



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 04:04 PM UTC

PDB ID : 2MF8 / pdb_00002mf8
BMRB ID : 19540
Title : HADDOCK model of MyT1 F4F5 - DNA complex
Authors : Gamsjaeger, R.; O'Connell, M.R.; Cubeddu, L.; Shepherd, N.E.; Lowry, J.A.;
Kwan, A.H.; Vandevenne, M.; Swanton, M.K.; Matthews, J.M.; Mackay, J.P.
Deposited on : 2013-10-08

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

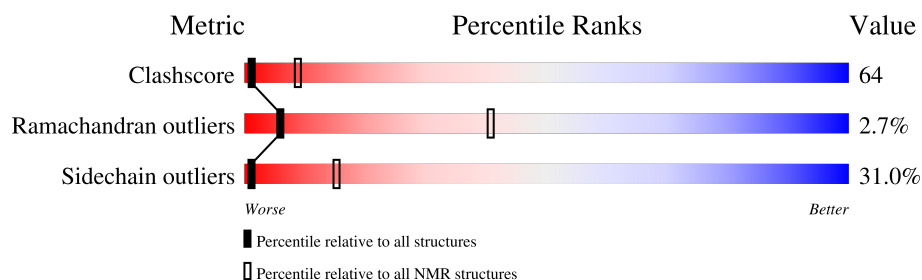
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 16%.

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	93	
2	B	13	
3	C	13	

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 4 unique types of molecules in this entry. The entry contains 1853 atoms, of which 796 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Myelin transcription factor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	75	Total	C	H	N	O	S	0
			1029	316	501	102	103	7	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	788	GLY	-	expression tag	UNP Q8CFC2
A	789	PRO	-	expression tag	UNP Q8CFC2
A	790	LEU	-	expression tag	UNP Q8CFC2
A	791	GLY	-	expression tag	UNP Q8CFC2
A	793	PHE	LYS	conflict	UNP Q8CFC2
A	879	ARG	LYS	conflict	UNP Q8CFC2

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*CP*CP*GP*AP*AP*AP*GP*TP*TP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms						Trace
2	B	13	Total	C	H	N	O	P	0
			408	126	146	51	73	12	

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*TP*GP*AP*AP*CP*TP*TP*TP*CP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms						Trace
3	C	13	Total	C	H	N	O	P	0
			414	128	149	46	79	12	

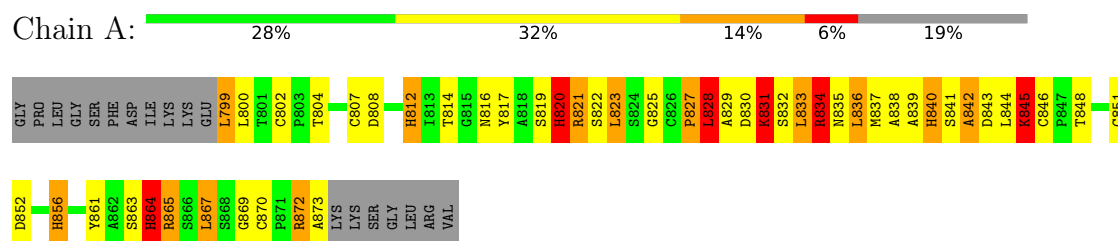
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
4	A	2	Total	Zn
			2	2

4 Residue-property plots [i](#)

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: Myelin transcription factor 1



- Molecule 2: DNA (5'-D(*AP*CP*CP*GP*AP*AP*AP*GP*TP*TP*CP*AP*C)-3')



- Molecule 3: DNA (5'-D(*GP*TP*GP*AP*AP*CP*TP*TP*TP*CP*GP*GP*T)-3')



5 Refinement protocol and experimental data overview

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

Of the 10 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
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	217
Number of shifts mapped to atoms	217
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	16%

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	3.63	74/540 (13.7%)	1.65	13/732 (1.8%)
2	B	2.16	6/294 (2.0%)	2.65	25/451 (5.5%)
3	C	2.22	6/296 (2.0%)	2.61	22/456 (4.8%)
All	All	2.97	86/1130 (7.6%)	2.25	60/1639 (3.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0	3
All	All	0	3

