Full wwPDB NMR Structure Validation Report

Jun 3, 2023 – 08:33 PM EDT

PDB ID	:	2MZU
BMRB ID	:	25502
Title	:	Extending the eNOE data set of large proteins by evaluation of NOEs with unresolved diagonals
Authors	:	Chi, C.N.; Strotz, D.; Riek, R.; Voegeli, B.
Deposited on	:	2015-02-24

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

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

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

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

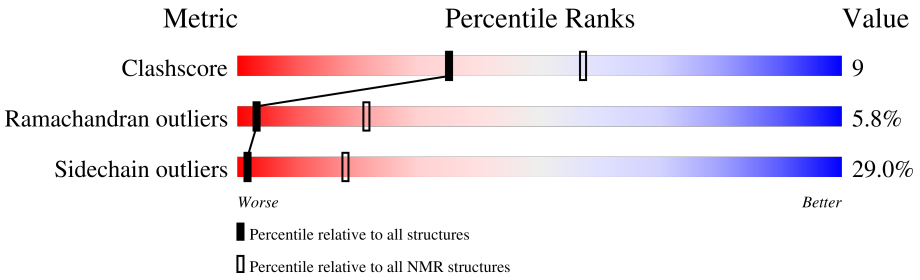
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 83%.

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	165	54% 35% · 8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:64, A:78-A:165 (151)	0.74	2

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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2500 atoms, of which 1235 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	165	2500	802	1235	218	236	9	0

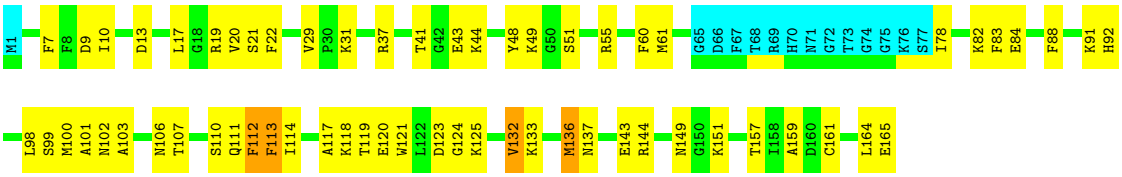
4 Residue-property plots

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: Peptidyl-prolyl cis-trans isomerase A

Chain A:



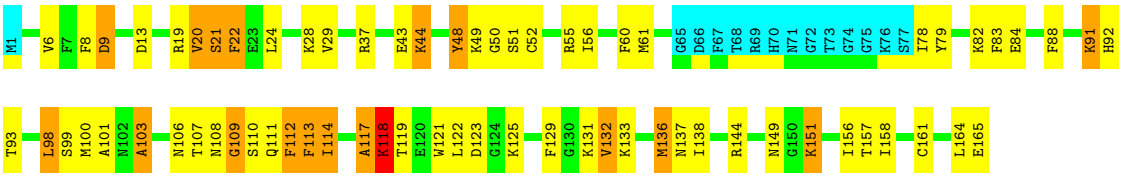
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

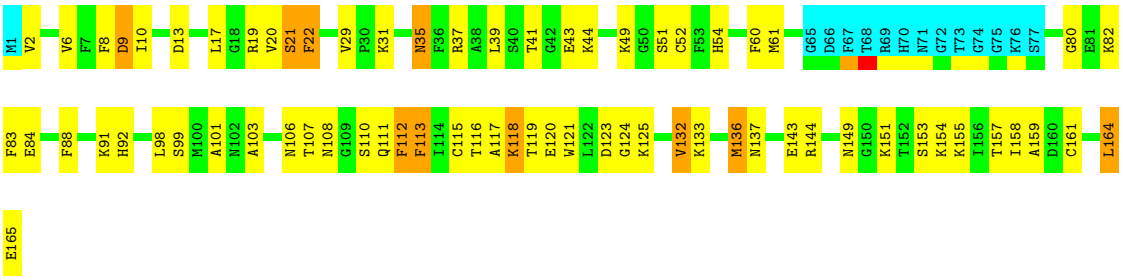
Chain A:



4.2.2 Score per residue for model 2 (medoid)

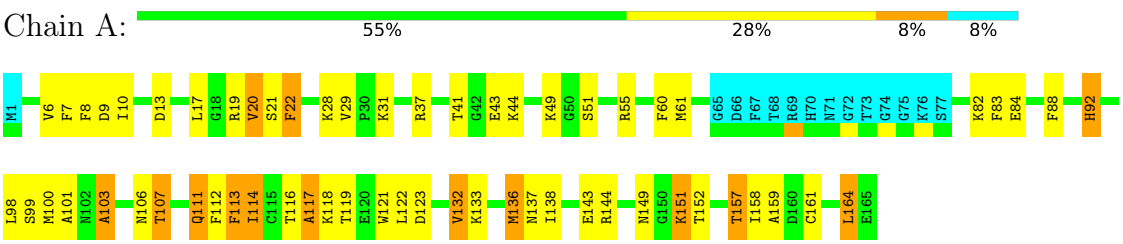
• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

Chain A:



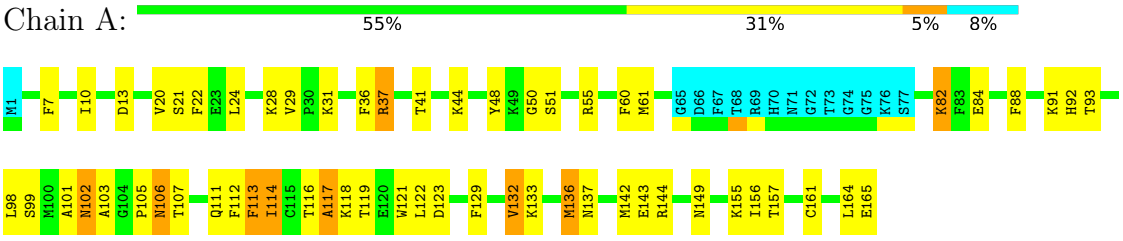
4.2.3 Score per residue for model 3

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A



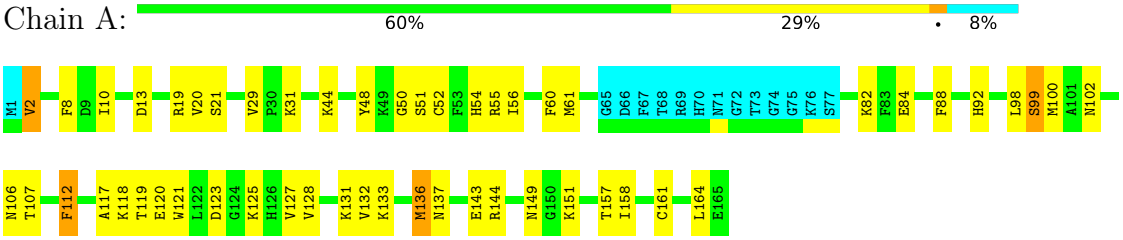
4.2.4 Score per residue for model 4

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A



4.2.5 Score per residue for model 5

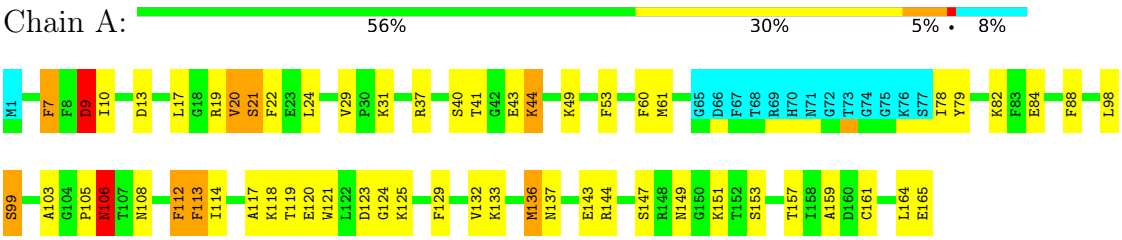
• Molecule 1: Peptidyl-prolyl cis-trans isomerase A



4.2.6 Score per residue for model 6

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

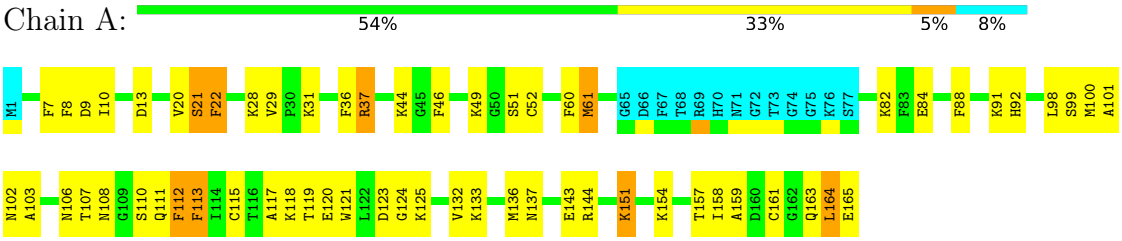
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

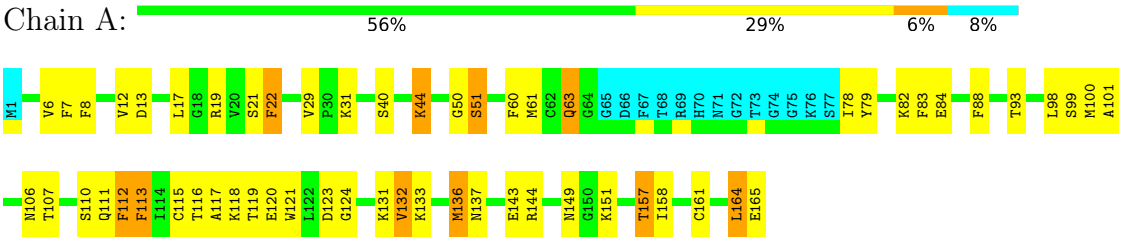
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

