



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:49 PM UTC

PDB ID : 9PQI / pdb_00009pqi
BMRB ID : 51821
Title : NMR Structure of Ca²⁺/Calmodulin bound to the GluN2A C0 domain of the NMDA receptor
Authors : Bej, A.; Ames, J.B.
Deposited on : 2025-07-22

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

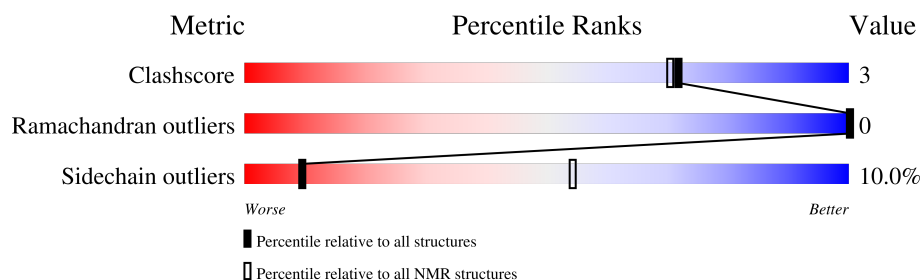
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	149	 38% 5% 54%
2	B	1464	 99%

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:83-A:147, B:1010-B:1021 (77)	0.54	2

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1368 atoms, of which 666 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	69	Total	C	H	N	O	S	0
			1063	337	510	91	121	4	

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms					Trace
2	B	18	Total	C	H	N	O	0
			303	91	156	30	26	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

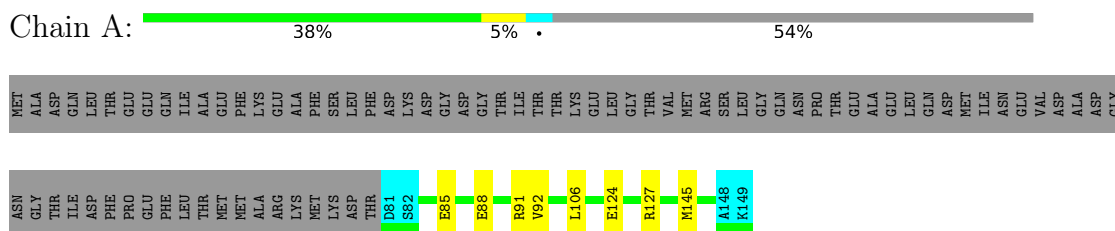
Mol	Chain	Residues	Atoms	
3	A	2	Total	Ca
			2	2

4 Residue-property plots

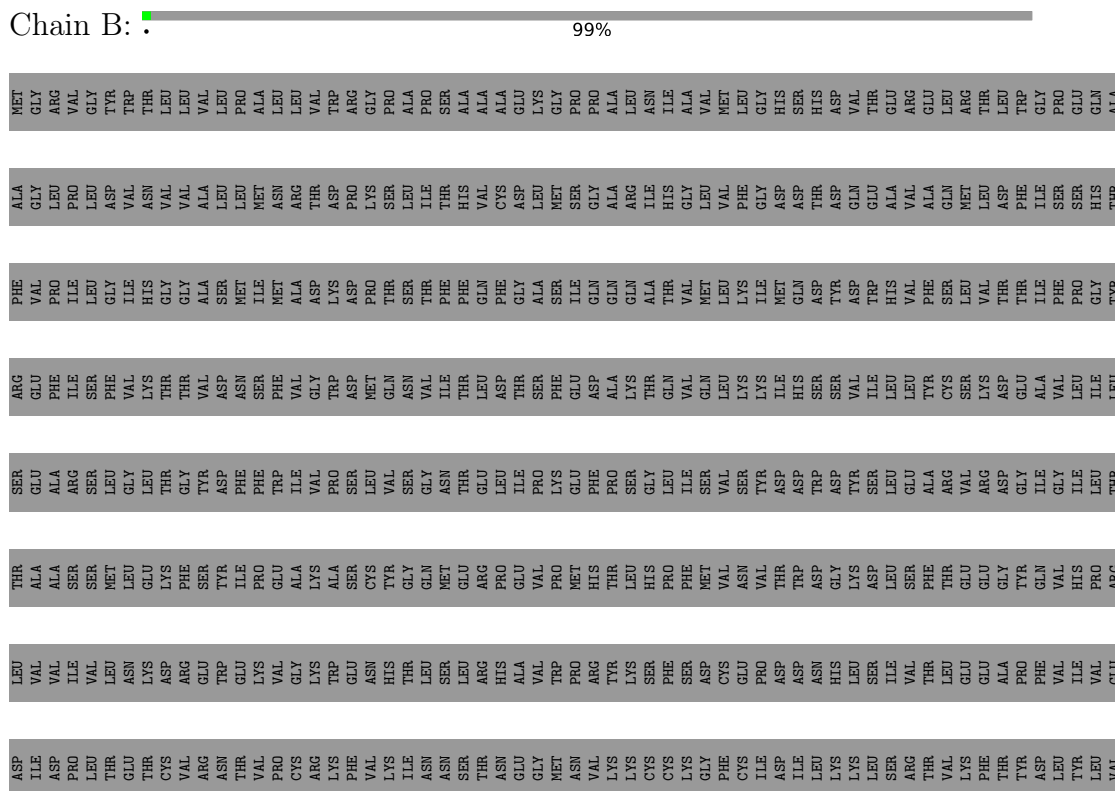
4.1 Average score per residue in the NMR ensemble

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: Calmodulin-1



- Molecule 2: Glutamate receptor ionotropic, NMDA 2A





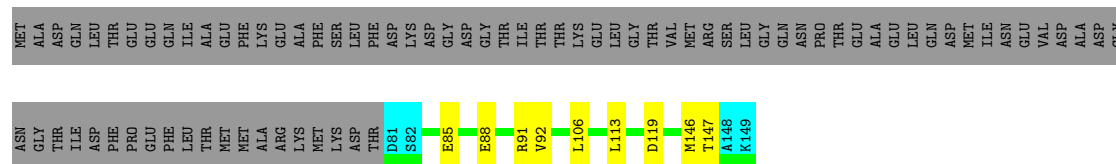
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

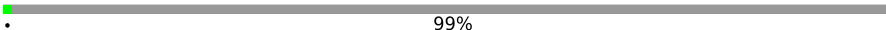
4.2.1 Score per residue for model 1

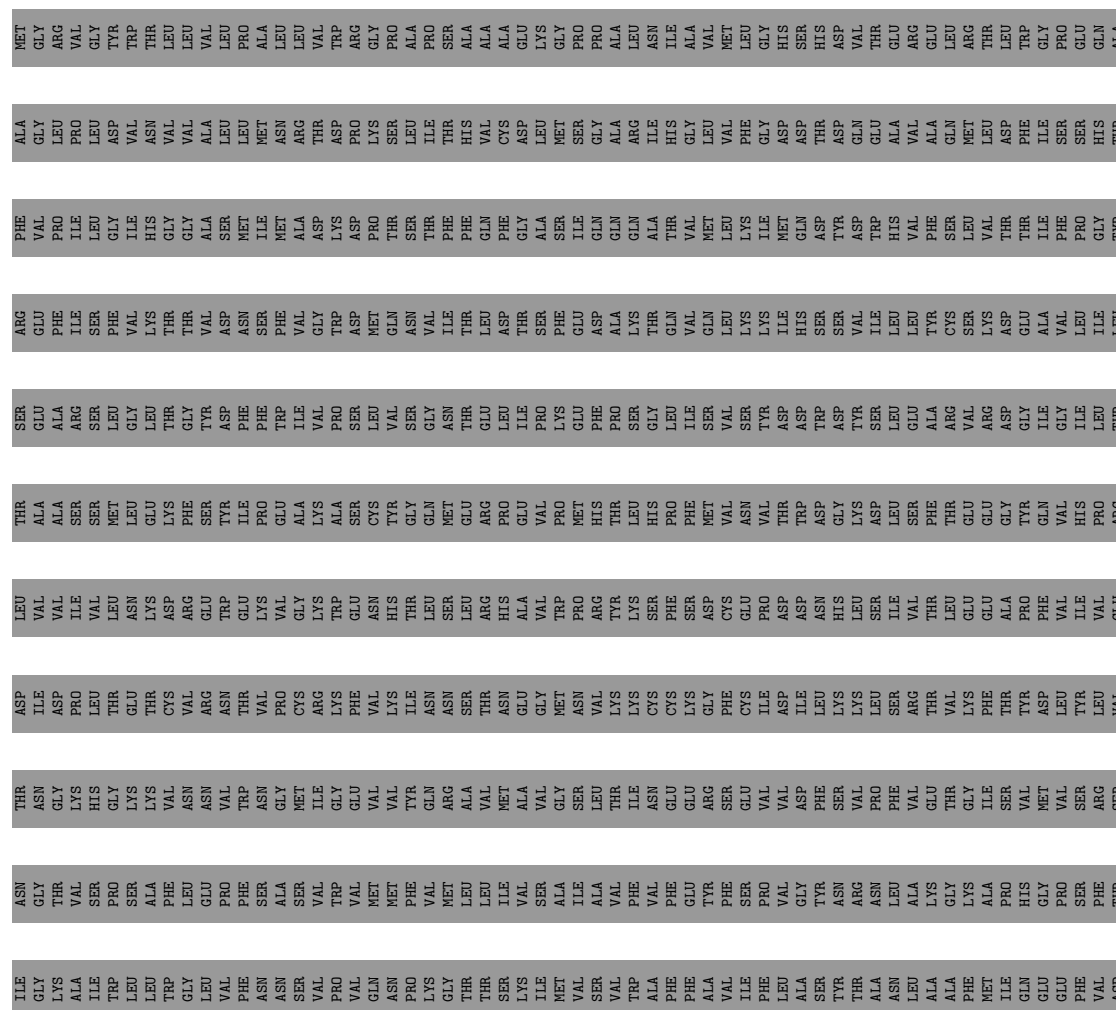
- Molecule 1: Calmodulin-1

Chain A:  38% 6% 54%



- Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain B:  99%





- Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain B: . 99%

[illegible]





SER	SER	TYR	SER
CYS	LEU	LYS	PHE
SER	ASN	HIS	SER
ARG	VAL	LEU	VAL
ARG	PRO	PRO	PRO
VAL	SER	SER	SER
TYR	GLN	GLN	SER
LYS	ALA	VAL	LYS
LYS	ASN	ASN	SER
MET	ASP	ASP	GLY
PRO	SER	SER	LYS
SER	ILE	TYR	LYS
ILE	GLU	LEU	SER
GLU	SER	ARG	SER
SER	ASP	SER	LEU
ASP	VAL	SER	PHE
VAL		LEU	PRO
		ARG	GLN
		ARG	GLY
		THR	LEU
		ALA	GLU
		SER	ASP
		ALA	SER
		TYR	LYS
		CYS	ARG
		SER	SER
		ARG	SER
		ASP	LYS
		SER	SER
		ARG	LEU
		GLY	LEU
		HIS	PRO
		ASN	ASP
		ASN	HIS
		VAL	THR
		THR	SER
		ILE	ASN
		TYR	LEU
		SER	HIS
		THR	SER
		PRO	HIS
		ARG	ARG
		VAL	LEU
		VAL	VAL
		LEU	ASP
		ASN	PRO

4.2.4 Score per residue for model 4

- Molecule 1: Calmodulin-1

Chain A: 35% 9% 1% 54%

[illegible]

- Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain B: . 99%

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







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

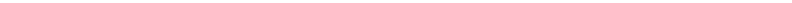
4.2.7 Score per residue for model 7

- Molecule 1: Calmodulin-1

Chain A:  37% 7% 54%

ASN	GLY	THR	ILE	ASP	PHE	PRO	GLU	PHE	LEU	THR	MET	MET	ALA	ARG	LYS	LYS	ASP	THR	D81	S82	ASP	ASP	E85	L106	R127	D132	Q136	Y139	F142	V143	Q144	M145	T147	A148	K149	ASN	GLY	THR	GLU	ALA	GLU	LEU	GLN	ASP	MET	GLY	THR	VAL	MET	ARG	SER	LEU	GLY	GLN	ASN	PRO	THR	GLU	ALA	GLU	LEU	GLN	ASP	ALA	ASP	GLY	THR	LYS	THR	THR	ILE	GLY	THR	GLY	ASP	GLY	ASP	ASP	LYS	ASP	ASP	LYS	ASP	LEU	SER	PHE	ALA	LYS	ARG	ALA	LYS	MET	LEU	THR	GLU	GLU	THR	THR	GLN	GLN	ASP	GLU	ASP	ALA	ALA	MET
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain B:  99%