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	844	LEU	C-N	-24.66	0.98	1.33
3	C	15	DT	O3'-P	-22.83	1.26	1.61
2	B	12	DA	O3'-P	-22.38	1.27	1.61
3	C	22	DT	O3'-P	-22.29	1.27	1.61
2	B	1	DA	O3'-P	-22.29	1.27	1.61
1	A	842	ALA	C-N	-17.95	1.03	1.33
1	A	836	LEU	C-N	-17.38	1.08	1.33
1	A	842	ALA	C-O	16.16	1.43	1.23
1	A	872	ARG	C-O	-14.48	1.05	1.24
1	A	841	SER	CA-CB	14.41	1.71	1.52
1	A	833	LEU	C-O	13.02	1.40	1.24
1	A	839	ALA	C-N	-12.88	1.16	1.33
1	A	828	LEU	CG-CD1	12.49	1.93	1.52
1	A	835	ASN	C-O	-12.29	1.08	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	872	ARG	CD-NE	-11.37	1.30	1.46
1	A	831	LYS	CD-CE	11.35	1.86	1.52
1	A	834	ARG	CB-CG	11.34	1.86	1.52
1	A	839	ALA	CA-CB	10.71	1.69	1.53
1	A	844	LEU	CA-CB	10.67	1.71	1.53
2	B	3	DC	O3'-P	-10.27	1.45	1.61
3	C	23	DC	O3'-P	-10.17	1.45	1.61
1	A	828	LEU	CG-CD2	10.03	1.85	1.52
2	B	2	DC	O3'-P	-9.92	1.46	1.61
1	A	872	ARG	CB-CG	9.78	1.81	1.52
1	A	872	ARG	NE-CZ	-9.64	1.22	1.33
1	A	833	LEU	CG-CD1	9.44	1.83	1.52
3	C	24	DG	O3'-P	-9.41	1.47	1.61
1	A	836	LEU	CG-CD2	9.27	1.83	1.52
1	A	829	ALA	CA-CB	9.25	1.68	1.53
3	C	14	DG	O3'-P	-9.25	1.47	1.61
1	A	836	LEU	C-O	9.20	1.36	1.23
3	C	25	DG	O3'-P	-9.18	1.47	1.61
1	A	838	ALA	CA-CB	9.11	1.68	1.53
1	A	831	LYS	CA-C	8.97	1.64	1.53
1	A	835	ASN	C-N	8.81	1.46	1.33
1	A	828	LEU	N-CA	8.78	1.57	1.46
1	A	840	HIS	C-N	-8.77	1.21	1.33
1	A	842	ALA	N-CA	8.63	1.56	1.46
1	A	838	ALA	C-O	-8.61	1.13	1.24
1	A	834	ARG	C-O	-8.42	1.13	1.24
1	A	829	ALA	N-CA	-8.36	1.35	1.46
1	A	835	ASN	N-CA	-8.06	1.35	1.46
1	A	834	ARG	CA-C	8.06	1.63	1.52
1	A	831	LYS	CB-CG	7.98	1.76	1.52
1	A	838	ALA	C-N	7.57	1.43	1.33
1	A	799	LEU	CB-CG	7.49	1.68	1.53
1	A	827	PRO	C-N	-7.49	1.23	1.33
1	A	800	LEU	C-N	-7.41	1.24	1.33
1	A	833	LEU	C-N	-7.34	1.23	1.33
1	A	834	ARG	NE-CZ	-7.28	1.25	1.33
1	A	844	LEU	CA-C	7.27	1.62	1.52
1	A	873	ALA	C-O	-6.98	1.09	1.23
1	A	828	LEU	CA-CB	6.98	1.65	1.53
1	A	864	HIS	CD2-NE2	6.96	1.45	1.37
2	B	11	DC	O3'-P	-6.85	1.50	1.61
1	A	799	LEU	C-N	-6.83	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	839	ALA	C-O	6.62	1.33	1.23
1	A	799	LEU	CA-C	6.40	1.66	1.52
1	A	831	LYS	CA-CB	6.34	1.67	1.53
1	A	833	LEU	CG-CD2	6.26	1.73	1.52
2	B	4	DG	O3'-P	-6.20	1.51	1.61
1	A	834	ARG	C-N	6.09	1.42	1.33
1	A	799	LEU	CG-CD1	6.03	1.72	1.52
1	A	844	LEU	CG-CD1	5.97	1.72	1.52
1	A	799	LEU	CG-CD2	5.92	1.72	1.52
1	A	831	LYS	C-N	-5.90	1.25	1.33
1	A	800	LEU	CA-CB	5.79	1.62	1.53
1	A	872	ARG	CG-CD	5.76	1.69	1.52
1	A	836	LEU	CA-CB	5.70	1.60	1.53
1	A	830	ASP	C-N	-5.64	1.24	1.34
1	A	800	LEU	CG-CD2	5.63	1.71	1.52
1	A	800	LEU	CG-CD1	5.61	1.71	1.52
1	A	834	ARG	CD-NE	5.56	1.54	1.46
1	A	833	LEU	CA-C	-5.55	1.45	1.52
1	A	836	LEU	CG-CD1	5.54	1.70	1.52
1	A	844	LEU	C-O	5.50	1.31	1.24
1	A	841	SER	C-O	5.50	1.30	1.23
1	A	864	HIS	CB-CG	5.49	1.57	1.50
1	A	837	MET	CB-CG	5.28	1.68	1.52
1	A	837	MET	C-N	-5.21	1.26	1.33
1	A	828	LEU	C-O	-5.13	1.17	1.24
1	A	841	SER	C-N	-5.12	1.26	1.33
1	A	832	SER	CA-CB	5.11	1.62	1.53
1	A	834	ARG	CZ-NH2	-5.03	1.26	1.33
1	A	828	LEU	CA-C	-5.03	1.46	1.52
1	A	845	LYS	CB-CG	5.03	1.67	1.52

