:HE1	1:A:30:GLN:HE21	6	0.13
(1,897)	1:A:23:MET:HE2	1:A:30:GLN:HE21	6	0.13
(1,897)	1:A:23:MET:HE3	1:A:30:GLN:HE21	6	0.13
(1,882)	1:A:15:ILE:HD11	1:A:75:LEU:HA	10	0.13
(1,882)	1:A:15:ILE:HD12	1:A:75:LEU:HA	10	0.13
(1,882)	1:A:15:ILE:HD13	1:A:75:LEU:HA	10	0.13
(1,875)	1:A:13:THR:HG21	1:A:9:LEU:H	19	0.13
(1,875)	1:A:13:THR:HG22	1:A:9:LEU:H	19	0.13
(1,875)	1:A:13:THR:HG23	1:A:9:LEU:H	19	0.13
(1,865)	1:A:9:LEU:HD11	1:A:7:ASN:HD22	9	0.13
(1,865)	1:A:9:LEU:HD12	1:A:7:ASN:HD22	9	0.13
(1,865)	1:A:9:LEU:HD13	1:A:7:ASN:HD22	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,853)	1:A:90:LYS:H	1:A:88:GLY:HA3	16	0.13
(1,818)	1:A:85:ARG:H	1:A:87:ILE:HD11	19	0.13
(1,818)	1:A:85:ARG:H	1:A:87:ILE:HD12	19	0.13
(1,818)	1:A:85:ARG:H	1:A:87:ILE:HD13	19	0.13
(1,789)	1:A:83:THR:H	1:A:87:ILE:H	1	0.13
(1,789)	1:A:83:THR:H	1:A:87:ILE:H	3	0.13
(1,725)	1:A:78:THR:H	1:A:76:LEU:HB3	12	0.13
(1,684)	1:A:71:ASP:H	1:A:70:LYS:HE2	1	0.13
(1,684)	1:A:71:ASP:H	1:A:70:LYS:HE3	1	0.13
(1,648)	1:A:69:ALA:H	1:A:65:ASN:H	8	0.13
(1,648)	1:A:69:ALA:H	1:A:65:ASN:H	13	0.13
(1,620)	1:A:67:VAL:H	1:A:65:ASN:HB2	13	0.13
(1,613)	1:A:67:VAL:H	1:A:70:LYS:HD2	8	0.13
(1,613)	1:A:67:VAL:H	1:A:70:LYS:HD3	8	0.13
(1,597)	1:A:65:ASN:H	1:A:66:GLN:HE22	10	0.13
(1,565)	1:A:62:GLU:H	1:A:63:LYS:HG2	9	0.13
(1,565)	1:A:62:GLU:H	1:A:63:LYS:HG3	9	0.13
(1,439)	1:A:46:ARG:H	1:A:50:ILE:HB	14	0.13
(1,425)	1:A:45:SER:H	1:A:84:MET:HB2	9	0.13
(1,425)	1:A:45:SER:H	1:A:84:MET:HB3	9	0.13
(1,422)	1:A:45:SER:H	1:A:47:ASP:HB2	5	0.13
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH11	19	0.13
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH12	19	0.13
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH21	19	0.13
(1,420)	1:A:45:SER:H	1:A:46:ARG:HH22	19	0.13
(1,398)	1:A:43:VAL:H	1:A:40:ASN:HB3	9	0.13
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD11	1	0.13
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD12	1	0.13
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD13	1	0.13
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD11	12	0.13
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD12	12	0.13
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD13	12	0.13
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	7	0.13
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	20	0.13
(1,338)	1:A:37:VAL:H	1:A:80:ILE:HD11	17	0.13
(1,338)	1:A:37:VAL:H	1:A:80:ILE:HD12	17	0.13
(1,338)	1:A:37:VAL:H	1:A:80:ILE:HD13	17	0.13
(1,304)	1:A:35:VAL:H	1:A:31:VAL:H	6	0.13
(1,304)	1:A:35:VAL:H	1:A:31:VAL:H	13	0.13
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	1	0.13
(1,244)	1:A:28:SER:H	1:A:24:ALA:H	13	0.13