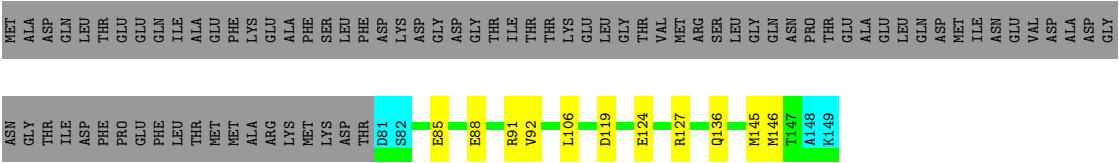
LEU	THR	SER	ARG	PHE	ALA	MET
VAL	ALA	GLU	GLU	VAL	GLY	GLY
VAL	ALA	ALA	PHE	PRO	LEU	ARG
ILE	SER	ARG	ILE	ILE	PRO	VAL
VAL	SER	SER	SER	LEU	LEU	GLY
ASN	MET	LEU	PHE	PHE	ASP	TYR
LEU	GLU	GLY	VAL	VAL	VAL	THR
LYS	LYS	LYS	LYS	HIS	ASN	THR
ASP	PHE	THR	THR	GLY	VAL	LEU
ARG	PHE	THR	THR	VAL	VAL	LEU
GLU	ILE	ASP	ASP	SER	ALA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



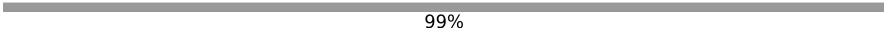
4.2.8 Score per residue for model 8

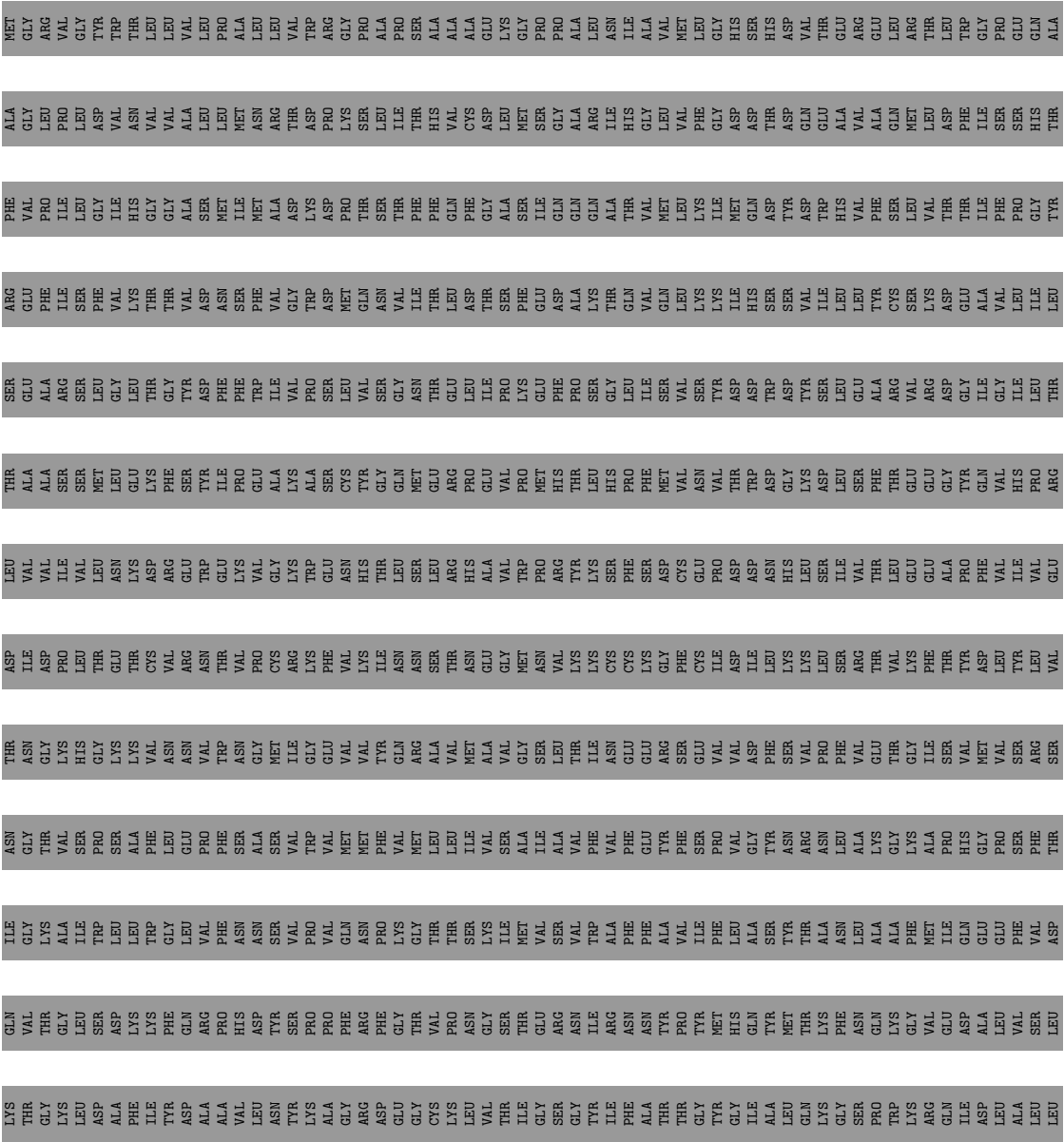
• Molecule 1: Calmodulin-1

Chain A:  36% 7% • 54%



• Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain B:  99%







[illegible]

4.2.10 Score per residue for model 10

- Molecule 1: Calmodulin-1

Chain A: 37% 7% 54%

[illegible]

- Molecule 2: Glutamate receptor ionotropic, NMDA 2A

Chain B: 99%

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



ASP	LEU
PRO	ASN
TYR	SER
LYS	CYS
HIS	SER
SER	ASN
LEU	ARG
PRO	ARG
SER	VAL
GLN	TYR
ALA	LYS
VAL	LYS
ASN	MET
ASP	PRO
SER	SER
TYR	ILE
LEU	GLU
ARG	SER
SER	ASP
SER	VAL
LEU	
ARG	
SER	
THR	
ALA	
SER	
TYR	
CYS	
SER	
ARG	
ASP	
SER	
ARG	
GLY	
HIS	
ASN	
ASP	
VAL	
TYR	
ILE	
SER	
GLU	
HIS	
VAL	
MET	
PRO	
TYR	
ALA	
ALA	
ASN	
LYS	
ASN	
ASN	
MET	
TYR	
SER	
THR	
PRO	
ARG	
VAL	

LEU
ASN
SER
CYS
SER
ASN
ARG
ARG
VAL
TYR
LYS
LYS
MET
PRO
SER
ILE
GLU
SER
ASP
VAL

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 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
HADDOCK	structure calculation	
HADDOCK	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	1097
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1097
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	525	483	483	4±1
2	B	102	109	109	1±1
All	All	6290	5920	5920	41

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:PHE:HA	1:A:145:MET:SD	0.65	2.32	7	1
1:A:124:GLU:OE2	1:A:127:ARG:HD2	0.58	1.98	5	4
1:A:146:MET:HE1	2:B:1014:TRP:HB3	0.54	1.80	2	4
1:A:100:TYR:CE1	1:A:138:ASN:HB3	0.53	2.39	9	1
1:A:88:GLU:O	1:A:92:VAL:HG23	0.49	2.08	1	6
1:A:83:GLU:HB2	1:A:87:ARG:NH2	0.49	2.23	4	3
1:A:116:LYS:HZ1	1:A:121:GLU:CD	0.48	2.17	3	1
1:A:124:GLU:HA	1:A:127:ARG:HD2	0.48	1.86	10	3
1:A:88:GLU:OE2	1:A:91:ARG:HD2	0.46	2.11	3	7
1:A:139:TYR:O	1:A:143:VAL:HG23	0.45	2.12	6	2
1:A:124:GLU:HA	1:A:124:GLU:OE2	0.44	2.12	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LYS:O	1:A:116:LYS:HE2	0.42	2.14	4	1
2:B:1015:LYS:O	2:B:1019:ASP:HB2	0.42	2.14	10	1
1:A:128:GLU:CD	2:B:1011:ARG:HH21	0.41	2.23	2	1
2:B:1014:TRP:CE3	2:B:1014:TRP:HA	0.41	2.51	10	1
1:A:142:PHE:O	1:A:145:MET:HG2	0.41	2.16	10	1
1:A:88:GLU:OE2	1:A:88:GLU:HA	0.40	2.16	3	1
1:A:145:MET:HB2	2:B:1011:ARG:NH1	0.40	2.31	8	1
1:A:145:MET:HE2	2:B:1014:TRP:CD1	0.40	2.51	6	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	65/149 (44%)	64±1 (99±2%)	1±1 (1±2%)	0±0 (0±0%)	100	100
2	B	11/1464 (1%)	11±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	760/16130 (5%)	751 (99%)	9 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	56/127 (44%)	52±2 (92±3%)	4±2 (8±3%)	13	60
2	B	12/1308 (1%)	10±1 (81±9%)	2±1 (19±9%)	3	34
All	All	680/14350 (5%)	612 (90%)	68 (10%)	9	54

All 22 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	106	LEU	10
2	B	1014	TRP	8
1	A	85	GLU	7
2	B	1016	LYS	7
1	A	147	THR	5
1	A	136	GLN	5
1	A	119	ASP	4
2	B	1020	SER	3
1	A	145	MET	3
1	A	84	GLU	2
2	B	1017	SER	2
2	B	1015	LYS	2
1	A	113	LEU	1
1	A	120	GLU	1
1	A	128	GLU	1
1	A	94	ASP	1
1	A	116	LYS	1
2	B	1019	ASP	1
1	A	108	HIS	1
1	A	127	ARG	1
1	A	132	ASP	1
1	A	110	MET	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1097
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	1097
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