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	842	ALA	CA-C-O	-15.52	101.98	120.60
2	B	1	DA	P-O3'-C3'	-14.31	98.73	120.20
2	B	12	DA	P-O3'-C3'	-14.22	98.86	120.20
2	B	12	DA	OP1-P-O3'	-14.18	65.46	108.00
3	C	22	DT	OP1-P-O3'	-14.18	65.47	108.00
2	B	1	DA	OP1-P-O3'	-14.16	65.50	108.00
2	B	2	DC	OP1-P-O3'	-14.03	65.92	108.00
3	C	15	DT	OP1-P-O3'	-13.94	66.19	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	24	DG	OP1-P-O3'	-13.87	66.38	108.00
2	B	3	DC	OP1-P-O3'	-13.85	66.46	108.00
3	C	23	DC	OP1-P-O3'	-13.80	66.58	108.00
3	C	22	DT	P-O3'-C3'	-13.46	100.02	120.20
2	B	2	DC	P-O3'-C3'	-12.97	100.74	120.20
3	C	24	DG	P-O3'-C3'	-12.83	100.95	120.20
3	C	15	DT	P-O3'-C3'	-12.74	101.09	120.20
2	B	3	DC	P-O3'-C3'	-12.45	101.53	120.20
3	C	23	DC	P-O3'-C3'	-12.43	101.56	120.20
1	A	836	LEU	CA-C-O	-11.13	107.37	121.17
2	B	1	DA	OP2-P-O3'	10.68	140.04	108.00
2	B	12	DA	OP2-P-O3'	10.64	139.92	108.00
3	C	25	DG	OP1-P-O3'	-10.60	76.20	108.00
3	C	14	DG	OP1-P-O3'	-10.57	76.30	108.00
3	C	22	DT	OP2-P-O3'	10.35	139.03	108.00
3	C	15	DT	OP2-P-O3'	10.11	138.34	108.00
2	B	4	DG	OP1-P-O3'	-10.07	77.77	108.00
2	B	11	DC	OP1-P-O3'	-10.00	78.00	108.00
3	C	24	DG	OP2-P-O3'	9.10	135.30	108.00
2	B	2	DC	OP2-P-O3'	8.97	134.91	108.00
3	C	23	DC	OP2-P-O3'	8.81	134.45	108.00
2	B	3	DC	OP2-P-O3'	8.81	134.42	108.00
1	A	844	LEU	CA-C-O	-8.21	109.66	119.27
1	A	835	ASN	CA-C-O	7.91	131.82	120.51
2	B	10	DT	OP1-P-O3'	-7.87	84.39	108.00
3	C	14	DG	P-O3'-C3'	-7.70	108.66	120.20
3	C	25	DG	P-O3'-C3'	-7.70	108.66	120.20
1	A	839	ALA	CA-C-O	-7.31	112.89	122.03
2	B	4	DG	P-O3'-C3'	-7.21	109.39	120.20
3	C	21	DT	OP1-P-O3'	-7.16	86.54	108.00
2	B	8	DG	C5'-C4'-C3'	-6.96	104.46	114.90
1	A	836	LEU	O-C-N	6.67	130.98	121.97
2	B	11	DC	P-O3'-C3'	-6.59	110.31	120.20
1	A	864	HIS	CE1-NE2-CD2	-6.57	102.43	109.00
3	C	21	DT	C5'-C4'-C3'	-6.56	105.06	114.90
1	A	864	HIS	CA-CB-CG	6.23	120.03	113.80
3	C	25	DG	O3'-P-O5'	6.11	113.17	104.00
3	C	14	DG	O3'-P-O5'	6.08	113.12	104.00
2	B	11	DC	O3'-P-O5'	6.07	113.11	104.00
1	A	820	HIS	CA-CB-CG	6.06	119.86	113.80
1	A	844	LEU	O-C-N	6.06	130.76	122.46
3	C	14	DG	OP2-P-O3'	5.93	125.80	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	25	DG	OP2-P-O3'	5.93	125.79	108.00
2	B	4	DG	OP2-P-O3'	5.92	125.75	108.00
1	A	829	ALA	N-CA-C	-5.80	103.69	112.04
2	B	9	DT	C5'-C4'-C3'	-5.76	106.27	114.90
2	B	11	DC	OP2-P-O3'	5.62	124.87	108.00
1	A	831	LYS	O-C-N	5.56	129.71	122.15
1	A	800	LEU	CA-C-O	-5.48	114.15	120.24
2	B	4	DG	O3'-P-O5'	5.46	112.19	104.00
2	B	10	DT	C5'-C4'-C3'	-5.42	106.78	114.90
2	B	10	DT	OP2-P-O3'	5.40	124.19	108.00

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	799	LEU	Mainchain
1	A	828	LEU	Mainchain
1	A	842	ALA	Mainchain

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	528	501	497	52
2	B	262	146	147	39
3	C	265	149	150	45
All	All	1057	796	794	118

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 64.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:831:LYS:CB	1:A:831:LYS:CG	1.58	1.76
1:A:836:LEU:CD2	1:A:836:LEU:CG	1.56	1.83
1:A:872:ARG:CB	1:A:872:ARG:CG	1.55	1.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:828:LEU:CD2	1:A:828:LEU:CG	1.54	1.85
1:A:833:LEU:CG	1:A:833:LEU:CD1	1.52	1.83
1:A:834:ARG:CB	1:A:834:ARG:CG	1.51	1.86
1:A:831:LYS:CD	1:A:831:LYS:CE	1.51	1.86
1:A:828:LEU:CG	1:A:828:LEU:CD1	1.43	1.93
1:A:864:HIS:NE2	1:A:870:CYS:SG	1.08	2.27
1:A:846:CYS:SG	1:A:864:HIS:NE2	1.03	2.32
3:C:16:DG:H2''	3:C:17:DA:OP2	0.92	1.64
1:A:867:LEU:HD11	2:B:10:DT:H71	0.91	1.41
2:B:8:DG:H2''	2:B:9:DT:OP2	0.87	1.68
3:C:20:DT:H2''	3:C:21:DT:OP2	0.83	1.73
2:B:9:DT:H2''	2:B:10:DT:OP2	0.83	1.74
2:B:8:DG:H1'	2:B:9:DT:H5'	0.82	1.51
2:B:5:DA:H2''	2:B:6:DA:OP2	0.79	1.75
3:C:18:DA:H2''	3:C:19:DC:OP2	0.79	1.76
3:C:19:DC:H2''	3:C:20:DT:H71	0.79	1.54
2:B:6:DA:H2''	2:B:7:DA:OP2	0.79	1.77
2:B:7:DA:H2''	2:B:8:DG:OP2	0.78	1.77
1:A:851:CYS:SG	1:A:864:HIS:CE1	0.78	2.76
3:C:17:DA:H2''	3:C:18:DA:OP2	0.77	1.77
3:C:23:DC:H2''	3:C:24:DG:OP2	0.77	1.71
1:A:861:TYR:CD1	3:C:16:DG:H5''	0.76	2.15
3:C:15:DT:H2''	3:C:16:DG:OP2	0.76	1.75
1:A:814:THR:HG22	2:B:5:DA:OP1	0.76	1.81
3:C:25:DG:H2''	3:C:26:DT:OP2	0.75	1.76
2:B:4:DG:H2''	2:B:5:DA:OP2	0.75	1.81
3:C:14:DG:H2''	3:C:15:DT:OP2	0.74	1.76
3:C:19:DC:H2''	3:C:20:DT:OP2	0.74	1.83
2:B:3:DC:H2''	2:B:4:DG:OP2	0.72	1.71
3:C:24:DG:H2''	3:C:25:DG:OP2	0.72	1.70
2:B:2:DC:H2''	2:B:3:DC:OP2	0.71	1.69
1:A:861:TYR:CE1	3:C:16:DG:H5''	0.69	2.21
1:A:816:ASN:HA	1:A:840:HIS:NE2	0.69	2.02
2:B:11:DC:H2''	2:B:12:DA:OP2	0.68	1.82
1:A:816:ASN:HA	1:A:840:HIS:CD2	0.67	2.24
1:A:823:LEU:HD11	3:C:21:DT:H71	0.65	1.69
3:C:16:DG:C2'	3:C:17:DA:OP2	0.64	2.45
1:A:823:LEU:HD21	3:C:21:DT:H71	0.63	1.70
3:C:21:DT:H2''	3:C:22:DT:OP2	0.62	1.95
1:A:817:TYR:CE1	2:B:5:DA:H4'	0.62	2.30
3:C:19:DC:C2'	3:C:20:DT:H71	0.61	2.25
1:A:821:ARG:HE	2:B:7:DA:H62	0.61	1.38

