



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 12:30 AM UTC

PDB ID : 2MLK / pdb_00002mlk
BMRB ID : 18200
Title : Three-dimensional structure of the C-terminal DNA-binding domain of RstA protein from *Klebsiella pneumoniae*
Authors : Fang, P.; Chen, S.; Cheng, Y.; Chang, C.; Yu, T.; Huang, T.
Deposited on : 2014-03-02

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

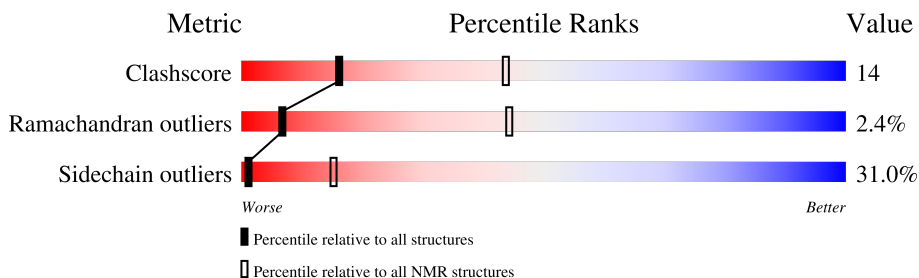
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	119	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:136-A:234 (99)	0.86	9

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1738 atoms, of which 873 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RstA.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	110	1738	546	873	156	161	2	0

There are 10 discrepancies between the modelled and reference sequences:

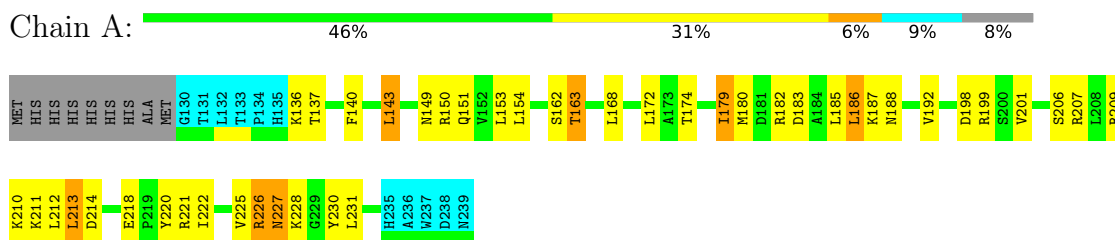
Chain	Residue	Modelled	Actual	Comment	Reference
A	121	MET	-	expression tag	UNP U5MDD9
A	122	HIS	-	expression tag	UNP U5MDD9
A	123	HIS	-	expression tag	UNP U5MDD9
A	124	HIS	-	expression tag	UNP U5MDD9
A	125	HIS	-	expression tag	UNP U5MDD9
A	126	HIS	-	expression tag	UNP U5MDD9
A	127	HIS	-	expression tag	UNP U5MDD9
A	128	ALA	-	expression tag	UNP U5MDD9
A	129	MET	-	expression tag	UNP U5MDD9
A	130	GLY	-	expression tag	UNP U5MDD9

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: RstA

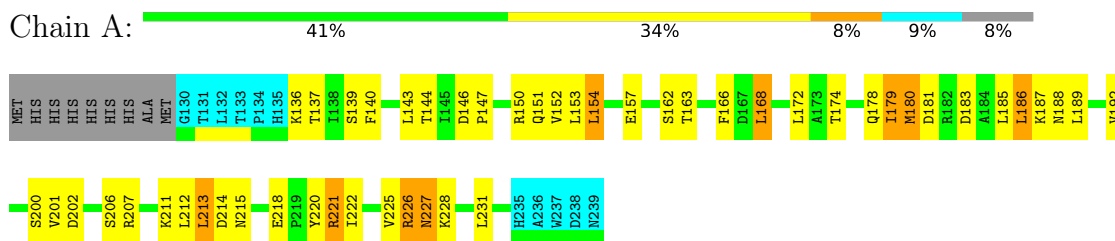


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

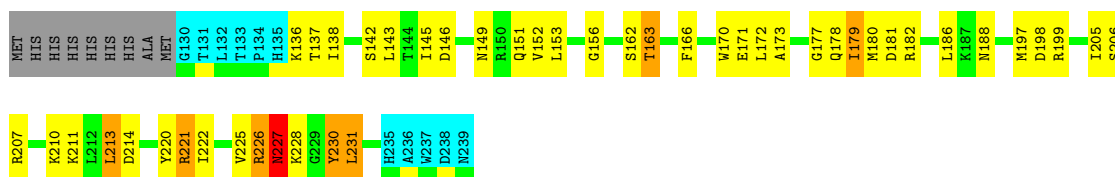
- Molecule 1: RstA



4.2.2 Score per residue for model 2

- Molecule 1: RstA

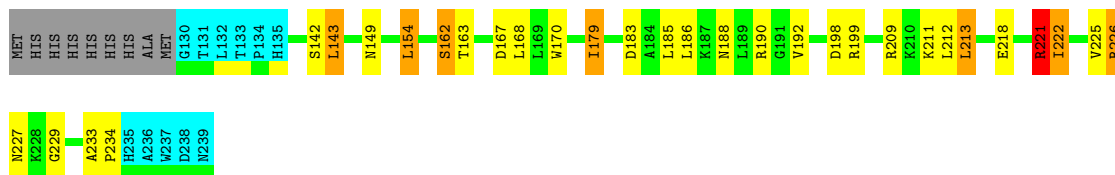




4.2.3 Score per residue for model 3

- Molecule 1: RstA

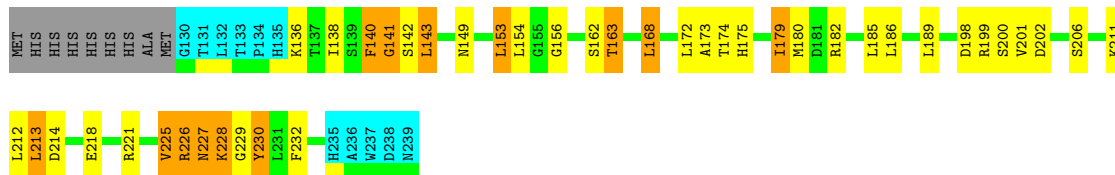
Chain A: 57% 19% 6% 9% 8%



4.2.4 Score per residue for model 4

- Molecule 1: RstA

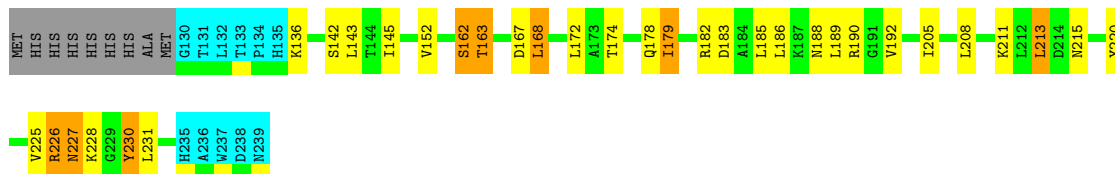
Chain A: 48% 24% 11% 9% 8%



4.2.5 Score per residue for model 5

- Molecule 1: RstA

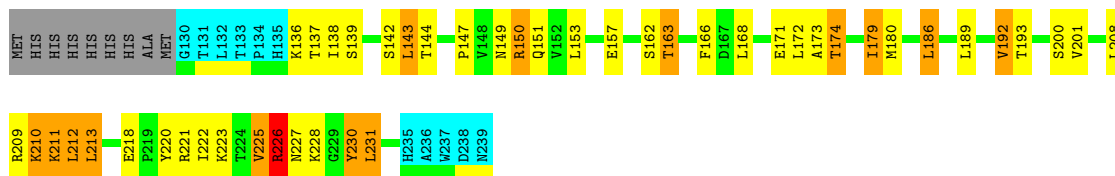
Chain A: 55% 21% 7% 9% 8%



4.2.6 Score per residue for model 6

- Molecule 1: RstA

Chain A: 



4.2.7 Score per residue for model 7

- Molecule 1: RstA

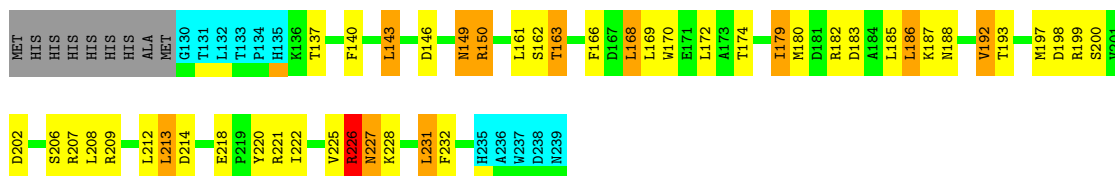
Chain A: 



4.2.8 Score per residue for model 8

- Molecule 1: RstA

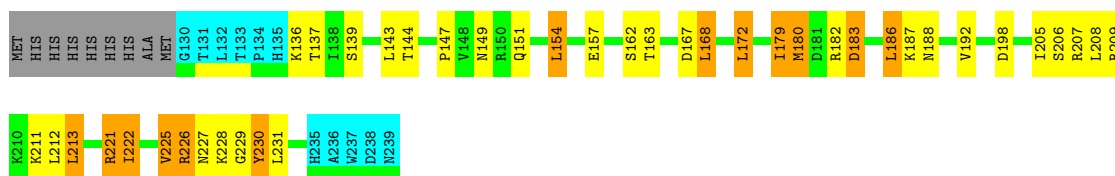
Chain A: 



4.2.9 Score per residue for model 9 (medoid)

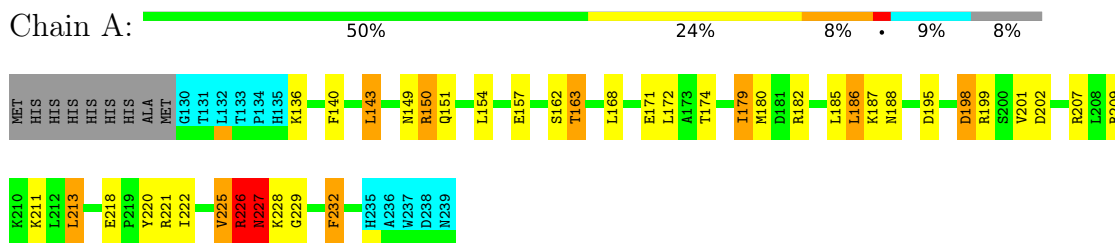
- Molecule 1: RstA

Chain A: 



