



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 10:19 PM UTC

PDB ID : 2MBB / pdb_00002mbb
BMRB ID : 19394
Title : Solution Structure of the human Polymerase iota UBM1-Ubiquitin Complex
Authors : Wang, S.; Zhou, P.
Deposited on : 2013-07-29

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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

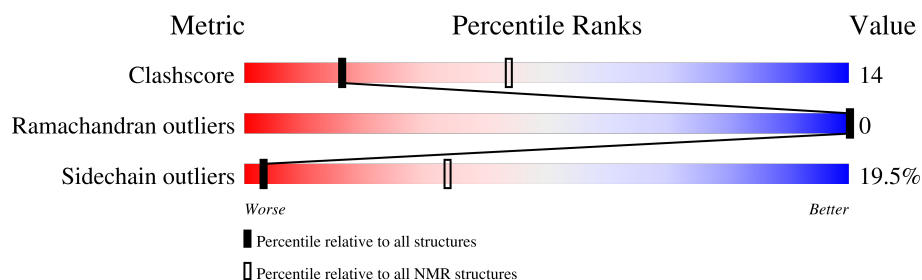
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	106	
2	B	78	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:66-A:90, B:201-B:272 (97)	0.21	6

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1835 atoms, of which 934 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	38	Total	C	H	N	O	S	0
			607	191	307	49	59	1	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P06654
A	2	GLN	-	expression tag	UNP P06654
A	57	GLY	-	linker	UNP P06654
A	58	SER	-	linker	UNP P06654
A	99	LEU	-	expression tag	UNP Q9UNA4
A	100	GLU	-	expression tag	UNP Q9UNA4
A	101	HIS	-	expression tag	UNP Q9UNA4
A	102	HIS	-	expression tag	UNP Q9UNA4
A	103	HIS	-	expression tag	UNP Q9UNA4
A	104	HIS	-	expression tag	UNP Q9UNA4
A	105	HIS	-	expression tag	UNP Q9UNA4
A	106	HIS	-	expression tag	UNP Q9UNA4

- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms						Trace
2	B	76	Total	C	H	N	O	S	0
			1228	378	627	105	117	1	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	199	SER	-	expression tag	UNP P0CG47
B	200	HIS	-	expression tag	UNP P0CG47

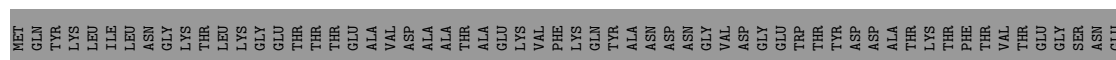
4 Residue-property plots

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: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

Chain A: 



- Molecule 2: Polyubiquitin-B

Chain B: 



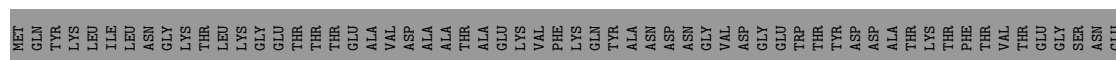
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

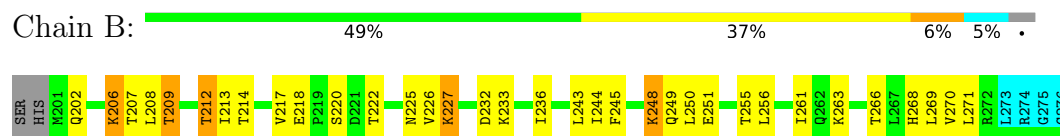
4.2.1 Score per residue for model 1

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

Chain A: 

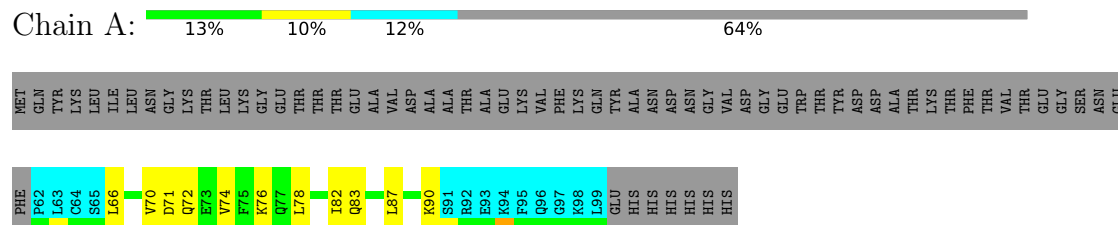


- Molecule 2: Polyubiquitin-B

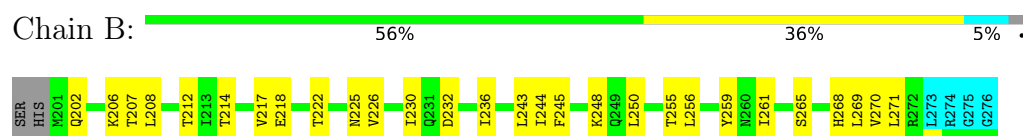


4.2.2 Score per residue for model 2

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

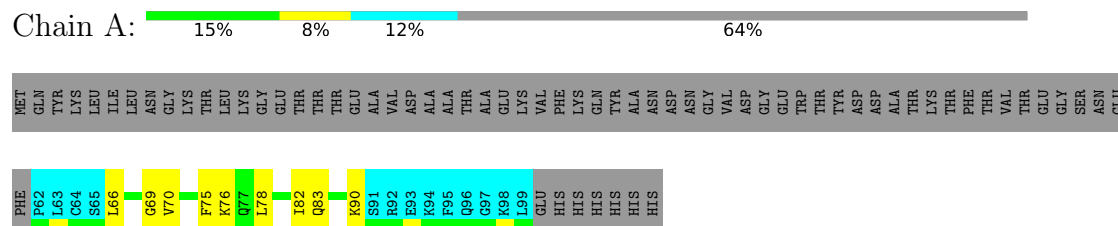


- Molecule 2: Polyubiquitin-B

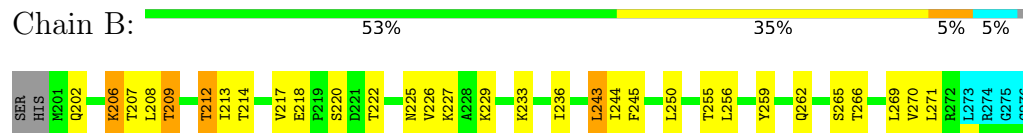


4.2.3 Score per residue for model 3

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein



- Molecule 2: Polyubiquitin-B



4.2.4 Score per residue for model 4

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

Chain A: 

MET GLN TYR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY GLU THR THR THR GLU ALA VAL R92 ASP ALA ALA THR ALA GLU VAL PHE LYS GLN TYR ASN ASP ASN GLY VAL ASP GLY TRP THR TYR ASP ASP THR LYS THR PHE THR VAL THR GLY SER ASN GLU

PHE P62 L63 C64 S65 L66 V70 V74 F75 K76 Q77 L78 I82 L87 S91 R92 E93 K94 F95 Q96 Q97 K98 L99 GLU HIS HIS HIS HIS HIS HIS

• Molecule 2: Polyubiquitin-B

Chain B: 

SER HIS Q201 Q202 K206 T207 L208 T212 I213 T214 V217 E218 P219 S220 D221 T222 N225 V226 L243 I244 F245 K248 Q249 L250 E251 R254 T255 L256 I261 Q262 K263 E264 S265 T266 L267 H268 L269 V270 L271 R272 L273 R274 G275 G276

4.2.5 Score per residue for model 5

• Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

Chain A: 

MET GLN TYR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY GLU THR THR THR GLU ALA VAL ASP ALA ALA THR ALA GLU VAL PHE LYS GLN TYR THR ASN ASP ASN GLY VAL ASP GLY TRP THR TYR ASP ASP THR LYS THR PHE THR VAL THR GLY SER ASN GLU

PHE P62 L63 C64 S65 L66 G69 V70 V74 F75 K76 Q77 L78 I82 Q83 L87 K90 R91 R92 E93 K94 F95 Q96 Q97 K98 L99 GLU HIS HIS HIS HIS HIS HIS HIS

• Molecule 2: Polyubiquitin-B

Chain B: 

SER HIS Q201 Q202 K206 T207 L208 T209 T212 I213 T214 V217 E218 T222 N225 V226 K233 Q241 R242 L243 I244 F245 K248 Q249 L250 T255 L256 Y259 R260 I261 Q262 K263 E264 S265 T266 L267 H268 L269 V270 L271 R272 L273 R274 G275 G276

4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

Chain A: 

MET GLN TYR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY GLU THR THR THR GLU ALA VAL ASP ALA ALA THR ALA GLU VAL PHE LYS GLN TYR THR ASN ASP ASN GLY VAL ASP GLY TRP THR TYR ASP ASP THR LYS THR PHE THR VAL THR GLY SER ASN GLU

PHE P62 L63 C64 S65 L66 P67 E68 G69 D71 V74 F75 K76 Q77 L78 I82 Q83 L87 K90 R91 R92 E93 K94 F95 Q96 Q97 K98 L99 GLU HIS HIS HIS HIS HIS HIS

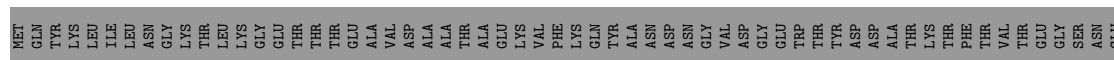
• Molecule 2: Polyubiquitin-B

Chain B: 



4.2.7 Score per residue for model 7

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

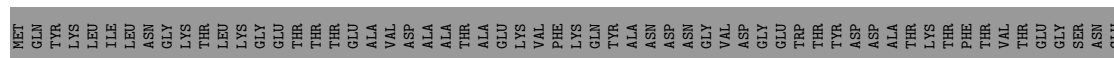


- Molecule 2: Polyubiquitin-B

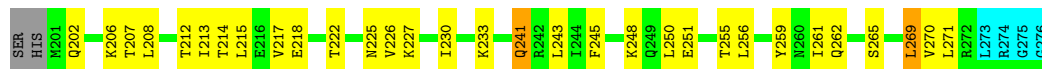


4.2.8 Score per residue for model 8

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein



- Molecule 2: Polyubiquitin-B



4.2.9 Score per residue for model 9

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein



MET GLN TYR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY THR THR THR GLU ALA VAL ASP ASP ALA ALA THR ALA GLU LYS VAL PHE PHE LYS GLN TYR ALA ALA ASN ASP ASP ASN GLY VAL ASP GLY GLU TRP THR TYR ASP ASP ALA THR LYS THR PHE THR VAL THR GLY SER ASN GLU

PHE P62 L63 C64 S65 L66 P67 E68 G69 V70 K76 Q77 L78 I82 Q83 E84 L87 K90 S91 R92 E93 K94 F95 Q96 Q97 K98 L99 GLU HIS HIS HIS HIS HIS HIS

• Molecule 2: Polyubiquitin-B

Chain B: 54% 33% 5% 5%

SER HIS Q201 Q202 K206 T207 L208 T209 T212 T213 T214 V217 E218 P219 S220 Q221 T222 N225 V226 K227 K228 K229 I230 K233 T236 F245 K248 Q249 L250 T255 T256 T261 S265 L269 V270 L271 R272 L273 R274 Q275 Q276

4.2.10 Score per residue for model 10

• Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

Chain A: 13% 10% 12% 64%

MET GLN TYR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY THR THR THR GLU ALA VAL ASP ASP ALA ALA THR ALA GLU LYS VAL PHE PHE LYS GLN TYR ALA ALA ASN ASP ASP ASN GLY VAL ASP GLY GLU TRP THR TYR ASP ASP ALA THR LYS THR PHE THR VAL THR GLY SER ASN GLU

PHE P62 L63 C64 S65 L66 P67 E68 G69 V70 D71 Q72 F73 V74 F75 K76 Q77 L78 I82 L87 K90 S91 R92 E93 K94 F95 Q96 Q97 K98 L99 GLU HIS HIS HIS HIS HIS HIS

• Molecule 2: Polyubiquitin-B

Chain B: 55% 36% 5%

SER HIS Q201 Q202 K206 T207 L208 T212 T213 T217 E218 T222 N225 V226 K227 K233 T236 L243 T244 F245 K248 Q249 L250 T255 T256 T261 S265 T266 L269 V270 L271 R272 L273 R274 Q275 Q276

4.2.11 Score per residue for model 11

• Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

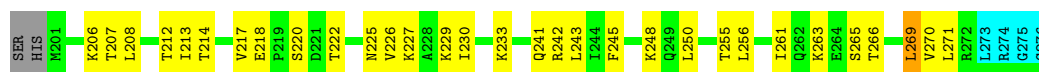
Chain A: 16% 8% 12% 64%

MET GLN TYR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY THR THR THR GLU ALA VAL ASP ASP ALA ALA THR ALA GLU LYS VAL PHE PHE LYS GLN TYR ALA ALA ASN ASP ASP ASN GLY VAL ASP GLY GLU TRP THR TYR ASP ASP ALA THR LYS THR PHE THR VAL THR GLY SER ASN GLU

PHE P62 L63 C64 S65 L66 V70 F75 K76 Q77 L78 I82 Q83 L87 S91 R92 E93 K94 F95 Q96 Q97 K98 L99 GLU HIS HIS HIS HIS HIS HIS

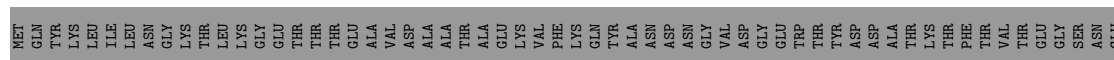
• Molecule 2: Polyubiquitin-B

Chain B: 53% 38% 5%

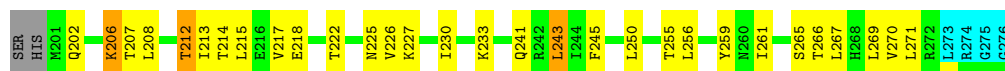


4.2.12 Score per residue for model 12

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

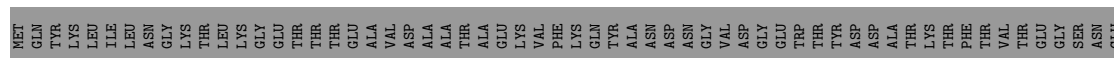


- Molecule 2: Polyubiquitin-B



4.2.13 Score per residue for model 13

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein



- Molecule 2: Polyubiquitin-B



4.2.14 Score per residue for model 14

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein



MET GLN TYR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY THR THR THR GLU ALA VAL ASP ALA ALA THR ALA GLU LYS VAL PHE GLN LYS TYR ALA ASN ASP ASN GLY VAL ASP GLY TRP THR TYR ASP ALA THR LYS THR PHE THR VAL THR GLY SER ASN GLU

PHE P62 L63 C64 S65 L66 P67 E68 G69 V70 D71 V74 F75 K76 Q77 L78 I82 L87 K90 S91 R92 E93 F95 Q96 G97 K98 L99 GLU HIS HIS HIS HIS HIS

• Molecule 2: Polyubiquitin-B

Chain B: 51% 38% 5%

SER HIS Q201 Q202 L203 K206 T207 L208 T212 T213 T214 V217 E218 E219 T222 N225 V226 K227 K233 K236 L243 L244 F245 Q249 L250 T255 L256 Y259 H260 L261 Q262 K263 E264 S265 T266 H268 L269 V270 L271 K272 L273 R274 Q275 Q276

4.2.15 Score per residue for model 15

• Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

Chain A: 14% 9% 12% 64%

MET GLN TYR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY THR THR THR GLU ALA VAL ASP ALA ALA THR ALA GLU LYS VAL PHE GLN LYS TYR ALA ASN ASP ASN GLY VAL ASP GLY TRP THR TYR ASP ALA THR LYS THR PHE THR VAL THR GLY SER ASN GLU