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:843:ASP:OD1	1:A:845:LYS:HG3	0.60	1.95
1:A:864:HIS:CD2	1:A:870:CYS:SG	0.59	2.94
1:A:831:LYS:CB	1:A:831:LYS:CD	0.59	2.79
1:A:831:LYS:CG	1:A:831:LYS:CA	0.58	2.79
1:A:865:ARG:NE	3:C:18:DA:H62	0.57	1.97
3:C:25:DG:C2'	3:C:26:DT:OP2	0.57	2.51
1:A:851:CYS:SG	1:A:864:HIS:NE2	0.56	2.77
3:C:23:DC:C2'	3:C:24:DG:OP2	0.56	2.47
3:C:24:DG:C2'	3:C:25:DG:OP2	0.56	2.46
3:C:14:DG:C2'	3:C:15:DT:OP2	0.56	2.50
1:A:828:LEU:CD2	1:A:828:LEU:CB	0.56	2.78
3:C:20:DT:H1'	3:C:21:DT:H5'	0.55	1.77
1:A:851:CYS:SG	1:A:864:HIS:HE1	0.55	2.24
3:C:17:DA:O5'	3:C:17:DA:C2'	0.55	2.54
2:B:8:DG:O5'	2:B:8:DG:H2'	0.55	2.02
1:A:872:ARG:CG	1:A:872:ARG:CA	0.55	2.80
1:A:807:CYS:SG	1:A:827:PRO:HD2	0.55	2.41
2:B:8:DG:O5'	2:B:8:DG:C2'	0.55	2.53
1:A:823:LEU:HD21	3:C:21:DT:C7	0.54	2.32
2:B:2:DC:C2'	2:B:3:DC:OP2	0.54	2.45
3:C:17:DA:O5'	3:C:17:DA:H2'	0.54	2.03
1:A:828:LEU:CD1	1:A:828:LEU:CB	0.54	2.81
2:B:9:DT:C2'	2:B:10:DT:OP2	0.54	2.54
1:A:822:SER:HB2	3:C:20:DT:H72	0.53	1.79
2:B:10:DT:O5'	2:B:10:DT:C2'	0.53	2.56
2:B:10:DT:O5'	2:B:10:DT:H2'	0.53	2.03
3:C:21:DT:O5'	3:C:21:DT:C2'	0.53	2.56
2:B:8:DG:C2'	2:B:9:DT:OP2	0.53	2.50
3:C:21:DT:O5'	3:C:21:DT:H2'	0.53	2.04
1:A:834:ARG:CB	1:A:834:ARG:CD	0.52	2.82
1:A:812:HIS:CD2	1:A:817:TYR:HB2	0.52	2.39
2:B:9:DT:C2'	2:B:9:DT:O5'	0.52	2.56
2:B:9:DT:O5'	2:B:9:DT:H2'	0.52	2.04
1:A:836:LEU:CD2	1:A:836:LEU:CD1	0.52	2.83
3:C:20:DT:C2'	3:C:21:DT:OP2	0.51	2.55
3:C:15:DT:C2'	3:C:16:DG:OP2	0.51	2.45
2:B:7:DA:C2'	2:B:8:DG:OP2	0.51	2.56
2:B:7:DA:H2''	2:B:8:DG:C8	0.51	2.41
2:B:5:DA:C2'	2:B:6:DA:OP2	0.50	2.53
1:A:865:ARG:HE	3:C:18:DA:H62	0.50	1.47
2:B:7:DA:O5'	2:B:7:DA:H2'	0.50	2.07
2:B:6:DA:C2'	2:B:7:DA:OP2	0.50	2.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:10:DT:H2''	2:B:11:DC:OP2	0.49	2.07
1:A:846:CYS:HB3	1:A:864:HIS:CD2	0.49	2.42
2:B:11:DC:C2'	2:B:12:DA:OP2	0.49	2.57
1:A:833:LEU:CD1	1:A:833:LEU:CD2	0.48	2.86
2:B:7:DA:C2'	2:B:7:DA:O5'	0.48	2.60
3:C:17:DA:C2'	3:C:18:DA:OP2	0.48	2.56
1:A:822:SER:CB	3:C:20:DT:C7	0.47	2.92
1:A:822:SER:HB3	3:C:20:DT:C7	0.46	2.39
2:B:4:DG:C2'	2:B:5:DA:OP2	0.46	2.57
1:A:821:ARG:NE	2:B:7:DA:H62	0.46	2.07
1:A:822:SER:CB	3:C:20:DT:H72	0.46	2.40
2:B:3:DC:C2'	2:B:4:DG:OP2	0.45	2.47
3:C:18:DA:C2'	3:C:19:DC:OP2	0.45	2.58
2:B:9:DT:H1'	2:B:10:DT:H5'	0.45	1.87
2:B:7:DA:H2''	2:B:8:DG:H8	0.44	1.71
3:C:16:DG:H1'	3:C:17:DA:H5'	0.44	1.89
1:A:807:CYS:SG	1:A:820:HIS:CE1	0.44	3.10
3:C:21:DT:H2''	3:C:22:DT:H71	0.44	1.89
1:A:814:THR:O	1:A:833:LEU:HD23	0.43	2.13
3:C:24:DG:H1'	3:C:25:DG:H5'	0.43	1.91
1:A:831:LYS:CD	1:A:831:LYS:NZ	0.42	2.68
3:C:19:DC:C2'	3:C:20:DT:OP2	0.42	2.63
3:C:23:DC:H1'	3:C:24:DG:H5'	0.42	1.91
2:B:2:DC:H1'	2:B:3:DC:H5'	0.42	1.91
1:A:856:HIS:CE1	3:C:16:DG:OP2	0.42	2.73
2:B:3:DC:H1'	2:B:4:DG:H5'	0.42	1.91
1:A:833:LEU:CD1	1:A:833:LEU:CB	0.41	2.84
1:A:846:CYS:SG	1:A:864:HIS:CD2	0.41	3.12
1:A:816:ASN:HA	1:A:840:HIS:CE1	0.41	2.49
1:A:861:TYR:CZ	3:C:16:DG:H4'	0.40	2.51
2:B:1:DA:H1'	2:B:2:DC:H5'	0.40	1.94