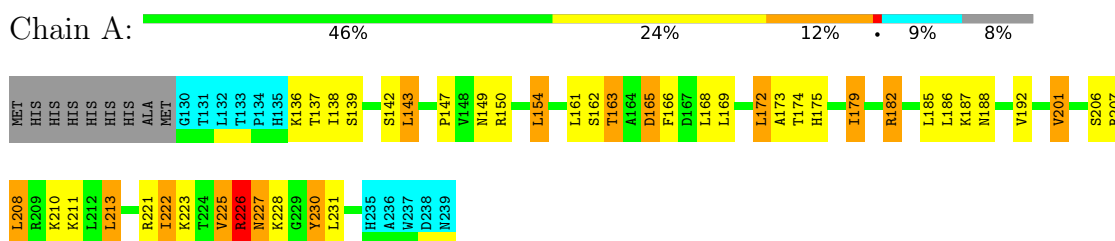
4.2.10 Score per residue for model 10

- Molecule 1: RstA



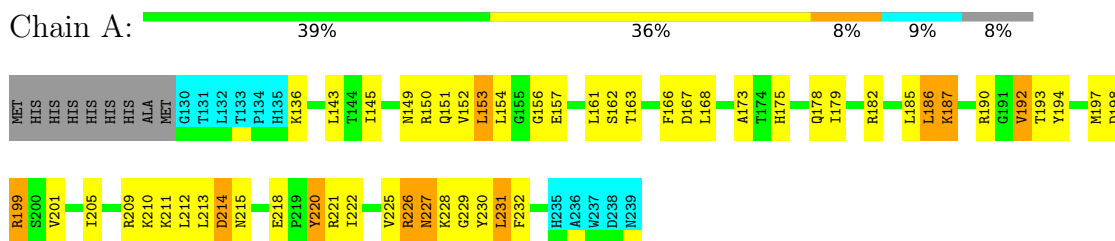
4.2.11 Score per residue for model 11

- Molecule 1: RstA



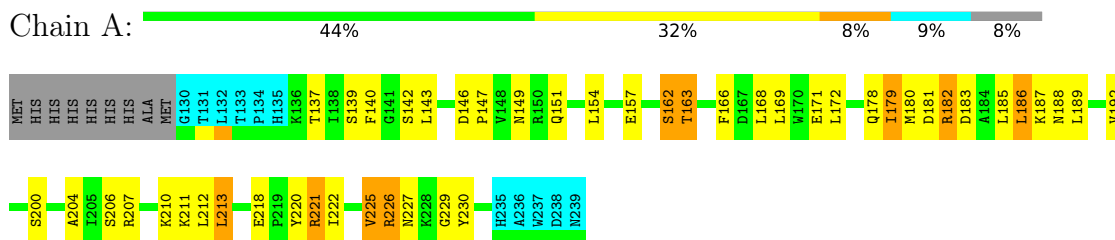
4.2.12 Score per residue for model 12

- Molecule 1: RstA



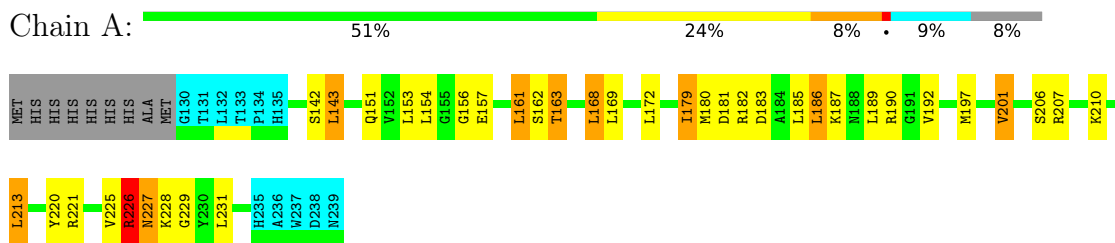
4.2.13 Score per residue for model 13

- Molecule 1: RstA



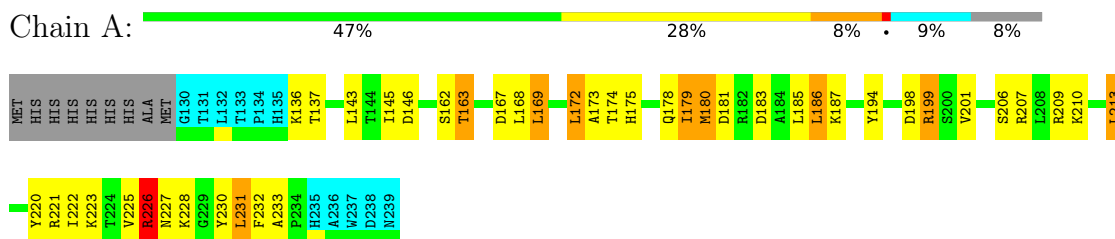
4.2.14 Score per residue for model 14

- Molecule 1: RstA



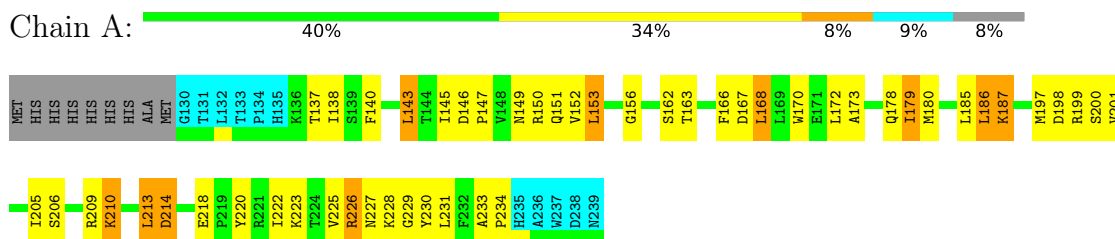
4.2.15 Score per residue for model 15

- Molecule 1: RstA



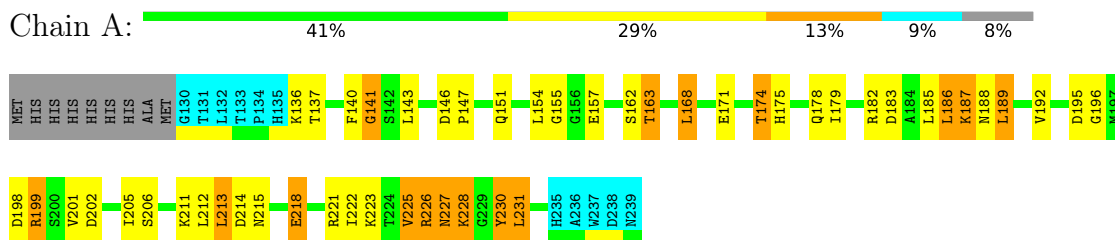
4.2.16 Score per residue for model 16

- Molecule 1: RstA



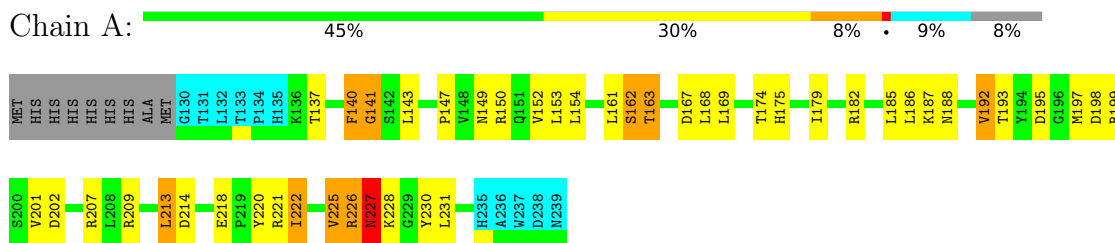
4.2.17 Score per residue for model 17

- Molecule 1: RstA



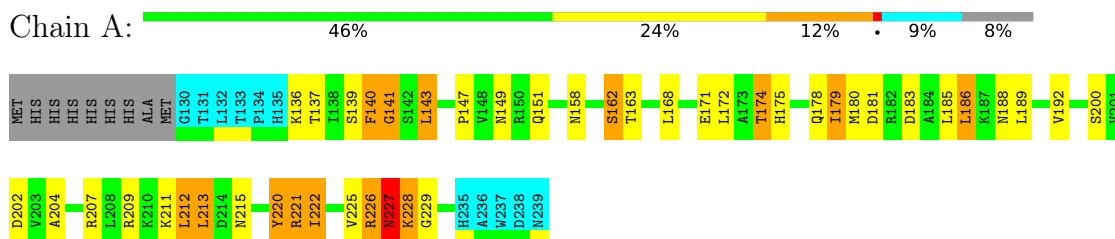
4.2.18 Score per residue for model 18

- Molecule 1: RstA



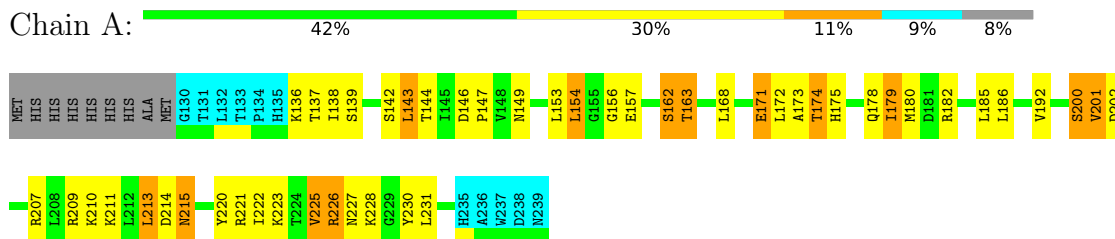
4.2.19 Score per residue for model 19

- Molecule 1: RstA



4.2.20 Score per residue for model 20

- Molecule 1: RstA



5 Refinement protocol and experimental data overview

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

Of the 150 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
CYANA	structure solution	
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1173
Number of shifts mapped to atoms	1156
Number of unparsed shifts	0
Number of shifts with mapping errors	17
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality i

6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	777	799	799	23±5
All	All	15540	15980	15980	452

