Full wwPDB NMR Structure Validation Report (i)

Jun 5, 2023 – 03:23 PM EDT

PDB ID	:	2M4K
BMRB ID	:	16912
Title	:	Solution structure of the delta subunit of RNA polymerase from Bacillus subtilis
Authors	:	Papouskova, V.; Novacek, J.; Kaderavek, P.; Zidek, L.; Rabatinova, A.; Sanderova, H.; Krasny, L.; Sklenar, V.
Deposited on	:	2013-02-07

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:

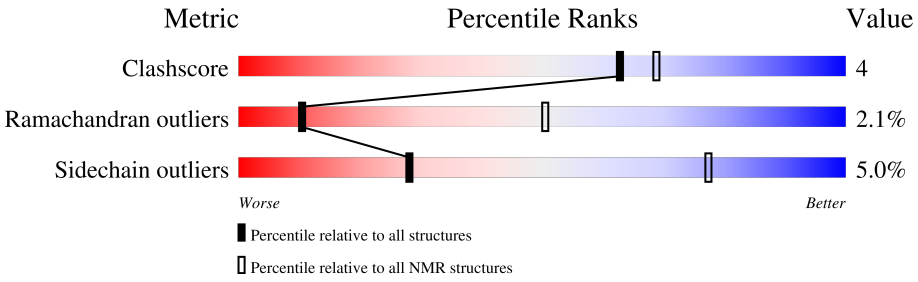
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 92%.

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	172	42% • • 53%

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:3-A:82 (80)	0.85	11

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1332 atoms, of which 663 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit delta.

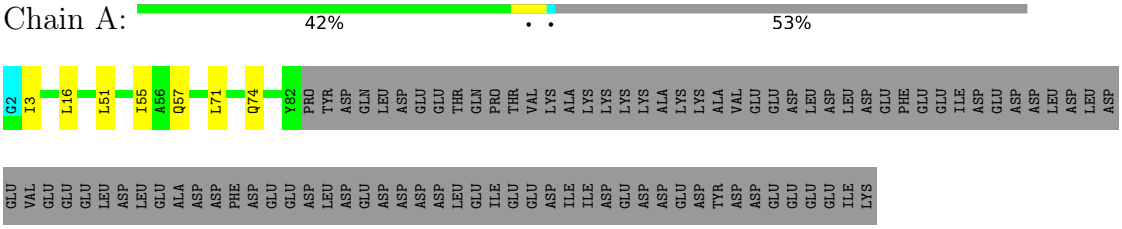
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	81	1332	432	663	109	127	1	0

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: DNA-directed RNA polymerase subunit delta

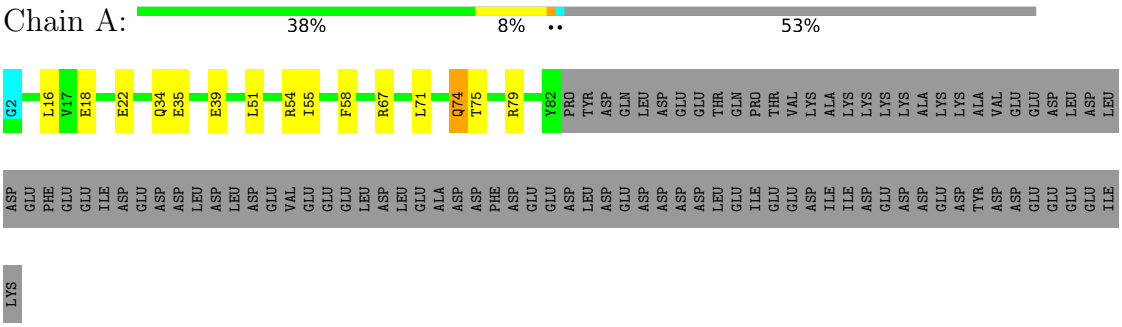


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

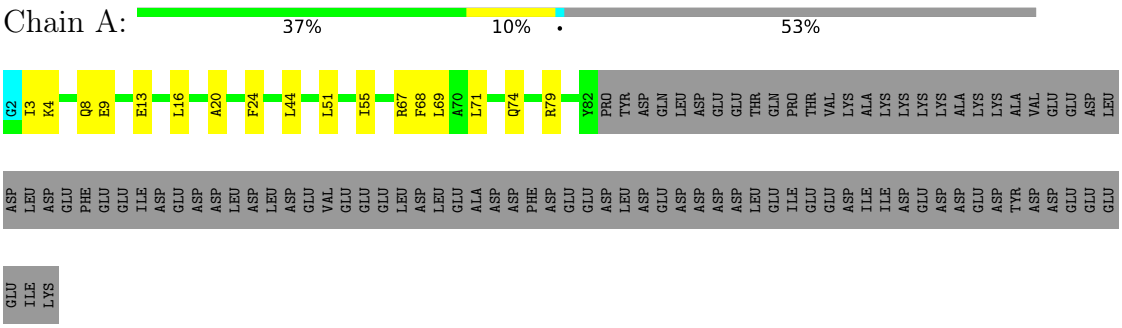
4.2.1 Score per residue for model 1

• Molecule 1: DNA-directed RNA polymerase subunit delta



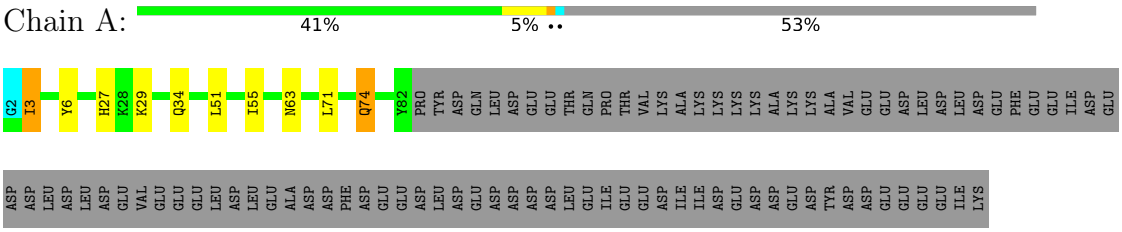
4.2.2 Score per residue for model 2

• Molecule 1: DNA-directed RNA polymerase subunit delta



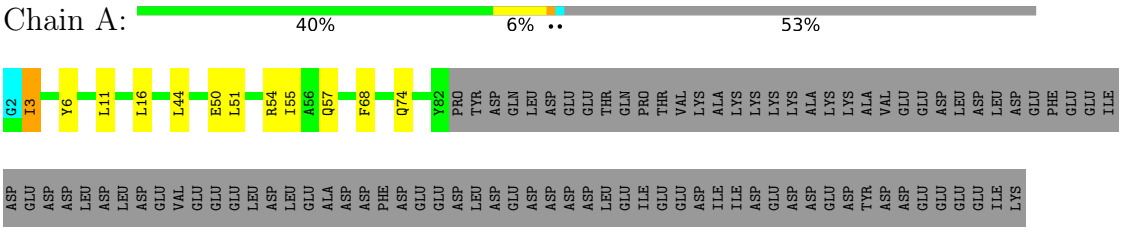
4.2.3 Score per residue for model 3

• Molecule 1: DNA-directed RNA polymerase subunit delta



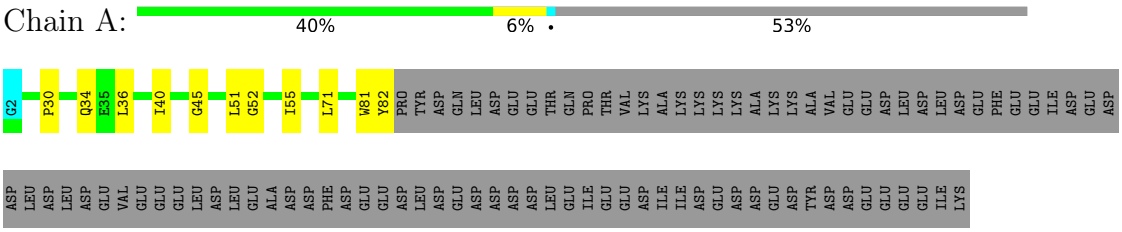
4.2.4 Score per residue for model 4

• Molecule 1: DNA-directed RNA polymerase subunit delta



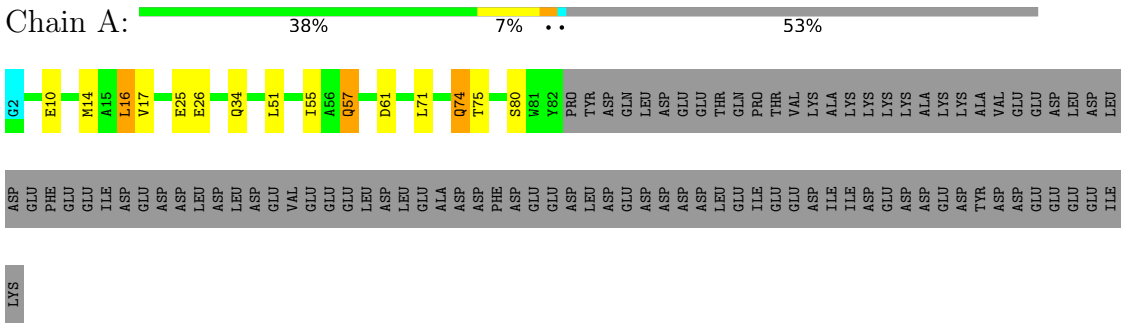
4.2.5 Score per residue for model 5

• Molecule 1: DNA-directed RNA polymerase subunit delta



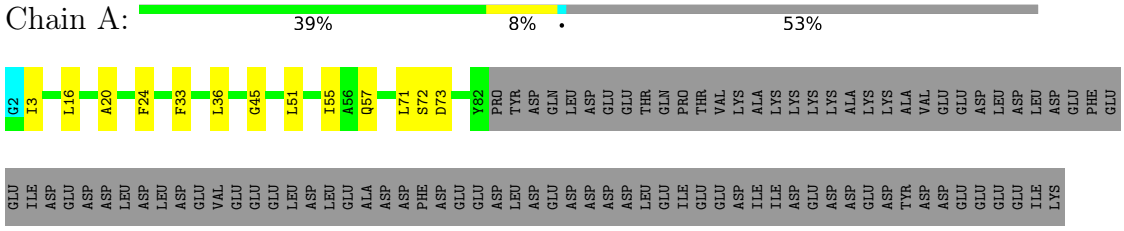
4.2.6 Score per residue for model 6

• Molecule 1: DNA-directed RNA polymerase subunit delta



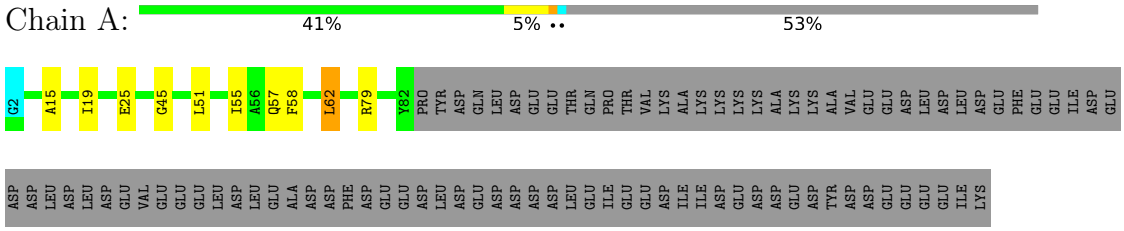
4.2.7 Score per residue for model 7

• Molecule 1: DNA-directed RNA polymerase subunit delta



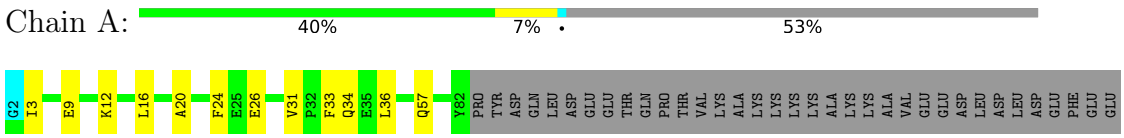
4.2.8 Score per residue for model 8

• Molecule 1: DNA-directed RNA polymerase subunit delta



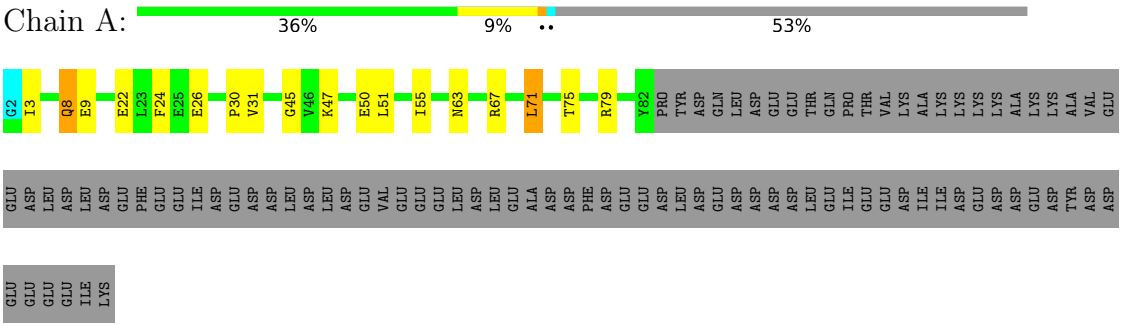
4.2.9 Score per residue for model 9

• Molecule 1: DNA-directed RNA polymerase subunit delta



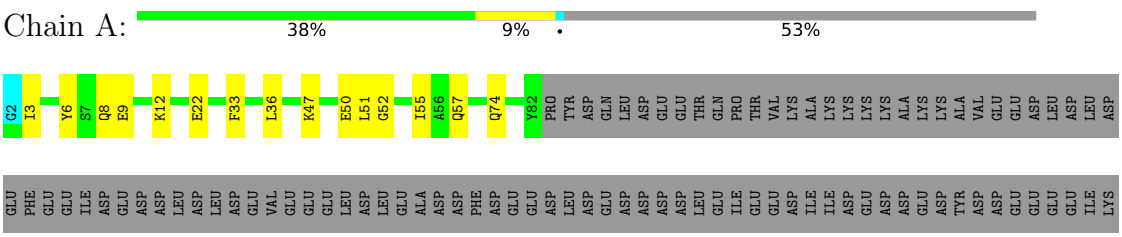
4.2.10 Score per residue for model 10

• Molecule 1: DNA-directed RNA polymerase subunit delta



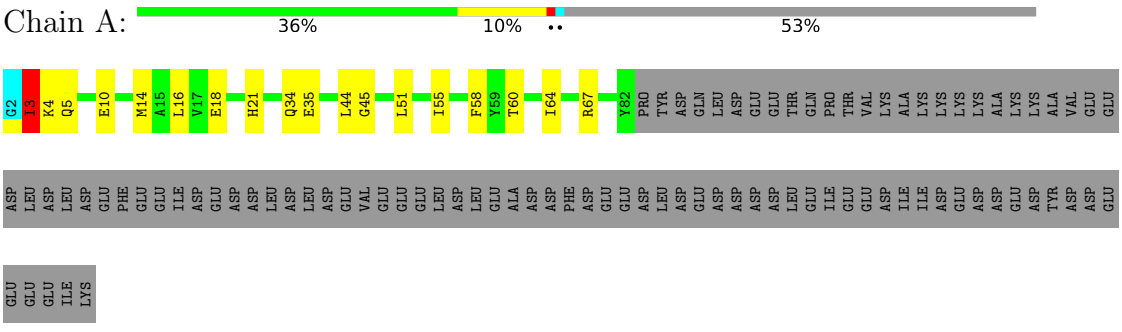
4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: DNA-directed RNA polymerase subunit delta



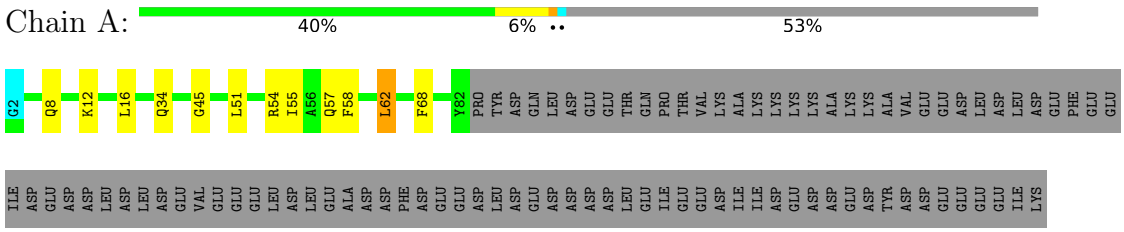
4.2.12 Score per residue for model 12

• Molecule 1: DNA-directed RNA polymerase subunit delta



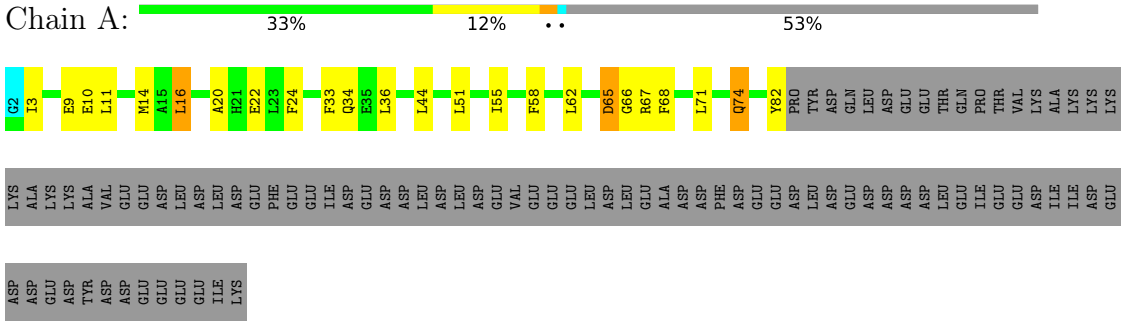
4.2.13 Score per residue for model 13

• Molecule 1: DNA-directed RNA polymerase subunit delta



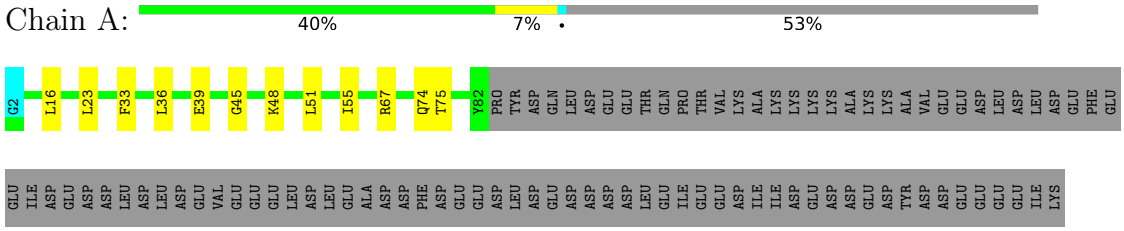
4.2.14 Score per residue for model 14

• Molecule 1: DNA-directed RNA polymerase subunit delta



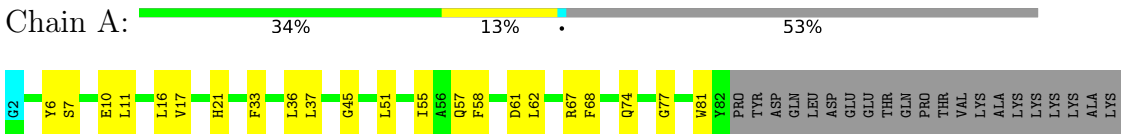
4.2.15 Score per residue for model 15

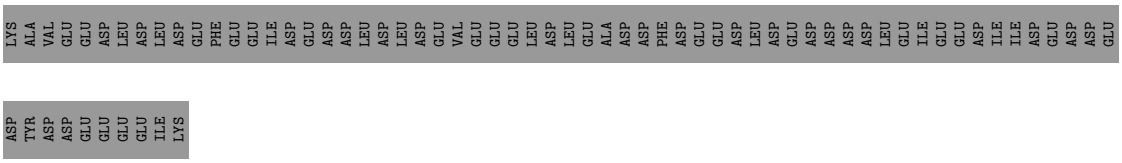
• Molecule 1: DNA-directed RNA polymerase subunit delta



