

Full wwPDB NMR Structure Validation Report (i)

Sep 4, 2024 – 01:21 pm BST

PDB ID : 8QAJ BMRB ID : 34847

Title : NMR solution structure of C-terminal domain of CDNF

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Deposited on : 2023-08-22

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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

wwPDB-RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

 $\begin{array}{ccc} wwPDB\text{-ShiftChecker} &:& v1.2\\ BMRB \ Restraints \ Analysis &:& v1.2 \end{array}$

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

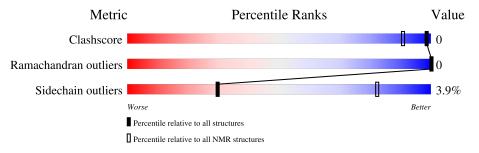
Validation Pipeline (wwPDB-VP) : 2.38.2

1 Overall quality at a glance (i)

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	NMR archive	
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries})$	
Clashscore	210492	14027	
Ramachandran outliers	207382	12486	
Sidechain outliers	206894	12463	

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 <=5%

Mol	Chain	Length	Quality of chain			
1	A	65	60%	5%	35%	



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: fewest violations.

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:107-A:131, A:136-A:152	0.43	17			
	(42)					

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 3 clusters and 4 single-model clusters were found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1049 atoms, of which 527 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Cerebral dopamine neurotrophic factor.

Mol	Chain	Residues		Atoms			Trace		
1	Λ	65	Total	С	Н	N	О	S	0
1	A	65	1049	328	527	91	99	4	U

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	GLY	-	expression tag	UNP Q49AH0
A	98	SER	-	expression tag	UNP Q49AH0
A	99	HIS	-	expression tag	UNP Q49AH0
A	100	MET	-	expression tag	UNP Q49AH0



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: Cerebral dopamine neurotrophic factor



4.2 Scores per residue for each member of the ensemble

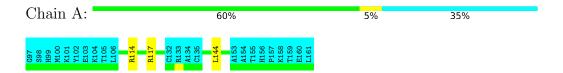
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Cerebral dopamine neurotrophic factor



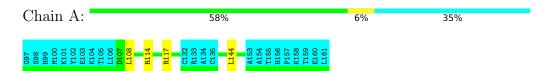
4.2.2 Score per residue for model 2





4.2.3 Score per residue for model 3

• Molecule 1: Cerebral dopamine neurotrophic factor



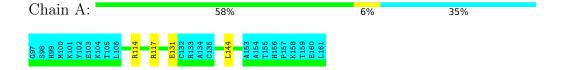
4.2.4 Score per residue for model 4

• Molecule 1: Cerebral dopamine neurotrophic factor



4.2.5 Score per residue for model 5

• Molecule 1: Cerebral dopamine neurotrophic factor

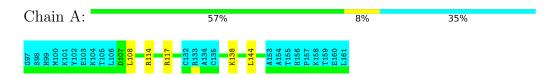


4.2.6 Score per residue for model 6

• Molecule 1: Cerebral dopamine neurotrophic factor



4.2.7 Score per residue for model 7





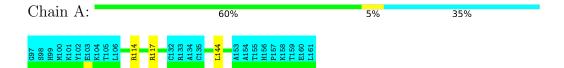
4.2.8 Score per residue for model 8

• Molecule 1: Cerebral dopamine neurotrophic factor



4.2.9 Score per residue for model 9

• Molecule 1: Cerebral dopamine neurotrophic factor



4.2.10 Score per residue for model 10

• Molecule 1: Cerebral dopamine neurotrophic factor

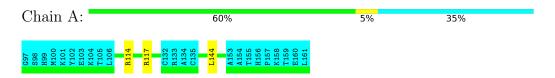


4.2.11 Score per residue for model 11

• Molecule 1: Cerebral dopamine neurotrophic factor



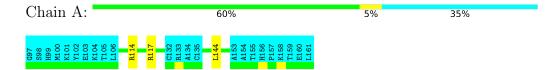
4.2.12 Score per residue for model 12





4.2.13 Score per residue for model 13

• Molecule 1: Cerebral dopamine neurotrophic factor



4.2.14 Score per residue for model 14

• Molecule 1: Cerebral dopamine neurotrophic factor



4.2.15 Score per residue for model 15

• Molecule 1: Cerebral dopamine neurotrophic factor



4.2.16 Score per residue for model 16

• Molecule 1: Cerebral dopamine neurotrophic factor



4.2.17 Score per residue for model 17 (medoid)





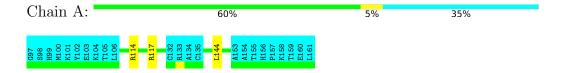
4.2.18 Score per residue for model 18

• Molecule 1: Cerebral dopamine neurotrophic factor



4.2.19 Score per residue for model 19

• Molecule 1: Cerebral dopamine neurotrophic factor



4.2.20 Score per residue for model 20





Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: simulated annealing, molecular dynamics.

