



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 06:59 AM UTC

PDB ID : 6WA4 / pdb_00006wa4
BMRB ID : 30739
Title : Solution NMR structure of the unmyristoylated feline immunodeficiency virus matrix protein
Authors : Brown, J.B.; Summers, H.R.; Brown, L.A.; Marchant, J.; Canova, P.N.; O'Hern, C.T.; Abbott, S.T.; Nyaunu, C.; Maxwell, S.; Johnson, T.; Moser, M.B.; Carter, H.; Ablan, S.; Freed, E.O.; Summers, M.F.
Deposited on : 2020-03-24

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

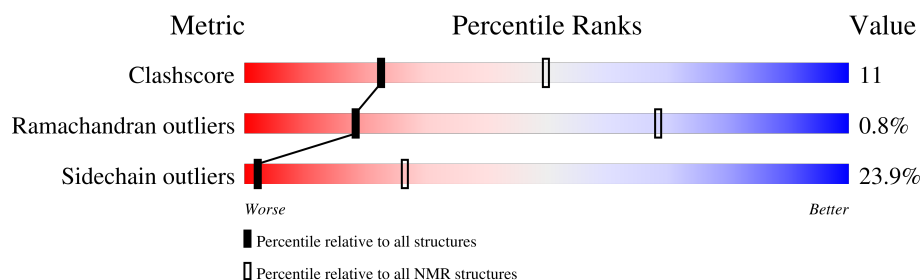
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	126	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:6-A:21, A:28-A:115 (104)	0.70	1

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1808 atoms, of which 911 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrix protein.

Mol	Chain	Residues	Atoms						Trace
1	A	118	Total	C	H	N	O	S	0
			1808	556	911	165	168	8	

There are 8 discrepancies between the modelled and reference sequences:

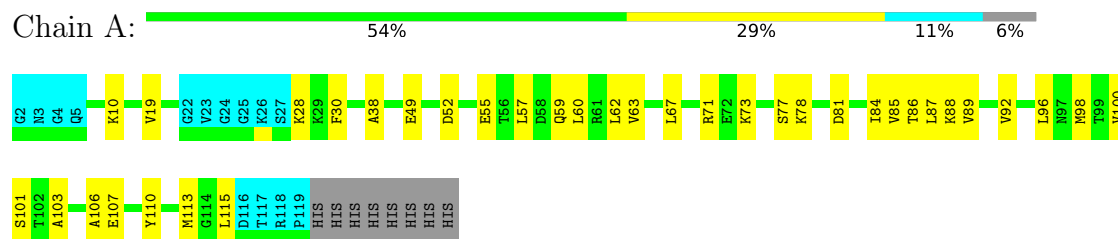
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	HIS	-	expression tag	UNP Q66971
A	121	HIS	-	expression tag	UNP Q66971
A	122	HIS	-	expression tag	UNP Q66971
A	123	HIS	-	expression tag	UNP Q66971
A	124	HIS	-	expression tag	UNP Q66971
A	125	HIS	-	expression tag	UNP Q66971
A	126	HIS	-	expression tag	UNP Q66971
A	127	HIS	-	expression tag	UNP Q66971

