



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 12:32 AM UTC

PDB ID : 9PQH / pdb_00009pqh
BMRB ID : 51715
Title : NMR Structure of Ca²⁺/Calmodulin bound to the GluN1 C0 domain of the NMDA receptor
Authors : Bej, A.; Ames, J.B.
Deposited on : 2025-07-22

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

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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

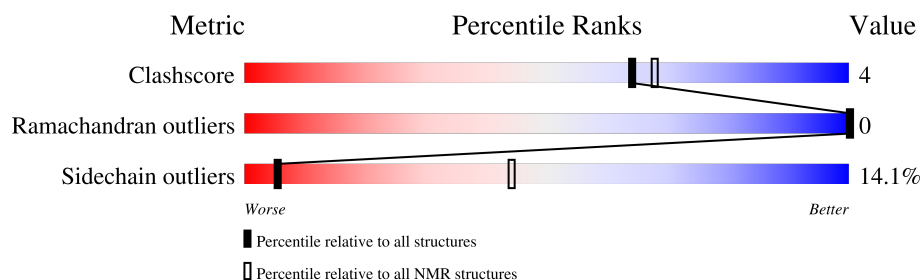
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 70%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	149	
2	B	938	

2 Ensemble composition and analysis

This entry contains 10 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:149, B:846-B:865 (162)	1.00	9

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 and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 6, 8, 9
2	3, 5, 10
Single-model clusters	7

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2585 atoms, of which 1260 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	146	Total	C	H	N	O	S	0
			2237	707	1085	186	250	9	

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms						Trace
2	B	20	Total	C	H	N	O	S	0
			344	107	175	34	27	1	

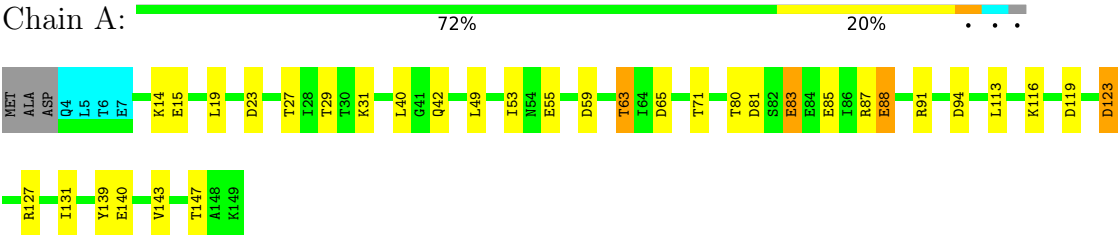
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
3	A	4	Total	Ca
			4	4

THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR</
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4.2.2 Score per residue for model 2

- Molecule 1: Calmodulin-1



- Molecule 2: Glutamate receptor ionotropic, NMDA 1



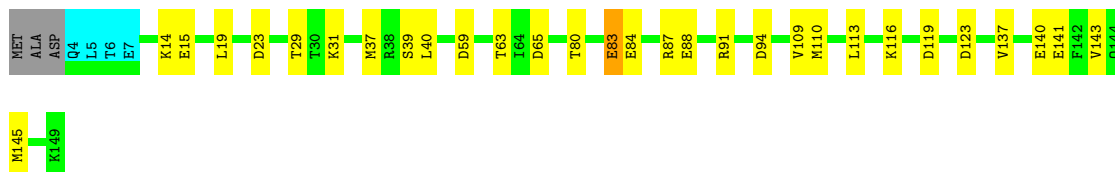


GLN	LYS	ASP	THR	VAL	LEU	PRO	ARG	ARG	ALA	ILE	GLU	ARG	GLU	GLU	GLY	GLN	LEU	GLN	LEU	CYS	SER	ARG	HIS	ARG	GLU	SER
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4.2.4 Score per residue for model 4

- Molecule 1: Calmodulin-1

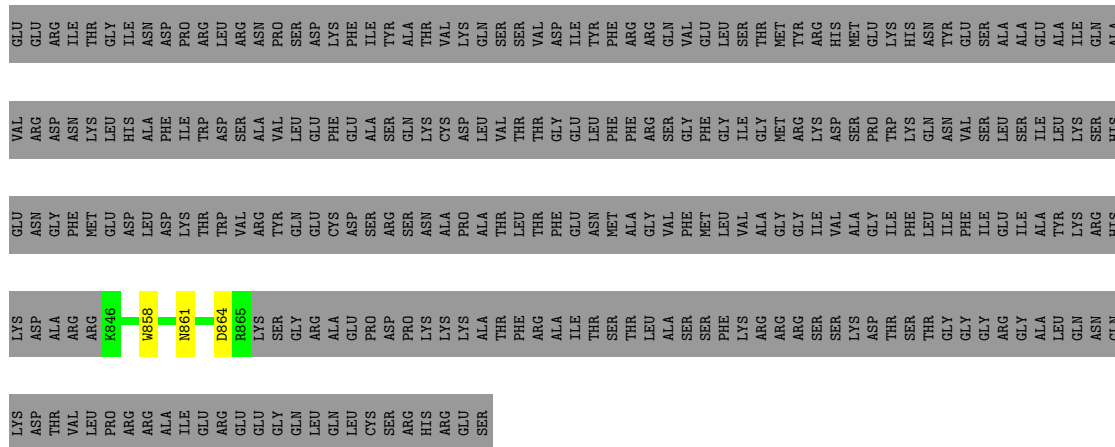
Chain A: 75% 19% ..



