



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 07:43 PM UTC

PDB ID : 2MZW / pdb_00002mzw
BMRB ID : 25504
Title : Staphylococcus aureus FusB:EF-GC3 complex
Authors : Tomlinson, J.H.; Thompson, G.S.; Kalverda, A.P.; Zhuravleva, A.; O'Neill, A.
Deposited on : 2015-02-25

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

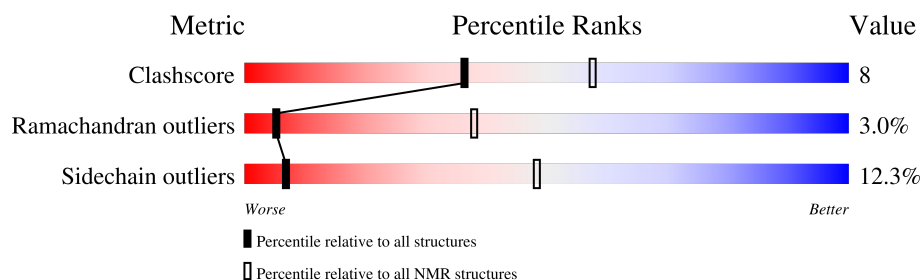
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 12%.

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	301	 65% 28% . .
2	B	233	 74% 16% . 9%

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8050 atoms, of which 4018 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms						Trace
1	A	292	Total	C	H	N	O	S	0
			4471	1417	2214	378	445	17	

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	693	GLU	-	expression tag	UNP W8UT26
A	694	LEU	-	expression tag	UNP W8UT26
A	695	GLU	-	expression tag	UNP W8UT26
A	696	HIS	-	expression tag	UNP W8UT26
A	697	HIS	-	expression tag	UNP W8UT26
A	698	HIS	-	expression tag	UNP W8UT26
A	699	HIS	-	expression tag	UNP W8UT26
A	700	HIS	-	expression tag	UNP W8UT26
A	701	HIS	-	expression tag	UNP W8UT26

- Molecule 2 is a protein called Far1.

Mol	Chain	Residues	Atoms						Trace
2	B	213	Total	C	H	N	O	S	0
			3578	1143	1804	291	332	8	

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q8GNY5
B	-18	GLY	-	expression tag	UNP Q8GNY5
B	-17	SER	-	expression tag	UNP Q8GNY5
B	-16	SER	-	expression tag	UNP Q8GNY5
B	-15	HIS	-	expression tag	UNP Q8GNY5
B	-14	HIS	-	expression tag	UNP Q8GNY5
B	-13	HIS	-	expression tag	UNP Q8GNY5
B	-12	HIS	-	expression tag	UNP Q8GNY5
B	-11	HIS	-	expression tag	UNP Q8GNY5
B	-10	HIS	-	expression tag	UNP Q8GNY5
B	-9	SER	-	expression tag	UNP Q8GNY5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	SER	-	expression tag	UNP Q8GNY5
B	-7	GLY	-	expression tag	UNP Q8GNY5
B	-6	LEU	-	expression tag	UNP Q8GNY5
B	-5	VAL	-	expression tag	UNP Q8GNY5
B	-4	PRO	-	expression tag	UNP Q8GNY5
B	-3	ASN	-	expression tag	UNP Q8GNY5
B	-2	GLY	-	expression tag	UNP Q8GNY5
B	-1	SER	-	expression tag	UNP Q8GNY5
B	0	HIS	-	expression tag	UNP Q8GNY5

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
3	B	1	Total	Zn
			1	1

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 1 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
X-PLOR NIH	structure solution	2.33.0
X-PLOR NIH	refinement	2.33.0
HADDOCK	structure solution	2.1
HADDOCK	refinement	2.1

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	2
Total number of shifts	812
Number of shifts mapped to atoms	808
Number of unparsed shifts	0
Number of shifts with mapping errors	4
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	12%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2257	2214	2204	52
2	B	1774	1804	1805	22
3	B	1	0	0	2
All	All	4032	4018	4009	62