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:222:ILE:O	1:A:222:ILE:HG23	0.90	1.64	19	4
1:A:186:LEU:HD13	1:A:187:LYS:N	0.90	1.81	13	1
1:A:168:LEU:HD13	1:A:185:LEU:HD21	0.89	1.44	8	2
1:A:143:LEU:HD12	1:A:154:LEU:HD12	0.87	1.46	14	2
1:A:168:LEU:HD12	1:A:189:LEU:HD11	0.78	1.55	1	2
1:A:143:LEU:HD12	1:A:212:LEU:HD21	0.77	1.53	19	2
1:A:186:LEU:HD22	1:A:186:LEU:O	0.77	1.79	13	1
1:A:225:VAL:HG11	1:A:231:LEU:HD12	0.76	1.56	17	4
1:A:186:LEU:HD23	1:A:187:LYS:N	0.76	1.95	17	4
1:A:180:MET:HE2	1:A:185:LEU:HD13	0.75	1.57	8	1
1:A:154:LEU:HD13	1:A:212:LEU:HD11	0.72	1.61	3	2
1:A:168:LEU:HD21	1:A:185:LEU:HD21	0.72	1.62	5	9
1:A:222:ILE:O	1:A:222:ILE:CG2	0.71	2.37	19	1
1:A:222:ILE:HG22	1:A:230:TYR:CE1	0.70	2.22	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:LEU:HD22	1:A:186:LEU:C	0.69	2.10	13	1
1:A:168:LEU:HD11	1:A:185:LEU:HD21	0.69	1.64	17	1
1:A:205:ILE:HG21	1:A:230:TYR:CZ	0.69	2.23	16	2
1:A:140:PHE:O	1:A:141:GLY:C	0.67	2.35	4	4
1:A:168:LEU:HD23	1:A:208:LEU:HD22	0.65	1.67	6	1
1:A:175:HIS:CG	1:A:175:HIS:O	0.64	2.50	19	1
1:A:168:LEU:HD23	1:A:189:LEU:HD11	0.63	1.70	17	1
1:A:143:LEU:HD13	1:A:220:TYR:CE1	0.63	2.28	8	1
1:A:209:ARG:O	1:A:213:LEU:N	0.63	2.32	12	10
1:A:185:LEU:HD22	1:A:230:TYR:CE2	0.62	2.29	4	1
1:A:168:LEU:HD12	1:A:204:ALA:HB1	0.62	1.71	19	2
1:A:168:LEU:CD2	1:A:185:LEU:HD11	0.61	2.24	3	1
1:A:185:LEU:HD23	1:A:201:VAL:HG13	0.61	1.70	7	3
1:A:172:LEU:HD21	1:A:230:TYR:CE2	0.61	2.30	11	1
1:A:168:LEU:HG	1:A:189:LEU:HD11	0.61	1.72	13	1
1:A:186:LEU:HD12	1:A:187:LYS:N	0.61	2.10	14	2
1:A:186:LEU:HB3	1:A:201:VAL:HG23	0.61	1.73	14	3
1:A:179:ILE:CD1	1:A:225:VAL:HG21	0.61	2.26	11	3
1:A:172:LEU:O	1:A:180:MET:HE1	0.60	1.95	15	1
1:A:192:VAL:HG11	1:A:194:TYR:CE2	0.60	2.31	7	1
1:A:143:LEU:CD1	1:A:212:LEU:HD21	0.60	2.24	19	3
1:A:220:TYR:O	1:A:221:ARG:C	0.60	2.44	10	9
1:A:169:LEU:HD22	1:A:220:TYR:OH	0.60	1.96	8	1
1:A:168:LEU:HG	1:A:185:LEU:HD11	0.59	1.74	11	3
1:A:186:LEU:HD13	1:A:186:LEU:C	0.59	2.21	13	1
1:A:168:LEU:CD2	1:A:189:LEU:HD11	0.59	2.27	17	1
1:A:205:ILE:HG23	1:A:230:TYR:CZ	0.59	2.32	2	4
1:A:213:LEU:O	1:A:214:ASP:C	0.59	2.45	7	2
1:A:143:LEU:HD21	1:A:152:VAL:HB	0.58	1.73	1	2
1:A:179:ILE:HD12	1:A:180:MET:N	0.58	2.13	19	4
1:A:139:SER:HB3	1:A:144:THR:HG23	0.58	1.74	9	4
1:A:143:LEU:HD12	1:A:154:LEU:HD13	0.58	1.75	11	2
1:A:165:ASP:OD2	1:A:208:LEU:HD12	0.58	1.97	11	1
1:A:220:TYR:CD2	1:A:222:ILE:HD11	0.58	2.34	15	1
1:A:192:VAL:HG23	1:A:194:TYR:H	0.57	1.59	12	1
1:A:205:ILE:HD13	1:A:230:TYR:CE1	0.57	2.34	16	1
1:A:172:LEU:HD13	1:A:230:TYR:CE2	0.57	2.34	15	3
1:A:168:LEU:HD21	1:A:185:LEU:HD11	0.57	1.76	3	1
1:A:154:LEU:HD22	1:A:212:LEU:HD23	0.57	1.75	4	1
1:A:225:VAL:CG1	1:A:231:LEU:HD12	0.57	2.29	17	1
1:A:154:LEU:HD13	1:A:212:LEU:CD1	0.57	2.30	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:ILE:HD11	1:A:228:LYS:O	0.56	1.99	19	10
1:A:222:ILE:HG22	1:A:230:TYR:OH	0.56	2.00	11	1
1:A:221:ARG:HD3	1:A:233:ALA:HB3	0.56	1.77	15	1
1:A:220:TYR:CE2	1:A:222:ILE:HD12	0.56	2.36	16	1
1:A:172:LEU:C	1:A:172:LEU:HD12	0.56	2.26	15	1
1:A:172:LEU:HD11	1:A:232:PHE:CZ	0.56	2.36	15	1
1:A:168:LEU:CD1	1:A:189:LEU:HD11	0.56	2.29	1	3
1:A:212:LEU:HD13	1:A:220:TYR:CD2	0.56	2.34	8	1
1:A:168:LEU:CD1	1:A:185:LEU:HD11	0.56	2.31	20	1
1:A:145:ILE:HG12	1:A:152:VAL:HG12	0.56	1.76	12	3
1:A:168:LEU:CD1	1:A:185:LEU:HD21	0.55	2.32	20	2
1:A:222:ILE:HG22	1:A:230:TYR:CE2	0.55	2.36	7	1
1:A:205:ILE:HG23	1:A:230:TYR:CE2	0.55	2.36	2	1
1:A:172:LEU:HA	1:A:180:MET:HE1	0.55	1.78	8	1
1:A:186:LEU:HA	1:A:189:LEU:HD12	0.55	1.78	17	1
1:A:183:ASP:HA	1:A:186:LEU:HD11	0.55	1.78	14	1
1:A:213:LEU:CG	1:A:213:LEU:O	0.54	2.56	16	1
1:A:168:LEU:HD13	1:A:189:LEU:HD11	0.54	1.79	6	2
1:A:232:PHE:C	1:A:232:PHE:CD1	0.54	2.84	10	1
1:A:225:VAL:O	1:A:227:ASN:N	0.54	2.41	4	20
1:A:154:LEU:HD22	1:A:212:LEU:CD2	0.54	2.32	4	2
1:A:192:VAL:HG23	1:A:194:TYR:N	0.54	2.18	12	1
1:A:168:LEU:HD22	1:A:208:LEU:CD2	0.53	2.32	7	2
1:A:185:LEU:HD22	1:A:230:TYR:CE1	0.53	2.38	13	1
1:A:168:LEU:HD12	1:A:189:LEU:HD21	0.53	1.79	14	1
1:A:149:ASN:O	1:A:150:ARG:C	0.53	2.52	11	5
1:A:153:LEU:HD11	1:A:156:GLY:O	0.53	2.04	14	2
1:A:185:LEU:HD23	1:A:201:VAL:CG1	0.53	2.33	15	2
1:A:168:LEU:CD2	1:A:185:LEU:HD21	0.53	2.34	1	3
1:A:179:ILE:HD11	1:A:225:VAL:HG21	0.53	1.78	11	1
1:A:137:THR:HG22	1:A:147:PRO:HD2	0.53	1.79	20	10
1:A:210:LYS:HG3	1:A:211:LYS:N	0.53	2.18	6	1
1:A:214:ASP:O	1:A:218:GLU:C	0.53	2.52	16	2
1:A:213:LEU:O	1:A:213:LEU:HG	0.52	2.04	16	16
1:A:179:ILE:HD13	1:A:180:MET:N	0.52	2.19	10	6
1:A:205:ILE:HG21	1:A:230:TYR:CE2	0.52	2.38	16	1
1:A:143:LEU:HD12	1:A:154:LEU:CD1	0.52	2.34	20	1
1:A:153:LEU:HD21	1:A:156:GLY:HA2	0.52	1.80	16	4
1:A:177:GLY:O	1:A:231:LEU:HD21	0.52	2.05	2	1
1:A:138:ILE:HD12	1:A:173:ALA:HB1	0.52	1.80	2	1
1:A:168:LEU:O	1:A:168:LEU:HD12	0.51	2.05	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:221:ARG:O	1:A:222:ILE:HG22	0.51	2.05	9	1
1:A:209:ARG:NH2	1:A:222:ILE:HD12	0.51	2.19	6	1
1:A:154:LEU:C	1:A:154:LEU:HD13	0.51	2.30	17	1
1:A:143:LEU:HD12	1:A:212:LEU:CD1	0.51	2.34	3	1
1:A:138:ILE:HD12	1:A:173:ALA:CB	0.51	2.36	20	5
1:A:222:ILE:C	1:A:222:ILE:HD13	0.51	2.30	19	1
1:A:149:ASN:C	1:A:150:ARG:HG2	0.51	2.31	8	1
1:A:182:ARG:O	1:A:186:LEU:HD12	0.51	2.06	13	1
1:A:168:LEU:CG	1:A:185:LEU:HD21	0.50	2.36	1	1
1:A:225:VAL:HG23	1:A:229:GLY:N	0.50	2.22	13	4
1:A:226:ARG:O	1:A:227:ASN:C	0.50	2.54	19	20
1:A:231:LEU:HD23	1:A:232:PHE:H	0.50	1.65	15	3
1:A:169:LEU:HA	1:A:172:LEU:HD23	0.50	1.83	15	1
1:A:212:LEU:HD13	1:A:220:TYR:CE2	0.50	2.40	8	1
1:A:231:LEU:HD23	1:A:232:PHE:N	0.50	2.22	15	2
1:A:145:ILE:HG13	1:A:152:VAL:HG12	0.49	1.83	5	1
1:A:183:ASP:HA	1:A:186:LEU:HD21	0.49	1.82	19	4
1:A:143:LEU:CD1	1:A:212:LEU:HD11	0.49	2.38	6	1
1:A:201:VAL:HG12	1:A:205:ILE:HD11	0.49	1.84	16	1
1:A:161:LEU:HD13	1:A:208:LEU:CD1	0.49	2.37	8	1
1:A:172:LEU:O	1:A:172:LEU:HD12	0.49	2.07	15	1
1:A:179:ILE:HD11	1:A:229:GLY:HA3	0.49	1.84	4	1
1:A:222:ILE:HG22	1:A:230:TYR:CD1	0.49	2.43	6	1
1:A:183:ASP:HA	1:A:186:LEU:HD22	0.49	1.84	15	1
1:A:210:LYS:O	1:A:213:LEU:HD13	0.49	2.08	16	1
1:A:222:ILE:C	1:A:222:ILE:CD1	0.49	2.86	19	1
1:A:205:ILE:HG23	1:A:230:TYR:OH	0.49	2.07	17	1
1:A:221:ARG:O	1:A:222:ILE:CG2	0.48	2.61	9	2
1:A:169:LEU:HD21	1:A:208:LEU:HG	0.48	1.84	8	1
1:A:152:VAL:HG21	1:A:161:LEU:CD1	0.48	2.37	18	1
1:A:213:LEU:O	1:A:213:LEU:CG	0.48	2.60	8	13
1:A:172:LEU:HD11	1:A:222:ILE:HD13	0.48	1.84	8	1
1:A:198:ASP:O	1:A:199:ARG:C	0.48	2.57	15	11
1:A:137:THR:HG21	1:A:146:ASP:OD2	0.48	2.08	2	4
1:A:172:LEU:CD1	1:A:222:ILE:HD11	0.48	2.38	9	1
1:A:169:LEU:HD23	1:A:172:LEU:HD23	0.47	1.85	13	1
1:A:168:LEU:HD21	1:A:185:LEU:HG	0.47	1.86	19	1
1:A:139:SER:CB	1:A:144:THR:HG23	0.47	2.39	1	1
1:A:225:VAL:HG22	1:A:229:GLY:C	0.47	2.35	12	5
1:A:168:LEU:HD22	1:A:208:LEU:HD22	0.47	1.85	7	2
1:A:230:TYR:CD1	1:A:230:TYR:C	0.47	2.93	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:HIS:O	1:A:180:MET:HE3	0.47	2.10	15	1
1:A:201:VAL:HG12	1:A:205:ILE:CD1	0.47	2.40	16	1
1:A:154:LEU:HD21	1:A:214:ASP:OD2	0.46	2.10	1	1
1:A:162:SER:O	1:A:163:THR:C	0.46	2.58	17	20
1:A:168:LEU:HD23	1:A:208:LEU:HD11	0.46	1.88	9	1
1:A:181:ASP:O	1:A:185:LEU:N	0.46	2.48	15	1
1:A:161:LEU:HD13	1:A:169:LEU:CD1	0.46	2.41	11	2
1:A:145:ILE:CD1	1:A:173:ALA:HB2	0.46	2.41	12	1
1:A:183:ASP:O	1:A:186:LEU:CD1	0.46	2.64	13	1
1:A:233:ALA:HB1	1:A:234:PRO:HD2	0.46	1.88	16	2
1:A:213:LEU:O	1:A:215:ASN:N	0.45	2.49	20	1
1:A:192:VAL:HG12	1:A:193:THR:H	0.45	1.72	8	3
1:A:220:TYR:CZ	1:A:222:ILE:HD12	0.45	2.46	16	1
1:A:143:LEU:HD12	1:A:154:LEU:HD22	0.45	1.88	10	1
1:A:208:LEU:O	1:A:212:LEU:HD12	0.45	2.12	8	1
1:A:186:LEU:HD23	1:A:186:LEU:C	0.45	2.35	17	2
1:A:182:ARG:O	1:A:186:LEU:HG	0.45	2.12	14	2
1:A:154:LEU:CD2	1:A:212:LEU:HD22	0.45	2.42	12	1
1:A:226:ARG:O	1:A:228:LYS:N	0.44	2.50	4	6
1:A:186:LEU:HD12	1:A:197:MET:C	0.44	2.37	16	1
1:A:172:LEU:HD12	1:A:172:LEU:O	0.44	2.12	20	1
1:A:161:LEU:HD13	1:A:208:LEU:HD11	0.44	1.90	8	1
1:A:186:LEU:CB	1:A:201:VAL:HG21	0.44	2.42	17	1
1:A:222:ILE:HG22	1:A:222:ILE:O	0.44	2.13	15	1
1:A:172:LEU:HD11	1:A:222:ILE:CD1	0.44	2.43	8	1
1:A:185:LEU:HD23	1:A:201:VAL:HG11	0.44	1.90	15	1
1:A:168:LEU:HG	1:A:185:LEU:HD21	0.44	1.90	1	1
1:A:149:ASN:O	1:A:150:ARG:HG2	0.43	2.13	6	1
1:A:138:ILE:HD12	1:A:173:ALA:HB3	0.43	1.89	20	4
1:A:171:GLU:O	1:A:174:THR:HG22	0.43	2.14	6	4
1:A:222:ILE:HG22	1:A:230:TYR:HE2	0.43	1.74	7	1
1:A:213:LEU:C	1:A:213:LEU:HD23	0.43	2.38	16	1
1:A:213:LEU:HD23	1:A:213:LEU:C	0.43	2.39	5	1
1:A:214:ASP:C	1:A:218:GLU:O	0.43	2.62	17	2
1:A:179:ILE:HD12	1:A:180:MET:H	0.43	1.74	19	1
1:A:168:LEU:CG	1:A:189:LEU:HD11	0.42	2.42	13	1
1:A:232:PHE:CD1	1:A:232:PHE:C	0.42	2.97	4	1
1:A:143:LEU:HD23	1:A:144:THR:N	0.42	2.29	1	1
1:A:154:LEU:HD23	1:A:212:LEU:HD22	0.42	1.89	12	1
1:A:168:LEU:HG	1:A:189:LEU:HD21	0.42	1.90	19	1
1:A:143:LEU:HD12	1:A:212:LEU:HD11	0.42	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:ARG:C	1:A:228:LYS:N	0.42	2.78	4	1
1:A:153:LEU:HD11	1:A:156:GLY:C	0.42	2.39	4	1
1:A:218:GLU:HB3	1:A:219:PRO:HD2	0.42	1.91	7	1
1:A:186:LEU:C	1:A:186:LEU:CD2	0.42	2.81	13	1
1:A:154:LEU:HD22	1:A:155:GLY:N	0.42	2.30	17	1
1:A:172:LEU:HG	1:A:173:ALA:N	0.42	2.29	15	1
1:A:221:ARG:C	1:A:222:ILE:HG22	0.41	2.40	9	2
1:A:171:GLU:HA	1:A:174:THR:HG22	0.41	1.92	10	1
1:A:225:VAL:HG22	1:A:229:GLY:O	0.41	2.14	12	1
1:A:186:LEU:HB3	1:A:201:VAL:HG21	0.41	1.91	12	1
1:A:183:ASP:O	1:A:186:LEU:CD2	0.41	2.68	17	1
1:A:186:LEU:HD23	1:A:201:VAL:HG21	0.41	1.92	1	2
1:A:221:ARG:O	1:A:222:ILE:C	0.41	2.64	3	1
1:A:179:ILE:HB	1:A:231:LEU:HD12	0.41	1.93	12	1
1:A:192:VAL:HG23	1:A:193:THR:N	0.41	2.30	12	1
1:A:186:LEU:HD12	1:A:197:MET:O	0.41	2.16	12	1
1:A:186:LEU:HD12	1:A:196:GLY:O	0.41	2.16	17	1
1:A:200:SER:O	1:A:201:VAL:C	0.40	2.65	20	1
1:A:168:LEU:HD23	1:A:168:LEU:C	0.40	2.41	7	1
1:A:186:LEU:HD13	1:A:197:MET:HE3	0.40	1.93	7	1
1:A:186:LEU:C	1:A:186:LEU:CD1	0.40	2.89	13	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	99/119 (83%)	83±2 (84±2%)	13±2 (14±2%)	2±1 (2±1%)	7	44
All	All	1980/2380 (83%)	1663 (84%)	269 (14%)	48 (2%)	7	44