4.2.16 Score per residue for model 16

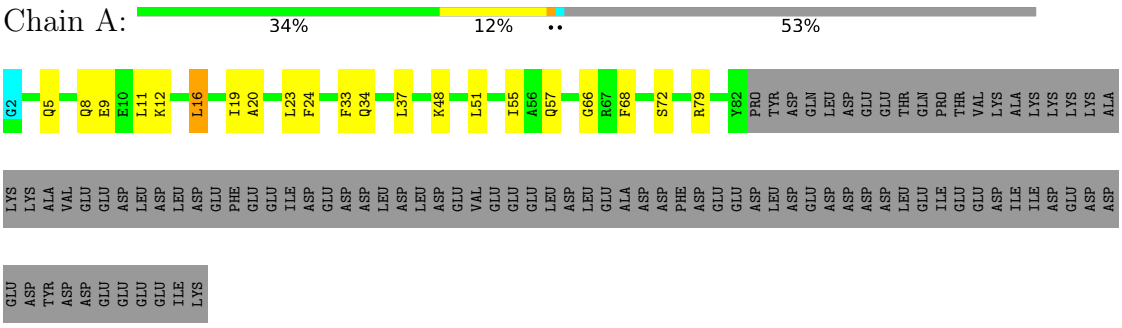
• Molecule 1: DNA-directed RNA polymerase subunit delta





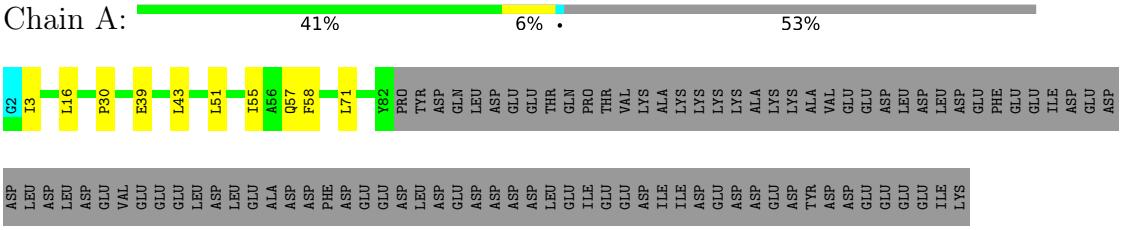
4.2.17 Score per residue for model 17

• Molecule 1: DNA-directed RNA polymerase subunit delta



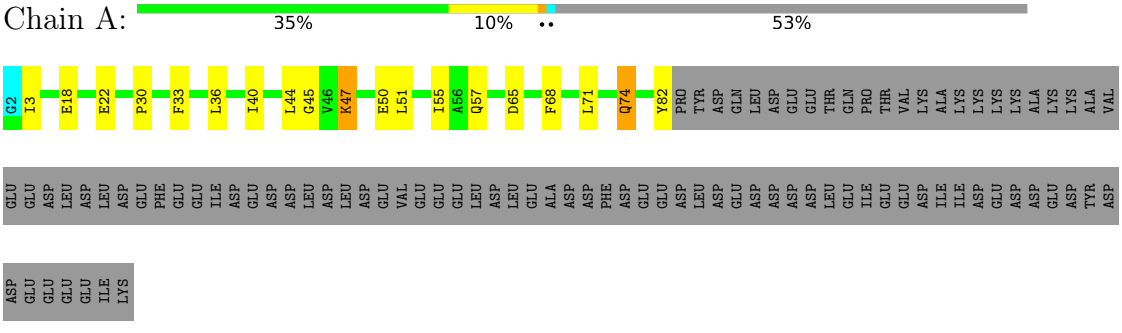
4.2.18 Score per residue for model 18

• Molecule 1: DNA-directed RNA polymerase subunit delta



4.2.19 Score per residue for model 19

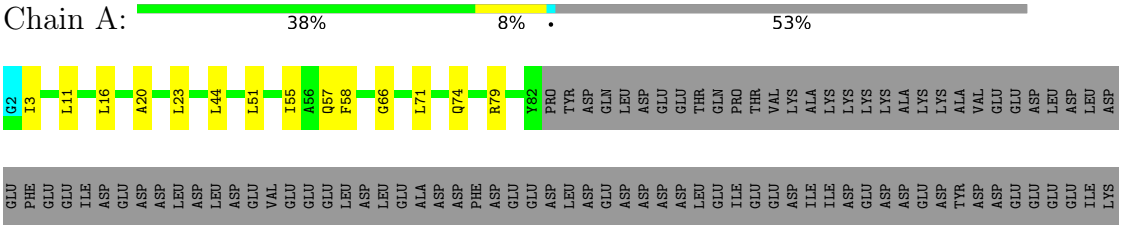
• Molecule 1: DNA-directed RNA polymerase subunit delta



4.2.20 Score per residue for model 20

• Molecule 1: DNA-directed RNA polymerase subunit delta

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	structure solution	
CNS	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	2126
Number of shifts mapped to atoms	1069
Number of unparsed shifts	0
Number of shifts with mapping errors	1057
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality

6.1 Standard geometry

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.4±0.7
All	All	0	8

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	67	ARG	Sidechain	5
1	A	79	ARG	Sidechain	3

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	665	658	656	6±2
All	All	13300	13160	13120	116

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:O	1:A:55:ILE:HG13	0.63	1.92	12	19
1:A:8:GLN:HB2	1:A:45:GLY:N	0.62	2.09	10	1
1:A:16:LEU:HG	1:A:58:PHE:CD1	0.60	2.31	12	3
1:A:16:LEU:H	1:A:16:LEU:HD23	0.56	1.61	14	9
1:A:9:GLU:O	1:A:13:GLU:HG2	0.55	2.01	2	1
1:A:3:ILE:H	1:A:3:ILE:HD13	0.54	1.61	3	1
1:A:8:GLN:HG3	1:A:44:LEU:O	0.54	2.03	2	1
1:A:17:VAL:HB	1:A:61:ASP:OD2	0.53	2.03	6	2
1:A:69:LEU:HD22	1:A:79:ARG:HA	0.52	1.81	2	1
1:A:30:PRO:HB3	1:A:71:LEU:CD1	0.52	2.34	18	4
1:A:3:ILE:HB	1:A:22:GLU:HB3	0.52	1.81	10	2
1:A:24:PHE:CE2	1:A:31:VAL:HB	0.51	2.41	9	2
1:A:3:ILE:HA	1:A:6:TYR:CE2	0.50	2.41	4	1
1:A:33:PHE:O	1:A:36:LEU:HG	0.50	2.06	11	7
1:A:35:GLU:O	1:A:39:GLU:HG2	0.50	2.06	1	1
1:A:58:PHE:O	1:A:62:LEU:HB2	0.50	2.07	13	2
1:A:58:PHE:O	1:A:62:LEU:HG	0.49	2.08	16	1
1:A:66:GLY:O	1:A:79:ARG:HD3	0.48	2.08	20	2
1:A:10:GLU:O	1:A:14:MET:HG2	0.48	2.08	6	1
1:A:50:GLU:O	1:A:54:ARG:HD3	0.48	2.09	4	1
1:A:20:ALA:O	1:A:24:PHE:HD1	0.48	1.90	9	5
1:A:52:GLY:O	1:A:55:ILE:HB	0.48	2.09	5	2
1:A:40:ILE:O	1:A:44:LEU:HB3	0.47	2.09	19	1
1:A:11:LEU:HB2	1:A:44:LEU:HD13	0.47	1.87	14	2
1:A:18:GLU:HA	1:A:21:HIS:ND1	0.46	2.25	12	1
1:A:47:LYS:O	1:A:50:GLU:HG2	0.46	2.10	19	2
1:A:25:GLU:HA	1:A:25:GLU:OE1	0.46	2.11	8	1
1:A:54:ARG:O	1:A:58:PHE:HB2	0.46	2.10	13	2
1:A:3:ILE:HA	1:A:6:TYR:CD2	0.46	2.46	3	1
1:A:66:GLY:O	1:A:67:ARG:HG2	0.45	2.12	14	1
1:A:18:GLU:O	1:A:22:GLU:HG2	0.45	2.11	19	2
1:A:20:ALA:O	1:A:23:LEU:HB3	0.44	2.12	17	2
1:A:58:PHE:CE2	1:A:62:LEU:HD22	0.44	2.47	14	1
1:A:15:ALA:O	1:A:19:ILE:HG13	0.44	2.12	8	1
1:A:11:LEU:HB3	1:A:44:LEU:HG	0.44	1.88	4	1
1:A:33:PHE:CE2	1:A:37:LEU:HD11	0.44	2.48	17	1
1:A:39:GLU:O	1:A:43:LEU:HG	0.43	2.13	18	1
1:A:58:PHE:CZ	1:A:62:LEU:HD21	0.43	2.48	16	1
1:A:8:GLN:O	1:A:12:LYS:HB2	0.43	2.13	17	1
1:A:4:LYS:HG3	1:A:5:GLN:OE1	0.43	2.14	12	1
1:A:21:HIS:NE2	1:A:67:ARG:HB2	0.43	2.29	16	1
1:A:10:GLU:O	1:A:14:MET:HG3	0.43	2.13	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:ILE:HA	1:A:6:TYR:CD1	0.42	2.49	11	1
1:A:10:GLU:OE2	1:A:14:MET:HG3	0.42	2.14	14	1
1:A:27:HIS:CE1	1:A:29:LYS:HB2	0.42	2.50	3	1
1:A:3:ILE:HB	1:A:22:GLU:CB	0.42	2.45	14	1
1:A:8:GLN:O	1:A:12:LYS:HG2	0.42	2.14	13	2
1:A:8:GLN:NE2	1:A:8:GLN:H	0.42	2.12	10	1
1:A:81:TRP:HE3	1:A:82:TYR:CE2	0.41	2.34	5	1
1:A:16:LEU:HB3	1:A:58:PHE:CD2	0.41	2.51	13	1
1:A:6:TYR:CD1	1:A:10:GLU:HG2	0.41	2.50	16	1
1:A:9:GLU:O	1:A:12:LYS:HB2	0.41	2.15	9	1
1:A:47:LYS:HE3	1:A:50:GLU:CD	0.41	2.36	11	1
1:A:16:LEU:HD23	1:A:16:LEU:H	0.41	1.76	7	1
1:A:36:LEU:O	1:A:40:ILE:HG13	0.41	2.16	5	1
1:A:7:SER:O	1:A:11:LEU:HG	0.40	2.16	16	1
1:A:37:LEU:HD13	1:A:55:ILE:HG12	0.40	1.92	16	1
1:A:16:LEU:HD21	1:A:57:GLN:OE1	0.40	2.16	6	1
1:A:71:LEU:C	1:A:73:ASP:H	0.40	2.20	7	1
1:A:60:THR:O	1:A:64:ILE:HG12	0.40	2.17	12	1
1:A:23:LEU:HD11	1:A:39:GLU:OE1	0.40	2.16	15	1
1:A:77:GLY:HA3	1:A:81:TRP:CZ3	0.40	2.52	16	1
1:A:11:LEU:HD23	1:A:19:ILE:HD12	0.40	1.93	17	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	79/172 (46%)	74±2 (94±2%)	3±2 (4±2%)	2±1 (2±1%)	10	50
All	All	1580/3440 (46%)	1482 (94%)	65 (4%)	33 (2%)	10	50

All 8 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	45	GLY	8

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Mol	Chain	Res	Type	Models (Total)
1	A	71	LEU	7
1	A	74	GLN	6
1	A	3	ILE	6
1	A	72	SER	2
1	A	65	ASP	2
1	A	4	LYS	1
1	A	80	SER	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	71/158 (45%)	67±2 (95±3%)	4±2 (5±3%)	28 77
All	All	1420/3160 (45%)	1349 (95%)	71 (5%)	28 77

All 20 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	57	GLN	12
1	A	74	GLN	10
1	A	34	GLN	9
1	A	68	PHE	7
1	A	75	THR	4
1	A	3	ILE	4
1	A	9	GLU	4
1	A	16	LEU	3
1	A	26	GLU	3
1	A	63	ASN	2
1	A	62	LEU	2
1	A	82	TYR	2
1	A	48	LYS	2
1	A	25	GLU	1
1	A	8	GLN	1
1	A	35	GLU	1
1	A	44	LEU	1
1	A	65	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	5	GLN	1
1	A	47	LYS	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 92% for the well-defined parts and 92% 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	2126
Number of shifts mapped to atoms	1069
Number of unparsed shifts	0
Number of shifts with mapping errors	1057
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