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	73/93 (78%)	48 (66%)	23 (32%)	2 (3%)	6	41
All	All	73/93 (78%)	48 (66%)	23 (32%)	2 (3%)	6	41

All 2 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	825	GLY
1	A	869	GLY

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	58/73 (79%)	40 (69%)	18 (31%)	1	15
All	All	58/73 (79%)	40 (69%)	18 (31%)	1	15

All 18 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	802	CYS
1	A	804	THR
1	A	808	ASP
1	A	812	HIS
1	A	819	SER
1	A	820	HIS
1	A	821	ARG
1	A	823	LEU
1	A	831	LYS
1	A	834	ARG
1	A	845	LYS
1	A	848	THR
1	A	852	ASP
1	A	856	HIS
1	A	863	SER
1	A	864	HIS
1	A	865	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	867	LEU

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
2	B	2
3	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1:DA	O3'	2:DC	P	1.27
1	B	12:DA	O3'	13:DC	P	1.27
1	C	22:DT	O3'	23:DC	P	1.27
1	C	15:DT	O3'	16:DG	P	1.26

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	839:ALA	C	840:HIS	N	1.16
1	A	836:LEU	C	837:MET	N	1.08
1	A	842:ALA	C	843:ASP	N	1.03
1	A	844:LEU	C	845:LYS	N	0.98

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 16% for the well-defined parts and 16% 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	217
Number of shifts mapped to atoms	217
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
$^{13}\text{C}_\alpha$	63	-0.24 ± 0.34	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	52	-0.01 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	51	0.06 ± 1.12	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 16%, i.e. 217 atoms were assigned a chemical shift out of a possible 1395. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	165/373 (44%)	51/154 (33%)	63/150 (42%)	51/69 (74%)
Sidechain	52/456 (11%)	0/300 (0%)	52/139 (37%)	0/17 (0%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	0/54 (0%)	0/28 (0%)	0/20 (0%)	0/6 (0%)
Sugar	0/312 (0%)	0/182 (0%)	0/130 (0%)	0/0 (—%)
Base	0/200 (0%)	0/122 (0%)	0/46 (0%)	0/32 (0%)
Overall	217/1395 (16%)	51/786 (6%)	115/485 (24%)	51/124 (41%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 16%, i.e. 217 atoms were assigned a chemical shift out of a possible 1395. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	165/373 (44%)	51/154 (33%)	63/150 (42%)	51/69 (74%)
Sidechain	52/456 (11%)	0/300 (0%)	52/139 (37%)	0/17 (0%)
Aromatic	0/54 (0%)	0/28 (0%)	0/20 (0%)	0/6 (0%)
Sugar	0/312 (0%)	0/182 (0%)	0/130 (0%)	0/0 (—%)
Base	0/200 (0%)	0/122 (0%)	0/46 (0%)	0/32 (0%)
Overall	217/1395 (16%)	51/786 (6%)	115/485 (24%)	51/124 (41%)

