



Full wwPDB NMR Structure Validation Report ⓘ

Mar 24, 2026 – 09:24 PM UTC

PDB ID : 5ISN / pdb_00005isn
BMRB ID : 25132
Title : NMR solution structure of macro domain from Venezuelan equine encephalitis virus
Authors : Makrynitsa, G.I.; Ntonti, D.; Marousis, K.D.; Tsika, A.C.; Papageorgiou, N.; Coutard, B.; Bentrop, D.; Spyroulias, G.A.
Deposited on : 2016-03-15

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

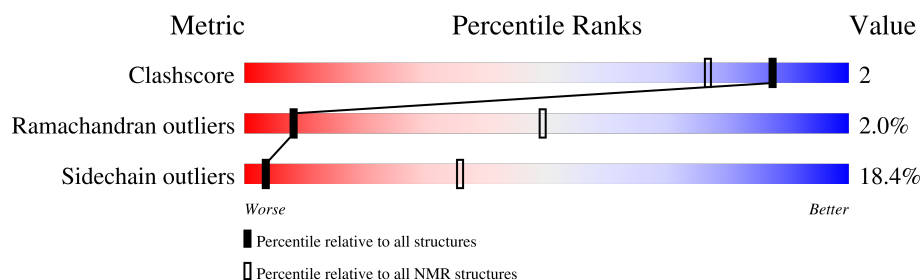
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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	168	

2 Ensemble composition and analysis

This entry contains 21 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:160 (158)	0.80	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 5, 7, 9, 10, 11, 13, 15, 16, 18, 19
2	2, 8, 12, 17, 21
3	3, 4, 6, 14
Single-model clusters	20

3 Entry composition

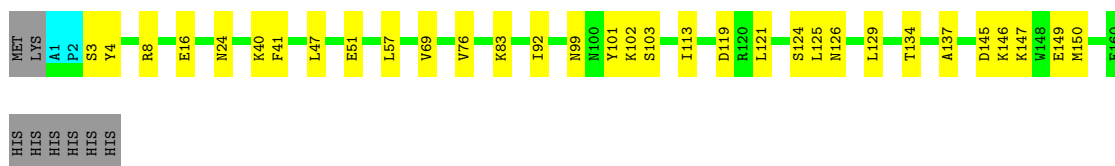
There is only 1 type of molecule in this entry. The entry contains 2441 atoms, of which 1227 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Non-structural polyprotein.

Mol	Chain	Residues	Atoms						Trace
1	A	160	Total	C	H	N	O	S	0
			2441	764	1227	214	233	3	

There are 8 discrepancies between the modelled and reference sequences:

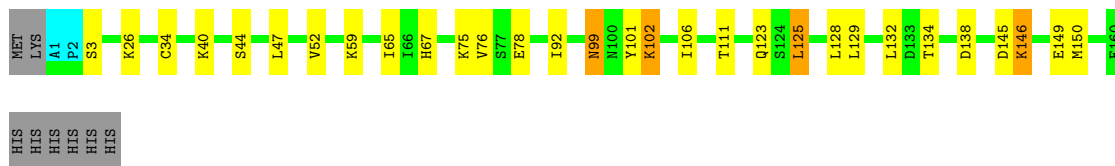
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P36328
A	0	LYS	-	expression tag	UNP P36328
A	161	HIS	-	expression tag	UNP P36328
A	162	HIS	-	expression tag	UNP P36328
A	163	HIS	-	expression tag	UNP P36328
A	164	HIS	-	expression tag	UNP P36328
A	165	HIS	-	expression tag	UNP P36328
A	166	HIS	-	expression tag	UNP P36328