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:169:PHE:HB2	2:B:188:ILE:HG12	0.90	1.40
2:B:195:CYS:HG	3:B:301:ZN:ZN	0.83	0.78
1:A:525:GLU:HG2	2:B:183:LYS:HB2	0.82	1.49
1:A:525:GLU:HA	2:B:183:LYS:HD3	0.73	1.58
2:B:195:CYS:SG	3:B:301:ZN:ZN	0.72	1.77
1:A:533:VAL:HB	1:A:534:PRO:HD3	0.70	1.63
1:A:606:LYS:HA	1:A:645:TYR:HB3	0.68	1.64
1:A:522:PHE:HB3	2:B:168:LEU:HD13	0.67	1.67
1:A:467:LYS:HA	1:A:467:LYS:HE2	0.65	1.68
2:B:157:CYS:SG	2:B:188:ILE:HA	0.65	2.31
1:A:519:GLY:HA3	2:B:158:THR:HG23	0.65	1.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:546:LYS:O	1:A:550:GLU:HG2	0.64	1.91
1:A:639:ALA:HB3	2:B:35:VAL:HG21	0.60	1.72
1:A:602:GLU:HB2	1:A:678:VAL:CG1	0.58	2.28
1:A:606:LYS:HA	1:A:645:TYR:CB	0.55	2.30
2:B:8:HIS:CD2	2:B:201:ASP:HA	0.55	2.37
1:A:612:PRO:HA	1:A:639:ALA:HA	0.54	1.77
1:A:665:ARG:HD2	2:B:29:ASP:OD1	0.54	2.02
1:A:522:PHE:HB2	2:B:187:TYR:HE1	0.54	1.62
1:A:482:TYR:O	1:A:483:ARG:HB2	0.53	2.02
1:A:609:ILE:HB	1:A:642:VAL:HB	0.53	1.78
1:A:604:MET:HA	1:A:647:PRO:HA	0.52	1.80
1:A:485:THR:O	1:A:486:PHE:HB2	0.52	2.05
2:B:23:VAL:HG21	2:B:36:ILE:HG13	0.52	1.81
1:A:628:GLY:HA2	1:A:646:VAL:HG22	0.51	1.83
1:A:629:ARG:HB3	1:A:645:TYR:CE1	0.50	2.42
1:A:523:GLU:O	1:A:563:LYS:HA	0.49	2.06
1:A:486:PHE:CE2	1:A:515:PRO:HA	0.49	2.42
1:A:631:ASP:HB2	1:A:645:TYR:CE2	0.49	2.42
1:A:487:LYS:HG3	1:A:600:ILE:HD12	0.49	1.84
1:A:636:ARG:HB3	2:B:35:VAL:HG22	0.48	1.85
2:B:157:CYS:O	2:B:161:ASN:HA	0.48	2.08
2:B:90:SER:HB2	2:B:92:GLN:OE1	0.48	2.08
1:A:535:ARG:O	1:A:538:ILE:HG12	0.47	2.09
1:A:678:VAL:HB	1:A:679:PRO:HD2	0.47	1.85
1:A:510:HIS:HB2	1:A:568:ASP:HB3	0.47	1.86
1:A:647:PRO:O	1:A:679:PRO:HD3	0.47	2.09
1:A:538:ILE:HG13	1:A:539:PRO:HD3	0.46	1.87
1:A:603:PRO:HA	1:A:676:ALA:O	0.46	2.11
2:B:63:MET:HA	2:B:63:MET:HE2	0.46	1.87
1:A:558:PRO:HA	2:B:156:PHE:N	0.46	2.25
1:A:484:GLU:HA	1:A:560:ILE:CG2	0.45	2.41
1:A:481:SER:HA	1:A:650:GLU:OE2	0.45	2.12
1:A:423:MET:O	1:A:427:LEU:HG	0.45	2.12
1:A:538:ILE:N	1:A:539:PRO:HD2	0.44	2.27
1:A:413:GLU:HG3	1:A:447:GLN:HB3	0.44	1.88
1:A:556:GLY:CA	2:B:153:VAL:HG21	0.44	2.43
1:A:602:GLU:HB2	1:A:678:VAL:HG11	0.44	1.89
1:A:406:PRO:O	1:A:453:MET:HA	0.44	2.12
1:A:684:GLU:HA	1:A:687:ILE:HG22	0.44	1.89
1:A:611:MET:HE1	1:A:658:LEU:HD11	0.43	1.90
1:A:639:ALA:HB3	2:B:35:VAL:CG2	0.43	2.41
1:A:486:PHE:CE2	1:A:562:VAL:HA	0.43	2.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:678:VAL:HB	1:A:679:PRO:CD	0.43	2.44
1:A:602:GLU:HB2	1:A:678:VAL:HG13	0.42	1.91
1:A:600:ILE:HG23	1:A:676:ALA:O	0.42	2.15
1:A:406:PRO:HB2	1:A:407:VAL:H	0.41	1.53
1:A:539:PRO:HA	1:A:542:GLU:HG2	0.41	1.91
1:A:554:LEU:H	1:A:554:LEU:HD23	0.41	1.75
2:B:121:GLY:HA2	2:B:131:TYR:O	0.41	2.16
1:A:522:PHE:CA	1:A:561:ASP:HB3	0.40	2.46
1:A:520:ALA:HB3	2:B:187:TYR:HB2	0.40	1.92