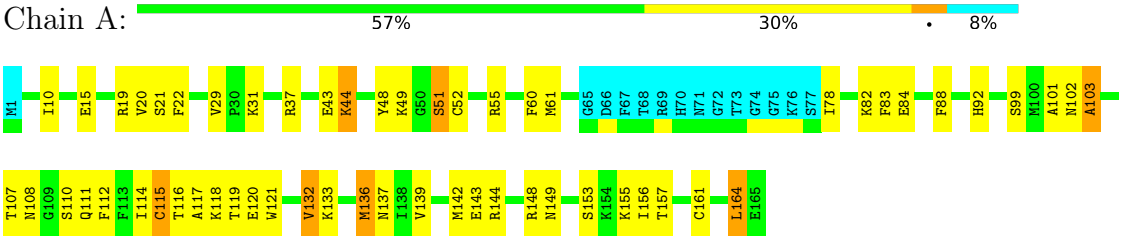
Chain A:



4.2.9 Score per residue for model 9

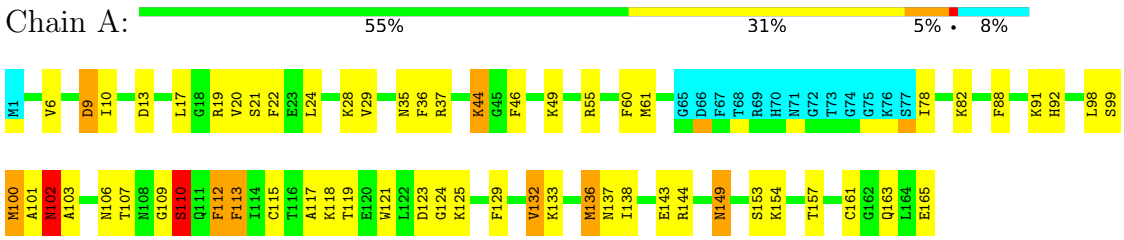
• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

Chain A:



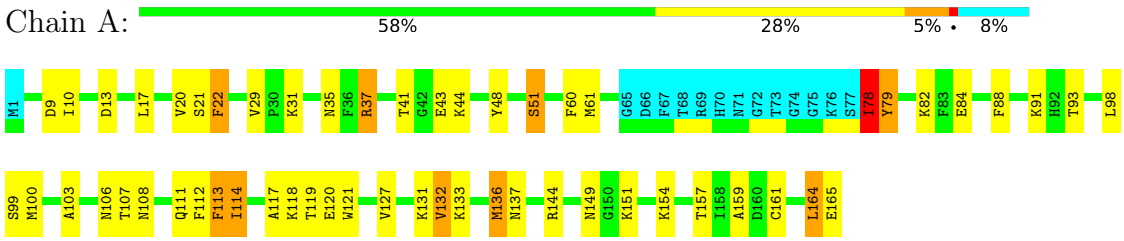
4.2.10 Score per residue for model 10

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A



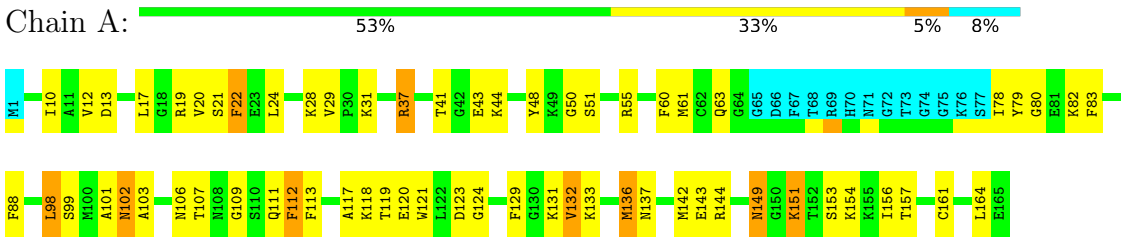
4.2.11 Score per residue for model 11

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A



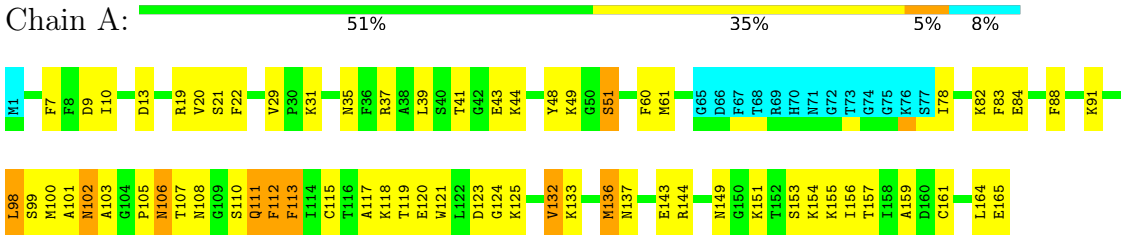
4.2.12 Score per residue for model 12

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A



4.2.13 Score per residue for model 13

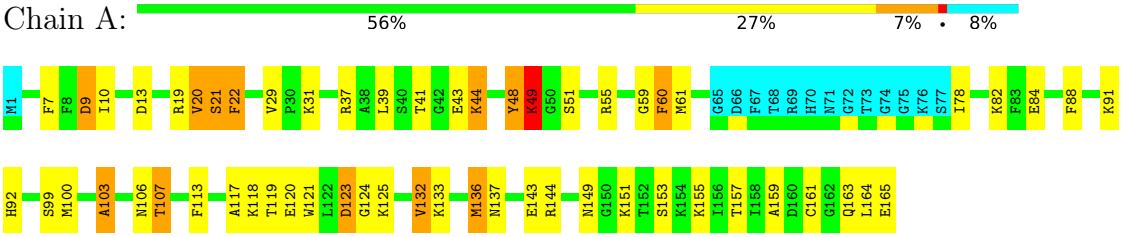
• Molecule 1: Peptidyl-prolyl cis-trans isomerase A



4.2.14 Score per residue for model 14

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

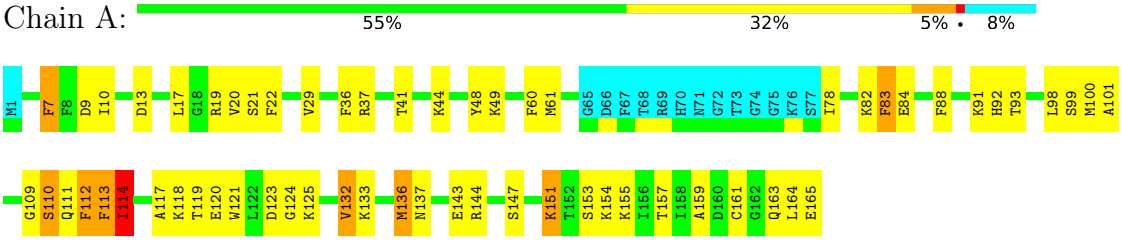
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

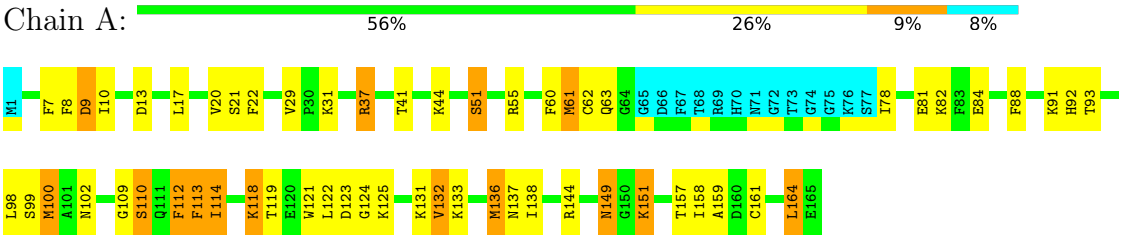
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

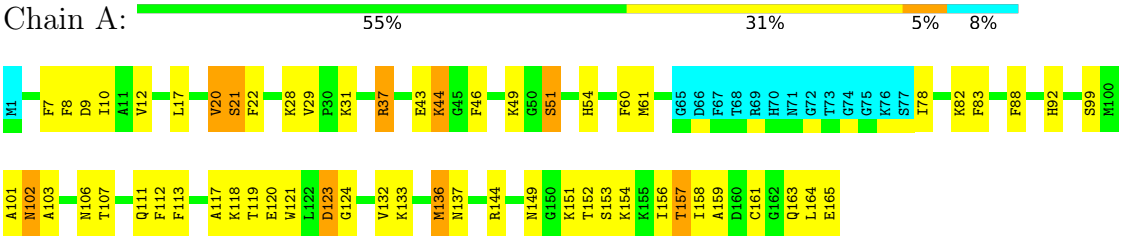
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

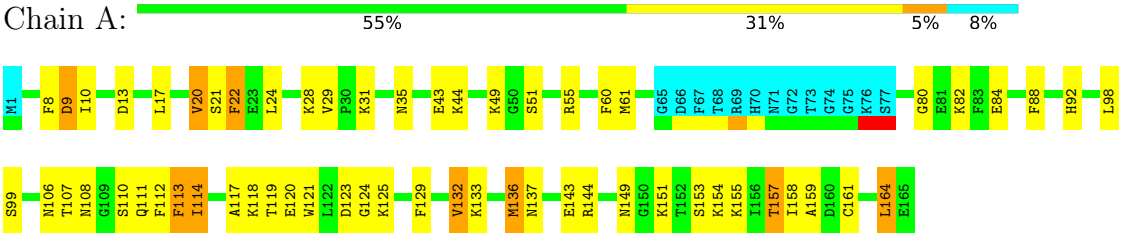
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