4.2.3 Score per residue for model 3

- Molecule 1: Non-structural polypeptide

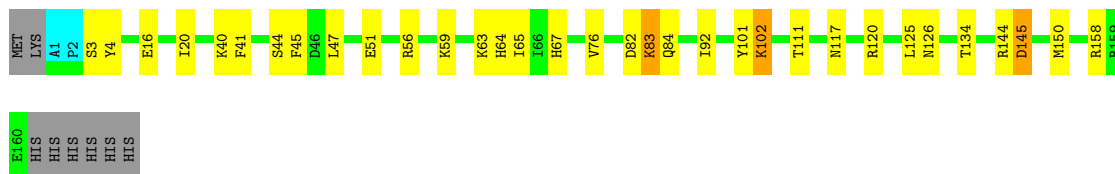
Chain A: 76% 15% •• 5%



4.2.4 Score per residue for model 4

- Molecule 1: Non-structural polypeptide

Chain A: 74% 18% •• 5%



4.2.5 Score per residue for model 5

- Molecule 1: Non-structural polypeptide

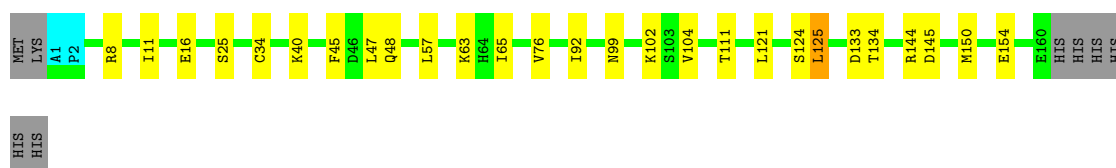
Chain A: 82% 10% •• 5%



4.2.6 Score per residue for model 6

- Molecule 1: Non-structural polypeptide

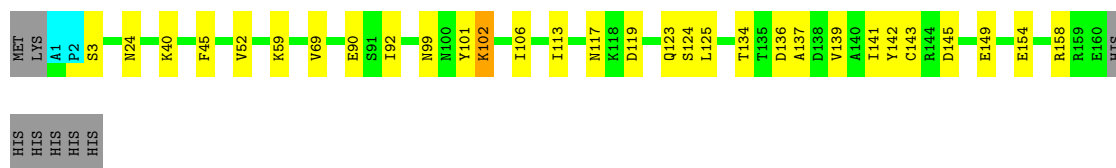
Chain A: 78% 15% •• 5%



4.2.7 Score per residue for model 7

- Molecule 1: Non-structural polypeptide

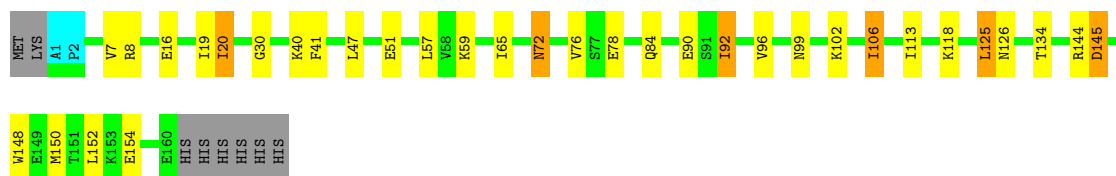
Chain A: 76% 17% 5%



4.2.8 Score per residue for model 8

- Molecule 1: Non-structural polypeptide

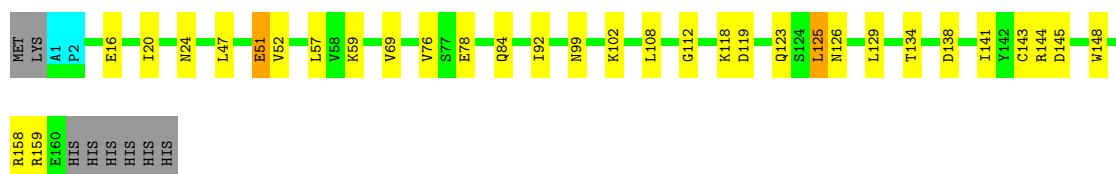
Chain A: 74% 17% 5%



4.2.9 Score per residue for model 9

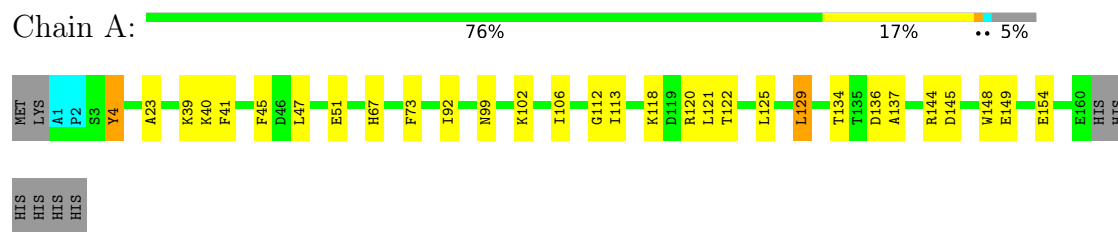
- Molecule 1: Non-structural polypeptide