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Matrix protein

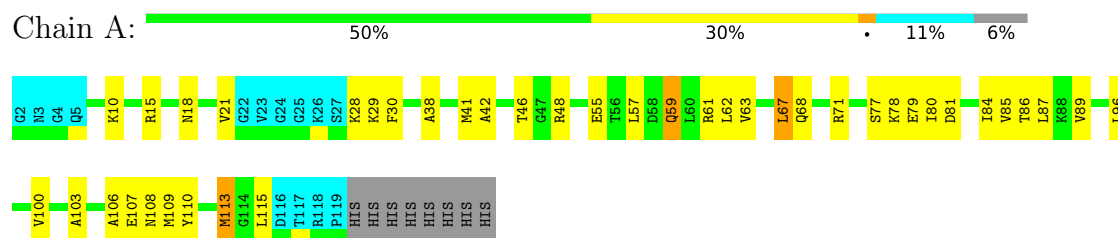


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

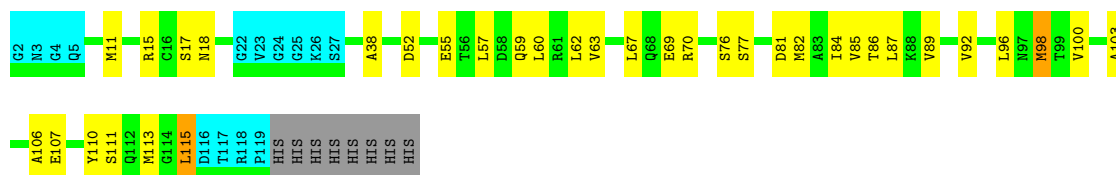
- Molecule 1: Matrix protein



4.2.2 Score per residue for model 2

- Molecule 1: Matrix protein

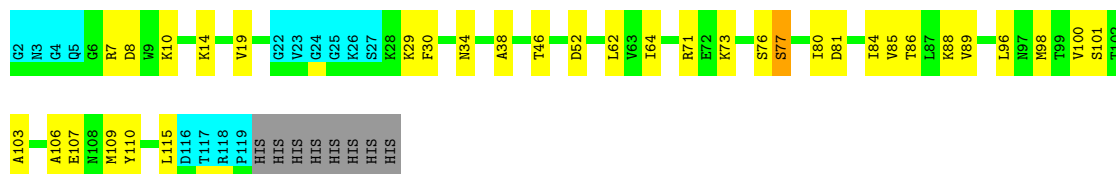




4.2.3 Score per residue for model 3

- Molecule 1: Matrix protein

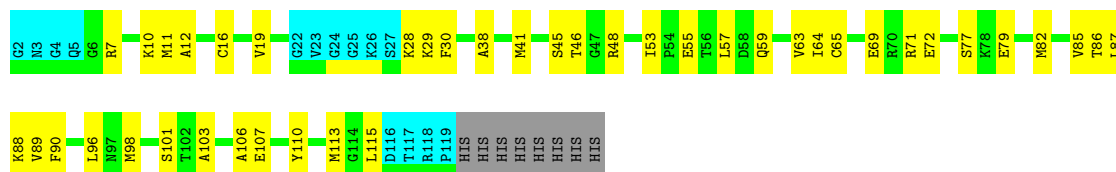
Chain A: 56% 26% 11% 6%



4.2.4 Score per residue for model 4

- Molecule 1: Matrix protein

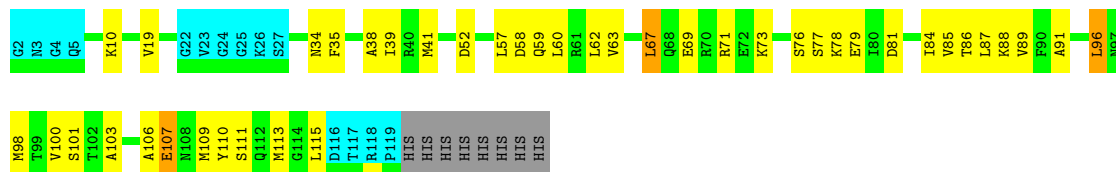
Chain A: 49% 33% 11% 6%



4.2.5 Score per residue for model 5

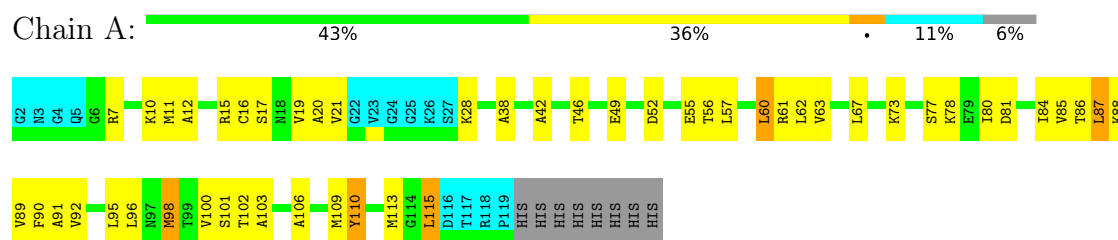
- Molecule 1: Matrix protein

Chain A: 49% 31% 11% 6%



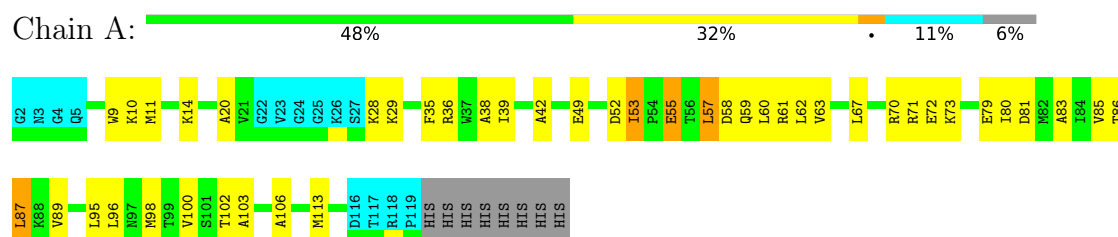
4.2.6 Score per residue for model 6

- Molecule 1: Matrix protein



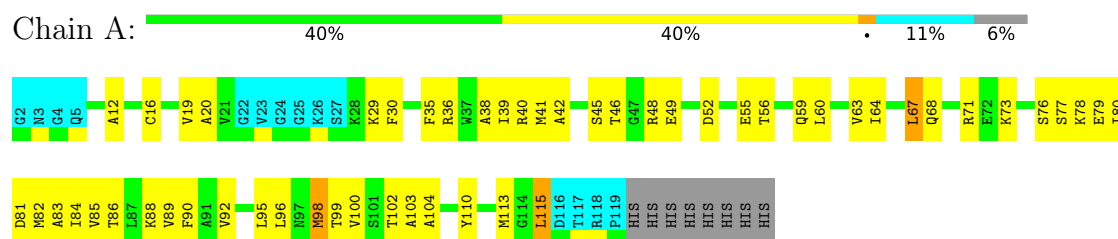
4.2.7 Score per residue for model 7

- Molecule 1: Matrix protein



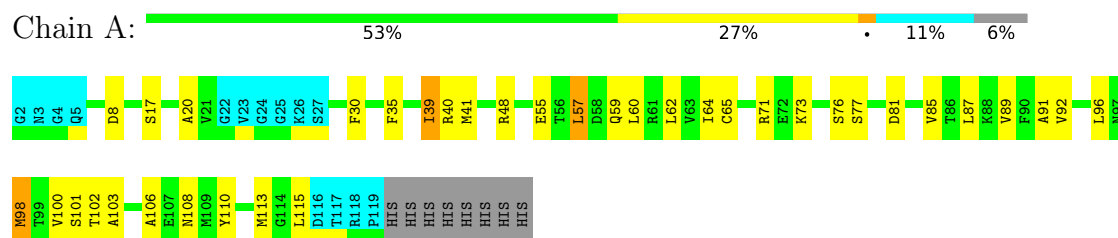