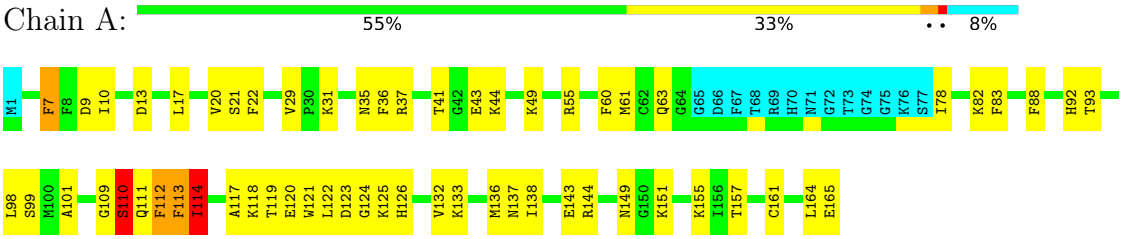
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

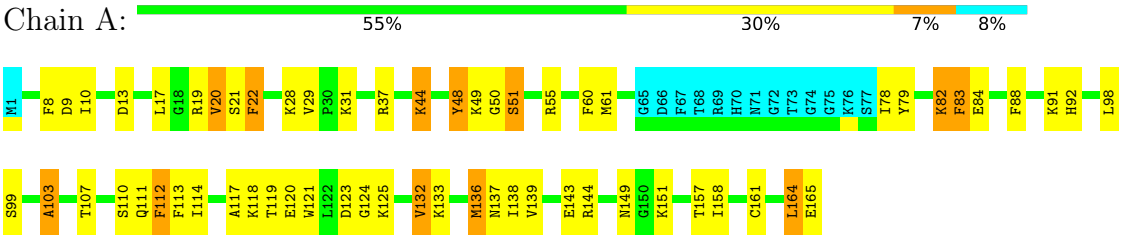
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing.*

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	Classification	Version
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1786
Number of shifts mapped to atoms	1786
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1164	1143	1143	20±3
All	All	23280	22860	22860	403

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:ALA:HB2	1:A:113:PHE:HB3	0.77	1.55	8	6
1:A:119:THR:HG22	1:A:121:TRP:CZ2	0.75	2.16	1	20
1:A:103:ALA:HB3	1:A:107:THR:OG1	0.73	1.82	10	11
1:A:98:LEU:HD11	1:A:112:PHE:CE2	0.70	2.21	13	1
1:A:117:ALA:O	1:A:119:THR:HG23	0.69	1.86	13	16
1:A:10:ILE:HG23	1:A:156:ILE:HG23	0.69	1.63	13	5
1:A:101:ALA:HB3	1:A:111:GLN:CG	0.69	2.18	19	2
1:A:101:ALA:HB3	1:A:111:GLN:O	0.69	1.88	1	6
1:A:39:LEU:HD21	1:A:78:ILE:HG22	0.69	1.64	14	1
1:A:111:GLN:O	1:A:112:PHE:CB	0.69	2.41	13	1
1:A:48:TYR:O	1:A:49:LYS:C	0.67	2.33	14	1
1:A:10:ILE:HG22	1:A:17:LEU:HD12	0.66	1.67	19	9
1:A:44:LYS:HD2	1:A:78:ILE:HG22	0.65	1.69	8	8
1:A:8:PHE:CD2	1:A:158:ILE:HD13	0.63	2.29	20	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:PHE:HB3	1:A:164:LEU:HD21	0.63	1.71	14	6
1:A:101:ALA:HB2	1:A:113:PHE:CE2	0.62	2.29	1	1
1:A:112:PHE:CD1	1:A:112:PHE:C	0.61	2.74	15	5
1:A:101:ALA:HB3	1:A:111:GLN:HG2	0.61	1.72	19	2
1:A:91:LYS:O	1:A:93:THR:HG23	0.61	1.95	16	4
1:A:41:THR:HG22	1:A:163:GLN:HG3	0.61	1.71	14	1
1:A:8:PHE:CE2	1:A:158:ILE:HD13	0.60	2.31	5	10
1:A:51:SER:O	1:A:157:THR:HG22	0.60	1.96	17	4
1:A:122:LEU:HD22	1:A:126:HIS:NE2	0.59	2.12	19	1
1:A:9:ASP:HB3	1:A:159:ALA:HB3	0.59	1.75	7	11
1:A:56:ILE:CD1	1:A:156:ILE:HD13	0.59	2.27	1	1
1:A:113:PHE:CD1	1:A:113:PHE:O	0.59	2.56	19	4
1:A:119:THR:OG1	1:A:122:LEU:HD12	0.58	1.98	1	3
1:A:103:ALA:HB3	1:A:107:THR:CB	0.57	2.29	1	4
1:A:35:ASN:O	1:A:39:LEU:HD12	0.57	1.99	13	2
1:A:122:LEU:HD13	1:A:126:HIS:CD2	0.57	2.35	19	1
1:A:113:PHE:O	1:A:114:ILE:C	0.56	2.44	15	7
1:A:132:VAL:HG11	1:A:136:MET:HG2	0.56	1.77	17	18
1:A:111:GLN:O	1:A:112:PHE:HB3	0.56	2.00	13	2
1:A:113:PHE:C	1:A:113:PHE:CD1	0.55	2.79	2	4
1:A:113:PHE:O	1:A:113:PHE:CD1	0.55	2.59	15	3
1:A:101:ALA:HB2	1:A:113:PHE:CB	0.55	2.32	13	3
1:A:10:ILE:CG2	1:A:17:LEU:HD12	0.55	2.32	15	10
1:A:61:MET:HE3	1:A:62:CYS:O	0.54	2.02	16	1
1:A:113:PHE:CD1	1:A:113:PHE:N	0.54	2.73	1	9
1:A:109:GLY:O	1:A:110:SER:CB	0.53	2.56	10	4
1:A:24:LEU:HD23	1:A:129:PHE:O	0.52	2.03	1	6
1:A:113:PHE:O	1:A:113:PHE:CG	0.51	2.63	13	4
1:A:106:ASN:C	1:A:107:THR:HG23	0.50	2.26	8	9
1:A:2:VAL:HG22	1:A:2:VAL:O	0.50	2.07	5	1
1:A:12:VAL:HG23	1:A:17:LEU:HD13	0.50	1.83	12	3
1:A:117:ALA:O	1:A:118:LYS:C	0.49	2.50	1	3
1:A:56:ILE:HD12	1:A:156:ILE:HD13	0.48	1.84	1	1
1:A:12:VAL:CG2	1:A:17:LEU:HD13	0.48	2.38	8	3
1:A:164:LEU:CD2	1:A:164:LEU:N	0.48	2.77	7	6
1:A:119:THR:HG22	1:A:121:TRP:HZ2	0.48	1.68	3	2
1:A:101:ALA:HB3	1:A:111:GLN:HB3	0.48	1.84	8	2
1:A:108:ASN:O	1:A:109:GLY:C	0.48	2.51	1	1
1:A:37:ARG:O	1:A:41:THR:HG23	0.48	2.09	19	10
1:A:102:ASN:CG	1:A:109:GLY:HA3	0.48	2.29	10	1
1:A:98:LEU:HD22	1:A:112:PHE:HB2	0.47	1.85	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LYS:O	1:A:132:VAL:C	0.47	2.53	8	5
1:A:78:ILE:O	1:A:78:ILE:HD12	0.47	2.09	12	2
1:A:164:LEU:N	1:A:164:LEU:CD2	0.47	2.78	8	7
1:A:142:MET:SD	1:A:156:ILE:HG21	0.47	2.49	12	3
1:A:114:ILE:HG21	1:A:139:VAL:CG1	0.47	2.39	20	1
1:A:98:LEU:HD22	1:A:112:PHE:CG	0.46	2.45	5	2
1:A:82:LYS:HD2	1:A:82:LYS:C	0.46	2.31	20	2
1:A:22:PHE:CZ	1:A:114:ILE:HD11	0.46	2.46	19	1
1:A:8:PHE:CD2	1:A:158:ILE:HG21	0.46	2.46	5	2
1:A:63:GLN:CG	1:A:101:ALA:HB1	0.46	2.40	8	1
1:A:101:ALA:HB3	1:A:111:GLN:HG3	0.46	1.87	19	1
1:A:21:SER:OG	1:A:22:PHE:N	0.46	2.49	8	18
1:A:114:ILE:HG22	1:A:114:ILE:O	0.45	2.10	6	1
1:A:101:ALA:O	1:A:102:ASN:CB	0.45	2.64	17	1
1:A:20:VAL:CG2	1:A:138:ILE:HG21	0.45	2.42	1	3
1:A:98:LEU:HD21	1:A:112:PHE:CD1	0.45	2.47	1	3
1:A:106:ASN:O	1:A:107:THR:HG23	0.45	2.12	13	2
1:A:114:ILE:O	1:A:114:ILE:HG22	0.45	2.12	4	1
1:A:116:THR:HG22	1:A:139:VAL:CG1	0.45	2.41	9	1
1:A:122:LEU:HD13	1:A:126:HIS:HD2	0.45	1.72	19	1
1:A:102:ASN:HB3	1:A:107:THR:O	0.44	2.12	10	1
1:A:17:LEU:HB3	1:A:138:ILE:HD12	0.44	1.89	19	4
1:A:113:PHE:CD1	1:A:113:PHE:C	0.44	2.89	15	5
1:A:44:LYS:CD	1:A:78:ILE:HG22	0.44	2.41	1	2
1:A:116:THR:O	1:A:117:ALA:HB2	0.44	2.11	3	4
1:A:99:SER:O	1:A:112:PHE:HB3	0.44	2.13	5	1
1:A:92:HIS:CE1	1:A:122:LEU:HD12	0.44	2.48	16	1
1:A:10:ILE:HG13	1:A:20:VAL:HG21	0.44	1.89	15	7
1:A:112:PHE:CZ	1:A:114:ILE:HD12	0.44	2.48	16	1
1:A:111:GLN:O	1:A:111:GLN:CG	0.44	2.65	20	1
1:A:10:ILE:CG1	1:A:20:VAL:HG21	0.44	2.43	6	5
1:A:98:LEU:HD23	1:A:113:PHE:O	0.43	2.13	6	1
1:A:105:PRO:O	1:A:107:THR:HG23	0.43	2.13	4	1
1:A:37:ARG:NH2	1:A:163:GLN:HG2	0.43	2.28	7	2
1:A:83:PHE:N	1:A:83:PHE:CD1	0.43	2.84	20	1
1:A:105:PRO:O	1:A:106:ASN:CB	0.43	2.67	6	1
1:A:78:ILE:HG13	1:A:79:TYR:CD2	0.43	2.49	11	1
1:A:22:PHE:N	1:A:22:PHE:CD1	0.43	2.86	8	3
1:A:78:ILE:HD12	1:A:78:ILE:O	0.43	2.14	19	1
1:A:83:PHE:CD1	1:A:83:PHE:N	0.43	2.84	15	1
1:A:123:ASP:O	1:A:124:GLY:C	0.42	2.57	20	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:PHE:HA	1:A:21:SER:HA	0.42	1.91	17	6
1:A:41:THR:HG22	1:A:163:GLN:CG	0.42	2.42	14	1
1:A:143:GLU:OE1	1:A:143:GLU:HA	0.42	2.14	20	1
1:A:105:PRO:O	1:A:106:ASN:C	0.42	2.58	4	2
1:A:100:MET:HE2	1:A:127:VAL:HB	0.42	1.92	11	2
1:A:39:LEU:CD2	1:A:78:ILE:HG22	0.41	2.42	14	1
1:A:100:MET:HE2	1:A:110:SER:HA	0.40	1.93	10	1
1:A:56:ILE:O	1:A:56:ILE:HG22	0.40	2.16	5	1
1:A:98:LEU:O	1:A:128:VAL:HG22	0.40	2.16	5	1
1:A:101:ALA:CB	1:A:111:GLN:O	0.40	2.69	4	1
1:A:44:LYS:CE	1:A:78:ILE:HG22	0.40	2.46	1	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	150/165 (91%)	107±3 (71±2%)	34±3 (23±2%)	9±3 (6±2%)	3	21
All	All	3000/3300 (91%)	2137 (71%)	689 (23%)	174 (6%)	3	21