Chain A: 75% 18% 5%



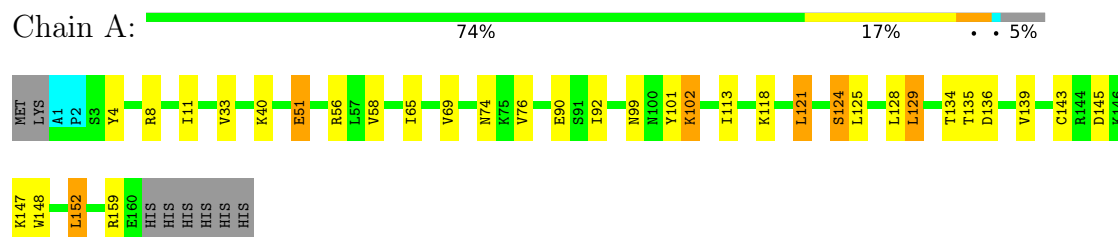
4.2.10 Score per residue for model 10

- Molecule 1: Non-structural polypeptide



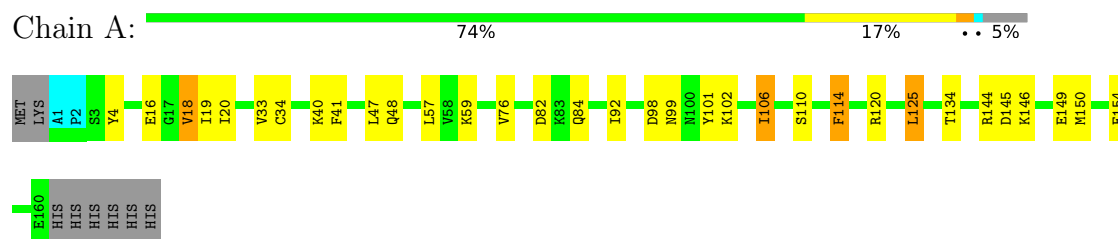
4.2.11 Score per residue for model 11

- Molecule 1: Non-structural polypeptide



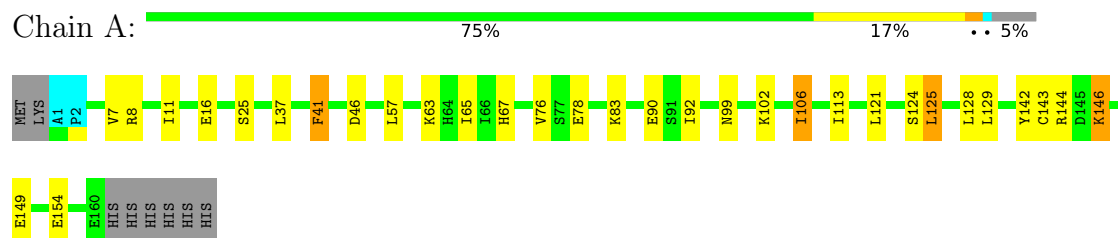
4.2.12 Score per residue for model 12

- Molecule 1: Non-structural polypeptide



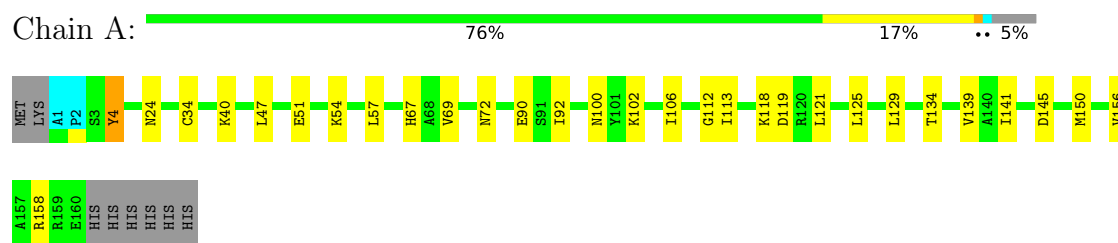
4.2.13 Score per residue for model 13

- Molecule 1: Non-structural polypeptide



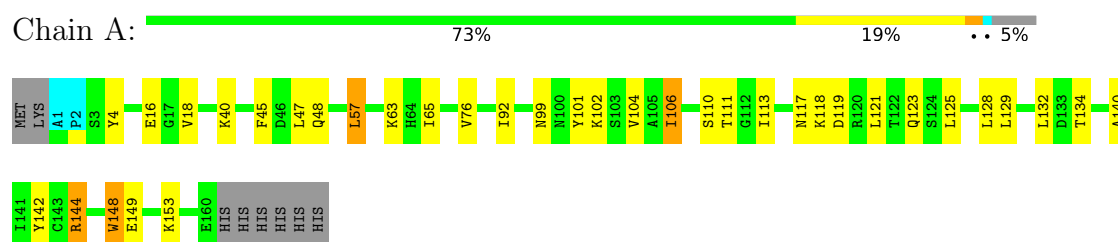
4.2.14 Score per residue for model 14

- Molecule 1: Non-structural polypeptide



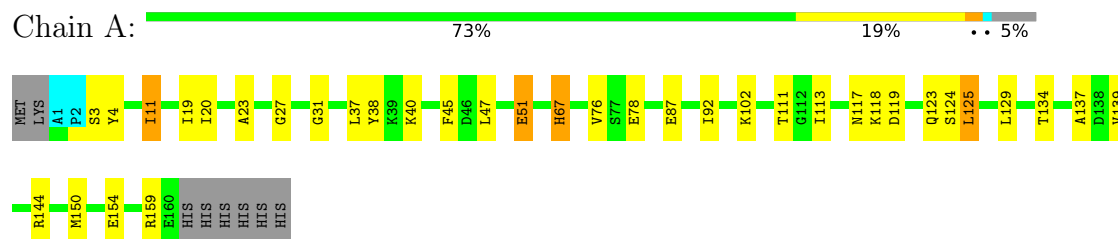
4.2.15 Score per residue for model 15

- Molecule 1: Non-structural polypeptide



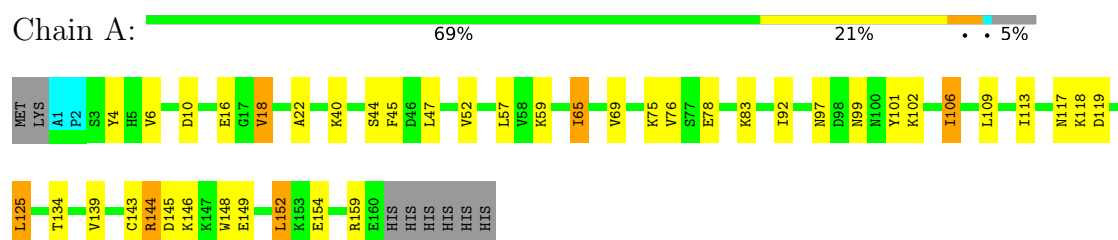
4.2.16 Score per residue for model 16

- Molecule 1: Non-structural polypeptide



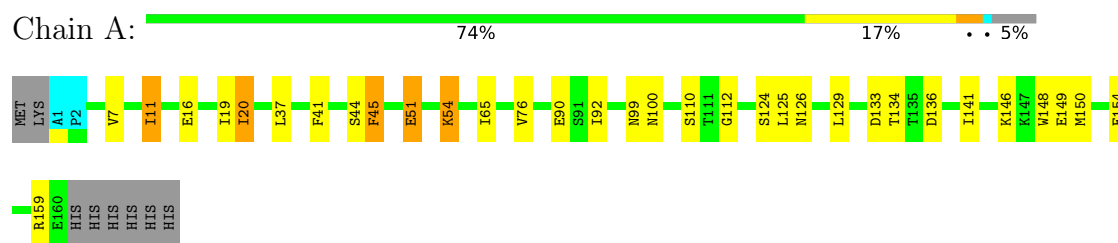
4.2.17 Score per residue for model 17