(1,192)	1:A:23:MET:H	1:A:21:ASN:HB2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG21	1	0.13
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG22	1	0.13
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG23	1	0.13
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG21	20	0.13
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG22	20	0.13
(1,159)	1:A:20:ALA:H	1:A:61:VAL:HG23	20	0.13
(1,136)	1:A:18:ALA:H	1:A:65:ASN:HB2	2	0.13
(1,120)	1:A:16:THR:H	1:A:20:ALA:HA	8	0.13
(1,1022)	1:A:84:MET:HE1	1:A:88:GLY:HA2	1	0.13
(1,1022)	1:A:84:MET:HE2	1:A:88:GLY:HA2	1	0.13
(1,1022)	1:A:84:MET:HE3	1:A:88:GLY:HA2	1	0.13
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE1	4	0.12
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE2	4	0.12
(1,953)	1:A:50:ILE:HD11	1:A:84:MET:HE3	4	0.12
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE1	4	0.12
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE2	4	0.12
(1,953)	1:A:50:ILE:HD12	1:A:84:MET:HE3	4	0.12
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE1	4	0.12
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE2	4	0.12
(1,953)	1:A:50:ILE:HD13	1:A:84:MET:HE3	4	0.12
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	10	0.12
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	10	0.12
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	10	0.12
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	16	0.12
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	16	0.12
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	16	0.12
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	17	0.12
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	17	0.12
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	17	0.12
(1,924)	1:A:38:MET:HE1	1:A:81:ASP:HB2	16	0.12
(1,924)	1:A:38:MET:HE2	1:A:81:ASP:HB2	16	0.12
(1,924)	1:A:38:MET:HE3	1:A:81:ASP:HB2	16	0.12
(1,865)	1:A:9:LEU:HD11	1:A:7:ASN:HD22	17	0.12
(1,865)	1:A:9:LEU:HD12	1:A:7:ASN:HD22	17	0.12
(1,865)	1:A:9:LEU:HD13	1:A:7:ASN:HD22	17	0.12
(1,853)	1:A:90:LYS:H	1:A:88:GLY:HA3	18	0.12
(1,776)	1:A:83:THR:H	1:A:64:LEU:HB2	1	0.12
(1,776)	1:A:83:THR:H	1:A:64:LEU:HB2	17	0.12
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE1	6	0.12
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE2	6	0.12
(1,773)	1:A:82:ASP:H	1:A:84:MET:HE3	6	0.12
(1,701)	1:A:74:MET:H	1:A:73:GLN:HE21	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,662)	1:A:70:LYS:H	1:A:66:GLN:HG2	18	0.12
(1,662)	1:A:70:LYS:H	1:A:66:GLN:HG3	18	0.12
(1,645)	1:A:69:ALA:H	1:A:18:ALA:H	19	0.12
(1,645)	1:A:69:ALA:H	1:A:18:ALA:H	20	0.12
(1,597)	1:A:65:ASN:H	1:A:66:GLN:HE22	20	0.12
(1,575)	1:A:63:LYS:H	1:A:83:THR:HG21	11	0.12