All 35 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	118	LYS	17
1	A	132	VAL	17
1	A	149	ASN	17
1	A	92	HIS	14
1	A	112	PHE	11
1	A	51	SER	8
1	A	103	ALA	8
1	A	110	SER	8
1	A	114	ILE	8
1	A	151	LYS	7
1	A	50	GLY	6

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Mol	Chain	Res	Type	Models (Total)
1	A	102	ASN	6
1	A	9	ASP	5
1	A	99	SER	5
1	A	79	TYR	3
1	A	117	ALA	3
1	A	123	ASP	3
1	A	80	GLY	3
1	A	46	PHE	3
1	A	48	TYR	2
1	A	109	GLY	2
1	A	2	VAL	2
1	A	52	CYS	2
1	A	55	ARG	2
1	A	111	GLN	2
1	A	106	ASN	1
1	A	61	MET	1
1	A	115	CYS	1
1	A	148	ARG	1
1	A	78	ILE	1
1	A	63	GLN	1
1	A	49	LYS	1
1	A	59	GLY	1
1	A	60	PHE	1
1	A	100	MET	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	123/133 (92%)	87±4 (71±3%)	36±4 (29±3%)	2 18
All	All	2460/2660 (92%)	1747 (71%)	713 (29%)	2 18

All 73 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	29	VAL	20

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Mol	Chain	Res	Type	Models (Total)
1	A	44	LYS	20
1	A	60	PHE	20
1	A	61	MET	20
1	A	82	LYS	20
1	A	88	PHE	20
1	A	133	LYS	20
1	A	136	MET	20
1	A	137	ASN	20
1	A	144	ARG	20
1	A	157	THR	20
1	A	161	CYS	20
1	A	13	ASP	18
1	A	113	PHE	18
1	A	31	LYS	17
1	A	84	GLU	16
1	A	99	SER	16
1	A	151	LYS	16
1	A	120	GLU	15
1	A	143	GLU	15
1	A	20	VAL	14
1	A	49	LYS	14
1	A	98	LEU	14
1	A	165	GLU	14
1	A	19	ARG	13
1	A	125	LYS	13
1	A	43	GLU	12
1	A	22	PHE	11
1	A	37	ARG	11
1	A	83	PHE	11
1	A	51	SER	11
1	A	48	TYR	10
1	A	55	ARG	10
1	A	153	SER	10
1	A	112	PHE	10
1	A	28	LYS	9
1	A	100	MET	9
1	A	154	LYS	9
1	A	164	LEU	9
1	A	91	LYS	8
1	A	155	LYS	8
1	A	9	ASP	7
1	A	21	SER	7

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Mol	Chain	Res	Type	Models (Total)
1	A	108	ASN	7
1	A	102	ASN	7
1	A	115	CYS	6
1	A	110	SER	6
1	A	6	VAL	5
1	A	35	ASN	5
1	A	36	PHE	5
1	A	106	ASN	5
1	A	118	LYS	4
1	A	149	ASN	4
1	A	52	CYS	3
1	A	54	HIS	3
1	A	111	GLN	3
1	A	123	ASP	3
1	A	7	PHE	3
1	A	79	TYR	3
1	A	63	GLN	3
1	A	93	THR	3
1	A	114	ILE	3
1	A	107	THR	2
1	A	152	THR	2
1	A	40	SER	2
1	A	147	SER	2
1	A	163	GLN	2
1	A	78	ILE	2
1	A	92	HIS	1
1	A	131	LYS	1
1	A	53	PHE	1
1	A	15	GLU	1
1	A	81	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 82% 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	1786
Number of shifts mapped to atoms	1786
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	87

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	164	0.11 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	138	0.46 ± 0.21	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	156	1.10 ± 0.28	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 83%, i.e. 1649 atoms were assigned a chemical shift out of a possible 1994. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	607/762 (80%)	314/315 (100%)	150/302 (50%)	143/145 (99%)
Sidechain	935/1041 (90%)	653/674 (97%)	267/328 (81%)	15/39 (38%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	107/191 (56%)	78/96 (81%)	28/91 (31%)	1/4 (25%)
Overall	1649/1994 (83%)	1045/1085 (96%)	445/721 (62%)	159/188 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1775 atoms were assigned a chemical shift out of a possible 2158. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	664/836 (79%)	344/347 (99%)	164/330 (50%)	156/159 (98%)
Sidechain	996/1114 (89%)	694/720 (96%)	286/350 (82%)	16/44 (36%)
Aromatic	115/208 (55%)	84/105 (80%)	30/98 (31%)	1/5 (20%)
Overall	1775/2158 (82%)	1122/1172 (96%)	480/778 (62%)	173/208 (83%)

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	53	PHE	CE2	1.01	124.80 – 136.72	-108.8
1	A	46	PHE	CE2	1.27	124.80 – 136.72	-108.6
1	A	129	PHE	CE2	2.81	124.80 – 136.72	-107.3
1	A	8	PHE	CD2	2.87	125.53 – 137.61	-106.5
1	A	8	PHE	CE2	5.54	124.80 – 136.72	-105.0
1	A	8	PHE	CD1	2.87	125.33 – 137.83	-103.0
1	A	22	PHE	CD2	8.19	125.53 – 137.61	-102.1
1	A	53	PHE	CE1	1.01	124.17 – 137.29	-98.9
1	A	22	PHE	CD1	8.19	125.33 – 137.83	-98.7
1	A	46	PHE	CE1	1.27	124.17 – 137.29	-98.7
1	A	8	PHE	CE1	5.54	124.17 – 137.29	-95.4
1	A	79	TYR	CE2	2.02	111.68 – 124.17	-92.8
1	A	79	TYR	CE1	2.02	111.24 – 124.66	-86.4
1	A	25	PHE	CZ	2.71	121.82 – 136.66	-85.3
1	A	67	PHE	CZ	3.15	121.82 – 136.66	-85.0
1	A	88	PHE	CZ	8.01	121.82 – 136.66	-81.7
1	A	8	PHE	CZ	9.27	121.82 – 136.66	-80.8
1	A	22	PHE	CE2	41.07	124.80 – 136.72	-75.2
1	A	7	PHE	CD2	42.95	125.53 – 137.61	-73.4
1	A	46	PHE	CD2	43.35	125.53 – 137.61	-73.0
1	A	7	PHE	CD1	42.95	125.33 – 137.83	-70.9
1	A	46	PHE	CD1	43.35	125.33 – 137.83	-70.6