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	290/301 (96%)	232 (80%)	44 (15%)	14 (5%)	3	25
2	B	211/233 (91%)	199 (94%)	11 (5%)	1 (0%)	26	74
All	All	501/534 (94%)	431 (86%)	55 (11%)	15 (3%)	5	38

All 15 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	406	PRO
1	A	442	ASP
1	A	483	ARG
1	A	486	PHE
1	A	501	GLY
1	A	520	ALA
1	A	522	PHE
1	A	533	VAL
1	A	558	PRO
1	A	561	ASP
1	A	572	HIS
1	A	597	ASP
1	A	633	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	650	GLU
2	B	159	ILE

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	243/252 (96%)	210 (86%)	33 (14%)	6	45
2	B	204/221 (92%)	182 (89%)	22 (11%)	8	52
All	All	447/473 (95%)	392 (88%)	55 (12%)	7	48

All 55 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	409	HIS
1	A	411	SER
1	A	412	VAL
1	A	431	GLN
1	A	436	THR
1	A	438	HIS
1	A	440	HIS
1	A	443	GLU
1	A	445	THR
1	A	449	ILE
1	A	458	LEU
1	A	472	GLU
1	A	489	SER
1	A	498	ARG
1	A	499	GLN
1	A	505	GLN
1	A	511	ILE
1	A	518	THR
1	A	540	SER
1	A	545	LEU
1	A	550	GLU
1	A	561	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	576	SER
1	A	610	GLU
1	A	613	GLU
1	A	624	THR
1	A	629	ARG
1	A	636	ARG
1	A	649	SER
1	A	652	PHE
1	A	656	THR
1	A	678	VAL
1	A	681	SER
2	B	8	HIS
2	B	43	ASP
2	B	52	ASP
2	B	53	ASP
2	B	54	ASP
2	B	60	LYS
2	B	87	GLU
2	B	106	ILE
2	B	123	ASN
2	B	124	GLU
2	B	127	SER
2	B	144	LEU
2	B	152	VAL
2	B	158	THR
2	B	161	ASN
2	B	163	GLU
2	B	175	THR
2	B	177	SER
2	B	184	LYS
2	B	186	ASP
2	B	188	ILE
2	B	200	THR

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](#)

Of 1 ligands modelled in this entry, 1 is 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 12% for the well-defined parts and 12% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *C3_assigned_chem_shift_list*