PHE P62 L63 C64 S65 L66 P67 E68 G69 V70 D71 V74 F75 K76 Q77 L78 I82 L87 K90 S91 R92 E93 F95 Q96 G97 K98 L99 GLU HIS HIS HIS HIS HIS

• Molecule 2: Polyubiquitin-B

Chain B: 53% 37% 5%

SER HIS Q201 Q202 L203 K206 T207 L208 T212 T213 T214 V217 E218 E219 T222 N225 V226 K227 K233 K236 L243 L244 F245 Q249 L250 T255 L256 Y259 H260 L261 Q262 K263 E264 S265 T266 H268 L269 V270 L271 K272 L273 R274 Q275 Q276

4.2.16 Score per residue for model 16

• Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

Chain A: 16% 8% 12% 64%

MET GLN TYR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY THR THR THR GLU ALA VAL ASP ALA ALA THR ALA GLU LYS VAL PHE GLN LYS TYR ALA ASN ASP ASN GLY VAL ASP GLY TRP THR TYR ASP ALA THR LYS THR PHE THR VAL THR GLY SER ASN GLU

PHE P62 L63 C64 S65 L66 P67 E68 G69 V70 D71 V74 F75 K76 Q77 L78 I82 L87 K90 S91 R92 E93 F95 Q96 G97 K98 L99 GLU HIS HIS HIS HIS HIS

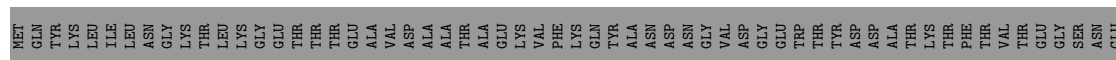
• Molecule 2: Polyubiquitin-B

Chain B: 49% 42% 5%

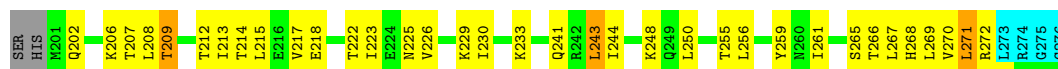


4.2.17 Score per residue for model 17

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

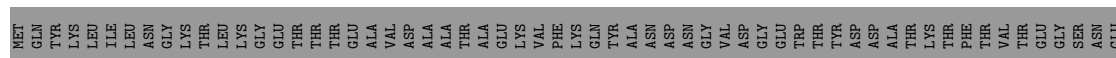


- Molecule 2: Polyubiquitin-B



4.2.18 Score per residue for model 18

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein



- Molecule 2: Polyubiquitin-B



4.2.19 Score per residue for model 19

- Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein



MET GLN TYR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY THR THR THR GLU ALA VAL ASP ALA ALA ALA ALA GLU LYS VAL PHE LYS GLN TYR ALA ALA ASN ASP ASN GLY VAL ASP GLY TRP THR TYR ASP ALA THR LYS THR PHE THR VAL THR THR GLY SER ASN GLU

PHE P62 L63 C64 S65 L66 P67 E68 V70 V74 F75 K76 Q77 L78 I82 L87 K90 S91 R92 E93 K94 F95 Q96 Q97 K98 L99 GLU HIS HIS HIS HIS HIS HIS

• Molecule 2: Polyubiquitin-B

Chain B: 49% 41% 5%

SER HIS Q201 Q202 K206 T207 L208 T209 T212 T213 T214 T215 E216 V217 E218 T222 N225 V226 K227 K230 K233 T236 Q241 R242 L243 T244 F245 K248 Q249 L250 T255 L256 Y259 Q260 L261 S265 T266 L267 H268 L269 V270 L271 L272 L273 R274 Q275 G276

4.2.20 Score per residue for model 20

• Molecule 1: Immunoglobulin G-binding protein G/DNA polymerase iota fusion protein

Chain A: 16% 7% 12% 64%

MET GLN TYR LYS LEU ILE LEU ASN GLY LYS THR LEU LYS GLY THR THR THR GLU ALA VAL ASP ALA ALA ALA GLU LYS VAL PHE LYS GLN TYR ALA ALA ASN ASP ASN GLY VAL ASP GLY TRP THR TYR ASP ALA THR LYS THR PHE THR VAL THR THR GLY SER ASN GLU

PHE P62 L63 C64 S65 L66 V70 V74 L78 I82 L87 S88 G89 K90 S91 R92 E93 K94 F95 Q96 K98 L99 GLU HIS HIS HIS HIS HIS HIS

• Molecule 2: Polyubiquitin-B

Chain B: 54% 37% 5%

SER HIS Q201 Q202 L203 K206 T207 L208 T212 T213 T214 V217 E218 T222 N225 V226 K229 K233 T236 T244 F245 L250 T255 L256 Y259 Q260 L261 Q262 K263 E264 S265 T266 L267 H268 L269 V270 L271 L272 L273 R274 Q275 G276

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

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

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

Software name	Classification	Version
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	2017
Number of shifts mapped to atoms	1333
Number of unparsed shifts	0
Number of shifts with mapping errors	684
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	197	198	198	8±1
2	B	574	597	596	18±3
All	All	15420	15900	15880	448

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
2:B:217:VAL:HG11	2:B:226:VAL:HG22	0.94	1.39	16	20
1:A:78:LEU:HD13	1:A:82:ILE:HG21	0.93	1.38	20	18
1:A:82:ILE:HG23	2:B:270:VAL:HG11	0.78	1.56	19	18
1:A:78:LEU:HD23	1:A:82:ILE:HG21	0.77	1.56	9	2
2:B:226:VAL:HG21	2:B:256:LEU:HD21	0.72	1.61	18	19
2:B:223:ILE:HD12	2:B:250:LEU:HD23	0.69	1.64	7	2
2:B:207:THR:HG22	2:B:269:LEU:HD23	0.69	1.63	12	18
2:B:226:VAL:HG21	2:B:256:LEU:HD11	0.67	1.67	16	1
1:A:74:VAL:HG13	2:B:268:HIS:CE1	0.66	2.26	20	11
1:A:66:LEU:CB	1:A:70:VAL:HG11	0.65	2.21	6	20
2:B:227:LYS:HG3	2:B:243:LEU:HD11	0.65	1.69	1	1
1:A:78:LEU:HD13	1:A:82:ILE:CG2	0.64	2.23	3	14
2:B:243:LEU:CD1	2:B:250:LEU:HD12	0.64	2.21	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:ILE:HD12	2:B:270:VAL:HG11	0.62	1.70	9	19
2:B:245:PHE:HB3	2:B:250:LEU:HD21	0.62	1.72	1	17
2:B:227:LYS:CG	2:B:243:LEU:HD11	0.61	2.25	1	3
1:A:66:LEU:HB3	1:A:70:VAL:HG11	0.61	1.73	13	20
2:B:217:VAL:HG12	2:B:229:LYS:HE3	0.60	1.74	17	8
2:B:250:LEU:HD22	2:B:259:TYR:CD1	0.60	2.32	16	11
2:B:221:ASP:O	2:B:255:THR:HG22	0.59	1.97	16	2
2:B:217:VAL:CG1	2:B:226:VAL:HG22	0.58	2.24	16	1
1:A:78:LEU:CD2	1:A:82:ILE:HG21	0.57	2.28	9	2
1:A:78:LEU:HD23	1:A:82:ILE:CG2	0.57	2.29	9	2
2:B:213:ILE:HG23	2:B:233:LYS:HE3	0.57	1.77	16	16
2:B:207:THR:CG2	2:B:269:LEU:HD23	0.55	2.30	12	16
2:B:214:THR:C	2:B:215:LEU:HD12	0.54	2.25	19	3
2:B:206:LYS:HG2	2:B:212:THR:HG23	0.54	1.78	6	8
2:B:243:LEU:HD13	2:B:250:LEU:CB	0.54	2.32	17	1
2:B:213:ILE:HG22	2:B:215:LEU:CD1	0.54	2.33	19	3
1:A:69:GLY:O	2:B:209:THR:HG22	0.53	2.02	17	6
2:B:250:LEU:HD22	2:B:259:TYR:CG	0.53	2.39	3	9
2:B:218:GLU:O	2:B:256:LEU:HD12	0.52	2.04	9	19
2:B:227:LYS:CE	2:B:243:LEU:HD11	0.52	2.34	19	2
2:B:243:LEU:O	2:B:244:ILE:HD13	0.52	2.04	4	9
2:B:215:LEU:HD21	2:B:230:ILE:HG13	0.52	1.81	17	1
2:B:215:LEU:HD22	2:B:229:LYS:HB2	0.52	1.82	18	1
1:A:71:ASP:CG	1:A:74:VAL:HG23	0.52	2.30	2	4
2:B:215:LEU:HD21	2:B:230:ILE:CG1	0.52	2.34	19	3
2:B:227:LYS:HA	2:B:230:ILE:HD12	0.51	1.82	18	5
1:A:83:GLN:O	1:A:87:LEU:HD23	0.51	2.06	6	6
2:B:256:LEU:HD12	2:B:261:ILE:HG21	0.51	1.82	16	1
2:B:230:ILE:HG21	2:B:269:LEU:CD1	0.50	2.37	2	1
2:B:213:ILE:HG22	2:B:215:LEU:HD21	0.50	1.84	16	2
1:A:82:ILE:HD11	2:B:244:ILE:HD11	0.49	1.84	20	2
2:B:207:THR:HG22	2:B:269:LEU:HB3	0.49	1.85	2	2
2:B:236:ILE:HD12	2:B:269:LEU:HD21	0.48	1.84	1	7
2:B:245:PHE:CD2	2:B:261:ILE:HD13	0.48	2.42	14	17
2:B:227:LYS:HE3	2:B:243:LEU:HD11	0.48	1.86	12	1
2:B:227:LYS:CD	2:B:243:LEU:HD11	0.47	2.40	10	1
2:B:265:SER:OG	2:B:267:LEU:HD12	0.47	2.10	14	1
2:B:243:LEU:HD13	2:B:250:LEU:HB2	0.47	1.85	17	1
1:A:82:ILE:HD11	2:B:242:ARG:HD3	0.47	1.85	19	2
2:B:203:ILE:HD11	2:B:226:VAL:HG13	0.47	1.85	20	3
2:B:223:ILE:HD11	2:B:259:TYR:CE1	0.47	2.45	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:226:VAL:CG2	2:B:256:LEU:HD11	0.46	2.40	18	9
2:B:215:LEU:HD22	2:B:229:LYS:CB	0.46	2.40	18	1
2:B:203:ILE:HD12	2:B:267:LEU:HD13	0.46	1.87	14	3
2:B:215:LEU:HD21	2:B:230:ILE:HG12	0.46	1.87	19	1
1:A:71:ASP:OD2	1:A:74:VAL:HG23	0.46	2.10	10	3
2:B:246:ALA:HB3	2:B:248:LYS:NZ	0.46	2.24	13	1
2:B:203:ILE:HD11	2:B:226:VAL:CG1	0.46	2.40	20	2
2:B:223:ILE:CD1	2:B:250:LEU:HD23	0.46	2.37	7	1
2:B:243:LEU:HD11	2:B:250:LEU:HD12	0.46	1.89	16	1
2:B:271:LEU:HD13	2:B:272:ARG:N	0.45	2.26	13	7
2:B:261:ILE:HD12	2:B:267:LEU:HD11	0.45	1.87	17	1
2:B:245:PHE:CE2	2:B:261:ILE:HD13	0.44	2.48	20	8
2:B:269:LEU:HD12	2:B:270:VAL:N	0.44	2.27	13	2
1:A:78:LEU:HD23	2:B:244:ILE:HG21	0.44	1.89	18	1
2:B:207:THR:HG22	2:B:269:LEU:CB	0.43	2.44	7	1
1:A:66:LEU:HD23	1:A:75:PHE:CZ	0.43	2.48	12	1
2:B:214:THR:O	2:B:215:LEU:HD12	0.43	2.13	19	3
1:A:66:LEU:HB2	1:A:70:VAL:HG11	0.43	1.90	18	1
2:B:241:GLN:HG3	2:B:269:LEU:HD13	0.43	1.90	8	1
2:B:227:LYS:HD3	2:B:243:LEU:HD22	0.43	1.90	16	1
2:B:269:LEU:HD23	2:B:270:VAL:N	0.42	2.28	7	1
2:B:246:ALA:HB3	2:B:248:LYS:HZ3	0.42	1.73	13	1
2:B:256:LEU:HD22	2:B:261:ILE:HG21	0.42	1.91	1	2
2:B:226:VAL:HG23	2:B:256:LEU:HD21	0.42	1.91	16	1
2:B:243:LEU:CB	2:B:250:LEU:HD12	0.42	2.44	11	1
2:B:227:LYS:HE2	2:B:243:LEU:HD11	0.42	1.92	19	1
1:A:82:ILE:CG2	2:B:270:VAL:HG11	0.42	2.45	9	2
2:B:222:THR:HG22	2:B:254:ARG:O	0.41	2.15	4	1
1:A:66:LEU:HD22	1:A:75:PHE:CD2	0.41	2.51	6	1
2:B:250:LEU:HD11	2:B:267:LEU:HD11	0.41	1.93	6	1
2:B:240:GLN:O	2:B:271:LEU:HD22	0.41	2.15	13	1
2:B:248:LYS:CE	2:B:250:LEU:HD23	0.40	2.45	1	1
2:B:243:LEU:H	2:B:243:LEU:HD12	0.40	1.77	17	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	25/106 (24%)	25±0 (99±2%)	0±0 (1±2%)	0±0 (0±0%)	100	100
2	B	71/78 (91%)	69±1 (97±1%)	2±1 (3±1%)	0±0 (0±0%)	100	100
All	All	1920/3680 (52%)	1869 (97%)	51 (3%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains ⓘ

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	23/92 (25%)	20±2 (86±9%)	3±1 (13±6%)	6	48
2	B	66/70 (94%)	52±2 (78±2%)	14±2 (22±2%)	2	30
All	All	1773/3240 (55%)	1427 (80%)	346 (20%)	3	33

All 38 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)
2	B	206	LYS	20
2	B	208	LEU	20
2	B	212	THR	20
2	B	225	ASN	20
2	B	255	THR	20
2	B	271	LEU	20
1	A	76	LYS	19
2	B	202	GLN	19
2	B	265	SER	19
2	B	222	THR	18
2	B	214	THR	16
2	B	248	LYS	15
1	A	87	LEU	14
2	B	266	THR	12
2	B	263	LYS	10
2	B	241	GLN	10
1	A	68	GLU	10

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Mol	Chain	Res	Type	Models (Total)
2	B	209	THR	7
2	B	220	SER	7
1	A	90	LYS	7
2	B	243	LEU	6
2	B	227	LYS	5
2	B	251	GLU	5
2	B	249	GLN	4
2	B	269	LEU	4
2	B	232	ASP	2
2	B	262	GLN	2
1	A	78	LEU	2
1	A	84	GLU	2
2	B	267	LEU	2
2	B	236	ILE	2
1	A	72	GLN	1
2	B	242	ARG	1
1	A	75	PHE	1
2	B	233	LYS	1
2	B	250	LEU	1
1	A	66	LEU	1
1	A	88	SER	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

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 83% 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	2017
Number of shifts mapped to atoms	1333
Number of unparsed shifts	0
Number of shifts with mapping errors	684
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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