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

- No matching atom found in the structure. All 1097 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	H	8.383	0.002	1
1	A	1	MET	HA	4.703	0.004	1
1	A	1	MET	HB2	2.697	0.008	1
1	A	1	MET	HB3	2.697	0.008	1
1	A	1	MET	C	176.553	0.000	1
1	A	1	MET	CA	54.602	0.183	1
1	A	1	MET	CB	41.397	0.044	1
1	A	1	MET	N	123.131	0.048	1
1	A	2	ALA	H	8.412	0.003	1
1	A	2	ALA	HA	4.456	0.004	1
1	A	2	ALA	HB1	3.955	0.002	1
1	A	2	ALA	HB2	4.069	0.009	1
1	A	2	ALA	HB3	3.955	0.002	1
1	A	2	ALA	C	175.434	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ALA	CA	59.052	0.100	1
1	A	2	ALA	CB	63.98	0.059	1
1	A	2	ALA	N	117.092	0.020	1
1	A	3	ASP	H	8.546	0.004	1
1	A	3	ASP	HA	4.63	0.005	1
1	A	3	ASP	HB2	2.694	0.004	2
1	A	3	ASP	HB3	2.55	0.005	2
1	A	3	ASP	HG2	2.344	0.000	1
1	A	3	ASP	HG3	2.344	0.000	1
1	A	3	ASP	C	175.609	0.000	1
1	A	3	ASP	CA	54.863	0.000	1
1	A	3	ASP	CB	41.448	0.044	1
1	A	3	ASP	CG	36.486	0.000	1
1	A	3	ASP	N	122.84	0.021	1
1	A	4	GLN	H	8.302	0.003	1
1	A	4	GLN	HA	4.379	0.004	1
1	A	4	GLN	HB2	1.972	0.011	2
1	A	4	GLN	HB3	2.088	0.003	2
1	A	4	GLN	HG2	2.351	0.000	1
1	A	4	GLN	HG3	2.351	0.000	1
1	A	4	GLN	C	175.593	0.000	1
1	A	4	GLN	CA	55.632	0.076	1
1	A	4	GLN	CB	29.832	0.064	1
1	A	4	GLN	CG	33.709	0.000	1
1	A	4	GLN	N	119.759	0.035	1
1	A	5	LEU	H	8.252	0.003	1
1	A	5	LEU	HA	4.665	0.006	1
1	A	5	LEU	HB2	1.728	0.006	2
1	A	5	LEU	HB3	1.513	0.005	2
1	A	5	LEU	HD11	0.946	0.000	1
1	A	5	LEU	HD12	0.946	0.000	1
1	A	5	LEU	HD13	0.946	0.000	1
1	A	5	LEU	HD21	0.948	0.000	1
1	A	5	LEU	HD22	0.948	0.000	1
1	A	5	LEU	HD23	0.948	0.000	1
1	A	5	LEU	C	177.663	0.000	1
1	A	5	LEU	CA	54.459	0.074	1
1	A	5	LEU	CB	43.609	0.038	1
1	A	5	LEU	CD1	23.764	0.005	1
1	A	5	LEU	CD2	26.854	0.006	1
1	A	5	LEU	CG	36.656	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LEU	N	123.145	0.032	1
1	A	6	THR	H	8.68	0.013	1
1	A	6	THR	HA	4.47	0.006	1
1	A	6	THR	HB	4.782	0.005	1
1	A	6	THR	HG12	1.773	0.004	1
1	A	6	THR	HG13	1.773	0.004	1
1	A	6	THR	HG21	1.333	0.003	1
1	A	6	THR	HG22	1.333	0.003	1
1	A	6	THR	HG23	1.333	0.003	1
1	A	6	THR	C	175.497	0.000	1
1	A	6	THR	CA	60.628	0.046	1
1	A	6	THR	CB	71.217	0.057	1
1	A	6	THR	CD1	12.878	0.000	1
1	A	6	THR	CG1	29.172	0.000	1
1	A	6	THR	CG2	21.842	0.038	1
1	A	6	THR	N	113.032	0.030	1
1	A	7	GLU	H	8.999	0.002	1
1	A	7	GLU	HA	3.978	0.005	1
1	A	7	GLU	HB2	2.053	0.005	1
1	A	7	GLU	HB3	2.053	0.005	1
1	A	7	GLU	HD2	3.009	0.000	1
1	A	7	GLU	HD3	3.009	0.000	1
1	A	7	GLU	HG2	2.371	0.000	1
1	A	7	GLU	HG3	2.371	0.000	1
1	A	7	GLU	C	179.48	0.000	1
1	A	7	GLU	CA	60.116	0.069	1
1	A	7	GLU	CB	29.226	0.052	1
1	A	7	GLU	CD	43.181	0.000	1
1	A	7	GLU	CG	36.565	0.000	1
1	A	7	GLU	N	120.471	0.020	1
1	A	8	GLU	H	8.714	0.003	1
1	A	8	GLU	HA	4.067	0.011	1
1	A	8	GLU	HB2	2.039	0.010	2
1	A	8	GLU	HB3	1.94	0.007	2
1	A	8	GLU	HG2	2.336	0.000	1
1	A	8	GLU	HG3	2.336	0.000	1
1	A	8	GLU	C	179.143	0.000	1
1	A	8	GLU	CA	60.051	0.022	1
1	A	8	GLU	CB	29.007	0.024	1
1	A	8	GLU	CG	36.805	0.000	1
1	A	8	GLU	N	119.462	0.013	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	9	GLN	H	7.714	0.002	1
1	A	9	GLN	HA	3.866	0.004	1
1	A	9	GLN	HB1	1.83	0.004	1
1	A	9	GLN	HB2	1.675	0.010	2
1	A	9	GLN	HB3	2.364	0.016	2
1	A	9	GLN	C	178.248	0.000	1
1	A	9	GLN	CA	58.658	0.000	1
1	A	9	GLN	CB	29.245	0.000	1
1	A	9	GLN	CG	34.914	0.000	1
1	A	9	GLN	N	120.357	0.055	1
1	A	10	ILE	H	8.365	0.001	1
1	A	10	ILE	HA	3.705	0.004	1
1	A	10	ILE	HB	1.962	0.006	1
1	A	10	ILE	HB2	3.024	0.006	1
1	A	10	ILE	HB3	3.024	0.006	1
1	A	10	ILE	HD1	6.585	0.002	1
1	A	10	ILE	HD11	0.865	0.000	1
1	A	10	ILE	HD12	0.865	0.000	1
1	A	10	ILE	HD13	0.865	0.000	1
1	A	10	ILE	HD2	6.585	0.002	1
1	A	10	ILE	HE1	7.001	0.000	1
1	A	10	ILE	HE2	7.001	0.000	1
1	A	10	ILE	HG12	1.815	0.000	1
1	A	10	ILE	HG13	1.815	0.000	1
1	A	10	ILE	HG21	1.118	0.000	1
1	A	10	ILE	HG22	1.118	0.000	1
1	A	10	ILE	HG23	1.118	0.000	1
1	A	10	ILE	C	177.778	0.000	1
1	A	10	ILE	CA	66.331	0.081	1
1	A	10	ILE	CB	37.805	0.032	1
1	A	10	ILE	CD1	13.006	0.071	1
1	A	10	ILE	CG1	30.199	0.000	1
1	A	10	ILE	CG2	17.459	0.012	1
1	A	10	ILE	N	119.53	0.034	1
1	A	11	ALA	H	7.985	0.003	1
1	A	11	ALA	HA	4.127	0.006	1
1	A	11	ALA	HB1	1.531	0.005	1
1	A	11	ALA	HB2	1.531	0.005	1
1	A	11	ALA	HB3	1.531	0.005	1
1	A	11	ALA	HD2	3.233	0.000	1
1	A	11	ALA	HD3	3.233	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	ALA	HG2	1.727	0.000	1
1	A	11	ALA	HG3	1.727	0.000	1
1	A	11	ALA	C	180.994	0.000	1
1	A	11	ALA	CA	55.569	0.025	1
1	A	11	ALA	CB	17.873	0.059	1
1	A	11	ALA	CD	43.579	0.000	1
1	A	11	ALA	CG	27.806	0.000	1
1	A	11	ALA	N	121.242	0.037	1
1	A	12	GLU	H	7.777	0.007	1
1	A	12	GLU	HA	4.146	0.007	1
1	A	12	GLU	HB	2.174	0.012	1
1	A	12	GLU	HB2	1.929	0.013	2
1	A	12	GLU	HB3	2.04	0.006	2
1	A	12	GLU	HG11	1.056	0.002	1
1	A	12	GLU	HG12	1.056	0.002	1
1	A	12	GLU	HG13	1.056	0.002	1
1	A	12	GLU	HG2	2.4	0.000	2
1	A	12	GLU	HG21	0.728	0.001	1
1	A	12	GLU	HG22	0.728	0.001	1
1	A	12	GLU	HG23	0.728	0.001	1
1	A	12	GLU	HG3	2.161	0.000	2
1	A	12	GLU	C	180.492	0.000	1
1	A	12	GLU	CA	59.467	0.072	1
1	A	12	GLU	CB	29.164	0.060	1
1	A	12	GLU	CG	35.926	0.000	1
1	A	12	GLU	CG1	22.825	0.009	1
1	A	12	GLU	CG2	21.12	0.022	1
1	A	12	GLU	N	119.685	0.042	1
1	A	13	PHE	H	8.583	0.008	1
1	A	13	PHE	HA	5.037	0.003	1
1	A	13	PHE	HB2	3.463	0.004	1
1	A	13	PHE	HB3	3.463	0.004	1
1	A	13	PHE	HD1	7.18	0.005	1
1	A	13	PHE	HD2	7.18	0.005	1
1	A	13	PHE	HE1	7.255	0.001	1
1	A	13	PHE	HE2	7.255	0.001	1
1	A	13	PHE	C	178.702	0.000	1
1	A	13	PHE	CA	59.239	0.049	1
1	A	13	PHE	CB	37.831	0.078	1
1	A	13	PHE	N	120.122	0.037	1
1	A	14	LYS	H	9.19	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	14	LYS	HA	4.033	0.005	1
1	A	14	LYS	HB2	1.942	0.002	1
1	A	14	LYS	HB3	1.942	0.002	1
1	A	14	LYS	C	179.361	0.000	1
1	A	14	LYS	CA	60.329	0.036	1
1	A	14	LYS	CB	31.945	0.072	1
1	A	14	LYS	N	123.535	0.045	1
1	A	15	GLU	H	7.796	0.009	1
1	A	15	GLU	HA	4.15	0.005	1
1	A	15	GLU	HB2	2.224	0.006	1
1	A	15	GLU	HB3	2.224	0.006	1
1	A	15	GLU	HG2	2.424	0.000	1
1	A	15	GLU	HG3	2.424	0.000	1
1	A	15	GLU	C	179.46	0.000	1
1	A	15	GLU	CA	59.476	0.081	1
1	A	15	GLU	CB	29.119	0.067	1
1	A	15	GLU	CG	35.982	0.000	1
1	A	15	GLU	N	120.383	0.053	1
1	A	16	ALA	H	8.009	0.006	1
1	A	16	ALA	HA	4.306	0.004	1
1	A	16	ALA	HB1	1.967	0.003	1
1	A	16	ALA	HB2	1.967	0.003	1
1	A	16	ALA	HB3	1.967	0.003	1
1	A	16	ALA	C	179.106	0.000	1
1	A	16	ALA	CA	55.431	0.084	1
1	A	16	ALA	CB	18.106	0.041	1
1	A	16	ALA	N	122.59	0.072	1
1	A	17	PHE	H	8.803	0.018	1
1	A	17	GLY	H	7.844	0.001	1
1	A	17	PHE	HA	3.238	0.014	1
1	A	17	GLY	HA2	3.855	0.006	1
1	A	17	GLY	HA3	3.855	0.006	1
1	A	17	PHE	HB2	2.952	0.007	1
1	A	17	PHE	HB3	2.952	0.007	1
1	A	17	PHE	HD1	6.637	0.014	1
1	A	17	PHE	HD2	6.637	0.014	1
1	A	17	PHE	HE1	7.02	0.000	1
1	A	17	PHE	HE2	7.02	0.000	1
1	A	17	PHE	C	177.317	0.000	1
1	A	17	GLY	C	175.141	0.000	1
1	A	17	PHE	CA	62.167	0.086	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	GLY	CA	47.209	0.044	1
1	A	17	PHE	CB	39.602	0.050	1
1	A	17	PHE	N	119.242	0.145	1
1	A	17	GLY	N	109.364	0.026	1
1	A	18	SER	H	7.92	0.016	1
1	A	18	SER	HA	4.152	0.014	1
1	A	18	SER	HB2	4.041	0.009	1
1	A	18	SER	HB3	4.041	0.009	1
1	A	18	SER	C	175.032	0.000	1
1	A	18	SER	CA	61.499	0.015	1
1	A	18	SER	CB	63.227	0.188	1
1	A	18	SER	N	112.646	0.045	1
1	A	19	LEU	H	7.44	0.012	1
1	A	19	GLY	H	10.683	0.002	1
1	A	19	LEU	HA	4.006	0.008	1
1	A	19	GLY	HA2	4.098	0.005	2
1	A	19	GLY	HA3	3.473	0.004	2
1	A	19	LEU	HB2	1.741	0.002	2
1	A	19	LEU	HB3	1.6	0.005	2
1	A	19	LEU	HD11	0.848	0.002	1
1	A	19	LEU	HD12	0.848	0.002	1
1	A	19	LEU	HD13	0.848	0.002	1
1	A	19	LEU	HD21	0.738	0.006	1
1	A	19	LEU	HD22	0.738	0.006	1
1	A	19	LEU	HD23	0.738	0.006	1
1	A	19	LEU	HG	1.474	0.000	1
1	A	19	LEU	C	178.063	0.000	1
1	A	19	GLY	C	172.792	0.000	1
1	A	19	LEU	CA	57.188	0.030	1
1	A	19	GLY	CA	45.01	0.051	1
1	A	19	LEU	CB	41.574	0.049	1
1	A	19	LEU	CD1	24.429	0.000	1
1	A	19	LEU	CD2	23.995	0.056	1
1	A	19	LEU	CG	26.659	0.000	1
1	A	19	LEU	N	120.875	0.065	1
1	A	19	GLY	N	112.82	0.023	1
1	A	20	PHE	H	7.331	0.008	1
1	A	20	PHE	HA	4.255	0.002	1
1	A	20	PHE	HB2	2.677	0.007	1
1	A	20	PHE	HB3	2.677	0.007	1
1	A	20	PHE	HD1	7.322	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	PHE	HD2	7.322	0.003	1
1	A	20	PHE	HE1	7.382	0.005	1
1	A	20	PHE	HE2	7.382	0.005	1
1	A	20	PHE	C	174.867	0.000	1
1	A	20	PHE	CA	59.455	0.069	1
1	A	20	PHE	CB	40.957	0.141	1
1	A	20	PHE	N	115.162	0.046	1
1	A	21	ASP	H	7.818	0.007	1
1	A	21	ASP	HA	4.549	0.000	1
1	A	21	ASP	HB	1.948	0.009	1
1	A	21	ASP	HB2	2.396	0.004	2
1	A	21	ASP	HB3	1.531	0.006	2
1	A	21	ASP	HD11	0.455	0.006	1
1	A	21	ASP	HD12	0.455	0.006	1
1	A	21	ASP	HD13	0.455	0.006	1
1	A	21	ASP	HG12	1.391	0.004	1
1	A	21	ASP	HG13	1.391	0.004	1