- Molecule 1: Non-structural polypeptide



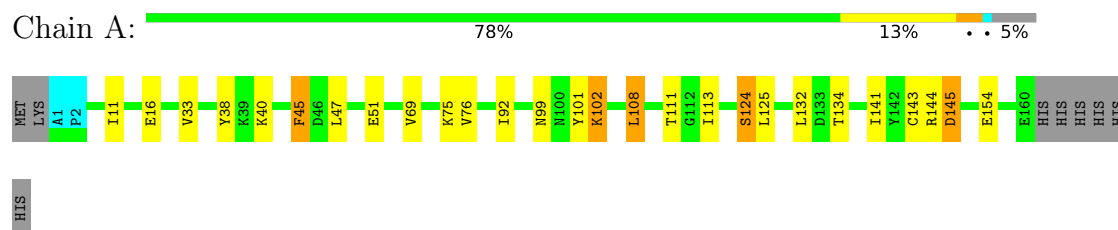
4.2.18 Score per residue for model 18

- Molecule 1: Non-structural polypeptide



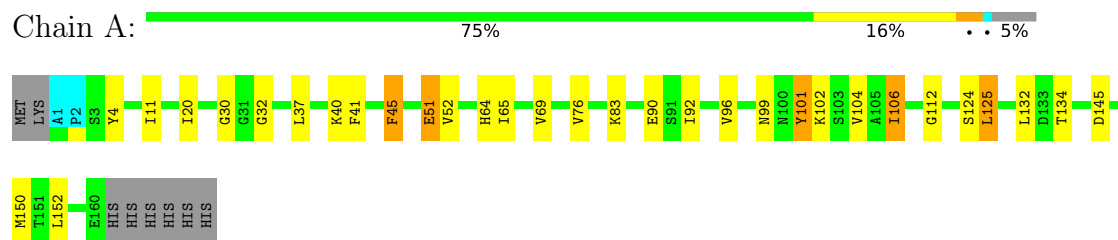
4.2.19 Score per residue for model 19

- Molecule 1: Non-structural polypeptide



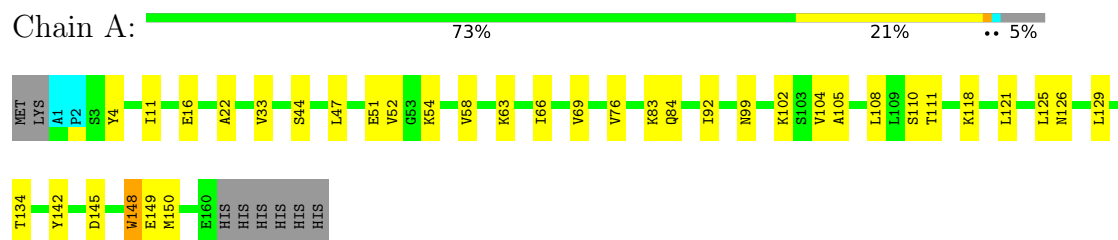
4.2.20 Score per residue for model 20

- Molecule 1: Non-structural polypeptide



4.2.21 Score per residue for model 21

- Molecule 1: Non-structural polypeptide



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 21 calculated structures, 21 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DYANA	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	1776
Number of shifts mapped to atoms	1776
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

6 Model quality

6.1 Standard geometry

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	0.63±0.01	0±0/1221 (0.0± 0.0%)	1.20±0.02	2±1/1650 (0.1± 0.1%)
All	All	0.63	0/25641 (0.0%)	1.20	48/34650 (0.1%)