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	226	ARG	20

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Mol	Chain	Res	Type	Models (Total)
1	A	227	ASN	10
1	A	222	ILE	5
1	A	221	ARG	4
1	A	141	GLY	4
1	A	214	ASP	3
1	A	219	PRO	1
1	A	194	TYR	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	84/101 (83%)	58±4 (69±4%)	26±4 (31±4%)	1 15
All	All	1680/2020 (83%)	1159 (69%)	521 (31%)	1 15

All 70 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	179	ILE	19
1	A	186	LEU	19
1	A	213	LEU	19
1	A	143	LEU	19
1	A	192	VAL	15
1	A	211	LYS	14
1	A	163	THR	14
1	A	136	LYS	13
1	A	172	LEU	13
1	A	207	ARG	13
1	A	231	LEU	13
1	A	182	ARG	13
1	A	174	THR	12
1	A	188	ASN	12
1	A	206	SER	12
1	A	151	GLN	11
1	A	178	GLN	10
1	A	142	SER	10

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Mol	Chain	Res	Type	Models (Total)
1	A	149	ASN	10
1	A	210	LYS	10
1	A	157	GLU	9
1	A	168	LEU	9
1	A	200	SER	9
1	A	221	ARG	9
1	A	230	TYR	9
1	A	225	VAL	9
1	A	228	LYS	9
1	A	140	PHE	8
1	A	166	PHE	8
1	A	187	LYS	8
1	A	202	ASP	8
1	A	167	ASP	8
1	A	218	GLU	8
1	A	162	SER	7
1	A	175	HIS	7
1	A	223	LYS	7
1	A	150	ARG	6
1	A	153	LEU	6
1	A	154	LEU	6
1	A	180	MET	6
1	A	215	ASN	6
1	A	227	ASN	6
1	A	226	ARG	6
1	A	181	ASP	5
1	A	214	ASP	5
1	A	146	ASP	5
1	A	170	TRP	4
1	A	197	MET	4
1	A	183	ASP	4
1	A	190	ARG	4
1	A	222	ILE	4
1	A	220	TYR	4
1	A	199	ARG	4
1	A	171	GLU	3
1	A	212	LEU	3
1	A	198	ASP	3
1	A	195	ASP	3
1	A	139	SER	3
1	A	201	VAL	3
1	A	208	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	209	ARG	2
1	A	161	LEU	2
1	A	169	LEU	2
1	A	217	THR	1
1	A	224	THR	1
1	A	232	PHE	1
1	A	165	ASP	1
1	A	145	ILE	1
1	A	189	LEU	1
1	A	158	ASN	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping i

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

Total number of shifts	1173
Number of shifts mapped to atoms	1156
Number of unparsed shifts	0
Number of shifts with mapping errors	17
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