1	A	21	ASP	HG21	1.054	0.006	1
1	A	21	ASP	HG22	1.054	0.006	1
1	A	21	ASP	HG23	1.054	0.006	1
1	A	21	ASP	C	177.203	0.000	1
1	A	21	ASP	CA	52.556	0.000	1
1	A	21	ASP	CB	38.927	0.020	1
1	A	21	ASP	CD1	15.637	0.000	1
1	A	21	ASP	CG1	26.902	0.000	1
1	A	21	ASP	CG2	17.555	0.039	1
1	A	21	ASP	N	117.812	0.057	1
1	A	22	LYS	H	7.67	0.009	1
1	A	22	LYS	HA	3.972	0.005	1
1	A	22	LYS	HB2	1.879	0.006	1
1	A	22	LYS	HB3	1.879	0.006	1
1	A	22	LYS	C	178.132	0.000	1
1	A	22	LYS	CA	58.504	0.003	1
1	A	22	LYS	CB	32.609	0.001	1
1	A	22	LYS	N	124.245	0.057	1
1	A	23	ASP	H	8.079	0.004	1
1	A	23	ASP	HA	4.592	0.004	1
1	A	23	ASP	HB1	1.486	0.003	1
1	A	23	ASP	HB2	3.061	0.005	2
1	A	23	ASP	HB3	2.615	0.003	2
1	A	23	ASP	C	177.684	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	23	ASP	CA	52.935	0.013	1
1	A	23	ASP	CB	39.644	0.017	1
1	A	23	ASP	N	114.042	0.102	1
1	A	24	GLY	H	7.675	0.007	1
1	A	24	ALA	H	8.233	0.001	1
1	A	24	ALA	HA	4.045	0.004	1
1	A	24	GLY	HA2	3.854	0.007	2
1	A	24	GLY	HA3	3.984	0.000	2
1	A	24	ALA	HB1	1.431	0.005	1
1	A	24	ALA	HB2	1.431	0.005	1
1	A	24	ALA	HB3	1.431	0.005	1
1	A	24	GLY	C	175.152	0.000	1
1	A	24	ALA	C	181.439	0.000	1
1	A	24	GLY	CA	47.424	0.075	1
1	A	24	ALA	CA	55.338	0.064	1
1	A	24	ALA	CB	18.368	0.054	1
1	A	24	GLY	N	109.203	0.037	1
1	A	24	ALA	N	118.487	0.023	1
1	A	25	ASP	H	8.377	0.002	1
1	A	25	ASP	HA	4.504	0.013	1
1	A	25	ASP	HB2	3.048	0.015	2
1	A	25	ASP	HB3	2.461	0.005	2
1	A	25	ASP	HG2	2.356	0.000	1
1	A	25	ASP	HG3	2.356	0.000	1
1	A	25	ASP	C	177.458	0.000	1
1	A	25	ASP	CA	53.822	0.040	1
1	A	25	ASP	CB	40.391	0.152	1
1	A	25	ASP	CG	38.098	0.000	1
1	A	25	ASP	N	120.705	0.067	1
1	A	26	GLY	H	10.608	0.003	1
1	A	26	LEU	H	8.489	0.002	1
1	A	26	LEU	HA	4.1	0.012	1
1	A	26	GLY	HA2	3.692	0.007	2
1	A	26	GLY	HA3	4.361	0.004	2
1	A	26	LEU	HB2	1.858	0.007	2
1	A	26	LEU	HB3	1.458	0.006	2
1	A	26	LEU	HD11	0.951	0.018	1
1	A	26	LEU	HD12	0.951	0.018	1
1	A	26	LEU	HD13	0.951	0.018	1
1	A	26	LEU	HD21	0.689	0.008	1
1	A	26	LEU	HD22	0.689	0.008	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	26	LEU	HD23	0.689	0.008	1
1	A	26	GLY	C	173.714	0.000	1
1	A	26	LEU	C	178.435	0.000	1
1	A	26	GLY	CA	45.552	0.030	1
1	A	26	LEU	CA	58.31	0.049	1
1	A	26	LEU	CB	42.301	0.057	1
1	A	26	LEU	CD1	24.917	0.000	1
1	A	26	LEU	CD2	26.306	0.042	1
1	A	26	GLY	N	113.234	0.012	1
1	A	26	LEU	N	121.172	0.018	1
1	A	27	THR	H	8.135	0.018	1
1	A	27	THR	HA	5.295	0.003	1
1	A	27	THR	HB	3.86	0.004	1
1	A	27	THR	HB2	1.943	0.007	1
1	A	27	THR	HB3	1.943	0.007	1
1	A	27	THR	HG2	1.633	0.000	1
1	A	27	THR	HG21	1.046	0.001	1
1	A	27	THR	HG22	1.046	0.001	1
1	A	27	THR	HG23	1.046	0.001	1
1	A	27	THR	HG3	1.633	0.000	1
1	A	27	THR	C	172.951	0.000	1
1	A	27	THR	CA	59.912	0.035	1
1	A	27	THR	CB	72.661	0.048	1
1	A	27	THR	CG	27.971	0.000	1
1	A	27	THR	CG2	21.572	0.048	1
1	A	27	THR	N	112.741	0.117	1
1	A	28	ILE	H	9.771	0.012	1
1	A	28	ILE	HA	4.975	0.009	1
1	A	28	ILE	HB	1.821	0.005	1
1	A	28	ILE	HB2	3.369	0.000	1
1	A	28	ILE	HB3	3.242	0.007	1
1	A	28	ILE	HD11	0.293	0.022	1
1	A	28	ILE	HD12	0.293	0.022	1
1	A	28	ILE	HD13	0.293	0.022	1
1	A	28	ILE	HG12	1.174	0.017	1
1	A	28	ILE	HG13	1.174	0.017	1
1	A	28	ILE	HG21	0.869	0.004	1
1	A	28	ILE	HG22	0.869	0.004	1
1	A	28	ILE	HG23	0.869	0.004	1
1	A	28	ILE	C	176.079	0.000	1
1	A	28	ILE	CA	60.593	0.137	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	28	ILE	CB	39.659	0.064	1
1	A	28	ILE	CD1	15.201	0.073	1
1	A	28	ILE	CG1	26.887	0.000	1
1	A	28	ILE	CG2	17.664	0.032	1
1	A	28	ILE	N	126.909	0.042	1
1	A	29	THR	H	8.465	0.010	1
1	A	29	THR	HA	4.826	0.010	1
1	A	29	THR	HB	2.028	0.016	1
1	A	29	THR	HG11	0.921	0.003	1
1	A	29	THR	HG12	0.921	0.003	1
1	A	29	THR	HG13	0.921	0.003	1
1	A	29	THR	HG21	1.311	0.000	1
1	A	29	THR	HG22	1.311	0.000	1
1	A	29	THR	HG23	1.311	0.000	1
1	A	29	THR	C	176.617	0.000	1
1	A	29	THR	CA	59.808	0.026	1
1	A	29	THR	CB	72.431	0.057	1
1	A	29	THR	CG1	23.547	0.194	1
1	A	29	THR	CG2	21.971	0.017	1
1	A	29	THR	N	116.421	0.030	1
1	A	30	THR	H	9.071	0.007	1
1	A	30	THR	HA	3.794	0.006	1
1	A	30	THR	HB	4.202	0.001	1
1	A	30	THR	HB2	2.075	0.004	2
1	A	30	THR	HB3	1.897	0.008	2
1	A	30	THR	HG2	2.668	0.000	1
1	A	30	THR	HG21	1.277	0.000	1
1	A	30	THR	HG22	1.277	0.000	1
1	A	30	THR	HG23	1.277	0.000	1
1	A	30	THR	HG3	2.668	0.000	1
1	A	30	THR	C	177.208	0.000	1
1	A	30	THR	CA	66.422	0.190	1
1	A	30	THR	CB	68.001	0.003	1
1	A	30	THR	CG	32.219	0.000	1
1	A	30	THR	CG2	23.269	0.109	1
1	A	30	THR	N	112.889	0.067	1
1	A	31	LYS	H	7.665	0.004	1
1	A	31	LYS	HA	4.138	0.009	1
1	A	31	LYS	HB	4.261	0.007	1
1	A	31	LYS	HB2	1.831	0.009	1
1	A	31	LYS	HB3	1.831	0.009	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	31	LYS	HG2	1.492	0.000	1
1	A	31	LYS	HG21	1.233	0.001	1
1	A	31	LYS	HG22	1.233	0.001	1
1	A	31	LYS	HG23	1.233	0.001	1
1	A	31	LYS	HG3	1.492	0.000	1
1	A	31	LYS	C	179.87	0.000	1
1	A	31	LYS	CA	59.229	0.032	1
1	A	31	LYS	CB	32.708	0.000	1
1	A	31	LYS	CG	24.943	0.000	1
1	A	31	LYS	CG2	21.46	0.055	1
1	A	31	LYS	N	120.679	0.032	1
1	A	32	GLU	H	7.652	0.009	1
1	A	32	GLU	HA	4.067	0.006	1
1	A	32	GLU	HB2	2.58	0.009	2
1	A	32	GLU	HB3	2.386	0.009	2
1	A	32	GLU	C	179.059	0.000	1
1	A	32	GLU	CA	59.451	0.117	1
1	A	32	GLU	CB	29.875	0.069	1
1	A	32	GLU	CG	38.169	0.000	1
1	A	32	GLU	N	121.547	0.063	1
1	A	33	LEU	H	8.686	0.005	1
1	A	33	LEU	HA	4.089	0.007	1
1	A	33	LEU	HB2	1.866	0.007	2
1	A	33	LEU	HB3	1.531	0.006	2
1	A	33	LEU	HD11	0.861	0.006	1
1	A	33	LEU	HD12	0.861	0.006	1
1	A	33	LEU	HD13	0.861	0.006	1
1	A	33	LEU	HD21	0.862	0.000	1
1	A	33	LEU	HD22	0.862	0.000	1
1	A	33	LEU	HD23	0.862	0.000	1
1	A	33	LEU	C	178.951	0.000	1
1	A	33	LEU	CA	58.172	0.095	1
1	A	33	LEU	CB	42.722	0.045	1
1	A	33	LEU	CD1	23.747	0.026	1
1	A	33	LEU	CD2	25.954	0.078	1
1	A	33	LEU	N	120.647	0.081	1
1	A	34	GLY	H	8.613	0.002	1
1	A	34	GLY	HA2	3.58	0.005	2
1	A	34	GLY	HA3	3.979	0.005	2
1	A	34	GLY	C	175.214	0.000	1
1	A	34	GLY	CA	48.501	0.030	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	34	GLY	N	105.403	0.042	1
1	A	35	THR	H	7.872	0.003	1
1	A	35	THR	HA	3.928	0.007	1
1	A	35	THR	HB	4.317	0.004	1
1	A	35	THR	HB2	1.613	0.000	2
1	A	35	THR	HB3	1.868	0.000	2
1	A	35	THR	HG21	1.281	0.001	1
1	A	35	THR	HG22	1.281	0.001	1
1	A	35	THR	HG23	1.281	0.001	1
1	A	35	THR	C	177.128	0.000	1
1	A	35	THR	CA	66.927	0.011	1
1	A	35	THR	CB	68.724	0.142	1
1	A	35	THR	CG2	21.63	0.044	1
1	A	35	THR	N	117.978	0.076	1
1	A	36	VAL	H	7.643	0.007	1
1	A	36	VAL	HA	3.482	0.005	1
1	A	36	VAL	HB	1.966	0.005	1
1	A	36	VAL	HB2	1.726	0.017	1
1	A	36	VAL	HB3	1.726	0.017	1
1	A	36	VAL	HG11	0.67	0.000	1
1	A	36	VAL	HG12	0.67	0.000	1
1	A	36	VAL	HG13	0.67	0.000	1
1	A	36	VAL	HG2	1.319	0.000	1
1	A	36	VAL	HG21	0.418	0.010	1
1	A	36	VAL	HG22	0.418	0.010	1
1	A	36	VAL	HG23	0.418	0.010	1
1	A	36	VAL	HG3	1.319	0.000	1
1	A	36	VAL	C	175.448	0.000	1
1	A	36	VAL	CA	66.414	0.107	1
1	A	36	VAL	CB	31.34	0.000	1
1	A	36	VAL	CG	24.466	0.000	1
1	A	36	VAL	CG1	22.861	0.014	1
1	A	36	VAL	CG2	20.579	0.002	1
1	A	36	VAL	N	122.195	0.031	1
1	A	37	MET	H	8.455	0.006	1
1	A	37	MET	HA	4.106	0.012	1
1	A	37	MET	HB2	2.012	0.008	2
1	A	37	MET	HB3	1.866	0.003	2
1	A	37	MET	HD11	0.691	0.006	1
1	A	37	MET	HD12	0.691	0.006	1
1	A	37	MET	HD13	0.691	0.006	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	37	MET	HD21	0.72	0.008	1
1	A	37	MET	HD22	0.72	0.008	1
1	A	37	MET	HD23	0.72	0.008	1
1	A	37	MET	HE1	1.987	0.002	1
1	A	37	MET	HE2	1.987	0.002	1
1	A	37	MET	HE3	1.987	0.002	1
1	A	37	MET	HG2	2.67	0.010	1
1	A	37	MET	HG3	2.67	0.010	1
1	A	37	MET	C	179.166	0.000	1
1	A	37	MET	CA	59.183	0.077	1
1	A	37	MET	CB	31.454	0.072	1
1	A	37	MET	CD1	27.44	0.067	1
1	A	37	MET	CD2	23.905	0.000	1
1	A	37	MET	CE	17.495	0.000	1
1	A	37	MET	CG	32.929	0.000	1
1	A	37	MET	N	118.479	0.039	1
1	A	38	ARG	H	8.465	0.007	1
1	A	38	ARG	HA	4.809	0.004	1
1	A	38	ARG	HB	4.742	0.007	1
1	A	38	ARG	HB2	1.919	0.009	1
1	A	38	ARG	HB3	1.919	0.009	1
1	A	38	ARG	HD2	3.309	0.000	1
1	A	38	ARG	HD3	3.309	0.000	1
1	A	38	ARG	HG21	1.331	0.000	1
1	A	38	ARG	HG22	1.331	0.000	1
1	A	38	ARG	HG23	1.331	0.000	1
1	A	38	ARG	C	181.219	0.000	1
1	A	38	ARG	CA	59.225	0.078	1
1	A	38	ARG	CB	30.002	0.059	1
1	A	38	ARG	CD	43.492	0.000	1
1	A	38	ARG	CG	29.325	0.000	1
1	A	38	ARG	CG2	21.878	0.000	1
1	A	38	ARG	N	118.92	0.043	1
1	A	39	SER	H	7.916	0.006	1
1	A	39	SER	HA	4.414	0.005	1
1	A	39	SER	HB2	4.097	0.008	1
1	A	39	SER	HB3	4.097	0.008	1
1	A	39	SER	C	174.991	0.000	1
1	A	39	SER	CA	61.578	0.108	1
1	A	39	SER	CB	62.843	0.077	1
1	A	39	SER	N	118.805	0.018	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	40	LEU	H	7.406	0.004	1
1	A	40	LEU	HA	4.501	0.007	1
1	A	40	LEU	HB2	1.909	0.011	2
1	A	40	LEU	HB3	1.793	0.007	2
1	A	40	LEU	HD11	0.847	0.000	1