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	560
Number of shifts mapped to atoms	560
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	129	0.36 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	117	0.12 ± 0.14	None needed (< 0.5 ppm)
^{15}N	157	-0.33 ± 0.25	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 8%, i.e. 560 atoms were assigned a chemical shift out of a possible 6939. 0 out of 72 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	560/2519 (22%)	157/1024 (15%)	246/1010 (24%)	157/485 (32%)
Sidechain	0/3884 (0%)	0/2511 (0%)	0/1230 (0%)	0/143 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/536 (0%)	0/255 (0%)	0/260 (0%)	0/21 (0%)
Overall	560/6939 (8%)	157/3790 (4%)	246/2500 (10%)	157/649 (24%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 560 atoms were assigned a chemical shift out of a possible 6939. 0 out of 72 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	560/2519 (22%)	157/1024 (15%)	246/1010 (24%)	157/485 (32%)
Sidechain	0/3884 (0%)	0/2511 (0%)	0/1230 (0%)	0/143 (0%)
Aromatic	0/536 (0%)	0/255 (0%)	0/260 (0%)	0/21 (0%)
Overall	560/6939 (8%)	157/3790 (4%)	246/2500 (10%)	157/649 (24%)

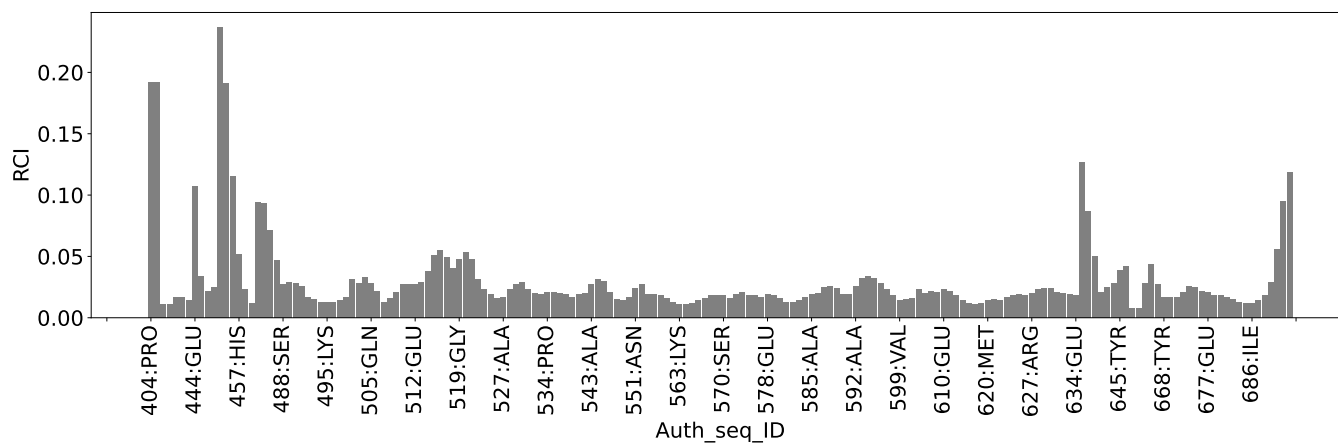
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *C3_assigned_chem_shift_list_dup*

7.2.1 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	252
Number of shifts mapped to atoms	248
Number of unparsed shifts	0
Number of shifts with mapping errors	4
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 4 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	B	-6	LEU	H	7.973	0.01	1
2	B	-6	LEU	N	122.04	0.02	1
2	B	-5	VAL	H	8.008	0.01	1
2	B	-5	VAL	N	122.816	0.02	1

7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	126	-0.23 ± 0.38	None needed (< 0.5 ppm)

7.2.3 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 4%, i.e. 248 atoms were assigned a chemical

shift out of a possible 6939. 0 out of 72 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	248/2519 (10%)	124/1024 (12%)	0/1010 (0%)	124/485 (26%)
Sidechain	0/3884 (0%)	0/2511 (0%)	0/1230 (0%)	0/143 (0%)
Aromatic	0/536 (0%)	0/255 (0%)	0/260 (0%)	0/21 (0%)
Overall	248/6939 (4%)	124/3790 (3%)	0/2500 (0%)	124/649 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 248 atoms were assigned a chemical shift out of a possible 6939. 0 out of 72 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	248/2519 (10%)	124/1024 (12%)	0/1010 (0%)	124/485 (26%)
Sidechain	0/3884 (0%)	0/2511 (0%)	0/1230 (0%)	0/143 (0%)
Aromatic	0/536 (0%)	0/255 (0%)	0/260 (0%)	0/21 (0%)
Overall	248/6939 (4%)	124/3790 (3%)	0/2500 (0%)	124/649 (19%)