- Molecule 2: Glutamate receptor ionotropic, NMDA 1

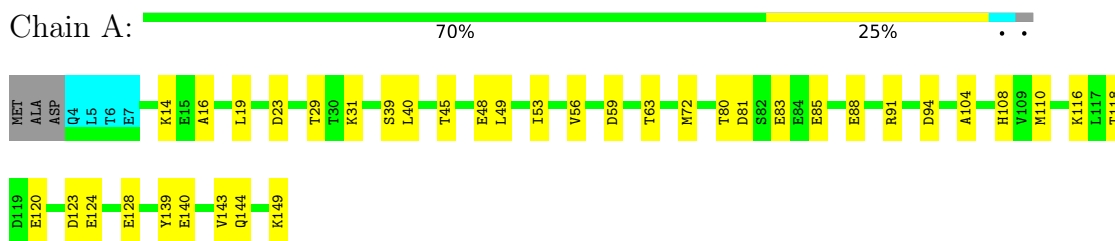
Chain B: 98%

[illegible]

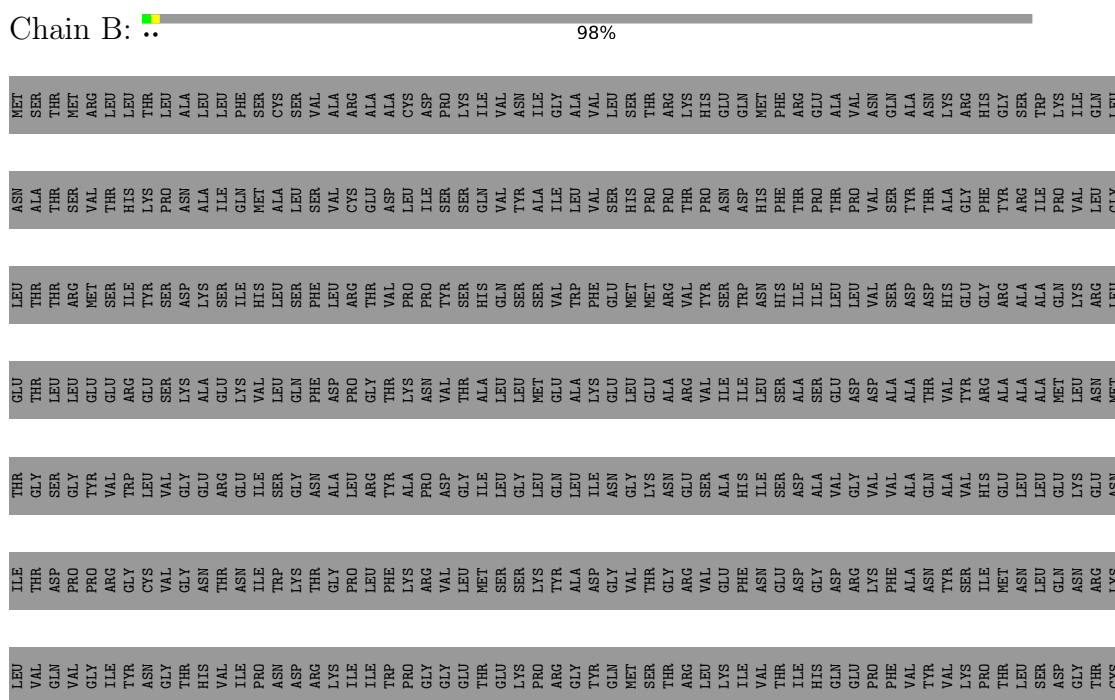


4.2.5 Score per residue for model 5

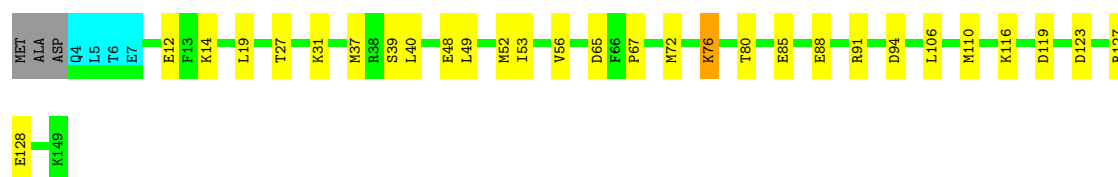
- Molecule 1: Calmodulin-1



- Molecule 2: Glutamate receptor ionotropic, NMDA 1

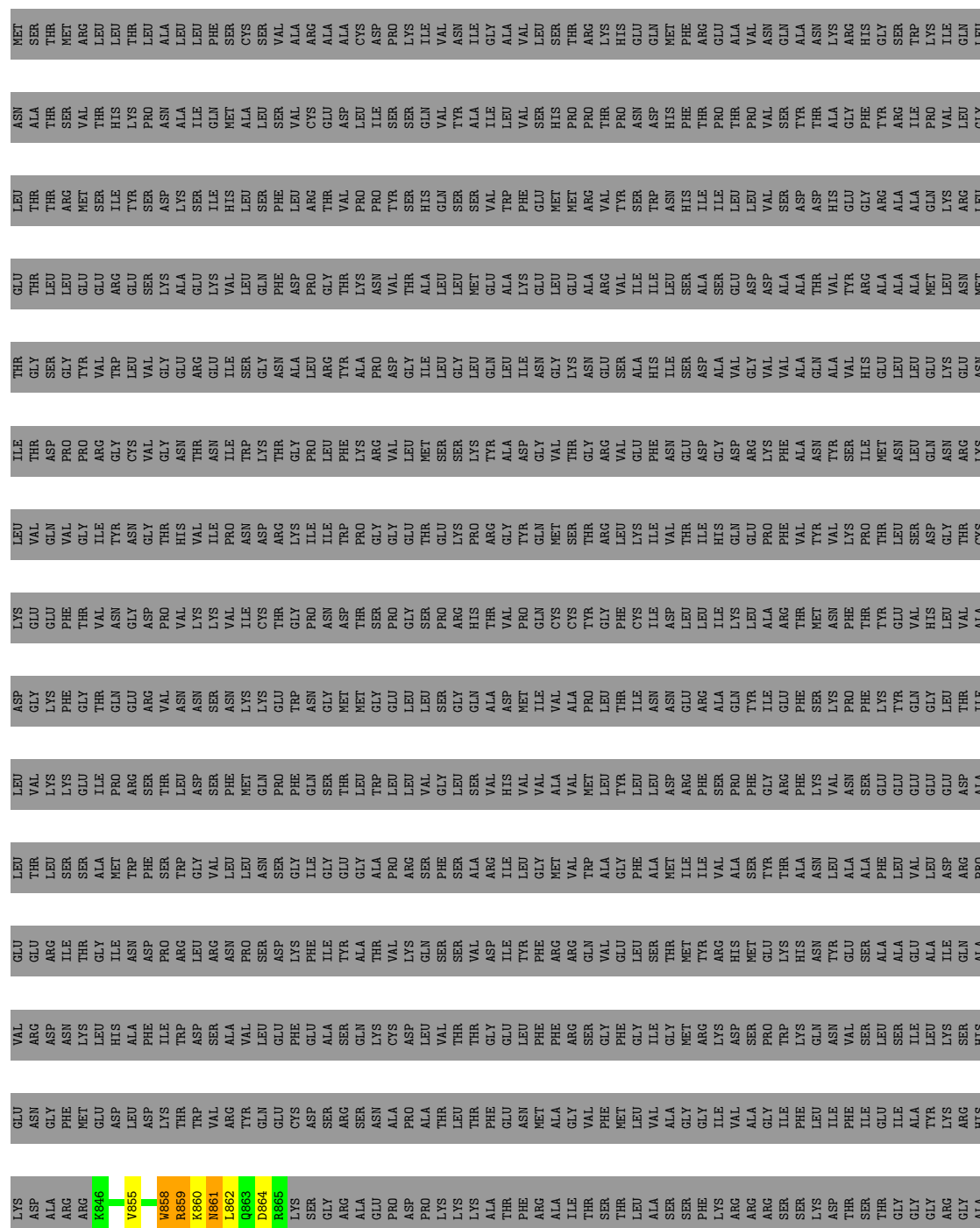