1	A	40	LEU	HD12	0.847	0.000	1
1	A	40	LEU	HD13	0.847	0.000	1
1	A	40	LEU	HD21	0.852	0.000	1
1	A	40	LEU	HD22	0.852	0.000	1
1	A	40	LEU	HD23	0.852	0.000	1
1	A	40	LEU	C	177.55	0.000	1
1	A	40	LEU	CA	54.665	0.070	1
1	A	40	LEU	CB	42.042	0.099	1
1	A	40	LEU	CD1	25.64	0.023	1
1	A	40	LEU	CD2	22.366	0.041	1
1	A	40	LEU	N	120.938	0.062	1
1	A	41	GLY	H	7.858	0.002	1
1	A	41	GLY	HA2	3.794	0.005	2
1	A	41	GLY	HA3	4.282	0.006	2
1	A	41	GLY	C	174.421	0.000	1
1	A	41	GLY	CA	45.63	0.023	1
1	A	41	GLY	N	106.903	0.058	1
1	A	42	GLN	H	7.78	0.002	1
1	A	42	GLN	HA	4.488	0.006	1
1	A	42	GLN	HB	2.191	0.007	1
1	A	42	GLN	HB2	1.656	0.007	2
1	A	42	GLN	HB3	2.127	0.009	2
1	A	42	GLN	HG11	0.875	0.002	1
1	A	42	GLN	HG12	0.875	0.002	1
1	A	42	GLN	HG13	0.875	0.002	1
1	A	42	GLN	HG2	2.244	0.000	1
1	A	42	GLN	HG21	0.962	0.000	1
1	A	42	GLN	HG22	0.962	0.000	1
1	A	42	GLN	HG23	0.962	0.000	1
1	A	42	GLN	HG3	2.244	0.000	1
1	A	42	GLN	C	174.17	0.000	1
1	A	42	GLN	CA	54.551	0.116	1
1	A	42	GLN	CB	30.593	0.054	1
1	A	42	GLN	CG	33.877	0.000	1
1	A	42	GLN	CG1	23.622	0.007	1
1	A	42	GLN	CG2	22.005	0.019	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	42	GLN	N	118.43	0.127	1
1	A	43	ASN	H	8.688	0.010	1
1	A	43	ASN	HA	5.179	0.000	1
1	A	43	ASN	HB2	2.786	0.000	2
1	A	43	ASN	HB3	2.514	0.000	2
1	A	43	ASN	C	179.121	0.000	1
1	A	43	ASN	CA	51.442	0.000	1
1	A	43	ASN	CB	39.228	0.000	1
1	A	43	ASN	N	116.472	0.027	1
1	A	44	PRO	H	8.226	0.002	1
1	A	44	PRO	HA	4.764	0.003	1
1	A	44	PRO	HB2	2.23	0.007	2
1	A	44	PRO	HB3	1.943	0.004	2
1	A	44	PRO	HG2	2.473	0.000	1
1	A	44	PRO	HG3	2.473	0.000	1
1	A	44	PRO	C	177.782	0.000	1
1	A	44	PRO	CA	62.467	0.049	1
1	A	44	PRO	CB	31.986	0.060	1
1	A	44	PRO	CG	27.422	0.000	1
1	A	44	PRO	N	119.491	0.047	1
1	A	45	THR	H	8.737	0.017	1
1	A	45	THR	HA	4.445	0.005	1
1	A	45	THR	HB	4.711	0.012	1
1	A	45	THR	HB2	2.214	0.000	2
1	A	45	THR	HB3	2.023	0.000	2
1	A	45	THR	HG21	1.365	0.001	1
1	A	45	THR	HG22	1.365	0.001	1
1	A	45	THR	HG23	1.365	0.001	1
1	A	45	THR	C	175.202	0.000	1
1	A	45	THR	CA	60.693	0.048	1
1	A	45	THR	CB	71.147	0.055	1
1	A	45	THR	CG2	21.929	0.013	1
1	A	45	THR	N	112.976	0.026	1
1	A	46	GLU	H	8.782	0.002	1
1	A	46	GLU	HA	3.979	0.007	1
1	A	46	GLU	HB	2.345	0.007	1
1	A	46	GLU	HB2	2.049	0.005	1
1	A	46	GLU	HB3	2.049	0.005	1
1	A	46	GLU	HD11	0.809	0.009	1
1	A	46	GLU	HD12	0.809	0.009	1
1	A	46	GLU	HD13	0.809	0.009	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	46	GLU	HG12	1.507	0.005	1
1	A	46	GLU	HG13	1.507	0.005	1
1	A	46	GLU	HG2	2.345	0.000	1
1	A	46	GLU	HG21	0.786	0.003	1
1	A	46	GLU	HG22	0.786	0.003	1
1	A	46	GLU	HG23	0.786	0.003	1
1	A	46	GLU	HG3	2.345	0.000	1
1	A	46	GLU	C	179.008	0.000	1
1	A	46	GLU	CA	60.149	0.056	1
1	A	46	GLU	CB	28.989	0.056	1
1	A	46	GLU	CD1	10.367	0.083	1
1	A	46	GLU	CG	36.277	0.000	1
1	A	46	GLU	CG2	16.351	0.045	1
1	A	46	GLU	N	120.569	0.033	1
1	A	47	ALA	H	8.22	0.008	1
1	A	47	ALA	HA	4.111	0.004	1
1	A	47	ALA	HB1	1.399	0.004	1
1	A	47	ALA	HB2	1.399	0.004	1
1	A	47	ALA	HB3	1.399	0.004	1
1	A	47	ALA	HG2	1.721	0.000	1
1	A	47	ALA	HG3	1.721	0.000	1
1	A	47	ALA	C	180.148	0.000	1
1	A	47	ALA	CA	55.138	0.022	1
1	A	47	ALA	CB	18.25	0.029	1
1	A	47	ALA	CG	27.965	0.000	1
1	A	47	ALA	N	120.808	0.048	1
1	A	48	GLU	H	7.671	0.002	1
1	A	48	GLU	HA	4.029	0.001	1
1	A	48	GLU	HB2	2.322	0.005	2
1	A	48	GLU	HB3	1.912	0.004	2
1	A	48	GLU	C	180.132	0.000	1
1	A	48	GLU	CA	59.142	0.071	1
1	A	48	GLU	CB	29.827	0.037	1
1	A	48	GLU	CG	37.353	0.000	1
1	A	48	GLU	N	118.682	0.019	1
1	A	49	LEU	H	8.142	0.006	1
1	A	49	LEU	HA	4.077	0.012	1
1	A	49	LEU	HB1	1.175	0.006	1
1	A	49	LEU	HB2	2.049	0.005	2
1	A	49	LEU	HB3	1.276	0.009	2
1	A	49	LEU	HD11	0.812	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	LEU	HD12	0.812	0.000	1
1	A	49	LEU	HD13	0.812	0.000	1
1	A	49	LEU	HD21	0.828	0.011	1
1	A	49	LEU	HD22	0.828	0.011	1
1	A	49	LEU	HD23	0.828	0.011	1
1	A	49	LEU	HG	1.768	0.000	1
1	A	49	LEU	C	178.482	0.000	1
1	A	49	LEU	CA	57.941	0.077	1
1	A	49	LEU	CB	42.37	0.034	1
1	A	49	LEU	CD1	25.904	0.078	1
1	A	49	LEU	CD2	23.545	0.050	1
1	A	49	LEU	N	120.279	0.044	1
1	A	50	GLN	H	8.137	0.005	1
1	A	50	GLN	HA	3.839	0.004	1
1	A	50	GLN	HB2	2.179	0.007	1
1	A	50	GLN	HB3	2.179	0.007	1
1	A	50	GLN	HG2	2.439	0.000	1
1	A	50	GLN	HG3	2.439	0.000	1
1	A	50	GLN	C	178.489	0.000	1
1	A	50	GLN	CA	58.629	0.033	1
1	A	50	GLN	CB	28.197	0.049	1
1	A	50	GLN	CG	34.121	0.000	1
1	A	50	GLN	N	118.251	0.028	1
1	A	51	ASP	H	8.076	0.005	1
1	A	51	ASP	HA	4.422	0.004	1
1	A	51	ASP	HB	1.964	0.006	1
1	A	51	ASP	HB2	2.802	0.003	2
1	A	51	ASP	HB3	2.666	0.012	2
1	A	51	ASP	HD11	0.867	0.001	1
1	A	51	ASP	HD12	0.867	0.001	1
1	A	51	ASP	HD13	0.867	0.001	1
1	A	51	ASP	HG12	1.281	0.013	2
1	A	51	ASP	HG13	1.668	0.006	2
1	A	51	ASP	HG21	0.924	0.001	1
1	A	51	ASP	HG22	0.924	0.001	1
1	A	51	ASP	HG23	0.924	0.001	1
1	A	51	ASP	C	178.726	0.000	1
1	A	51	ASP	CA	57.562	0.098	1
1	A	51	ASP	CB	40.298	0.048	1
1	A	51	ASP	CD1	12.576	0.000	1
1	A	51	ASP	CG1	27.777	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	ASP	CG2	17.377	0.005	1
1	A	51	ASP	N	119.967	0.017	1
1	A	52	MET	H	7.86	0.004	1
1	A	52	MET	HA	4.039	0.009	1
1	A	52	MET	HB2	2.288	0.008	2
1	A	52	MET	HB3	1.976	0.009	2
1	A	52	MET	HE1	2.034	0.001	1
1	A	52	MET	HE2	2.034	0.001	1
1	A	52	MET	HE3	2.034	0.001	1
1	A	52	MET	HG2	2.537	0.000	1
1	A	52	MET	HG3	2.537	0.000	1
1	A	52	MET	C	178.898	0.000	1
1	A	52	MET	CA	59.512	0.117	1
1	A	52	MET	CB	32.609	0.000	1
1	A	52	MET	CE	17.313	0.000	1
1	A	52	MET	N	119.338	0.018	1
1	A	53	ILE	H	7.718	0.003	1
1	A	53	GLY	H	7.627	0.002	1
1	A	53	ILE	HA	3.517	0.005	1
1	A	53	GLY	HA2	3.82	0.000	2
1	A	53	GLY	HA3	3.982	0.000	2
1	A	53	ILE	HB	1.945	0.014	1
1	A	53	ILE	HD11	0.744	0.000	1
1	A	53	ILE	HD12	0.744	0.000	1
1	A	53	ILE	HD13	0.744	0.000	1
1	A	53	ILE	HG12	1.673	0.000	2
1	A	53	ILE	HG13	1.015	0.000	2
1	A	53	ILE	HG21	0.707	0.000	1
1	A	53	ILE	HG22	0.707	0.000	1
1	A	53	ILE	HG23	0.707	0.000	1
1	A	53	ILE	C	177.746	0.000	1
1	A	53	ILE	CA	64.943	0.046	1
1	A	53	GLY	CA	47.506	0.000	1
1	A	53	ILE	CB	37.283	0.029	1
1	A	53	ILE	CD1	13.039	0.058	1
1	A	53	ILE	CG1	29.05	0.000	1
1	A	53	ILE	CG2	16.102	0.017	1
1	A	53	ILE	N	118.301	0.060	1
1	A	53	GLY	N	108.615	0.019	1
1	A	54	ASN	H	8.546	0.004	1
1	A	54	ASN	HA	4.378	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	ASN	HB2	2.989	0.005	2
1	A	54	ASN	HB3	2.882	0.014	2
1	A	54	ASN	C	177.391	0.000	1
1	A	54	ASN	CA	56.043	0.044	1
1	A	54	ASN	CB	38.069	0.021	1
1	A	54	ASN	N	117.726	0.030	1
1	A	55	GLU	H	7.586	0.003	1
1	A	55	GLY	H	10.223	0.001	1
1	A	55	GLU	HA	4.037	0.005	1
1	A	55	GLY	HA2	3.439	0.008	2
1	A	55	GLY	HA3	4.051	0.008	2
1	A	55	GLU	HB2	2.141	0.004	2
1	A	55	GLU	HB3	2.011	0.005	2
1	A	55	GLU	HG2	2.436	0.000	2
1	A	55	GLU	HG3	2.27	0.000	2
1	A	55	GLU	C	177.577	0.000	1
1	A	55	GLY	C	172.796	0.000	1
1	A	55	GLU	CA	58.923	0.000	1
1	A	55	GLY	CA	46.005	0.056	1
1	A	55	GLU	CB	30.379	0.000	1
1	A	55	GLU	CG	36.229	0.000	1
1	A	55	GLU	N	116.424	0.025	1
1	A	55	GLY	N	112.653	0.017	1
1	A	56	VAL	H	7.228	0.003	1
1	A	56	VAL	HA	4.471	0.007	1
1	A	56	VAL	HB	2.392	0.004	1
1	A	56	VAL	HB2	1.769	0.002	2
1	A	56	VAL	HB3	2.05	0.002	2
1	A	56	VAL	HG11	0.811	0.002	1
1	A	56	VAL	HG12	0.811	0.002	1
1	A	56	VAL	HG13	0.811	0.002	1
1	A	56	VAL	HG21	0.903	0.005	1
1	A	56	VAL	HG22	0.903	0.005	1
1	A	56	VAL	HG23	0.903	0.005	1
1	A	56	VAL	C	175.777	0.000	1
1	A	56	VAL	CA	60.865	0.078	1
1	A	56	VAL	CB	32.723	0.086	1
1	A	56	VAL	CG1	21.765	0.035	1
1	A	56	VAL	CG2	19.408	0.048	1
1	A	56	VAL	N	108.413	0.021	1
1	A	57	ASP	H	7.68	0.010	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	57	ASP	HA	4.648	0.004	1
1	A	57	ASP	HB	2.35	0.005	1
1	A	57	ASP	HB2	2.75	0.003	2
1	A	57	ASP	HB3	2.567	0.002	2
1	A	57	ASP	HG11	1.111	0.006	1
1	A	57	ASP	HG12	1.111	0.006	1
1	A	57	ASP	HG13	1.111	0.006	1
1	A	57	ASP	HG21	1.072	0.003	1
1	A	57	ASP	HG22	1.072	0.003	1
1	A	57	ASP	HG23	1.072	0.003	1
1	A	57	ASP	C	176.265	0.000	1
1	A	57	ASP	CA	53.81	0.094	1
1	A	57	ASP	CB	40.196	0.027	1
1	A	57	ASP	CG1	22.771	0.018	1
1	A	57	ASP	CG2	21.532	0.063	1
1	A	57	ASP	N	121.825	0.052	1
1	A	58	ALA	H	8.459	0.016	1
1	A	58	ALA	HA	4.199	0.005	1
1	A	58	ALA	HB1	1.527	0.004	1
1	A	58	ALA	HB2	1.527	0.004	1
1	A	58	ALA	HB3	1.527	0.004	1
1	A	58	ALA	C	178.643	0.000	1
1	A	58	ALA	CA	54.392	0.012	1
1	A	58	ALA	CB	19.502	0.085	1
1	A	58	ALA	N	131.719	0.014	1
1	A	59	ASP	H	8.155	0.011	1
1	A	59	ASP	HA	4.64	0.007	1
1	A	59	ASP	HB2	3.038	0.004	2
1	A	59	ASP	HB3	2.652	0.009	2
1	A	59	ASP	HD1	6.297	0.002	1
1	A	59	ASP	HD2	6.297	0.002	1
1	A	59	ASP	HE1	6.521	0.000	1
1	A	59	ASP	HE2	6.521	0.000	1
1	A	59	ASP	C	177.851	0.000	1
1	A	59	ASP	CA	52.763	0.042	1
1	A	59	ASP	CB	39.823	0.032	1
1	A	59	ASP	N	113.759	0.060	1