(1,575)	1:A:63:LYS:H	1:A:83:THR:HG22	11	0.12
(1,575)	1:A:63:LYS:H	1:A:83:THR:HG23	11	0.12
(1,522)	1:A:57:SER:H	1:A:53:SER:HA	19	0.12
(1,487)	1:A:51:GLU:H	1:A:52:GLN:HG2	13	0.12
(1,487)	1:A:51:GLU:H	1:A:52:GLN:HG3	13	0.12
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	15	0.12
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	15	0.12
(1,439)	1:A:46:ARG:H	1:A:50:ILE:HB	12	0.12
(1,427)	1:A:46:ARG:H	1:A:43:VAL:HB	14	0.12
(1,349)	1:A:38:MET:H	1:A:40:ASN:HB3	8	0.12
(1,304)	1:A:35:VAL:H	1:A:31:VAL:H	5	0.12
(1,304)	1:A:35:VAL:H	1:A:31:VAL:H	8	0.12
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG11	10	0.12
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG12	10	0.12
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG13	10	0.12
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG11	16	0.12
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG12	16	0.12
(1,286)	1:A:32:ALA:H	1:A:35:VAL:HG13	16	0.12
(1,243)	1:A:27:ASP:H	1:A:30:GLN:HG2	14	0.12
(1,243)	1:A:27:ASP:H	1:A:30:GLN:HG3	14	0.12
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE1	5	0.12
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE2	5	0.12
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE3	5	0.12
(1,136)	1:A:18:ALA:H	1:A:65:ASN:HB2	12	0.12
(1,100)	1:A:14:TYR:H	1:A:77:ILE:HD11	10	0.12
(1,100)	1:A:14:TYR:H	1:A:77:ILE:HD12	10	0.12
(1,100)	1:A:14:TYR:H	1:A:77:ILE:HD13	10	0.12
(1,981)	1:A:74:MET:HE1	1:A:71:ASP:HB2	3	0.11
(1,981)	1:A:74:MET:HE1	1:A:71:ASP:HB3	3	0.11
(1,981)	1:A:74:MET:HE2	1:A:71:ASP:HB2	3	0.11
(1,981)	1:A:74:MET:HE2	1:A:71:ASP:HB3	3	0.11
(1,981)	1:A:74:MET:HE3	1:A:71:ASP:HB2	3	0.11
(1,981)	1:A:74:MET:HE3	1:A:71:ASP:HB3	3	0.11
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	2	0.11
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	2	0.11
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	11	0.11
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	11	0.11
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	11	0.11
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	18	0.11
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	18	0.11
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	18	0.11
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB1	20	0.11
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB2	20	0.11
(1,927)	1:A:40:ASN:HD21	1:A:44:ALA:HB3	20	0.11
(1,907)	1:A:32:ALA:HB1	1:A:58:ALA:H	10	0.11
(1,907)	1:A:32:ALA:HB2	1:A:58:ALA:H	10	0.11
(1,907)	1:A:32:ALA:HB3	1:A:58:ALA:H	10	0.11
(1,887)	1:A:16:THR:HG21	1:A:68:CYS:HA	7	0.11
(1,887)	1:A:16:THR:HG22	1:A:68:CYS:HA	7	0.11
(1,887)	1:A:16:THR:HG23	1:A:68:CYS:HA	7	0.11
(1,887)	1:A:16:THR:HG21	1:A:68:CYS:HA	18	0.11