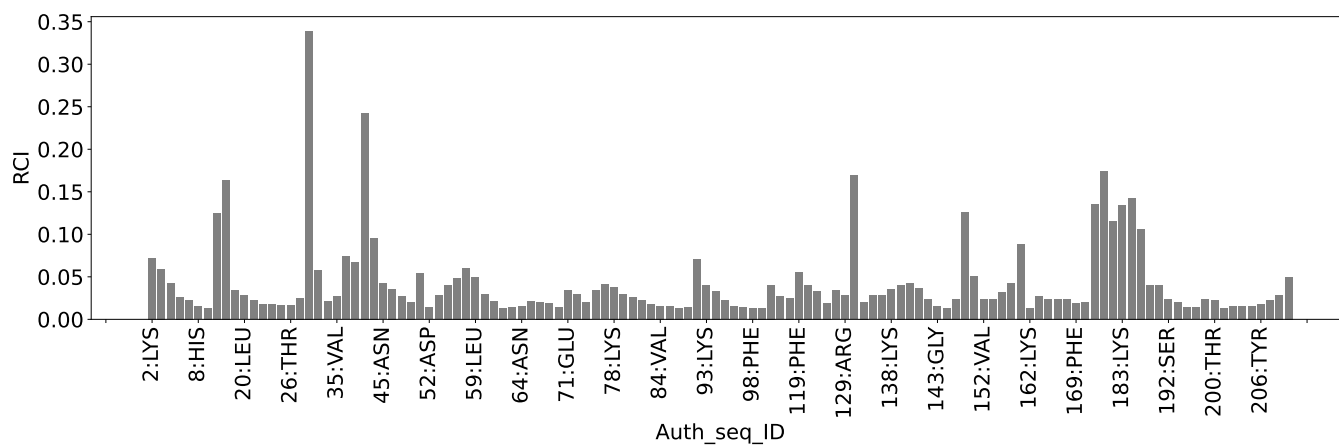
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 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 B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	173
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	173
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.3
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)	4.0	0.2
0.2-0.5 (Medium)	3.0	0.31
>0.5 (Large)	20.0	11.76