1	A	60	GLY	H	7.567	0.003	1
1	A	60	GLU	H	8.034	0.003	1
1	A	60	GLU	HA	3.616	0.008	1
1	A	60	GLY	HA2	3.886	0.010	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	GLY	HA3	3.808	0.008	2
1	A	60	GLU	HB2	2.057	0.006	2
1	A	60	GLU	HB3	1.925	0.002	2
1	A	60	GLU	HG2	2.303	0.000	1
1	A	60	GLU	HG3	2.303	0.000	1
1	A	60	GLY	C	174.942	0.000	1
1	A	60	GLU	C	180.128	0.000	1
1	A	60	GLY	CA	47.315	0.051	1
1	A	60	GLU	CA	60.237	0.028	1
1	A	60	GLU	CB	28.859	0.059	1
1	A	60	GLU	CG	36.938	0.000	1
1	A	60	GLY	N	108.321	0.037	1
1	A	60	GLU	N	118.516	0.018	1
1	A	61	ASN	H	8.07	0.004	1
1	A	61	ASN	HA	4.643	0.006	1
1	A	61	ASN	HB2	3.306	0.004	2
1	A	61	ASN	HB3	2.65	0.004	2
1	A	61	ASN	C	176.863	0.000	1
1	A	61	ASN	CA	52.599	0.058	1
1	A	61	ASN	CB	37.727	0.083	1
1	A	61	ASN	CG	37.237	0.000	1
1	A	61	ASN	N	118.395	0.034	1
1	A	62	GLY	H	10.581	0.008	1
1	A	62	PHE	H	8.487	0.002	1
1	A	62	PHE	HA	3.523	0.007	1
1	A	62	GLY	HA2	3.495	0.005	2
1	A	62	GLY	HA3	4.198	0.006	2
1	A	62	PHE	HB2	3.225	0.007	2
1	A	62	PHE	HB3	2.982	0.008	2
1	A	62	PHE	HD1	6.676	0.002	1
1	A	62	PHE	HD2	6.676	0.002	1
1	A	62	PHE	HE1	6.972	0.017	1
1	A	62	PHE	HE2	6.972	0.017	1
1	A	62	GLY	C	173.29	0.000	1
1	A	62	PHE	C	176.774	0.000	1
1	A	62	GLY	CA	45.823	0.061	1
1	A	62	PHE	CA	61.857	0.087	1
1	A	62	PHE	CB	40.101	0.059	1
1	A	62	GLY	N	113.454	0.018	1
1	A	62	PHE	N	123.433	0.031	1
1	A	63	THR	H	7.681	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	63	THR	HA	4.756	0.006	1
1	A	63	THR	HB	4.016	0.004	1
1	A	63	THR	HG11	0.451	0.002	1
1	A	63	THR	HG12	0.451	0.002	1
1	A	63	THR	HG13	0.451	0.002	1
1	A	63	THR	HG21	1.115	0.003	1
1	A	63	THR	HG22	1.115	0.003	1
1	A	63	THR	HG23	1.115	0.003	1
1	A	63	THR	C	173.191	0.000	1
1	A	63	THR	CA	59.623	0.061	1
1	A	63	THR	CB	72.048	0.087	1
1	A	63	THR	CG1	23.003	0.106	1
1	A	63	THR	CG2	22.356	0.071	1
1	A	63	THR	N	108.982	0.098	1
1	A	64	ILE	H	8.916	0.011	1
1	A	64	ILE	HA	5.179	0.004	1
1	A	64	ILE	HB	2.074	0.007	1
1	A	64	ILE	HB2	2.033	0.007	1
1	A	64	ILE	HB3	2.033	0.007	1
1	A	64	ILE	HD11	0.819	0.008	1
1	A	64	ILE	HD12	0.819	0.008	1
1	A	64	ILE	HD13	0.819	0.008	1
1	A	64	ILE	HG12	1.569	0.005	1
1	A	64	ILE	HG13	1.569	0.005	1
1	A	64	ILE	HG2	2.379	0.000	1
1	A	64	ILE	HG21	1.211	0.011	1
1	A	64	ILE	HG22	1.211	0.011	1
1	A	64	ILE	HG23	1.211	0.011	1
1	A	64	ILE	HG3	2.379	0.000	1
1	A	64	ILE	C	175.519	0.000	1
1	A	64	ILE	CA	60.003	0.004	1
1	A	64	ILE	CB	39.693	0.080	1
1	A	64	ILE	CD1	13.622	0.013	1
1	A	64	ILE	CG	34.095	0.000	1
1	A	64	ILE	CG1	27.334	0.000	1
1	A	64	ILE	CG2	18.376	0.006	1
1	A	64	ILE	N	123.926	0.026	1
1	A	65	ASP	H	8.816	0.004	1
1	A	65	ASP	HA	5.365	0.004	1
1	A	65	ASP	HB2	3.1	0.006	2
1	A	65	ASP	HB3	2.838	0.002	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	65	ASP	C	176.356	0.000	1
1	A	65	ASP	CA	52.268	0.085	1
1	A	65	ASP	CB	42.26	0.025	1
1	A	65	ASP	N	128.211	0.035	1
1	A	66	PHE	H	8.915	0.003	1
1	A	66	PHE	HA	4.001	0.000	1
1	A	66	PHE	HB2	2.842	0.015	2
1	A	66	PHE	HB3	2.155	0.009	2
1	A	66	PHE	HD1	6.756	0.011	1
1	A	66	PHE	HD2	6.756	0.011	1
1	A	66	PHE	HE1	7.206	0.000	1
1	A	66	PHE	HE2	7.206	0.000	1
1	A	66	PHE	C	177.877	0.000	1
1	A	66	PHE	CA	63.502	0.000	1
1	A	66	PHE	CB	36.017	0.080	1
1	A	66	PHE	N	118.744	0.072	1
1	A	67	PRO	H	7.627	0.003	1
1	A	67	PRO	HA	3.892	0.001	1
1	A	67	PRO	HB2	2.243	0.012	2
1	A	67	PRO	HB3	1.918	0.000	2
1	A	67	PRO	HG21	1.138	0.001	1
1	A	67	PRO	HG22	1.138	0.001	1
1	A	67	PRO	HG23	1.138	0.001	1
1	A	67	PRO	C	180.08	0.000	1
1	A	67	PRO	CA	66.655	0.163	1
1	A	67	PRO	CB	30.615	0.167	1
1	A	67	PRO	CG	28.185	0.000	1
1	A	67	PRO	CG2	21.298	0.077	1
1	A	67	PRO	N	109.153	0.042	1
1	A	68	GLU	H	7.916	0.008	1
1	A	68	GLU	HA	4.111	0.005	1
1	A	68	GLU	HB1	1.413	0.003	1
1	A	68	GLU	HB2	2.584	0.013	2
1	A	68	GLU	HB3	2.073	0.009	2
1	A	68	GLU	HG2	2.929	0.000	1
1	A	68	GLU	HG3	2.929	0.000	1
1	A	68	GLU	C	178.793	0.000	1
1	A	68	GLU	CA	58.783	0.054	1
1	A	68	GLU	CB	29.55	0.070	1
1	A	68	GLU	CG	36.881	0.000	1
1	A	68	GLU	N	117.62	0.049	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	69	PHE	H	8.828	0.011	1
1	A	69	PHE	HA	3.953	0.005	1
1	A	69	PHE	HB2	3.486	0.005	2
1	A	69	PHE	HB3	3.173	0.008	2
1	A	69	PHE	HD1	6.92	0.006	1
1	A	69	PHE	HD2	6.92	0.006	1
1	A	69	PHE	C	177.062	0.000	1
1	A	69	PHE	CA	61.191	0.000	1
1	A	69	PHE	CB	40.016	0.013	1
1	A	69	PHE	N	123.583	0.029	1
1	A	70	LEU	H	8.344	0.005	1
1	A	70	LEU	HA	3.365	0.020	1
1	A	70	LEU	HB2	1.571	0.007	2
1	A	70	LEU	HB3	1.164	0.006	2
1	A	70	LEU	HD11	0.625	0.001	1
1	A	70	LEU	HD12	0.625	0.001	1
1	A	70	LEU	HD13	0.625	0.001	1
1	A	70	LEU	HD21	0.635	0.000	1
1	A	70	LEU	HD22	0.635	0.000	1
1	A	70	LEU	HD23	0.635	0.000	1
1	A	70	LEU	HG	1.019	0.001	1
1	A	70	LEU	C	179.234	0.000	1
1	A	70	LEU	CA	58.071	0.063	1
1	A	70	LEU	CB	40.933	0.050	1
1	A	70	LEU	CD1	25.502	0.008	1
1	A	70	LEU	CD2	24.067	0.084	1
1	A	70	LEU	N	118.918	0.035	1
1	A	71	THR	H	7.493	0.005	1
1	A	71	THR	HA	3.793	0.003	1
1	A	71	THR	HB	4.327	0.005	1
1	A	71	THR	HG21	1.205	0.001	1
1	A	71	THR	HG22	1.205	0.001	1
1	A	71	THR	HG23	1.205	0.001	1
1	A	71	THR	C	176.088	0.000	1
1	A	71	THR	CA	66.43	0.000	1
1	A	71	THR	CB	68.364	0.000	1
1	A	71	THR	CG2	22.12	0.032	1
1	A	71	THR	N	115.482	0.028	1
1	A	72	MET	H	7.766	0.003	1
1	A	72	MET	HA	3.756	0.008	1
1	A	72	MET	HB2	2.113	0.010	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	MET	HB3	1.953	0.006	2
1	A	72	MET	HE1	1.742	0.001	1
1	A	72	MET	HE2	1.742	0.001	1
1	A	72	MET	HE3	1.742	0.001	1
1	A	72	MET	HG2	2.41	0.000	1
1	A	72	MET	HG3	2.41	0.000	1
1	A	72	MET	C	178.163	0.000	1
1	A	72	MET	CA	58.993	0.000	1
1	A	72	MET	CB	33.395	0.000	1
1	A	72	MET	CE	17.362	0.000	1
1	A	72	MET	CG	31.388	0.000	1
1	A	72	MET	N	121.752	0.022	1
1	A	73	MET	H	8.04	0.003	1
1	A	73	MET	HA	3.996	0.006	1
1	A	73	MET	HB2	1.079	0.019	1
1	A	73	MET	HB3	1.079	0.019	1
1	A	73	MET	HE1	1.688	0.003	1
1	A	73	MET	HE2	1.688	0.003	1
1	A	73	MET	HE3	1.688	0.003	1
1	A	73	MET	HG2	1.301	0.000	1
1	A	73	MET	HG3	1.301	0.000	1
1	A	73	MET	C	178.53	0.000	1
1	A	73	MET	CA	55.853	0.020	1
1	A	73	MET	CB	30.978	0.050	1
1	A	73	MET	CE	17.602	0.000	1
1	A	73	MET	CG	32.246	0.000	1
1	A	73	MET	N	116.685	0.043	1
1	A	74	ALA	H	8.162	0.004	1
1	A	74	ALA	HA	4.088	0.007	1
1	A	74	ALA	HB1	1.418	0.003	1
1	A	74	ALA	HB2	1.418	0.003	1
1	A	74	ALA	HB3	1.418	0.003	1
1	A	74	ALA	C	179.764	0.000	1
1	A	74	ALA	CA	54.611	0.008	1
1	A	74	ALA	CB	18.28	0.048	1
1	A	74	ALA	N	122.206	0.103	1
1	A	75	ARG	H	7.551	0.006	1
1	A	75	ARG	HA	4.089	0.005	1
1	A	75	ARG	HB2	1.867	0.017	1
1	A	75	ARG	HB3	1.867	0.017	1
1	A	75	ARG	C	177.715	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	75	ARG	CA	58.089	0.000	1
1	A	75	ARG	CB	29.998	0.000	1
1	A	75	ARG	N	116.705	0.022	1
1	A	76	LYS	H	7.625	0.005	1
1	A	76	LYS	HB2	1.841	0.016	1
1	A	76	LYS	HB3	1.841	0.016	1
1	A	76	LYS	HG2	1.45	0.000	1
1	A	76	LYS	HG3	1.45	0.000	1
1	A	76	LYS	C	177.574	0.000	1
1	A	76	LYS	CA	57.209	0.000	1
1	A	76	LYS	CB	32.444	0.000	1
1	A	76	LYS	CG	24.683	0.000	1
1	A	76	LYS	N	118.653	0.020	1
1	A	77	MET	H	7.82	0.003	1
1	A	77	MET	HA	4.376	0.007	1
1	A	77	MET	HB2	2.163	0.021	1
1	A	77	MET	HB3	2.163	0.021	1
1	A	77	MET	HE1	2.125	0.004	1
1	A	77	MET	HE2	2.125	0.004	1
1	A	77	MET	HE3	2.125	0.004	1
1	A	77	MET	HG2	2.679	0.003	1
1	A	77	MET	HG3	2.679	0.003	1
1	A	77	MET	C	176.431	0.000	1
1	A	77	MET	CA	56.482	0.085	1
1	A	77	MET	CB	32.967	0.000	1
1	A	77	MET	CE	17.091	0.000	1
1	A	77	MET	CG	32.057	0.000	1
1	A	77	MET	N	118.692	0.023	1
1	A	78	LYS	H	7.841	0.005	1
1	A	78	LYS	HA	4.348	0.010	1
1	A	78	LYS	HB2	1.851	0.007	1
1	A	78	LYS	HB3	1.851	0.007	1
1	A	78	LYS	HG2	1.472	0.000	1
1	A	78	LYS	HG3	1.472	0.000	1
1	A	78	LYS	C	176.399	0.000	1
1	A	78	LYS	CA	56.658	0.035	1
1	A	78	LYS	CB	33.174	0.018	1
1	A	78	LYS	CG	24.586	0.000	1
1	A	78	LYS	N	120.746	0.040	1
1	A	79	ASP	H	8.259	0.004	1
1	A	79	ASP	HA	4.678	0.004	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	ASP	HB2	2.749	0.020	2
1	A	79	ASP	HB3	2.668	0.004	2
1	A	79	ASP	C	176.602	0.000	1
1	A	79	ASP	CA	54.976	0.259	1
1	A	79	ASP	CB	41.16	0.035	1
1	A	79	ASP	N	121.766	0.041	1
1	A	80	THR	H	8.057	0.009	1
1	A	80	THR	HA	4.32	0.001	1
1	A	80	THR	HB	4.231	0.016	1
1	A	80	THR	HG21	1.217	0.000	1
1	A	80	THR	HG22	1.217	0.000	1
1	A	80	THR	HG23	1.217	0.000	1
1	A	80	THR	C	174.455	0.000	1
1	A	80	THR	CA	62.431	0.009	1
1	A	80	THR	CB	69.838	0.069	1
1	A	80	THR	CG2	21.673	0.005	1
1	A	80	THR	N	114.492	0.078	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
$^{13}\text{C}_\alpha$	88	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	78	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	87	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
^{15}N	88	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)