- No matching atom found in the structure. All 684 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HA	4.155	0.020	1
1	A	1	MET	HB2	2.083	0.020	2
1	A	1	MET	HB3	2.209	0.020	2
1	A	1	MET	HE1	2.11	0.020	1
1	A	1	MET	HE2	2.11	0.020	1
1	A	1	MET	HE3	2.11	0.020	1
1	A	1	MET	HG2	2.17	0.020	2
1	A	1	MET	HG3	2.407	0.020	2
1	A	1	MET	CA	54.073	0.400	1
1	A	1	MET	CB	32.187	0.400	1
1	A	1	MET	CE	15.833	0.400	1
1	A	1	MET	CG	30.268	0.400	1
1	A	2	GLN	H	8.338	0.020	1
1	A	2	GLN	HA	4.954	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	GLN	HB2	1.955	0.020	2
1	A	2	GLN	HB3	2.018	0.020	2
1	A	2	GLN	HE21	6.887	0.020	2
1	A	2	GLN	HE22	7.827	0.020	2
1	A	2	GLN	HG2	2.341	0.020	2
1	A	2	GLN	HG3	2.114	0.020	2
1	A	2	GLN	CA	55.411	0.400	1
1	A	2	GLN	CB	29.995	0.400	1
1	A	2	GLN	CG	34.639	0.400	1
1	A	2	GLN	N	123.406	0.400	1
1	A	2	GLN	NE2	112.352	0.400	1
1	A	3	TYR	H	9.082	0.020	1
1	A	3	TYR	HA	5.35	0.020	1
1	A	3	TYR	HB2	2.708	0.020	2
1	A	3	TYR	HB3	3.383	0.020	2
1	A	3	TYR	HD1	7.13	0.020	1
1	A	3	TYR	HD2	7.13	0.020	1
1	A	3	TYR	HE1	6.908	0.020	1
1	A	3	TYR	HE2	6.908	0.020	1
1	A	3	TYR	CA	56.595	0.400	1
1	A	3	TYR	CB	42.987	0.400	1
1	A	3	TYR	CD1	133.033	0.400	1
1	A	3	TYR	CE1	117.444	0.400	1
1	A	3	TYR	N	124.395	0.400	1
1	A	4	LYS	H	9.088	0.020	1
1	A	4	LYS	HA	5.209	0.020	1
1	A	4	LYS	HB2	1.876	0.020	2
1	A	4	LYS	HB3	2.013	0.020	2
1	A	4	LYS	HD2	1.605	0.020	1
1	A	4	LYS	HD3	1.605	0.020	1
1	A	4	LYS	HE2	2.775	0.020	1
1	A	4	LYS	HE3	2.775	0.020	1
1	A	4	LYS	HG2	1.327	0.020	2
1	A	4	LYS	HG3	1.448	0.020	2
1	A	4	LYS	CA	54.057	0.400	1
1	A	4	LYS	CB	35.465	0.400	1
1	A	4	LYS	CD	28.441	0.400	1
1	A	4	LYS	CE	41.265	0.400	1
1	A	4	LYS	CG	25.103	0.400	1
1	A	4	LYS	N	122.232	0.400	1
1	A	5	LEU	H	8.608	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LEU	HA	4.934	0.020	1
1	A	5	LEU	HB2	0.736	0.020	2
1	A	5	LEU	HB3	-1.157	0.020	2
1	A	5	LEU	HD11	0.526	0.020	2
1	A	5	LEU	HD12	0.526	0.020	2
1	A	5	LEU	HD13	0.526	0.020	2
1	A	5	LEU	HD21	0.561	0.020	2
1	A	5	LEU	HD22	0.561	0.020	2
1	A	5	LEU	HD23	0.561	0.020	2
1	A	5	LEU	HG	0.849	0.020	1
1	A	5	LEU	CA	52.143	0.400	1
1	A	5	LEU	CB	42.147	0.400	1
1	A	5	LEU	CD1	24.28	0.400	1
1	A	5	LEU	CD2	25.395	0.400	1
1	A	5	LEU	CG	26.677	0.400	1
1	A	5	LEU	N	126.362	0.400	1
1	A	6	ILE	H	9.073	0.020	1
1	A	6	ILE	HA	4.308	0.020	1
1	A	6	ILE	HB	1.942	0.020	1
1	A	6	ILE	HD11	0.742	0.020	1
1	A	6	ILE	HD12	0.742	0.020	1
1	A	6	ILE	HD13	0.742	0.020	1
1	A	6	ILE	HG12	1.069	0.020	2
1	A	6	ILE	HG13	1.394	0.020	2
1	A	6	ILE	HG21	0.772	0.020	1
1	A	6	ILE	HG22	0.772	0.020	1
1	A	6	ILE	HG23	0.772	0.020	1
1	A	6	ILE	CA	59.636	0.400	1
1	A	6	ILE	CB	37.669	0.400	1
1	A	6	ILE	CD1	12.225	0.400	1
1	A	6	ILE	CG1	26.797	0.400	1
1	A	6	ILE	CG2	16.602	0.400	1
1	A	6	ILE	N	126.117	0.400	1
1	A	7	LEU	H	8.702	0.020	1
1	A	7	LEU	HA	4.462	0.020	1
1	A	7	LEU	HB2	1.421	0.020	2
1	A	7	LEU	HB3	1.332	0.020	2
1	A	7	LEU	HD11	0.736	0.020	2
1	A	7	LEU	HD12	0.736	0.020	2
1	A	7	LEU	HD13	0.736	0.020	2
1	A	7	LEU	HD21	0.746	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	LEU	HD22	0.746	0.020	2
1	A	7	LEU	HD23	0.746	0.020	2
1	A	7	LEU	HG	1.269	0.020	1
1	A	7	LEU	CA	53.842	0.400	1
1	A	7	LEU	CB	41.737	0.400	1
1	A	7	LEU	CD1	25.139	0.400	1
1	A	7	LEU	CD2	25.384	0.400	1
1	A	7	LEU	CG	27.043	0.400	1
1	A	7	LEU	N	125.509	0.400	1
1	A	8	ASN	H	8.831	0.020	1
1	A	8	ASN	HA	5.223	0.020	1
1	A	8	ASN	HB2	2.495	0.020	2
1	A	8	ASN	HB3	2.944	0.020	2
1	A	8	ASN	HD21	7.11	0.020	2
1	A	8	ASN	HD22	6.761	0.020	2
1	A	8	ASN	CA	50.535	0.400	1
1	A	8	ASN	CB	37.815	0.400	1
1	A	8	ASN	N	125.475	0.400	1
1	A	8	ASN	ND2	111.3	0.400	1
1	A	9	GLY	H	7.92	0.020	1
1	A	9	GLY	HA2	4.422	0.020	2
1	A	9	GLY	HA3	4.021	0.020	2
1	A	9	GLY	CA	44.266	0.400	1
1	A	9	GLY	N	109.755	0.400	1
1	A	10	LYS	H	9.283	0.020	1
1	A	10	LYS	HA	4.026	0.020	1
1	A	10	LYS	HB2	1.792	0.020	1
1	A	10	LYS	HB3	1.792	0.020	1
1	A	10	LYS	HD2	1.671	0.020	1
1	A	10	LYS	HD3	1.671	0.020	1
1	A	10	LYS	HE2	2.923	0.020	1
1	A	10	LYS	HE3	2.923	0.020	1
1	A	10	LYS	HG2	1.421	0.020	1
1	A	10	LYS	HG3	1.421	0.020	1
1	A	10	LYS	CA	58.515	0.400	1
1	A	10	LYS	CB	31.958	0.400	1
1	A	10	LYS	CD	28.434	0.400	1
1	A	10	LYS	CE	41.279	0.400	1
1	A	10	LYS	CG	24.774	0.400	1
1	A	10	LYS	N	121.086	0.400	1
1	A	11	THR	H	8.803	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	THR	HA	4.353	0.020	1
1	A	11	THR	HB	4.207	0.020	1
1	A	11	THR	HG21	1.125	0.020	1
1	A	11	THR	HG22	1.125	0.020	1
1	A	11	THR	HG23	1.125	0.020	1
1	A	11	THR	CA	61.46	0.400	1
1	A	11	THR	CB	69.112	0.400	1
1	A	11	THR	CG2	21.314	0.400	1
1	A	11	THR	N	108.583	0.400	1
1	A	12	LEU	H	7.306	0.020	1
1	A	12	LEU	HA	4.432	0.020	1
1	A	12	LEU	HB2	1.405	0.020	2
1	A	12	LEU	HB3	1.53	0.020	2
1	A	12	LEU	HD11	0.863	0.020	2
1	A	12	LEU	HD12	0.863	0.020	2
1	A	12	LEU	HD13	0.863	0.020	2
1	A	12	LEU	HD21	0.78	0.020	2
1	A	12	LEU	HD22	0.78	0.020	2
1	A	12	LEU	HD23	0.78	0.020	2
1	A	12	LEU	HG	1.394	0.020	1
1	A	12	LEU	CA	54.61	0.400	1
1	A	12	LEU	CB	42.938	0.400	1
1	A	12	LEU	CD1	23.754	0.400	1
1	A	12	LEU	CD2	24.863	0.400	1
1	A	12	LEU	CG	27.012	0.400	1
1	A	12	LEU	N	124.89	0.400	1
1	A	13	LYS	H	8.095	0.020	1
1	A	13	LYS	HA	5.114	0.020	1
1	A	13	LYS	HB2	1.877	0.020	2
1	A	13	LYS	HB3	1.705	0.020	2
1	A	13	LYS	HD2	1.72	0.020	1
1	A	13	LYS	HD3	1.72	0.020	1
1	A	13	LYS	HE2	2.902	0.020	2
1	A	13	LYS	HE3	2.986	0.020	2
1	A	13	LYS	HG2	1.435	0.020	1
1	A	13	LYS	HG3	1.435	0.020	1
1	A	13	LYS	CA	53.297	0.400	1
1	A	13	LYS	CB	34.391	0.400	1
1	A	13	LYS	CD	28.678	0.400	1
1	A	13	LYS	CE	42.079	0.400	1
1	A	13	LYS	CG	24.585	0.400	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	LYS	N	123.767	0.400	1
1	A	14	GLY	H	8.386	0.020	1
1	A	14	GLY	HA2	4.136	0.020	2
1	A	14	GLY	HA3	4.247	0.020	2
1	A	14	GLY	CA	44.568	0.400	1
1	A	14	GLY	N	109.323	0.400	1
1	A	15	GLU	H	8.376	0.020	1
1	A	15	GLU	HA	5.591	0.020	1
1	A	15	GLU	HB2	1.893	0.020	2
1	A	15	GLU	HB3	1.993	0.020	2
1	A	15	GLU	HG2	2.126	0.020	1
1	A	15	GLU	HG3	2.126	0.020	1
1	A	15	GLU	CA	54.057	0.400	1
1	A	15	GLU	CB	33.327	0.400	1
1	A	15	GLU	CG	35.58	0.400	1
1	A	15	GLU	N	118.548	0.400	1
1	A	16	THR	H	8.759	0.020	1
1	A	16	THR	HA	4.719	0.020	1
1	A	16	THR	HB	3.888	0.020	1
1	A	16	THR	HG21	0.414	0.020	1
1	A	16	THR	HG22	0.414	0.020	1
1	A	16	THR	HG23	0.414	0.020	1
1	A	16	THR	CA	59.943	0.400	1
1	A	16	THR	CB	68.911	0.400	1
1	A	16	THR	CG2	18.828	0.400	1
1	A	16	THR	N	115.84	0.400	1
1	A	17	THR	H	8.059	0.020	1
1	A	17	THR	HA	5.793	0.020	1
1	A	17	THR	HB	4.276	0.020	1
1	A	17	THR	HG21	1.17	0.020	1
1	A	17	THR	HG22	1.17	0.020	1
1	A	17	THR	HG23	1.17	0.020	1
1	A	17	THR	CA	59.295	0.400	1
1	A	17	THR	CB	72.719	0.400	1
1	A	17	THR	CG2	21.011	0.400	1
1	A	17	THR	N	111.797	0.400	1
1	A	18	THR	H	8.954	0.020	1
1	A	18	THR	HA	4.647	0.020	1
1	A	18	THR	HB	3.822	0.020	1
1	A	18	THR	HG21	0.458	0.020	1
1	A	18	THR	HG22	0.458	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	THR	HG23	0.458	0.020	1
1	A	18	THR	CA	61.725	0.400	1
1	A	18	THR	CB	69.521	0.400	1
1	A	18	THR	CG2	18.557	0.400	1
1	A	18	THR	N	114.492	0.400	1
1	A	19	GLU	H	7.92	0.020	1
1	A	19	GLU	HA	5.155	0.020	1
1	A	19	GLU	HB2	1.919	0.020	1
1	A	19	GLU	HB3	1.919	0.020	1
1	A	19	GLU	HG2	2.031	0.020	2
1	A	19	GLU	HG3	2.263	0.020	2
1	A	19	GLU	CA	53.843	0.400	1
1	A	19	GLU	CB	29.809	0.400	1
1	A	19	GLU	CG	35.232	0.400	1
1	A	19	GLU	N	125.896	0.400	1
1	A	20	ALA	H	9.32	0.020	1
1	A	20	ALA	HA	4.919	0.020	1
1	A	20	ALA	HB1	1.325	0.020	1
1	A	20	ALA	HB2	1.325	0.020	1
1	A	20	ALA	HB3	1.325	0.020	1
1	A	20	ALA	CA	50.26	0.400	1
1	A	20	ALA	CB	23.199	0.400	1
1	A	20	ALA	N	127.308	0.400	1
1	A	21	VAL	H	8.474	0.020	1
1	A	21	VAL	HA	4.082	0.020	1
1	A	21	VAL	HB	2.183	0.020	1
1	A	21	VAL	HG11	0.989	0.020	2
1	A	21	VAL	HG12	0.989	0.020	2
1	A	21	VAL	HG13	0.989	0.020	2
1	A	21	VAL	HG21	0.981	0.020	2
1	A	21	VAL	HG22	0.981	0.020	2
1	A	21	VAL	HG23	0.981	0.020	2
1	A	21	VAL	CA	62.975	0.400	1
1	A	21	VAL	CB	31.421	0.400	1
1	A	21	VAL	CG1	20.424	0.400	1
1	A	21	VAL	CG2	19.662	0.400	1
1	A	21	VAL	N	115.712	0.400	1
1	A	22	ASP	H	7.296	0.020	1
1	A	22	ASP	HA	4.74	0.020	1
1	A	22	ASP	HB2	2.944	0.020	2
1	A	22	ASP	HB3	3.026	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	ASP	CA	51.939	0.400	1
1	A	22	ASP	CB	41.543	0.400	1
1	A	22	ASP	N	115.055	0.400	1
1	A	23	ALA	H	8.276	0.020	1
1	A	23	ALA	HA	3.301	0.020	1
1	A	23	ALA	HB1	1.161	0.020	1
1	A	23	ALA	HB2	1.161	0.020	1
1	A	23	ALA	HB3	1.161	0.020	1
1	A	23	ALA	CA	54.038	0.400	1
1	A	23	ALA	CB	16.945	0.400	1
1	A	23	ALA	N	121.34	0.400	1
1	A	24	ALA	H	8.034	0.020	1
1	A	24	ALA	HA	3.943	0.020	1
1	A	24	ALA	HB1	1.27	0.020	1
1	A	24	ALA	HB2	1.27	0.020	1
1	A	24	ALA	HB3	1.27	0.020	1
1	A	24	ALA	CA	54.14	0.400	1
1	A	24	ALA	CB	17.275	0.400	1
1	A	24	ALA	N	120.414	0.400	1
1	A	25	THR	H	8.269	0.020	1
1	A	25	THR	HA	3.683	0.020	1
1	A	25	THR	HB	3.998	0.020	1
1	A	25	THR	HG21	1.207	0.020	1
1	A	25	THR	HG22	1.207	0.020	1
1	A	25	THR	HG23	1.207	0.020	1
1	A	25	THR	CA	66.348	0.400	1
1	A	25	THR	CB	67.268	0.400	1
1	A	25	THR	CG2	20.488	0.400	1
1	A	25	THR	N	116.322	0.400	1
1	A	26	ALA	H	7.135	0.020	1
1	A	26	ALA	HA	3.057	0.020	1
1	A	26	ALA	HB1	0.488	0.020	1
1	A	26	ALA	HB2	0.488	0.020	1
1	A	26	ALA	HB3	0.488	0.020	1
1	A	26	ALA	CA	54.338	0.400	1
1	A	26	ALA	CB	16.929	0.400	1
1	A	26	ALA	N	123.563	0.400	1
1	A	27	GLU	H	8.299	0.020	1
1	A	27	GLU	HA	2.608	0.020	1
1	A	27	GLU	HB2	1.829	0.020	2
1	A	27	GLU	HB3	1.931	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	27	GLU	HG2	1.603	0.020	1
1	A	27	GLU	HG3	1.603	0.020	1
1	A	27	GLU	CA	59.053	0.400	1
1	A	27	GLU	CB	28.681	0.400	1
1	A	27	GLU	CG	35.265	0.400	1
1	A	27	GLU	N	116.527	0.400	1
1	A	28	LYS	H	6.924	0.020	1
1	A	28	LYS	HA	3.705	0.020	1
1	A	28	LYS	HB2	1.813	0.020	1
1	A	28	LYS	HB3	1.813	0.020	1
1	A	28	LYS	HD2	1.592	0.020	1
1	A	28	LYS	HD3	1.592	0.020	1
1	A	28	LYS	HE2	2.874	0.020	1
1	A	28	LYS	HE3	2.874	0.020	1
1	A	28	LYS	HG2	1.305	0.020	2
1	A	28	LYS	HG3	1.527	0.020	2
1	A	28	LYS	CA	59.095	0.400	1
1	A	28	LYS	CB	31.691	0.400	1
1	A	28	LYS	CD	28.719	0.400	1
1	A	28	LYS	CE	41.425	0.400	1
1	A	28	LYS	CG	24.598	0.400	1
1	A	28	LYS	N	116.49	0.400	1
1	A	29	VAL	H	7.306	0.020	1
1	A	29	VAL	HA	3.619	0.020	1
1	A	29	VAL	HB	1.73	0.020	1
1	A	29	VAL	HG11	0.768	0.020	2
1	A	29	VAL	HG12	0.768	0.020	2
1	A	29	VAL	HG13	0.768	0.020	2
1	A	29	VAL	HG21	0.877	0.020	2
1	A	29	VAL	HG22	0.877	0.020	2
1	A	29	VAL	HG23	0.877	0.020	2
1	A	29	VAL	CA	65.349	0.400	1
1	A	29	VAL	CB	31.179	0.400	1
1	A	29	VAL	CG1	19.923	0.400	1
1	A	29	VAL	CG2	21.099	0.400	1
1	A	29	VAL	N	120.468	0.400	1
1	A	30	PHE	H	8.498	0.020	1
1	A	30	PHE	HA	4.755	0.020	1
1	A	30	PHE	HB2	2.812	0.020	2
1	A	30	PHE	HB3	3.3	0.020	2
1	A	30	PHE	HD1	6.899	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	30	PHE	HD2	6.899	0.020	1
1	A	30	PHE	HE1	7.078	0.020	1
1	A	30	PHE	HE2	7.078	0.020	1
1	A	30	PHE	HZ	7.168	0.020	1