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

- No matching atom found in the structure. All 17 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	128	ALA	H	8.519	0.020	1
1	A	128	ALA	HA	4.266	0.020	1
1	A	128	ALA	HB1	1.337	0.020	1
1	A	128	ALA	HB2	1.337	0.020	1
1	A	128	ALA	HB3	1.337	0.020	1
1	A	128	ALA	C	177.63	0.300	1
1	A	128	ALA	CA	52.427	0.300	1
1	A	128	ALA	CB	19.104	0.300	1
1	A	128	ALA	N	126.301	0.300	1
1	A	129	MET	H	8.522	0.020	1
1	A	129	MET	HA	4.445	0.020	1
1	A	129	MET	HB2	2.542	0.020	2
1	A	129	MET	HB3	2.034	0.020	2
1	A	129	MET	C	176.804	0.300	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	129	MET	CA	55.487	0.300	1
1	A	129	MET	CB	32.031	0.300	1
1	A	129	MET	N	120.529	0.300	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	104	-0.10 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	95	0.24 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	101	0.10 ± 0.14	None needed (< 0.5 ppm)
^{15}N	102	-0.32 ± 0.29	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1078 atoms were assigned a chemical shift out of a possible 1383. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	473/496 (95%)	194/202 (96%)	186/198 (94%)	93/96 (97%)
Sidechain	579/811 (71%)	415/528 (79%)	163/246 (66%)	1/37 (3%)
Aromatic	26/76 (34%)	18/37 (49%)	8/37 (22%)	0/2 (0%)
Overall	1078/1383 (78%)	627/767 (82%)	357/481 (74%)	94/135 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1155 atoms were assigned a chemical shift out of a possible 1521. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	511/550 (93%)	210/224 (94%)	201/220 (91%)	100/106 (94%)
Sidechain	616/869 (71%)	442/566 (78%)	173/265 (65%)	1/38 (3%)
Aromatic	28/102 (27%)	19/51 (37%)	9/46 (20%)	0/5 (0%)
Overall	1155/1521 (76%)	671/841 (80%)	383/531 (72%)	101/149 (68%)

7.1.4 Statistically unusual chemical shifts [i](#)

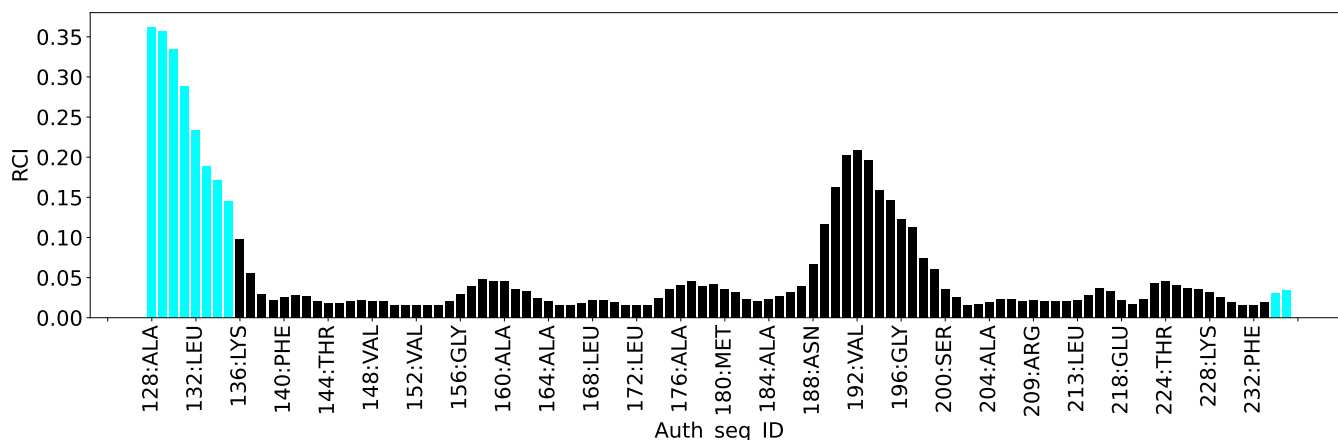
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	133	THR	HG1	4.11	0.08 – 2.19	14.1
1	A	221	ARG	HG3	-0.63	0.15 – 2.94	-7.8
1	A	221	ARG	HD3	1.28	1.81 – 4.39	-7.1
1	A	221	ARG	HG2	-0.04	0.26 – 2.87	-6.2
1	A	221	ARG	HD2	1.75	1.97 – 4.26	-6.0
1	A	174	THR	HG21	-0.05	0.08 – 2.19	-5.6
1	A	174	THR	HG22	-0.05	0.08 – 2.19	-5.6
1	A	174	THR	HG23	-0.05	0.08 – 2.19	-5.6
1	A	209	ARG	HB2	3.11	0.52 – 3.08	5.2
1	A	209	ARG	HB3	3.11	0.43 – 3.11	5.0

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	922
Intra-residue ($ i-j =0$)	233
Sequential ($ i-j =1$)	278
Medium range ($ i-j >1$ and $ i-j <5$)	155
Long range ($ i-j \geq 5$)	197
Inter-chain	0
Hydrogen bond restraints	59
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	7.7
Number of long range restraints per residue ¹	1.8

¹Long 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)	3.6	0.2
0.2-0.5 (Medium)	0.6	0.5
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

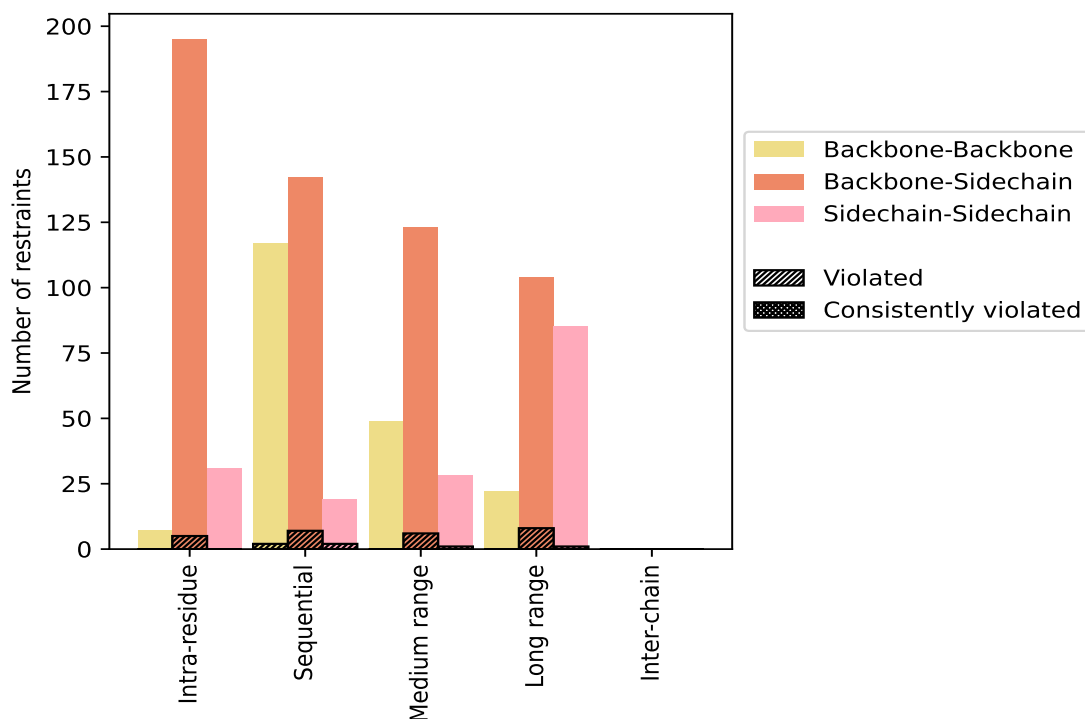
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	233	25.3	5	2.1	0.5	0	0.0	0.0
Backbone-Backbone	7	0.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	195	21.1	5	2.6	0.5	0	0.0	0.0
Sidechain-Sidechain	31	3.4	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	278	30.2	11	4.0	1.2	0	0.0	0.0
Backbone-Backbone	117	12.7	2	1.7	0.2	0	0.0	0.0
Backbone-Sidechain	142	15.4	7	4.9	0.8	0	0.0	0.0
Sidechain-Sidechain	19	2.1	2	10.5	0.2	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	155	16.8	2	1.3	0.2	0	0.0	0.0
Backbone-Backbone	49	5.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	78	8.5	1	1.3	0.1	0	0.0	0.0
Sidechain-Sidechain	28	3.0	1	3.6	0.1	0	0.0	0.0
Long range (i-j ≥5)	197	21.4	8	4.1	0.9	0	0.0	0.0
Backbone-Backbone	22	2.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	90	9.8	7	7.8	0.8	0	0.0	0.0
Sidechain-Sidechain	85	9.2	1	1.2	0.1	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	59	6.4	6	10.2	0.7	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	922	100.0	32	3.5	3.5	0	0.0	0.0
Backbone-Backbone	195	21.1	2	1.0	0.2	0	0.0	0.0
Backbone-Sidechain	564	61.2	26	4.6	2.8	0	0.0	0.0
Sidechain-Sidechain	163	17.7	4	2.5	0.4	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	1	2	2	0	6	0.12	0.17	0.02	0.11
2	1	1	1	2	0	5	0.12	0.16	0.02	0.11
3	1	2	1	1	0	5	0.12	0.14	0.01	0.13
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	1	0	0	1	0	2	0.14	0.17	0.03	0.14
6	0	0	1	0	0	1	0.14	0.14	0.0	0.14
7	1	1	1	3	0	6	0.15	0.2	0.03	0.16
8	1	1	0	1	0	3	0.19	0.2	0.01	0.19
9	1	1	0	1	0	3	0.11	0.14	0.02	0.1
10	0	2	2	1	0	5	0.13	0.15	0.02	0.13