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	0.3±0.5
All	All	0	6

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	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	41	PHE	CA-CB-CG	7.42	121.22	113.80	1	8
1	A	106	ILE	CB-CA-C	6.39	116.62	110.16	12	2
1	A	128	LEU	CA-C-N	6.08	128.43	120.28	13	2
1	A	128	LEU	C-N-CA	6.08	128.43	120.28	13	2
1	A	45	PHE	CA-CB-CG	5.77	119.57	113.80	18	1
1	A	124	SER	CA-C-N	5.55	128.17	120.29	11	7
1	A	124	SER	C-N-CA	5.55	128.17	120.29	11	7
1	A	142	TYR	CA-CB-CG	5.45	123.71	113.90	1	1
1	A	45	PHE	CA-C-N	5.33	127.69	120.44	5	2
1	A	45	PHE	C-N-CA	5.33	127.69	120.44	5	2
1	A	22	ALA	CA-C-N	5.32	127.85	120.29	21	2
1	A	22	ALA	C-N-CA	5.32	127.85	120.29	21	2
1	A	137	ALA	CA-C-O	5.32	121.03	117.94	2	1
1	A	119	ASP	CA-CB-CG	-5.32	107.28	112.60	9	1
1	A	52	VAL	CB-CA-C	5.32	117.75	111.32	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	72	ASN	CA-CB-CG	5.23	117.83	112.60	8	1
1	A	73	PHE	CA-CB-CG	5.10	118.90	113.80	1	2
1	A	118	LYS	CA-C-N	5.10	131.28	121.54	15	1
1	A	118	LYS	C-N-CA	5.10	131.28	121.54	15	1
1	A	97	ASN	CA-C-N	5.07	127.07	120.28	17	1
1	A	97	ASN	C-N-CA	5.07	127.07	120.28	17	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	144	ARG	Sidechain	4
1	A	142	TYR	Peptide	1
1	A	101	TYR	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	1202	1215	1215	5±2
All	All	25242	25515	25515	100

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ALA:HB3	1:A:67:HIS:CD2	0.81	2.10	16	2
1:A:57:LEU:H	1:A:57:LEU:HD13	0.61	1.54	15	1
1:A:41:PHE:CZ	1:A:63:LYS:HE2	0.60	2.31	4	1
1:A:140:ALA:HB1	1:A:142:TYR:CE2	0.59	2.33	15	1
1:A:101:TYR:C	1:A:102:LYS:HE3	0.57	2.25	7	3
1:A:146:LYS:CE	1:A:149:GLU:OE1	0.55	2.54	13	1
1:A:121:LEU:C	1:A:121:LEU:HD22	0.55	2.27	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:HD12	1:A:37:LEU:HD13	0.54	1.78	18	2
1:A:125:LEU:C	1:A:125:LEU:HD12	0.54	2.27	3	8
1:A:37:LEU:HD23	1:A:45:PHE:CE1	0.52	2.39	20	1
1:A:106:ILE:HD11	1:A:139:VAL:HG22	0.52	1.82	17	1
1:A:106:ILE:HB	1:A:128:LEU:HD21	0.51	1.82	15	1
1:A:44:SER:HB3	1:A:65:ILE:HD13	0.50	1.83	3	1
1:A:105:ALA:HB1	1:A:142:TYR:CD2	0.50	2.42	21	1
1:A:64:HIS:C	1:A:65:ILE:HD12	0.50	2.32	20	2
1:A:108:LEU:HD12	1:A:148:TRP:CZ3	0.50	2.42	21	1
1:A:51:GLU:O	1:A:69:VAL:HG21	0.49	2.06	2	5
1:A:37:LEU:HD11	1:A:41:PHE:CE2	0.49	2.42	13	1
1:A:6:VAL:HG23	1:A:148:TRP:CH2	0.49	2.43	17	1
1:A:11:ILE:HD11	1:A:19:ILE:HG21	0.49	1.84	18	2
1:A:102:LYS:N	1:A:102:LYS:HE2	0.49	2.22	3	1
1:A:11:ILE:HD13	1:A:11:ILE:O	0.49	2.08	18	1