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

- No matching atom found in the structure. All 1057 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	83	PRO	HA	4.466	0.005	1
1	A	83	PRO	HB2	2.276	0.004	2
1	A	83	PRO	HB3	1.883	0.005	2
1	A	83	PRO	HD2	3.765	0.005	2
1	A	83	PRO	HD3	3.659	0.005	2
1	A	83	PRO	HG2	2.012	0.026	2
1	A	83	PRO	HG3	1.959	0.008	2
1	A	83	PRO	C	177.097	0.004	1
1	A	83	PRO	CA	63.307	0.112	1
1	A	83	PRO	CB	32.114	0.090	1
1	A	83	PRO	CD	50.659	0.021	1
1	A	83	PRO	CG	27.253	0.000	1
1	A	83	PRO	N	136.054	0.005	1
1	A	84	TYR	H	8.264	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	84	TYR	HA	4.601	0.001	1
1	A	84	TYR	HB2	3.124	0.003	2
1	A	84	TYR	HB3	2.996	0.005	2
1	A	84	TYR	HD1	7.122	0.000	3
1	A	84	TYR	HD2	7.122	0.000	3
1	A	84	TYR	HE1	6.767	0.000	3
1	A	84	TYR	HE2	6.767	0.000	3
1	A	84	TYR	C	175.665	0.002	1
1	A	84	TYR	CA	57.916	0.000	1
1	A	84	TYR	CB	39.335	0.314	1
1	A	84	TYR	CE1	118.8	0.000	.
1	A	84	TYR	CE2	118.8	0.000	.
1	A	84	TYR	N	120.321	0.050	1
1	A	85	ASP	H	8.237	0.001	1
1	A	85	ASP	HA	4.536	0.000	1
1	A	85	ASP	HB2	2.602	0.000	2
1	A	85	ASP	HB3	2.602	0.000	2
1	A	85	ASP	C	175.78	0.007	1
1	A	85	ASP	CA	54.312	0.102	1
1	A	85	ASP	CB	41.144	0.035	1
1	A	85	ASP	N	121.037	0.006	1
1	A	86	GLN	H	8.105	0.001	1
1	A	86	GLN	HA	4.27	0.013	1
1	A	86	GLN	HB2	2.075	0.032	2
1	A	86	GLN	HB3	1.932	0.009	2
1	A	86	GLN	HE21	7.57	0.000	2
1	A	86	GLN	HE22	6.765	0.000	2
1	A	86	GLN	HG2	2.352	0.007	2
1	A	86	GLN	HG3	2.281	0.006	2
1	A	86	GLN	C	175.695	0.002	1
1	A	86	GLN	CA	55.812	0.065	1
1	A	86	GLN	CB	29.4	0.066	1
1	A	86	GLN	CG	33.964	0.074	1
1	A	86	GLN	N	119.939	0.034	1
1	A	86	GLN	NE2	112.606	0.021	1
1	A	87	LEU	H	8.247	0.003	1
1	A	87	LEU	HA	4.304	0.004	1
1	A	87	LEU	HB2	1.624	0.009	2
1	A	87	LEU	HB3	1.543	0.003	2
1	A	87	LEU	HD11	0.889	0.013	2
1	A	87	LEU	HD12	0.889	0.013	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	87	LEU	HD13	0.889	0.013	2
1	A	87	LEU	HD21	0.827	0.010	2
1	A	87	LEU	HD22	0.827	0.010	2
1	A	87	LEU	HD23	0.827	0.010	2
1	A	87	LEU	HG	1.577	0.004	1
1	A	87	LEU	C	177.086	0.011	1
1	A	87	LEU	CA	55.171	0.071	1
1	A	87	LEU	CB	42.47	0.114	1
1	A	87	LEU	CD1	24.984	0.035	2
1	A	87	LEU	CD2	23.455	0.030	2
1	A	87	LEU	CG	26.962	0.015	1
1	A	87	LEU	N	123.207	0.057	1
1	A	88	ASP	H	8.293	0.002	1
1	A	88	ASP	HA	4.599	0.000	1
1	A	88	ASP	HB2	2.712	0.000	2
1	A	88	ASP	HB3	2.548	0.000	2
1	A	88	ASP	C	176.264	0.002	1
1	A	88	ASP	CA	54.277	0.092	1
1	A	88	ASP	CB	41.253	0.054	1
1	A	88	ASP	N	121.266	0.035	1
1	A	89	GLU	H	8.325	0.000	1
1	A	89	GLU	HA	4.229	0.001	1
1	A	89	GLU	HB2	2.048	0.000	2
1	A	89	GLU	HB3	1.915	0.000	2
1	A	89	GLU	HG2	2.235	0.000	2
1	A	89	GLU	HG3	2.235	0.000	2
1	A	89	GLU	C	176.642	0.003	1
1	A	89	GLU	CA	56.81	0.061	1
1	A	89	GLU	CB	30.438	0.076	1
1	A	89	GLU	CG	36.159	0.000	1
1	A	89	GLU	N	121.069	0.023	1
1	A	90	GLU	H	8.416	0.001	1
1	A	90	GLU	HA	4.294	0.003	1
1	A	90	GLU	HB2	2.014	0.000	2
1	A	90	GLU	HB3	2.014	0.000	2
1	A	90	GLU	HG2	2.251	0.000	2
1	A	90	GLU	HG3	2.251	0.000	2
1	A	90	GLU	C	176.778	0.003	1
1	A	90	GLU	CA	56.788	0.076	1
1	A	90	GLU	CB	30.227	0.074	1
1	A	90	GLU	CG	36.212	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	90	GLU	N	121.274	0.068	1
1	A	91	THR	H	8.124	0.004	1
1	A	91	THR	HA	4.28	0.002	1
1	A	91	THR	HB	4.149	0.002	1
1	A	91	THR	HG21	1.185	0.001	.
1	A	91	THR	HG22	1.185	0.001	.
1	A	91	THR	HG23	1.185	0.001	.
1	A	91	THR	C	174.413	0.003	1
1	A	91	THR	CA	62.11	0.094	1
1	A	91	THR	CB	69.693	0.239	1
1	A	91	THR	CG2	21.703	0.028	1
1	A	91	THR	N	115.374	0.044	1
1	A	92	GLN	H	8.353	0.004	1
1	A	92	GLN	HA	4.283	0.000	1
1	A	92	GLN	HB2	2.091	0.000	2
1	A	92	GLN	HB3	1.939	0.000	2
1	A	92	GLN	HE21	7.47	0.000	2
1	A	92	GLN	HG2	2.304	0.003	2
1	A	92	GLN	HG3	2.304	0.003	2
1	A	92	GLN	C	173.924	0.004	1
1	A	92	GLN	CA	53.73	0.042	1
1	A	92	GLN	CB	28.852	0.059	1
1	A	92	GLN	CG	33.842	0.011	1
1	A	92	GLN	N	123.797	0.028	1
1	A	92	GLN	NE2	112.645	0.000	1
1	A	93	PRO	HA	4.466	0.002	1
1	A	93	PRO	HB2	2.273	0.000	2
1	A	93	PRO	HB3	1.843	0.000	2
1	A	93	PRO	HG2	1.994	0.000	2
1	A	93	PRO	HG3	1.994	0.000	2
1	A	93	PRO	C	177.093	0.005	1
1	A	93	PRO	CA	63.196	0.088	1
1	A	93	PRO	CB	32.193	0.111	1
1	A	93	PRO	CG	27.369	0.000	1
1	A	93	PRO	N	136.912	0.000	1
1	A	94	THR	H	8.285	0.002	1
1	A	94	THR	HA	4.28	0.003	1
1	A	94	THR	HB	4.15	0.002	1
1	A	94	THR	HG21	1.195	0.011	.
1	A	94	THR	HG22	1.195	0.011	.
1	A	94	THR	HG23	1.195	0.011	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	94	THR	C	174.62	0.006	1
1	A	94	THR	CA	62.231	0.174	1
1	A	94	THR	CB	69.827	0.071	1
1	A	94	THR	CG2	21.493	0.000	1
1	A	94	THR	N	115.161	0.038	1
1	A	95	VAL	H	8.139	0.004	1
1	A	95	VAL	HA	4.073	0.000	1
1	A	95	VAL	HB	2.018	0.000	1
1	A	95	VAL	HG11	0.895	0.000	2
1	A	95	VAL	HG12	0.895	0.000	2
1	A	95	VAL	HG13	0.895	0.000	2
1	A	95	VAL	HG21	0.911	0.000	2
1	A	95	VAL	HG22	0.911	0.000	2
1	A	95	VAL	HG23	0.911	0.000	2
1	A	95	VAL	C	175.93	0.005	1
1	A	95	VAL	CA	62.332	0.103	1
1	A	95	VAL	CB	32.772	0.037	1
1	A	95	VAL	CG1	21.032	0.000	2
1	A	95	VAL	CG2	20.739	0.000	2
1	A	95	VAL	N	123.172	0.039	1
1	A	96	LYS	H	8.354	0.004	1
1	A	96	LYS	HA	4.28	0.000	1
1	A	96	LYS	HB2	1.766	0.000	2
1	A	96	LYS	HB3	1.766	0.000	2
1	A	96	LYS	HD2	1.65	0.000	2
1	A	96	LYS	HD3	1.65	0.000	2
1	A	96	LYS	HE2	2.962	0.000	2
1	A	96	LYS	HE3	2.962	0.000	2
1	A	96	LYS	HG2	1.395	0.000	2
1	A	96	LYS	HG3	1.395	0.000	2
1	A	96	LYS	C	176.077	0.005	1
1	A	96	LYS	CA	56.244	0.027	1
1	A	96	LYS	CB	33.13	0.067	1
1	A	96	LYS	CD	29.084	0.000	1
1	A	96	LYS	CE	42.078	0.000	1
1	A	96	LYS	CG	24.795	0.000	1
1	A	96	LYS	N	125.671	0.021	1
1	A	97	ALA	H	8.28	0.006	1
1	A	97	ALA	HA	4.261	0.000	1
1	A	97	ALA	HB1	1.345	0.000	1
1	A	97	ALA	HB2	1.345	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	97	ALA	HB3	1.345	0.000	1
1	A	97	ALA	C	177.501	0.004	1
1	A	97	ALA	CA	52.199	0.040	1
1	A	97	ALA	CB	19.411	0.107	1
1	A	97	ALA	N	125.788	0.044	1
1	A	98	LYS	H	8.295	0.000	1
1	A	98	LYS	HA	4.272	0.000	1
1	A	98	LYS	HB2	1.728	0.000	2
1	A	98	LYS	HB3	1.728	0.000	2
1	A	98	LYS	HD2	1.639	0.000	2
1	A	98	LYS	HD3	1.639	0.000	2
1	A	98	LYS	HE2	2.967	0.000	2
1	A	98	LYS	HE3	2.967	0.000	2
1	A	98	LYS	HG2	1.407	0.000	2
1	A	98	LYS	HG3	1.407	0.000	2
1	A	98	LYS	C	176.514	0.007	1
1	A	98	LYS	CA	56.275	0.006	1
1	A	98	LYS	CB	33.39	0.030	1
1	A	98	LYS	CD	29.073	0.000	1
1	A	98	LYS	CE	42.142	0.000	1
1	A	98	LYS	CG	24.89	0.000	1
1	A	98	LYS	N	121.177	0.026	1
1	A	99	LYS	H	8.383	0.000	1
1	A	99	LYS	HA	4.295	0.000	1
1	A	99	LYS	HB2	1.76	0.000	2
1	A	99	LYS	HB3	1.76	0.000	2
1	A	99	LYS	HD2	1.646	0.000	2
1	A	99	LYS	HD3	1.646	0.000	2
1	A	99	LYS	HE2	2.95	0.000	2
1	A	99	LYS	HE3	2.95	0.000	2
1	A	99	LYS	HG2	1.387	0.000	2
1	A	99	LYS	HG3	1.387	0.000	2
1	A	99	LYS	C	176.37	0.025	1
1	A	99	LYS	CA	56.329	0.006	1
1	A	99	LYS	CB	33.398	0.032	1
1	A	99	LYS	CD	29.11	0.000	1
1	A	99	LYS	CE	42.125	0.000	1
1	A	99	LYS	CG	24.857	0.000	1
1	A	99	LYS	N	123.012	0.004	1
1	A	100	LYS	H	8.399	0.001	1
1	A	100	LYS	HA	4.292	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	LYS	HB2	1.732	0.000	2
1	A	100	LYS	HB3	1.732	0.000	2
1	A	100	LYS	HD2	1.625	0.000	2
1	A	100	LYS	HD3	1.625	0.000	2
1	A	100	LYS	HE2	2.953	0.000	2
1	A	100	LYS	HE3	2.953	0.000	2
1	A	100	LYS	HG2	1.383	0.000	2
1	A	100	LYS	HG3	1.383	0.000	2
1	A	100	LYS	C	176.405	0.005	1
1	A	100	LYS	CA	56.299	0.017	1
1	A	100	LYS	CB	33.377	0.044	1
1	A	100	LYS	CD	29.126	0.000	1
1	A	100	LYS	CE	42.144	0.000	1
1	A	100	LYS	CG	24.928	0.000	1
1	A	100	LYS	N	123.274	0.025	1
1	A	101	LYS	H	8.433	0.000	1
1	A	101	LYS	HA	4.265	0.000	1
1	A	101	LYS	HB2	1.726	0.000	2
1	A	101	LYS	HB3	1.726	0.000	2
1	A	101	LYS	HD2	1.645	0.000	2
1	A	101	LYS	HD3	1.645	0.000	2
1	A	101	LYS	HE2	2.964	0.000	2
1	A	101	LYS	HE3	2.964	0.000	2
1	A	101	LYS	HG2	1.388	0.000	2
1	A	101	LYS	HG3	1.388	0.000	2
1	A	101	LYS	C	176.072	0.007	1
1	A	101	LYS	CA	56.245	0.056	1
1	A	101	LYS	CB	33.354	0.013	1
1	A	101	LYS	CD	29.239	0.000	1
1	A	101	LYS	CE	42.077	0.000	1
1	A	101	LYS	CG	24.799	0.000	1
1	A	101	LYS	N	123.387	0.036	1
1	A	102	ALA	H	8.378	0.003	1
1	A	102	ALA	HA	4.272	0.000	1
1	A	102	ALA	HB1	1.347	0.000	1
1	A	102	ALA	HB2	1.347	0.000	1
1	A	102	ALA	HB3	1.347	0.000	1
1	A	102	ALA	C	177.495	0.006	1
1	A	102	ALA	CA	52.26	0.162	1
1	A	102	ALA	CB	19.523	0.091	1
1	A	102	ALA	N	126.052	0.025	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	LYS	H	8.333	0.000	1
1	A	103	LYS	HA	4.259	0.000	1
1	A	103	LYS	HB2	1.75	0.000	2
1	A	103	LYS	HB3	1.75	0.000	2
1	A	103	LYS	HD2	1.65	0.000	2
1	A	103	LYS	HD3	1.65	0.000	2
1	A	103	LYS	HE2	2.966	0.000	2
1	A	103	LYS	HE3	2.966	0.000	2
1	A	103	LYS	HG2	1.402	0.000	2
1	A	103	LYS	HG3	1.402	0.000	2
1	A	103	LYS	C	176.513	0.007	1
1	A	103	LYS	CA	56.287	0.087	1
1	A	103	LYS	CB	33.23	0.032	1
1	A	103	LYS	CD	29.149	0.000	1
1	A	103	LYS	CE	42.138	0.000	1
1	A	103	LYS	CG	24.823	0.000	1
1	A	103	LYS	N	121.384	0.037	1
1	A	104	LYS	H	8.365	0.001	1
1	A	104	LYS	HA	4.267	0.000	1
1	A	104	LYS	HB2	1.753	0.000	2
1	A	104	LYS	HB3	1.753	0.000	2
1	A	104	LYS	HD2	1.653	0.000	2
1	A	104	LYS	HD3	1.653	0.000	2
1	A	104	LYS	HE2	2.97	0.000	2
1	A	104	LYS	HE3	2.97	0.000	2
1	A	104	LYS	HG2	1.405	0.000	2
1	A	104	LYS	HG3	1.405	0.000	2
1	A	104	LYS	C	176.156	0.004	1
1	A	104	LYS	CA	56.282	0.014	1
1	A	104	LYS	CB	33.363	0.055	1
1	A	104	LYS	CD	29.15	0.000	1
1	A	104	LYS	CE	42.108	0.000	1
1	A	104	LYS	CG	24.769	0.000	1
1	A	104	LYS	N	123.013	0.005	1
1	A	105	ALA	H	8.371	0.001	1
1	A	105	ALA	HA	4.315	0.000	1
1	A	105	ALA	HB1	1.377	0.000	1
1	A	105	ALA	HB2	1.377	0.000	1
1	A	105	ALA	HB3	1.377	0.000	1
1	A	105	ALA	C	177.697	0.002	1
1	A	105	ALA	CA	52.585	0.102	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	105	ALA	CB	19.257	0.077	1
1	A	105	ALA	N	125.783	0.053	1
1	A	106	VAL	H	8.034	0.001	1
1	A	106	VAL	HA	4.09	0.000	1
1	A	106	VAL	HB	2.088	0.000	1
1	A	106	VAL	HG11	0.918	0.000	2
1	A	106	VAL	HG12	0.918	0.000	2
1	A	106	VAL	HG13	0.918	0.000	2
1	A	106	VAL	HG21	0.917	0.000	2
1	A	106	VAL	HG22	0.917	0.000	2
1	A	106	VAL	HG23	0.917	0.000	2
1	A	106	VAL	C	176.288	0.002	1
1	A	106	VAL	CA	62.457	0.043	1
1	A	106	VAL	CB	32.789	0.060	1
1	A	106	VAL	CG1	21.356	0.000	2
1	A	106	VAL	CG2	20.583	0.000	2
1	A	106	VAL	N	118.428	0.016	1
1	A	107	GLU	H	8.442	0.000	1
1	A	107	GLU	HA	4.248	0.000	1
1	A	107	GLU	HB2	2.038	0.000	2
1	A	107	GLU	HB3	1.925	0.000	2
1	A	107	GLU	HG2	2.25	0.000	2
1	A	107	GLU	HG3	2.25	0.000	2
1	A	107	GLU	C	176.418	0.004	1
1	A	107	GLU	CA	56.827	0.147	1
1	A	107	GLU	CB	30.131	0.032	1
1	A	107	GLU	CG	36.231	0.000	1
1	A	107	GLU	N	123.222	0.021	1
1	A	108	GLU	H	8.268	0.001	1
1	A	108	GLU	HA	4.24	0.003	1
1	A	108	GLU	HB2	2.018	0.000	2
1	A	108	GLU	HB3	1.907	0.000	2
1	A	108	GLU	HG2	2.228	0.000	2
1	A	108	GLU	HG3	2.228	0.000	2
1	A	108	GLU	C	175.909	0.007	1
1	A	108	GLU	CA	56.761	0.057	1
1	A	108	GLU	CB	30.471	0.087	1
1	A	108	GLU	CG	36.222	0.000	1
1	A	108	GLU	N	120.709	0.008	1
1	A	109	ASP	H	8.308	0.001	1
1	A	109	ASP	HA	4.569	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	109	ASP	HB2	2.721	0.000	2
1	A	109	ASP	HB3	2.584	0.000	2
1	A	109	ASP	C	175.901	0.001	1
1	A	109	ASP	CA	54.36	0.012	1
1	A	109	ASP	CB	40.528	0.520	1
1	A	109	ASP	N	120.703	0.036	1
1	A	110	LEU	H	8.04	0.001	1
1	A	110	LEU	HA	4.299	0.000	1
1	A	110	LEU	HB2	1.567	0.000	2
1	A	110	LEU	HB3	1.567	0.000	2
1	A	110	LEU	HD11	0.878	0.000	2
1	A	110	LEU	HD12	0.878	0.000	2
1	A	110	LEU	HD13	0.878	0.000	2
1	A	110	LEU	HD21	0.825	0.000	2
1	A	110	LEU	HD22	0.825	0.000	2
1	A	110	LEU	HD23	0.825	0.000	2
1	A	110	LEU	HG	1.569	0.000	1
1	A	110	LEU	C	176.923	0.006	1
1	A	110	LEU	CA	55.116	0.034	1
1	A	110	LEU	CB	42.616	0.130	1
1	A	110	LEU	CD1	25.054	0.000	2
1	A	110	LEU	CD2	23.483	0.000	2
1	A	110	LEU	CG	26.967	0.000	1
1	A	110	LEU	N	122.123	0.039	1
1	A	111	ASP	H	8.358	0.001	1
1	A	111	ASP	HA	4.589	0.000	1
1	A	111	ASP	HB2	2.716	0.000	2
1	A	111	ASP	HB3	2.583	0.000	2
1	A	111	ASP	C	175.99	0.006	1
1	A	111	ASP	CA	54.213	0.033	1
1	A	111	ASP	CB	40.918	0.049	1
1	A	111	ASP	N	121.043	0.053	1
1	A	112	LEU	H	8.047	0.003	1
1	A	112	LEU	HA	4.289	0.000	1
1	A	112	LEU	HB2	1.587	0.000	2
1	A	112	LEU	HB3	1.587	0.000	2
1	A	112	LEU	HD11	0.891	0.000	2
1	A	112	LEU	HD12	0.891	0.000	2
1	A	112	LEU	HD13	0.891	0.000	2
1	A	112	LEU	HD21	0.83	0.000	2
1	A	112	LEU	HD22	0.83	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	112	LEU	HD23	0.83	0.000	2
1	A	112	LEU	HG	1.578	0.000	1
1	A	112	LEU	C	177.228	0.003	1
1	A	112	LEU	CA	55.261	0.328	1
1	A	112	LEU	CB	42.599	0.048	1
1	A	112	LEU	CD1	25.116	0.000	2
1	A	112	LEU	CD2	23.448	0.000	2
1	A	112	LEU	CG	26.891	0.000	1
1	A	112	LEU	N	122.357	0.014	1
1	A	113	ASP	H	8.325	0.001	1
1	A	113	ASP	HA	4.549	0.000	1
1	A	113	ASP	HB2	2.6	0.000	2
1	A	113	ASP	HB3	2.6	0.000	2
1	A	113	ASP	C	176.144	0.004	1
1	A	113	ASP	CA	54.56	0.035	1
1	A	113	ASP	CB	41.203	0.076	1
1	A	113	ASP	N	121.055	0.005	1
1	A	114	GLU	H	8.14	0.001	1
1	A	114	GLU	HA	4.204	0.002	1
1	A	114	GLU	HB2	1.833	0.000	2
1	A	114	GLU	HB3	1.833	0.000	2
1	A	114	GLU	HG2	2.061	0.000	2
1	A	114	GLU	HG3	2.061	0.000	2
1	A	114	GLU	C	175.949	0.019	1
1	A	114	GLU	CA	56.551	0.066	1
1	A	114	GLU	CB	30.437	0.035	1
1	A	114	GLU	CG	35.864	0.000	1
1	A	114	GLU	N	120.518	0.005	1
1	A	115	PHE	H	8.188	0.006	1
1	A	115	PHE	HA	4.639	0.001	1
1	A	115	PHE	HB2	3.119	0.000	2
1	A	115	PHE	HB3	2.987	0.002	2
1	A	115	PHE	C	175.369	0.005	1
1	A	115	PHE	CA	57.481	0.040	1
1	A	115	PHE	CB	39.892	0.029	1
1	A	115	PHE	N	120.56	0.048	1
1	A	116	GLU	H	8.174	0.006	1
1	A	116	GLU	HA	4.274	0.000	1
1	A	116	GLU	HB2	1.922	0.000	2
1	A	116	GLU	HB3	1.922	0.000	2
1	A	116	GLU	HG2	2.194	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	GLU	HG3	2.194	0.000	2
1	A	116	GLU	C	175.651	0.003	1
1	A	116	GLU	CA	56.107	0.069	1
1	A	116	GLU	CB	30.877	0.028	1
1	A	116	GLU	CG	35.902	0.000	1
1	A	116	GLU	N	122.511	0.033	1
1	A	117	GLU	H	8.384	0.001	1
1	A	117	GLU	HA	4.312	0.002	1
1	A	117	GLU	HB2	1.967	0.000	2
1	A	117	GLU	HB3	1.919	0.000	2
1	A	117	GLU	HG2	2.245	0.000	2
1	A	117	GLU	HG3	2.245	0.000	2
1	A	117	GLU	C	175.991	0.002	1
1	A	117	GLU	CA	56.189	0.081	1
1	A	117	GLU	CB	30.415	0.037	1
1	A	117	GLU	CG	36.027	0.000	1
1	A	117	GLU	N	122.8	0.018	1
1	A	118	ILE	H	8.233	0.006	1
1	A	118	ILE	HA	4.188	0.000	1
1	A	118	ILE	HB	1.818	0.000	1
1	A	118	ILE	HD11	0.817	0.000	.
1	A	118	ILE	HD12	0.817	0.000	.
1	A	118	ILE	HD13	0.817	0.000	.
1	A	118	ILE	HG12	1.419	0.000	2
1	A	118	ILE	HG13	1.122	0.000	2
1	A	118	ILE	HG21	0.867	0.000	.
1	A	118	ILE	HG22	0.867	0.000	.
1	A	118	ILE	HG23	0.867	0.000	.
1	A	118	ILE	C	175.59	0.003	1
1	A	118	ILE	CA	60.738	0.057	1
1	A	118	ILE	CB	39.358	0.042	1
1	A	118	ILE	CD1	12.935	0.000	1
1	A	118	ILE	CG1	27.142	0.014	1
1	A	118	ILE	CG2	17.611	0.000	1
1	A	118	ILE	N	122.509	0.020	1
1	A	119	ASP	H	8.481	0.001	1
1	A	119	ASP	HA	4.647	0.000	1
1	A	119	ASP	HB2	2.721	0.000	2
1	A	119	ASP	HB3	2.555	0.000	2
1	A	119	ASP	C	176.109	0.003	1
1	A	119	ASP	CA	54.055	0.034	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	119	ASP	CB	41.331	0.044	1
1	A	119	ASP	N	125.291	0.015	1
1	A	120	GLU	H	8.433	0.001	1
1	A	120	GLU	HA	4.248	0.000	1
1	A	120	GLU	HB2	2.053	0.000	2
1	A	120	GLU	HB3	1.897	0.000	2
1	A	120	GLU	HG2	2.249	0.000	2
1	A	120	GLU	HG3	2.249	0.000	2
1	A	120	GLU	C	176.235	0.002	1
1	A	120	GLU	CA	56.636	0.097	1
1	A	120	GLU	CB	30.477	0.079	1
1	A	120	GLU	CG	36.012	0.000	1
1	A	120	GLU	N	122.271	0.005	1
1	A	121	ASP	H	8.405	0.002	1
1	A	121	ASP	HA	4.571	0.000	1
1	A	121	ASP	HB2	2.624	0.000	2
1	A	121	ASP	HB3	2.624	0.000	2
1	A	121	ASP	C	175.969	0.003	1
1	A	121	ASP	CA	54.603	0.038	1
1	A	121	ASP	CB	41.242	0.019	1
1	A	121	ASP	N	121.098	0.021	1
1	A	122	ASP	H	8.224	0.003	1
1	A	122	ASP	HA	4.569	0.000	1
1	A	122	ASP	HB2	2.721	0.000	2
1	A	122	ASP	HB3	2.584	0.000	2
1	A	122	ASP	C	176.0	0.007	1
1	A	122	ASP	CA	54.384	0.034	1
1	A	122	ASP	CB	40.852	0.044	1
1	A	122	ASP	N	120.532	0.041	1
1	A	123	LEU	H	8.041	0.001	1
1	A	123	LEU	HA	4.279	0.000	1
1	A	123	LEU	HB2	1.608	0.000	2
1	A	123	LEU	HB3	1.538	0.000	2
1	A	123	LEU	HD11	0.891	0.000	2
1	A	123	LEU	HD12	0.891	0.000	2
1	A	123	LEU	HD13	0.891	0.000	2
1	A	123	LEU	HD21	0.835	0.000	2
1	A	123	LEU	HD22	0.835	0.000	2
1	A	123	LEU	HD23	0.835	0.000	2
1	A	123	LEU	HG	1.584	0.000	1
1	A	123	LEU	C	176.999	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	123	LEU	CA	55.243	0.071	1
1	A	123	LEU	CB	42.649	0.050	1
1	A	123	LEU	CD1	25.033	0.000	2
1	A	123	LEU	CD2	23.512	0.000	2
1	A	123	LEU	CG	26.921	0.000	1
1	A	123	LEU	N	122.187	0.038	1
1	A	124	ASP	H	8.354	0.002	1
1	A	124	ASP	HA	4.598	0.000	1
1	A	124	ASP	HB2	2.731	0.000	2
1	A	124	ASP	HB3	2.551	0.000	2
1	A	124	ASP	C	176.019	0.002	1
1	A	124	ASP	CA	53.97	0.117	1
1	A	124	ASP	CB	40.835	0.033	1
1	A	124	ASP	N	121.276	0.074	1
1	A	125	LEU	H	8.12	0.000	1
1	A	125	LEU	HA	4.298	0.000	1
1	A	125	LEU	HB2	1.587	0.002	2
1	A	125	LEU	HB3	1.587	0.002	2
1	A	125	LEU	HD11	0.895	0.000	2
1	A	125	LEU	HD12	0.895	0.000	2
1	A	125	LEU	HD13	0.895	0.000	2
1	A	125	LEU	HD21	0.834	0.000	2
1	A	125	LEU	HD22	0.834	0.000	2
1	A	125	LEU	HD23	0.834	0.000	2
1	A	125	LEU	HG	1.587	0.000	1
1	A	125	LEU	C	177.24	0.012	1
1	A	125	LEU	CA	55.111	0.067	1
1	A	125	LEU	CB	42.503	0.036	1
1	A	125	LEU	CD1	25.115	0.000	2
1	A	125	LEU	CD2	23.362	0.000	2
1	A	125	LEU	CG	26.856	0.000	1
1	A	125	LEU	N	122.718	0.015	1
1	A	126	ASP	H	8.317	0.001	1
1	A	126	ASP	HA	4.568	0.000	1
1	A	126	ASP	HB2	2.655	0.000	2
1	A	126	ASP	HB3	2.599	0.000	2
1	A	126	ASP	C	176.062	0.011	1
1	A	126	ASP	CA	54.441	0.083	1
1	A	126	ASP	CB	41.157	0.058	1
1	A	126	ASP	N	121.059	0.004	1