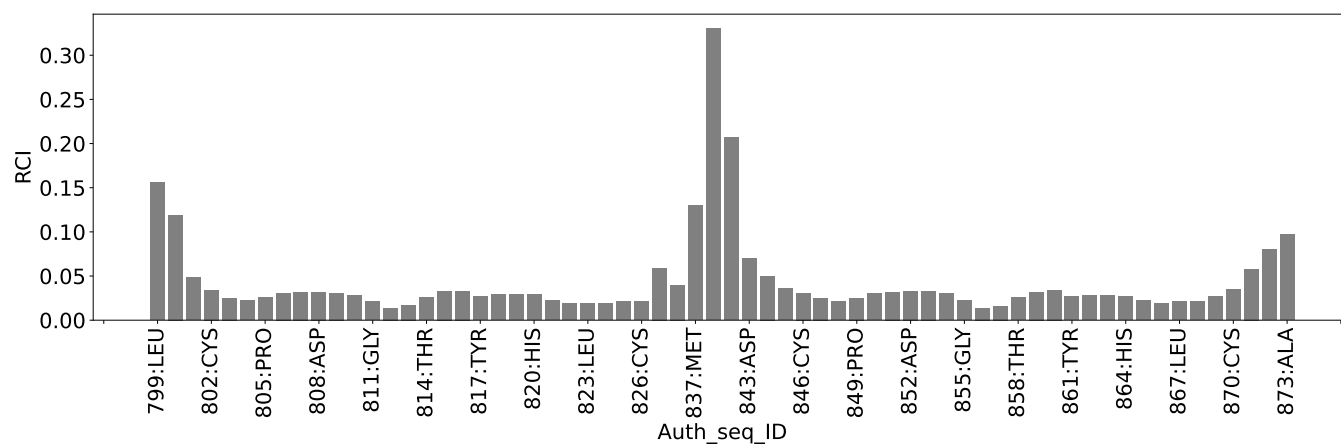
7.1.4 Statistically unusual chemical shifts [i](#)

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:



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	6
Hydrogen bond restraints	42
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.4
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)	3.0	0.19
0.2-0.5 (Medium)	17.0	0.47
>0.5 (Large)	17.0	20.14

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 ⓘ

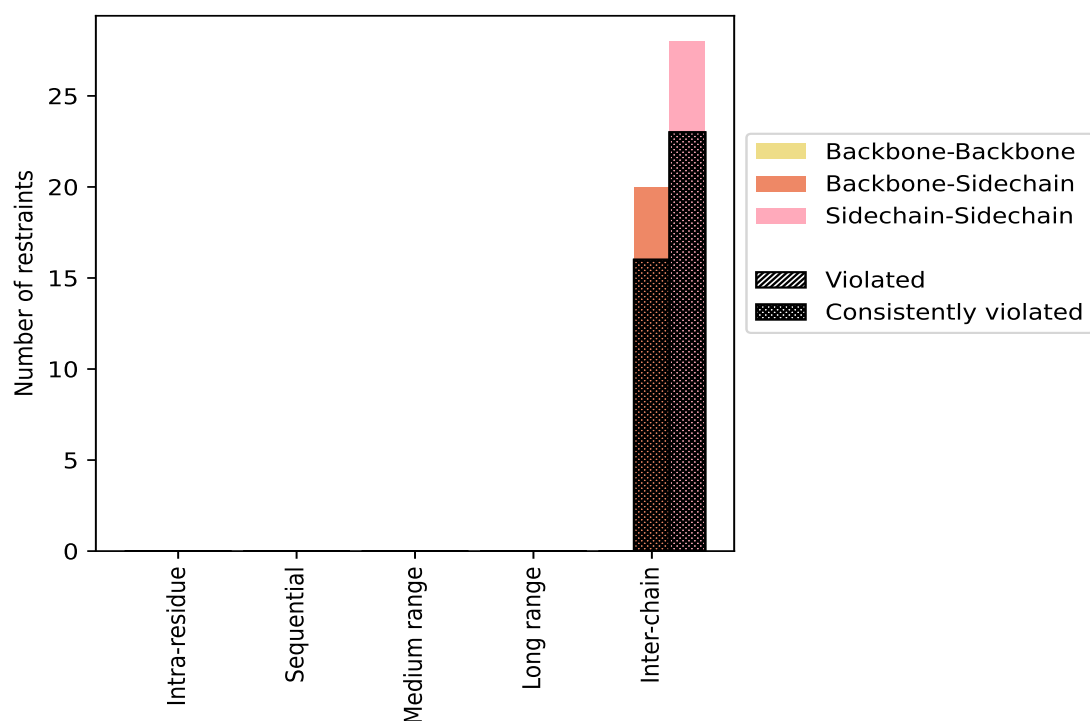
9.1 Summary of distance violations ⓘ

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	6	12.5	6	100.0	12.5	6	100.0	12.5
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	4	8.3	4	100.0	8.3	4	100.0	8.3
Sidechain-Sidechain	2	4.2	2	100.0	4.2	2	100.0	4.2
Hydrogen bond	42	87.5	33	78.6	68.8	33	78.6	68.8
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	48	100.0	39	81.2	81.2	39	81.2	81.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	20	41.7	16	80.0	33.3	16	80.0	33.3
Sidechain-Sidechain	28	58.3	23	82.1	47.9	23	82.1	47.9

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](#)