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 ⓘ

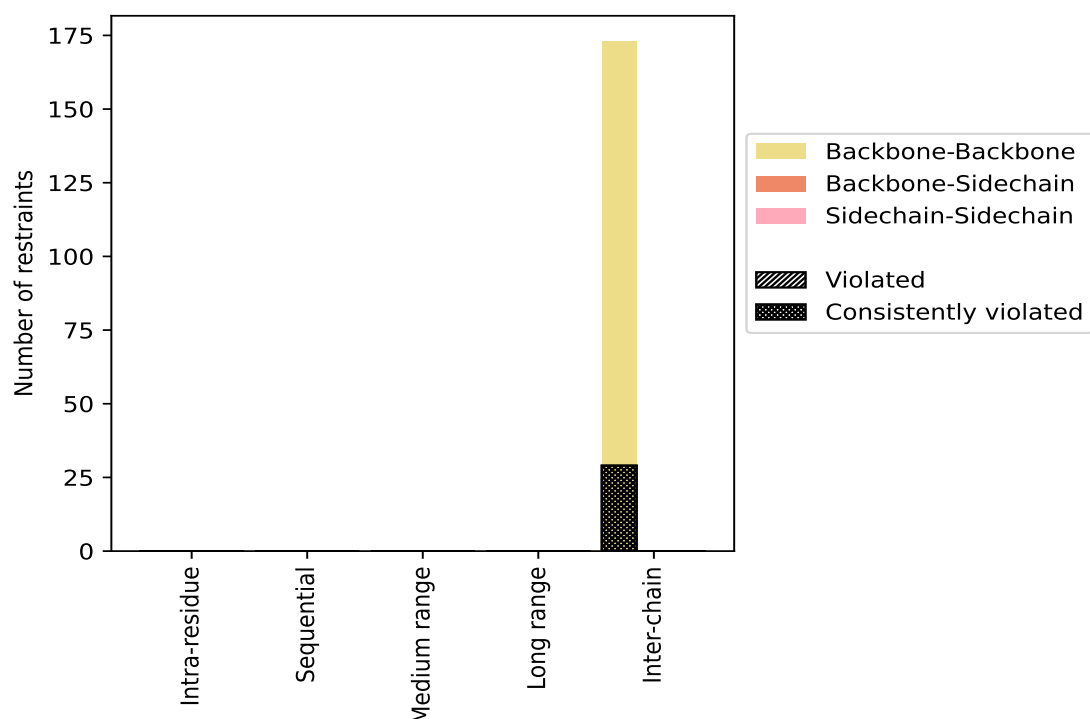
9.1 Summary of distance violations ⓘ

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 \geq 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	173	100.0	29	16.8	16.8	29	16.8	16.8
Backbone-Backbone	173	100.0	29	16.8	16.8	29	16.8	16.8
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	173	100.0	29	16.8	16.8	29	16.8	16.8
Backbone-Backbone	173	100.0	29	16.8	16.8	29	16.8	16.8
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

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

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



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

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

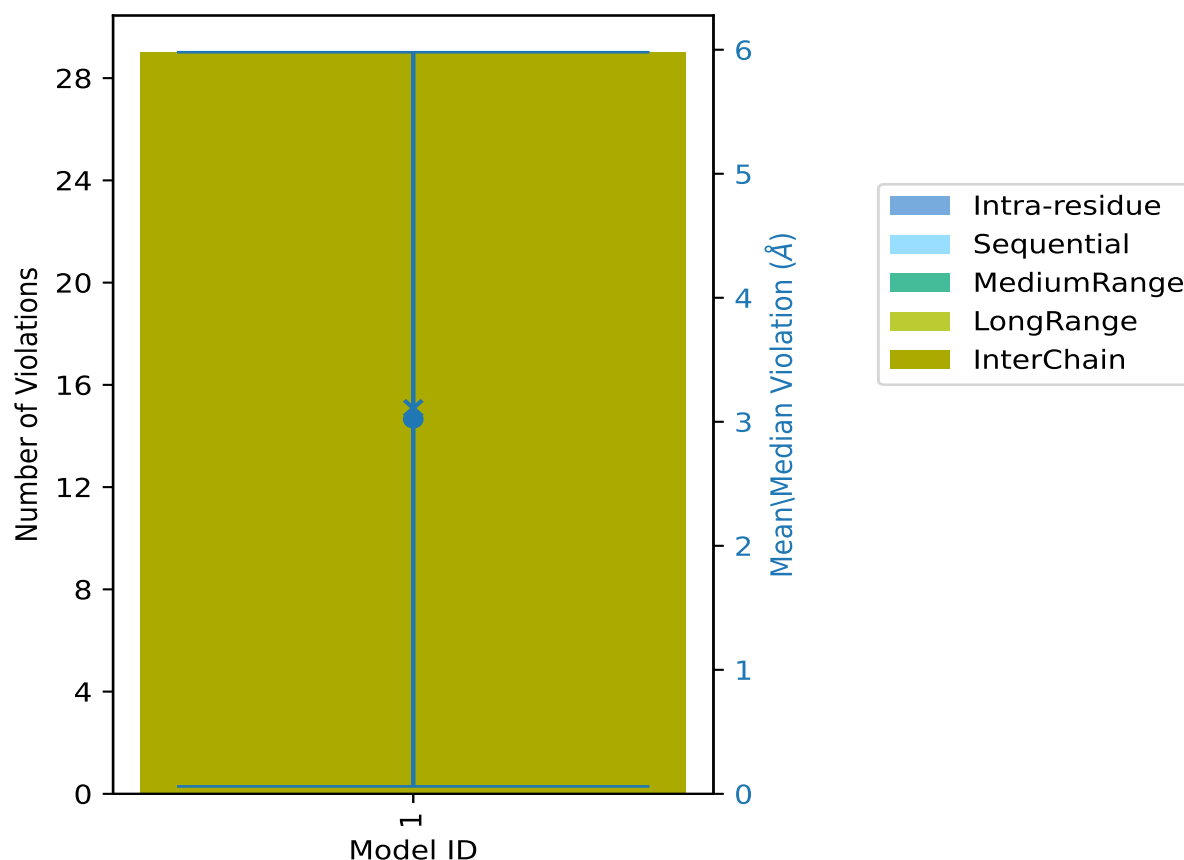
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	0	29	29	3.02	11.76	2.96	3.11