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	22	PHE	CE1	41.07	124.17 – 137.29	-68.3
1	A	7	PHE	CE2	53.44	124.80 – 136.72	-64.9
1	A	53	PHE	CZ	41.16	121.82 – 136.66	-59.4
1	A	7	PHE	CE1	53.44	124.17 – 137.29	-58.9
1	A	92	HIS	CE1	5.32	126.08 – 149.12	-57.4
1	A	70	HIS	CD2	2.17	103.95 – 136.66	-36.1
1	A	92	HIS	CD2	8.29	103.95 – 136.66	-34.2
1	A	54	HIS	CD2	8.73	103.95 – 136.66	-34.1
1	A	32	THR	HG1	7.75	0.08 – 2.19	31.4
1	A	31	LYS	CG	59.57	19.35 – 30.45	31.2
1	A	68	THR	CG2	52.78	16.06 – 27.03	28.5
1	A	93	THR	CG2	52.57	16.06 – 27.03	28.3
1	A	31	LYS	CD	59.57	23.50 – 34.42	28.0
1	A	32	THR	CG2	52.17	16.06 – 27.03	27.9
1	A	5	THR	CG2	52.13	16.06 – 27.03	27.9
1	A	41	THR	CG2	52.06	16.06 – 27.03	27.8
1	A	76	LYS	CD	59.27	23.50 – 34.42	27.8
1	A	95	PRO	CG	57.29	21.69 – 32.72	27.3
1	A	73	THR	CG2	50.55	16.06 – 27.03	26.4
1	A	41	THR	HG1	6.69	0.08 – 2.19	26.3
1	A	16	PRO	CB	62.11	26.06 – 37.61	26.2
1	A	95	PRO	CB	61.95	26.06 – 37.61	26.1
1	A	55	ARG	CG	58.00	21.24 – 33.19	25.8
1	A	56	ILE	CG2	47.56	10.93 – 24.12	22.8
1	A	100	MET	CG	61.92	25.46 – 38.60	22.7
1	A	73	THR	HG1	5.77	0.08 – 2.19	22.0
1	A	11	ALA	CB	52.56	10.19 – 27.75	19.1
1	A	56	ILE	CD1	44.28	5.18 – 21.60	18.8
1	A	78	ILE	CD1	44.02	5.18 – 21.60	18.6
1	A	152	THR	HG1	5.01	0.08 – 2.19	18.4
1	A	21	SER	CB	36.77	56.28 – 71.32	-18.0
1	A	32	THR	CB	38.88	61.12 – 78.27	-18.0
1	A	107	THR	CB	39.20	61.12 – 78.27	-17.8
1	A	69	ARG	CB	61.53	21.74 – 39.52	17.4
1	A	57	ILE	CG1	57.09	19.24 – 36.26	17.2
1	A	10	ILE	CD1	41.27	5.18 – 21.60	17.0
1	A	73	THR	CB	40.76	61.12 – 78.27	-16.9
1	A	107	THR	HG1	4.67	0.08 – 2.19	16.8
1	A	5	THR	CB	41.14	61.12 – 78.27	-16.6
1	A	34	GLU	CB	57.90	21.56 – 38.37	16.6
1	A	77	SER	CB	38.96	56.28 – 71.32	-16.5
1	A	37	ARG	CG	45.21	21.24 – 33.19	15.1

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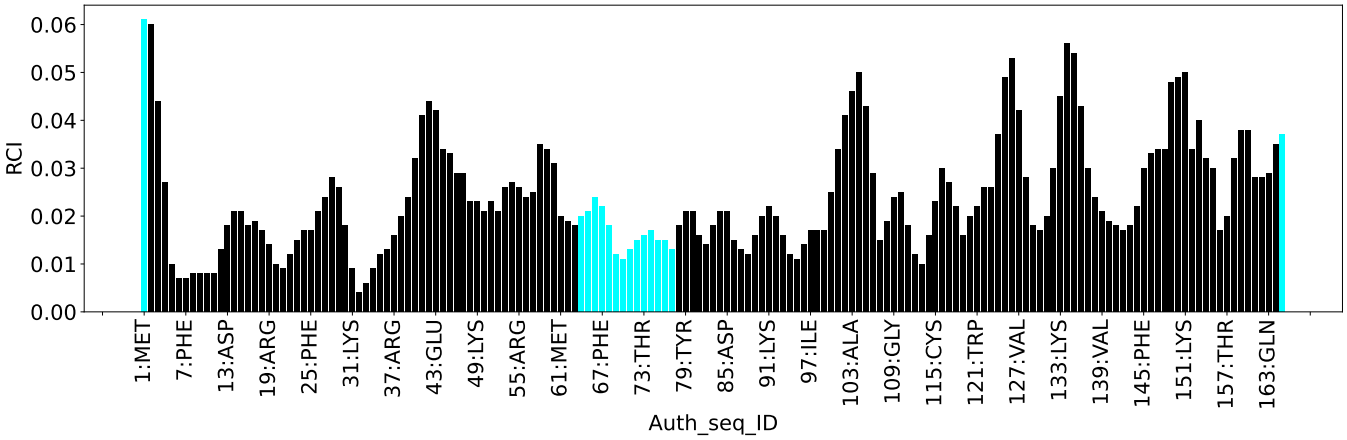
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	29	VAL	CG1	40.20	14.71 – 28.29	13.8
1	A	70	HIS	CB	58.43	19.76 – 40.75	13.4
1	A	20	VAL	CG1	37.22	14.71 – 28.29	11.6
1	A	6	VAL	CG1	36.66	14.71 – 28.29	11.2
1	A	90	LEU	CD1	41.73	16.71 – 32.55	10.8
1	A	12	VAL	CG1	36.14	14.71 – 28.29	10.8
1	A	2	VAL	CG1	35.83	14.71 – 28.29	10.6
1	A	20	VAL	CG2	36.85	13.71 – 28.88	10.2
1	A	12	VAL	CG2	36.53	13.71 – 28.88	10.0
1	A	39	LEU	CD1	40.37	16.71 – 32.55	9.9
1	A	24	LEU	CD1	39.82	16.71 – 32.55	9.6
1	A	32	THR	CA	37.68	49.41 – 75.05	-9.6
1	A	98	LEU	CD1	39.58	16.71 – 32.55	9.4
1	A	6	VAL	CG2	35.60	13.71 – 28.88	9.4
1	A	29	VAL	CG2	35.55	13.71 – 28.88	9.4
1	A	98	LEU	CD2	39.53	15.73 – 32.47	9.2
1	A	119	THR	HG1	3.05	0.08 – 2.19	9.1
1	A	17	LEU	CD2	39.12	15.73 – 32.47	9.0
1	A	90	LEU	CD2	37.46	15.73 – 32.47	8.0
1	A	76	LYS	HE3	1.51	1.92 – 3.89	-7.1
1	A	108	ASN	HB3	0.92	1.12 – 4.38	-5.6
1	A	31	LYS	HE3	1.86	1.92 – 3.89	-5.3
1	A	39	LEU	HB3	-0.33	-0.26 – 3.31	-5.2

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
0.06
0.05
0.04
0.03
0.02
0.01
0.00
1:MET
7:PHE
13:ASP
19:ARG
25:PHE
31:LYS
37:ARG
43:GLU
49:LYS
55:ARG
61:MET
67:PHE
73:THR
79:TYR
85:ASP
91:LYS
97:ILE
103:ALA
109:GLY
115:CYS
121:TRP
127:VAL
133:LYS
139:VAL
145:PHE
151:LYS
157:THR
163:GLN
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	281
Intra-residue (|i-j|=0)	281
Sequential (|i-j|=1)	0
Medium range (|i-j|>1 and |i-j|<5)	0
Long range (|i-j|≥5)	0
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	1.7
Number of long range restraints per residue[1]	0.0

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.9	0.19
0.2-0.5 (Medium)	14.1	0.5
>0.5 (Large)	14.1	1.47

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

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

9 Distance violation analysis (i)

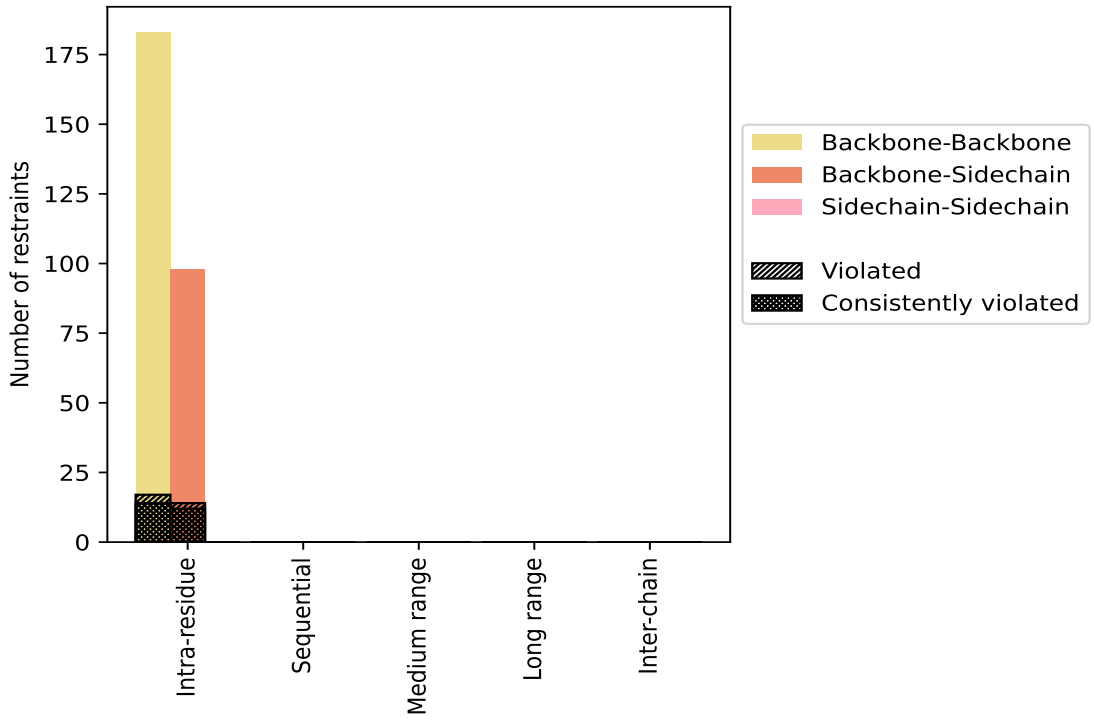
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	281	100.0	31	11.0	11.0	26	9.3	9.3
Backbone-Backbone	183	65.1	17	9.3	6.0	14	7.7	5.0
Backbone-Sidechain	98	34.9	14	14.3	5.0	12	12.2	4.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	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
Medium range (|i-j|>1 & |i-j|<5)	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
Long range (|i-j|≥5)	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
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	281	100.0	31	11.0	11.0	26	9.3	9.3
Backbone-Backbone	183	65.1	17	9.3	6.0	14	7.7	5.0
Backbone-Sidechain	98	34.9	14	14.3	5.0	12	12.2	4.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	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	31	0	0	0	0	31	0.63	1.45	0.33	0.49
2	27	0	0	0	0	27	0.67	1.44	0.31	0.53
3	29	0	0	0	0	29	0.64	1.44	0.32	0.5
4	31	0	0	0	0	31	0.62	1.43	0.31	0.47
5	27	0	0	0	0	27	0.67	1.42	0.32	0.54
6	30	0	0	0	0	30	0.63	1.41	0.34	0.48
7	30	0	0	0	0	30	0.63	1.43	0.34	0.47
8	30	0	0	0	0	30	0.62	1.47	0.32	0.53
9	29	0	0	0	0	29	0.62	1.43	0.32	0.52
10	29	0	0	0	0	29	0.62	1.43	0.31	0.49
11	29	0	0	0	0	29	0.63	1.45	0.31	0.52