- Molecule 2: Glutamate receptor ionotropic, NMDA 1

Chain B: 98%

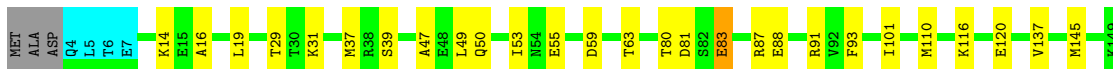


LEU GLN ASN GLN LYS THR VAL LEU PRO ARG ARG ALA ILE GLU ARG GLU GLU GLY GLN LEU GLN LEU CYS SER ARG HIS ARG GLU SER

4.2.9 Score per residue for model 9 (medoid)

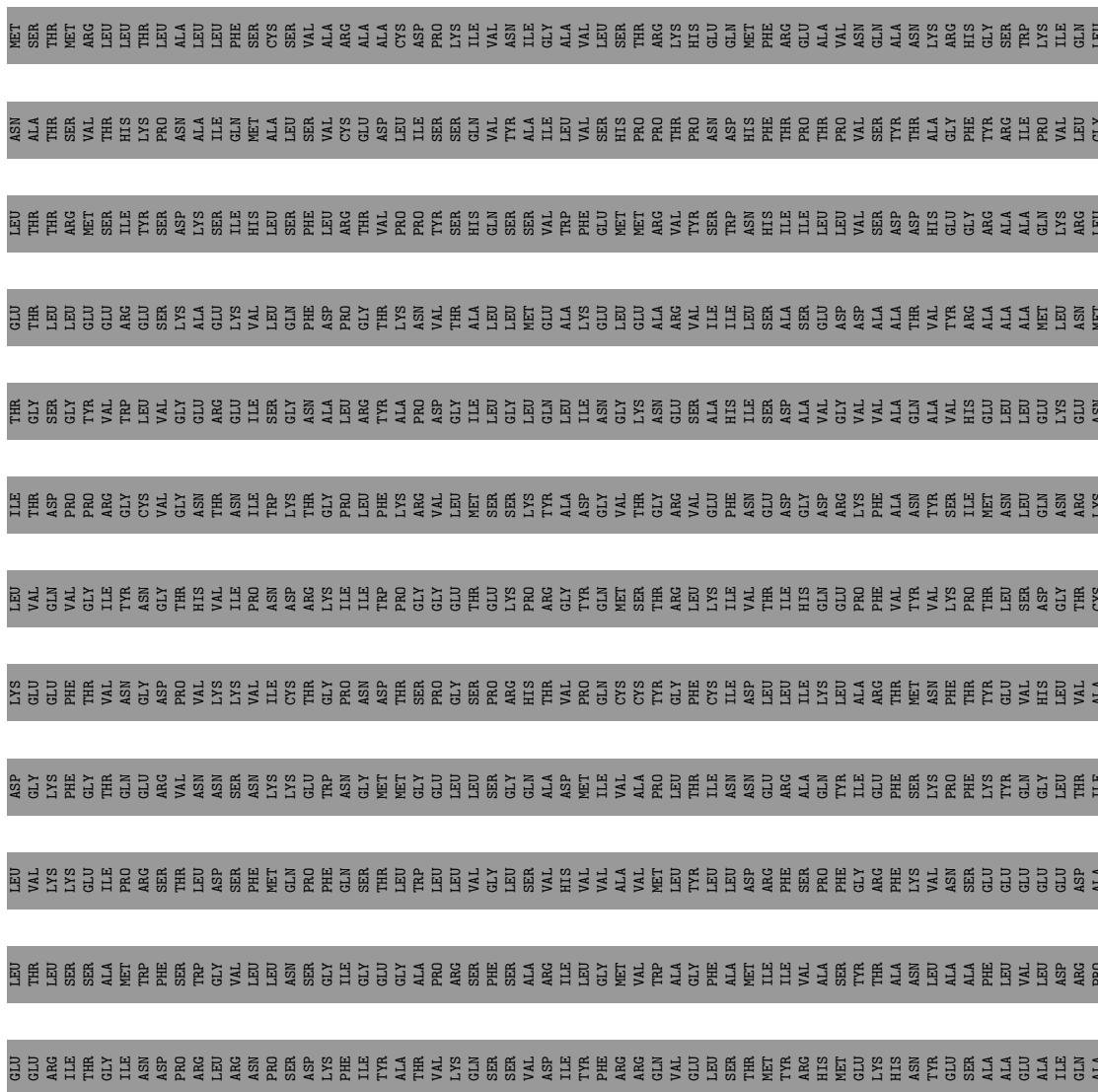
- Molecule 1: Calmodulin-1

Chain A: 77% 17% ..