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](#)

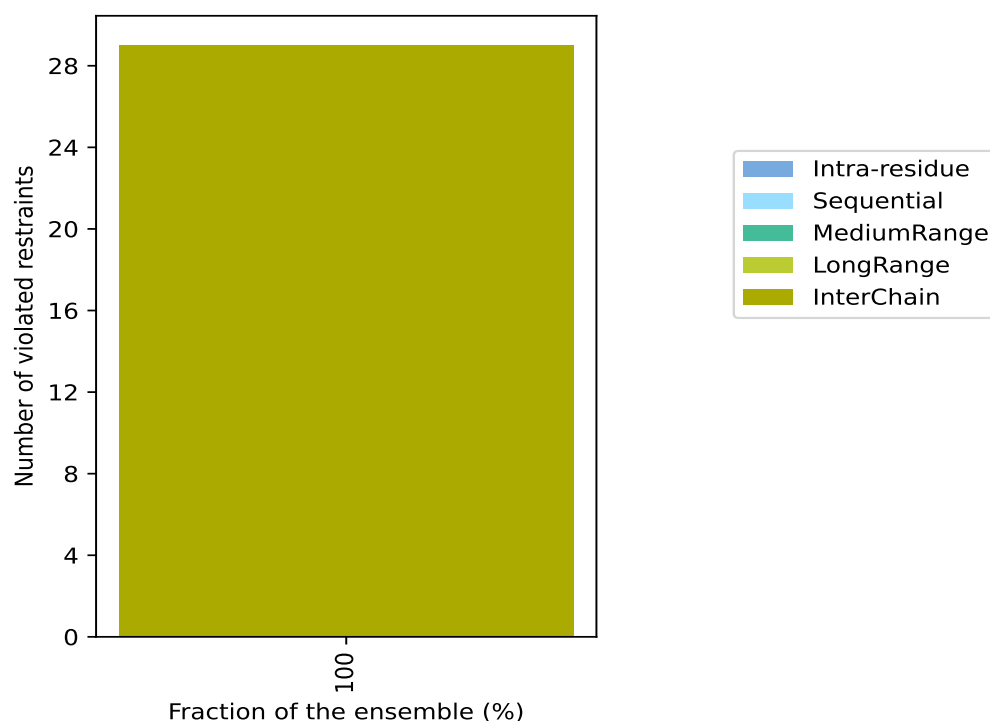
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 144(IR:0, SQ:0, MR:0, LR:0, IC:144) restraints are not violated 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	29	29	1	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