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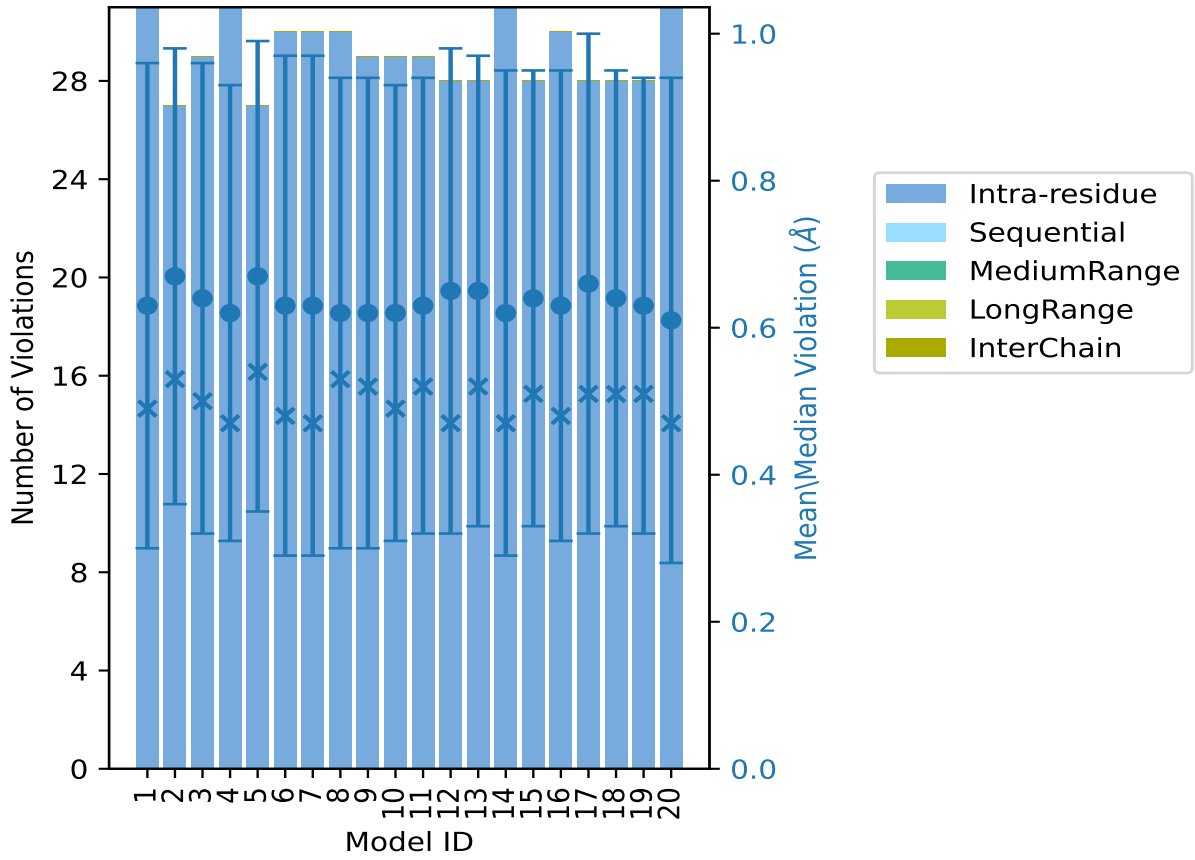
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	28	0	0	0	0	28	0.65	1.45	0.33	0.47
13	28	0	0	0	0	28	0.65	1.44	0.32	0.52
14	31	0	0	0	0	31	0.62	1.43	0.33	0.47
15	28	0	0	0	0	28	0.64	1.43	0.31	0.51
16	30	0	0	0	0	30	0.63	1.44	0.32	0.48
17	28	0	0	0	0	28	0.66	1.41	0.34	0.51
18	28	0	0	0	0	28	0.64	1.44	0.31	0.51
19	28	0	0	0	0	28	0.63	1.43	0.31	0.51
20	31	0	0	0	0	31	0.61	1.43	0.33	0.47

[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

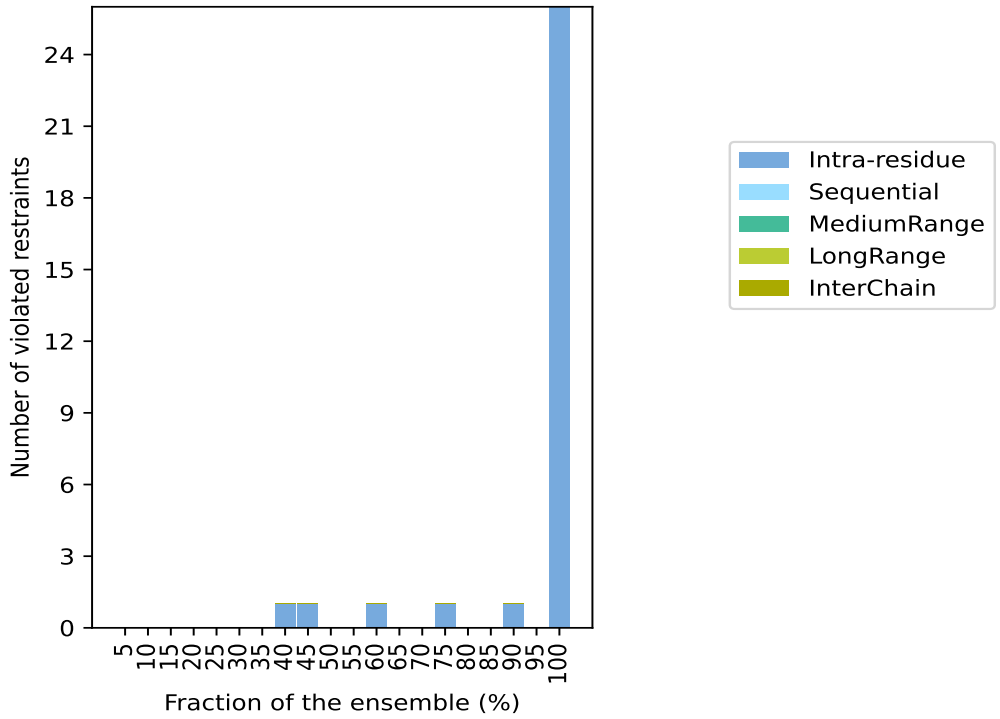
9.3 Distance violation statistics for the ensemble (i)

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, 250(IR:250, SQ:0, MR:0, LR:0, 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	0	0	0	0	0	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
1	0	0	0	0	1	8	40.0
1	0	0	0	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
1	0	0	0	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
1	0	0	0	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
1	0	0	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
26	0	0	0	0	26	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

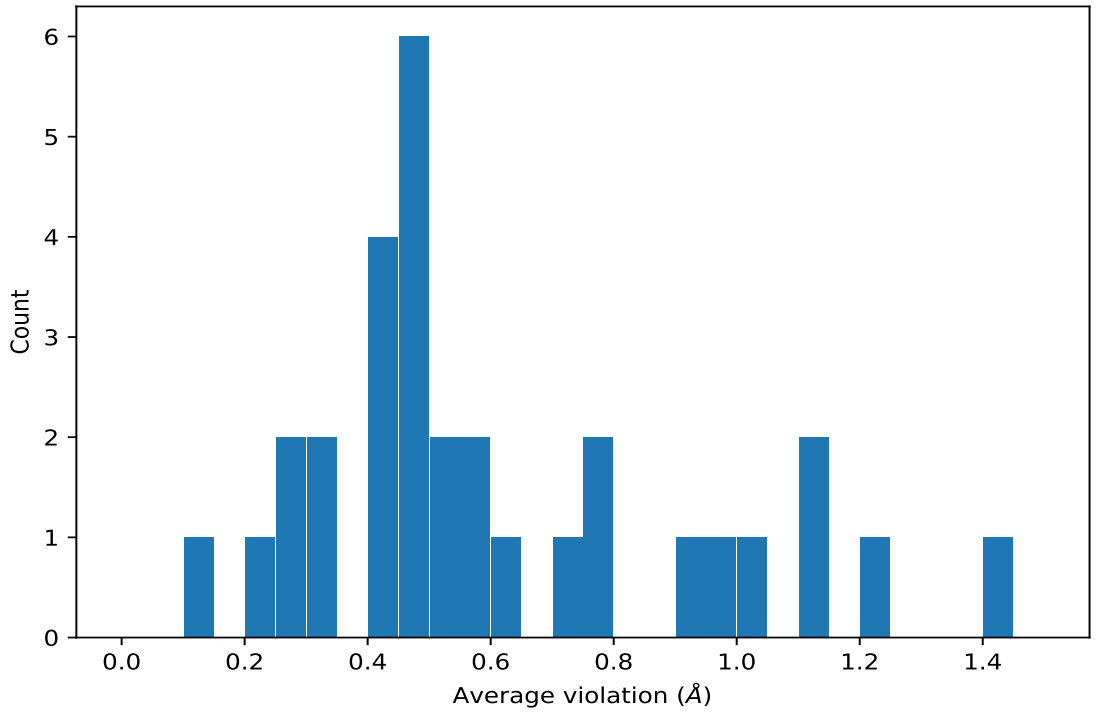
9.3.1 Bar graph : Distance violation statistics for the ensemble