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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1054. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/388 (0%)	0/158 (0%)	0/154 (0%)	0/76 (0%)
Sidechain	0/599 (0%)	0/382 (0%)	0/192 (0%)	0/25 (0%)
Aromatic	0/67 (0%)	0/33 (0%)	0/32 (0%)	0/2 (0%)
Overall	0/1054 (0%)	0/573 (0%)	0/378 (0%)	0/103 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1176. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/438 (0%)	0/178 (0%)	0/174 (0%)	0/86 (0%)
Sidechain	0/671 (0%)	0/427 (0%)	0/213 (0%)	0/31 (0%)
Aromatic	0/67 (0%)	0/33 (0%)	0/32 (0%)	0/2 (0%)
Overall	0/1176 (0%)	0/638 (0%)	0/419 (0%)	0/119 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

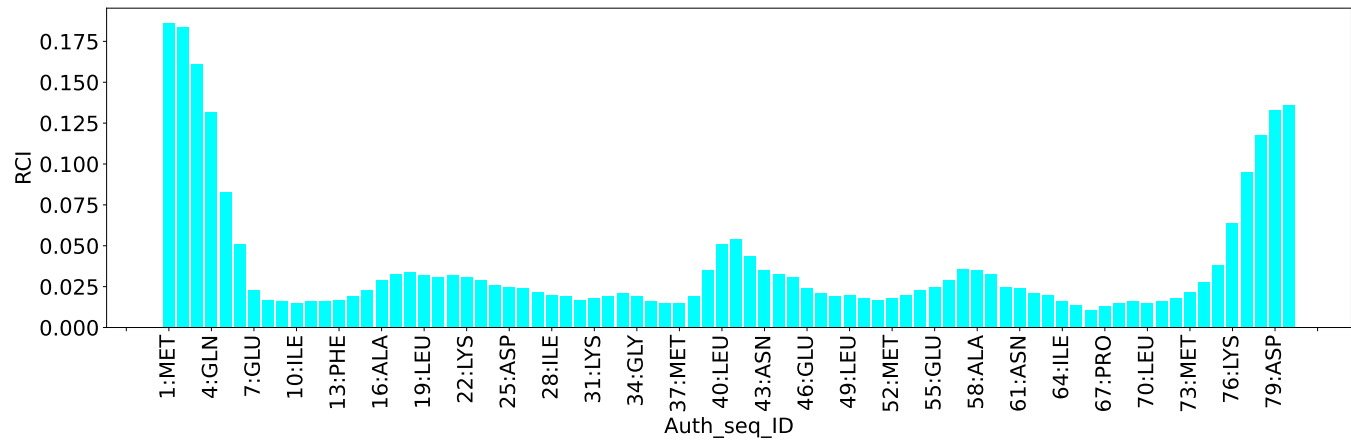
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	7	GLU	CD	43.18	171.45 – 193.13	-64.2
1	A	61	ASN	CG	37.24	164.52 – 188.90	-57.2
1	A	2	ALA	CB	63.98	10.19 – 27.75	25.6
1	A	3	ASP	CG	36.49	149.18 – 208.82	-23.9
1	A	25	ASP	CG	38.10	149.18 – 208.82	-23.6
1	A	2	ALA	HB2	4.07	0.14 – 2.58	11.1
1	A	2	ALA	HB1	3.96	0.14 – 2.58	10.7
1	A	2	ALA	HB3	3.96	0.14 – 2.58	10.7
1	A	5	LEU	CG	36.66	21.37 – 32.19	9.1
1	A	30	THR	HG2	2.67	0.08 – 2.19	7.2
1	A	30	THR	HG3	2.67	0.08 – 2.19	7.2
1	A	29	THR	HB	2.03	2.57 – 5.77	-6.7
1	A	64	ILE	HG2	2.38	-0.56 – 2.11	6.0
1	A	64	ILE	HG3	2.38	-0.56 – 2.11	6.0

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:



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	48
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	48
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	12
Number of restraints per residue	0.0
Number of long range restraints per residue ¹	0.0

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)	0.6	0.15
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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

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

9 Distance violation analysis ⓘ

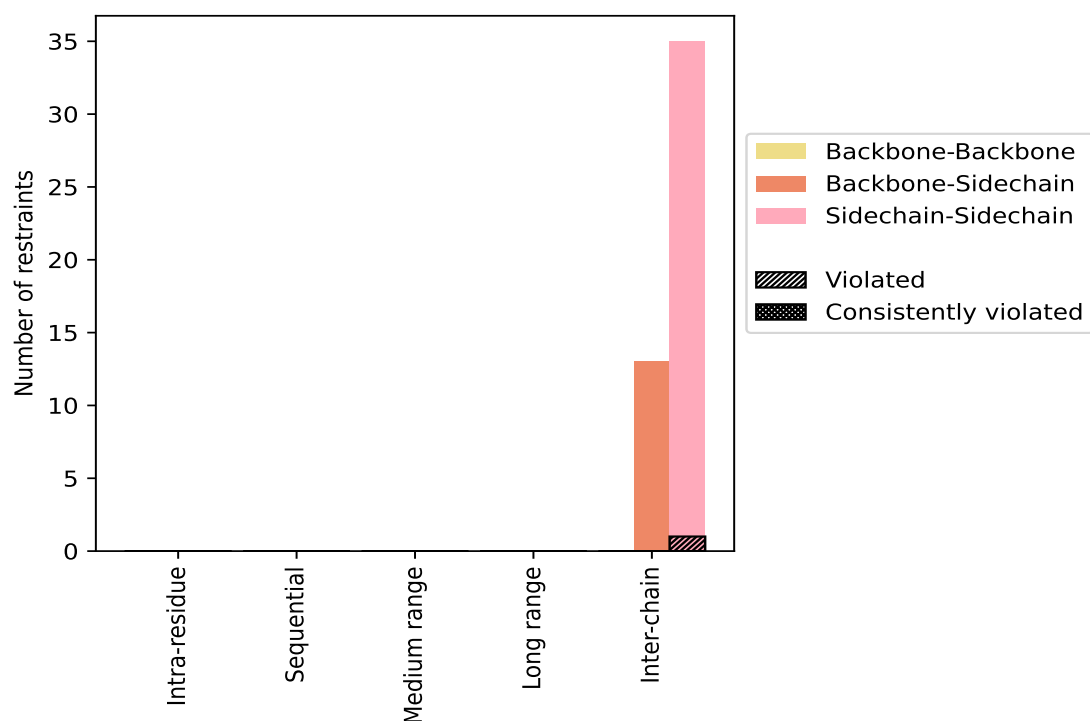
9.1 Summary of distance violations ⓘ

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)	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
Sequential (i-j =1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	48	100.0	1	2.1	2.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	13	27.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	35	72.9	1	2.9	2.1	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	48	100.0	1	2.1	2.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	13	27.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	35	72.9	1	2.9	2.1	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 disulfide bonds are counted in their appropriate category on the x-axis