1	A	30	PHE	CA	55.977	0.400	1
1	A	30	PHE	CB	36.854	0.400	1
1	A	30	PHE	CD1	129.211	0.400	1
1	A	30	PHE	CE1	130.036	0.400	1
1	A	30	PHE	CZ	129.763	0.400	1
1	A	30	PHE	N	120.532	0.400	1
1	A	31	LYS	H	9.058	0.020	1
1	A	31	LYS	HA	4.148	0.020	1
1	A	31	LYS	HB2	1.606	0.020	2
1	A	31	LYS	HB3	1.54	0.020	2
1	A	31	LYS	HD2	1.028	0.020	2
1	A	31	LYS	HD3	1.086	0.020	2
1	A	31	LYS	HE2	1.639	0.020	2
1	A	31	LYS	HE3	1.861	0.020	2
1	A	31	LYS	HG2	0.445	0.020	2
1	A	31	LYS	HG3	0.779	0.020	2
1	A	31	LYS	CA	59.299	0.400	1
1	A	31	LYS	CB	31.118	0.400	1
1	A	31	LYS	CD	28.182	0.400	1
1	A	31	LYS	CE	40.67	0.400	1
1	A	31	LYS	CG	25.363	0.400	1
1	A	31	LYS	N	122.701	0.400	1
1	A	32	GLN	H	7.423	0.020	1
1	A	32	GLN	HA	4.024	0.020	1
1	A	32	GLN	HB2	2.184	0.020	2
1	A	32	GLN	HB3	2.231	0.020	2
1	A	32	GLN	HE21	6.863	0.020	2
1	A	32	GLN	HE22	7.918	0.020	2
1	A	32	GLN	HG2	2.397	0.020	2
1	A	32	GLN	HG3	2.427	0.020	2
1	A	32	GLN	CA	57.95	0.400	1
1	A	32	GLN	CB	27.592	0.400	1
1	A	32	GLN	CG	32.832	0.400	1
1	A	32	GLN	N	119.507	0.400	1
1	A	32	GLN	NE2	115.204	0.400	1
1	A	33	TYR	H	8.232	0.020	1
1	A	33	TYR	HA	4.255	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	33	TYR	HB2	3.287	0.020	1
1	A	33	TYR	HB3	3.287	0.020	1
1	A	33	TYR	HD1	6.968	0.020	1
1	A	33	TYR	HD2	6.968	0.020	1
1	A	33	TYR	HE1	6.714	0.020	1
1	A	33	TYR	HE2	6.714	0.020	1
1	A	33	TYR	CA	61.241	0.400	1
1	A	33	TYR	CB	38.192	0.400	1
1	A	33	TYR	CD1	132.213	0.400	1
1	A	33	TYR	CE1	117.726	0.400	1
1	A	33	TYR	N	120.872	0.400	1
1	A	34	ALA	H	9.16	0.020	1
1	A	34	ALA	HA	3.774	0.020	1
1	A	34	ALA	HB1	1.821	0.020	1
1	A	34	ALA	HB2	1.821	0.020	1
1	A	34	ALA	HB3	1.821	0.020	1
1	A	34	ALA	CA	55.731	0.400	1
1	A	34	ALA	CB	17.381	0.400	1
1	A	34	ALA	N	122.479	0.400	1
1	A	35	ASN	H	8.229	0.020	1
1	A	35	ASN	HA	4.42	0.020	1
1	A	35	ASN	HB2	2.9	0.020	2
1	A	35	ASN	HB3	2.943	0.020	2
1	A	35	ASN	HD21	7.601	0.020	2
1	A	35	ASN	HD22	6.955	0.020	2
1	A	35	ASN	CA	56.368	0.400	1
1	A	35	ASN	CB	38.301	0.400	1
1	A	35	ASN	N	117.521	0.400	1
1	A	35	ASN	ND2	112.17	0.400	1
1	A	36	ASP	H	8.917	0.020	1
1	A	36	ASP	HA	4.345	0.020	1
1	A	36	ASP	HB2	2.713	0.020	2
1	A	36	ASP	HB3	2.542	0.020	2
1	A	36	ASP	CA	56.333	0.400	1
1	A	36	ASP	CB	39.413	0.400	1
1	A	36	ASP	N	121.311	0.400	1
1	A	37	ASN	H	7.357	0.020	1
1	A	37	ASN	HA	4.575	0.020	1
1	A	37	ASN	HB2	2.077	0.020	2
1	A	37	ASN	HB3	2.667	0.020	2
1	A	37	ASN	HD21	6.253	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	37	ASN	HD22	6.619	0.020	2
1	A	37	ASN	CA	53.194	0.400	1
1	A	37	ASN	CB	39.449	0.400	1
1	A	37	ASN	N	115.211	0.400	1
1	A	37	ASN	ND2	114.79	0.400	1
1	A	38	GLY	H	7.772	0.020	1
1	A	38	GLY	HA2	3.897	0.020	1
1	A	38	GLY	HA3	3.897	0.020	1
1	A	38	GLY	CA	46.224	0.400	1
1	A	38	GLY	N	108.012	0.400	1
1	A	39	VAL	H	8.099	0.020	1
1	A	39	VAL	HA	4.124	0.020	1
1	A	39	VAL	HB	1.711	0.020	1
1	A	39	VAL	HG11	0.615	0.020	2
1	A	39	VAL	HG12	0.615	0.020	2
1	A	39	VAL	HG13	0.615	0.020	2
1	A	39	VAL	HG21	0.784	0.020	2
1	A	39	VAL	HG22	0.784	0.020	2
1	A	39	VAL	HG23	0.784	0.020	2
1	A	39	VAL	CA	61.42	0.400	1
1	A	39	VAL	CB	32.712	0.400	1
1	A	39	VAL	CG1	21.005	0.400	1
1	A	39	VAL	CG2	21.289	0.400	1
1	A	39	VAL	N	120.706	0.400	1
1	A	40	ASP	H	8.468	0.020	1
1	A	40	ASP	HA	4.863	0.020	1
1	A	40	ASP	HB2	2.574	0.020	2
1	A	40	ASP	HB3	2.702	0.020	2
1	A	40	ASP	CA	51.913	0.400	1
1	A	40	ASP	CB	42.636	0.400	1
1	A	40	ASP	N	127.304	0.400	1
1	A	41	GLY	H	7.912	0.020	1
1	A	41	GLY	HA2	3.731	0.020	2
1	A	41	GLY	HA3	4.216	0.020	2
1	A	41	GLY	CA	44.866	0.400	1
1	A	41	GLY	N	107.327	0.400	1
1	A	42	GLU	H	8.024	0.020	1
1	A	42	GLU	HA	4.674	0.020	1
1	A	42	GLU	HB2	2.028	0.020	2
1	A	42	GLU	HB3	1.95	0.020	2
1	A	42	GLU	HG2	2.245	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	42	GLU	HG3	2.338	0.020	2
1	A	42	GLU	CA	54.95	0.400	1
1	A	42	GLU	CB	30.956	0.400	1
1	A	42	GLU	CG	35.811	0.400	1
1	A	42	GLU	N	120.524	0.400	1
1	A	43	TRP	H	9.294	0.020	1
1	A	43	TRP	HA	5.354	0.020	1
1	A	43	TRP	HB2	3.141	0.020	2
1	A	43	TRP	HB3	3.351	0.020	2
1	A	43	TRP	HD1	7.554	0.020	1
1	A	43	TRP	HE3	7.601	0.020	1
1	A	43	TRP	HH2	6.727	0.020	1
1	A	43	TRP	HZ2	7.322	0.020	1
1	A	43	TRP	HZ3	6.595	0.020	1
1	A	43	TRP	CA	57.201	0.400	1
1	A	43	TRP	CB	30.057	0.400	1
1	A	43	TRP	CD1	126.469	0.400	1
1	A	43	TRP	CE3	118.812	0.400	1
1	A	43	TRP	CH2	122.367	0.400	1
1	A	43	TRP	CZ2	113.889	0.400	1
1	A	43	TRP	CZ3	120.179	0.400	1
1	A	43	TRP	N	128.082	0.400	1
1	A	44	THR	H	9.247	0.020	1
1	A	44	THR	HA	4.803	0.020	1
1	A	44	THR	HB	4.215	0.020	1
1	A	44	THR	HG21	1.167	0.020	1
1	A	44	THR	HG22	1.167	0.020	1
1	A	44	THR	HG23	1.167	0.020	1
1	A	44	THR	CA	59.89	0.400	1
1	A	44	THR	CB	71.686	0.400	1
1	A	44	THR	CG2	21.312	0.400	1
1	A	44	THR	N	114.405	0.400	1
1	A	45	TYR	H	8.559	0.020	1
1	A	45	TYR	HA	4.946	0.020	1
1	A	45	TYR	HB2	2.48	0.020	2
1	A	45	TYR	HB3	2.854	0.020	2
1	A	45	TYR	HD1	7.791	0.020	1
1	A	45	TYR	HD2	7.791	0.020	1
1	A	45	TYR	HE1	6.335	0.020	1
1	A	45	TYR	HE2	6.335	0.020	1
1	A	45	TYR	CA	56.317	0.400	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	45	TYR	CB	41.007	0.400	1
1	A	45	TYR	CD1	131.666	0.400	1
1	A	45	TYR	CE1	116.897	0.400	1
1	A	45	TYR	N	120.527	0.400	1
1	A	46	ASP	H	7.604	0.020	1
1	A	46	ASP	HA	4.564	0.020	1
1	A	46	ASP	HB2	2.244	0.020	2
1	A	46	ASP	HB3	2.582	0.020	2
1	A	46	ASP	CA	51.153	0.400	1
1	A	46	ASP	CB	42.435	0.400	1
1	A	46	ASP	N	128.305	0.400	1
1	A	47	ASP	H	8.55	0.020	1
1	A	47	ASP	HA	4.115	0.020	1
1	A	47	ASP	HB2	2.502	0.020	2
1	A	47	ASP	HB3	2.806	0.020	2
1	A	47	ASP	CA	55.741	0.400	1
1	A	47	ASP	CB	41.549	0.400	1
1	A	47	ASP	N	124.821	0.400	1
1	A	48	ALA	H	8.319	0.020	1
1	A	48	ALA	HA	4.105	0.020	1
1	A	48	ALA	HB1	1.482	0.020	1
1	A	48	ALA	HB2	1.482	0.020	1
1	A	48	ALA	HB3	1.482	0.020	1
1	A	48	ALA	CA	54.624	0.400	1
1	A	48	ALA	CB	17.741	0.400	1
1	A	48	ALA	N	119.765	0.400	1
1	A	49	THR	H	6.989	0.020	1
1	A	49	THR	HA	4.38	0.020	1
1	A	49	THR	HB	4.384	0.020	1
1	A	49	THR	HG21	1.061	0.020	1
1	A	49	THR	HG22	1.061	0.020	1
1	A	49	THR	HG23	1.061	0.020	1
1	A	49	THR	CA	59.812	0.400	1
1	A	49	THR	CB	69.519	0.400	1
1	A	49	THR	CG2	20.533	0.400	1
1	A	49	THR	N	103.111	0.400	1
1	A	50	LYS	H	7.84	0.020	1
1	A	50	LYS	HA	4.167	0.020	1
1	A	50	LYS	HB2	2.08	0.020	2
1	A	50	LYS	HB3	2.022	0.020	2
1	A	50	LYS	HD2	1.418	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	50	LYS	HD3	1.677	0.020	2
1	A	50	LYS	HE2	2.934	0.020	2
1	A	50	LYS	HE3	3.084	0.020	2
1	A	50	LYS	HG2	1.22	0.020	2
1	A	50	LYS	HG3	1.397	0.020	2
1	A	50	LYS	CA	56.039	0.400	1
1	A	50	LYS	CB	28.705	0.400	1
1	A	50	LYS	CD	27.791	0.400	1
1	A	50	LYS	CG	24.059	0.400	1
1	A	50	LYS	N	123.033	0.400	1
1	A	51	THR	H	7.356	0.020	1
1	A	51	THR	HA	5.477	0.020	1
1	A	51	THR	HB	3.742	0.020	1
1	A	51	THR	HG21	0.97	0.020	1
1	A	51	THR	HG22	0.97	0.020	1
1	A	51	THR	HG23	0.97	0.020	1
1	A	51	THR	CA	61.62	0.400	1
1	A	51	THR	CB	71.382	0.400	1
1	A	51	THR	CG2	20.235	0.400	1
1	A	51	THR	N	111.03	0.400	1
1	A	52	PHE	H	10.378	0.020	1
1	A	52	PHE	HA	5.66	0.020	1
1	A	52	PHE	HB2	3.221	0.020	2
1	A	52	PHE	HB3	3.288	0.020	2
1	A	52	PHE	HD1	7.781	0.020	1
1	A	52	PHE	HD2	7.781	0.020	1
1	A	52	PHE	HE1	7.207	0.020	1
1	A	52	PHE	HE2	7.207	0.020	1
1	A	52	PHE	HZ	6.984	0.020	1
1	A	52	PHE	CA	56.579	0.400	1
1	A	52	PHE	CB	42.155	0.400	1
1	A	52	PHE	CD1	131.677	0.400	1
1	A	52	PHE	CE1	130.845	0.400	1
1	A	52	PHE	CZ	130.572	0.400	1
1	A	52	PHE	N	130.82	0.400	1
1	A	53	THR	H	9.087	0.020	1
1	A	53	THR	HA	5.194	0.020	1
1	A	53	THR	HB	3.803	0.020	1
1	A	53	THR	HG21	0.933	0.020	1
1	A	53	THR	HG22	0.933	0.020	1
1	A	53	THR	HG23	0.933	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	53	THR	CA	60.937	0.400	1
1	A	53	THR	CB	70.455	0.400	1
1	A	53	THR	CG2	19.978	0.400	1
1	A	53	THR	N	116.885	0.400	1
1	A	54	VAL	H	8.177	0.020	1
1	A	54	VAL	HA	4.463	0.020	1
1	A	54	VAL	HB	-0.324	0.020	1
1	A	54	VAL	HG11	0.365	0.020	2
1	A	54	VAL	HG12	0.365	0.020	2
1	A	54	VAL	HG13	0.365	0.020	2
1	A	54	VAL	HG21	-0.364	0.020	2
1	A	54	VAL	HG22	-0.364	0.020	2
1	A	54	VAL	HG23	-0.364	0.020	2
1	A	54	VAL	CA	57.398	0.400	1
1	A	54	VAL	CB	31.788	0.400	1
1	A	54	VAL	CG1	19.166	0.400	1
1	A	54	VAL	CG2	20.192	0.400	1
1	A	54	VAL	N	123.065	0.400	1
1	A	55	THR	H	8.322	0.020	1
1	A	55	THR	HA	4.691	0.020	1
1	A	55	THR	HB	3.826	0.020	1
1	A	55	THR	HG21	1.143	0.020	1
1	A	55	THR	HG22	1.143	0.020	1
1	A	55	THR	HG23	1.143	0.020	1
1	A	55	THR	CA	60.411	0.400	1
1	A	55	THR	CB	69.948	0.400	1
1	A	55	THR	CG2	20.761	0.400	1
1	A	55	THR	N	123.192	0.400	1
1	A	56	GLU	H	8.086	0.020	1
1	A	56	GLU	HA	4.517	0.020	1
1	A	56	GLU	HB2	1.984	0.020	2
1	A	56	GLU	HB3	2.146	0.020	2
1	A	56	GLU	HG2	2.388	0.020	1
1	A	56	GLU	HG3	2.388	0.020	1
1	A	56	GLU	CA	55.735	0.400	1
1	A	56	GLU	CB	31.402	0.400	1
1	A	56	GLU	CG	36.079	0.400	1
1	A	56	GLU	N	128.667	0.400	1
1	A	57	GLY	H	8.762	0.020	1
1	A	57	GLY	HA2	4.051	0.020	2
1	A	57	GLY	HA3	3.928	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	GLY	CA	44.569	0.400	1
1	A	57	GLY	N	112.349	0.400	1
1	A	58	SER	H	8.306	0.020	1
1	A	58	SER	HA	4.43	0.020	1
1	A	58	SER	HB2	3.811	0.020	1
1	A	58	SER	HB3	3.811	0.020	1
1	A	58	SER	CA	57.476	0.400	1
1	A	58	SER	CB	63.353	0.400	1
1	A	58	SER	N	115.095	0.400	1
1	A	59	ASN	HA	4.661	0.020	1
1	A	59	ASN	HB2	2.663	0.020	2
1	A	59	ASN	HB3	2.74	0.020	2
1	A	59	ASN	HD21	6.87	0.020	2
1	A	59	ASN	HD22	7.554	0.020	2
1	A	59	ASN	CA	52.684	0.400	1
1	A	59	ASN	CB	38.28	0.400	1
1	A	59	ASN	ND2	112.729	0.400	1
1	A	60	GLU	H	8.254	0.020	1
1	A	60	GLU	HA	4.157	0.020	1
1	A	60	GLU	HB2	1.76	0.020	2
1	A	60	GLU	HB3	1.846	0.020	2
1	A	60	GLU	HG2	2.017	0.020	1
1	A	60	GLU	CA	56.05	0.400	1
1	A	60	GLU	CB	30.054	0.400	1
1	A	60	GLU	CG	35.557	0.400	1
1	A	60	GLU	N	120.738	0.400	1
1	A	61	PHE	H	8.227	0.020	1
1	A	61	PHE	HA	4.836	0.020	1
1	A	61	PHE	HB2	2.913	0.020	2
1	A	61	PHE	HB3	3.079	0.020	2
1	A	61	PHE	HD1	7.247	0.020	1
1	A	61	PHE	HD2	7.247	0.020	1
1	A	61	PHE	HE1	7.436	0.020	1
1	A	61	PHE	HE2	7.436	0.020	1
1	A	61	PHE	HZ	7.228	0.020	1
1	A	61	PHE	CA	54.935	0.400	1
1	A	61	PHE	CB	38.54	0.400	1
1	A	61	PHE	CD1	131.392	0.400	1
1	A	61	PHE	CE1	129.478	0.400	1
1	A	61	PHE	CZ	129.204	0.400	1
1	A	61	PHE	N	121.332	0.400	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	100	GLU	H	8.339	0.020	1
1	A	100	GLU	HB2	1.842	0.020	1
1	A	100	GLU	HB3	1.842	0.020	1
1	A	100	GLU	HG2	2.112	0.020	1
1	A	100	GLU	HG3	2.112	0.020	1
1	A	100	GLU	CB	29.695	0.400	1
1	A	100	GLU	CG	35.547	0.400	1
1	A	100	GLU	N	121.442	0.400	1
1	B	200	HIS	HA	4.701	0.020	1
1	B	200	HIS	HB2	3.027	0.020	1
1	B	200	HIS	HB3	3.027	0.020	1
1	B	200	HIS	HD2	6.896	0.020	1
1	B	200	HIS	CA	55.778	0.400	1
1	B	200	HIS	CB	30.309	0.400	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	175	0.56 ± 0.10	Should be applied
$^{13}\text{C}_\beta$	160	0.62 ± 0.14	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	166	0.60 ± 0.39	None needed (imprecise)