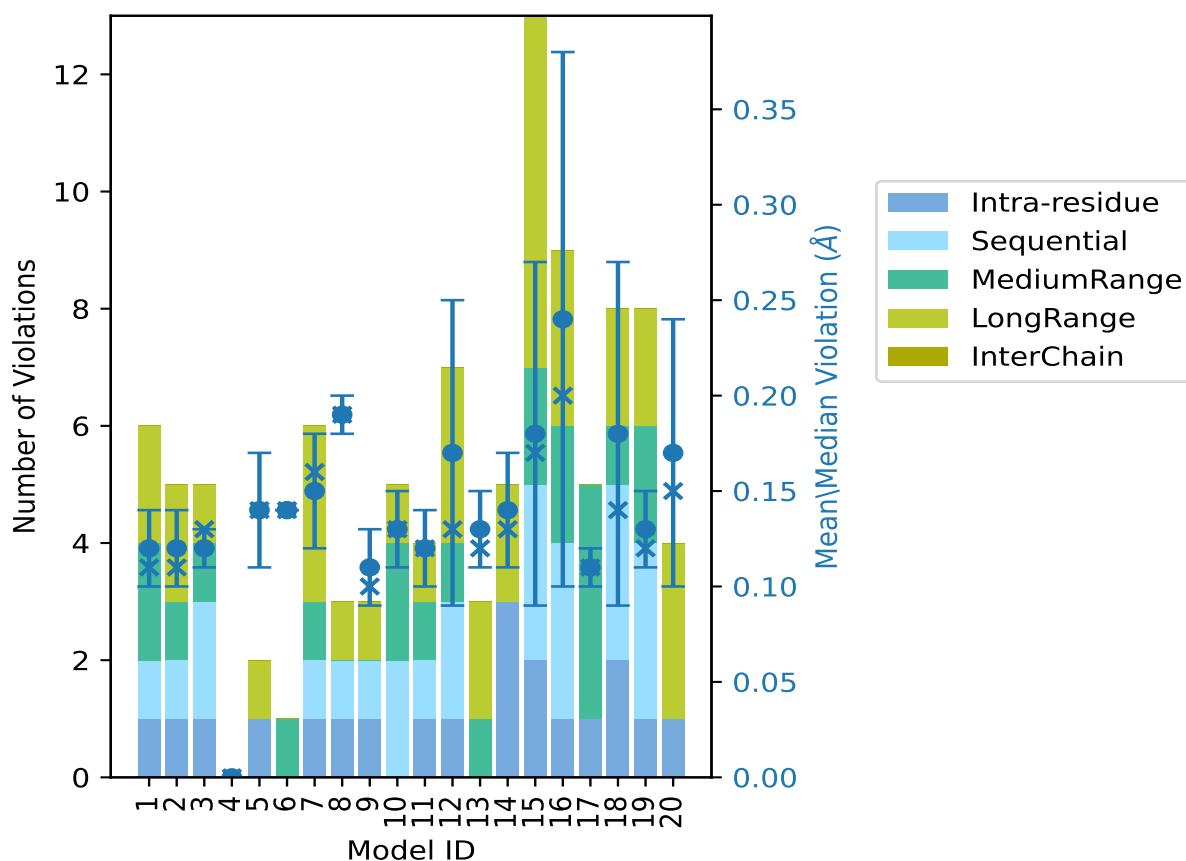
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
11	1	1	1	1	0	4	0.12	0.15	0.02	0.12
12	1	2	1	3	0	7	0.17	0.37	0.08	0.13
13	0	0	1	2	0	3	0.13	0.16	0.02	0.12
14	3	0	0	2	0	5	0.14	0.2	0.03	0.13
15	2	3	2	6	0	13	0.18	0.42	0.09	0.17
16	1	3	2	3	0	9	0.24	0.5	0.14	0.2
17	1	0	4	0	0	5	0.11	0.12	0.01	0.11
18	2	3	1	2	0	8	0.18	0.38	0.09	0.14
19	1	3	2	2	0	8	0.13	0.18	0.02	0.12
20	1	0	0	3	0	4	0.17	0.29	0.07	0.15

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

9.2.1 Bar graph : Distance Violation statistics for each model [\(i\)](#)



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

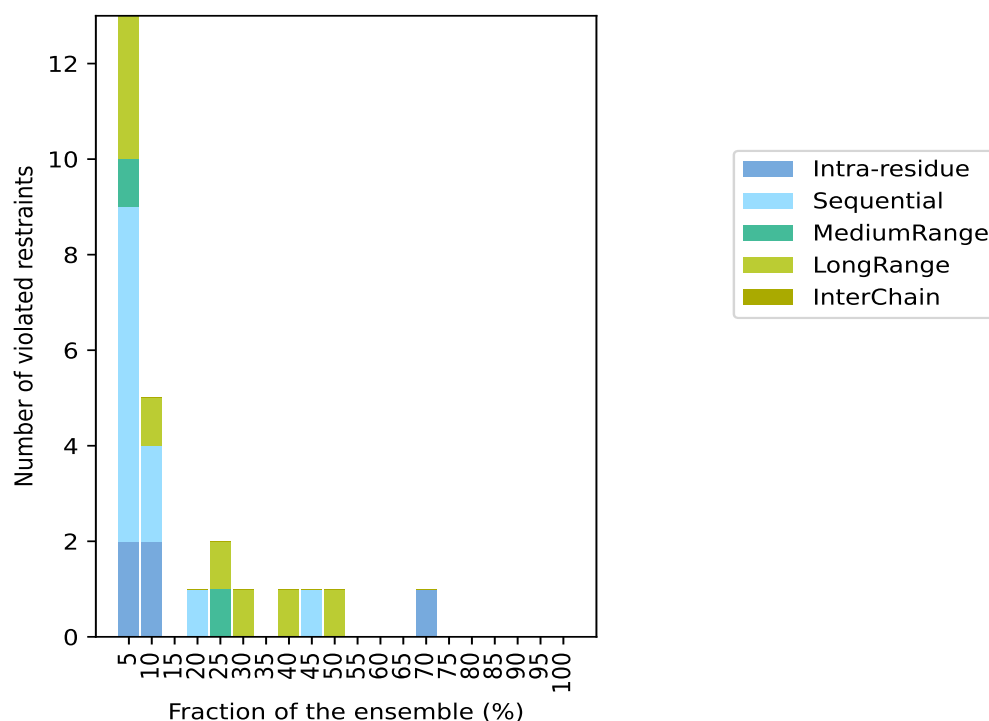
9.3 Distance violation statistics for the ensemble

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, 837(IR:228, SQ:267, MR:153, LR:189, 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	%
2	7	1	3	0	13	1	5.0
2	2	0	1	0	5	2	10.0
0	0	0	0	0	0	3	15.0
0	1	0	0	0	1	4	20.0
0	0	1	1	0	2	5	25.0
0	0	0	1	0	1	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	1	0	1	8	40.0
0	1	0	0	0	1	9	45.0
0	0	0	1	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
1	0	0	0	0	1	14	70.0
0	0	0	0	0	0	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

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

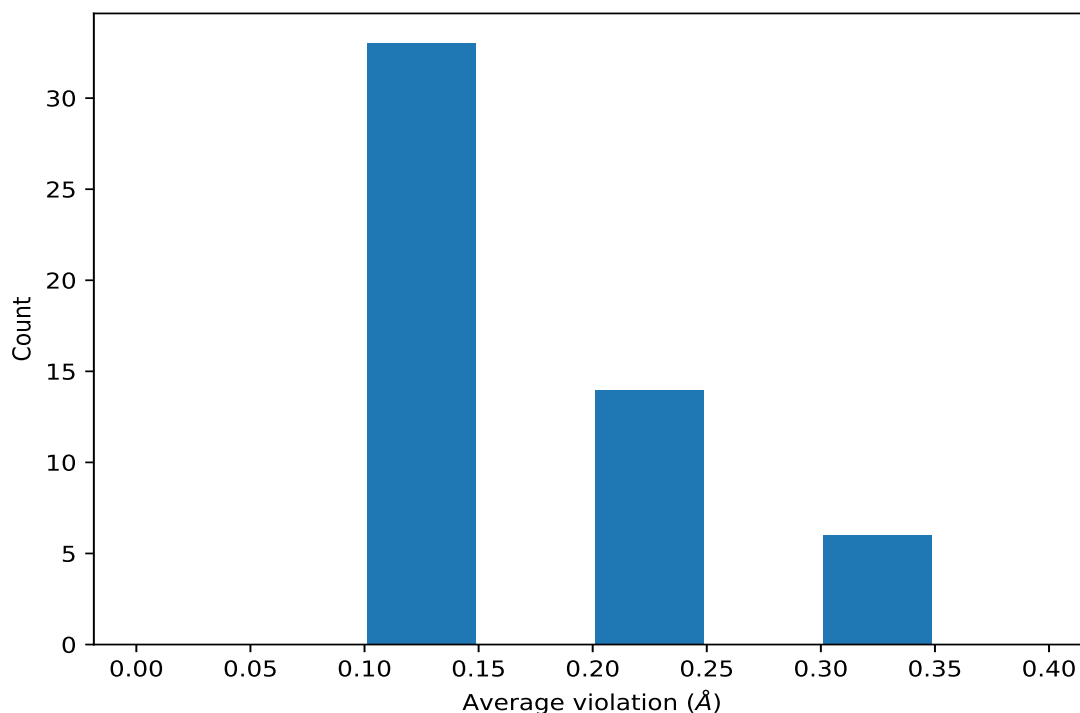
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	14	0.2	0.09	0.18
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	14	0.2	0.09	0.18
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD2	10	0.15	0.04	0.15
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD3	10	0.15	0.04	0.15
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD11	9	0.14	0.03	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD12	9	0.14	0.03	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD13	9	0.14	0.03	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD21	9	0.14	0.03	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD22	9	0.14	0.03	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD23	9	0.14	0.03	0.13
(1,862)	1:209:A:ARG:HB2	1:220:A:TYR:HB3	8	0.13	0.03	0.13
(1,862)	1:209:A:ARG:HB3	1:220:A:TYR:HB3	8	0.13	0.03	0.13
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD2	6	0.13	0.02	0.14
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD3	6	0.13	0.02	0.14
(2,54)	1:206:A:SER:O	1:210:A:LYS:H	6	0.12	0.01	0.12
(2,34)	1:171:A:GLU:O	1:175:A:HIS:H	6	0.11	0.01	0.11