Of the 300 calculated structures, 20 were deposited, based on the following criterion: structures with the least restraint violations.

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

Software name	Classification	Version
CYANA	structure calculation	_
Amber	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	111
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	111
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%



6 Model quality (i)

6.1 Standard geometry (i)

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	
IVIOI	Chain	RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.67 ± 0.01	$0\pm0/350~(~0.0\pm~0.0\%)$	1.05 ± 0.04	$2\pm0/473~(~0.4\pm~0.1\%)$
All	All	0.67	0/7000 (0.0%)	1.05	37/9460 (0.4%)

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	0.0 ± 0.0	0.1 ± 0.2
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Pag	Tuno	Atoma	Z	$\mathbf{Z} = \mathbf{Observed}(^{o})$	$Ideal(^{o})$	Models	
MIOI	Chain	nes	Type	Atoms		Observed()	ideai()	Worst	Total
1	A	117	ARG	NE-CZ-NH1	9.46	125.03	120.30	2	17
1	A	114	ARG	NE-CZ-NH1	8.92	124.76	120.30	13	18
1	A	130	GLU	N-CA-CB	-5.08	101.46	110.60	6	1
1	A	117	ARG	NE-CZ-NH2	-5.08	117.76	120.30	15	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	117	ARG	Sidechain	1



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	344	348	348	0±0
All	All	6880	6960	6960	1

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 0.

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

Atom-1	Atom-2	Clack(Å)	$\operatorname{Distance}(\mathring{\mathrm{A}})$	Mod	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:108:LEU:HD22	1:A:108:LEU:H	0.43	1.74	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	Perce	entiles
1	A	42/65 (65%)	41±1 (98±2%)	1±1 (2±2%)	0±0 (0±0%)	100	100
All	All	840/1300 (65%)	822 (98%)	18 (2%)	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	37/56 (66%)	36±1 (96±2%)	1±1 (4±2%)	30 82
All	All	740/1120 (66%)	711 (96%)	29 (4%)	30 82

All 5 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	144	LEU	20
1	A	108	LEU	6
1	A	131	GLU	1
1	A	138	LYS	1
1	A	127	SER	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

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 (i)

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	111
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	111
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 111 occurrences are reported below.

T:-4 ID	Cl :	D	Т	A 4	Shift Data				
List ID	Chain	Res	туре	Type	Type	Atom	Value	Uncertainty	Ambiguity
1	A	124	SER	CA	59.715	0.013	1		
1	A	124	SER	CB	65.272	0.02	1		
1	A	124	SER	HA	4.552	0.001	1		
1	A	124	SER	HB2	3.905	0.002	1		
1	A	124	SER	HB3	3.905	0.002	1		
1	A	125	HIS	С	175.128	0	1		
1	A	125	HIS	CA	57.718	0.033	1		
1	A	125	HIS	СВ	32.024	0.008	1		
1	A	125	HIS	CD2	121.306	0	1		
1	A	125	HIS	HA	4.709	0.003	1		
1	A	125	HIS	HB2	3.205	0	2		
1	A	125	HIS	HB3	3.144	0.007	2		
1	A	125	HIS	HD2	7.084	0	1		
1	A	126	MET	CE	18.298	0	1		



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Continue				A 4		Shift Data	l
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	A	126	MET	HE1	2.122	0	1
1	A	126	MET	HE2	2.122	0	1
1	A	126	MET	HE3	2.122	0	1
1	A	127	LYS	С	175.943	0	1
1	A	127	LYS	CA	57.583	0.123	1
1	A	127	LYS	СВ	34.475	0.091	1
1	A	127	LYS	CD	30.482	0.053	1
1	A	127	LYS	CE	43.612	0	1
1	A	127	LYS	CG	26.012	0.052	1
1	A	127	LYS	HA	4.333	0.004	1
1	A	127	LYS	HB2	1.76	0.001	2
1	A	127	LYS	HB3	1.734	0.001	2
1	A	127	LYS	HD2	1.696	0.001	1
1	A	127	LYS	HD3	1.696	0.001	1
1	A	127	LYS	HE2	3.025	0	1
1	A	127	LYS	HE3	3.025	0	1
1	A	127	LYS	HG2	1.383	0	2
1	A	127	LYS	HG3	1.316	0.001	2
1	A	128	TYR	С	175.56	0.049	1
1	A	128	TYR	CA	59.049	0.114	1
1	A	128	TYR	СВ	40.12	0.098	1
1	A	128	TYR	CD1	134.659	0	1
1	A	128	TYR	CD2	134.659	0	1
1	A	128	TYR	CE1	119.418	0	1
1	A	128	TYR	CE2	119.418	0	1
1	A	128	TYR	Н	8.303	0.004	1
1	A	128	TYR	HA	4.657	0.004	1
1	A	128	TYR	HB2	3.124	0.006	2
1	A	128	TYR	HB3	2.971	0.003	2
1	A	128	TYR	HD1	7.159	0.016	1
1	A	128	TYR	HD2	7.159	0.016	1
1	A	128	TYR	HE1	6.852	0.028	1
1	A	128	TYR	HE2	6.852	0.028	1
1	A	128	TYR	N	120.942	0.066	1
1	A	129	GLU	С	176.035	0	1
1	A	129	GLU	CA	57.687	0.102	1
1	A	129	GLU	СВ	31.93	0.099	1
1	A	129	GLU	CG	37.547	0.053	1
1	A	129	GLU	Н	8.395	0.005	1
1	A	129	GLU	HA	4.368	0.003	1
1	A	129	GLU	HB2	2.102	0	2