4.2.8 Score per residue for model 8

- Molecule 1: Matrix protein



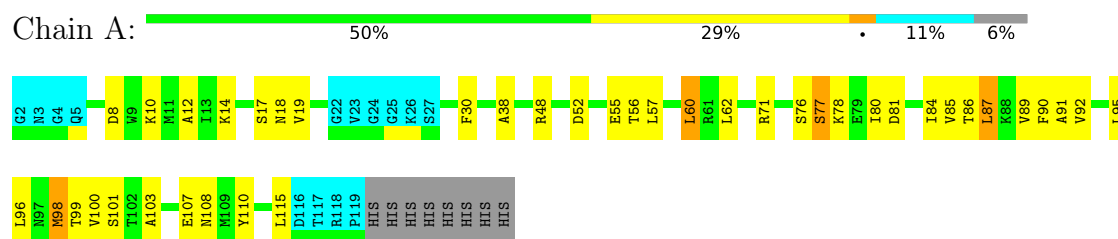
4.2.9 Score per residue for model 9

- Molecule 1: Matrix protein



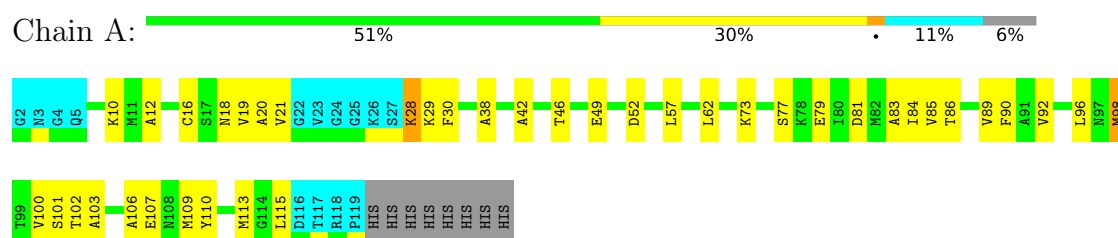
4.2.14 Score per residue for model 14

- Molecule 1: Matrix protein



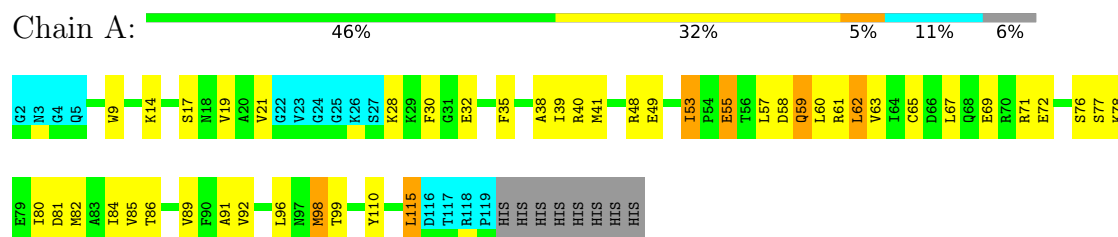
4.2.15 Score per residue for model 15

- Molecule 1: Matrix protein



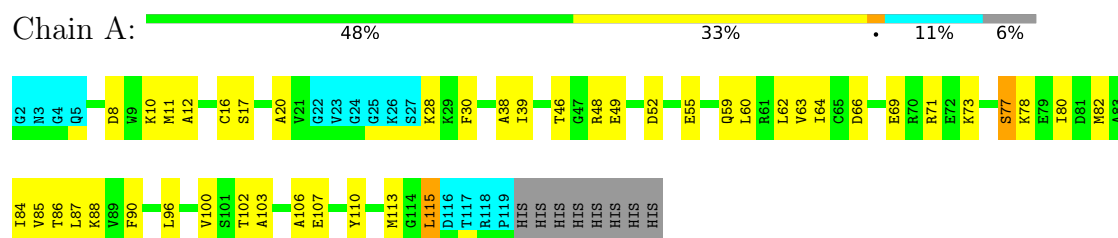
4.2.16 Score per residue for model 16

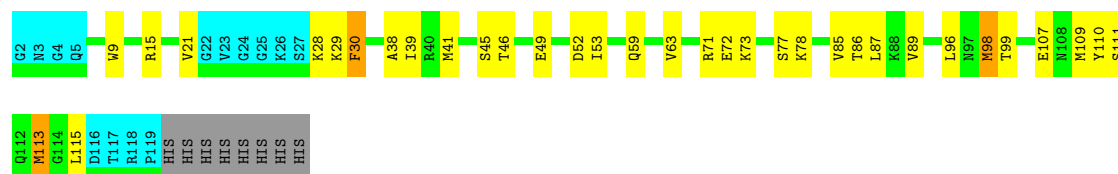
- Molecule 1: Matrix protein



4.2.17 Score per residue for model 17

- Molecule 1: Matrix protein





5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 160 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	
CYANA	structure calculation	

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	1208
Number of shifts mapped to atoms	1208
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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	805	824	824	18±6
All	All	16100	16480	16480	367