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

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)
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	20	1.44	0.01	1.43
(1,94)	1:A:116:THR:H	1:A:116:THR:C	20	1.23	0.08	1.2
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	20	1.14	0.05	1.12
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	20	1.11	0.11	1.1
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	20	1.02	0.0	1.02
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	20	0.98	0.01	0.98
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	20	0.95	0.14	1.04
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	20	0.79	0.2	0.68
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	20	0.76	0.09	0.78
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	20	0.71	0.2	0.63
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	20	0.61	0.05	0.6
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	20	0.58	0.06	0.57
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	20	0.51	0.02	0.5
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	20	0.51	0.04	0.52
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	20	0.49	0.06	0.46
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	20	0.47	0.0	0.47

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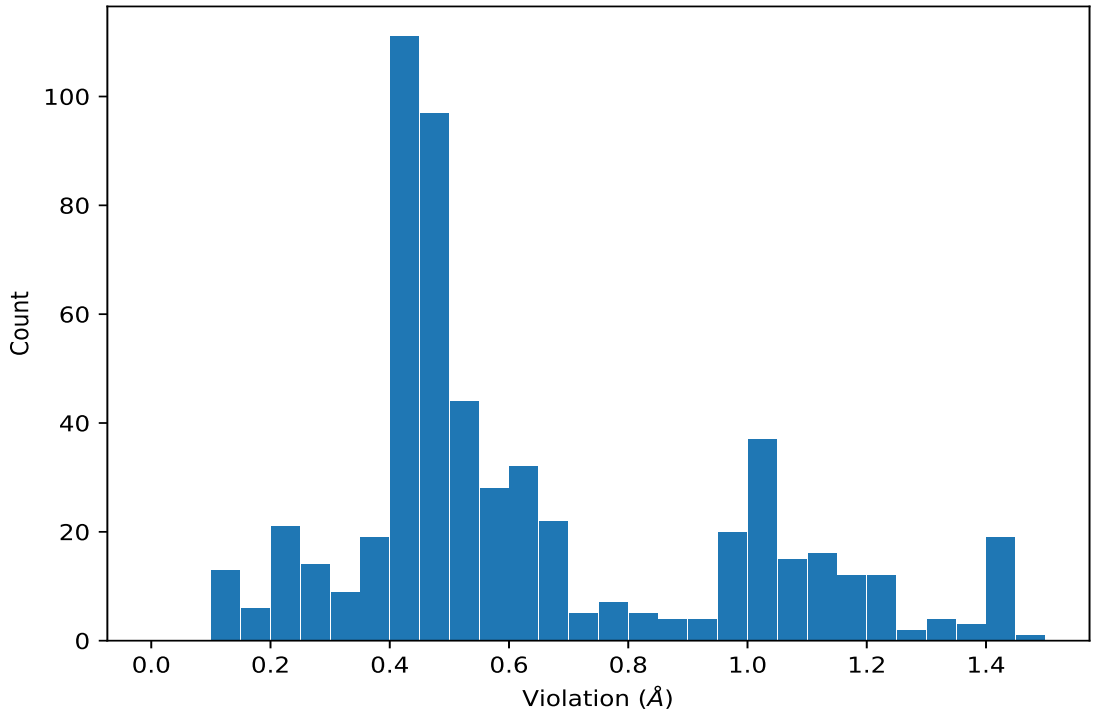
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	20	0.47	0.0	0.47
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	20	0.45	0.0	0.45
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	20	0.45	0.01	0.44
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	20	0.45	0.01	0.45
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	20	0.44	0.02	0.44
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	20	0.43	0.0	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	20	0.43	0.0	0.43
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	20	0.42	0.0	0.42
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	20	0.28	0.1	0.3
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	20	0.23	0.01	0.23
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	18	0.57	0.1	0.58
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	15	0.33	0.07	0.36
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	12	0.31	0.1	0.36
(1,113)	1:A:78:ILE:H	1:A:78:ILE:CB	9	0.29	0.04	0.28
(1,91)	1:A:78:ILE:H	1:A:78:ILE:C	8	0.14	0.01	0.14