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Continue	Shift Data			A 4		Shift Data	1
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	A	129	GLU	HB3	1.989	0	2
1	A	129	GLU	HG2	2.32	0.005	1
1	A	129	GLU	HG3	2.32	0.005	1
1	A	129	GLU	N	122.426	0.024	1
1	A	130	LYS	С	176.448	0.005	1
1	A	130	LYS	CA	57.791	0.11	1
1	A	130	LYS	CB	34.243	0.095	1
1	A	130	LYS	CD	30.558	0	1
1	A	130	LYS	CE	43.639	0	1
1	A	130	LYS	CG	26.162	0.004	1
1	A	130	LYS	Н	8.344	0.003	1
1	A	130	LYS	HA	4.432	0.002	1
1	A	130	LYS	HB2	1.915	0.003	2
1	A	130	LYS	HB3	1.847	0	2
1	A	130	LYS	HE2	3.071	0.003	1
1	A	130	LYS	HE3	3.071	0.003	1
1	A	130	LYS	HG2	1.522	0	2
1	A	130	LYS	HG3	1.475	0.002	2
1	A	130	LYS	N	121.322	0.05	1
1	A	131	THR	С	174.201	0	1
1	A	131	THR	CA	63.345	0.046	1
1	A	131	THR	СВ	71.261	0.078	1
1	A	131	THR	CG2	23.113	0.069	1
1	A	131	THR	Н	8.187	0.004	1
1	A	131	THR	HA	4.427	0.002	1
1	A	131	THR	НВ	4.272	0.001	1
1	A	131	THR	HG21	1.292	0	1
1	A	131	THR	HG22	1.292	0	1
1	A	131	THR	HG23	1.292	0	1
1	A	131	THR	N	114.902	0.074	1
1	A	132	LEU	С	175.758	0.028	1
1	A	132	LEU	CA	56.526	0.104	1
1	A	132	LEU	СВ	44.367	0.088	1
1	A	132	LEU	CD1	25.852	0	2
1	A	132	LEU	CD2	26.182	0	2
1	A	132	LEU	CG	28.477	0.04	1
1	A	132	LEU	Н	8.413	0.003	1
1	A	132	LEU	HA	4.399	0.003	1
1	A	132	LEU	HB2	1.73	0.005	2
1	A	132	LEU	HB3	1.684	0.008	2
1	A	132	LEU	HD11	0.933	0	2



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	.,	10	1

List ID	Chain	Res	Trino	Atom	Shift Data		
LIST ID	Chain	nes	Type	Atom	Value	Uncertainty	Ambiguity
1	A	132	LEU	HD12	0.933	0	2
1	A	132	LEU	HD13	0.933	0	2
1	A	132	LEU	HD21	0.929	0.003	2
1	A	132	LEU	HD22	0.929	0.003	2
1	A	132	LEU	HD23	0.929	0.003	2
1	A	132	LEU	HG	1.594	0.001	1
1	A	132	LEU	N	124.59	0.057	1
1	A	133	ASP	С	176.825	0	1
1	A	133	ASP	CA	54.251	0.187	1
1	A	133	ASP	СВ	42.254	0.138	1
1	A	133	ASP	Н	8.496	0.003	1
1	A	133	ASP	HA	4.883	0.004	1
1	A	133	ASP	HB2	2.929	0.004	2
1	A	133	ASP	HB3	2.675	0.004	2
1	A	133	ASP	N	123.279	0.059	1

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments (i)