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ILE:HG23	1:A:84:ILE:HG23	0.87	1.47	8	2
1:A:19:VAL:HG11	1:A:89:VAL:HG11	0.83	1.50	13	3
1:A:85:VAL:HG11	1:A:103:ALA:HB1	0.81	1.52	5	9
1:A:85:VAL:HG21	1:A:103:ALA:HB1	0.78	1.54	7	1
1:A:38:ALA:HB3	1:A:86:THR:HG21	0.78	1.55	7	19
1:A:89:VAL:HG22	1:A:106:ALA:HB3	0.78	1.55	5	7
1:A:100:VAL:HG11	1:A:106:ALA:HB2	0.77	1.56	9	11
1:A:113:MET:HE3	1:A:115:LEU:HD11	0.69	1.64	20	1
1:A:42:ALA:HB1	1:A:67:LEU:HD11	0.68	1.65	6	2
1:A:60:LEU:HD23	1:A:87:LEU:HD13	0.67	1.67	11	1
1:A:110:TYR:CE2	1:A:115:LEU:HD11	0.66	2.26	6	1
1:A:71:ARG:HB3	1:A:80:ILE:HG21	0.66	1.67	19	1
1:A:85:VAL:CG1	1:A:103:ALA:HB1	0.66	2.21	13	15
1:A:63:VAL:HG12	1:A:67:LEU:HD12	0.65	1.67	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:TRP:CZ2	1:A:53:ILE:HD11	0.64	2.27	16	1
1:A:16:CYS:O	1:A:19:VAL:HG12	0.63	1.92	6	2
1:A:89:VAL:HG23	1:A:100:VAL:HG21	0.63	1.70	14	2
1:A:59:GLN:O	1:A:63:VAL:HG23	0.63	1.94	13	13
1:A:80:ILE:HG22	1:A:84:ILE:HD11	0.63	1.69	3	6
1:A:92:VAL:HG12	1:A:98:MET:HB2	0.63	1.71	12	3
1:A:60:LEU:HD13	1:A:87:LEU:HD23	0.63	1.70	7	1
1:A:89:VAL:HG22	1:A:106:ALA:CB	0.62	2.24	13	7
1:A:96:LEU:HD23	1:A:99:THR:HB	0.62	1.70	20	2
1:A:85:VAL:HG22	1:A:107:GLU:OE1	0.61	1.95	1	2
1:A:71:ARG:HD2	1:A:80:ILE:HD12	0.61	1.71	17	4
1:A:9:TRP:CH2	1:A:53:ILE:HD11	0.61	2.31	7	2
1:A:9:TRP:CH2	1:A:53:ILE:HG23	0.61	2.30	20	2
1:A:81:ASP:O	1:A:85:VAL:HG23	0.61	1.96	3	12
1:A:67:LEU:HD12	1:A:84:ILE:HD12	0.61	1.72	5	1
1:A:71:ARG:CD	1:A:80:ILE:HD12	0.60	2.26	17	4
1:A:42:ALA:HB1	1:A:67:LEU:CD1	0.60	2.26	6	1
1:A:71:ARG:CB	1:A:80:ILE:HG21	0.60	2.26	19	2
1:A:92:VAL:HG22	1:A:98:MET:CB	0.60	2.26	15	1
1:A:19:VAL:HG11	1:A:89:VAL:HG21	0.60	1.72	15	6
1:A:56:THR:O	1:A:60:LEU:HD12	0.59	1.97	8	4
1:A:21:VAL:HG22	1:A:28:LYS:C	0.59	2.23	15	3
1:A:35:PHE:CZ	1:A:39:ILE:HD11	0.59	2.33	8	2
1:A:60:LEU:HD13	1:A:91:ALA:CB	0.59	2.27	9	1
1:A:64:ILE:HG12	1:A:87:LEU:HD11	0.59	1.74	13	1
1:A:81:ASP:HA	1:A:84:ILE:HD12	0.58	1.76	6	1
1:A:60:LEU:HD12	1:A:87:LEU:O	0.58	1.99	10	3
1:A:35:PHE:CE2	1:A:39:ILE:HD11	0.58	2.34	8	1
1:A:100:VAL:CG1	1:A:106:ALA:HB2	0.58	2.28	9	3
1:A:80:ILE:HG22	1:A:84:ILE:CD1	0.57	2.30	3	5
1:A:100:VAL:HG11	1:A:106:ALA:CB	0.57	2.28	2	1
1:A:35:PHE:CE1	1:A:39:ILE:HD11	0.57	2.34	7	1
1:A:85:VAL:HG22	1:A:103:ALA:HB1	0.56	1.75	19	2
1:A:19:VAL:HG11	1:A:89:VAL:CG2	0.56	2.30	18	3
1:A:85:VAL:O	1:A:89:VAL:HG12	0.56	2.01	20	6
1:A:67:LEU:HD23	1:A:84:ILE:HD13	0.56	1.78	11	1
1:A:19:VAL:HG23	1:A:100:VAL:O	0.56	2.01	6	1