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 86%, i.e. 1173 atoms were assigned a chemical shift out of a possible 1362. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	381/481 (79%)	194/195 (99%)	97/194 (50%)	90/92 (98%)
Sidechain	758/835 (91%)	519/539 (96%)	228/267 (85%)	11/29 (38%)
Aromatic	34/46 (74%)	21/23 (91%)	13/22 (59%)	0/1 (0%)
Overall	1173/1362 (86%)	734/757 (97%)	338/483 (70%)	101/122 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1333 atoms were assigned a chemical shift out of a possible 1597. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	447/567 (79%)	228/231 (99%)	113/228 (50%)	106/108 (98%)
Sidechain	845/974 (87%)	577/628 (92%)	256/308 (83%)	12/38 (32%)
Aromatic	41/56 (73%)	26/28 (93%)	15/27 (56%)	0/1 (0%)
Overall	1333/1597 (83%)	831/887 (94%)	384/563 (68%)	118/147 (80%)

7.1.4 Statistically unusual chemical shifts ⓘ

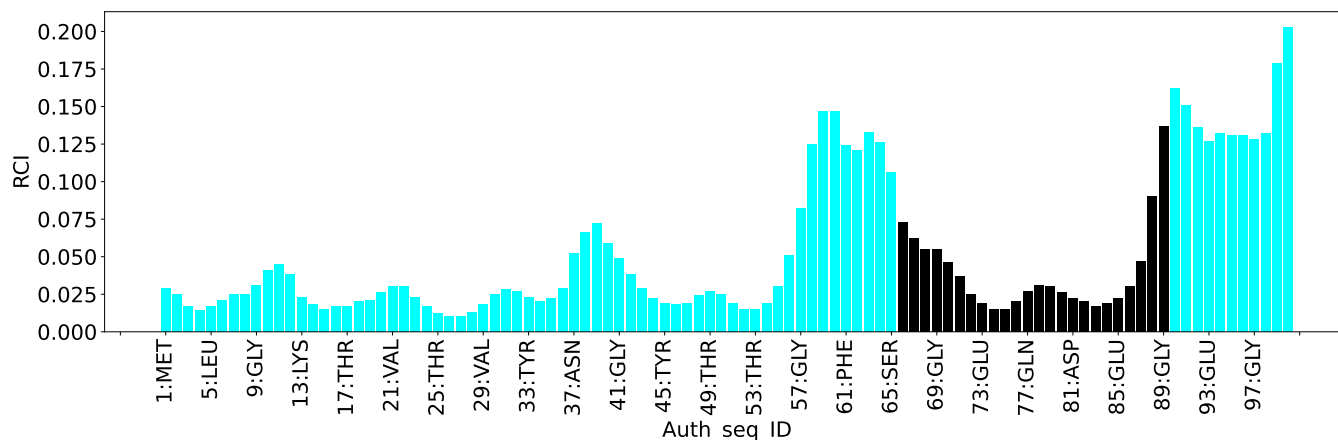
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	5	LEU	HB3	-1.16	-0.26 – 3.31	-7.5
1	A	54	VAL	HB	-0.32	0.43 – 3.54	-7.4
1	A	31	LYS	HE2	1.64	1.95 – 3.88	-6.6
1	A	31	LYS	HE3	1.86	1.92 – 3.89	-5.3

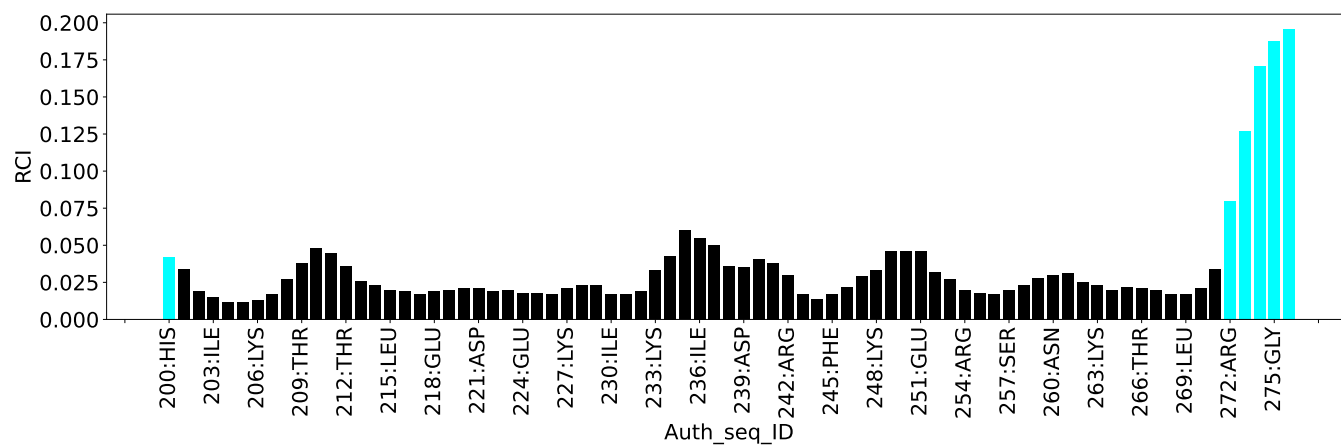
7.1.5 Random Coil Index (RCI) plots ⓘ

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:



Random coil index (RCI) for chain B:



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	3742
Intra-residue ($ i-j =0$)	514
Sequential ($ i-j =1$)	793
Medium range ($ i-j >1$ and $ i-j <5$)	842
Long range ($ i-j \geq 5$)	1273
Inter-chain	230
Hydrogen bond restraints	90
Disulfide bond restraints	0
Total dihedral-angle restraints	188
Number of unmapped restraints	0
Number of restraints per residue	21.4
Number of long range restraints per residue ¹	7.1

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)	2.1	0.19
0.2-0.5 (Medium)	0.3	0.45
>0.5 (Large)	2.4	2.06

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.9	2.27
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

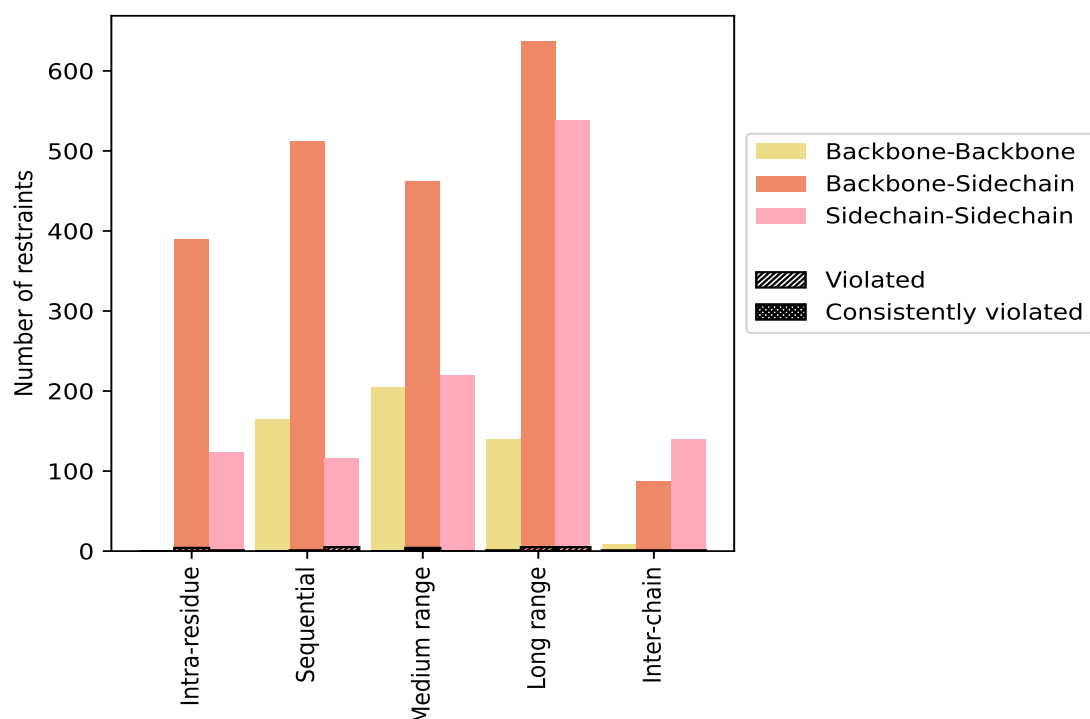
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	514	13.7	5	1.0	0.1	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	390	10.4	4	1.0	0.1	0	0.0	0.0
Sidechain-Sidechain	123	3.3	1	0.8	0.0	0	0.0	0.0
Sequential ($i-j =1$)	793	21.2	6	0.8	0.2	0	0.0	0.0
Backbone-Backbone	165	4.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	512	13.7	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	116	3.1	5	4.3	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	842	22.5	1	0.1	0.0	0	0.0	0.0
Backbone-Backbone	205	5.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	418	11.2	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	219	5.9	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	1273	34.0	9	0.7	0.2	0	0.0	0.0
Backbone-Backbone	140	3.7	1	0.7	0.0	0	0.0	0.0
Backbone-Sidechain	600	16.0	5	0.8	0.1	0	0.0	0.0
Sidechain-Sidechain	533	14.2	3	0.6	0.1	0	0.0	0.0
Inter-chain	230	6.1	2	0.9	0.1	0	0.0	0.0
Backbone-Backbone	8	0.2	1	12.5	0.0	0	0.0	0.0
Backbone-Sidechain	85	2.3	1	1.2	0.0	0	0.0	0.0
Sidechain-Sidechain	137	3.7	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	90	2.4	6	6.7	0.2	2	2.2	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3742	100.0	29	0.8	0.8	2	0.1	0.1
Backbone-Backbone	519	13.9	2	0.4	0.1	0	0.0	0.0
Backbone-Sidechain	2088	55.8	15	0.7	0.4	2	0.1	0.1
Sidechain-Sidechain	1135	30.3	12	1.1	0.3	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	2	2	0	4	1.0	1.91	0.72	0.96
2	0	0	2	2	0	4	0.93	1.96	0.81	0.82
3	0	0	2	3	0	5	0.88	1.92	0.69	0.92
4	0	1	2	2	0	5	0.88	2.06	0.79	0.37
5	0	1	2	0	1	4	1.04	1.95	0.71	1.04
6	0	0	2	1	0	3	1.15	1.99	0.78	1.35
7	0	0	2	2	1	5	0.97	1.89	0.71	1.26
8	0	0	2	0	2	4	0.9	1.93	0.75	0.78
9	0	0	2	1	0	3	1.19	1.94	0.76	1.48
10	0	0	2	4	1	7	0.62	1.91	0.64	0.38