(1,887)	1:A:16:THR:HG22	1:A:68:CYS:HA	18	0.11
(1,887)	1:A:16:THR:HG23	1:A:68:CYS:HA	18	0.11
(1,882)	1:A:15:ILE:HD11	1:A:75:LEU:HA	7	0.11
(1,882)	1:A:15:ILE:HD12	1:A:75:LEU:HA	7	0.11
(1,882)	1:A:15:ILE:HD13	1:A:75:LEU:HA	7	0.11
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE1	19	0.11
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE2	19	0.11
(1,836)	1:A:88:GLY:H	1:A:84:MET:HE3	19	0.11
(1,789)	1:A:83:THR:H	1:A:87:ILE:H	13	0.11
(1,776)	1:A:83:THR:H	1:A:64:LEU:HB2	11	0.11
(1,74)	1:A:12:GLU:H	1:A:15:ILE:HG21	8	0.11
(1,74)	1:A:12:GLU:H	1:A:15:ILE:HG22	8	0.11
(1,74)	1:A:12:GLU:H	1:A:15:ILE:HG23	8	0.11
(1,701)	1:A:74:MET:H	1:A:73:GLN:HE21	1	0.11
(1,675)	1:A:71:ASP:H	1:A:67:VAL:HB	5	0.11
(1,630)	1:A:68:CYS:H	1:A:18:ALA:H	9	0.11
(1,495)	1:A:53:SER:H	1:A:51:GLU:HG2	19	0.11
(1,495)	1:A:53:SER:H	1:A:51:GLU:HG3	19	0.11
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE2	18	0.11
(1,450)	1:A:47:ASP:H	1:A:49:LYS:HE3	18	0.11
(1,439)	1:A:46:ARG:H	1:A:50:ILE:HB	2	0.11
(1,439)	1:A:46:ARG:H	1:A:50:ILE:HB	6	0.11
(1,425)	1:A:45:SER:H	1:A:84:MET:HB2	3	0.11
(1,425)	1:A:45:SER:H	1:A:84:MET:HB3	3	0.11
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD11	4	0.11
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD12	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD13	4	0.11
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD11	9	0.11
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD12	9	0.11
(1,351)	1:A:38:MET:H	1:A:77:ILE:HD13	9	0.11
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE1	6	0.11
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE2	6	0.11
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE3	6	0.11
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE1	7	0.11
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE2	7	0.11
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE3	7	0.11
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE1	11	0.11
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE2	11	0.11
(1,157)	1:A:20:ALA:H	1:A:23:MET:HE3	11	0.11
(1,120)	1:A:16:THR:H	1:A:20:ALA:HA	5	0.11
(1,120)	1:A:16:THR:H	1:A:20:ALA:HA	16	0.11
(1,1022)	1:A:84:MET:HE1	1:A:88:GLY:HA2	17	0.11
(1,1022)	1:A:84:MET:HE2	1:A:88:GLY:HA2	17	0.11
(1,1022)	1:A:84:MET:HE3	1:A:88:GLY:HA2	17	0.11
(1,100)	1:A:14:TYR:H	1:A:77:ILE:HD11	1	0.11
(1,100)	1:A:14:TYR:H	1:A:77:ILE:HD12	1	0.11
(1,100)	1:A:14:TYR:H	1:A:77:ILE:HD13	1	0.11

10 Dihedral-angle violation analysis (i)

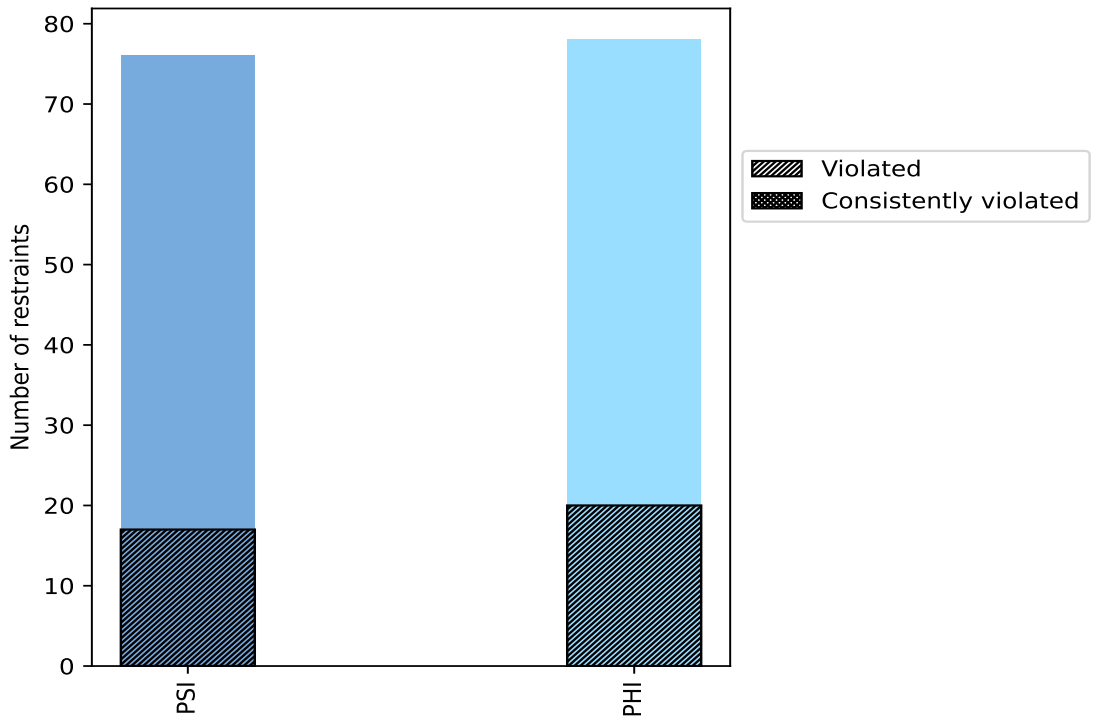
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	76	49.4	17	22.4	11.0	0	0.0	0.0
PHI	78	50.6	20	25.6	13.0	0	0.0	0.0