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



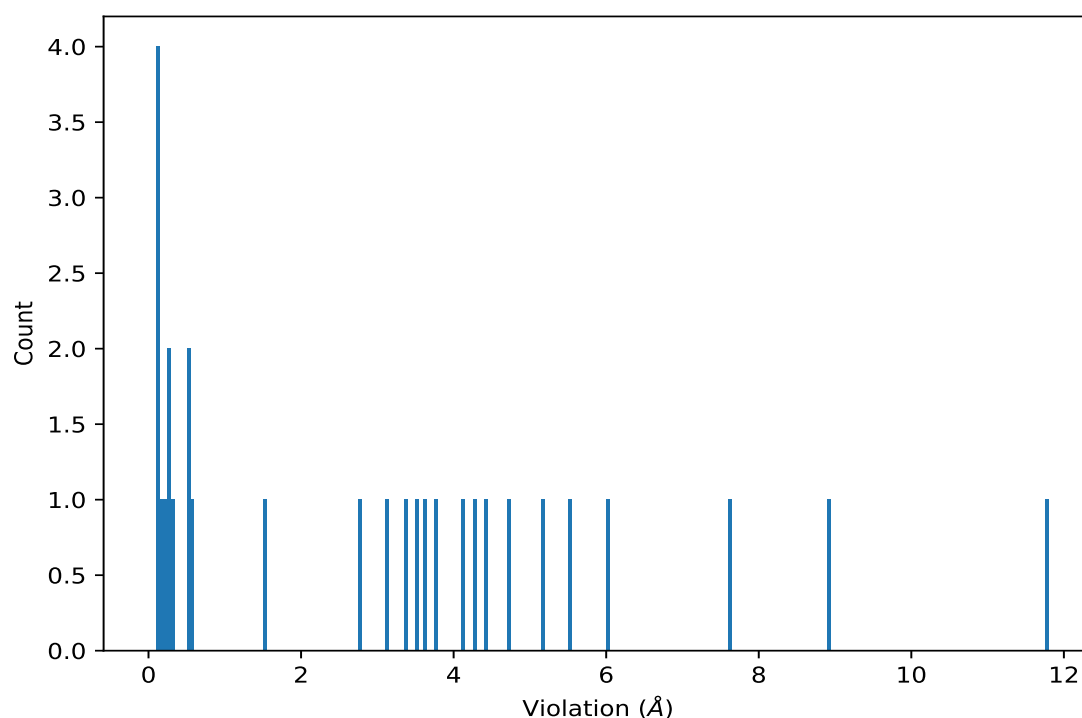
9.4 Most violated distance restraints in the ensemble [i](#)

No violations found

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)
(1,1)	1:490:A:ALA:H	2:182:B:VAL:HG11	1	11.76
(1,35)	2:200:B:THR:HG1	1:519:A:GLY:HA2	1	8.91
(1,12)	1:529:A:VAL:H	2:183:B:LYS:HD2	1	7.63
(1,2)	1:514:A:THR:HG1	2:183:B:LYS:O	1	6.03
(1,18)	2:152:B:VAL:HA	1:522:A:PHE:HE2	1	5.53
(1,26)	2:162:B:LYS:H	1:519:A:GLY:HA2	1	5.17
(1,20)	2:155:B:GLY:C	1:519:A:GLY:O	1	4.7
(1,10)	1:527:A:ALA:N	2:183:B:LYS:HD2	1	4.41
(3,12)	2:19:B:ARG:CA	1:615:A:TYR:H	1	4.25
(1,16)	1:566:A:LEU:H	2:183:B:LYS:HD3	1	4.11
(1,11)	1:528:A:ILE:HD13	2:172:B:LYS:HZ1	1	3.77
(3,3)	2:26:B:THR:CA	1:615:A:TYR:H	1	3.6
(1,15)	1:564:A:ALA:O	2:183:B:LYS:HB2	1	3.51
(1,24)	2:159:B:ILE:H	1:519:A:GLY:O	1	3.39
(1,19)	2:153:B:VAL:HG23	1:522:A:PHE:HE2	1	3.11
(1,27)	2:167:B:SER:C	1:522:A:PHE:HD2	1	2.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	2:157:B:CYS:C	1:519:A:GLY:O	1	1.51
(1,21)	2:156:B:PHE:O	1:519:A:GLY:O	1	0.59
(1,30)	2:172:B:LYS:HZ1	1:526:A:ASN:HD22	1	0.54
(1,9)	1:526:A:ASN:HD22	2:183:B:LYS:HD2	1	0.52
(3,19)	2:19:B:ARG:CA	1:645:A:TYR:H	1	0.31
(1,36)	2:211:B:LYS:HZ1	1:516:A:ASN:OD1	1	0.3
(1,3)	1:516:A:ASN:OD1	2:211:B:LYS:HZ1	1	0.3
(3,20)	2:19:B:ARG:CA	1:664:A:GLY:H	1	0.2
(3,13)	2:19:B:ARG:CA	1:631:A:ASP:H	1	0.19
(1,7)	1:524:A:PHE:O	2:183:B:LYS:HZ1	1	0.15
(2,86)	2:150:B:ASN:CA	1:519:A:GLY:H	1	0.14
(3,4)	2:26:B:THR:CA	1:650:A:GLU:H	1	0.1
(1,29)	2:170:B:MET:HG3	1:523:A:GLU:OE2	1	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found