[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)
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	8	1.47
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	1	1.45
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	11	1.45
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	12	1.45
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	2	1.44
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	3	1.44
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	13	1.44
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	16	1.44
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	18	1.44
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	4	1.43
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	7	1.43
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	9	1.43
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	10	1.43
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	14	1.43
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	15	1.43
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	19	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	20	1.43
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	5	1.42
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	6	1.41
(1,98)	1:A:132:VAL:H	1:A:132:VAL:C	17	1.41
(1,94)	1:A:116:THR:H	1:A:116:THR:C	6	1.37
(1,94)	1:A:116:THR:H	1:A:116:THR:C	17	1.37
(1,94)	1:A:116:THR:H	1:A:116:THR:C	12	1.35
(1,94)	1:A:116:THR:H	1:A:116:THR:C	14	1.34
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	14	1.34
(1,94)	1:A:116:THR:H	1:A:116:THR:C	5	1.33
(1,94)	1:A:116:THR:H	1:A:116:THR:C	20	1.33
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	17	1.26
(1,94)	1:A:116:THR:H	1:A:116:THR:C	13	1.25
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	8	1.24
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	12	1.24
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	3	1.23
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	17	1.23
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	9	1.23
(1,94)	1:A:116:THR:H	1:A:116:THR:C	1	1.22
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	19	1.22
(1,94)	1:A:116:THR:H	1:A:116:THR:C	7	1.21
(1,94)	1:A:116:THR:H	1:A:116:THR:C	10	1.21
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	6	1.21
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	10	1.21
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	18	1.21
(1,94)	1:A:116:THR:H	1:A:116:THR:C	2	1.2
(1,94)	1:A:116:THR:H	1:A:116:THR:C	4	1.19
(1,94)	1:A:116:THR:H	1:A:116:THR:C	8	1.19
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	2	1.19
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	6	1.19
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	15	1.19
(1,94)	1:A:116:THR:H	1:A:116:THR:C	3	1.18
(1,94)	1:A:116:THR:H	1:A:116:THR:C	9	1.17
(1,94)	1:A:116:THR:H	1:A:116:THR:C	16	1.17
(1,94)	1:A:116:THR:H	1:A:116:THR:C	15	1.16
(1,94)	1:A:116:THR:H	1:A:116:THR:C	19	1.16
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	16	1.16
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	4	1.15
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	7	1.15
(1,94)	1:A:116:THR:H	1:A:116:THR:C	18	1.14
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	7	1.14
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	11	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	13	1.14
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	13	1.13
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	5	1.13
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	14	1.12
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	20	1.12
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	1	1.11
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	3	1.11
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	10	1.11
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	16	1.11
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	18	1.11
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	19	1.1
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	2	1.09
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	15	1.09
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	1	1.09
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	20	1.09
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	9	1.08
(1,94)	1:A:116:THR:H	1:A:116:THR:C	11	1.07
(1,84)	1:A:14:GLY:H	1:A:14:GLY:C	6	1.07
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	2	1.06
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	18	1.06
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	5	1.06
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	7	1.06
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	1	1.05
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	11	1.05
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	12	1.05
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	14	1.05
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	8	1.04
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	3	1.04
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	5	1.04
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	9	1.04
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	20	1.04
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	7	1.03
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	16	1.03
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	1	1.03
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	6	1.03
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	7	1.03
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	8	1.03
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	11	1.03
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	14	1.03
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	15	1.03
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	16	1.03
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	1	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	4	1.02
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	5	1.02
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	20	1.02
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	8	1.02
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	17	1.02
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	4	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	2	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	3	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	4	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	5	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	9	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	10	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	12	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	13	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	17	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	18	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	19	1.02
(1,101)	1:A:143:GLU:H	1:A:143:GLU:C	20	1.02
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	15	1.01
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	1	1.0
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	17	1.0
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	4	0.99
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	8	0.99
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	11	0.99
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	12	0.99
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	12	0.98
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	2	0.98
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	3	0.98
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	5	0.98
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	6	0.98
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	9	0.98
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	13	0.98
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	16	0.98
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	18	0.98
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	11	0.97
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	7	0.97
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	10	0.97
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	14	0.97
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	15	0.97
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	19	0.97
(1,100)	1:A:141:ALA:H	1:A:141:ALA:C	20	0.97
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	2	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:A:49:LYS:H	1:A:49:LYS:C	7	0.94
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	11	0.92
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	13	0.9
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	17	0.89
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	16	0.89
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	12	0.88
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	1	0.86
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	18	0.83
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	3	0.82
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	10	0.82
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	16	0.82
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	13	0.8
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	19	0.79
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	10	0.79
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	8	0.78
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	19	0.77
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	4	0.77
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	5	0.77
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	12	0.75
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	13	0.74
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	15	0.73
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	4	0.72
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	6	0.72
(1,83)	1:A:7:PHE:H	1:A:7:PHE:C	19	0.72
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	2	0.69
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	15	0.69
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	16	0.68
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	20	0.68
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	4	0.68
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	10	0.68
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	14	0.67
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	4	0.66
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	1	0.66
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	6	0.66
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	2	0.66
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	14	0.66
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	8	0.66
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	13	0.65
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	3	0.65
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	4	0.65
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	9	0.65
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	6	0.65
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	7	0.65
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	15	0.65
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	6	0.65
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	12	0.64
(1,89)	1:A:56:ILE:H	1:A:56:ILE:C	9	0.64
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	13	0.64
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	14	0.64
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	19	0.64
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	2	0.63
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	15	0.63
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	17	0.63
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	18	0.63
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	1	0.63
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	2	0.63
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	3	0.63
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	4	0.63
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	8	0.63
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	11	0.63
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	12	0.63
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	13	0.63
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	17	0.63
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	18	0.63
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	20	0.63
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	3	0.62
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	18	0.62
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	13	0.62
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	9	0.62
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	5	0.62
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	9	0.62
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	10	0.62
(1,103)	1:A:149:ASN:H	1:A:149:ASN:C	16	0.62
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	9	0.61
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	11	0.61
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	8	0.61
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	11	0.61
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	1	0.6
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	5	0.6
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	14	0.6
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	7	0.6
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	11	0.6
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	6	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	14	0.6
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	10	0.59
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	2	0.59
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	15	0.59
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	19	0.59
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	7	0.58
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	20	0.58
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	8	0.58
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	16	0.58
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	19	0.58
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	3	0.58
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	11	0.58
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	3	0.58
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	8	0.57
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	18	0.57
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	19	0.57
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	17	0.57
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	5	0.56
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	8	0.56
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	17	0.55
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	10	0.55
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	15	0.55
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	12	0.54
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	5	0.54
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	5	0.54
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	9	0.54
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	18	0.54
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	17	0.54
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	8	0.54
(1,99)	1:A:135:GLY:H	1:A:135:GLY:C	6	0.53
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	2	0.53
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	6	0.53
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	10	0.53
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	13	0.53
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	16	0.53
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	9	0.53
(1,110)	1:A:48:TYR:H	1:A:48:TYR:CB	10	0.53
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	14	0.52
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	3	0.52
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	4	0.52
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	8	0.52
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	9	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	11	0.52
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	14	0.52
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	15	0.52
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	18	0.52
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	19	0.52
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	1	0.52
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	7	0.52
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	11	0.52
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	12	0.52
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	16	0.52
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	7	0.51
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	20	0.51
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	1	0.51
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	14	0.51
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	2	0.5
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	2	0.5
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	3	0.5
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	4	0.5
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	5	0.5
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	9	0.5
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	13	0.5
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	15	0.5
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	18	0.5
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	19	0.5
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	1	0.49
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	1	0.49
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	6	0.49
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	10	0.49
(1,106)	1:A:10:ILE:H	1:A:10:ILE:CB	20	0.49
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	17	0.48
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	20	0.48
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	16	0.48
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	3	0.48
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	20	0.47
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	7	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	1	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	2	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	3	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	4	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	5	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	6	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	8	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	9	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	10	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	11	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	12	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	13	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	14	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	15	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	16	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	17	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	18	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	19	0.47
(1,119)	1:A:138:ILE:H	1:A:138:ILE:CB	20	0.47
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	3	0.47
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	4	0.47
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	14	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	1	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	2	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	3	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	4	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	5	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	6	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	7	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	8	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	9	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	10	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	11	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	12	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	13	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	14	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	15	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	16	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	17	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	18	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	19	0.47
(1,115)	1:A:89:ILE:H	1:A:89:ILE:CB	20	0.47
(1,114)	1:A:86:GLU:H	1:A:86:GLU:CB	12	0.47
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	2	0.47
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	5	0.46
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	17	0.46
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	3	0.46
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	6	0.46
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	7	0.46
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	1	0.46
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	4	0.46
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	2	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	3	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	5	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	6	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	7	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	9	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	10	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	11	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	13	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	14	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	15	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	16	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	18	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	19	0.45
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	20	0.45
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	1	0.45
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	3	0.45
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	4	0.45
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	6	0.45
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	8	0.45
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	9	0.45
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	12	0.45
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	14	0.45
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	20	0.45
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	15	0.45
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	16	0.45
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	17	0.45
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	19	0.45
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	7	0.45
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	11	0.45
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	18	0.45
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	19	0.45
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	14	0.45
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	4	0.44
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	14	0.44
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	15	0.44
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	16	0.44
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	4	0.44
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	8	0.44
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	12	0.44
(1,120)	1:A:141:ALA:H	1:A:141:ALA:CB	17	0.44
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	2	0.44
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	7	0.44
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	10	0.44
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	11	0.44
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	13	0.44
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	15	0.44
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	16	0.44
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	18	0.44
(1,118)	1:A:133:LYS:H	1:A:133:LYS:CB	19	0.44
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	7	0.44
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	8	0.44
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	9	0.44
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	11	0.44
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	13	0.44
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	16	0.44
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	19	0.44
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	1	0.44
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	10	0.44
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	12	0.44
(1,116)	1:A:108:ASN:H	1:A:108:ASN:CB	20	0.44
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	5	0.44
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	6	0.44
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	8	0.44
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	10	0.44
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	12	0.44
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	13	0.44
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	14	0.44
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	15	0.44
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	16	0.44
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	17	0.44
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	20	0.44
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	5	0.44
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	1	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	2	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	3	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	5	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	6	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	8	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	9	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	10	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	11	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	12	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	13	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	17	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	18	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	19	0.43
(1,121)	1:A:142:MET:H	1:A:142:MET:CB	20	0.43
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	2	0.43
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	5	0.43
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	6	0.43
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	10	0.43
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	12	0.43
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	14	0.43
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	15	0.43
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	17	0.43
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	18	0.43
(1,117)	1:A:118:LYS:H	1:A:118:LYS:CB	20	0.43
(1,108)	1:A:37:ARG:H	1:A:37:ARG:CB	9	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	1	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	2	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	3	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	4	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	6	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	7	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	8	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	9	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	10	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	11	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	12	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	13	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	14	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	15	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	16	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	17	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	18	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	19	0.43
(1,107)	1:A:33:ALA:H	1:A:33:ALA:CB	20	0.43
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	5	0.43
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	2	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	3	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	5	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	6	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	8	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	9	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	10	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	11	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	12	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	13	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	15	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	16	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	17	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	18	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	19	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	20	0.42
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	4	0.42
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	20	0.42
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	4	0.41
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	7	0.41
(1,97)	1:A:131:LYS:H	1:A:131:LYS:C	14	0.41
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	7	0.4
(1,113)	1:A:78:ILE:H	1:A:78:ILE:CB	11	0.39
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	4	0.39
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	10	0.39
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	11	0.39
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	14	0.39
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	13	0.37
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	6	0.37
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	8	0.37
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	13	0.37
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	14	0.37
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	15	0.37
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	20	0.37
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	18	0.37
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	1	0.37
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	4	0.36
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	11	0.36
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	12	0.36
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	17	0.36
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	3	0.36
(1,86)	1:A:43:GLU:H	1:A:43:GLU:C	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	1	0.35
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	19	0.35
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	3	0.33
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	10	0.33
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	18	0.33
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	18	0.32
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	16	0.32
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	16	0.32
(1,93)	1:A:112:PHE:H	1:A:112:PHE:C	5	0.29
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	9	0.29
(1,113)	1:A:78:ILE:H	1:A:78:ILE:CB	1	0.29
(1,113)	1:A:78:ILE:H	1:A:78:ILE:CB	6	0.29
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	1	0.29
(1,113)	1:A:78:ILE:H	1:A:78:ILE:CB	14	0.28
(1,113)	1:A:78:ILE:H	1:A:78:ILE:CB	16	0.28
(1,113)	1:A:78:ILE:H	1:A:78:ILE:CB	20	0.28
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	2	0.28
(1,113)	1:A:78:ILE:H	1:A:78:ILE:CB	4	0.27
(1,113)	1:A:78:ILE:H	1:A:78:ILE:CB	8	0.27
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	6	0.27
(1,113)	1:A:78:ILE:H	1:A:78:ILE:CB	7	0.26
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	6	0.26
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	3	0.24
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	10	0.24
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	19	0.24
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	12	0.24
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	2	0.23
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	4	0.23
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	5	0.23
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	13	0.23
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	15	0.23
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	16	0.23
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	17	0.23
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	18	0.23
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	1	0.22
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	8	0.22
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	9	0.22
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	11	0.22
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	12	0.22
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	14	0.22
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	20	0.22
(1,105)	1:A:161:CYS:H	1:A:161:CYS:C	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	8	0.21
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	15	0.19
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	10	0.18
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	9	0.18
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	17	0.17
(1,35)	1:A:70:HIS:H	1:A:70:HIS:HA	3	0.16
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	20	0.16
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	11	0.15
(1,91)	1:A:78:ILE:H	1:A:78:ILE:C	4	0.14
(1,91)	1:A:78:ILE:H	1:A:78:ILE:C	7	0.14
(1,91)	1:A:78:ILE:H	1:A:78:ILE:C	8	0.14
(1,91)	1:A:78:ILE:H	1:A:78:ILE:C	14	0.14
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	19	0.14
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	7	0.14
(1,91)	1:A:78:ILE:H	1:A:78:ILE:C	1	0.13
(1,91)	1:A:78:ILE:H	1:A:78:ILE:C	6	0.13
(1,91)	1:A:78:ILE:H	1:A:78:ILE:C	16	0.13
(1,91)	1:A:78:ILE:H	1:A:78:ILE:C	20	0.13
(1,104)	1:A:154:LYS:H	1:A:154:LYS:C	13	0.13
(1,111)	1:A:69:ARG:H	1:A:69:ARG:CB	9	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found