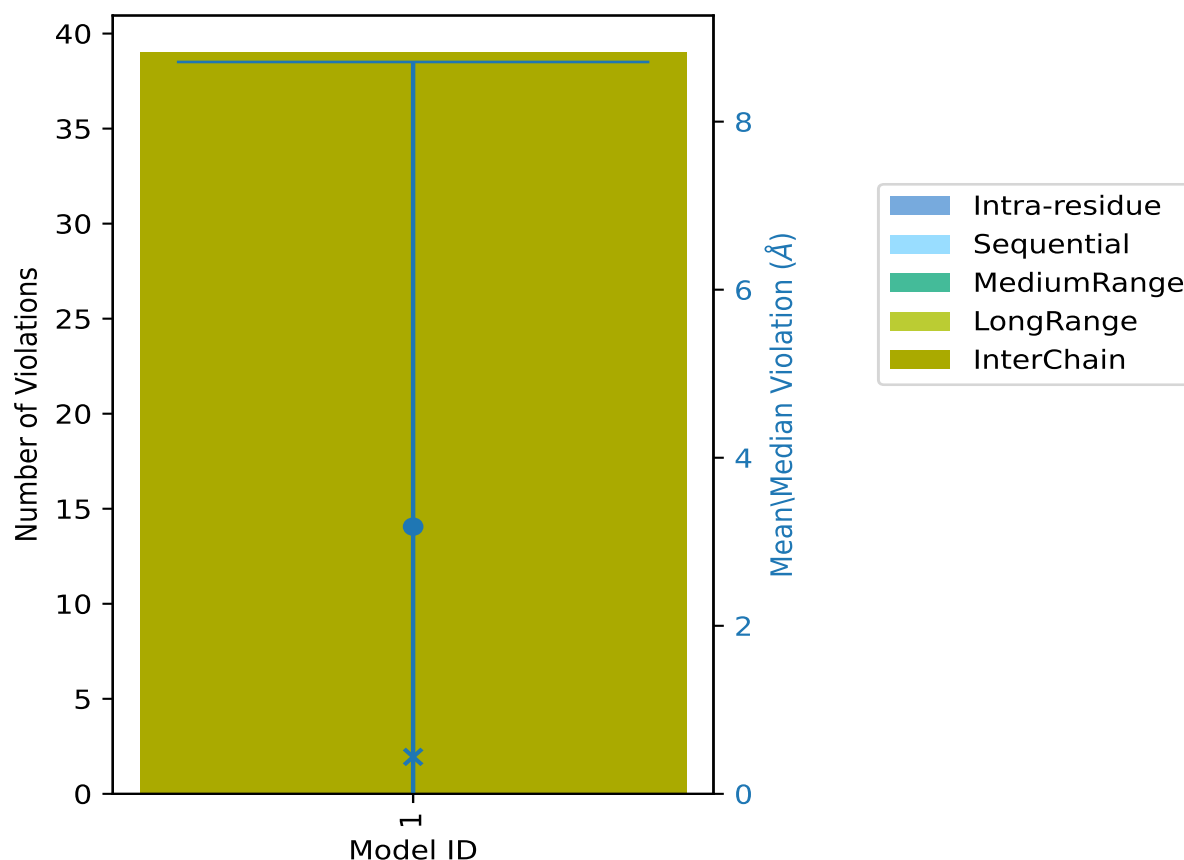
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	39	39	3.18	20.14	5.53	0.44

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](#)

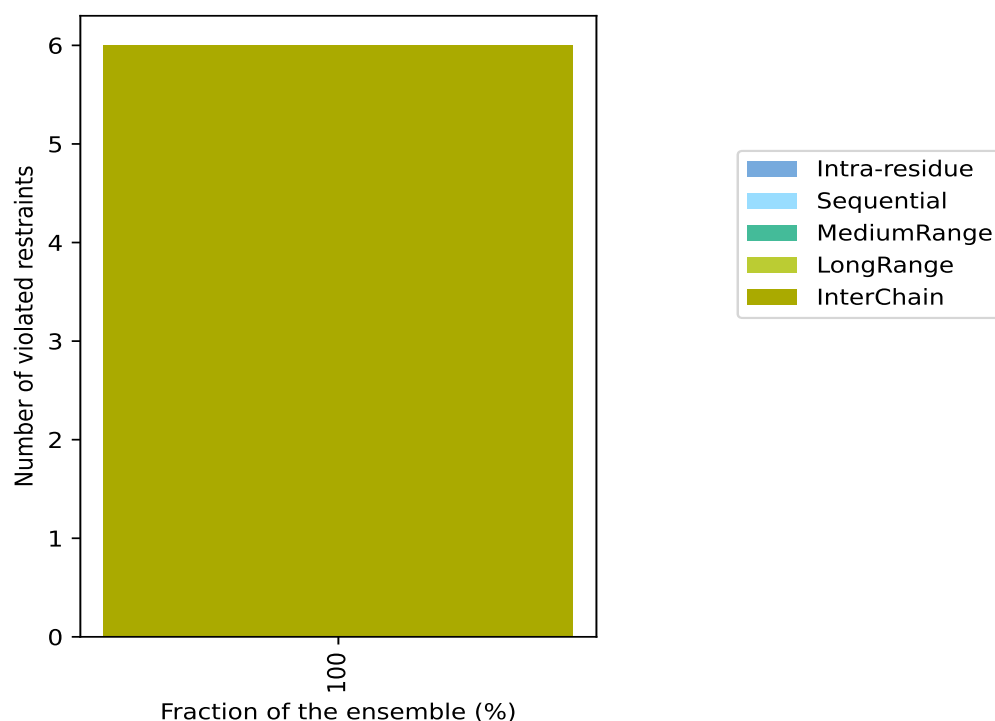
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 0(IR:0, SQ:0, MR:0, LR:0, IC:0) restraints are not violated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

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	6	6	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](#)