1:A:44:SER:CB	1:A:65:ILE:HD13	0.49	2.37	17	2
1:A:18:VAL:HG21	1:A:101:TYR:CZ	0.49	2.41	17	1
1:A:146:LYS:HE3	1:A:149:GLU:OE1	0.49	2.08	17	1
1:A:4:TYR:CD1	1:A:156:VAL:HG13	0.48	2.44	14	1
1:A:92:ILE:O	1:A:96:VAL:HG23	0.47	2.09	8	1
1:A:20:ILE:HD12	1:A:20:ILE:N	0.47	2.24	18	6
1:A:24:ASN:CA	1:A:69:VAL:HG22	0.47	2.40	14	1
1:A:24:ASN:HA	1:A:69:VAL:HG22	0.46	1.87	14	2
1:A:129:LEU:HD21	1:A:139:VAL:HG11	0.46	1.87	14	1
1:A:23:ALA:HB1	1:A:27:GLY:C	0.46	2.35	16	1
1:A:52:VAL:HA	1:A:69:VAL:HG11	0.46	1.87	21	2
1:A:19:ILE:C	1:A:20:ILE:HD12	0.45	2.36	8	2
1:A:67:HIS:CD2	1:A:67:HIS:C	0.45	2.94	16	2
1:A:129:LEU:O	1:A:129:LEU:HD22	0.45	2.11	11	1
1:A:108:LEU:HD21	1:A:141:ILE:CG2	0.45	2.42	19	1
1:A:38:TYR:CD2	1:A:45:PHE:CE1	0.45	3.05	16	1
1:A:6:VAL:HG21	1:A:152:LEU:HD21	0.45	1.89	17	1
1:A:57:LEU:HD12	1:A:57:LEU:H	0.44	1.72	8	1
1:A:146:LYS:CE	1:A:149:GLU:OE2	0.44	2.65	5	1
1:A:121:LEU:HD12	1:A:122:THR:N	0.44	2.27	10	1
1:A:24:ASN:C	1:A:69:VAL:HG22	0.44	2.37	7	1
1:A:99:ASN:HB3	1:A:101:TYR:CE1	0.44	2.48	15	1
1:A:45:PHE:O	1:A:45:PHE:CG	0.43	2.70	19	1
1:A:110:SER:O	1:A:111:THR:HG23	0.43	2.13	21	1
1:A:41:PHE:CZ	1:A:63:LYS:CE	0.43	3.01	4	1
1:A:125:LEU:O	1:A:125:LEU:HD22	0.43	2.13	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:LEU:HD22	1:A:108:LEU:N	0.43	2.28	19	1
1:A:20:ILE:HD13	1:A:106:ILE:CG2	0.43	2.44	20	1
1:A:99:ASN:HB3	1:A:101:TYR:CE2	0.43	2.49	17	2
1:A:20:ILE:HD13	1:A:106:ILE:HB	0.43	1.91	8	1
1:A:148:TRP:CD1	1:A:149:GLU:N	0.42	2.88	10	1
1:A:11:ILE:CD1	1:A:33:VAL:HG11	0.42	2.45	11	1
1:A:51:GLU:OE1	1:A:54:LYS:NZ	0.42	2.51	18	1
1:A:148:TRP:C	1:A:148:TRP:CD1	0.42	2.98	15	1
1:A:59:LYS:HE2	1:A:59:LYS:O	0.41	2.15	9	1
1:A:152:LEU:HD12	1:A:152:LEU:C	0.41	2.40	11	1
1:A:11:ILE:HD13	1:A:33:VAL:HG21	0.41	1.92	21	1
1:A:57:LEU:H	1:A:57:LEU:CD1	0.41	2.26	15	1
1:A:101:TYR:C	1:A:102:LYS:CE	0.41	2.94	19	1
1:A:145:ASP:CG	1:A:148:TRP:CD1	0.41	2.99	8	1
1:A:38:TYR:CD2	1:A:45:PHE:CZ	0.41	3.08	19	1
1:A:146:LYS:HE3	1:A:149:GLU:OE2	0.40	2.16	3	1
1:A:82:ASP:OD1	1:A:83:LYS:CE	0.40	2.69	4	1
1:A:18:VAL:HG21	1:A:101:TYR:CE1	0.40	2.51	12	1
1:A:101:TYR:O	1:A:102:LYS:HE2	0.40	2.16	2	1
1:A:125:LEU:HD13	1:A:125:LEU:C	0.40	2.42	16	1
1:A:102:LYS:N	1:A:102:LYS:CE	0.40	2.84	5	1
1:A:4:TYR:CE2	1:A:129:LEU:HD21	0.40	2.51	10	1
1:A:11:ILE:O	1:A:11:ILE:HD13	0.40	2.17	16	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/168 (93%)	137±3 (87±2%)	17±3 (11±2%)	3±1 (2±1%)	8	49
All	All	3297/3528 (93%)	2883 (87%)	347 (11%)	67 (2%)	8	49