Total	154	100.0	37	24.0	24.0	0	0.0	0.0

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

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



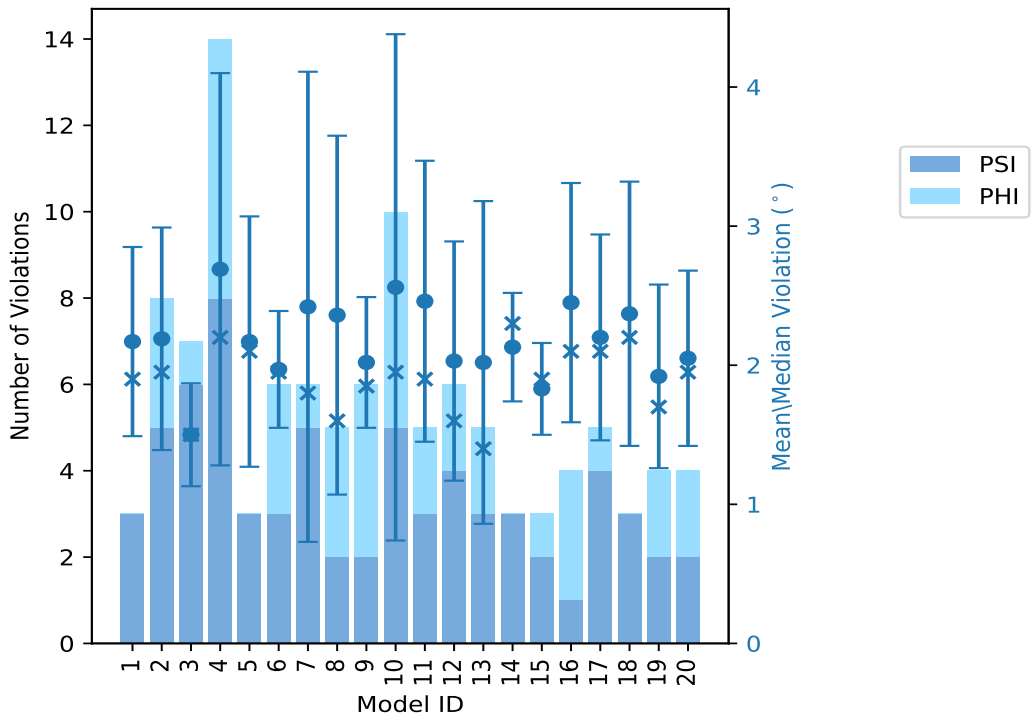
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	3	0	3	2.17	3.1	0.68	1.9
2	5	3	8	2.19	3.5	0.8	1.95
3	6	1	7	1.5	2.2	0.37	1.5
4	8	6	14	2.69	5.5	1.41	2.2
5	3	0	3	2.17	3.3	0.9	2.1
6	3	3	6	1.97	2.8	0.42	1.95
7	5	1	6	2.42	6.1	1.69	1.8
8	2	3	5	2.36	4.6	1.29	1.6
9	2	4	6	2.02	2.9	0.47	1.85
10	5	5	10	2.56	7.7	1.82	1.95
11	3	2	5	2.46	4.2	1.01	1.9
12	4	2	6	2.03	3.9	0.86	1.6
13	3	2	5	2.02	4.2	1.16	1.4
14	3	0	3	2.13	2.5	0.39	2.3
15	2	1	3	1.83	2.2	0.33	1.9
16	1	3	4	2.45	3.9	0.86	2.1
17	4	1	5	2.2	3.4	0.74	2.1
18	3	0	3	2.37	3.6	0.95	2.2
19	2	2	4	1.92	3.0	0.66	1.7
20	2	2	4	2.05	3.0	0.63	1.95

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
7	12	19	1	5.0
4	4	8	2	10.0
1	1	2	3	15.0
0	1	1	4	20.0
0	0	0	5	25.0
2	0	2	6	30.0
1	2	3	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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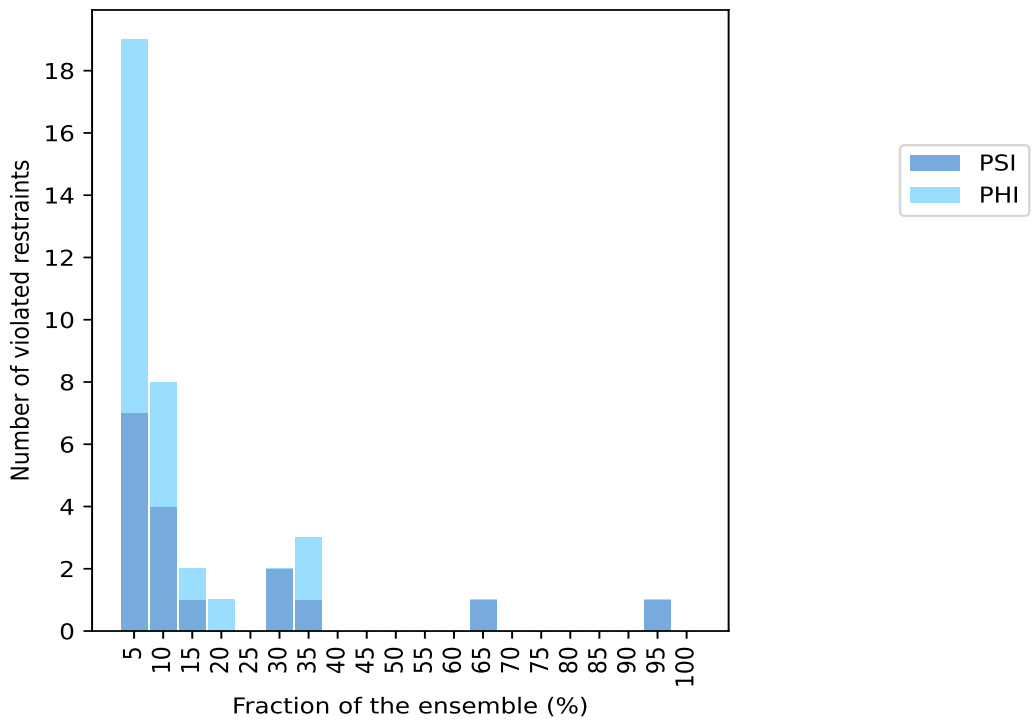
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
1	0	1	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
1	0	1	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

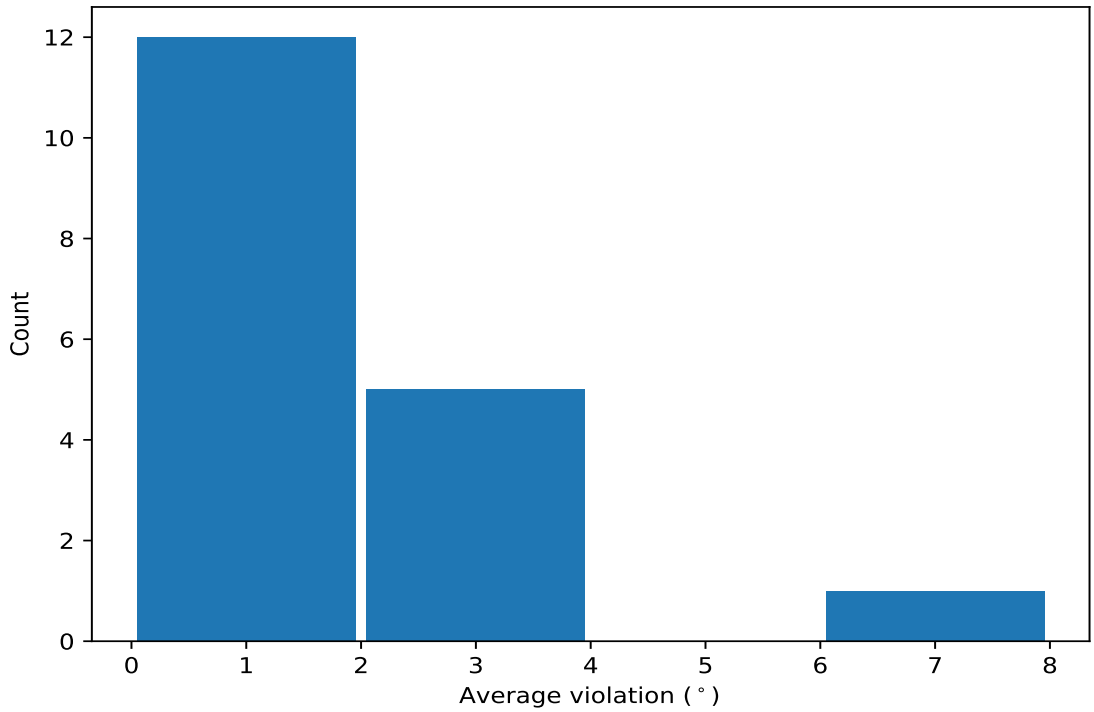


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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

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

in the ensemble



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

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

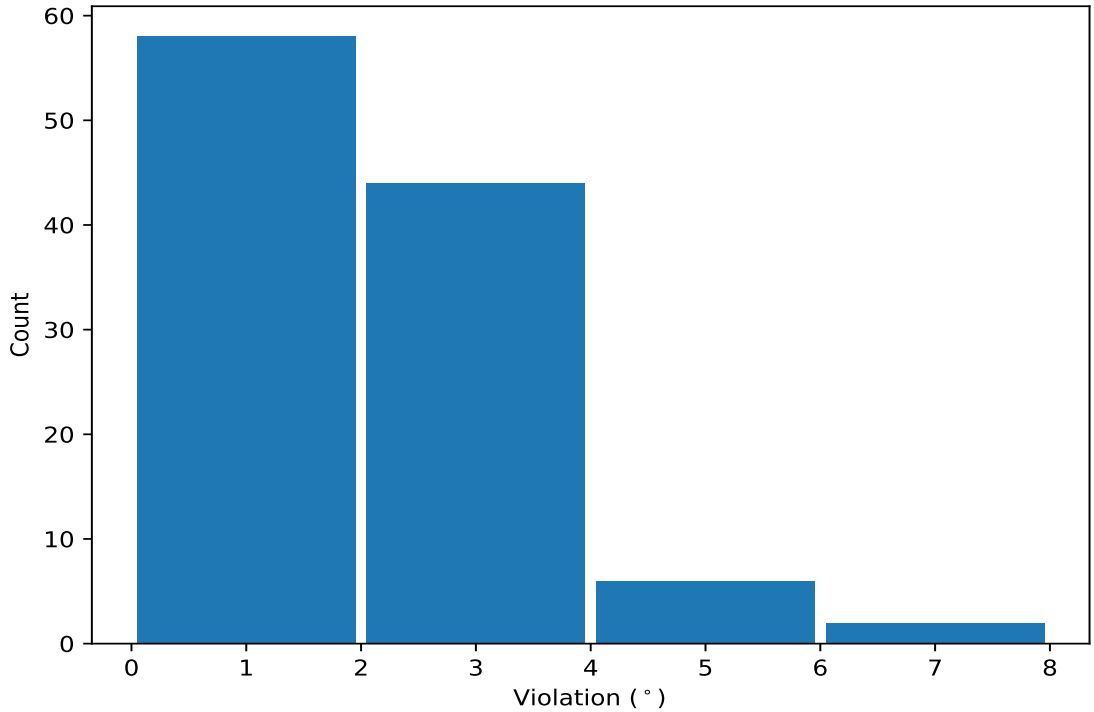
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	19	3.34	1.02	3.3
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	13	1.97	0.44	1.9
(1,82)	1:A:44:ALA:C	1:A:45:SER:N	1:A:45:SER:CA	1:A:45:SER:C	7	2.04	0.7	1.9
(1,81)	1:A:44:ALA:N	1:A:44:ALA:CA	1:A:44:ALA:C	1:A:45:SER:N	7	2.0	0.43	2.2
(1,107)	1:A:60:VAL:C	1:A:61:VAL:N	1:A:61:VAL:CA	1:A:61:VAL:C	7	1.63	0.39	1.6
(1,106)	1:A:60:VAL:N	1:A:60:VAL:CA	1:A:60:VAL:C	1:A:61:VAL:N	6	2.35	0.36	2.3
(1,31)	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	1:A:20:ALA:N	6	1.92	0.78	1.7
(1,111)	1:A:62:GLU:C	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	4	1.68	0.53	1.65
(1,14)	1:A:10:PRO:N	1:A:10:PRO:CA	1:A:10:PRO:C	1:A:11:SER:N	3	1.57	0.37	1.6
(1,101)	1:A:57:SER:C	1:A:58:ALA:N	1:A:58:ALA:CA	1:A:58:ALA:C	3	1.47	0.17	1.4
(1,114)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	2	6.5	1.2	6.5
(1,115)	1:A:64:LEU:C	1:A:65:ASN:N	1:A:65:ASN:CA	1:A:65:ASN:C	2	3.7	1.8	3.7
(1,121)	1:A:69:ALA:C	1:A:70:LYS:N	1:A:70:LYS:CA	1:A:70:LYS:C	2	1.9	0.0	1.9