1:A:42:ALA:O	1:A:46:THR:HG23	0.56	2.01	12	3
1:A:92:VAL:HG22	1:A:98:MET:HB2	0.55	1.79	15	1
1:A:67:LEU:HD22	1:A:84:ILE:CG1	0.55	2.31	2	2
1:A:92:VAL:HG12	1:A:98:MET:CB	0.55	2.31	11	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ARG:HA	1:A:39:ILE:HD12	0.55	1.77	7	2
1:A:89:VAL:HG23	1:A:100:VAL:HG11	0.55	1.78	1	3
1:A:21:VAL:HG22	1:A:28:LYS:O	0.55	2.01	20	4
1:A:85:VAL:O	1:A:89:VAL:HG23	0.54	2.02	3	7
1:A:45:SER:HB2	1:A:67:LEU:HD21	0.54	1.78	8	1
1:A:60:LEU:HD12	1:A:87:LEU:HB3	0.54	1.78	17	1
1:A:12:ALA:HB1	1:A:90:PHE:CE2	0.54	2.37	6	4
1:A:67:LEU:HD22	1:A:84:ILE:HG12	0.54	1.78	2	1
1:A:110:TYR:HA	1:A:115:LEU:HD12	0.54	1.80	15	7
1:A:63:VAL:HG12	1:A:67:LEU:HD23	0.54	1.79	5	1
1:A:109:MET:HE3	1:A:113:MET:HE2	0.53	1.79	1	2
1:A:64:ILE:HD13	1:A:88:LYS:CG	0.53	2.33	8	1
1:A:63:VAL:HG12	1:A:67:LEU:CD1	0.53	2.33	6	2
1:A:85:VAL:CG2	1:A:103:ALA:HB1	0.53	2.34	19	3
1:A:60:LEU:HD22	1:A:87:LEU:O	0.53	2.04	9	1
1:A:110:TYR:O	1:A:115:LEU:HD12	0.53	2.04	16	7
1:A:60:LEU:HD11	1:A:95:LEU:CD2	0.53	2.34	6	2
1:A:110:TYR:CD2	1:A:115:LEU:HD21	0.53	2.39	6	1
1:A:60:LEU:HD22	1:A:91:ALA:HB2	0.52	1.81	11	4
1:A:85:VAL:HG12	1:A:103:ALA:HB1	0.52	1.80	17	5
1:A:64:ILE:HD13	1:A:110:TYR:CE2	0.52	2.39	10	1
1:A:12:ALA:HB1	1:A:90:PHE:CE1	0.52	2.39	13	3
1:A:89:VAL:HG13	1:A:100:VAL:HG21	0.52	1.81	2	2
1:A:85:VAL:HG22	1:A:107:GLU:HG3	0.52	1.80	5	1
1:A:55:GLU:O	1:A:95:LEU:HD11	0.51	2.04	6	3
1:A:113:MET:HB2	1:A:115:LEU:HD12	0.51	1.83	5	1
1:A:21:VAL:HG12	1:A:28:LYS:C	0.51	2.30	6	1
1:A:71:ARG:HB2	1:A:84:ILE:HD11	0.51	1.83	16	1
1:A:85:VAL:O	1:A:89:VAL:HG22	0.51	2.05	10	1
1:A:84:ILE:HG22	1:A:88:LYS:HD2	0.51	1.82	19	4
1:A:60:LEU:HD23	1:A:87:LEU:CD1	0.50	2.35	11	3
1:A:64:ILE:HD12	1:A:88:LYS:HG3	0.50	1.82	17	1
1:A:110:TYR:CD1	1:A:115:LEU:HD13	0.50	2.42	5	1
1:A:96:LEU:HD23	1:A:99:THR:CB	0.50	2.37	20	2
1:A:89:VAL:HG23	1:A:100:VAL:CG2	0.49	2.37	14	2
1:A:67:LEU:HD11	1:A:80:ILE:HD11	0.49	1.84	13	1
1:A:20:ALA:HB3	1:A:102:THR:HG22	0.49	1.83	8	5
1:A:64:ILE:HB	1:A:87:LEU:HD13	0.49	1.84	18	1
1:A:64:ILE:CG1	1:A:87:LEU:HD11	0.49	2.37	13	1
1:A:46:THR:HG23	1:A:67:LEU:HG	0.49	1.85	8	1
1:A:60:LEU:HD12	1:A:91:ALA:HB2	0.48	1.85	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ILE:HG21	1:A:88:LYS:HE3	0.48	1.85	8	1
1:A:20:ALA:HB3	1:A:102:THR:HA	0.48	1.85	6	2
1:A:64:ILE:CD1	1:A:87:LEU:HD11	0.48	2.37	13	1
1:A:35:PHE:CZ	1:A:39:ILE:HD12	0.48	2.44	5	2
1:A:110:TYR:O	1:A:115:LEU:HD22	0.48	2.08	6	1