- Molecule 2: Glutamate receptor ionotropic, NMDA 1

Chain B: 98%



[illegible]

5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
HADDOCK	structure calculation	
HADDOCK	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1586
Number of shifts mapped to atoms	1580
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	70%

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:
CA

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [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	1119	1053	1053	9±2
2	B	169	175	174	3±2
All	All	12920	12280	12270	104

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:861:ASN:HA	2:B:864:ASP:OD1	0.65	1.90	2	4
1:A:29:THR:HA	1:A:63:THR:HG22	0.60	1.74	2	6
1:A:85:GLU:OE1	2:B:860:LYS:HB3	0.57	1.99	8	1
1:A:48:GLU:O	1:A:52:MET:HG3	0.53	2.04	8	1
1:A:93:PHE:CE1	1:A:106:LEU:HA	0.51	2.41	7	1
1:A:118:THR:HB	1:A:120:GLU:OE2	0.51	2.06	5	1
1:A:123:ASP:O	1:A:127:ARG:HG3	0.51	2.06	8	4
1:A:81:ASP:O	1:A:85:GLU:HG2	0.49	2.07	2	1
1:A:47:ALA:O	1:A:50:GLN:HG2	0.49	2.07	6	2
1:A:65:ASP:OD1	1:A:67:PRO:HD2	0.48	2.08	3	5
2:B:855:VAL:O	2:B:859:ARG:HB3	0.48	2.08	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:GLU:O	1:A:144:GLN:HB2	0.48	2.08	5	1
1:A:84:GLU:O	1:A:88:GLU:HG2	0.48	2.07	7	1
1:A:16:ALA:HB2	2:B:854:ALA:HB1	0.48	1.86	5	2
1:A:88:GLU:OE1	1:A:91:ARG:HD2	0.48	2.09	4	5
1:A:83:GLU:O	1:A:87:ARG:HG3	0.47	2.09	9	5
1:A:49:LEU:O	1:A:53:ILE:HG12	0.47	2.09	9	4
2:B:856:ASN:O	2:B:859:ARG:HG3	0.47	2.09	2	1
2:B:852:PHE:O	2:B:856:ASN:HB2	0.47	2.09	2	1
1:A:20:PHE:HA	1:A:36:VAL:HG21	0.47	1.87	3	1
1:A:149:LYS:N	1:A:149:LYS:HD2	0.47	2.25	7	1
1:A:83:GLU:OE1	1:A:87:ARG:HD3	0.47	2.10	1	2
1:A:15:GLU:OE1	1:A:15:GLU:HA	0.46	2.10	3	1
1:A:56:VAL:HG22	1:A:72:MET:HG3	0.45	1.89	8	2
1:A:128:GLU:OE1	2:B:846:LYS:HE2	0.45	2.11	7	1
1:A:45:THR:OG1	1:A:48:GLU:HB2	0.45	2.12	3	4
1:A:109:VAL:O	1:A:113:LEU:HG	0.45	2.12	4	2
1:A:137:VAL:HG23	1:A:141:GLU:HB2	0.45	1.88	6	2
1:A:55:GLU:CD	2:B:865:ARG:HE	0.45	2.20	10	1
1:A:140:GLU:O	1:A:143:VAL:HG22	0.45	2.12	2	2
1:A:82:SER:HA	1:A:85:GLU:CD	0.45	2.37	10	2
1:A:146:MET:SD	2:B:853:ALA:HB2	0.45	2.52	6	2
1:A:93:PHE:HE2	2:B:852:PHE:CE2	0.45	2.30	9	1
1:A:85:GLU:OE1	2:B:857:VAL:HA	0.44	2.12	5	1
1:A:128:GLU:HG3	2:B:846:LYS:HE2	0.44	1.89	7	1
1:A:123:ASP:OD2	1:A:127:ARG:NH1	0.44	2.51	1	3
1:A:139:TYR:O	1:A:143:VAL:HG22	0.44	2.13	5	1
1:A:8:GLU:O	1:A:12:GLU:HG2	0.44	2.13	7	1
2:B:856:ASN:O	2:B:859:ARG:HG2	0.43	2.13	7	4
1:A:139:TYR:O	1:A:143:VAL:HG13	0.43	2.14	2	1
2:B:858:TRP:O	2:B:862:LEU:HG	0.43	2.14	2	1
1:A:107:ARG:HB2	1:A:122:VAL:HG11	0.43	1.91	7	2
2:B:858:TRP:CE3	2:B:862:LEU:HD11	0.42	2.49	2	2
1:A:141:GLU:O	1:A:145:MET:HG3	0.42	2.14	3	1
1:A:88:GLU:OE1	1:A:91:ARG:HD3	0.42	2.14	8	1
1:A:95:LYS:HE2	1:A:108:HIS:ND1	0.42	2.29	6	1
1:A:137:VAL:HG21	1:A:145:MET:SD	0.42	2.55	4	4
1:A:66:PHE:HB3	1:A:67:PRO:HD3	0.42	1.92	6	1
1:A:101:ILE:HB	1:A:137:VAL:CG1	0.42	2.45	9	1
1:A:128:GLU:OE1	2:B:846:LYS:NZ	0.41	2.52	5	1
2:B:858:TRP:CZ3	2:B:862:LEU:HD11	0.41	2.50	2	1
1:A:85:GLU:OE2	2:B:857:VAL:HA	0.40	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:GLU:O	1:A:19:LEU:HG	0.40	2.17	2	1
1:A:104:ALA:O	1:A:108:HIS:HB2	0.40	2.16	5	1
1:A:72:MET:SD	1:A:76:LYS:HG3	0.40	2.56	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	141/149 (95%)	138±1 (98±1%)	3±1 (2±1%)	0±0 (0±0%)	100	100
2	B	18/938 (2%)	18±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1590/10870 (15%)	1556 (98%)	34 (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	121/127 (95%)	104±3 (86±2%)	17±3 (14±2%)	5	44
2	B	17/806 (2%)	15±1 (87±8%)	2±1 (13±8%)	6	47
All	All	1380/9330 (15%)	1186 (86%)	194 (14%)	5	44