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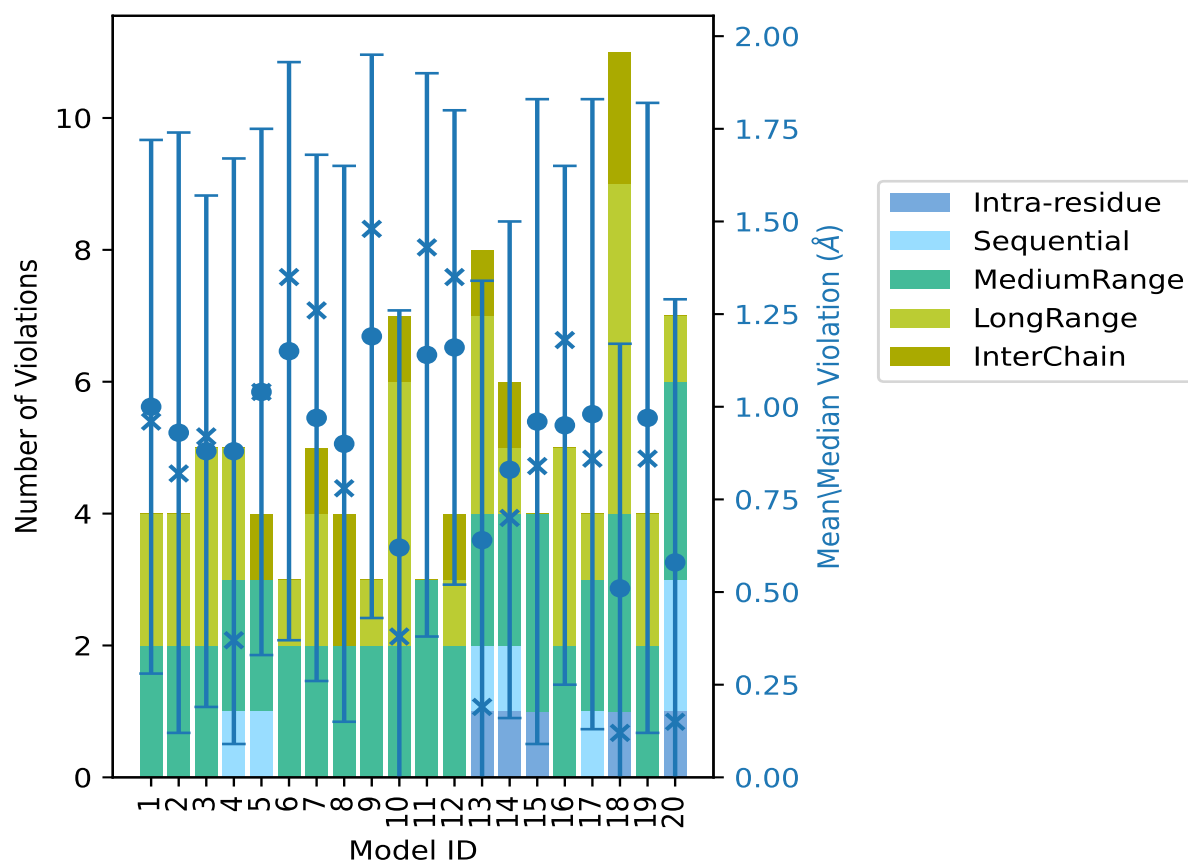
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	3	0	0	3	1.14	1.88	0.76	1.43
12	0	0	2	1	1	4	1.16	1.83	0.64	1.35
13	1	1	2	3	1	8	0.64	2.01	0.7	0.19
14	1	1	2	1	1	6	0.83	1.89	0.67	0.7
15	1	0	3	0	0	4	0.96	2.05	0.87	0.84
16	0	0	2	3	0	5	0.95	1.87	0.7	1.18
17	0	1	2	1	0	4	0.98	2.06	0.85	0.86
18	1	0	3	5	2	11	0.51	1.98	0.66	0.12
19	0	0	2	2	0	4	0.97	2.05	0.85	0.86
20	1	2	3	1	0	7	0.58	1.92	0.71	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 ⓘ



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

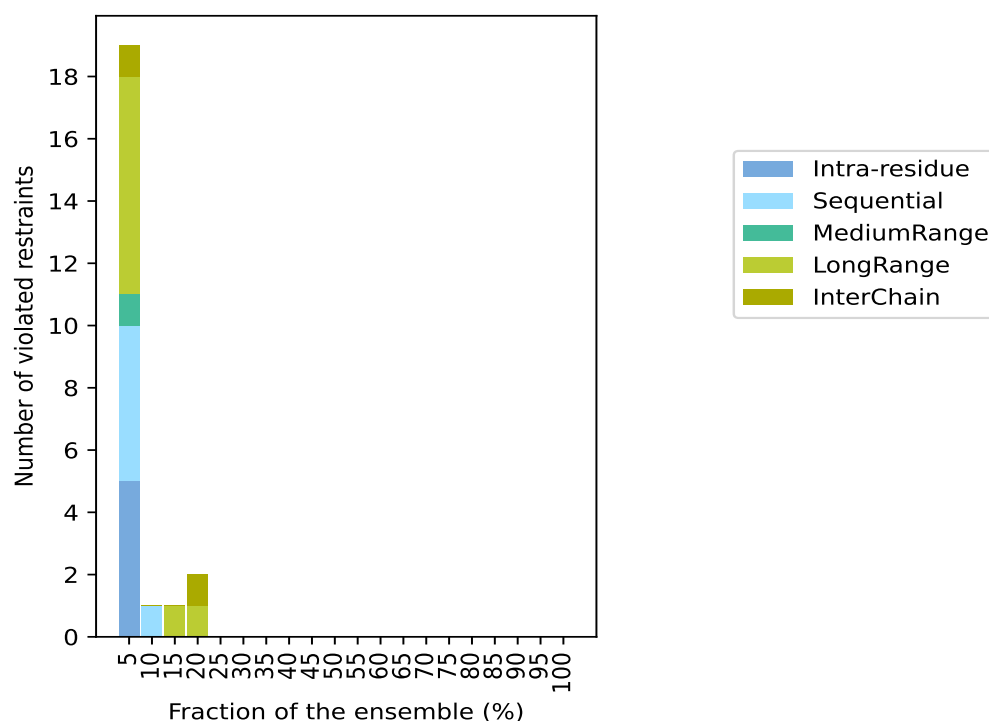
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3629(IR:509, SQ:787, MR:841, LR:1264, IC:228) restraints 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	%
5	5	1	7	1	19	1	5.0
0	1	0	0	0	1	2	10.0
0	0	0	1	0	1	3	15.0
0	0	0	1	1	2	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
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	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
0	0	0	0	0	0	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

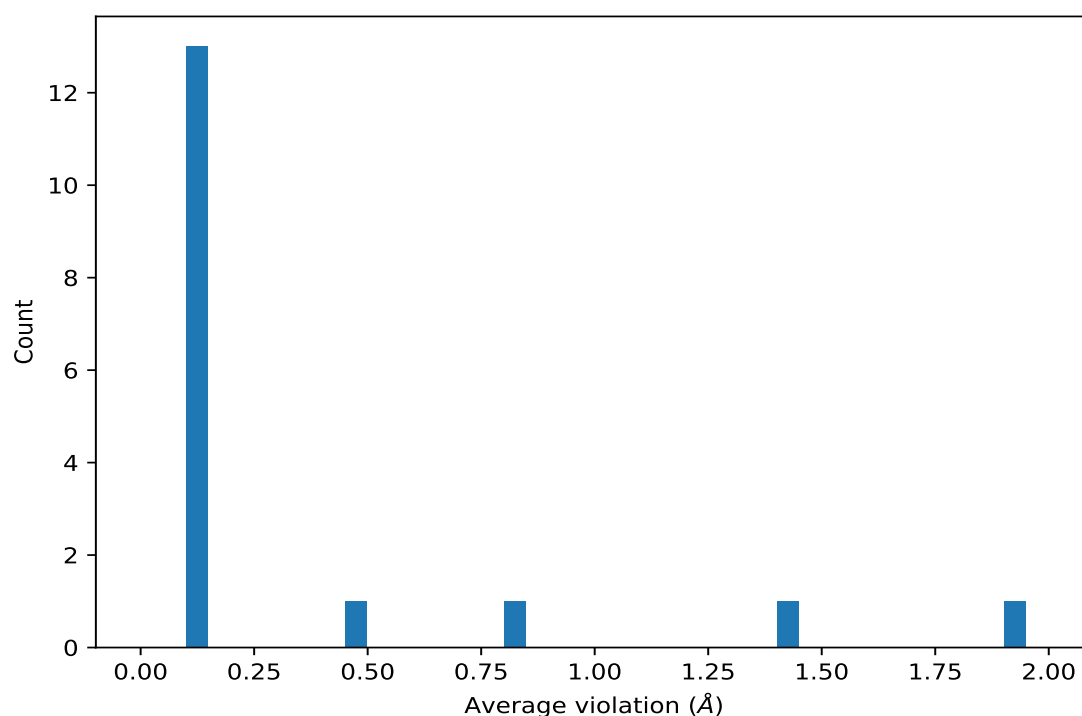
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	20	1.95	0.07	1.94
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	20	1.45	0.09	1.46
(3,64)	2:211:B:LYS:NZ	2:234:B:GLU:OE2	10	0.8	0.41	0.88
(3,67)	2:236:B:ILE:O	2:241:B:GLN:HE22	10	0.15	0.02	0.15
(3,88)	1:85:A:GLU:OE1	2:242:B:ARG:NH1	5	0.48	0.3	0.42
(1,746)	2:201:B:MET:HB2	2:263:B:LYS:HG2	4	0.12	0.01	0.12
(1,746)	2:201:B:MET:HB2	2:263:B:LYS:HG3	4	0.12	0.01	0.12
(1,746)	2:201:B:MET:HB3	2:263:B:LYS:HG2	4	0.12	0.01	0.12
(1,746)	2:201:B:MET:HB3	2:263:B:LYS:HG3	4	0.12	0.01	0.12
(1,2830)	1:71:A:ASP:H	2:208:B:LEU:HA	4	0.12	0.02	0.12
(1,739)	2:201:B:MET:HA	2:263:B:LYS:HG2	3	0.12	0.01	0.12
(1,739)	2:201:B:MET:HA	2:263:B:LYS:HG3	3	0.12	0.01	0.12
(3,58)	2:228:B:ALA:O	2:232:B:ASP:H	3	0.11	0.01	0.11
(1,604)	1:94:A:LYS:HD2	1:95:A:PHE:HD1	2	0.15	0.02	0.15
(1,604)	1:94:A:LYS:HD2	1:95:A:PHE:HD2	2	0.15	0.02	0.15
(1,604)	1:94:A:LYS:HD3	1:95:A:PHE:HD1	2	0.15	0.02	0.15

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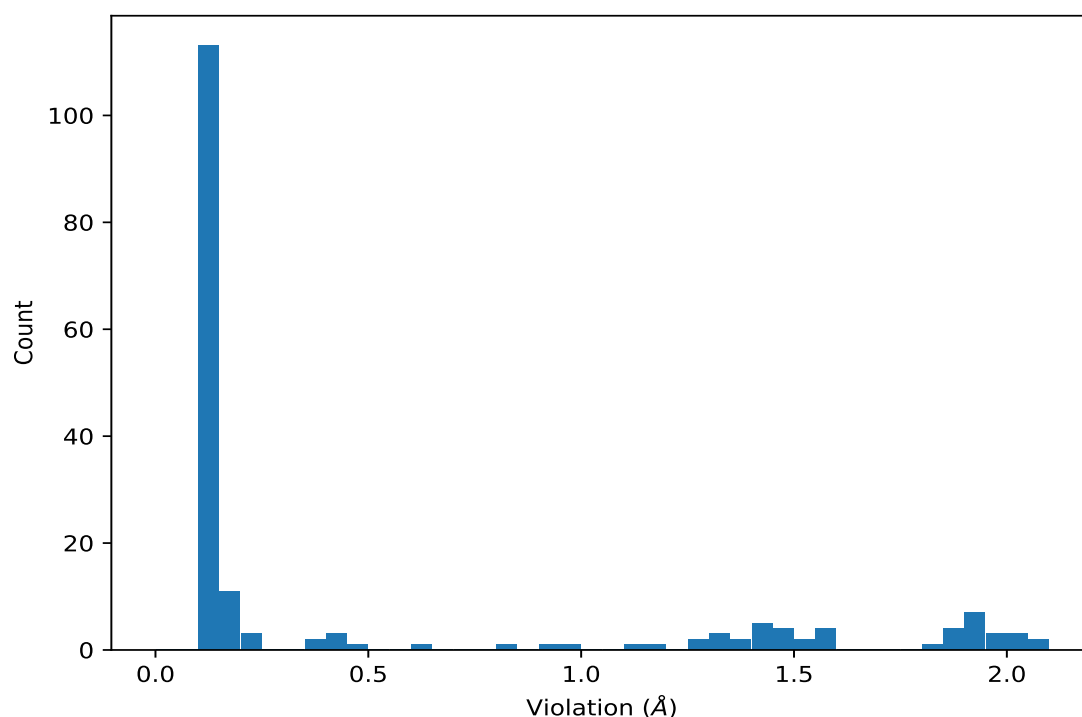
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,604)	1:94:A:LYS:HD3	1:95:A:PHE:HD2	2	0.15	0.02	0.15