1	A	127	GLU	H	8.198	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	127	GLU	HA	4.301	0.000	1
1	A	127	GLU	HB2	2.018	0.000	2
1	A	127	GLU	HB3	1.891	0.000	2
1	A	127	GLU	HG2	2.228	0.000	2
1	A	127	GLU	HG3	2.228	0.000	2
1	A	127	GLU	C	176.204	0.003	1
1	A	127	GLU	CA	56.308	0.044	1
1	A	127	GLU	CB	30.389	0.093	1
1	A	127	GLU	CG	35.962	0.000	1
1	A	127	GLU	N	121.082	0.026	1
1	A	128	VAL	H	8.151	0.008	1
1	A	128	VAL	HA	4.099	0.000	1
1	A	128	VAL	HB	2.039	0.000	1
1	A	128	VAL	HG11	0.897	0.000	2
1	A	128	VAL	HG12	0.897	0.000	2
1	A	128	VAL	HG13	0.897	0.000	2
1	A	128	VAL	HG21	0.911	0.000	2
1	A	128	VAL	HG22	0.911	0.000	2
1	A	128	VAL	HG23	0.911	0.000	2
1	A	128	VAL	C	176.035	0.007	1
1	A	128	VAL	CA	62.194	0.074	1
1	A	128	VAL	CB	33.004	0.055	1
1	A	128	VAL	CG1	21.265	0.000	2
1	A	128	VAL	CG2	20.787	0.000	2
1	A	128	VAL	N	121.666	0.038	1
1	A	129	GLU	H	8.471	0.000	1
1	A	129	GLU	HA	4.29	0.000	1
1	A	129	GLU	HB2	1.983	0.000	2
1	A	129	GLU	HB3	1.908	0.000	2
1	A	129	GLU	HG2	2.252	0.000	2
1	A	129	GLU	HG3	2.252	0.000	2
1	A	129	GLU	C	176.2	0.002	1
1	A	129	GLU	CA	56.439	0.149	1
1	A	129	GLU	CB	30.404	0.105	1
1	A	129	GLU	CG	35.985	0.000	1
1	A	129	GLU	N	125.352	0.029	1
1	A	130	GLU	H	8.415	0.001	1
1	A	130	GLU	HA	4.261	0.001	1
1	A	130	GLU	HB2	1.93	0.000	2
1	A	130	GLU	HB3	1.93	0.000	2
1	A	130	GLU	HG2	2.231	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	130	GLU	HG3	2.231	0.000	2
1	A	130	GLU	C	176.124	0.002	1
1	A	130	GLU	CA	56.41	0.045	1
1	A	130	GLU	CB	30.625	0.098	1
1	A	130	GLU	CG	36.018	0.000	1
1	A	130	GLU	N	122.876	0.026	1
1	A	131	GLU	H	8.477	0.002	1
1	A	131	GLU	HA	4.267	0.000	1
1	A	131	GLU	HB2	1.941	0.000	2
1	A	131	GLU	HB3	1.941	0.000	2
1	A	131	GLU	HG2	2.243	0.000	2
1	A	131	GLU	HG3	2.243	0.000	2
1	A	131	GLU	C	176.093	0.002	1
1	A	131	GLU	CA	56.386	0.051	1
1	A	131	GLU	CB	30.44	0.030	1
1	A	131	GLU	CG	35.995	0.000	1
1	A	131	GLU	N	122.909	0.019	1
1	A	132	LEU	H	8.282	0.000	1
1	A	132	LEU	HA	4.322	0.000	1
1	A	132	LEU	HB2	1.554	0.002	2
1	A	132	LEU	HB3	1.554	0.002	2
1	A	132	LEU	HD11	0.889	0.000	2
1	A	132	LEU	HD12	0.889	0.000	2
1	A	132	LEU	HD13	0.889	0.000	2
1	A	132	LEU	HD21	0.834	0.000	2
1	A	132	LEU	HD22	0.834	0.000	2
1	A	132	LEU	HD23	0.834	0.000	2
1	A	132	LEU	HG	1.572	0.000	1
1	A	132	LEU	C	176.815	0.003	1
1	A	132	LEU	CA	55.014	0.041	1
1	A	132	LEU	CB	42.884	0.032	1
1	A	132	LEU	CD1	24.924	0.000	2
1	A	132	LEU	CD2	23.527	0.000	2
1	A	132	LEU	CG	27.0	0.000	1
1	A	132	LEU	N	124.118	0.025	1
1	A	133	ASP	H	8.413	0.001	1
1	A	133	ASP	HA	4.609	0.000	1
1	A	133	ASP	HB2	2.721	0.000	2
1	A	133	ASP	HB3	2.551	0.000	2
1	A	133	ASP	C	175.958	0.004	1
1	A	133	ASP	CA	53.929	0.058	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	133	ASP	CB	40.827	0.030	1
1	A	133	ASP	N	121.868	0.008	1
1	A	134	LEU	H	8.176	0.001	1
1	A	134	LEU	HA	4.292	0.000	1
1	A	134	LEU	HB2	1.589	0.000	2
1	A	134	LEU	HB3	1.589	0.000	2
1	A	134	LEU	HD11	0.895	0.000	2
1	A	134	LEU	HD12	0.895	0.000	2
1	A	134	LEU	HD13	0.895	0.000	2
1	A	134	LEU	HD21	0.841	0.000	2
1	A	134	LEU	HD22	0.841	0.000	2
1	A	134	LEU	HD23	0.841	0.000	2
1	A	134	LEU	HG	1.593	0.000	1
1	A	134	LEU	C	177.486	0.004	1
1	A	134	LEU	CA	55.319	0.152	1
1	A	134	LEU	CB	42.527	0.030	1
1	A	134	LEU	CD1	25.028	0.000	2
1	A	134	LEU	CD2	23.384	0.000	2
1	A	134	LEU	CG	26.933	0.000	1
1	A	134	LEU	N	123.211	0.014	1
1	A	135	GLU	H	8.364	0.002	1
1	A	135	GLU	HA	4.252	0.000	1
1	A	135	GLU	HB2	2.048	0.000	2
1	A	135	GLU	HB3	1.908	0.000	2
1	A	135	GLU	HG2	2.248	0.000	2
1	A	135	GLU	HG3	2.248	0.000	2
1	A	135	GLU	C	176.06	0.002	1
1	A	135	GLU	CA	56.236	0.101	1
1	A	135	GLU	CB	30.058	0.052	1
1	A	135	GLU	CG	35.989	0.000	1
1	A	135	GLU	N	121.501	0.039	1
1	A	136	ALA	H	8.16	0.007	1
1	A	136	ALA	HA	4.262	0.000	1
1	A	136	ALA	HB1	1.356	0.000	1
1	A	136	ALA	HB2	1.356	0.000	1
1	A	136	ALA	HB3	1.356	0.000	1
1	A	136	ALA	C	177.36	0.002	1
1	A	136	ALA	CA	52.392	0.162	1
1	A	136	ALA	CB	19.502	0.117	1
1	A	136	ALA	N	125.249	0.040	1
1	A	137	ASP	H	8.264	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	137	ASP	HA	4.538	0.000	1
1	A	137	ASP	HB2	2.541	0.000	2
1	A	137	ASP	HB3	2.541	0.000	2
1	A	137	ASP	C	175.719	0.001	1
1	A	137	ASP	CA	54.145	0.056	1
1	A	137	ASP	CB	41.299	0.025	1
1	A	137	ASP	N	120.084	0.016	1
1	A	138	ASP	H	8.146	0.001	1
1	A	138	ASP	HA	4.557	0.000	1
1	A	138	ASP	HB2	2.551	0.000	2
1	A	138	ASP	HB3	2.551	0.000	2
1	A	138	ASP	C	175.679	0.004	1
1	A	138	ASP	CA	54.043	0.038	1
1	A	138	ASP	CB	41.299	0.151	1
1	A	138	ASP	N	120.495	0.018	1
1	A	139	PHE	H	8.092	0.004	1
1	A	139	PHE	HA	4.58	0.000	1
1	A	139	PHE	HB2	3.114	0.000	2
1	A	139	PHE	HB3	3.003	0.000	2
1	A	139	PHE	C	175.271	0.008	1
1	A	139	PHE	CA	57.552	0.059	1
1	A	139	PHE	CB	39.712	0.063	1
1	A	139	PHE	N	120.536	0.020	1
1	A	140	ASP	H	8.288	0.000	1
1	A	140	ASP	HA	4.588	0.000	1
1	A	140	ASP	HB2	2.658	0.000	2
1	A	140	ASP	HB3	2.547	0.000	2
1	A	140	ASP	C	175.762	0.003	1
1	A	140	ASP	CA	54.07	0.016	1
1	A	140	ASP	CB	41.243	0.092	1
1	A	140	ASP	N	122.708	0.008	1
1	A	141	GLU	H	8.26	0.001	1
1	A	141	GLU	HA	4.238	0.002	1
1	A	141	GLU	HB2	2.047	0.000	2
1	A	141	GLU	HB3	1.89	0.000	2
1	A	141	GLU	HG2	2.257	0.000	2
1	A	141	GLU	HG3	2.257	0.000	2
1	A	141	GLU	C	176.346	0.004	1
1	A	141	GLU	CA	56.507	0.084	1
1	A	141	GLU	CB	30.39	0.025	1
1	A	141	GLU	CG	35.93	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	141	GLU	N	121.792	0.048	1
1	A	142	GLU	H	8.396	0.000	1
1	A	142	GLU	HA	4.246	0.003	1
1	A	142	GLU	HB2	1.999	0.000	2
1	A	142	GLU	HB3	1.899	0.000	2
1	A	142	GLU	HG2	2.238	0.000	2
1	A	142	GLU	HG3	2.238	0.000	2
1	A	142	GLU	C	175.963	0.004	1
1	A	142	GLU	CA	56.49	0.056	1
1	A	142	GLU	CB	30.491	0.070	1
1	A	142	GLU	CG	35.955	0.000	1
1	A	142	GLU	N	121.938	0.045	1
1	A	143	ASP	H	8.383	0.001	1
1	A	143	ASP	HA	4.605	0.000	1
1	A	143	ASP	HB2	2.72	0.000	2
1	A	143	ASP	HB3	2.554	0.000	2
1	A	143	ASP	C	175.843	0.002	1
1	A	143	ASP	CA	54.137	0.024	1
1	A	143	ASP	CB	40.948	0.053	1
1	A	143	ASP	N	121.91	0.017	1
1	A	144	LEU	H	8.188	0.000	1
1	A	144	LEU	HA	4.309	0.000	1
1	A	144	LEU	HB2	1.585	0.000	2
1	A	144	LEU	HB3	1.585	0.000	2
1	A	144	LEU	HD11	0.889	0.000	2
1	A	144	LEU	HD12	0.889	0.000	2
1	A	144	LEU	HD13	0.889	0.000	2
1	A	144	LEU	HD21	0.835	0.000	2
1	A	144	LEU	HD22	0.835	0.000	2
1	A	144	LEU	HD23	0.835	0.000	2
1	A	144	LEU	HG	1.573	0.000	1
1	A	144	LEU	C	177.056	0.002	1
1	A	144	LEU	CA	55.277	0.438	1
1	A	144	LEU	CB	42.585	0.060	1
1	A	144	LEU	CD1	25.018	0.000	2
1	A	144	LEU	CD2	23.37	0.000	2
1	A	144	LEU	CG	26.963	0.000	1
1	A	144	LEU	N	123.121	0.007	1
1	A	145	ASP	H	8.367	0.000	1
1	A	145	ASP	HA	4.598	0.000	1
1	A	145	ASP	HB2	2.715	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	145	ASP	HB3	2.564	0.000	2
1	A	145	ASP	C	176.001	0.003	1
1	A	145	ASP	CA	54.253	0.015	1
1	A	145	ASP	CB	41.073	0.019	1
1	A	145	ASP	N	121.786	0.030	1
1	A	146	GLU	H	8.311	0.000	1
1	A	146	GLU	HA	4.293	0.003	1
1	A	146	GLU	HB2	2.039	0.000	2
1	A	146	GLU	HB3	1.877	0.000	2
1	A	146	GLU	HG2	2.241	0.000	2
1	A	146	GLU	HG3	2.241	0.000	2
1	A	146	GLU	C	176.024	0.003	1
1	A	146	GLU	CA	56.202	0.062	1
1	A	146	GLU	CB	30.461	0.135	1
1	A	146	GLU	CG	35.818	0.000	1
1	A	146	GLU	N	121.501	0.007	1
1	A	147	ASP	H	8.408	0.000	1
1	A	147	ASP	HA	4.6	0.000	1
1	A	147	ASP	HB2	2.706	0.000	2
1	A	147	ASP	HB3	2.586	0.000	2
1	A	147	ASP	C	175.857	0.002	1
1	A	147	ASP	CA	54.138	0.121	1
1	A	147	ASP	CB	41.267	0.018	1
1	A	147	ASP	N	121.906	0.015	1
1	A	148	ASP	H	8.32	0.002	1
1	A	148	ASP	HA	4.591	0.000	1
1	A	148	ASP	HB2	2.687	0.000	2
1	A	148	ASP	HB3	2.608	0.000	2
1	A	148	ASP	C	176.01	0.004	1
1	A	148	ASP	CA	54.218	0.022	1
1	A	148	ASP	CB	41.123	0.084	1
1	A	148	ASP	N	121.368	0.023	1
1	A	149	ASP	H	8.323	0.001	1
1	A	149	ASP	HA	4.565	0.000	1
1	A	149	ASP	HB2	2.628	0.000	2
1	A	149	ASP	HB3	2.628	0.000	2
1	A	149	ASP	C	175.983	0.008	1
1	A	149	ASP	CA	54.385	0.141	1
1	A	149	ASP	CB	41.167	0.025	1
1	A	149	ASP	N	121.116	0.007	1
1	A	150	ASP	H	8.308	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	150	ASP	HA	4.589	0.000	1
1	A	150	ASP	HB2	2.716	0.000	2
1	A	150	ASP	HB3	2.583	0.000	2
1	A	150	ASP	C	175.989	0.006	1
1	A	150	ASP	CA	54.225	0.021	1
1	A	150	ASP	CB	40.896	0.019	1
1	A	150	ASP	N	120.68	0.013	1
1	A	151	LEU	H	8.043	0.002	1
1	A	151	LEU	HA	4.284	0.000	1
1	A	151	LEU	HB2	1.584	0.002	2
1	A	151	LEU	HB3	1.584	0.002	2
1	A	151	LEU	HD11	0.9	0.000	2
1	A	151	LEU	HD12	0.9	0.000	2
1	A	151	LEU	HD13	0.9	0.000	2
1	A	151	LEU	HD21	0.844	0.000	2
1	A	151	LEU	HD22	0.844	0.000	2
1	A	151	LEU	HD23	0.844	0.000	2
1	A	151	LEU	HG	1.566	0.000	1
1	A	151	LEU	C	177.259	0.003	1
1	A	151	LEU	CA	55.209	0.062	1
1	A	151	LEU	CB	42.533	0.042	1
1	A	151	LEU	CD1	24.922	0.000	2
1	A	151	LEU	CD2	23.639	0.000	2
1	A	151	LEU	CG	26.93	0.000	1
1	A	151	LEU	N	122.351	0.008	1
1	A	152	GLU	H	8.345	0.001	1
1	A	152	GLU	HA	4.29	0.002	1
1	A	152	GLU	HB2	1.949	0.000	2
1	A	152	GLU	HB3	1.949	0.000	2
1	A	152	GLU	HG2	2.227	0.000	2
1	A	152	GLU	HG3	2.227	0.000	2
1	A	152	GLU	C	176.022	0.003	1
1	A	152	GLU	CA	56.172	0.119	1
1	A	152	GLU	CB	30.044	0.030	1
1	A	152	GLU	CG	35.858	0.000	1
1	A	152	GLU	N	122.509	0.007	1
1	A	153	ILE	H	8.157	0.001	1
1	A	153	ILE	HA	4.152	0.000	1
1	A	153	ILE	HB	1.815	0.000	1
1	A	153	ILE	HD11	0.833	0.000	.
1	A	153	ILE	HD12	0.833	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	153	ILE	HD13	0.833	0.000	.
1	A	153	ILE	HG12	1.426	0.000	2
1	A	153	ILE	HG13	1.146	0.000	2
1	A	153	ILE	HG21	0.862	0.000	.
1	A	153	ILE	HG22	0.862	0.000	.
1	A	153	ILE	HG23	0.862	0.000	.
1	A	153	ILE	C	176.058	0.006	1
1	A	153	ILE	CA	60.796	0.057	1
1	A	153	ILE	CB	38.973	0.089	1
1	A	153	ILE	CD1	12.761	0.000	1
1	A	153	ILE	CG1	27.096	0.032	1
1	A	153	ILE	CG2	17.528	0.000	1
1	A	153	ILE	N	122.733	0.011	1
1	A	154	GLU	H	8.476	0.006	1
1	A	154	GLU	HA	4.313	0.003	1
1	A	154	GLU	HB2	1.991	0.000	2
1	A	154	GLU	HB3	1.902	0.000	2
1	A	154	GLU	HG2	2.251	0.000	2
1	A	154	GLU	HG3	2.251	0.000	2
1	A	154	GLU	C	176.072	0.006	1
1	A	154	GLU	CA	56.286	0.080	1
1	A	154	GLU	CB	30.403	0.047	1
1	A	154	GLU	CG	35.929	0.000	1
1	A	154	GLU	N	126.025	0.082	1
1	A	155	GLU	H	8.425	0.001	1
1	A	155	GLU	HA	4.272	0.001	1
1	A	155	GLU	HB2	2.005	0.000	2
1	A	155	GLU	HB3	1.873	0.000	2
1	A	155	GLU	HG2	2.233	0.000	2
1	A	155	GLU	HG3	2.233	0.000	2
1	A	155	GLU	C	175.858	0.006	1
1	A	155	GLU	CA	56.235	0.055	1
1	A	155	GLU	CB	30.887	0.031	1
1	A	155	GLU	CG	36.018	0.000	1
1	A	155	GLU	N	122.904	0.026	1
1	A	156	ASP	H	8.436	0.001	1
1	A	156	ASP	HA	4.588	0.000	1
1	A	156	ASP	HB2	2.621	0.000	2
1	A	156	ASP	HB3	2.554	0.000	2
1	A	156	ASP	C	175.705	0.007	1
1	A	156	ASP	CA	54.175	0.074	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	156	ASP	CB	41.124	0.065	1
1	A	156	ASP	N	122.353	0.026	1
1	A	157	ILE	H	8.156	0.008	1
1	A	157	ILE	HA	4.136	0.000	1
1	A	157	ILE	HB	1.814	0.000	1
1	A	157	ILE	HD11	0.828	0.000	.
1	A	157	ILE	HD12	0.828	0.000	.
1	A	157	ILE	HD13	0.828	0.000	.
1	A	157	ILE	HG12	1.44	0.000	2
1	A	157	ILE	HG13	1.16	0.000	2
1	A	157	ILE	HG21	0.84	0.000	.
1	A	157	ILE	HG22	0.84	0.000	.
1	A	157	ILE	HG23	0.84	0.000	.
1	A	157	ILE	C	176.048	0.002	1
1	A	157	ILE	CA	60.959	0.030	1
1	A	157	ILE	CB	38.605	0.107	1
1	A	157	ILE	CD1	12.691	0.000	1
1	A	157	ILE	CG1	27.163	0.005	1
1	A	157	ILE	CG2	17.558	0.000	1
1	A	157	ILE	N	122.016	0.042	1
1	A	158	ILE	H	8.258	0.001	1
1	A	158	ILE	HA	4.171	0.000	1
1	A	158	ILE	HB	1.822	0.000	1
1	A	158	ILE	HD11	0.816	0.000	.
1	A	158	ILE	HD12	0.816	0.000	.
1	A	158	ILE	HD13	0.816	0.000	.
1	A	158	ILE	HG12	1.41	0.000	2
1	A	158	ILE	HG13	1.14	0.000	2
1	A	158	ILE	HG21	0.855	0.000	.
1	A	158	ILE	HG22	0.855	0.000	.
1	A	158	ILE	HG23	0.855	0.000	.
1	A	158	ILE	C	175.62	0.002	1
1	A	158	ILE	CA	60.621	0.091	1
1	A	158	ILE	CB	38.814	0.099	1
1	A	158	ILE	CD1	12.64	0.000	1
1	A	158	ILE	CG1	27.101	0.027	1
1	A	158	ILE	CG2	17.487	0.000	1
1	A	158	ILE	N	126.22	0.034	1
1	A	159	ASP	H	8.439	0.003	1
1	A	159	ASP	HA	4.62	0.000	1
1	A	159	ASP	HB2	2.7	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	159	ASP	HB3	2.538	0.000	2
1	A	159	ASP	C	175.892	0.005	1
1	A	159	ASP	CA	54.1	0.033	1
1	A	159	ASP	CB	41.321	0.032	1
1	A	159	ASP	N	125.723	0.092	1
1	A	160	GLU	H	8.385	0.001	1
1	A	160	GLU	HA	4.275	0.002	1
1	A	160	GLU	HB2	2.039	0.000	2
1	A	160	GLU	HB3	1.876	0.000	2
1	A	160	GLU	HG2	2.24	0.000	2
1	A	160	GLU	HG3	2.24	0.000	2
1	A	160	GLU	C	176.003	0.005	1
1	A	160	GLU	CA	56.559	0.211	1
1	A	160	GLU	CB	30.548	0.065	1
1	A	160	GLU	CG	35.863	0.000	1
1	A	160	GLU	N	122.221	0.022	1
1	A	161	ASP	H	8.417	0.000	1
1	A	161	ASP	HA	4.607	0.000	1
1	A	161	ASP	HB2	2.707	0.000	2
1	A	161	ASP	HB3	2.597	0.000	2
1	A	161	ASP	C	175.854	0.003	1
1	A	161	ASP	CA	54.282	0.020	1
1	A	161	ASP	CB	41.194	0.032	1
1	A	161	ASP	N	121.726	0.013	1
1	A	162	ASP	H	8.284	0.002	1
1	A	162	ASP	HA	4.591	0.000	1
1	A	162	ASP	HB2	2.639	0.000	2
1	A	162	ASP	HB3	2.639	0.000	2
1	A	162	ASP	C	176.16	0.002	1
1	A	162	ASP	CA	54.248	0.022	1
1	A	162	ASP	CB	41.199	0.009	1
1	A	162	ASP	N	121.406	0.024	1
1	A	163	GLU	H	8.267	0.000	1
1	A	163	GLU	HA	4.201	0.001	1
1	A	163	GLU	HB2	1.885	0.000	2
1	A	163	GLU	HB3	1.885	0.000	2
1	A	163	GLU	HG2	2.198	0.000	2
1	A	163	GLU	HG3	2.198	0.000	2
1	A	163	GLU	C	175.765	0.004	1
1	A	163	GLU	CA	56.529	0.137	1
1	A	163	GLU	CB	30.327	0.022	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	163	GLU	CG	35.736	0.000	1
1	A	163	GLU	N	121.198	0.025	1
1	A	164	ASP	H	8.266	0.000	1
1	A	164	ASP	HA	4.587	0.000	1
1	A	164	ASP	HB2	2.637	0.000	2
1	A	164	ASP	HB3	2.508	0.000	2
1	A	164	ASP	C	175.567	0.003	1
1	A	164	ASP	CA	53.827	0.063	1
1	A	164	ASP	CB	41.141	0.037	1
1	A	164	ASP	N	121.407	0.011	1
1	A	165	TYR	H	8.069	0.005	1
1	A	165	TYR	HA	4.548	0.000	1
1	A	165	TYR	HB2	3.034	0.000	2
1	A	165	TYR	HB3	2.893	0.000	2
1	A	165	TYR	C	175.364	0.002	1
1	A	165	TYR	CA	57.727	0.032	1
1	A	165	TYR	CB	39.054	0.032	1
1	A	165	TYR	N	121.215	0.020	1
1	A	166	ASP	H	8.28	0.002	1
1	A	166	ASP	HA	4.596	0.000	1
1	A	166	ASP	HB2	2.664	0.000	2
1	A	166	ASP	HB3	2.554	0.000	2
1	A	166	ASP	C	175.509	0.004	1
1	A	166	ASP	CA	54.02	0.011	1
1	A	166	ASP	CB	41.315	0.021	1
1	A	166	ASP	N	122.778	0.016	1
1	A	167	ASP	H	8.218	0.002	1
1	A	167	ASP	HA	4.557	0.000	1
1	A	167	ASP	HB2	2.644	0.000	2
1	A	167	ASP	HB3	2.644	0.000	2
1	A	167	ASP	C	176.233	0.004	1
1	A	167	ASP	CA	54.258	0.058	1
1	A	167	ASP	CB	41.175	0.022	1
1	A	167	ASP	N	121.556	0.036	1
1	A	168	GLU	H	8.325	0.000	1
1	A	168	GLU	HA	4.252	0.001	1
1	A	168	GLU	HB2	2.045	0.000	2
1	A	168	GLU	HB3	1.931	0.000	2
1	A	168	GLU	HG2	2.26	0.000	2
1	A	168	GLU	HG3	2.26	0.000	2
1	A	168	GLU	C	176.534	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	168	GLU	CA	56.602	0.075	1
1	A	168	GLU	CB	30.205	0.064	1
1	A	168	GLU	CG	35.912	0.000	1
1	A	168	GLU	N	121.133	0.023	1
1	A	169	GLU	H	8.344	0.001	1
1	A	169	GLU	HA	4.249	0.001	1
1	A	169	GLU	HB2	2.008	0.000	2
1	A	169	GLU	HB3	1.934	0.000	2
1	A	169	GLU	HG2	2.255	0.000	2
1	A	169	GLU	HG3	2.255	0.000	2
1	A	169	GLU	C	176.404	0.001	1
1	A	169	GLU	CA	56.507	0.060	1
1	A	169	GLU	CB	30.339	0.042	1
1	A	169	GLU	CG	35.973	0.000	1
1	A	169	GLU	N	121.871	0.004	1
1	A	170	GLU	H	8.345	0.001	1
1	A	170	GLU	HA	4.238	0.001	1
1	A	170	GLU	HB2	1.989	0.000	2
1	A	170	GLU	HB3	1.925	0.000	2
1	A	170	GLU	HG2	2.247	0.000	2
1	A	170	GLU	HG3	2.247	0.000	2
1	A	170	GLU	C	176.233	0.005	1
1	A	170	GLU	CA	56.463	0.042	1
1	A	170	GLU	CB	30.519	0.091	1
1	A	170	GLU	CG	35.982	0.000	1
1	A	170	GLU	N	122.3	0.023	1
1	A	171	GLU	H	8.394	0.001	1
1	A	171	GLU	HA	4.255	0.003	1
1	A	171	GLU	HB2	1.941	0.000	2
1	A	171	GLU	HB3	1.941	0.000	2
1	A	171	GLU	HG2	2.177	0.000	2
1	A	171	GLU	HG3	2.255	0.000	2
1	A	171	GLU	C	176.044	0.002	1
1	A	171	GLU	CA	56.434	0.040	1
1	A	171	GLU	CB	30.48	0.040	1
1	A	171	GLU	CG	36.04	0.000	1
1	A	171	GLU	N	122.846	0.004	1
1	A	172	ILE	H	8.263	0.001	1
1	A	172	ILE	HA	4.115	0.000	1
1	A	172	ILE	HB	1.844	0.000	1
1	A	172	ILE	HD11	0.831	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	172	ILE	HD12	0.831	0.000	.
1	A	172	ILE	HD13	0.831	0.000	.
1	A	172	ILE	HG12	1.482	0.000	2
1	A	172	ILE	HG13	1.178	0.000	2
1	A	172	ILE	HG21	0.886	0.000	.
1	A	172	ILE	HG22	0.886	0.000	.
1	A	172	ILE	HG23	0.886	0.000	.
1	A	172	ILE	C	175.367	0.004	1
1	A	172	ILE	CA	61.236	0.044	1
1	A	172	ILE	CB	38.174	0.050	1
1	A	172	ILE	CD1	12.514	0.000	1
1	A	172	ILE	CG1	27.209	0.002	1
1	A	172	ILE	CG2	17.465	0.000	1
1	A	172	ILE	N	124.073	0.012	1
1	A	173	LYS	H	7.966	0.003	1
1	A	173	LYS	CA	57.493	0.000	1
1	A	173	LYS	CB	33.9	0.000	1
1	A	173	LYS	N	131.653	0.032	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	172	-0.34 ± 0.20	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	167	0.27 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	170	-0.24 ± 0.16	None needed (< 0.5 ppm)
^{15}N	171	1.16 ± 0.37	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 92%, i.e. 1063 atoms were assigned a chemical shift out of a possible 1152. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	398/400 (100%)	161/162 (99%)	159/160 (99%)	78/78 (100%)
Sidechain	581/645 (90%)	397/417 (95%)	176/206 (85%)	8/22 (36%)
Aromatic	84/107 (79%)	42/52 (81%)	40/49 (82%)	2/6 (33%)
Overall	1063/1152 (92%)	600/631 (95%)	375/415 (90%)	88/106 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1067 atoms were assigned a chemical shift out of a possible 1158. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	402/406 (99%)	163/165 (99%)	161/162 (99%)	78/79 (99%)
Sidechain	581/645 (90%)	397/417 (95%)	176/206 (85%)	8/22 (36%)
Aromatic	84/107 (79%)	42/52 (81%)	40/49 (82%)	2/6 (33%)
Overall	1067/1158 (92%)	602/634 (95%)	377/417 (90%)	88/107 (82%)