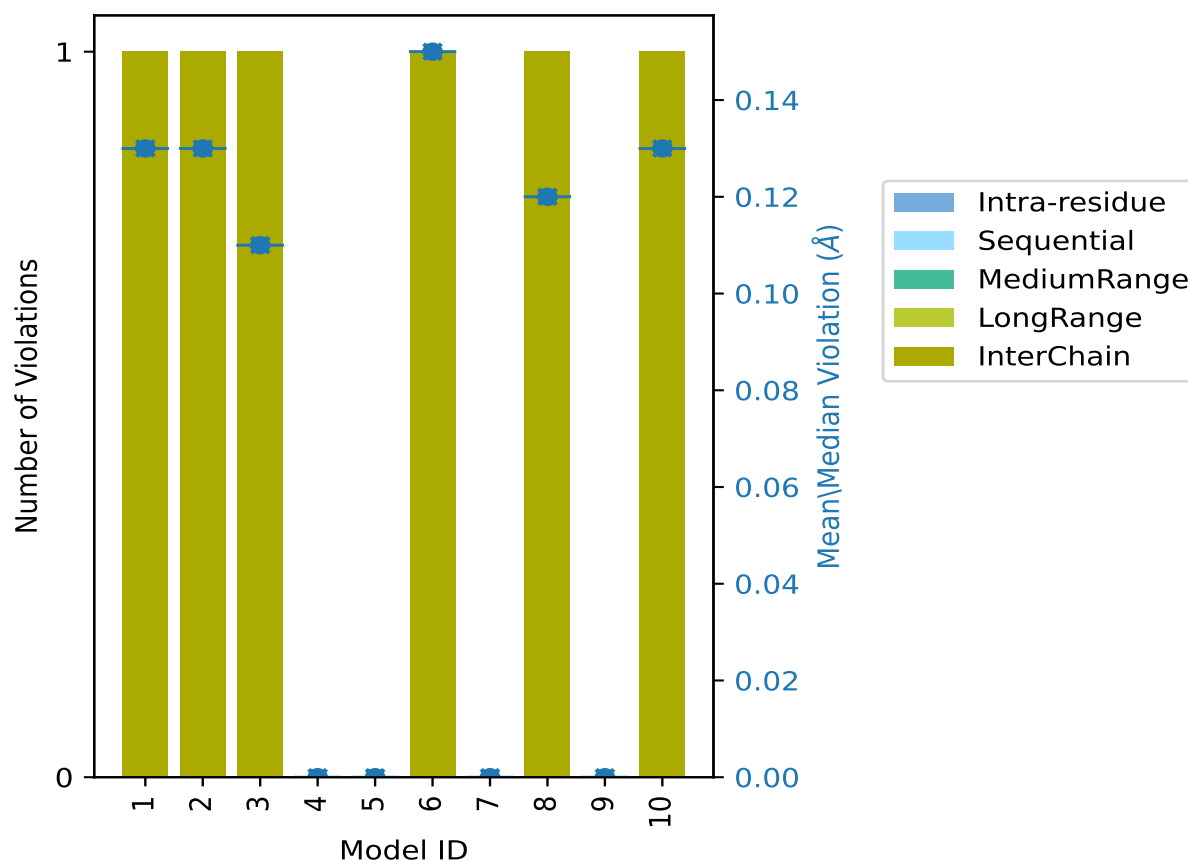
9.2 Distance violation statistics for each model [i](#)

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	0	0	1	1	0.13	0.13	0.0	0.13
2	0	0	0	0	1	1	0.13	0.13	0.0	0.13
3	0	0	0	0	1	1	0.11	0.11	0.0	0.11
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	1	1	0.15	0.15	0.0	0.15
7	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	1	1	0.12	0.12	0.0	0.12
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	1	1	0.13	0.13	0.0	0.13

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 [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 47(IR:0, SQ:0, MR:0, LR:0, IC:47) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	1	10.0
0	0	0	0	0	0	2	20.0
0	0	0	0	0	0	3	30.0

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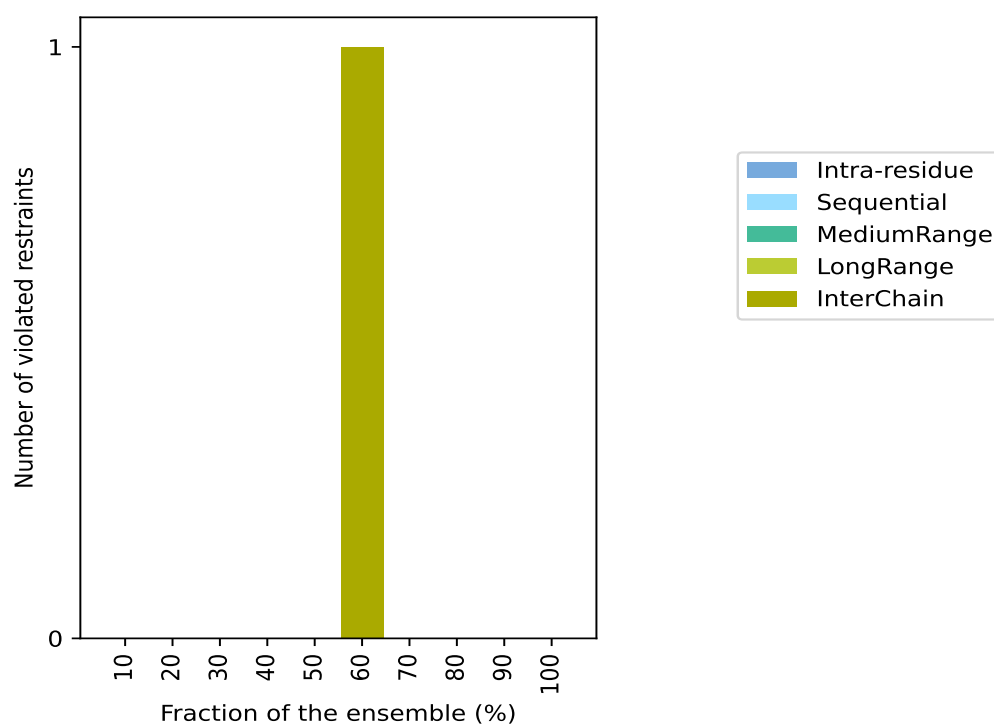
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	1	1	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	0	0	9	90.0
0	0	0	0	0	0	10	100.0

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 ⓘ

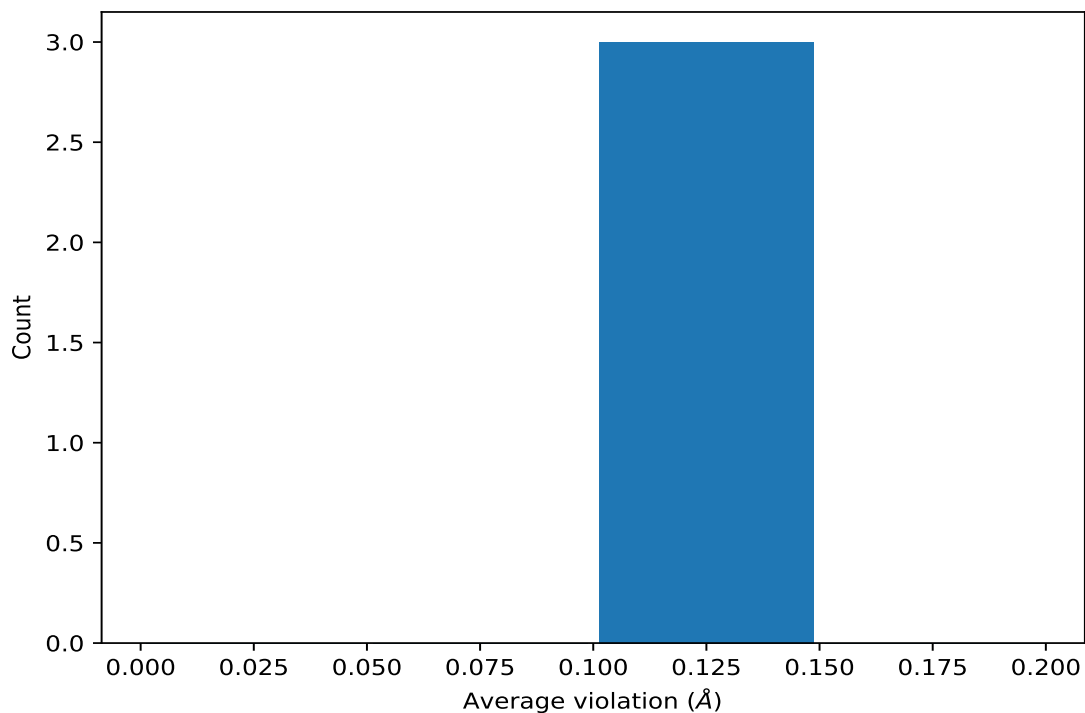


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

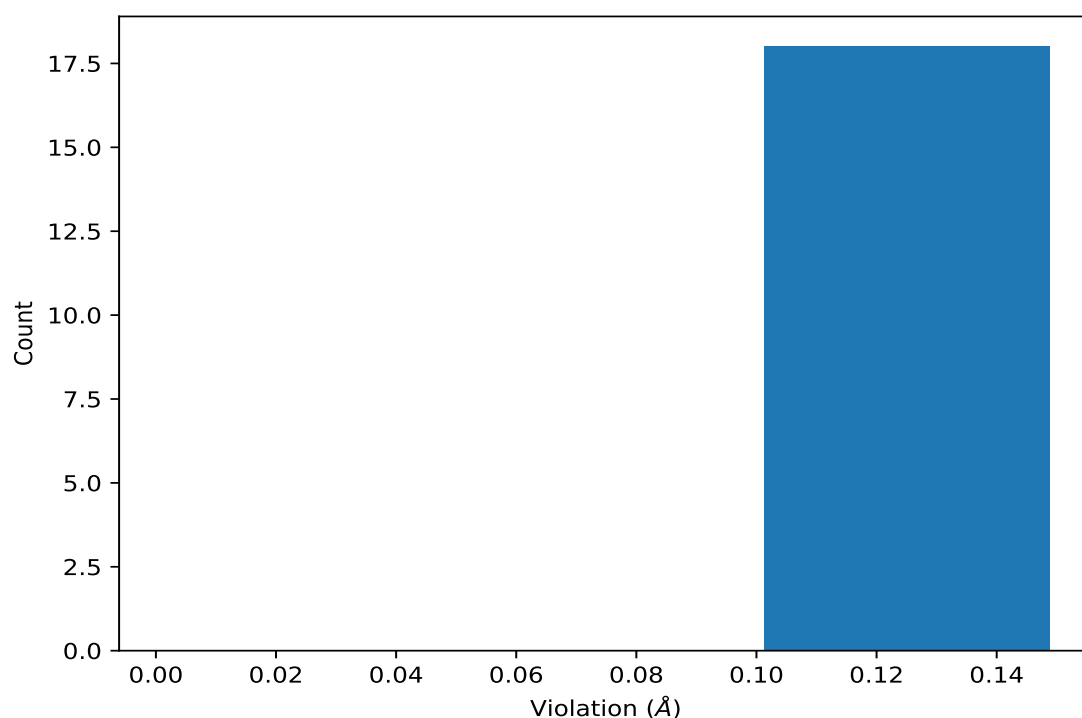
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,36)	1:146:A:MET:HE1	2:1014:B:TRP:HD1	6	0.13	0.01	0.13
(1,36)	1:146:A:MET:HE2	2:1014:B:TRP:HD1	6	0.13	0.01	0.13
(1,36)	1:146:A:MET:HE3	2:1014:B:TRP:HD1	6	0.13	0.01	0.13

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)
(1,36)	1:146:A:MET:HE1	2:1014:B:TRP:HD1	6	0.15
(1,36)	1:146:A:MET:HE2	2:1014:B:TRP:HD1	6	0.15
(1,36)	1:146:A:MET:HE3	2:1014:B:TRP:HD1	6	0.15
(1,36)	1:146:A:MET:HE1	2:1014:B:TRP:HD1	1	0.13
(1,36)	1:146:A:MET:HE2	2:1014:B:TRP:HD1	1	0.13
(1,36)	1:146:A:MET:HE3	2:1014:B:TRP:HD1	1	0.13
(1,36)	1:146:A:MET:HE1	2:1014:B:TRP:HD1	2	0.13
(1,36)	1:146:A:MET:HE2	2:1014:B:TRP:HD1	2	0.13
(1,36)	1:146:A:MET:HE3	2:1014:B:TRP:HD1	2	0.13
(1,36)	1:146:A:MET:HE1	2:1014:B:TRP:HD1	10	0.13
(1,36)	1:146:A:MET:HE2	2:1014:B:TRP:HD1	10	0.13
(1,36)	1:146:A:MET:HE3	2:1014:B:TRP:HD1	10	0.13
(1,36)	1:146:A:MET:HE1	2:1014:B:TRP:HD1	8	0.12
(1,36)	1:146:A:MET:HE2	2:1014:B:TRP:HD1	8	0.12
(1,36)	1:146:A:MET:HE3	2:1014:B:TRP:HD1	8	0.12
(1,36)	1:146:A:MET:HE1	2:1014:B:TRP:HD1	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:146:A:MET:HE2	2:1014:B:TRP:HD1	3	0.11
(1,36)	1:146:A:MET:HE3	2:1014:B:TRP:HD1	3	0.11

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found