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 601. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	0/209 (0%)	0/84 (0%)	0/84 (0%)	0/41 (0%)
Sidechain	0/355~(0%)	0/230~(0%)	0/112 (0%)	0/13 (0%)
Aromatic	0/37 (0%)	0/18 (0%)	0/17 (0%)	0/2 (0%)
Overall	0/601 (0%)	0/332 (0%)	0/213 (0%)	0/56 (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 902. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathbf{C}$	$^{15}\mathbf{N}$
Backbone	0/323 (0%)	0/130 (0%)	0/130 (0%)	0/63 (0%)
Sidechain	0/519 (0%)	0/337~(0%)	0/163~(0%)	0/19 (0%)



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	Total	$^{1}{ m H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Aromatic	0/60 (0%)	0/30 (0%)	0/26~(0%)	0/4~(0%)
Overall	0/902 (0%)	0/497 (0%)	0/319 (0%)	0/86 (0%)

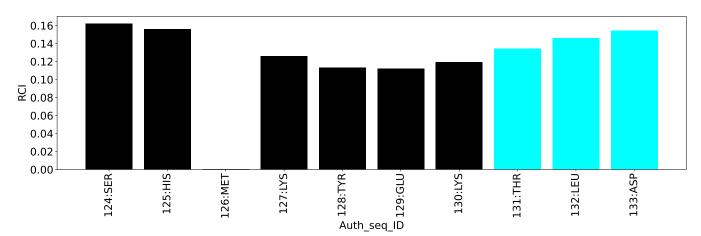
7.1.4 Statistically unusual chemical shifts (i)

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 (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	977
Intra-residue ($ i-j =0$)	267
Sequential (i-j =1)	241
Medium range ($ i-j >1$ and $ i-j <5$)	277
Long range (i-j ≥5)	192
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	83
Number of unmapped restraints	1060
Number of restraints per residue	16.3
Number of long range restraints per residue ¹	3.0

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 (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 (i)

9.1 Summary of distance violations (i)

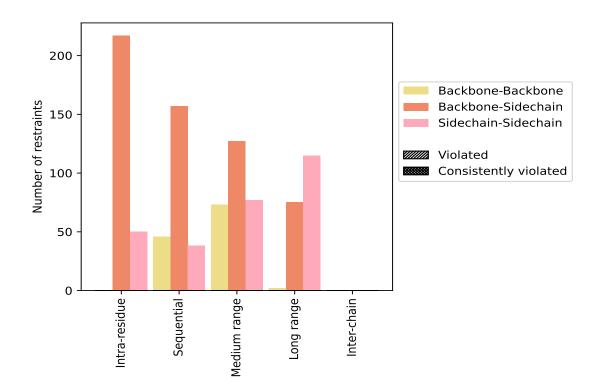
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1~Å are not included in the statistics.

Dantuninta tema	Count	% ¹	${f Violated}^3$			Consistently Violated ⁴		
Restraints type			Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
Intra-residue (i-j =0)	267	27.3	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	217	22.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	50	5.1	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	241	24.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	46	4.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	157	16.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	38	3.9	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1 \& i-j <5$)	277	28.4	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	73	7.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	127	13.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	77	7.9	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \ge 5$)	192	19.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	2	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	75	7.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	115	11.8	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	977	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	121	12.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	576	59.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	280	28.7	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 disulfied 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 (i)

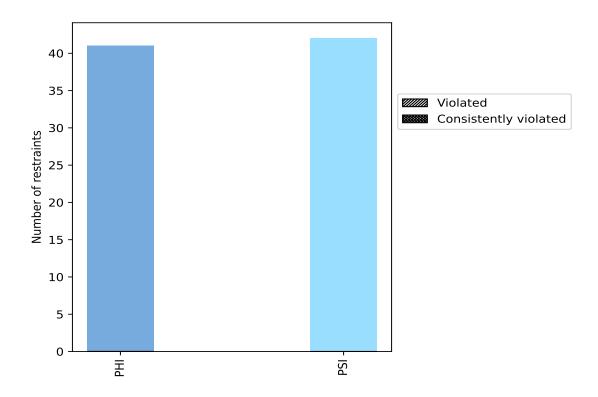
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	$\%^1$	${f Violated^3}$			Consistently Violated ⁴			
			Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$	
PHI	41	49.4	0	0.0	0.0	0	0.0	0.0	
PSI	42	50.6	0	0.0	0.0	0	0.0	0.0	
Total	83	100.0	0	0.0	0.0	0	0.0	0.0	

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

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



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



10.2	Dihedral-angle	violation	statistics	for	each model	(i)

No violations found

Dihedral-angle violation statistics for the ensemble (i) 10.3

No violations found

Most violated dihedral-angle restraints in the ensemble (i)

No violations found

All violated dihedral-angle restraints (i) 10.5

No violations found