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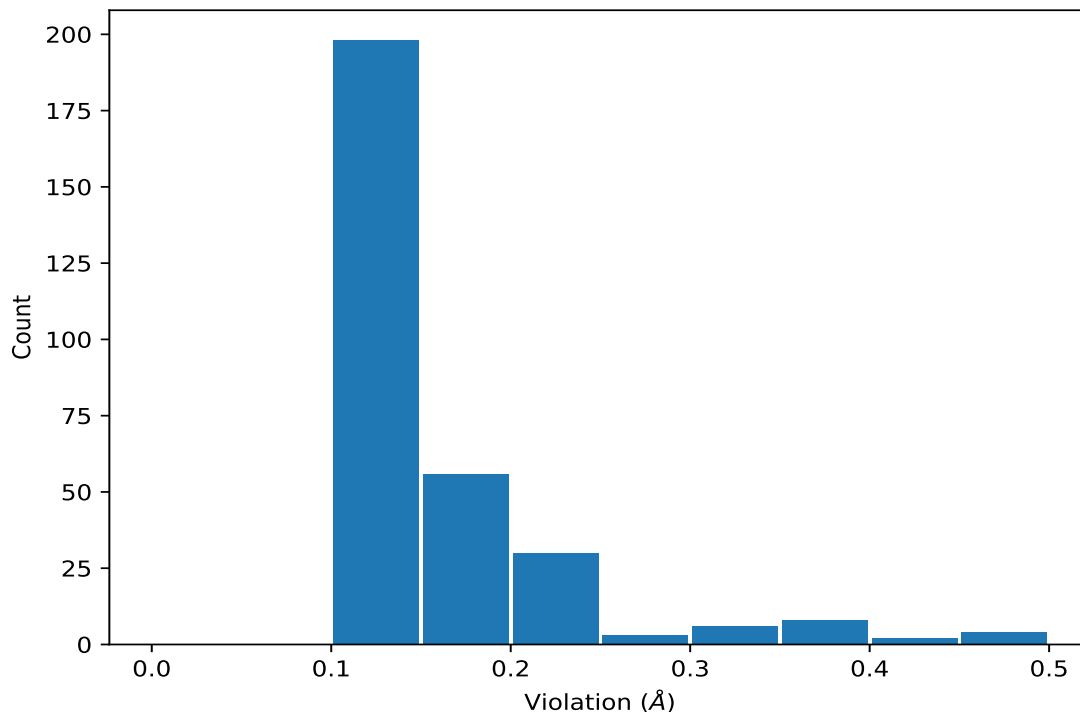
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,91)	1:192:A:VAL:HG11	1:194:A:TYR:HB3	5	0.13	0.02	0.12
(1,91)	1:192:A:VAL:HG12	1:194:A:TYR:HB3	5	0.13	0.02	0.12
(1,91)	1:192:A:VAL:HG13	1:194:A:TYR:HB3	5	0.13	0.02	0.12
(1,91)	1:192:A:VAL:HG21	1:194:A:TYR:HB3	5	0.13	0.02	0.12
(1,91)	1:192:A:VAL:HG22	1:194:A:TYR:HB3	5	0.13	0.02	0.12
(1,91)	1:192:A:VAL:HG23	1:194:A:TYR:HB3	5	0.13	0.02	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD11	5	0.12	0.01	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD12	5	0.12	0.01	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD13	5	0.12	0.01	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD21	5	0.12	0.01	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD22	5	0.12	0.01	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD23	5	0.12	0.01	0.12
(1,245)	1:220:A:TYR:H	1:221:A:ARG:H	4	0.12	0.01	0.12
(1,791)	1:213:A:LEU:HD11	1:214:A:ASP:HA	2	0.35	0.03	0.35
(1,791)	1:213:A:LEU:HD12	1:214:A:ASP:HA	2	0.35	0.03	0.35
(1,791)	1:213:A:LEU:HD13	1:214:A:ASP:HA	2	0.35	0.03	0.35
(1,791)	1:213:A:LEU:HD21	1:214:A:ASP:HA	2	0.35	0.03	0.35
(1,791)	1:213:A:LEU:HD22	1:214:A:ASP:HA	2	0.35	0.03	0.35
(1,791)	1:213:A:LEU:HD23	1:214:A:ASP:HA	2	0.35	0.03	0.35
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD11	2	0.22	0.01	0.22
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD12	2	0.22	0.01	0.22
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD13	2	0.22	0.01	0.22
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD21	2	0.22	0.01	0.22
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD22	2	0.22	0.01	0.22
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD23	2	0.22	0.01	0.22
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD11	2	0.21	0.03	0.21
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD12	2	0.21	0.03	0.21
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD13	2	0.21	0.03	0.21
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD21	2	0.21	0.03	0.21
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD22	2	0.21	0.03	0.21
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD23	2	0.21	0.03	0.21
(2,58)	1:208:A:LEU:O	1:212:A:LEU:H	2	0.15	0.03	0.15
(2,17)	1:223:A:LYS:H	1:231:A:LEU:O	2	0.11	0.01	0.11
(1,399)	1:224:A:THR:H	1:224:A:THR:HB	2	0.11	0.0	0.11
(1,861)	1:212:A:LEU:HA	1:143:A:LEU:HD11	2	0.11	0.0	0.11
(1,861)	1:212:A:LEU:HA	1:143:A:LEU:HD12	2	0.11	0.0	0.11
(1,861)	1:212:A:LEU:HA	1:143:A:LEU:HD13	2	0.11	0.0	0.11