7.1.4 Statistically unusual chemical shifts (i)

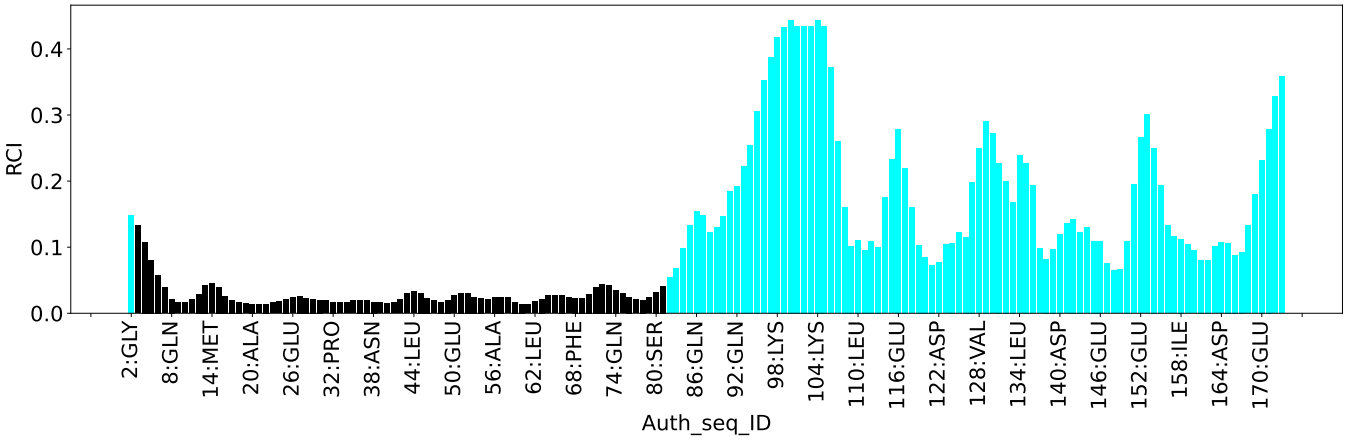
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	78	LEU	H	4.08	5.09 – 11.34	-6.6
1	A	78	LEU	HB3	-0.73	-0.26 – 3.31	-6.3
1	A	62	LEU	HD11	-0.77	-0.61 – 2.12	-5.6
1	A	62	LEU	HD12	-0.77	-0.61 – 2.12	-5.6
1	A	62	LEU	HD13	-0.77	-0.61 – 2.12	-5.6
1	A	62	LEU	HD21	-0.80	-0.65 – 2.13	-5.5
1	A	62	LEU	HD22	-0.80	-0.65 – 2.13	-5.5
1	A	62	LEU	HD23	-0.80	-0.65 – 2.13	-5.5

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.0
0.1
0.2
0.3
0.4
2:GLY
8:GLN
14:MET
20:ALA
26:GLU
32:PRO
38:ASN
44:LEU
50:GLU
56:ALA
62:LEU
68:PHE
74:GLN
80:SER
86:GLN
92:GLN
98:LYS
104:LYS
110:LEU
116:GLU
122:ASP
128:VAL
134:LEU
140:ASP
146:GLU
152:GLU
158:ILE
164:ASP
170:GLU
Auth_seq_ID

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	2520
Intra-residue (|i-j|=0)	836
Sequential (|i-j|=1)	574
Medium range (|i-j|>1 and |i-j|<5)	585
Long range (|i-j|≥5)	525
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	125
Number of unmapped restraints	200
Number of restraints per residue	15.4
Number of long range restraints per residue[1]	3.1

[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)	5.0	0.2
0.2-0.5 (Medium)	0.8	0.5
>0.5 (Large)	0.8	1.67

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)	5.7	4.9
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

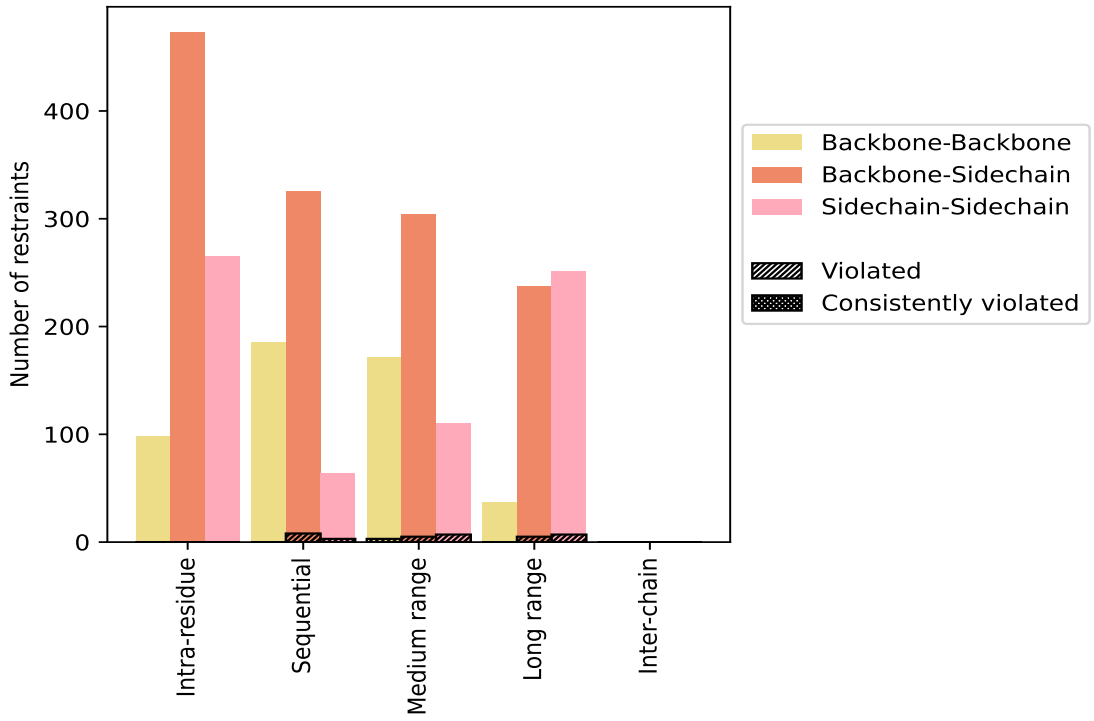
9.1 Summary of distance violations (i)

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)	836	33.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	98	3.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	473	18.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	265	10.5	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	574	22.8	11	1.9	0.4	0	0.0	0.0
Backbone-Backbone	185	7.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	325	12.9	8	2.5	0.3	0	0.0	0.0
Sidechain-Sidechain	64	2.5	3	4.7	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	585	23.2	15	2.6	0.6	0	0.0	0.0
Backbone-Backbone	171	6.8	3	1.8	0.1	0	0.0	0.0
Backbone-Sidechain	304	12.1	5	1.6	0.2	0	0.0	0.0
Sidechain-Sidechain	110	4.4	7	6.4	0.3	0	0.0	0.0
Long range (|i-j|≥5)	525	20.8	12	2.3	0.5	0	0.0	0.0
Backbone-Backbone	37	1.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	237	9.4	5	2.1	0.2	0	0.0	0.0
Sidechain-Sidechain	251	10.0	7	2.8	0.3	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	2520	100.0	38	1.5	1.5	0	0.0	0.0
Backbone-Backbone	491	19.5	3	0.6	0.1	0	0.0	0.0
Backbone-Sidechain	1339	53.1	18	1.3	0.7	0	0.0	0.0
Sidechain-Sidechain	690	27.4	17	2.5	0.7	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	0	1	2	2	0	5	0.3	0.63	0.23	0.12
2	0	0	4	1	0	5	0.15	0.17	0.02	0.16
3	0	1	2	0	0	3	0.63	1.08	0.32	0.47
4	0	1	3	2	0	6	0.19	0.49	0.14	0.12
5	0	0	2	3	0	5	0.26	0.7	0.22	0.15
6	0	2	4	1	0	7	0.32	0.89	0.27	0.17
7	0	3	5	0	0	8	0.25	0.79	0.21	0.15
8	0	2	4	2	0	8	0.16	0.24	0.04	0.16
9	0	0	2	3	0	5	0.14	0.21	0.04	0.13
10	0	1	3	4	0	8	0.14	0.17	0.02	0.14
11	0	0	5	1	0	6	0.26	0.75	0.22	0.15