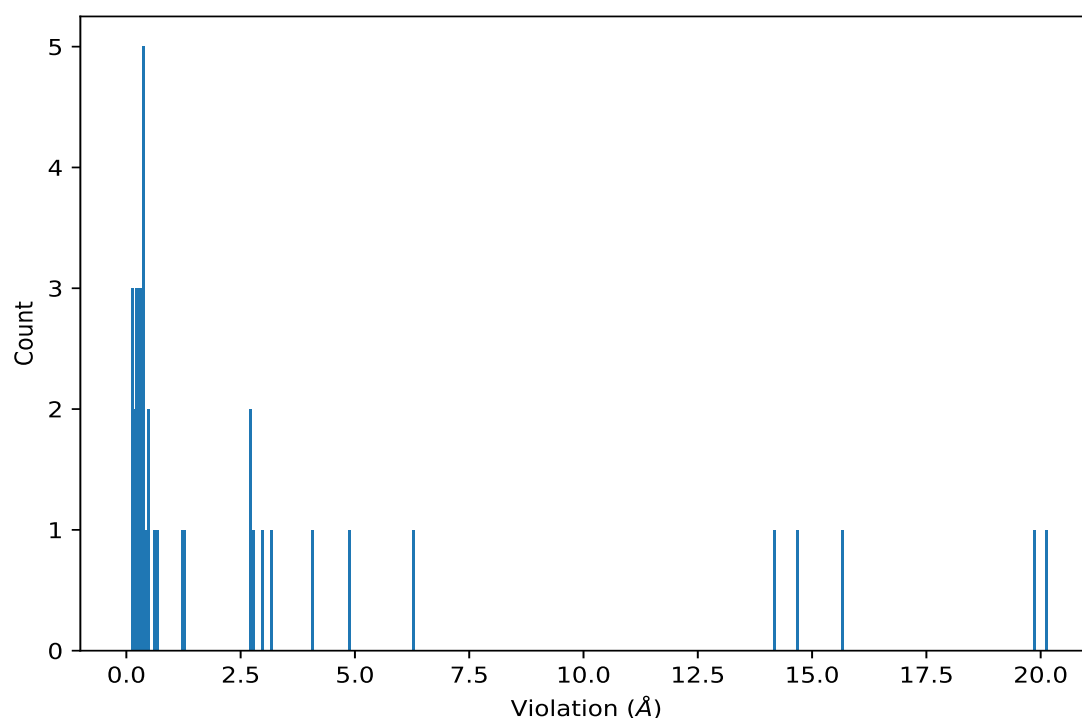
9.4 Most violated distance restraints in the ensemble [i](#)

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)
(1,19)	1:861:A:TYR:HH	3:20:C:DT:O4	1	20.14
(1,18)	1:861:A:TYR:OH	2:7:B:DA:H61	1	19.85
(1,16)	1:856:A:HIS:ND1	2:7:B:DA:H8	1	15.66
(1,15)	1:856:A:HIS:NE2	2:7:B:DA:H61	1	14.69
(1,17)	1:856:A:HIS:HE2	2:7:B:DA:N7	1	14.15
(1,4)	1:817:A:TYR:OH	2:6:B:DA:H8	1	6.27
(1,2)	1:812:A:HIS:ND1	2:6:B:DA:H8	1	4.86
(1,5)	1:817:A:TYR:HH	2:6:B:DA:OP1	1	4.05
(1,47)	2:10:B:DT:H3	1:866:A:SER:OG	1	3.15
(1,1)	1:812:A:HIS:NE2	2:6:B:DA:H8	1	2.98
(1,37)	3:21:C:DT:H3	1:822:A:SER:OG	1	2.77
(1,44)	2:9:B:DT:H3	1:866:A:SER:OG	1	2.74
(1,34)	3:20:C:DT:H3	1:822:A:SER:OG	1	2.71
(1,20)	1:863:A:SER:OG	3:17:C:DA:H8	1	1.27
(1,6)	1:819:A:SER:OG	2:6:B:DA:H8	1	1.22
(1,24)	1:866:A:SER:OG	3:17:C:DA:H62	1	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	2:10:B:DT:O4	1:867:A:LEU:HG	1	0.62
(1,10)	1:822:A:SER:OG	2:6:B:DA:H62	1	0.47
(1,36)	3:21:C:DT:O4	1:823:A:LEU:HG	1	0.46
(1,45)	2:9:B:DT:C7	1:866:A:SER:HB2	1	0.44
(1,25)	1:866:A:SER:HG	2:9:B:DT:O4	1	0.39
(1,35)	3:20:C:DT:C7	1:822:A:SER:HB3	1	0.38
(1,14)	1:824:A:SER:HG	2:6:B:DA:N7	1	0.38
(1,29)	2:6:B:DA:N6	1:822:A:SER:HG	1	0.37
(1,11)	1:822:A:SER:HG	2:6:B:DA:N6	1	0.37
(1,3)	1:812:A:HIS:HE2	2:6:B:DA:OP2	1	0.34
(1,39)	3:17:C:DA:N6	1:868:A:SER:HG	1	0.33
(1,28)	1:868:A:SER:HG	3:17:C:DA:N6	1	0.33
(1,48)	2:10:B:DT:C7	1:867:A:LEU:HD12	1	0.25
(1,43)	2:9:B:DT:O4	1:866:A:SER:HB3	1	0.25
(1,26)	1:867:A:LEU:HD12	2:10:B:DT:C7	1	0.25
(1,38)	3:21:C:DT:C7	1:823:A:LEU:HD21	1	0.23
(1,33)	3:20:C:DT:O4	1:822:A:SER:HB3	1	0.23
(1,12)	1:823:A:LEU:HD21	3:21:C:DT:C7	1	0.23
(1,41)	3:18:C:DA:N6	1:865:A:ARG:HE	1	0.19
(1,22)	1:865:A:ARG:HE	3:18:C:DA:N6	1	0.19
(1,7)	1:819:A:SER:HG	2:6:B:DA:OP2	1	0.14
(1,31)	2:7:B:DA:N6	1:821:A:ARG:HE	1	0.1
(1,9)	1:821:A:ARG:HE	2:7:B:DA:N6	1	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found