All 51 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	31	LYS	10
1	A	116	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	14	LYS	9
1	A	40	LEU	9
1	A	59	ASP	9
1	A	94	ASP	9
2	B	858	TRP	9
1	A	80	THR	9
1	A	39	SER	8
1	A	110	MET	8
1	A	123	ASP	8
1	A	83	GLU	8
1	A	19	LEU	8
1	A	23	ASP	7
1	A	37	MET	6
1	A	55	GLU	4
1	A	63	THR	4
1	A	119	ASP	4
1	A	27	THR	4
2	B	850	LEU	4
1	A	15	GLU	3
1	A	113	LEU	3
1	A	128	GLU	3
1	A	65	ASP	3
2	B	856	ASN	3
1	A	149	LYS	3
1	A	71	THR	2
2	B	857	VAL	2
1	A	81	ASP	2
1	A	120	GLU	2
1	A	54	ASN	1
1	A	42	GLN	1
1	A	88	GLU	1
1	A	131	ILE	1
1	A	147	THR	1
2	B	860	LYS	1
2	B	863	GLN	1
1	A	18	SER	1
1	A	85	GLU	1
1	A	112	ASN	1
1	A	84	GLU	1
1	A	124	GLU	1
1	A	46	GLU	1
1	A	73	MET	1

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Mol	Chain	Res	Type	Models (Total)
1	A	52	MET	1
1	A	115	GLU	1
1	A	12	GLU	1
1	A	76	LYS	1
1	A	106	LEU	1
2	B	859	ARG	1
2	B	861	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 70% for the well-defined parts and 71% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1586
Number of shifts mapped to atoms	1580
Number of unparsed shifts	0
Number of shifts with mapping errors	6
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 6 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	ASP	HA	4.623	0.004	1
1	A	3	ASP	HB2	2.684	0.008	2
1	A	3	ASP	HB3	2.531	0.003	2
1	A	3	ASP	C	175.607	0.000	1
1	A	3	ASP	CA	54.845	0.000	1
1	A	3	ASP	CB	41.44	0.038	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
$^{13}\text{C}_\alpha$	146	-0.32 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	135	0.19 ± 0.07	None needed (< 0.5 ppm)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}'$	142	-0.47 ± 0.11	None needed (< 0.5 ppm)
^{15}N	143	0.27 ± 0.19	None needed (< 0.5 ppm)

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 70%, i.e. 1531 atoms were assigned a chemical shift out of a possible 2173. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	709/817 (87%)	292/333 (88%)	278/324 (86%)	139/160 (87%)
Sidechain	786/1229 (64%)	534/786 (68%)	252/393 (64%)	0/50 (0%)
Aromatic	36/127 (28%)	36/63 (57%)	0/62 (0%)	0/2 (0%)
Overall	1531/2173 (70%)	862/1182 (73%)	530/779 (68%)	139/212 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 1580 atoms were assigned a chemical shift out of a possible 2229. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	729/837 (87%)	300/341 (88%)	286/332 (86%)	143/164 (87%)
Sidechain	815/1265 (64%)	554/809 (68%)	261/405 (64%)	0/51 (0%)
Aromatic	36/127 (28%)	36/63 (57%)	0/62 (0%)	0/2 (0%)
Overall	1580/2229 (71%)	890/1213 (73%)	547/799 (68%)	143/217 (66%)

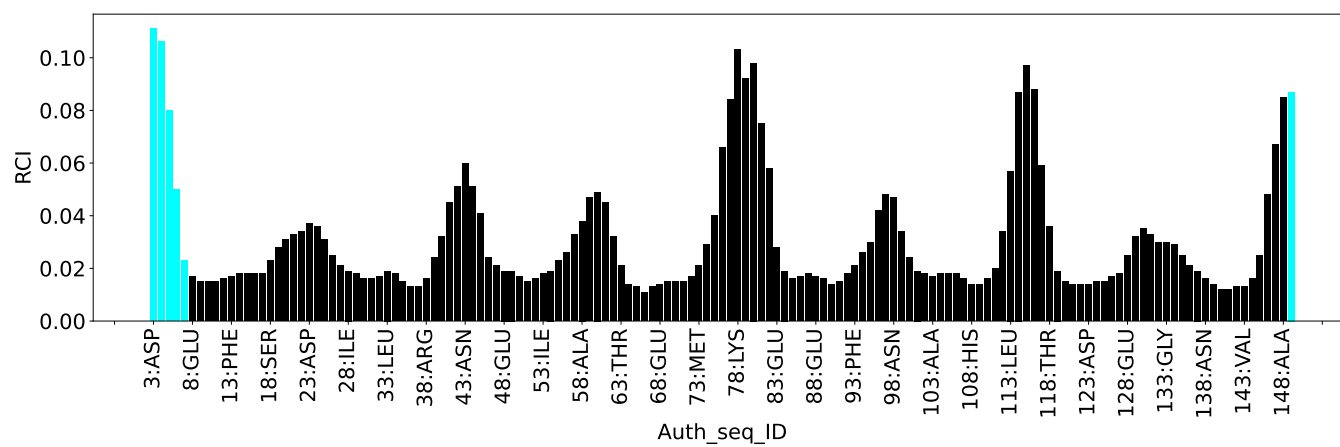
7.1.4 Statistically unusual chemical shifts [i](#)

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	60
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	60
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
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)	1.0	0.16
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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