1:A:38:ALA:HB1	1:A:83:ALA:HA	0.48	1.86	7	1
1:A:53:ILE:HG23	1:A:53:ILE:O	0.47	2.09	4	3
1:A:56:THR:C	1:A:60:LEU:HD12	0.47	2.33	11	1
1:A:42:ALA:HB2	1:A:83:ALA:HB1	0.47	1.85	8	3
1:A:89:VAL:HG23	1:A:106:ALA:HB2	0.47	1.84	15	1
1:A:87:LEU:HD12	1:A:88:LYS:N	0.47	2.24	4	2
1:A:92:VAL:HG12	1:A:98:MET:HB3	0.47	1.86	6	3
1:A:60:LEU:O	1:A:64:ILE:HG22	0.47	2.09	17	1
1:A:64:ILE:HD13	1:A:88:LYS:HG2	0.47	1.85	3	1
1:A:19:VAL:HG22	1:A:100:VAL:HG23	0.47	1.87	3	1
1:A:89:VAL:HG23	1:A:100:VAL:CG1	0.46	2.39	1	1
1:A:39:ILE:HA	1:A:87:LEU:HD21	0.46	1.88	17	1
1:A:60:LEU:HD11	1:A:87:LEU:CB	0.46	2.40	19	1
1:A:63:VAL:HG11	1:A:87:LEU:HD22	0.46	1.86	20	1
1:A:67:LEU:CD2	1:A:80:ILE:HG23	0.46	2.41	8	1
1:A:19:VAL:HG11	1:A:89:VAL:CG1	0.46	2.34	13	1
1:A:60:LEU:HD23	1:A:87:LEU:HD22	0.45	1.88	9	1
1:A:89:VAL:HG12	1:A:106:ALA:HB3	0.45	1.88	10	1
1:A:55:GLU:CG	1:A:95:LEU:HD21	0.45	2.41	19	1
1:A:64:ILE:HD11	1:A:88:LYS:HZ2	0.45	1.72	18	1
1:A:89:VAL:HA	1:A:106:ALA:HB1	0.45	1.88	15	4
1:A:20:ALA:O	1:A:103:ALA:HB2	0.44	2.11	10	1
1:A:30:PHE:CZ	1:A:89:VAL:HG11	0.44	2.48	11	1
1:A:59:GLN:NE2	1:A:60:LEU:HD22	0.43	2.28	2	1
1:A:19:VAL:HG11	1:A:89:VAL:HG23	0.43	1.90	18	1
1:A:55:GLU:C	1:A:95:LEU:HD11	0.43	2.39	6	1
1:A:55:GLU:H	1:A:59:GLN:NE2	0.43	2.11	7	1
1:A:109:MET:SD	1:A:113:MET:HE2	0.43	2.54	6	1
1:A:60:LEU:HG	1:A:91:ALA:HB2	0.42	1.91	19	1
1:A:53:ILE:O	1:A:53:ILE:HG23	0.42	2.14	7	1
1:A:64:ILE:HD13	1:A:88:LYS:HG3	0.42	1.91	8	1
1:A:35:PHE:O	1:A:39:ILE:HG22	0.42	2.13	13	2
1:A:46:THR:HG21	1:A:63:VAL:HG13	0.42	1.90	17	1
1:A:38:ALA:CB	1:A:86:THR:HG21	0.42	2.43	19	3
1:A:30:PHE:CE2	1:A:89:VAL:HG11	0.42	2.49	20	1
1:A:57:LEU:HD22	1:A:95:LEU:HD12	0.42	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:VAL:HG13	1:A:100:VAL:HG11	0.42	1.92	5	1
1:A:57:LEU:HD13	1:A:57:LEU:O	0.42	2.15	9	1
1:A:46:THR:HG23	1:A:67:LEU:CD2	0.41	2.45	6	1
1:A:64:ILE:HG23	1:A:84:ILE:CG2	0.41	2.32	8	1
1:A:92:VAL:HG13	1:A:96:LEU:CD2	0.41	2.45	16	1
1:A:92:VAL:HG22	1:A:98:MET:HB3	0.41	1.91	13	1
1:A:61:ARG:NH2	1:A:62:LEU:HD22	0.41	2.31	16	1
1:A:57:LEU:CD1	1:A:96:LEU:HD23	0.41	2.45	5	1
1:A:64:ILE:HG13	1:A:84:ILE:HG23	0.41	1.91	19	1
1:A:64:ILE:HD12	1:A:87:LEU:CD1	0.40	2.46	4	1
1:A:85:VAL:HG22	1:A:107:GLU:CD	0.40	2.42	1	1
1:A:64:ILE:HD12	1:A:87:LEU:HD11	0.40	1.92	4	1
1:A:89:VAL:HG23	1:A:106:ALA:CB	0.40	2.47	15	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	104/126 (83%)	93±2 (90±2%)	10±2 (9±2%)	1±1 (1±1%)	18	68
All	All	2080/2520 (83%)	1866 (90%)	197 (9%)	17 (1%)	18	68