(1,112)	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	1:A:64:LEU:N	2	1.75	0.05	1.75
(1,10)	1:A:7:ASN:N	1:A:7:ASN:CA	1:A:7:ASN:C	1:A:8:GLY:N	2	1.7	0.2	1.7
(1,109)	1:A:61:VAL:C	1:A:62:GLU:N	1:A:62:GLU:CA	1:A:62:GLU:C	2	1.5	0.2	1.5
(1,146)	1:A:84:MET:N	1:A:84:MET:CA	1:A:84:MET:C	1:A:85:ARG:N	2	1.5	0.2	1.5
(1,64)	1:A:35:VAL:C	1:A:36:ALA:N	1:A:36:ALA:CA	1:A:36:ALA:C	2	1.35	0.05	1.35

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,114)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	10	7.7
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	7	6.1
(1,115)	1:A:64:LEU:C	1:A:65:ASN:N	1:A:65:ASN:CA	1:A:65:ASN:C	4	5.5
(1,114)	1:A:64:LEU:N	1:A:64:LEU:CA	1:A:64:LEU:C	1:A:65:ASN:N	4	5.3
(1,116)	1:A:65:ASN:N	1:A:65:ASN:CA	1:A:65:ASN:C	1:A:66:GLN:N	4	4.9
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	8	4.6
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	11	4.2
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	13	4.2
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	12	3.9
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	16	3.9
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	18	3.6
(1,82)	1:A:44:ALA:C	1:A:45:SER:N	1:A:45:SER:CA	1:A:45:SER:C	10	3.5
(1,31)	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	1:A:20:ALA:N	2	3.5
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	2	3.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	17	3.4
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	5	3.3
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	1	3.1
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	19	3.0
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	20	3.0
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	11	3.0
(1,106)	1:A:60:VAL:N	1:A:60:VAL:CA	1:A:60:VAL:C	1:A:61:VAL:N	8	3.0
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	9	2.9
(1,84)	1:A:45:SER:C	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	4	2.9
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	6	2.8
(1,81)	1:A:44:ALA:N	1:A:44:ALA:CA	1:A:44:ALA:C	1:A:45:SER:N	17	2.6
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	14	2.5
(1,106)	1:A:60:VAL:N	1:A:60:VAL:CA	1:A:60:VAL:C	1:A:61:VAL:N	4	2.5
(1,82)	1:A:44:ALA:C	1:A:45:SER:N	1:A:45:SER:CA	1:A:45:SER:C	2	2.4
(1,81)	1:A:44:ALA:N	1:A:44:ALA:CA	1:A:44:ALA:C	1:A:45:SER:N	4	2.4
(1,117)	1:A:65:ASN:C	1:A:66:GLN:N	1:A:66:GLN:CA	1:A:66:GLN:C	10	2.4
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	4	2.3
(1,111)	1:A:62:GLU:C	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	16	2.3
(1,107)	1:A:60:VAL:C	1:A:61:VAL:N	1:A:61:VAL:CA	1:A:61:VAL:C	9	2.3