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

9 Distance violation analysis [i](#)

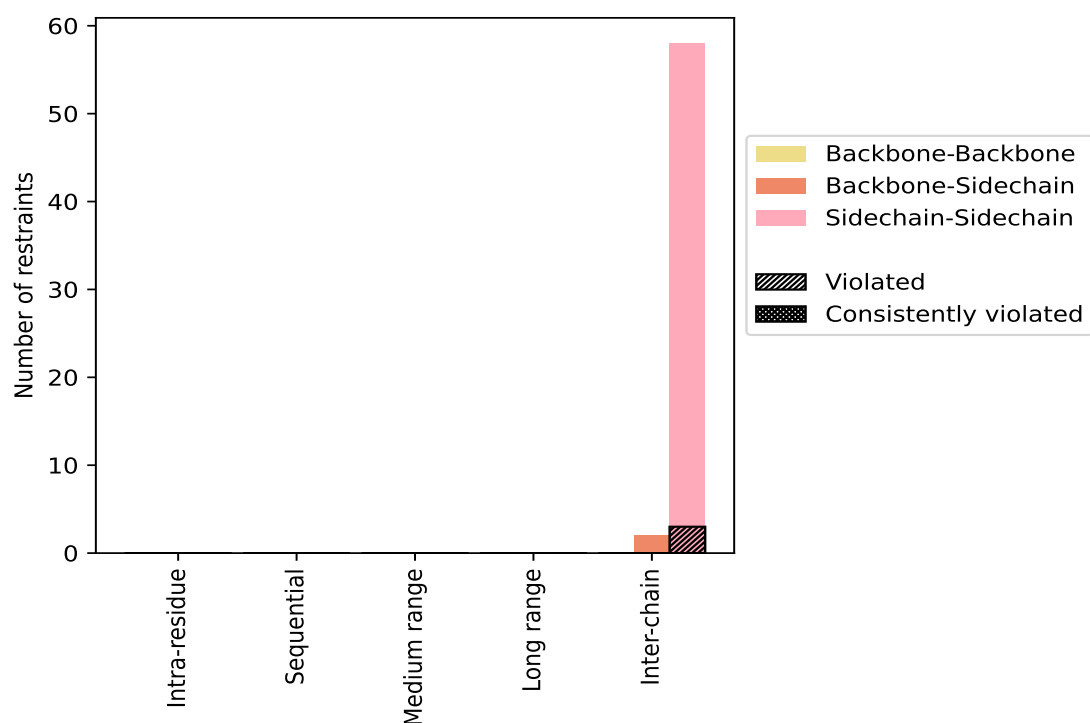
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	60	100.0	3	5.0	5.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	3.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	58	96.7	3	5.2	5.0	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	60	100.0	3	5.0	5.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	3.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	58	96.7	3	5.2	5.0	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

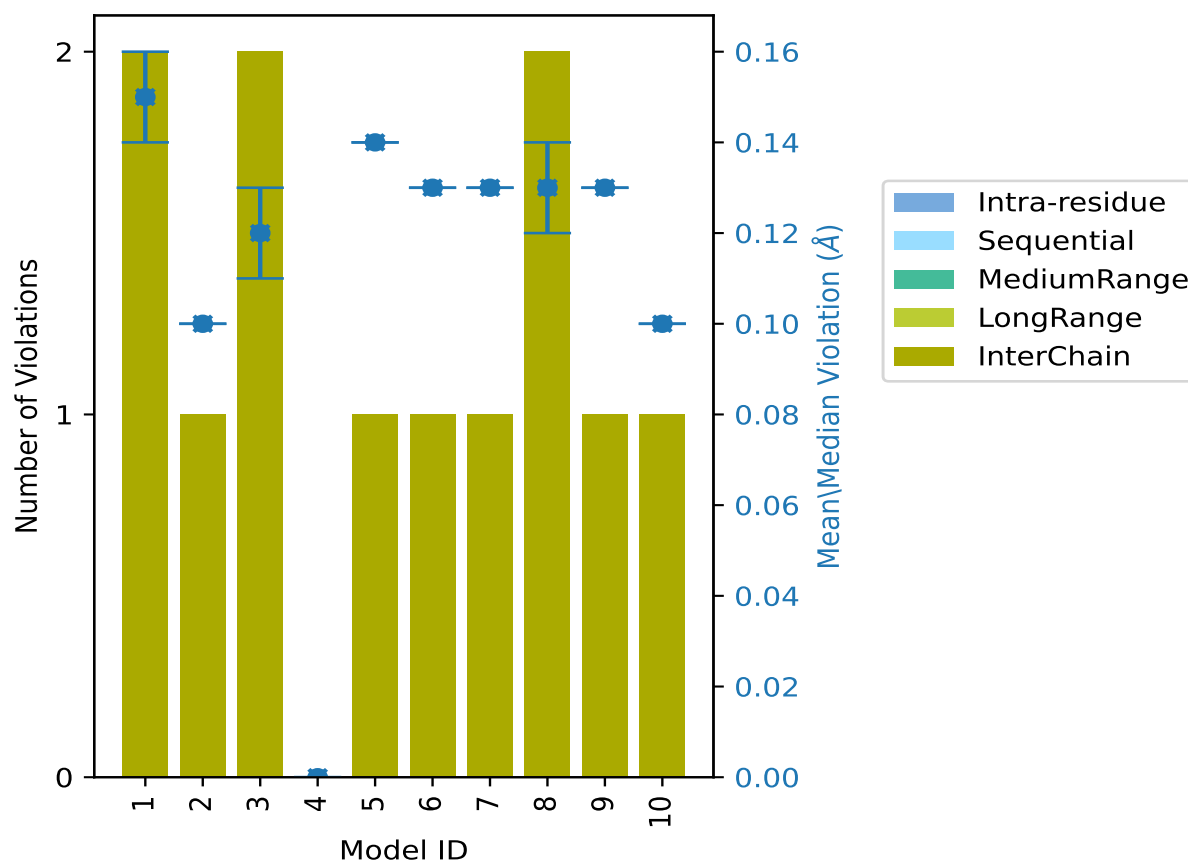
9.2 Distance violation statistics for each model [i](#)