¹Number of violated models, ²Standard 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)
(1,516)	1:190:A:ARG:HB2	1:191:A:GLY:H	16	0.5
(1,516)	1:190:A:ARG:HB3	1:191:A:GLY:H	16	0.5
(1,547)	1:190:A:ARG:HG2	1:191:A:GLY:H	16	0.47
(1,547)	1:190:A:ARG:HG3	1:191:A:GLY:H	16	0.47
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	15	0.42
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	15	0.42
(1,791)	1:213:A:LEU:HD11	1:214:A:ASP:HA	18	0.38
(1,791)	1:213:A:LEU:HD12	1:214:A:ASP:HA	18	0.38
(1,791)	1:213:A:LEU:HD13	1:214:A:ASP:HA	18	0.38
(1,791)	1:213:A:LEU:HD21	1:214:A:ASP:HA	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	1:213:A:LEU:HD22	1:214:A:ASP:HA	18	0.38
(1,791)	1:213:A:LEU:HD23	1:214:A:ASP:HA	18	0.38
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	12	0.37
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	12	0.37
(1,791)	1:213:A:LEU:HD11	1:214:A:ASP:HA	15	0.32
(1,791)	1:213:A:LEU:HD12	1:214:A:ASP:HA	15	0.32
(1,791)	1:213:A:LEU:HD13	1:214:A:ASP:HA	15	0.32
(1,791)	1:213:A:LEU:HD21	1:214:A:ASP:HA	15	0.32
(1,791)	1:213:A:LEU:HD22	1:214:A:ASP:HA	15	0.32
(1,791)	1:213:A:LEU:HD23	1:214:A:ASP:HA	15	0.32
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	20	0.29
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	20	0.29
(1,287)	1:190:A:ARG:H	1:191:A:GLY:H	16	0.26
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD11	18	0.24
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD12	18	0.24
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD13	18	0.24
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD21	18	0.24
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD22	18	0.24
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD23	18	0.24
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD2	15	0.23
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD3	15	0.23
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD11	15	0.22
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD12	15	0.22
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD13	15	0.22
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD21	15	0.22
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD22	15	0.22
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD23	15	0.22
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD11	18	0.21
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD12	18	0.21
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD13	18	0.21
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD21	18	0.21
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD22	18	0.21
(1,787)	1:212:A:LEU:H	1:213:A:LEU:HD23	18	0.21
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD2	7	0.2
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD3	7	0.2
(1,543)	1:190:A:ARG:HG2	1:192:A:VAL:H	16	0.2
(1,543)	1:190:A:ARG:HG3	1:192:A:VAL:H	16	0.2
(1,515)	1:190:A:ARG:H	1:190:A:ARG:HB2	14	0.2
(1,515)	1:190:A:ARG:H	1:190:A:ARG:HB3	14	0.2
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	8	0.2
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	8	0.2
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	16	0.2
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD11	8	0.19
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD12	8	0.19
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD13	8	0.19
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD21	8	0.19
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD22	8	0.19
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD23	8	0.19
(2,58)	1:208:A:LEU:O	1:212:A:LEU:H	15	0.18
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD11	15	0.18
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD12	15	0.18
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD13	15	0.18
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD21	15	0.18
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD22	15	0.18
(1,788)	1:213:A:LEU:H	1:213:A:LEU:HD23	15	0.18
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	7	0.18
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	7	0.18
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	19	0.18
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	19	0.18
(1,862)	1:209:A:ARG:HB2	1:220:A:TYR:HB3	15	0.17
(1,862)	1:209:A:ARG:HB3	1:220:A:TYR:HB3	15	0.17
(1,862)	1:209:A:ARG:HB2	1:220:A:TYR:HB3	20	0.17
(1,862)	1:209:A:ARG:HB3	1:220:A:TYR:HB3	20	0.17
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD2	8	0.17
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD3	8	0.17
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD11	1	0.17
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD12	1	0.17
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD13	1	0.17
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD21	1	0.17
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD22	1	0.17
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD23	1	0.17
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	5	0.17
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	5	0.17
(1,862)	1:209:A:ARG:HB2	1:220:A:TYR:HB3	7	0.16
(1,862)	1:209:A:ARG:HB3	1:220:A:TYR:HB3	7	0.16
(1,829)	1:137:A:THR:HG21	1:146:A:ASP:H	14	0.16
(1,829)	1:137:A:THR:HG22	1:146:A:ASP:H	14	0.16
(1,829)	1:137:A:THR:HG23	1:146:A:ASP:H	14	0.16
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD11	19	0.16
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD12	19	0.16
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD13	19	0.16
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD21	19	0.16
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD22	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD23	19	0.16
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	2	0.16
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	2	0.16
(1,91)	1:192:A:VAL:HG11	1:194:A:TYR:HB3	13	0.16
(1,91)	1:192:A:VAL:HG12	1:194:A:TYR:HB3	13	0.16
(1,91)	1:192:A:VAL:HG13	1:194:A:TYR:HB3	13	0.16
(1,91)	1:192:A:VAL:HG21	1:194:A:TYR:HB3	13	0.16
(1,91)	1:192:A:VAL:HG22	1:194:A:TYR:HB3	13	0.16
(1,91)	1:192:A:VAL:HG23	1:194:A:TYR:HB3	13	0.16
(1,91)	1:192:A:VAL:HG11	1:194:A:TYR:HB3	18	0.16
(1,91)	1:192:A:VAL:HG12	1:194:A:TYR:HB3	18	0.16
(1,91)	1:192:A:VAL:HG13	1:194:A:TYR:HB3	18	0.16
(1,91)	1:192:A:VAL:HG21	1:194:A:TYR:HB3	18	0.16
(1,91)	1:192:A:VAL:HG22	1:194:A:TYR:HB3	18	0.16
(1,91)	1:192:A:VAL:HG23	1:194:A:TYR:HB3	18	0.16
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD2	7	0.15
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD3	7	0.15
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD2	10	0.15
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD3	10	0.15
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD2	11	0.15
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD3	11	0.15
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD2	12	0.15
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD3	12	0.15
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD2	19	0.15
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD3	19	0.15
(1,184)	1:192:A:VAL:HG11	1:193:A:THR:HG21	12	0.15
(1,184)	1:192:A:VAL:HG11	1:193:A:THR:HG22	12	0.15
(1,184)	1:192:A:VAL:HG11	1:193:A:THR:HG23	12	0.15
(1,184)	1:192:A:VAL:HG12	1:193:A:THR:HG21	12	0.15
(1,184)	1:192:A:VAL:HG12	1:193:A:THR:HG22	12	0.15
(1,184)	1:192:A:VAL:HG12	1:193:A:THR:HG23	12	0.15
(1,184)	1:192:A:VAL:HG13	1:193:A:THR:HG21	12	0.15
(1,184)	1:192:A:VAL:HG13	1:193:A:THR:HG22	12	0.15
(1,184)	1:192:A:VAL:HG13	1:193:A:THR:HG23	12	0.15
(1,184)	1:192:A:VAL:HG21	1:193:A:THR:HG21	12	0.15
(1,184)	1:192:A:VAL:HG21	1:193:A:THR:HG22	12	0.15
(1,184)	1:192:A:VAL:HG21	1:193:A:THR:HG23	12	0.15
(1,184)	1:192:A:VAL:HG22	1:193:A:THR:HG21	12	0.15
(1,184)	1:192:A:VAL:HG22	1:193:A:THR:HG22	12	0.15
(1,184)	1:192:A:VAL:HG22	1:193:A:THR:HG23	12	0.15
(1,184)	1:192:A:VAL:HG23	1:193:A:THR:HG21	12	0.15
(1,184)	1:192:A:VAL:HG23	1:193:A:THR:HG22	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,184)	1:192:A:VAL:HG23	1:193:A:THR:HG23	12	0.15
(2,34)	1:171:A:GLU:O	1:175:A:HIS:H	6	0.14
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD2	16	0.14
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD3	16	0.14
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD11	9	0.14
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD12	9	0.14
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD13	9	0.14
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD21	9	0.14
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD22	9	0.14
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD23	9	0.14
(1,628)	1:167:A:ASP:H	1:189:A:LEU:HD11	3	0.14
(1,628)	1:167:A:ASP:H	1:189:A:LEU:HD12	3	0.14
(1,628)	1:167:A:ASP:H	1:189:A:LEU:HD13	3	0.14
(1,628)	1:167:A:ASP:H	1:189:A:LEU:HD21	3	0.14
(1,628)	1:167:A:ASP:H	1:189:A:LEU:HD22	3	0.14
(1,628)	1:167:A:ASP:H	1:189:A:LEU:HD23	3	0.14
(2,54)	1:206:A:SER:O	1:210:A:LYS:H	10	0.13
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD2	16	0.13
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD3	16	0.13
(1,862)	1:209:A:ARG:HB2	1:220:A:TYR:HB3	12	0.13
(1,862)	1:209:A:ARG:HB3	1:220:A:TYR:HB3	12	0.13
(1,862)	1:209:A:ARG:HB2	1:220:A:TYR:HB3	16	0.13
(1,862)	1:209:A:ARG:HB3	1:220:A:TYR:HB3	16	0.13
(1,758)	1:185:A:LEU:HG	1:186:A:LEU:HD11	15	0.13
(1,758)	1:185:A:LEU:HG	1:186:A:LEU:HD12	15	0.13
(1,758)	1:185:A:LEU:HG	1:186:A:LEU:HD13	15	0.13
(1,758)	1:185:A:LEU:HG	1:186:A:LEU:HD21	15	0.13
(1,758)	1:185:A:LEU:HG	1:186:A:LEU:HD22	15	0.13
(1,758)	1:185:A:LEU:HG	1:186:A:LEU:HD23	15	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD11	3	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD12	3	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD13	3	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD21	3	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD22	3	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD23	3	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD11	10	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD12	10	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD13	10	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD21	10	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD22	10	0.13
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD23	10	0.13
(1,673)	1:145:A:ILE:HD11	1:174:A:THR:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:145:A:ILE:HD12	1:174:A:THR:H	12	0.13
(1,673)	1:145:A:ILE:HD13	1:174:A:THR:H	12	0.13
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	11	0.13
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	11	0.13
(1,245)	1:220:A:TYR:H	1:221:A:ARG:H	3	0.13
(1,136)	1:190:A:ARG:HA	1:190:A:ARG:HG2	14	0.13
(1,136)	1:190:A:ARG:HA	1:190:A:ARG:HG3	14	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD11	15	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD12	15	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD13	15	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD21	15	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD22	15	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD23	15	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD11	20	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD12	20	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD13	20	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD21	20	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD22	20	0.13
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD23	20	0.13
(2,58)	1:208:A:LEU:O	1:212:A:LEU:H	16	0.12
(2,54)	1:206:A:SER:O	1:210:A:LYS:H	1	0.12
(2,54)	1:206:A:SER:O	1:210:A:LYS:H	7	0.12
(2,54)	1:206:A:SER:O	1:210:A:LYS:H	19	0.12
(2,34)	1:171:A:GLU:O	1:175:A:HIS:H	12	0.12
(2,17)	1:223:A:LYS:H	1:231:A:LEU:O	18	0.12
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD2	19	0.12
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD3	19	0.12
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD2	13	0.12
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD3	13	0.12
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD11	11	0.12
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD12	11	0.12
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD13	11	0.12
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD21	11	0.12
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD22	11	0.12
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD23	11	0.12
(1,609)	1:145:A:ILE:HG12	1:146:A:ASP:H	19	0.12
(1,609)	1:145:A:ILE:HG13	1:146:A:ASP:H	19	0.12
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	18	0.12
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	18	0.12
(1,245)	1:220:A:TYR:H	1:221:A:ARG:H	10	0.12
(1,91)	1:192:A:VAL:HG11	1:194:A:TYR:HB3	17	0.12
(1,91)	1:192:A:VAL:HG12	1:194:A:TYR:HB3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:192:A:VAL:HG13	1:194:A:TYR:HB3	17	0.12
(1,91)	1:192:A:VAL:HG21	1:194:A:TYR:HB3	17	0.12
(1,91)	1:192:A:VAL:HG22	1:194:A:TYR:HB3	17	0.12
(1,91)	1:192:A:VAL:HG23	1:194:A:TYR:HB3	17	0.12
(1,91)	1:192:A:VAL:HG11	1:194:A:TYR:HB3	19	0.12
(1,91)	1:192:A:VAL:HG12	1:194:A:TYR:HB3	19	0.12
(1,91)	1:192:A:VAL:HG13	1:194:A:TYR:HB3	19	0.12
(1,91)	1:192:A:VAL:HG21	1:194:A:TYR:HB3	19	0.12
(1,91)	1:192:A:VAL:HG22	1:194:A:TYR:HB3	19	0.12
(1,91)	1:192:A:VAL:HG23	1:194:A:TYR:HB3	19	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD11	13	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD12	13	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD13	13	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD21	13	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD22	13	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD23	13	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD11	14	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD12	14	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD13	14	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD21	14	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD22	14	0.12
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD23	14	0.12
(2,34)	1:171:A:GLU:O	1:175:A:HIS:H	2	0.11
(2,34)	1:171:A:GLU:O	1:175:A:HIS:H	17	0.11
(1,861)	1:212:A:LEU:HA	1:143:A:LEU:HD11	5	0.11
(1,861)	1:212:A:LEU:HA	1:143:A:LEU:HD12	5	0.11
(1,861)	1:212:A:LEU:HA	1:143:A:LEU:HD13	5	0.11
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD2	1	0.11
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD3	1	0.11
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD2	18	0.11
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD3	18	0.11
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD11	7	0.11
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD12	7	0.11
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD13	7	0.11
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD21	7	0.11
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD22	7	0.11
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD23	7	0.11
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	14	0.11
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	14	0.11
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	17	0.11
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	17	0.11
(1,399)	1:224:A:THR:H	1:224:A:THR:HB	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,245)	1:220:A:TYR:H	1:221:A:ARG:H	12	0.11
(1,91)	1:192:A:VAL:HG11	1:194:A:TYR:HB3	1	0.11
(1,91)	1:192:A:VAL:HG12	1:194:A:TYR:HB3	1	0.11
(1,91)	1:192:A:VAL:HG13	1:194:A:TYR:HB3	1	0.11
(1,91)	1:192:A:VAL:HG21	1:194:A:TYR:HB3	1	0.11
(1,91)	1:192:A:VAL:HG22	1:194:A:TYR:HB3	1	0.11
(1,91)	1:192:A:VAL:HG23	1:194:A:TYR:HB3	1	0.11
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD11	2	0.11
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD12	2	0.11
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD13	2	0.11
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD21	2	0.11
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD22	2	0.11
(1,68)	1:172:A:LEU:HA	1:185:A:LEU:HD23	2	0.11
(2,54)	1:206:A:SER:O	1:210:A:LYS:H	11	0.1
(2,54)	1:206:A:SER:O	1:210:A:LYS:H	15	0.1
(2,46)	1:202:A:ASP:O	1:206:A:SER:H	17	0.1
(2,38)	1:198:A:ASP:O	1:202:A:ASP:H	17	0.1
(2,34)	1:171:A:GLU:O	1:175:A:HIS:H	3	0.1
(2,34)	1:171:A:GLU:O	1:175:A:HIS:H	10	0.1
(2,17)	1:223:A:LYS:H	1:231:A:LEU:O	15	0.1
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD2	15	0.1
(1,863)	1:214:A:ASP:H	1:209:A:ARG:HD3	15	0.1
(1,862)	1:209:A:ARG:HB2	1:220:A:TYR:HB3	1	0.1
(1,862)	1:209:A:ARG:HB3	1:220:A:TYR:HB3	1	0.1
(1,862)	1:209:A:ARG:HB2	1:220:A:TYR:HB3	2	0.1
(1,862)	1:209:A:ARG:HB3	1:220:A:TYR:HB3	2	0.1
(1,862)	1:209:A:ARG:HB2	1:220:A:TYR:HB3	9	0.1
(1,862)	1:209:A:ARG:HB3	1:220:A:TYR:HB3	9	0.1
(1,861)	1:212:A:LEU:HA	1:143:A:LEU:HD11	15	0.1
(1,861)	1:212:A:LEU:HA	1:143:A:LEU:HD12	15	0.1
(1,861)	1:212:A:LEU:HA	1:143:A:LEU:HD13	15	0.1
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD2	20	0.1
(1,859)	1:224:A:THR:H	1:209:A:ARG:HD3	20	0.1
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD11	2	0.1
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD12	2	0.1
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD13	2	0.1
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD21	2	0.1
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD22	2	0.1
(1,757)	1:185:A:LEU:H	1:186:A:LEU:HD23	2	0.1
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD2	1	0.1
(1,420)	1:209:A:ARG:H	1:209:A:ARG:HD3	1	0.1
(1,399)	1:224:A:THR:H	1:224:A:THR:HB	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,245)	1:220:A:TYR:H	1:221:A:ARG:H	19	0.1
(1,160)	1:231:A:LEU:HB2	1:232:A:PHE:HA	18	0.1
(1,160)	1:231:A:LEU:HB3	1:232:A:PHE:HA	18	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found