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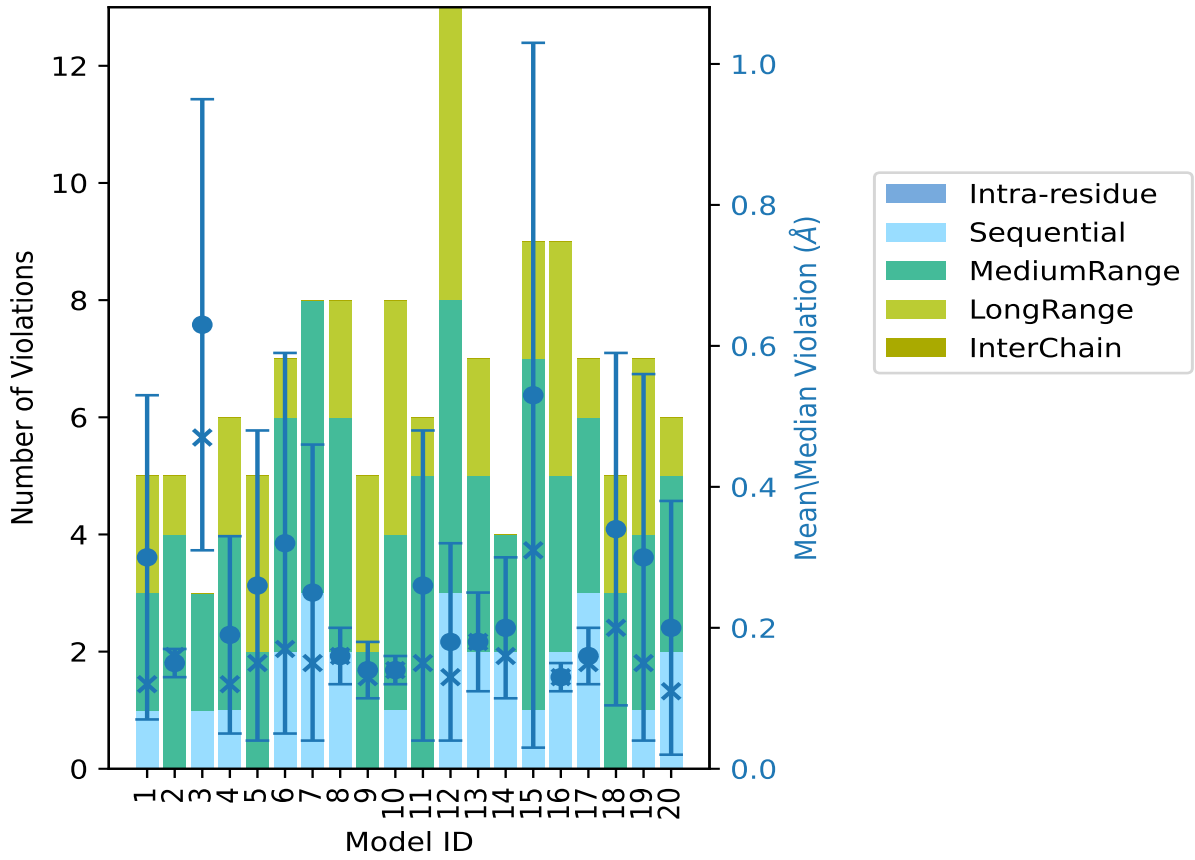
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	3	5	5	0	13	0.18	0.68	0.14	0.13
13	0	2	3	2	0	7	0.18	0.32	0.07	0.18
14	0	2	2	0	0	4	0.2	0.38	0.1	0.16
15	0	1	6	2	0	9	0.53	1.67	0.5	0.31
16	0	2	3	4	0	9	0.13	0.16	0.02	0.13
17	0	3	3	1	0	7	0.16	0.25	0.04	0.15
18	0	0	3	2	0	5	0.34	0.77	0.25	0.2
19	0	1	3	3	0	7	0.3	0.72	0.26	0.15
20	0	2	3	1	0	6	0.2	0.59	0.18	0.11

[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

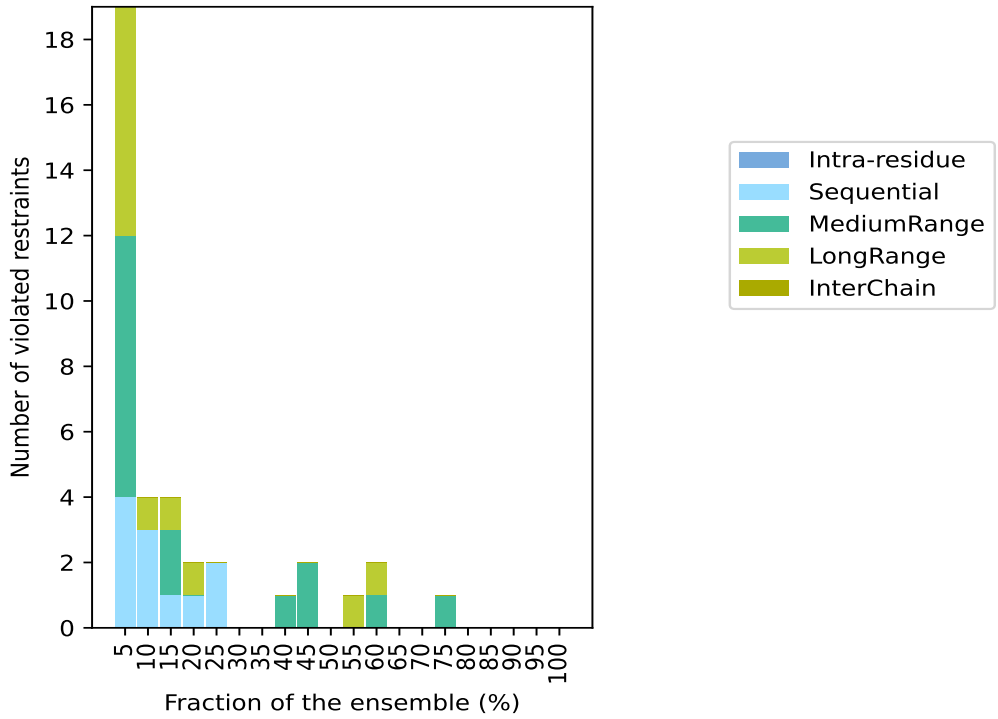
9.3 Distance violation statistics for the ensemble (i)

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, 2482(IR:836, SQ:563, MR:570, LR:513, 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	8	7	0	19	1	5.0
0	3	0	1	0	4	2	10.0
0	1	2	1	0	4	3	15.0
0	1	0	1	0	2	4	20.0
0	2	0	0	0	2	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	1	0	0	1	8	40.0
0	0	2	0	0	2	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	1	0	1	11	55.0
0	0	1	1	0	2	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	1	0	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

[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

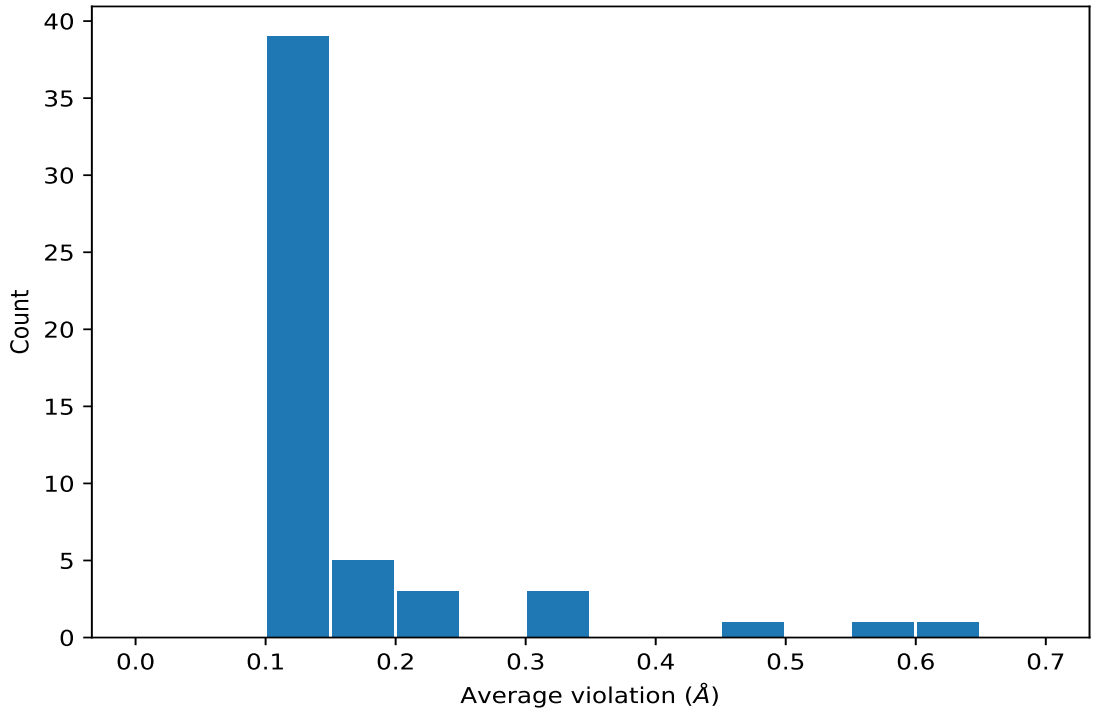
9.3.1 Bar graph : Distance violation statistics for the ensemble



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)
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	15	0.46	0.23	0.38
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	12	0.64	0.42	0.62
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	12	0.13	0.02	0.12
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	11	0.15	0.02	0.15
(1,1002)	1:A:70:ALA:HB2	1:A:73:ASP:HA	9	0.2	0.05	0.17
(1,1002)	1:A:70:ALA:HB1	1:A:73:ASP:HA	9	0.2	0.05	0.17
(1,1002)	1:A:70:ALA:HB3	1:A:73:ASP:HA	9	0.2	0.05	0.17
(1,1737)	1:A:45:GLY:H	1:A:42:SER:HA	9	0.15	0.02	0.16
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD22	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD21	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD23	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD12	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD11	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD13	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD22	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD21	8	0.14	0.02	0.15