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	2	2	0.15	0.16	0.01	0.15
2	0	0	0	0	1	1	0.1	0.1	0.0	0.1
3	0	0	0	0	2	2	0.12	0.13	0.01	0.12
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	1	1	0.14	0.14	0.0	0.14
6	0	0	0	0	1	1	0.13	0.13	0.0	0.13
7	0	0	0	0	1	1	0.13	0.13	0.0	0.13
8	0	0	0	0	2	2	0.13	0.14	0.01	0.13
9	0	0	0	0	1	1	0.13	0.13	0.0	0.13
10	0	0	0	0	1	1	0.1	0.1	0.0	0.1

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, 57(IR:0, SQ:0, MR:0, LR:0, IC:57) 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	1	1	1	10.0
0	0	0	0	0	0	2	20.0
0	0	0	0	1	1	3	30.0

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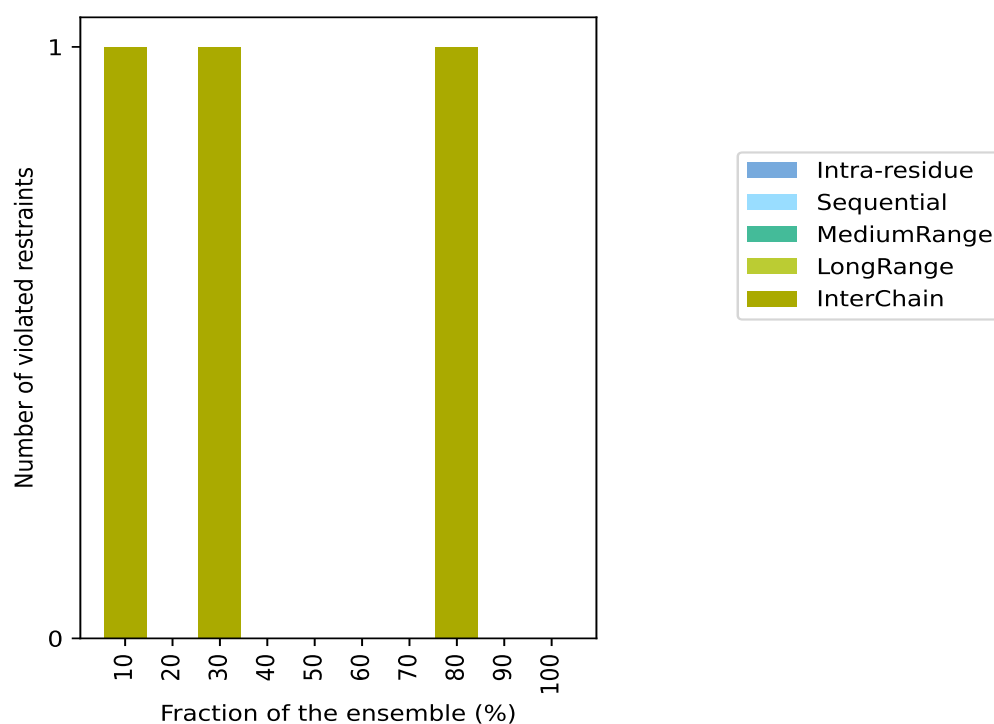
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	4	40.0
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	1	1	8	80.0
0	0	0	0	0	0	9	90.0
0	0	0	0	0	0	10	100.0