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)
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	4	2.06
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	17	2.06
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	15	2.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	19	2.05
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	13	2.01
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	6	1.99
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	18	1.98
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	2	1.96
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	5	1.95
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	9	1.94
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	8	1.93
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	3	1.92
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	20	1.92
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	1	1.91
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	10	1.91
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	7	1.89
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	14	1.89
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	11	1.88
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	16	1.87
(3,69)	1:71:A:ASP:OD2	1:73:A:GLU:H	12	1.83
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	4	1.57
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	19	1.57
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	15	1.56
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	17	1.56
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	13	1.53
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	18	1.53
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	2	1.48
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	5	1.48
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	9	1.48
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	1	1.47
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	20	1.45
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	7	1.43
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	11	1.43
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	14	1.42
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	16	1.42
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	12	1.38
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	6	1.35
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	3	1.32
(3,64)	2:211:B:LYS:NZ	2:234:B:GLU:OE2	12	1.32
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	8	1.31
(3,68)	1:71:A:ASP:OD2	1:73:A:GLU:N	10	1.27
(3,64)	2:211:B:LYS:NZ	2:234:B:GLU:OE2	7	1.26
(3,64)	2:211:B:LYS:NZ	2:234:B:GLU:OE2	16	1.18
(3,64)	2:211:B:LYS:NZ	2:234:B:GLU:OE2	18	1.13
(3,88)	1:85:A:GLU:OE1	2:242:B:ARG:NH1	14	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,64)	2:211:B:LYS:NZ	2:234:B:GLU:OE2	3	0.92
(3,64)	2:211:B:LYS:NZ	2:234:B:GLU:OE2	13	0.84
(3,88)	1:85:A:GLU:OE1	2:242:B:ARG:NH1	5	0.61
(3,64)	2:211:B:LYS:NZ	2:234:B:GLU:OE2	1	0.45
(3,88)	1:85:A:GLU:OE1	2:242:B:ARG:NH1	10	0.42
(1,628)	1:96:A:GLN:HA	1:96:A:GLN:HG2	14	0.41
(1,628)	1:96:A:GLN:HA	1:96:A:GLN:HG3	14	0.41
(3,64)	2:211:B:LYS:NZ	2:234:B:GLU:OE2	10	0.38
(3,64)	2:211:B:LYS:NZ	2:234:B:GLU:OE2	4	0.37
(3,88)	1:85:A:GLU:OE1	2:242:B:ARG:NH1	8	0.24
(2,351)	2:224:B:GLU:HB2	2:225:B:ASN:HD22	4	0.21
(2,351)	2:224:B:GLU:HB3	2:225:B:ASN:HD22	4	0.21
(3,67)	2:236:B:ILE:O	2:241:B:GLN:HE22	13	0.19
(1,2748)	2:271:B:LEU:HA	2:272:B:ARG:HD2	13	0.19
(1,2748)	2:271:B:LEU:HA	2:272:B:ARG:HD3	13	0.19
(3,67)	2:236:B:ILE:O	2:241:B:GLN:HE22	4	0.17
(1,604)	1:94:A:LYS:HD2	1:95:A:PHE:HD1	17	0.17
(1,604)	1:94:A:LYS:HD2	1:95:A:PHE:HD2	17	0.17
(1,604)	1:94:A:LYS:HD3	1:95:A:PHE:HD1	17	0.17
(1,604)	1:94:A:LYS:HD3	1:95:A:PHE:HD2	17	0.17
(3,67)	2:236:B:ILE:O	2:241:B:GLN:HE22	2	0.16
(1,280)	1:76:A:LYS:HA	1:76:A:LYS:HD2	20	0.16
(1,280)	1:76:A:LYS:HA	1:76:A:LYS:HD3	20	0.16
(3,88)	1:85:A:GLU:OE1	2:242:B:ARG:NH1	18	0.15
(3,67)	2:236:B:ILE:O	2:241:B:GLN:HE22	1	0.15
(3,67)	2:236:B:ILE:O	2:241:B:GLN:HE22	3	0.15
(3,67)	2:236:B:ILE:O	2:241:B:GLN:HE22	9	0.15
(3,67)	2:236:B:ILE:O	2:241:B:GLN:HE22	20	0.15
(1,2179)	2:243:B:LEU:HB2	2:268:B:HIS:H	18	0.15
(1,2179)	2:243:B:LEU:HB3	2:268:B:HIS:H	18	0.15
(1,1727)	2:226:B:VAL:H	2:256:B:LEU:HG	16	0.15
(1,213)	1:73:A:GLU:HA	1:76:A:LYS:HD2	20	0.15
(1,213)	1:73:A:GLU:HA	1:76:A:LYS:HD3	20	0.15
(3,67)	2:236:B:ILE:O	2:241:B:GLN:HE22	10	0.14
(3,67)	2:236:B:ILE:O	2:241:B:GLN:HE22	14	0.14
(1,2830)	1:71:A:ASP:H	2:208:B:LEU:HA	8	0.14
(1,1596)	2:223:B:ILE:HD11	2:250:B:LEU:HD11	7	0.14
(1,1596)	2:223:B:ILE:HD11	2:250:B:LEU:HD12	7	0.14
(1,1596)	2:223:B:ILE:HD11	2:250:B:LEU:HD13	7	0.14
(1,1596)	2:223:B:ILE:HD12	2:250:B:LEU:HD11	7	0.14
(1,1596)	2:223:B:ILE:HD12	2:250:B:LEU:HD12	7	0.14
(1,1596)	2:223:B:ILE:HD12	2:250:B:LEU:HD13	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1596)	2:223:B:ILE:HD13	2:250:B:LEU:HD11	7	0.14
(1,1596)	2:223:B:ILE:HD13	2:250:B:LEU:HD12	7	0.14
(1,1596)	2:223:B:ILE:HD13	2:250:B:LEU:HD13	7	0.14
(1,1438)	2:217:B:VAL:HA	2:256:B:LEU:HD11	16	0.14
(1,1438)	2:217:B:VAL:HA	2:256:B:LEU:HD12	16	0.14
(1,1438)	2:217:B:VAL:HA	2:256:B:LEU:HD13	16	0.14
(1,1438)	2:217:B:VAL:HA	2:256:B:LEU:HD21	16	0.14
(1,1438)	2:217:B:VAL:HA	2:256:B:LEU:HD22	16	0.14
(1,1438)	2:217:B:VAL:HA	2:256:B:LEU:HD23	16	0.14
(1,746)	2:201:B:MET:HB2	2:263:B:LYS:HG2	19	0.14
(1,746)	2:201:B:MET:HB2	2:263:B:LYS:HG3	19	0.14
(1,746)	2:201:B:MET:HB3	2:263:B:LYS:HG2	19	0.14
(1,746)	2:201:B:MET:HB3	2:263:B:LYS:HG3	19	0.14
(1,255)	1:75:A:PHE:HB2	1:76:A:LYS:HD2	20	0.14
(1,255)	1:75:A:PHE:HB2	1:76:A:LYS:HD3	20	0.14
(1,255)	1:75:A:PHE:HB3	1:76:A:LYS:HD2	20	0.14
(1,255)	1:75:A:PHE:HB3	1:76:A:LYS:HD3	20	0.14
(2,447)	2:240:B:GLN:HA	2:273:B:LEU:HD11	13	0.13
(2,447)	2:240:B:GLN:HA	2:273:B:LEU:HD12	13	0.13
(2,447)	2:240:B:GLN:HA	2:273:B:LEU:HD13	13	0.13
(1,2830)	1:71:A:ASP:H	2:208:B:LEU:HA	7	0.13
(1,746)	2:201:B:MET:HB2	2:263:B:LYS:HG2	10	0.13
(1,746)	2:201:B:MET:HB2	2:263:B:LYS:HG3	10	0.13
(1,746)	2:201:B:MET:HB3	2:263:B:LYS:HG2	10	0.13
(1,746)	2:201:B:MET:HB3	2:263:B:LYS:HG3	10	0.13
(1,739)	2:201:B:MET:HA	2:263:B:LYS:HG2	19	0.13
(1,739)	2:201:B:MET:HA	2:263:B:LYS:HG3	19	0.13
(1,604)	1:94:A:LYS:HD2	1:95:A:PHE:HD1	5	0.13
(1,604)	1:94:A:LYS:HD2	1:95:A:PHE:HD2	5	0.13
(1,604)	1:94:A:LYS:HD3	1:95:A:PHE:HD1	5	0.13
(1,604)	1:94:A:LYS:HD3	1:95:A:PHE:HD2	5	0.13
(3,58)	2:228:B:ALA:O	2:232:B:ASP:H	18	0.12
(1,739)	2:201:B:MET:HA	2:263:B:LYS:HG2	10	0.12
(1,739)	2:201:B:MET:HA	2:263:B:LYS:HG3	10	0.12
(1,566)	1:92:A:ARG:HB2	1:92:A:ARG:HD2	18	0.12
(1,566)	1:92:A:ARG:HB2	1:92:A:ARG:HD3	18	0.12
(3,67)	2:236:B:ILE:O	2:241:B:GLN:HE22	18	0.11
(3,64)	2:211:B:LYS:NZ	2:234:B:GLU:OE2	2	0.11
(3,58)	2:228:B:ALA:O	2:232:B:ASP:H	15	0.11
(1,2976)	1:92:A:ARG:H	2:271:B:LEU:HG	18	0.11
(1,2830)	1:71:A:ASP:H	2:208:B:LEU:HA	12	0.11
(1,2705)	2:266:B:THR:HB	2:267:B:LEU:HD11	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2705)	2:266:B:THR:HB	2:267:B:LEU:HD12	14	0.11
(1,2705)	2:266:B:THR:HB	2:267:B:LEU:HD13	14	0.11
(1,2705)	2:266:B:THR:HB	2:267:B:LEU:HD21	14	0.11
(1,2705)	2:266:B:THR:HB	2:267:B:LEU:HD22	14	0.11
(1,2705)	2:266:B:THR:HB	2:267:B:LEU:HD23	14	0.11
(1,2173)	2:243:B:LEU:HD11	2:261:B:ILE:HD11	18	0.11
(1,2173)	2:243:B:LEU:HD11	2:261:B:ILE:HD12	18	0.11
(1,2173)	2:243:B:LEU:HD11	2:261:B:ILE:HD13	18	0.11
(1,2173)	2:243:B:LEU:HD12	2:261:B:ILE:HD11	18	0.11
(1,2173)	2:243:B:LEU:HD12	2:261:B:ILE:HD12	18	0.11
(1,2173)	2:243:B:LEU:HD12	2:261:B:ILE:HD13	18	0.11
(1,2173)	2:243:B:LEU:HD13	2:261:B:ILE:HD11	18	0.11
(1,2173)	2:243:B:LEU:HD13	2:261:B:ILE:HD12	18	0.11
(1,2173)	2:243:B:LEU:HD13	2:261:B:ILE:HD13	18	0.11
(1,2173)	2:243:B:LEU:HD21	2:261:B:ILE:HD11	18	0.11
(1,2173)	2:243:B:LEU:HD21	2:261:B:ILE:HD12	18	0.11
(1,2173)	2:243:B:LEU:HD21	2:261:B:ILE:HD13	18	0.11
(1,2173)	2:243:B:LEU:HD22	2:261:B:ILE:HD11	18	0.11
(1,2173)	2:243:B:LEU:HD22	2:261:B:ILE:HD12	18	0.11
(1,2173)	2:243:B:LEU:HD22	2:261:B:ILE:HD13	18	0.11
(1,2173)	2:243:B:LEU:HD23	2:261:B:ILE:HD11	18	0.11
(1,2173)	2:243:B:LEU:HD23	2:261:B:ILE:HD12	18	0.11
(1,2173)	2:243:B:LEU:HD23	2:261:B:ILE:HD13	18	0.11
(1,746)	2:201:B:MET:HB2	2:263:B:LYS:HG2	6	0.11
(1,746)	2:201:B:MET:HB2	2:263:B:LYS:HG3	6	0.11
(1,746)	2:201:B:MET:HB3	2:263:B:LYS:HG2	6	0.11
(1,746)	2:201:B:MET:HB3	2:263:B:LYS:HG3	6	0.11
(1,746)	2:201:B:MET:HB2	2:263:B:LYS:HG2	17	0.11
(1,746)	2:201:B:MET:HB2	2:263:B:LYS:HG3	17	0.11
(1,746)	2:201:B:MET:HB3	2:263:B:LYS:HG2	17	0.11
(1,746)	2:201:B:MET:HB3	2:263:B:LYS:HG3	17	0.11
(1,739)	2:201:B:MET:HA	2:263:B:LYS:HG2	3	0.11
(1,739)	2:201:B:MET:HA	2:263:B:LYS:HG3	3	0.11
(1,662)	1:99:A:LEU:HA	1:99:A:LEU:HD11	13	0.11
(1,662)	1:99:A:LEU:HA	1:99:A:LEU:HD12	13	0.11
(1,662)	1:99:A:LEU:HA	1:99:A:LEU:HD13	13	0.11
(1,662)	1:99:A:LEU:HA	1:99:A:LEU:HD21	13	0.11
(1,662)	1:99:A:LEU:HA	1:99:A:LEU:HD22	13	0.11
(1,662)	1:99:A:LEU:HA	1:99:A:LEU:HD23	13	0.11
(1,252)	1:75:A:PHE:HD1	1:76:A:LYS:HD2	20	0.11
(1,252)	1:75:A:PHE:HD1	1:76:A:LYS:HD3	20	0.11
(1,252)	1:75:A:PHE:HD2	1:76:A:LYS:HD2	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:75:A:PHE:HD2	1:76:A:LYS:HD3	20	0.11
(1,12)	1:63:A:LEU:HA	1:63:A:LEU:HD11	15	0.11
(1,12)	1:63:A:LEU:HA	1:63:A:LEU:HD12	15	0.11
(1,12)	1:63:A:LEU:HA	1:63:A:LEU:HD13	15	0.11
(1,12)	1:63:A:LEU:HA	1:63:A:LEU:HD21	15	0.11
(1,12)	1:63:A:LEU:HA	1:63:A:LEU:HD22	15	0.11
(1,12)	1:63:A:LEU:HA	1:63:A:LEU:HD23	15	0.11
(3,58)	2:228:B:ALA:O	2:232:B:ASP:H	11	0.1
(2,99)	1:85:A:GLU:HA	1:91:A:SER:H	18	0.1
(1,2830)	1:71:A:ASP:H	2:208:B:LEU:HA	13	0.1

10 Dihedral-angle violation analysis [i](#)

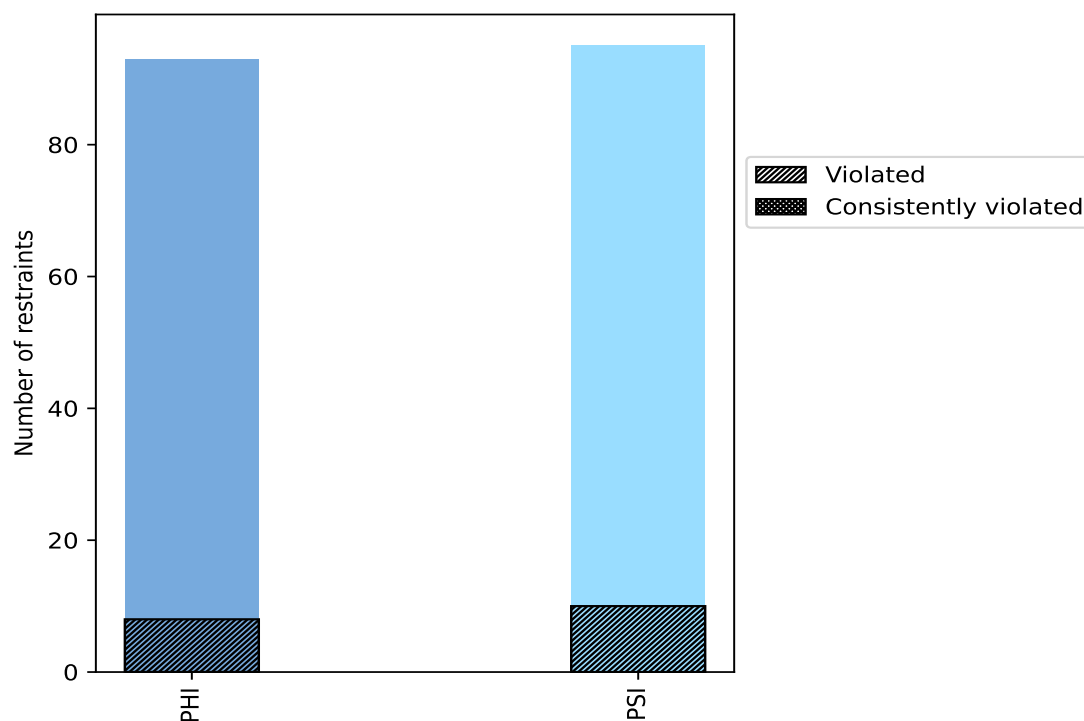
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	93	49.5	8	8.6	4.3	0	0.0	0.0
PSI	95	50.5	10	10.5	5.3	0	0.0	0.0
Total	188	100.0	18	9.6	9.6	0	0.0	0.0