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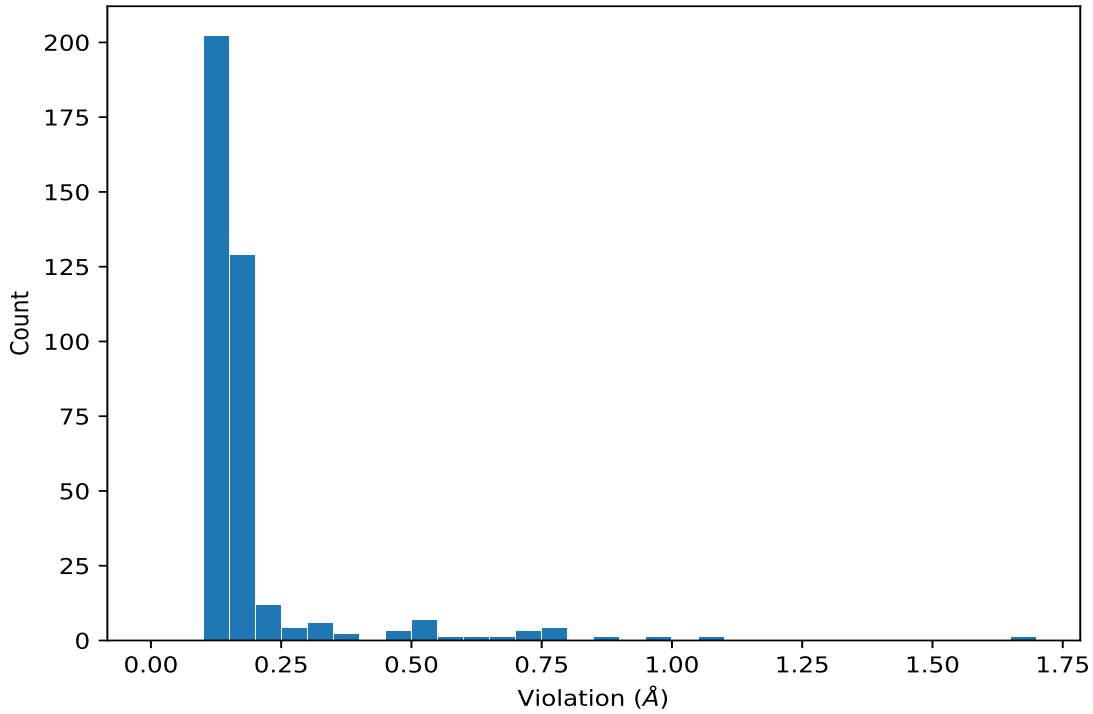
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD23	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD12	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD11	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD13	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD22	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD21	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD23	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD12	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD11	8	0.14	0.02	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD13	8	0.14	0.02	0.15
(1,792)	1:A:3:ILE:HG22	1:A:2:GLY:HA2	5	0.31	0.17	0.23
(1,792)	1:A:3:ILE:HG21	1:A:2:GLY:HA2	5	0.31	0.17	0.23
(1,792)	1:A:3:ILE:HG23	1:A:2:GLY:HA2	5	0.31	0.17	0.23
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB2	5	0.12	0.01	0.12
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB3	5	0.12	0.01	0.12
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB2	5	0.12	0.01	0.12
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB3	5	0.12	0.01	0.12
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB2	5	0.12	0.01	0.12
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB3	5	0.12	0.01	0.12
(1,811)	1:A:10:GLU:H	1:A:9:GLU:HG3	4	0.13	0.02	0.12
(1,1154)	1:A:38:ASN:HD21	1:A:48:LYS:HE2	4	0.12	0.01	0.12
(1,1154)	1:A:38:ASN:HD21	1:A:48:LYS:HE3	4	0.12	0.01	0.12
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD22	3	0.14	0.01	0.13
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD21	3	0.14	0.01	0.13
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD23	3	0.14	0.01	0.13
(1,509)	1:A:48:LYS:HG2	1:A:50:GLU:HG2	3	0.13	0.02	0.14
(1,509)	1:A:48:LYS:HG3	1:A:50:GLU:HG2	3	0.13	0.02	0.14
(1,1816)	1:A:74:GLN:HE22	1:A:75:THR:H	3	0.12	0.01	0.12
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD12	3	0.12	0.01	0.11
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD11	3	0.12	0.01	0.11
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD13	3	0.12	0.01	0.11
(1,5)	1:A:3:ILE:HB	1:A:2:GLY:HA2	2	0.57	0.11	0.57
(1,145)	1:A:16:LEU:HD22	1:A:17:VAL:HB	2	0.17	0.01	0.17
(1,145)	1:A:16:LEU:HD21	1:A:17:VAL:HB	2	0.17	0.01	0.17
(1,145)	1:A:16:LEU:HD23	1:A:17:VAL:HB	2	0.17	0.01	0.17
(1,806)	1:A:8:GLN:HG3	1:A:7:SER:HA	2	0.13	0.02	0.13
(1,2058)	1:A:81:TRP:HE3	1:A:71:LEU:HB2	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)
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	15	1.67
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	3	1.08
(1,1085)	1:A:2:GLY:HA3	1:A:5:GLN:HG2	15	0.99
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	6	0.89
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	7	0.79
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	18	0.77
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	15	0.76
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	11	0.75
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	19	0.72
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	19	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	5	0.7
(1,5)	1:A:3:ILE:HB	1:A:2:GLY:HA2	12	0.68
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	1	0.63
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	20	0.59
(1,792)	1:A:3:ILE:HG22	1:A:2:GLY:HA2	15	0.54
(1,792)	1:A:3:ILE:HG21	1:A:2:GLY:HA2	15	0.54
(1,792)	1:A:3:ILE:HG23	1:A:2:GLY:HA2	15	0.54
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	1	0.53
(1,792)	1:A:3:ILE:HG22	1:A:2:GLY:HA2	6	0.5
(1,792)	1:A:3:ILE:HG21	1:A:2:GLY:HA2	6	0.5
(1,792)	1:A:3:ILE:HG23	1:A:2:GLY:HA2	6	0.5
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	4	0.49
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	18	0.49
(1,5)	1:A:3:ILE:HB	1:A:2:GLY:HA2	3	0.47
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	14	0.38
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	6	0.37
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	3	0.34
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	13	0.32
(1,1002)	1:A:70:ALA:HB2	1:A:73:ASP:HA	7	0.31
(1,1002)	1:A:70:ALA:HB1	1:A:73:ASP:HA	7	0.31
(1,1002)	1:A:70:ALA:HB3	1:A:73:ASP:HA	7	0.31
(1,1)	1:A:2:GLY:HA3	1:A:5:GLN:H	15	0.31
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	11	0.28
(1,1002)	1:A:70:ALA:HB2	1:A:73:ASP:HA	17	0.25
(1,1002)	1:A:70:ALA:HB1	1:A:73:ASP:HA	17	0.25
(1,1002)	1:A:70:ALA:HB3	1:A:73:ASP:HA	17	0.25
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	8	0.24
(1,792)	1:A:3:ILE:HG22	1:A:2:GLY:HA2	13	0.23
(1,792)	1:A:3:ILE:HG21	1:A:2:GLY:HA2	13	0.23
(1,792)	1:A:3:ILE:HG23	1:A:2:GLY:HA2	13	0.23
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	7	0.23
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	5	0.22
(1,1002)	1:A:70:ALA:HB2	1:A:73:ASP:HA	9	0.21
(1,1002)	1:A:70:ALA:HB1	1:A:73:ASP:HA	9	0.21
(1,1002)	1:A:70:ALA:HB3	1:A:73:ASP:HA	9	0.21
(1,1002)	1:A:70:ALA:HB2	1:A:73:ASP:HA	18	0.2
(1,1002)	1:A:70:ALA:HB1	1:A:73:ASP:HA	18	0.2
(1,1002)	1:A:70:ALA:HB3	1:A:73:ASP:HA	18	0.2
(1,1737)	1:A:45:GLY:H	1:A:42:SER:HA	19	0.19
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	13	0.18
(1,145)	1:A:16:LEU:HD22	1:A:17:VAL:HB	13	0.18
(1,145)	1:A:16:LEU:HD21	1:A:17:VAL:HB	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,145)	1:A:16:LEU:HD23	1:A:17:VAL:HB	13	0.18
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	12	0.18
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD22	8	0.17
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD21	8	0.17
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD23	8	0.17
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD12	8	0.17
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD11	8	0.17
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD13	8	0.17
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD22	8	0.17
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD21	8	0.17
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD23	8	0.17
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD12	8	0.17
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD11	8	0.17
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD13	8	0.17
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD22	8	0.17
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD21	8	0.17
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD23	8	0.17
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD12	8	0.17
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD11	8	0.17
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD13	8	0.17
(1,811)	1:A:10:GLU:H	1:A:9:GLU:HG3	14	0.17
(1,792)	1:A:3:ILE:HG22	1:A:2:GLY:HA2	12	0.17
(1,792)	1:A:3:ILE:HG21	1:A:2:GLY:HA2	12	0.17
(1,792)	1:A:3:ILE:HG23	1:A:2:GLY:HA2	12	0.17
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	2	0.17
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	8	0.17
(1,1737)	1:A:45:GLY:H	1:A:42:SER:HA	10	0.17
(1,1737)	1:A:45:GLY:H	1:A:42:SER:HA	17	0.17
(1,1170)	1:A:49:GLU:HG3	1:A:47:LYS:HD2	6	0.17
(1,1170)	1:A:49:GLU:HG3	1:A:47:LYS:HD3	6	0.17
(1,1002)	1:A:70:ALA:HB2	1:A:73:ASP:HA	8	0.17
(1,1002)	1:A:70:ALA:HB1	1:A:73:ASP:HA	8	0.17
(1,1002)	1:A:70:ALA:HB3	1:A:73:ASP:HA	8	0.17
(1,1002)	1:A:70:ALA:HB2	1:A:73:ASP:HA	12	0.17
(1,1002)	1:A:70:ALA:HB1	1:A:73:ASP:HA	12	0.17
(1,1002)	1:A:70:ALA:HB3	1:A:73:ASP:HA	12	0.17
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD22	7	0.16
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD21	7	0.16
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD23	7	0.16
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD12	7	0.16
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD11	7	0.16
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD13	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD22	7	0.16
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD21	7	0.16
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD23	7	0.16
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD12	7	0.16
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD11	7	0.16
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD13	7	0.16
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD22	7	0.16
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD21	7	0.16
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD23	7	0.16
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD12	7	0.16
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD11	7	0.16
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD13	7	0.16
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	17	0.16
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	20	0.16
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	2	0.16
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	10	0.16
(1,1737)	1:A:45:GLY:H	1:A:42:SER:HA	4	0.16
(1,1737)	1:A:45:GLY:H	1:A:42:SER:HA	12	0.16
(1,145)	1:A:16:LEU:HD22	1:A:17:VAL:HB	8	0.16
(1,145)	1:A:16:LEU:HD21	1:A:17:VAL:HB	8	0.16
(1,145)	1:A:16:LEU:HD23	1:A:17:VAL:HB	8	0.16
(1,1086)	1:A:2:GLY:HA3	1:A:5:GLN:HG3	2	0.16
(1,1002)	1:A:70:ALA:HB2	1:A:73:ASP:HA	16	0.16
(1,1002)	1:A:70:ALA:HB1	1:A:73:ASP:HA	16	0.16
(1,1002)	1:A:70:ALA:HB3	1:A:73:ASP:HA	16	0.16
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD22	12	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD21	12	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD23	12	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD12	12	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD11	12	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD13	12	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD22	12	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD21	12	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD23	12	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD12	12	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD11	12	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD13	12	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD22	12	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD21	12	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD23	12	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD12	12	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD11	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD13	12	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD22	16	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD21	16	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD23	16	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD12	16	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD11	16	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD13	16	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD22	16	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD21	16	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD23	16	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD12	16	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD11	16	0.15
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD13	16	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD22	16	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD21	16	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD23	16	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD12	16	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD11	16	0.15
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD13	16	0.15
(1,806)	1:A:8:GLN:HG3	1:A:7:SER:HA	17	0.15
(1,509)	1:A:48:LYS:HG2	1:A:50:GLU:HG2	2	0.15
(1,509)	1:A:48:LYS:HG3	1:A:50:GLU:HG2	2	0.15
(1,49)	1:A:8:GLN:HG2	1:A:44:LEU:HD22	10	0.15
(1,49)	1:A:8:GLN:HG2	1:A:44:LEU:HD21	10	0.15
(1,49)	1:A:8:GLN:HG2	1:A:44:LEU:HD23	10	0.15
(1,49)	1:A:8:GLN:HG2	1:A:44:LEU:HD12	10	0.15
(1,49)	1:A:8:GLN:HG2	1:A:44:LEU:HD11	10	0.15
(1,49)	1:A:8:GLN:HG2	1:A:44:LEU:HD13	10	0.15
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	15	0.15
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	19	0.15
(1,1737)	1:A:45:GLY:H	1:A:42:SER:HA	11	0.15
(1,1737)	1:A:45:GLY:H	1:A:42:SER:HA	16	0.15
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD22	5	0.15
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD21	5	0.15
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD23	5	0.15
(1,1002)	1:A:70:ALA:HB2	1:A:73:ASP:HA	11	0.15
(1,1002)	1:A:70:ALA:HB1	1:A:73:ASP:HA	11	0.15
(1,1002)	1:A:70:ALA:HB3	1:A:73:ASP:HA	11	0.15
(1,1002)	1:A:70:ALA:HB2	1:A:73:ASP:HA	13	0.15
(1,1002)	1:A:70:ALA:HB1	1:A:73:ASP:HA	13	0.15
(1,1002)	1:A:70:ALA:HB3	1:A:73:ASP:HA	13	0.15
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD22	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD21	9	0.14
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD23	9	0.14
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD12	9	0.14
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD11	9	0.14
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD13	9	0.14
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD22	9	0.14
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD21	9	0.14
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD23	9	0.14
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD12	9	0.14
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD11	9	0.14
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD13	9	0.14
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD22	9	0.14
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD21	9	0.14
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD23	9	0.14
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD12	9	0.14
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD11	9	0.14
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD13	9	0.14
(1,924)	1:A:46:VAL:HG22	1:A:42:SER:HA	7	0.14
(1,924)	1:A:46:VAL:HG21	1:A:42:SER:HA	7	0.14
(1,924)	1:A:46:VAL:HG23	1:A:42:SER:HA	7	0.14
(1,509)	1:A:48:LYS:HG2	1:A:50:GLU:HG2	10	0.14
(1,509)	1:A:48:LYS:HG3	1:A:50:GLU:HG2	10	0.14
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	5	0.14
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	11	0.14
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	16	0.14
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB2	14	0.14
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB3	14	0.14
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB2	14	0.14
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB3	14	0.14
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB2	14	0.14
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB3	14	0.14
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD22	10	0.13
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD21	10	0.13
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD23	10	0.13
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD12	10	0.13
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD11	10	0.13
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD13	10	0.13
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD22	10	0.13
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD21	10	0.13
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD23	10	0.13
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD12	10	0.13
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD11	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD13	10	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD22	10	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD21	10	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD23	10	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD12	10	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD11	10	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD13	10	0.13
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD22	17	0.13
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD21	17	0.13
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD23	17	0.13
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD12	17	0.13
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD11	17	0.13
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD13	17	0.13
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD22	17	0.13
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD21	17	0.13
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD23	17	0.13
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD12	17	0.13
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD11	17	0.13
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD13	17	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD22	17	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD21	17	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD23	17	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD12	17	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD11	17	0.13
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD13	17	0.13
(1,811)	1:A:10:GLU:H	1:A:9:GLU:HG3	12	0.13
(1,656)	1:A:68:PHE:HA	1:A:79:ARG:HB3	12	0.13
(1,53)	1:A:8:GLN:HG3	1:A:44:LEU:HD22	4	0.13
(1,53)	1:A:8:GLN:HG3	1:A:44:LEU:HD21	4	0.13
(1,53)	1:A:8:GLN:HG3	1:A:44:LEU:HD23	4	0.13
(1,53)	1:A:8:GLN:HG3	1:A:44:LEU:HD12	4	0.13
(1,53)	1:A:8:GLN:HG3	1:A:44:LEU:HD11	4	0.13
(1,53)	1:A:8:GLN:HG3	1:A:44:LEU:HD13	4	0.13
(1,510)	1:A:38:ASN:H	1:A:48:LYS:HD2	12	0.13
(1,510)	1:A:38:ASN:H	1:A:48:LYS:HD3	12	0.13
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD12	14	0.13
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD11	14	0.13
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD13	14	0.13
(1,2340)	1:A:82:TYR:H	1:A:79:ARG:HD2	12	0.13
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	9	0.13
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	12	0.13
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1816)	1:A:74:GLN:HE22	1:A:75:THR:H	8	0.13
(1,1154)	1:A:38:ASN:HD21	1:A:48:LYS:HE2	16	0.13
(1,1154)	1:A:38:ASN:HD21	1:A:48:LYS:HE3	16	0.13
(1,1154)	1:A:38:ASN:HD21	1:A:48:LYS:HE2	18	0.13
(1,1154)	1:A:38:ASN:HD21	1:A:48:LYS:HE3	18	0.13
(1,1082)	1:A:62:LEU:HD22	1:A:33:PHE:HB2	16	0.13
(1,1082)	1:A:62:LEU:HD21	1:A:33:PHE:HB2	16	0.13
(1,1082)	1:A:62:LEU:HD23	1:A:33:PHE:HB2	16	0.13
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD22	8	0.13
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD21	8	0.13
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD23	8	0.13
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD22	10	0.13
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD21	10	0.13
(1,1019)	1:A:30:PRO:HB2	1:A:71:LEU:HD23	10	0.13
(1,811)	1:A:10:GLU:H	1:A:9:GLU:HG3	7	0.12
(1,792)	1:A:3:ILE:HG22	1:A:2:GLY:HA2	7	0.12
(1,792)	1:A:3:ILE:HG21	1:A:2:GLY:HA2	7	0.12
(1,792)	1:A:3:ILE:HG23	1:A:2:GLY:HA2	7	0.12
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	15	0.12
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	16	0.12
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	19	0.12
(1,2058)	1:A:81:TRP:HE3	1:A:71:LEU:HB2	12	0.12
(1,1816)	1:A:74:GLN:HE22	1:A:75:THR:H	4	0.12
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	1	0.12
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	9	0.12
(1,1737)	1:A:45:GLY:H	1:A:42:SER:HA	8	0.12
(1,1737)	1:A:45:GLY:H	1:A:42:SER:HA	15	0.12
(1,1304)	1:A:54:ARG:HD3	1:A:51:LEU:HB3	6	0.12
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB2	1	0.12
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB3	1	0.12
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB2	1	0.12
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB3	1	0.12
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB2	1	0.12
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB3	1	0.12
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB2	17	0.12
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB3	17	0.12
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB2	17	0.12
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB3	17	0.12
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB2	17	0.12
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB3	17	0.12
(1,935)	1:A:48:LYS:HD2	1:A:37:LEU:HD22	10	0.11
(1,935)	1:A:48:LYS:HD2	1:A:37:LEU:HD21	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,935)	1:A:48:LYS:HD2	1:A:37:LEU:HD23	10	0.11
(1,935)	1:A:48:LYS:HD2	1:A:37:LEU:HD12	10	0.11
(1,935)	1:A:48:LYS:HD2	1:A:37:LEU:HD11	10	0.11
(1,935)	1:A:48:LYS:HD2	1:A:37:LEU:HD13	10	0.11
(1,935)	1:A:48:LYS:HD3	1:A:37:LEU:HD22	10	0.11
(1,935)	1:A:48:LYS:HD3	1:A:37:LEU:HD21	10	0.11
(1,935)	1:A:48:LYS:HD3	1:A:37:LEU:HD23	10	0.11
(1,935)	1:A:48:LYS:HD3	1:A:37:LEU:HD12	10	0.11
(1,935)	1:A:48:LYS:HD3	1:A:37:LEU:HD11	10	0.11
(1,935)	1:A:48:LYS:HD3	1:A:37:LEU:HD13	10	0.11
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD22	4	0.11
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD21	4	0.11
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD23	4	0.11
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD12	4	0.11
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD11	4	0.11
(1,927)	1:A:41:ALA:HB2	1:A:44:LEU:HD13	4	0.11
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD22	4	0.11
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD21	4	0.11
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD23	4	0.11
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD12	4	0.11
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD11	4	0.11
(1,927)	1:A:41:ALA:HB1	1:A:44:LEU:HD13	4	0.11
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD22	4	0.11
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD21	4	0.11
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD23	4	0.11
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD12	4	0.11
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD11	4	0.11
(1,927)	1:A:41:ALA:HB3	1:A:44:LEU:HD13	4	0.11
(1,811)	1:A:10:GLU:H	1:A:9:GLU:HG3	19	0.11
(1,806)	1:A:8:GLN:HG3	1:A:7:SER:HA	6	0.11
(1,711)	1:A:74:GLN:H	1:A:75:THR:HG21	7	0.11
(1,711)	1:A:74:GLN:H	1:A:75:THR:HG22	7	0.11
(1,711)	1:A:74:GLN:H	1:A:75:THR:HG23	7	0.11
(1,509)	1:A:48:LYS:HG2	1:A:50:GLU:HG2	20	0.11
(1,509)	1:A:48:LYS:HG3	1:A:50:GLU:HG2	20	0.11
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD12	2	0.11
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD11	2	0.11
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD13	2	0.11
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD12	20	0.11
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD11	20	0.11
(1,48)	1:A:8:GLN:HG2	1:A:11:LEU:HD13	20	0.11
(1,2319)	1:A:48:LYS:H	1:A:55:ILE:HD12	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2319)	1:A:48:LYS:H	1:A:55:ILE:HD11	9	0.11
(1,2319)	1:A:48:LYS:H	1:A:55:ILE:HD13	9	0.11
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	1	0.11
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	4	0.11
(1,2248)	1:A:35:GLU:H	1:A:23:LEU:HG	6	0.11
(1,2171)	1:A:39:GLU:H	1:A:40:ILE:HB	20	0.11
(1,2074)	1:A:6:TYR:H	1:A:2:GLY:HA3	13	0.11
(1,2058)	1:A:81:TRP:HE3	1:A:71:LEU:HB2	19	0.11
(1,1816)	1:A:74:GLN:HE22	1:A:75:THR:H	17	0.11
(1,1795)	1:A:5:GLN:HE21	1:A:6:TYR:HD1	16	0.11
(1,1795)	1:A:5:GLN:HE21	1:A:6:TYR:HD2	16	0.11
(1,1740)	1:A:45:GLY:H	1:A:10:GLU:HB3	12	0.11
(1,1578)	1:A:10:GLU:HB2	1:A:6:TYR:HD1	15	0.11
(1,1578)	1:A:10:GLU:HB2	1:A:6:TYR:HD2	15	0.11
(1,1270)	1:A:47:LYS:HD2	1:A:50:GLU:HG2	11	0.11
(1,1270)	1:A:47:LYS:HD3	1:A:50:GLU:HG2	11	0.11
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB2	10	0.11
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB3	10	0.11
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB2	10	0.11
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB3	10	0.11
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB2	10	0.11
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB3	10	0.11
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB2	20	0.11
(1,1197)	1:A:23:LEU:HD22	1:A:22:GLU:HB3	20	0.11
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB2	20	0.11
(1,1197)	1:A:23:LEU:HD21	1:A:22:GLU:HB3	20	0.11
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB2	20	0.11
(1,1197)	1:A:23:LEU:HD23	1:A:22:GLU:HB3	20	0.11
(1,1154)	1:A:38:ASN:HD21	1:A:48:LYS:HE2	5	0.11
(1,1154)	1:A:38:ASN:HD21	1:A:48:LYS:HE3	5	0.11
(1,1154)	1:A:38:ASN:HD21	1:A:48:LYS:HE2	13	0.11
(1,1154)	1:A:38:ASN:HD21	1:A:48:LYS:HE3	13	0.11
(1,1109)	1:A:5:GLN:HG2	1:A:6:TYR:HA	16	0.11

10 Dihedral-angle violation analysis

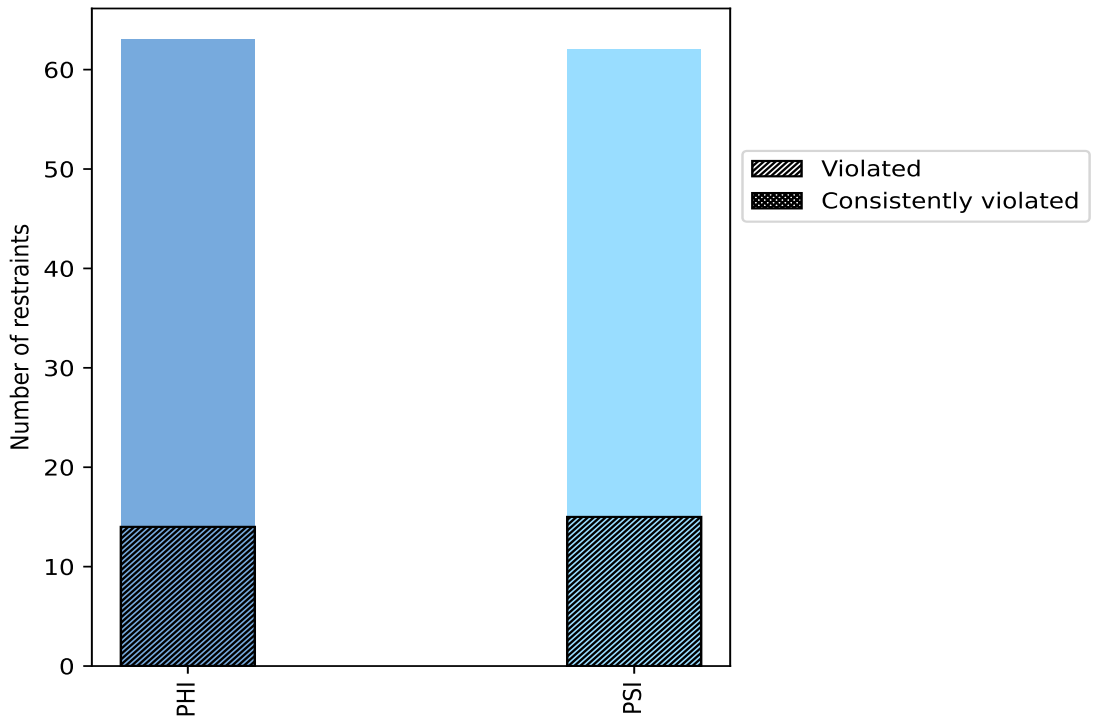
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	63	50.4	14	22.2	11.2	0	0.0	0.0
PSI	62	49.6	15	24.2	12.0	0	0.0	0.0
Total	125	100.0	29	23.2	23.2	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



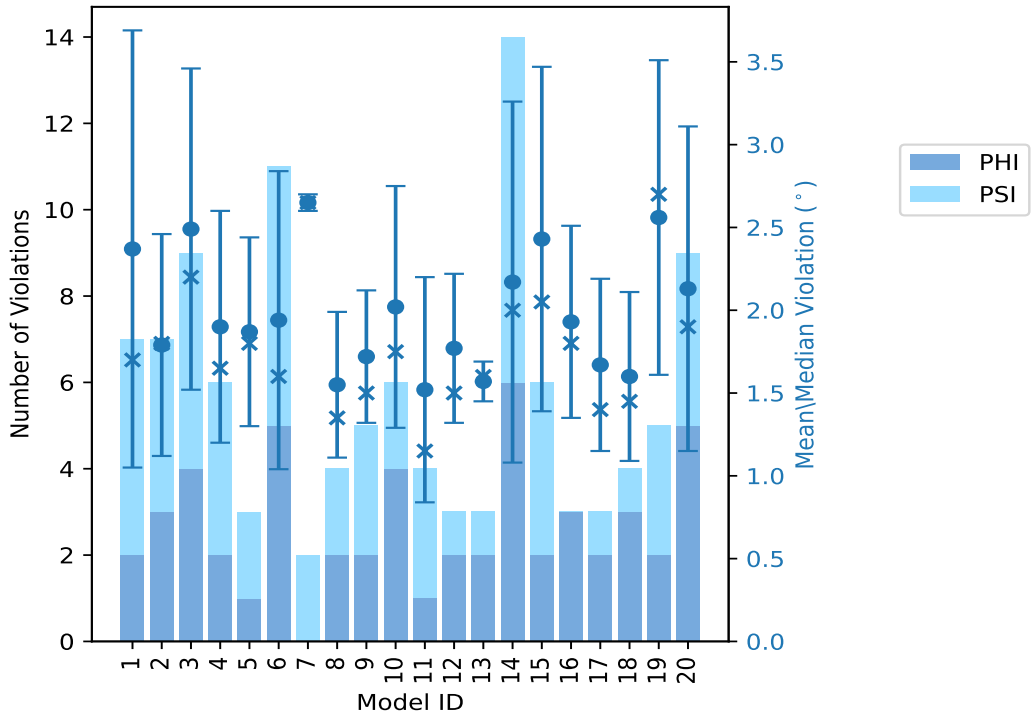
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	2	5	7	2.37	4.9	1.32	1.7
2	3	4	7	1.79	3.2	0.67	1.8
3	4	5	9	2.49	4.2	0.97	2.2
4	2	4	6	1.9	3.2	0.7	1.65
5	1	2	3	1.87	2.6	0.57	1.8
6	5	6	11	1.94	4.2	0.9	1.6
7	0	2	2	2.65	2.7	0.05	2.65
8	2	2	4	1.55	2.3	0.44	1.35
9	2	3	5	1.72	2.5	0.4	1.5
10	4	2	6	2.02	3.5	0.73	1.75
11	1	3	4	1.52	2.7	0.68	1.15
12	2	1	3	1.77	2.4	0.45	1.5
13	2	1	3	1.57	1.7	0.12	1.6
14	6	8	14	2.17	4.8	1.09	2.0
15	2	4	6	2.43	4.0	1.04	2.05
16	3	0	3	1.93	2.7	0.58	1.8
17	2	1	3	1.67	2.4	0.52	1.4
18	3	1	4	1.6	2.4	0.51	1.45
19	2	3	5	2.56	3.8	0.95	2.7
20	5	4	9	2.13	4.5	0.98	1.9