All 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	145	ASP	17
1	A	113	ILE	9
1	A	118	LYS	7
1	A	112	GLY	6
1	A	119	ASP	5
1	A	146	LYS	3
1	A	137	ALA	3
1	A	16	GLU	3
1	A	32	GLY	2
1	A	30	GLY	2
1	A	51	GLU	2
1	A	47	LEU	1
1	A	120	ARG	1
1	A	3	SER	1
1	A	136	ASP	1
1	A	114	PHE	1
1	A	31	GLY	1
1	A	45	PHE	1
1	A	117	ASN	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/136 (93%)	104±3 (82±2%)	23±3 (18±2%)	3	36
All	All	2667/2856 (93%)	2176 (82%)	491 (18%)	3	36

All 92 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	92	ILE	21
1	A	125	LEU	21
1	A	134	THR	20
1	A	102	LYS	19
1	A	76	VAL	18
1	A	40	LYS	16
1	A	47	LEU	15

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Mol	Chain	Res	Type	Models (Total)
1	A	99	ASN	15
1	A	106	ILE	12
1	A	129	LEU	11
1	A	4	TYR	11
1	A	150	MET	11
1	A	16	GLU	10
1	A	144	ARG	10
1	A	154	GLU	10
1	A	57	LEU	9
1	A	121	LEU	9
1	A	51	GLU	9
1	A	65	ILE	8
1	A	111	THR	8
1	A	8	ARG	7
1	A	143	CYS	7
1	A	83	LYS	7
1	A	149	GLU	7
1	A	11	ILE	7
1	A	45	PHE	7
1	A	90	GLU	7
1	A	148	TRP	6
1	A	126	ASN	6
1	A	59	LYS	6
1	A	78	GLU	6
1	A	3	SER	5
1	A	67	HIS	5
1	A	123	GLN	5
1	A	84	GLN	5
1	A	104	VAL	5
1	A	124	SER	5
1	A	159	ARG	5
1	A	34	CYS	4
1	A	132	LEU	4
1	A	146	LYS	4
1	A	117	ASN	4
1	A	158	ARG	4
1	A	18	VAL	4
1	A	63	LYS	4
1	A	141	ILE	4
1	A	152	LEU	4
1	A	44	SER	3
1	A	113	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	133	ASP	3
1	A	142	TYR	3
1	A	52	VAL	3
1	A	75	LYS	3
1	A	48	GLN	3
1	A	139	VAL	3
1	A	7	VAL	3
1	A	118	LYS	3
1	A	110	SER	3
1	A	54	LYS	3
1	A	98	ASP	2
1	A	147	LYS	2
1	A	138	ASP	2
1	A	56	ARG	2
1	A	145	ASP	2
1	A	25	SER	2
1	A	136	ASP	2
1	A	20	ILE	2
1	A	72	ASN	2
1	A	108	LEU	2
1	A	120	ARG	2
1	A	58	VAL	2
1	A	33	VAL	2
1	A	100	ASN	2
1	A	69	VAL	2
1	A	103	SER	1
1	A	26	LYS	1
1	A	128	LEU	1
1	A	24	ASN	1
1	A	39	LYS	1
1	A	74	ASN	1
1	A	135	THR	1
1	A	82	ASP	1
1	A	114	PHE	1
1	A	46	ASP	1
1	A	153	LYS	1
1	A	87	GLU	1
1	A	10	ASP	1
1	A	109	LEU	1
1	A	119	ASP	1
1	A	96	VAL	1
1	A	101	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	66	ILE	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

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `start_cs.str`

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	1776
Number of shifts mapped to atoms	1776
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	154	0.06 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	144	0.08 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	154	0.23 ± 0.10	None needed (< 0.5 ppm)
^{15}N	147	0.57 ± 0.60	None needed (imprecise)

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 83%, i.e. 1749 atoms were assigned a chemical shift out of a possible 2096. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	746/793 (94%)	302/324 (93%)	304/316 (96%)	140/153 (92%)
Sidechain	1003/1178 (85%)	686/767 (89%)	317/366 (87%)	0/45 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/125 (0%)	0/62 (0%)	0/58 (0%)	0/5 (0%)
Overall	1749/2096 (83%)	988/1153 (86%)	621/740 (84%)	140/203 (69%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1770 atoms were assigned a chemical shift out of a possible 2117. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	754/801 (94%)	305/327 (93%)	308/320 (96%)	141/154 (92%)
Sidechain	1016/1191 (85%)	695/776 (90%)	321/370 (87%)	0/45 (0%)
Aromatic	0/125 (0%)	0/62 (0%)	0/58 (0%)	0/5 (0%)
Overall	1770/2117 (84%)	1000/1165 (86%)	629/748 (84%)	141/204 (69%)

7.1.4 Statistically unusual chemical shifts ⓘ

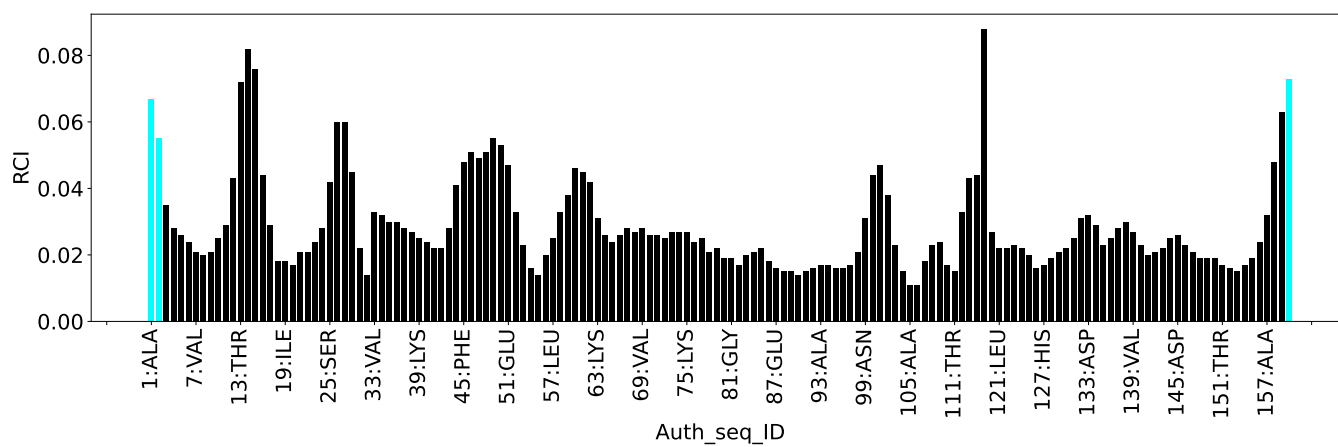
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	29	PRO	CD	42.09	45.11 – 55.58	-7.9
1	A	121	LEU	CD1	16.19	16.71 – 32.55	-5.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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	1413
Intra-residue ($ i-j =0$)	292
Sequential ($ i-j =1$)	535
Medium range ($ i-j >1$ and $ i-j <5$)	363
Long range ($ i-j \geq 5$)	223
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	1
Number of restraints per residue	8.4
Number of long range restraints per residue ¹	1.3