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

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

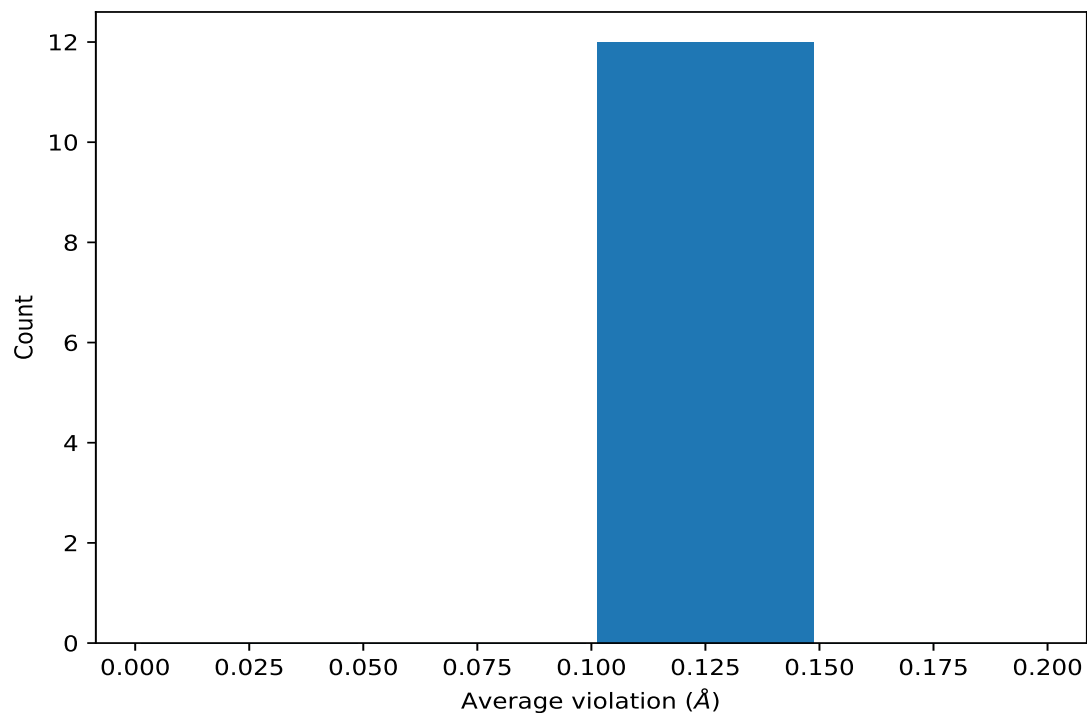


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

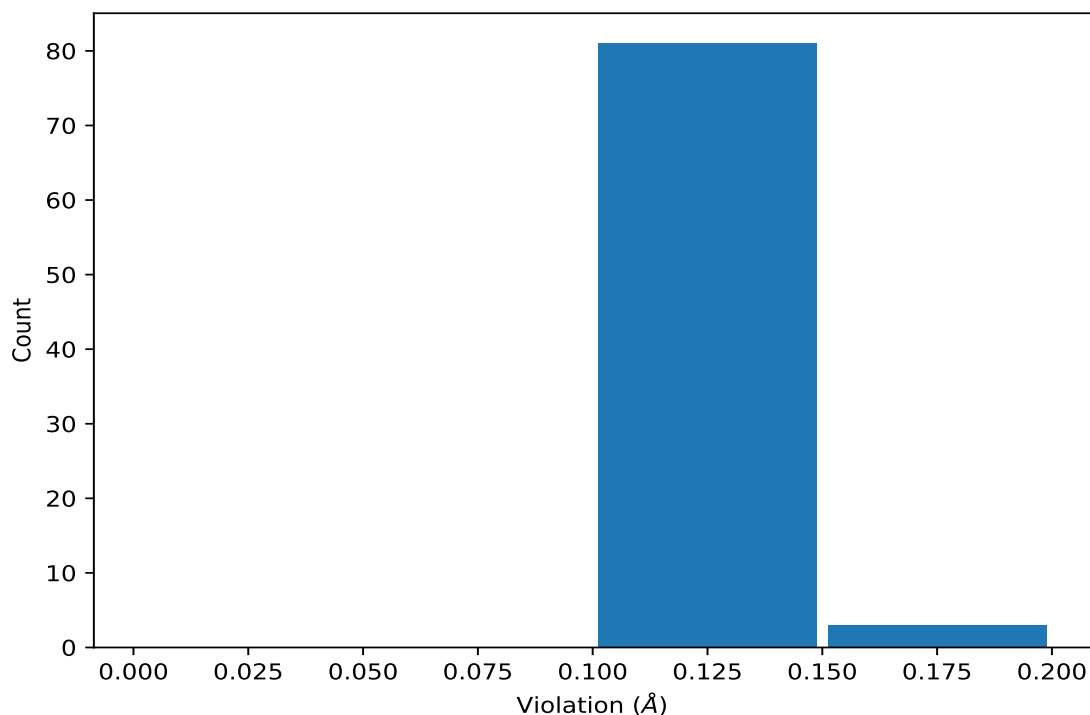
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG11	8	0.13	0.02	0.13
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG12	8	0.13	0.02	0.13
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG13	8	0.13	0.02	0.13
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG11	8	0.13	0.02	0.13
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG12	8	0.13	0.02	0.13
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG13	8	0.13	0.02	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG11	8	0.13	0.02	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG12	8	0.13	0.02	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG13	8	0.13	0.02	0.13
(1,2)	1:16:A:ALA:HB1	2:858:B:TRP:HE3	3	0.13	0.02	0.12
(1,2)	1:16:A:ALA:HB2	2:858:B:TRP:HE3	3	0.13	0.02	0.12
(1,2)	1:16:A:ALA:HB3	2:858:B:TRP:HE3	3	0.13	0.02	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:16:A:ALA:HB1	2:858:B:TRP:HE3	1	0.16
(1,2)	1:16:A:ALA:HB2	2:858:B:TRP:HE3	1	0.16
(1,2)	1:16:A:ALA:HB3	2:858:B:TRP:HE3	1	0.16
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG11	1	0.14
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG12	1	0.14
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG13	1	0.14
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG11	1	0.14
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG12	1	0.14
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG13	1	0.14
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG11	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG12	1	0.14
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG13	1	0.14
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG11	5	0.14
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG12	5	0.14
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG13	5	0.14
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG11	5	0.14
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG12	5	0.14
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG13	5	0.14
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG11	5	0.14
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG12	5	0.14
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG13	5	0.14
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG11	8	0.14
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG12	8	0.14
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG13	8	0.14
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG11	8	0.14
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG12	8	0.14
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG13	8	0.14
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG11	8	0.14
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG12	8	0.14
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG13	8	0.14
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG11	3	0.13
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG12	3	0.13
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG13	3	0.13
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG11	3	0.13
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG12	3	0.13
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG13	3	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG11	3	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG12	3	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG13	3	0.13
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG11	6	0.13
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG12	6	0.13
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG13	6	0.13
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG11	6	0.13
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG12	6	0.13
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG13	6	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG11	6	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG12	6	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG13	6	0.13
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG11	9	0.13
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG12	9	0.13
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG13	9	0.13
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG11	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG12	9	0.13
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG13	9	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG11	9	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG12	9	0.13
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG13	9	0.13
(1,27)	1:72:A:MET:HE1	2:858:B:TRP:HZ2	7	0.13
(1,27)	1:72:A:MET:HE2	2:858:B:TRP:HZ2	7	0.13
(1,27)	1:72:A:MET:HE3	2:858:B:TRP:HZ2	7	0.13
(1,2)	1:16:A:ALA:HB1	2:858:B:TRP:HE3	3	0.12
(1,2)	1:16:A:ALA:HB2	2:858:B:TRP:HE3	3	0.12
(1,2)	1:16:A:ALA:HB3	2:858:B:TRP:HE3	3	0.12
(1,2)	1:16:A:ALA:HB1	2:858:B:TRP:HE3	8	0.12
(1,2)	1:16:A:ALA:HB2	2:858:B:TRP:HE3	8	0.12
(1,2)	1:16:A:ALA:HB3	2:858:B:TRP:HE3	8	0.12
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG11	2	0.1
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG12	2	0.1
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG13	2	0.1
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG11	2	0.1
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG12	2	0.1
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG13	2	0.1
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG11	2	0.1
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG12	2	0.1
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG13	2	0.1
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG11	10	0.1
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG12	10	0.1
(1,60)	1:147:A:THR:HG21	2:857:B:VAL:HG13	10	0.1
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG11	10	0.1
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG12	10	0.1
(1,60)	1:147:A:THR:HG22	2:857:B:VAL:HG13	10	0.1
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG11	10	0.1
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG12	10	0.1
(1,60)	1:147:A:THR:HG23	2:857:B:VAL:HG13	10	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found