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

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

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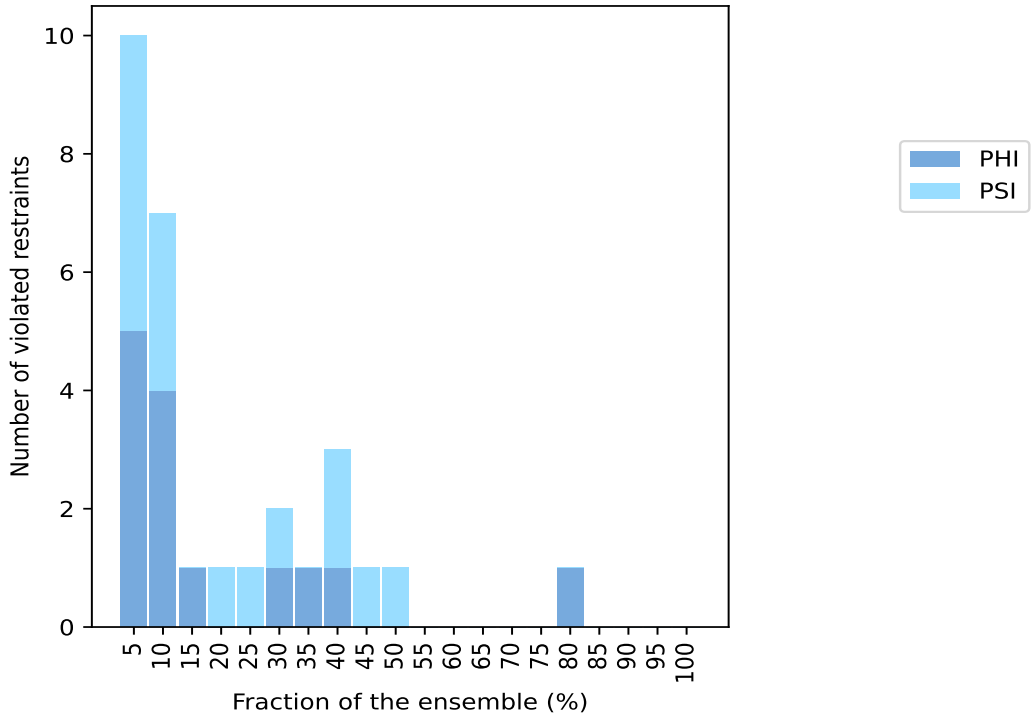
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

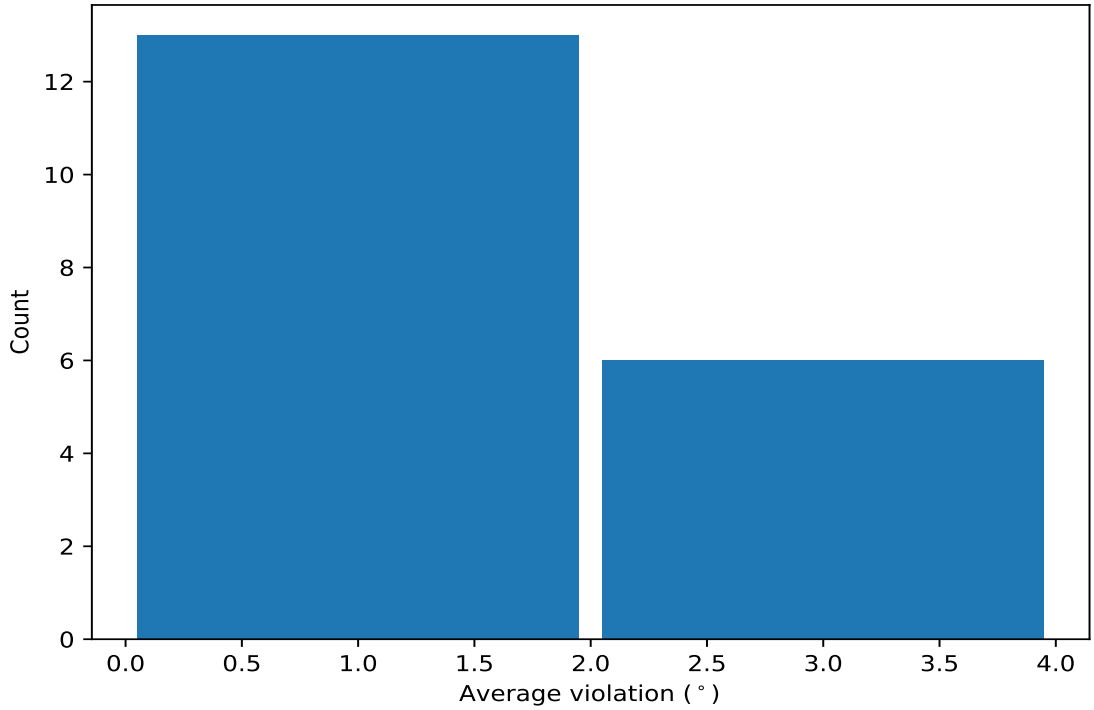


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

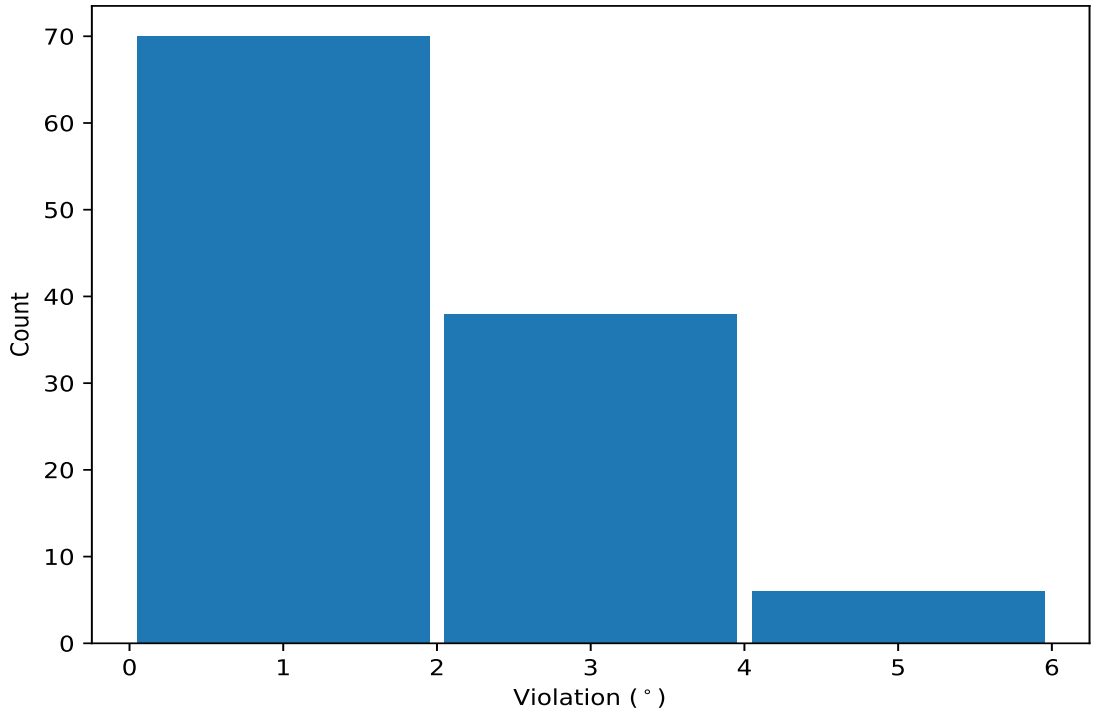
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	16	2.08	0.54	1.95
(1,97)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:SER:N	10	1.94	0.61	1.85
(1,106)	1:A:54:ARG:N	1:A:54:ARG:CA	1:A:54:ARG:C	1:A:55:ILE:N	9	1.68	0.5	1.6
(1,120)	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	1:A:74:GLN:N	8	3.48	1.09	3.5
(1,119)	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	1:A:73:ASP:N	8	3.31	0.79	3.7
(1,58)	1:A:72:SER:C	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	8	2.79	1.17	2.85
(1,59)	1:A:75:THR:C	1:A:76:TRP:N	1:A:76:TRP:CA	1:A:76:TRP:C	7	1.47	0.23	1.5
(1,57)	1:A:71:LEU:C	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	6	1.85	0.38	1.9
(1,66)	1:A:8:GLN:N	1:A:8:GLN:CA	1:A:8:GLN:C	1:A:9:GLU:N	6	1.57	0.35	1.5
(1,101)	1:A:48:LYS:N	1:A:48:LYS:CA	1:A:48:LYS:C	1:A:49:GLU:N	5	2.16	0.53	2.4
(1,72)	1:A:15:ALA:N	1:A:15:ALA:CA	1:A:15:ALA:C	1:A:16:LEU:N	4	2.17	0.79	1.9
(1,28)	1:A:34:GLN:C	1:A:35:GLU:N	1:A:35:GLU:CA	1:A:35:GLU:C	3	1.3	0.08	1.3
(1,60)	1:A:78:LEU:C	1:A:79:ARG:N	1:A:79:ARG:CA	1:A:79:ARG:C	2	1.55	0.15	1.55
(1,68)	1:A:10:GLU:N	1:A:10:GLU:CA	1:A:10:GLU:C	1:A:11:LEU:N	2	1.45	0.15	1.45
(1,70)	1:A:12:LYS:N	1:A:12:LYS:CA	1:A:12:LYS:C	1:A:13:GLU:N	2	1.45	0.35	1.45
(1,10)	1:A:15:ALA:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	2	1.3	0.2	1.3
(1,98)	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	1:A:43:LEU:N	2	1.3	0.0	1.3
(1,22)	1:A:28:LYS:C	1:A:29:LYS:N	1:A:29:LYS:CA	1:A:29:LYS:C	2	1.15	0.05	1.15
(1,53)	1:A:61:ASP:C	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	2	1.15	0.05	1.15

[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 (°)
(1,120)	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	1:A:74:GLN:N	1	4.9
(1,120)	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	1:A:74:GLN:N	14	4.8
(1,58)	1:A:72:SER:C	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	20	4.5
(1,120)	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	1:A:74:GLN:N	3	4.2
(1,119)	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	1:A:73:ASP:N	6	4.2
(1,58)	1:A:72:SER:C	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	15	4.0
(1,119)	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	1:A:73:ASP:N	1	3.9
(1,119)	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	1:A:73:ASP:N	3	3.9
(1,120)	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	1:A:74:GLN:N	19	3.8
(1,58)	1:A:72:SER:C	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	14	3.7
(1,119)	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	1:A:73:ASP:N	14	3.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,119)	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	1:A:73:ASP:N	15	3.7
(1,72)	1:A:15:ALA:N	1:A:15:ALA:CA	1:A:15:ALA:C	1:A:16:LEU:N	10	3.5
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	19	3.3
(1,97)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:SER:N	4	3.2
(1,58)	1:A:72:SER:C	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	3	3.2
(1,120)	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	1:A:74:GLN:N	2	3.2
(1,120)	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	1:A:74:GLN:N	6	3.0
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	11	2.7
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	16	2.7
(1,119)	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	1:A:73:ASP:N	19	2.7
(1,101)	1:A:48:LYS:N	1:A:48:LYS:CA	1:A:48:LYS:C	1:A:49:GLU:N	7	2.7
(1,97)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:SER:N	7	2.6
(1,119)	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	1:A:73:ASP:N	20	2.6
(1,106)	1:A:54:ARG:N	1:A:54:ARG:CA	1:A:54:ARG:C	1:A:55:ILE:N	5	2.6
(1,58)	1:A:72:SER:C	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	6	2.5
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	9	2.5
(1,101)	1:A:48:LYS:N	1:A:48:LYS:CA	1:A:48:LYS:C	1:A:49:GLU:N	20	2.5
(1,57)	1:A:71:LEU:C	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	20	2.4
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	12	2.4
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	17	2.4
(1,106)	1:A:54:ARG:N	1:A:54:ARG:CA	1:A:54:ARG:C	1:A:55:ILE:N	18	2.4
(1,101)	1:A:48:LYS:N	1:A:48:LYS:CA	1:A:48:LYS:C	1:A:49:GLU:N	4	2.4
(1,97)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:SER:N	8	2.3
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	10	2.3
(1,3)	1:A:7:SER:C	1:A:8:GLN:N	1:A:8:GLN:CA	1:A:8:GLN:C	14	2.3
(1,97)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:SER:N	3	2.2
(1,66)	1:A:8:GLN:N	1:A:8:GLN:CA	1:A:8:GLN:C	1:A:9:GLU:N	3	2.2
(1,120)	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	1:A:74:GLN:N	15	2.2
(1,57)	1:A:71:LEU:C	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	2	2.1
(1,72)	1:A:15:ALA:N	1:A:15:ALA:CA	1:A:15:ALA:C	1:A:16:LEU:N	14	2.0
(1,57)	1:A:71:LEU:C	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	14	2.0
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	14	2.0
(1,101)	1:A:48:LYS:N	1:A:48:LYS:CA	1:A:48:LYS:C	1:A:49:GLU:N	14	2.0
(1,97)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:SER:N	15	1.9
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	3	1.9
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	20	1.9
(1,97)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:SER:N	5	1.8
(1,72)	1:A:15:ALA:N	1:A:15:ALA:CA	1:A:15:ALA:C	1:A:16:LEU:N	6	1.8
(1,70)	1:A:12:LYS:N	1:A:12:LYS:CA	1:A:12:LYS:C	1:A:13:GLU:N	3	1.8
(1,66)	1:A:8:GLN:N	1:A:8:GLN:CA	1:A:8:GLN:C	1:A:9:GLU:N	6	1.8
(1,6)	1:A:10:GLU:C	1:A:11:LEU:N	1:A:11:LEU:CA	1:A:11:LEU:C	2	1.8
(1,59)	1:A:75:THR:C	1:A:76:TRP:N	1:A:76:TRP:CA	1:A:76:TRP:C	16	1.8
(1,58)	1:A:72:SER:C	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	19	1.8
(1,57)	1:A:71:LEU:C	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	10	1.8
(1,119)	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	1:A:73:ASP:N	2	1.8
(1,106)	1:A:54:ARG:N	1:A:54:ARG:CA	1:A:54:ARG:C	1:A:55:ILE:N	1	1.8
(1,106)	1:A:54:ARG:N	1:A:54:ARG:CA	1:A:54:ARG:C	1:A:55:ILE:N	14	1.8
(1,87)	1:A:31:VAL:N	1:A:31:VAL:CA	1:A:31:VAL:C	1:A:32:PRO:N	9	1.7
(1,60)	1:A:78:LEU:C	1:A:79:ARG:N	1:A:79:ARG:CA	1:A:79:ARG:C	1	1.7
(1,59)	1:A:75:THR:C	1:A:76:TRP:N	1:A:76:TRP:CA	1:A:76:TRP:C	13	1.7
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	4	1.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	18	1.7
(1,120)	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	1:A:74:GLN:N	10	1.7
(1,68)	1:A:10:GLU:N	1:A:10:GLU:CA	1:A:10:GLU:C	1:A:11:LEU:N	14	1.6
(1,66)	1:A:8:GLN:N	1:A:8:GLN:CA	1:A:8:GLN:C	1:A:9:GLU:N	1	1.6
(1,59)	1:A:75:THR:C	1:A:76:TRP:N	1:A:76:TRP:CA	1:A:76:TRP:C	4	1.6
(1,57)	1:A:71:LEU:C	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	3	1.6
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	13	1.6
(1,106)	1:A:54:ARG:N	1:A:54:ARG:CA	1:A:54:ARG:C	1:A:55:ILE:N	6	1.6
(1,67)	1:A:9:GLU:N	1:A:9:GLU:CA	1:A:9:GLU:C	1:A:10:GLU:N	9	1.5
(1,59)	1:A:75:THR:C	1:A:76:TRP:N	1:A:76:TRP:CA	1:A:76:TRP:C	9	1.5
(1,19)	1:A:24:PHE:C	1:A:25:GLU:N	1:A:25:GLU:CA	1:A:25:GLU:C	12	1.5
(1,10)	1:A:15:ALA:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	10	1.5
(1,97)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:SER:N	12	1.4
(1,97)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:SER:N	13	1.4
(1,97)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:SER:N	20	1.4
(1,72)	1:A:15:ALA:N	1:A:15:ALA:CA	1:A:15:ALA:C	1:A:16:LEU:N	9	1.4
(1,66)	1:A:8:GLN:N	1:A:8:GLN:CA	1:A:8:GLN:C	1:A:9:GLU:N	17	1.4
(1,60)	1:A:78:LEU:C	1:A:79:ARG:N	1:A:79:ARG:CA	1:A:79:ARG:C	6	1.4
(1,58)	1:A:72:SER:C	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	1	1.4
(1,39)	1:A:47:LYS:C	1:A:48:LYS:N	1:A:48:LYS:CA	1:A:48:LYS:C	3	1.4
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	6	1.4
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	8	1.4
(1,35)	1:A:41:ALA:C	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	15	1.4
(1,28)	1:A:34:GLN:C	1:A:35:GLU:N	1:A:35:GLU:CA	1:A:35:GLU:C	20	1.4
(1,106)	1:A:54:ARG:N	1:A:54:ARG:CA	1:A:54:ARG:C	1:A:55:ILE:N	15	1.4
(1,98)	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	1:A:43:LEU:N	1	1.3
(1,98)	1:A:42:SER:N	1:A:42:SER:CA	1:A:42:SER:C	1:A:43:LEU:N	6	1.3
(1,68)	1:A:10:GLU:N	1:A:10:GLU:CA	1:A:10:GLU:C	1:A:11:LEU:N	4	1.3
(1,59)	1:A:75:THR:C	1:A:76:TRP:N	1:A:76:TRP:CA	1:A:76:TRP:C	8	1.3
(1,59)	1:A:75:THR:C	1:A:76:TRP:N	1:A:76:TRP:CA	1:A:76:TRP:C	10	1.3
(1,45)	1:A:53:ASP:C	1:A:54:ARG:N	1:A:54:ARG:CA	1:A:54:ARG:C	20	1.3
(1,28)	1:A:34:GLN:C	1:A:35:GLU:N	1:A:35:GLU:CA	1:A:35:GLU:C	16	1.3
(1,97)	1:A:41:ALA:N	1:A:41:ALA:CA	1:A:41:ALA:C	1:A:42:SER:N	14	1.2
(1,66)	1:A:8:GLN:N	1:A:8:GLN:CA	1:A:8:GLN:C	1:A:9:GLU:N	8	1.2
(1,66)	1:A:8:GLN:N	1:A:8:GLN:CA	1:A:8:GLN:C	1:A:9:GLU:N	11	1.2
(1,58)	1:A:72:SER:C	1:A:73:ASP:N	1:A:73:ASP:CA	1:A:73:ASP:C	2	1.2
(1,57)	1:A:71:LEU:C	1:A:72:SER:N	1:A:72:SER:CA	1:A:72:SER:C	6	1.2
(1,53)	1:A:61:ASP:C	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	17	1.2
(1,28)	1:A:34:GLN:C	1:A:35:GLU:N	1:A:35:GLU:CA	1:A:35:GLU:C	18	1.2
(1,22)	1:A:28:LYS:C	1:A:29:LYS:N	1:A:29:LYS:CA	1:A:29:LYS:C	5	1.2
(1,112)	1:A:60:THR:N	1:A:60:THR:CA	1:A:60:THR:C	1:A:61:ASP:N	2	1.2
(1,106)	1:A:54:ARG:N	1:A:54:ARG:CA	1:A:54:ARG:C	1:A:55:ILE:N	2	1.2
(1,106)	1:A:54:ARG:N	1:A:54:ARG:CA	1:A:54:ARG:C	1:A:55:ILE:N	20	1.2
(1,102)	1:A:49:GLU:N	1:A:49:GLU:CA	1:A:49:GLU:C	1:A:50:GLU:N	4	1.2
(1,101)	1:A:48:LYS:N	1:A:48:LYS:CA	1:A:48:LYS:C	1:A:49:GLU:N	19	1.2
(1,70)	1:A:12:LYS:N	1:A:12:LYS:CA	1:A:12:LYS:C	1:A:13:GLU:N	11	1.1
(1,69)	1:A:11:LEU:N	1:A:11:LEU:CA	1:A:11:LEU:C	1:A:12:LYS:N	14	1.1
(1,59)	1:A:75:THR:C	1:A:76:TRP:N	1:A:76:TRP:CA	1:A:76:TRP:C	14	1.1
(1,53)	1:A:61:ASP:C	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	18	1.1
(1,22)	1:A:28:LYS:C	1:A:29:LYS:N	1:A:29:LYS:CA	1:A:29:LYS:C	6	1.1
(1,106)	1:A:54:ARG:N	1:A:54:ARG:CA	1:A:54:ARG:C	1:A:55:ILE:N	11	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:A:15:ALA:C	1:A:16:LEU:N	1:A:16:LEU:CA	1:A:16:LEU:C	14	1.1