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	55	GLU	6
1	A	77	SER	5
1	A	98	MET	4
1	A	20	ALA	1
1	A	99	THR	1

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	85/102 (83%)	65±2 (76±3%)	20±2 (24±3%)	2	26
All	All	1700/2040 (83%)	1293 (76%)	407 (24%)	2	26

All 62 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	96	LEU	17
1	A	62	LEU	16
1	A	77	SER	15
1	A	113	MET	14
1	A	52	ASP	14
1	A	98	MET	14
1	A	57	LEU	13
1	A	73	LYS	13
1	A	10	LYS	12
1	A	78	LYS	12
1	A	30	PHE	11
1	A	101	SER	11
1	A	49	GLU	11
1	A	48	ARG	10
1	A	76	SER	10
1	A	29	LYS	9
1	A	41	MET	9
1	A	87	LEU	9
1	A	107	GLU	9
1	A	71	ARG	8
1	A	79	GLU	8
1	A	59	GLN	7
1	A	17	SER	7
1	A	115	LEU	7
1	A	55	GLU	7
1	A	72	GLU	7
1	A	58	ASP	7
1	A	15	ARG	6
1	A	11	MET	6

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Mol	Chain	Res	Type	Models (Total)
1	A	69	GLU	6
1	A	82	MET	6
1	A	28	LYS	6
1	A	67	LEU	5
1	A	7	ARG	5
1	A	14	LYS	5
1	A	109	MET	5
1	A	18	ASN	4
1	A	61	ARG	4
1	A	111	SER	4
1	A	8	ASP	4
1	A	46	THR	4
1	A	40	ARG	4
1	A	68	GLN	3
1	A	108	ASN	3
1	A	70	ARG	3
1	A	34	ASN	3
1	A	45	SER	3
1	A	65	CYS	3
1	A	88	LYS	3
1	A	60	LEU	3
1	A	16	CYS	3
1	A	84	ILE	3
1	A	80	ILE	2
1	A	53	ILE	2
1	A	99	THR	2
1	A	39	ILE	2
1	A	112	GLN	2
1	A	66	ASP	2
1	A	110	TYR	1
1	A	81	ASP	1
1	A	36	ARG	1
1	A	32	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [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 78% for the well-defined parts and 77% 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	1208
Number of shifts mapped to atoms	1208
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	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
$^{13}\text{C}_\alpha$	117	-1.15 ± 0.05	Should be checked
$^{13}\text{C}_\beta$	104	-0.35 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	117	-0.24 ± 0.06	None needed (< 0.5 ppm)
^{15}N	113	0.66 ± 0.32	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1115 atoms were assigned a chemical shift out of a possible 1425. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	515/524 (98%)	206/214 (96%)	208/208 (100%)	101/102 (99%)
Sidechain	554/828 (67%)	342/539 (63%)	204/250 (82%)	8/39 (21%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	46/73 (63%)	23/36 (64%)	21/35 (60%)	2/2 (100%)
Overall	1115/1425 (78%)	571/789 (72%)	433/493 (88%)	111/143 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1208 atoms were assigned a chemical shift out of a possible 1578. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	576/597 (96%)	229/246 (93%)	234/236 (99%)	113/115 (98%)
Sidechain	586/908 (65%)	360/589 (61%)	217/274 (79%)	9/45 (20%)
Aromatic	46/73 (63%)	23/36 (64%)	21/35 (60%)	2/2 (100%)
Overall	1208/1578 (77%)	612/871 (70%)	472/545 (87%)	124/162 (77%)