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

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



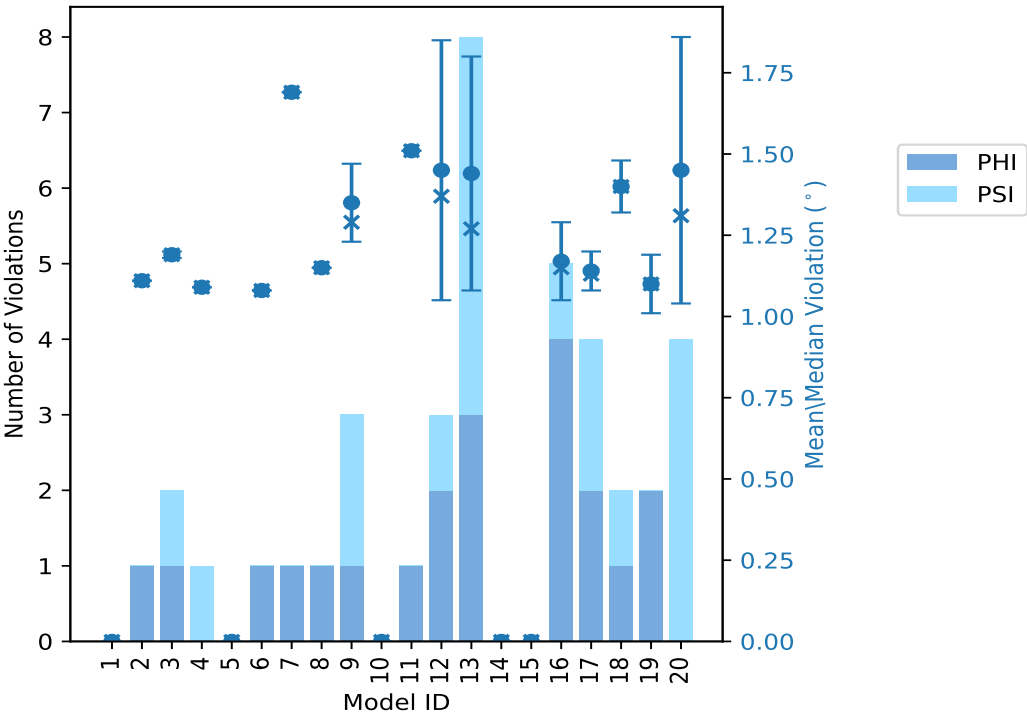
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	1	0	1	1.11	1.11	0.0	1.11
3	1	1	2	1.19	1.2	0.01	1.19
4	0	1	1	1.09	1.09	0.0	1.09
5	0	0	0	0.0	0.0	0.0	0.0
6	1	0	1	1.08	1.08	0.0	1.08
7	1	0	1	1.69	1.69	0.0	1.69
8	1	0	1	1.15	1.15	0.0	1.15
9	1	2	3	1.35	1.51	0.12	1.29
10	0	0	0	0.0	0.0	0.0	0.0
11	1	0	1	1.51	1.51	0.0	1.51
12	2	1	3	1.45	1.98	0.4	1.37
13	3	5	8	1.44	2.27	0.36	1.27
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0
16	4	1	5	1.17	1.33	0.12	1.15
17	2	2	4	1.14	1.23	0.06	1.13
18	1	1	2	1.4	1.48	0.08	1.4
19	2	0	2	1.1	1.19	0.09	1.1
20	0	4	4	1.45	2.14	0.41	1.31

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

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

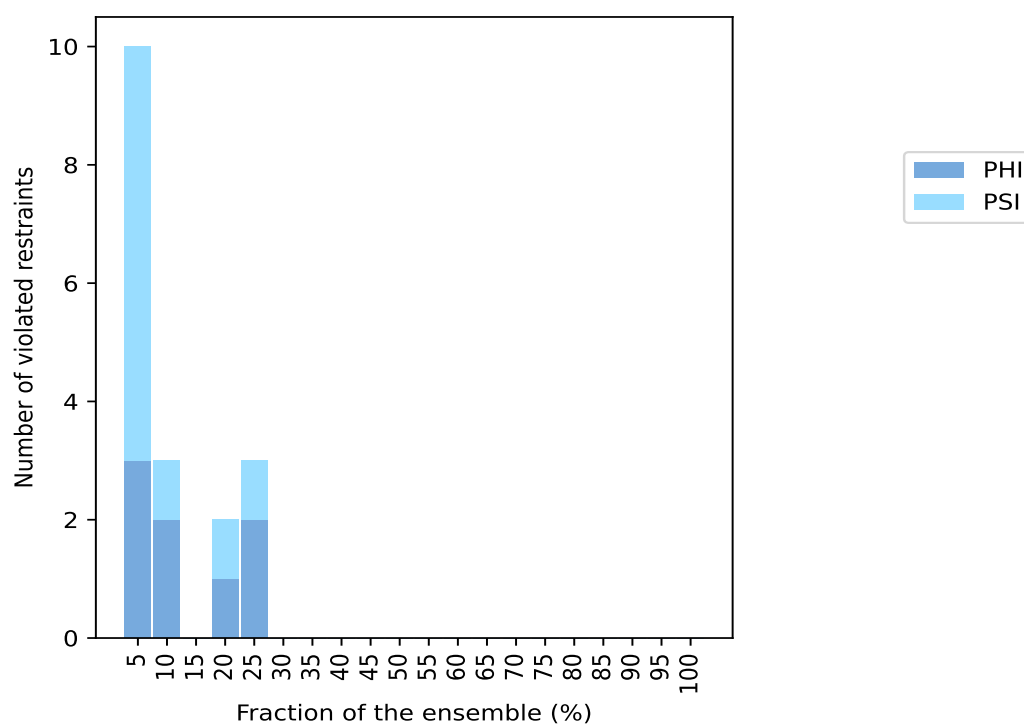
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

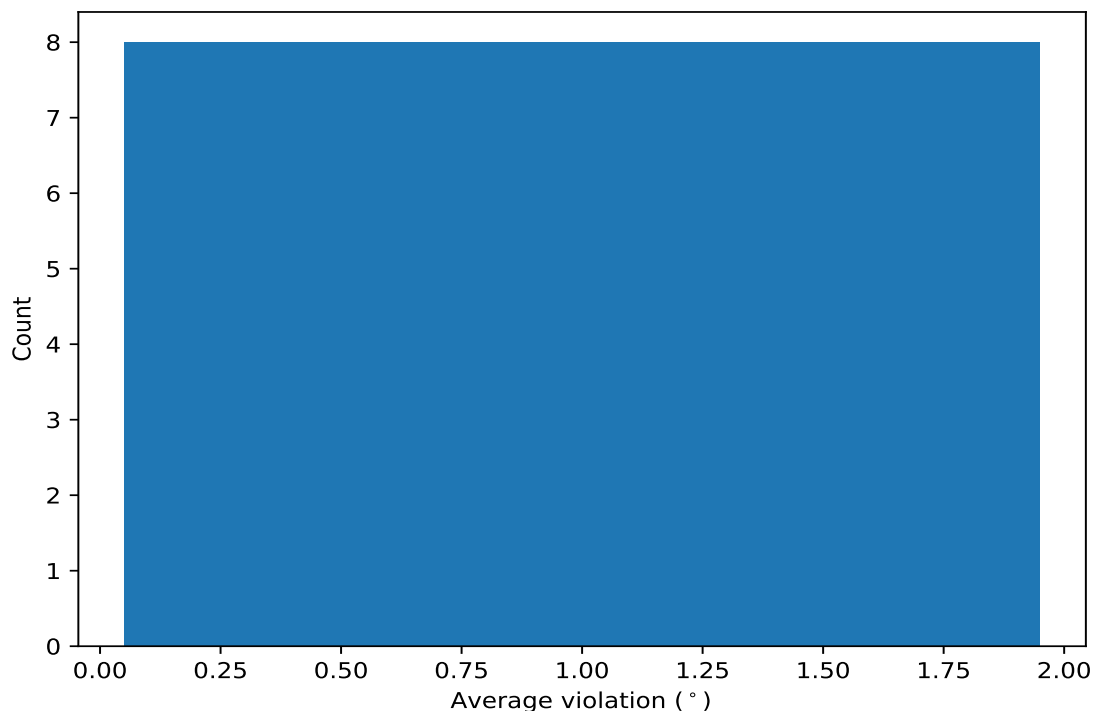


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

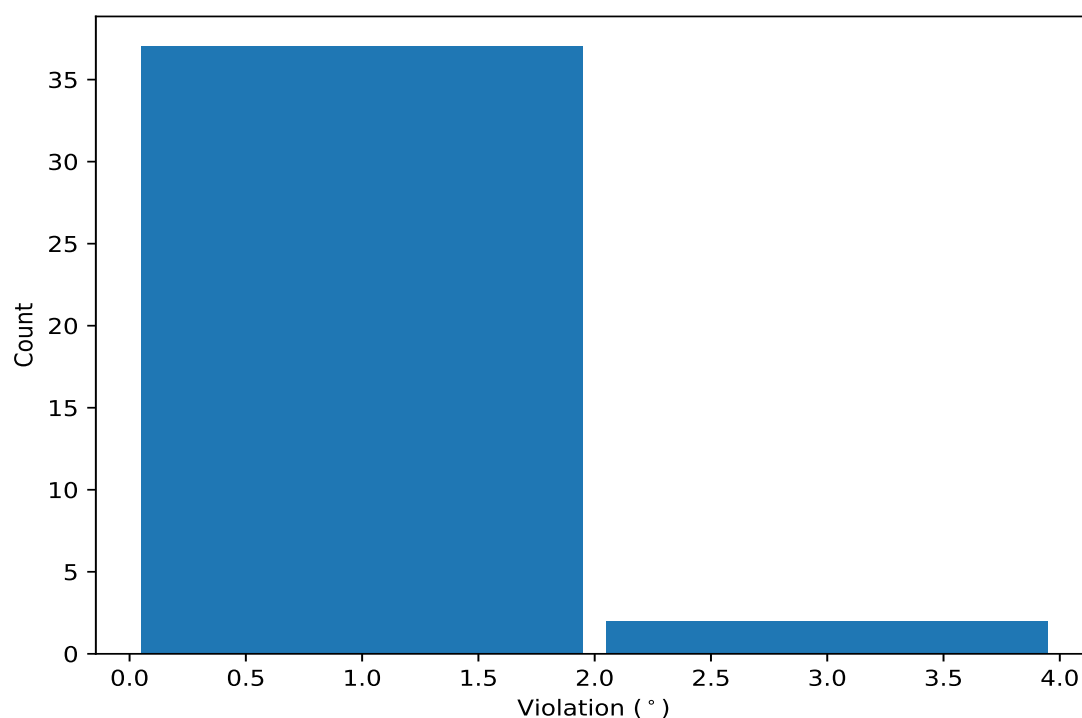
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,23)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LYS:N	5	1.54	0.43	1.29
(1,129)	2:239:B:ASP:C	2:240:B:GLN:N	2:240:B:GLN:CA	2:240:B:GLN:C	5	1.21	0.19	1.23
(1,55)	1:91:A:SER:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	5	1.18	0.08	1.18
(1,124)	2:234:B:GLU:N	2:234:B:GLU:CA	2:234:B:GLU:C	2:235:B:GLY:N	4	1.24	0.15	1.22
(1,125)	2:234:B:GLU:C	2:235:B:GLY:N	2:235:B:GLY:CA	2:235:B:GLY:C	4	1.18	0.11	1.13
(1,83)	2:211:B:LYS:C	2:212:B:THR:N	2:212:B:THR:CA	2:212:B:THR:C	2	1.51	0.0	1.51
(1,133)	2:241:B:GLN:C	2:242:B:ARG:N	2:242:B:ARG:CA	2:242:B:ARG:C	2	1.4	0.29	1.4
(1,52)	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	1:91:A:SER:N	2	1.18	0.09	1.18

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,184)	2:272:B:ARG:N	2:272:B:ARG:CA	2:272:B:ARG:C	2:273:B:LEU:N	13	2.27
(1,23)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LYS:N	20	2.14
(1,23)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LYS:N	12	1.98
(1,133)	2:241:B:GLN:C	2:242:B:ARG:N	2:242:B:ARG:CA	2:242:B:ARG:C	7	1.69
(1,5)	1:65:A:SER:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	13	1.69
(1,129)	2:239:B:ASP:C	2:240:B:GLN:N	2:240:B:GLN:CA	2:240:B:GLN:C	13	1.53
(1,83)	2:211:B:LYS:C	2:212:B:THR:N	2:212:B:THR:CA	2:212:B:THR:C	9	1.51
(1,83)	2:211:B:LYS:C	2:212:B:THR:N	2:212:B:THR:CA	2:212:B:THR:C	11	1.51
(1,124)	2:234:B:GLU:N	2:234:B:GLU:CA	2:234:B:GLU:C	2:235:B:GLY:N	18	1.48
(1,125)	2:234:B:GLU:C	2:235:B:GLY:N	2:235:B:GLY:CA	2:235:B:GLY:C	12	1.37
(1,111)	2:227:B:LYS:C	2:228:B:ALA:N	2:228:B:ALA:CA	2:228:B:ALA:C	16	1.33
(1,55)	1:91:A:SER:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	18	1.32
(1,21)	1:74:A:VAL:N	1:74:A:VAL:CA	1:74:A:VAL:C	1:75:A:PHE:N	20	1.32
(1,23)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LYS:N	9	1.29
(1,17)	1:72:A:GLN:N	1:72:A:GLN:CA	1:72:A:GLN:C	1:73:A:GLU:N	20	1.29
(1,129)	2:239:B:ASP:C	2:240:B:GLN:N	2:240:B:GLN:CA	2:240:B:GLN:C	16	1.27
(1,52)	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	1:91:A:SER:N	13	1.27
(1,180)	2:270:B:VAL:N	2:270:B:VAL:CA	2:270:B:VAL:C	2:271:B:LEU:N	13	1.26
(1,132)	2:241:B:GLN:N	2:241:B:GLN:CA	2:241:B:GLN:C	2:242:B:ARG:N	13	1.25
(1,124)	2:234:B:GLU:N	2:234:B:GLU:CA	2:234:B:GLU:C	2:235:B:GLY:N	9	1.24
(1,129)	2:239:B:ASP:C	2:240:B:GLN:N	2:240:B:GLN:CA	2:240:B:GLN:C	17	1.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,124)	2:234:B:GLU:N	2:234:B:GLU:CA	2:234:B:GLU:C	2:235:B:GLY:N	3	1.2
(1,55)	1:91:A:SER:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	19	1.19
(1,55)	1:91:A:SER:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	3	1.18
(1,23)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LYS:N	13	1.18
(1,138)	2:244:B:ILE:N	2:244:B:ILE:CA	2:244:B:ILE:C	2:245:B:PHE:N	17	1.15
(1,125)	2:234:B:GLU:C	2:235:B:GLY:N	2:235:B:GLY:CA	2:235:B:GLY:C	8	1.15
(1,55)	1:91:A:SER:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	16	1.15
(1,125)	2:234:B:GLU:C	2:235:B:GLY:N	2:235:B:GLY:CA	2:235:B:GLY:C	2	1.11
(1,23)	1:75:A:PHE:N	1:75:A:PHE:CA	1:75:A:PHE:C	1:76:A:LYS:N	17	1.11
(1,133)	2:241:B:GLN:C	2:242:B:ARG:N	2:242:B:ARG:CA	2:242:B:ARG:C	13	1.1
(1,52)	1:90:A:LYS:N	1:90:A:LYS:CA	1:90:A:LYS:C	1:91:A:SER:N	4	1.09
(1,125)	2:234:B:GLU:C	2:235:B:GLY:N	2:235:B:GLY:CA	2:235:B:GLY:C	6	1.08
(1,55)	1:91:A:SER:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	17	1.06
(1,150)	2:254:B:ARG:N	2:254:B:ARG:CA	2:254:B:ARG:C	2:255:B:THR:N	16	1.05
(1,124)	2:234:B:GLU:N	2:234:B:GLU:CA	2:234:B:GLU:C	2:235:B:GLY:N	20	1.05
(1,93)	2:216:B:GLU:C	2:217:B:VAL:N	2:217:B:VAL:CA	2:217:B:VAL:C	16	1.03
(1,129)	2:239:B:ASP:C	2:240:B:GLN:N	2:240:B:GLN:CA	2:240:B:GLN:C	12	1.01
(1,129)	2:239:B:ASP:C	2:240:B:GLN:N	2:240:B:GLN:CA	2:240:B:GLN:C	19	1.01