(1,106)	1:A:60:VAL:N	1:A:60:VAL:CA	1:A:60:VAL:C	1:A:61:VAL:N	7	2.3
(1,106)	1:A:60:VAL:N	1:A:60:VAL:CA	1:A:60:VAL:C	1:A:61:VAL:N	14	2.3
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	3	2.2
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	15	2.2
(1,81)	1:A:44:ALA:N	1:A:44:ALA:CA	1:A:44:ALA:C	1:A:45:SER:N	13	2.2
(1,81)	1:A:44:ALA:N	1:A:44:ALA:CA	1:A:44:ALA:C	1:A:45:SER:N	20	2.2
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	18	2.2
(1,106)	1:A:60:VAL:N	1:A:60:VAL:CA	1:A:60:VAL:C	1:A:61:VAL:N	10	2.2
(1,31)	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	1:A:20:ALA:N	12	2.1
(1,24)	1:A:15:ILE:N	1:A:15:ILE:CA	1:A:15:ILE:C	1:A:16:THR:N	17	2.1
(1,20)	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	1:A:14:TYR:N	5	2.1
(1,111)	1:A:62:GLU:C	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	4	2.1
(1,93)	1:A:53:SER:C	1:A:54:PRO:N	1:A:54:PRO:CA	1:A:54:PRO:C	6	2.0
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	4	2.0
(1,82)	1:A:44:ALA:C	1:A:45:SER:N	1:A:45:SER:CA	1:A:45:SER:C	4	2.0
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	9	2.0
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	10	2.0
(1,14)	1:A:10:PRO:N	1:A:10:PRO:CA	1:A:10:PRO:C	1:A:11:SER:N	6	2.0
(1,107)	1:A:60:VAL:C	1:A:61:VAL:N	1:A:61:VAL:CA	1:A:61:VAL:C	2	2.0
(1,82)	1:A:44:ALA:C	1:A:45:SER:N	1:A:45:SER:CA	1:A:45:SER:C	6	1.9
(1,82)	1:A:44:ALA:C	1:A:45:SER:N	1:A:45:SER:CA	1:A:45:SER:C	16	1.9
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	1	1.9
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	2	1.9
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	15	1.9
(1,31)	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	1:A:20:ALA:N	4	1.9
(1,121)	1:A:69:ALA:C	1:A:70:LYS:N	1:A:70:LYS:CA	1:A:70:LYS:C	11	1.9
(1,121)	1:A:69:ALA:C	1:A:70:LYS:N	1:A:70:LYS:CA	1:A:70:LYS:C	19	1.9
(1,115)	1:A:64:LEU:C	1:A:65:ASN:N	1:A:65:ASN:CA	1:A:65:ASN:C	10	1.9
(1,10)	1:A:7:ASN:N	1:A:7:ASN:CA	1:A:7:ASN:C	1:A:8:GLY:N	7	1.9
(1,112)	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	1:A:64:LEU:N	10	1.8
(1,106)	1:A:60:VAL:N	1:A:60:VAL:CA	1:A:60:VAL:C	1:A:61:VAL:N	3	1.8
(1,76)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	10	1.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,19)	1:A:12:GLU:C	1:A:13:THR:N	1:A:13:THR:CA	1:A:13:THR:C	9	1.7
(1,146)	1:A:84:MET:N	1:A:84:MET:CA	1:A:84:MET:C	1:A:85:ARG:N	7	1.7
(1,112)	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	1:A:64:LEU:N	11	1.7
(1,109)	1:A:61:VAL:C	1:A:62:GLU:N	1:A:62:GLU:CA	1:A:62:GLU:C	16	1.7
(1,107)	1:A:60:VAL:C	1:A:61:VAL:N	1:A:61:VAL:CA	1:A:61:VAL:C	20	1.7
(1,101)	1:A:57:SER:C	1:A:58:ALA:N	1:A:58:ALA:CA	1:A:58:ALA:C	9	1.7