7.1.4 Statistically unusual chemical shifts [i](#)

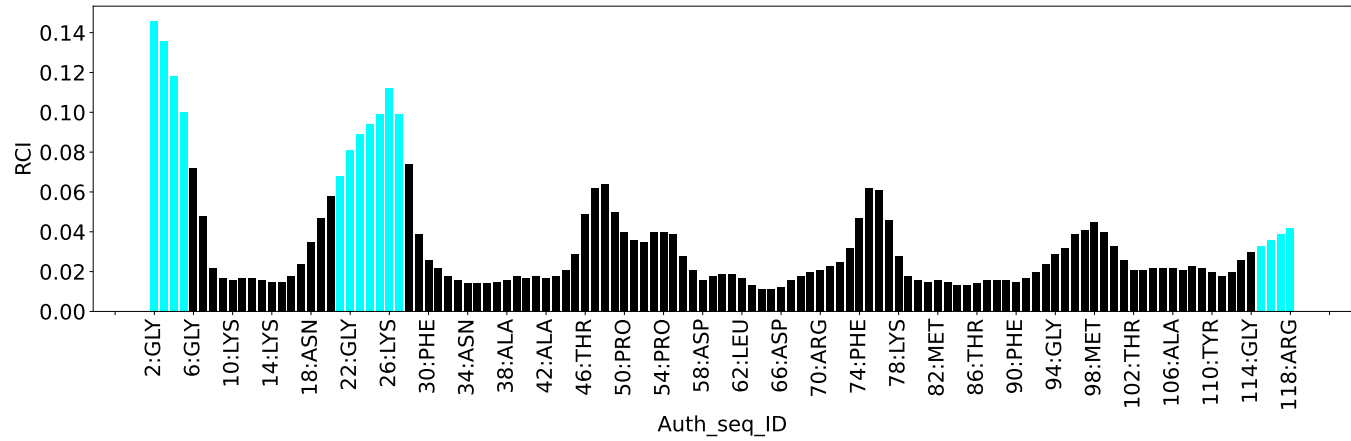
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	71	ARG	HD2	4.37	1.97 – 4.26	5.5

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis [i](#)

8.1 Conformationally restricting restraints [i](#)

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	464
Intra-residue ($ i-j =0$)	2
Sequential ($ i-j =1$)	108
Medium range ($ i-j >1$ and $ i-j <5$)	244
Long range ($ i-j \geq 5$)	110
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	3.7
Number of long range restraints per residue ¹	0.9

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 [i](#)

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 [i](#)

Distance violations less than 0.1 Å are not included in the calculation. There are no distance violations

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

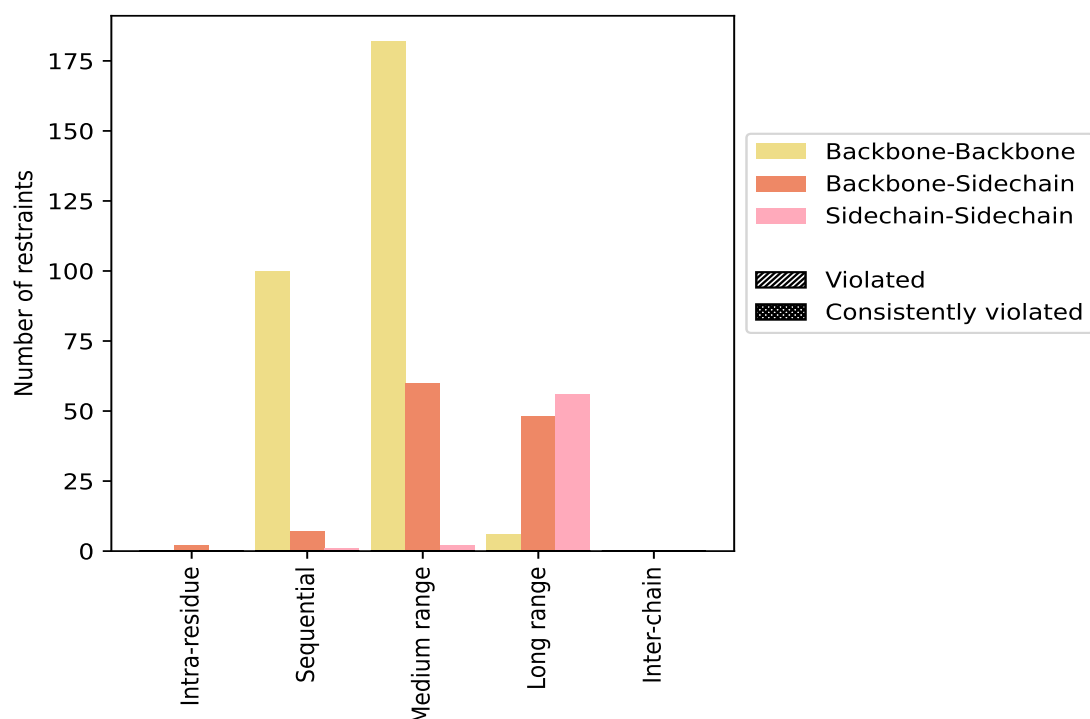
9.1 Summary of distance violations

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$)	2	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	0.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	108	23.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	100	21.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	7	1.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1	0.2	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	244	52.6	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	182	39.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	60	12.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	2	0.4	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	110	23.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	6	1.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	48	10.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	56	12.1	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	464	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	288	62.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	117	25.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	59	12.7	0	0.0	0.0	0	0.0	0.0

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

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

No violations found

9.3 Distance violation statistics for the ensemble [i](#)

No violations found

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

No violations found

9.5 All violated distance restraints [i](#)

No violations found

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found