(1,85)	1:A:46:ARG:N	1:A:46:ARG:CA	1:A:46:ARG:C	1:A:47:ASP:N	14	1.6
(1,81)	1:A:44:ALA:N	1:A:44:ALA:CA	1:A:44:ALA:C	1:A:45:SER:N	6	1.6
(1,81)	1:A:44:ALA:N	1:A:44:ALA:CA	1:A:44:ALA:C	1:A:45:SER:N	12	1.6
(1,44)	1:A:25:LYS:C	1:A:26:THR:N	1:A:26:THR:CA	1:A:26:THR:C	8	1.6
(1,14)	1:A:10:PRO:N	1:A:10:PRO:CA	1:A:10:PRO:C	1:A:11:SER:N	2	1.6
(1,107)	1:A:60:VAL:C	1:A:61:VAL:N	1:A:61:VAL:CA	1:A:61:VAL:C	12	1.6
(1,90)	1:A:51:GLU:N	1:A:51:GLU:CA	1:A:51:GLU:C	1:A:52:GLN:N	1	1.5
(1,89)	1:A:50:ILE:C	1:A:51:GLU:N	1:A:51:GLU:CA	1:A:51:GLU:C	9	1.5
(1,82)	1:A:44:ALA:C	1:A:45:SER:N	1:A:45:SER:CA	1:A:45:SER:C	8	1.5
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	3	1.5
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	12	1.5
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	17	1.5
(1,31)	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	1:A:20:ALA:N	19	1.5
(1,26)	1:A:16:THR:C	1:A:17:CYS:N	1:A:17:CYS:CA	1:A:17:CYS:C	12	1.5
(1,13)	1:A:9:LEU:C	1:A:10:PRO:N	1:A:10:PRO:CA	1:A:10:PRO:C	6	1.5
(1,107)	1:A:60:VAL:C	1:A:61:VAL:N	1:A:61:VAL:CA	1:A:61:VAL:C	11	1.5
(1,10)	1:A:7:ASN:N	1:A:7:ASN:CA	1:A:7:ASN:C	1:A:8:GLY:N	3	1.5
(1,81)	1:A:44:ALA:N	1:A:44:ALA:CA	1:A:44:ALA:C	1:A:45:SER:N	2	1.4
(1,67)	1:A:37:VAL:N	1:A:37:VAL:CA	1:A:37:VAL:C	1:A:38:MET:N	13	1.4
(1,64)	1:A:35:VAL:C	1:A:36:ALA:N	1:A:36:ALA:CA	1:A:36:ALA:C	17	1.4
(1,56)	1:A:31:VAL:C	1:A:32:ALA:N	1:A:32:ALA:CA	1:A:32:ALA:C	4	1.4
(1,101)	1:A:57:SER:C	1:A:58:ALA:N	1:A:58:ALA:CA	1:A:58:ALA:C	15	1.4
(1,69)	1:A:38:MET:N	1:A:38:MET:CA	1:A:38:MET:C	1:A:39:GLY:N	18	1.3
(1,64)	1:A:35:VAL:C	1:A:36:ALA:N	1:A:36:ALA:CA	1:A:36:ALA:C	2	1.3
(1,31)	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	1:A:20:ALA:N	3	1.3
(1,146)	1:A:84:MET:N	1:A:84:MET:CA	1:A:84:MET:C	1:A:85:ARG:N	4	1.3
(1,141)	1:A:81:ASP:C	1:A:82:ASP:N	1:A:82:ASP:CA	1:A:82:ASP:C	7	1.3
(1,109)	1:A:61:VAL:C	1:A:62:GLU:N	1:A:62:GLU:CA	1:A:62:GLU:C	19	1.3
(1,101)	1:A:57:SER:C	1:A:58:ALA:N	1:A:58:ALA:CA	1:A:58:ALA:C	20	1.3
(1,31)	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	1:A:20:ALA:N	10	1.2
(1,16)	1:A:11:SER:N	1:A:11:SER:CA	1:A:11:SER:C	1:A:12:GLU:N	7	1.2
(1,111)	1:A:62:GLU:C	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	10	1.2
(1,107)	1:A:60:VAL:C	1:A:61:VAL:N	1:A:61:VAL:CA	1:A:61:VAL:C	13	1.2
(1,86)	1:A:48:LEU:C	1:A:49:LYS:N	1:A:49:LYS:CA	1:A:49:LYS:C	3	1.1
(1,82)	1:A:44:ALA:C	1:A:45:SER:N	1:A:45:SER:CA	1:A:45:SER:C	13	1.1
(1,63)	1:A:35:VAL:N	1:A:35:VAL:CA	1:A:35:VAL:C	1:A:36:ALA:N	5	1.1
(1,14)	1:A:10:PRO:N	1:A:10:PRO:CA	1:A:10:PRO:C	1:A:11:SER:N	3	1.1
(1,111)	1:A:62:GLU:C	1:A:63:LYS:N	1:A:63:LYS:CA	1:A:63:LYS:C	8	1.1
(1,107)	1:A:60:VAL:C	1:A:61:VAL:N	1:A:61:VAL:CA	1:A:61:VAL:C	4	1.1