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)	10.5	0.19
0.2-0.5 (Medium)	0.4	0.32
>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

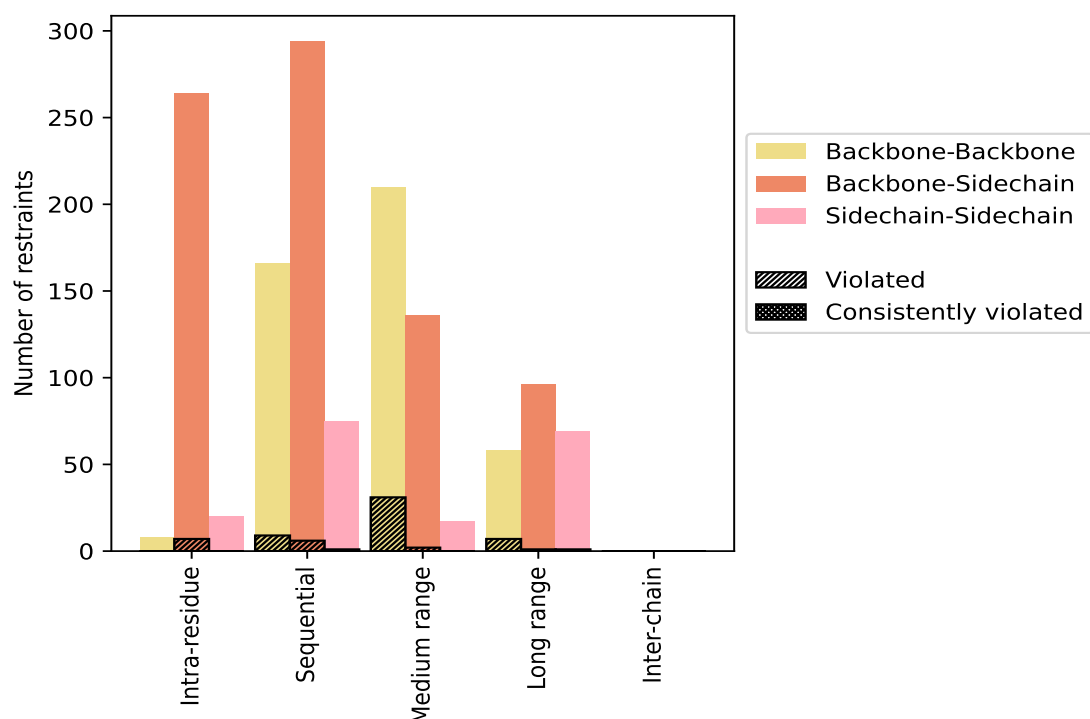
9.1 Summary of distance violations

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 ($i-j =0$)	292	20.7	7	2.4	0.5	0	0.0	0.0
Backbone-Backbone	8	0.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	264	18.7	7	2.7	0.5	0	0.0	0.0
Sidechain-Sidechain	20	1.4	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	535	37.9	16	3.0	1.1	0	0.0	0.0
Backbone-Backbone	166	11.7	9	5.4	0.6	0	0.0	0.0
Backbone-Sidechain	294	20.8	6	2.0	0.4	0	0.0	0.0
Sidechain-Sidechain	75	5.3	1	1.3	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	363	25.7	33	9.1	2.3	0	0.0	0.0
Backbone-Backbone	210	14.9	31	14.8	2.2	0	0.0	0.0
Backbone-Sidechain	136	9.6	2	1.5	0.1	0	0.0	0.0
Sidechain-Sidechain	17	1.2	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	223	15.8	9	4.0	0.6	0	0.0	0.0
Backbone-Backbone	58	4.1	7	12.1	0.5	0	0.0	0.0
Backbone-Sidechain	96	6.8	1	1.0	0.1	0	0.0	0.0
Sidechain-Sidechain	69	4.9	1	1.4	0.1	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	1413	100.0	65	4.6	4.6	0	0.0	0.0
Backbone-Backbone	442	31.3	47	10.6	3.3	0	0.0	0.0
Backbone-Sidechain	790	55.9	16	2.0	1.1	0	0.0	0.0
Sidechain-Sidechain	181	12.8	2	1.1	0.1	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	4	7	2	0	13	0.12	0.16	0.02	0.12
2	0	3	5	2	0	10	0.12	0.14	0.01	0.12
3	0	3	7	3	0	13	0.12	0.16	0.02	0.11
4	0	5	3	1	0	9	0.13	0.22	0.03	0.12
5	0	4	8	5	0	17	0.12	0.16	0.02	0.12
6	1	3	7	1	0	12	0.12	0.15	0.01	0.12
7	0	3	6	2	0	11	0.12	0.19	0.03	0.11
8	0	6	7	3	0	16	0.14	0.21	0.03	0.14
9	1	4	3	2	0	10	0.12	0.14	0.01	0.11
10	0	2	6	2	0	10	0.14	0.22	0.03	0.13

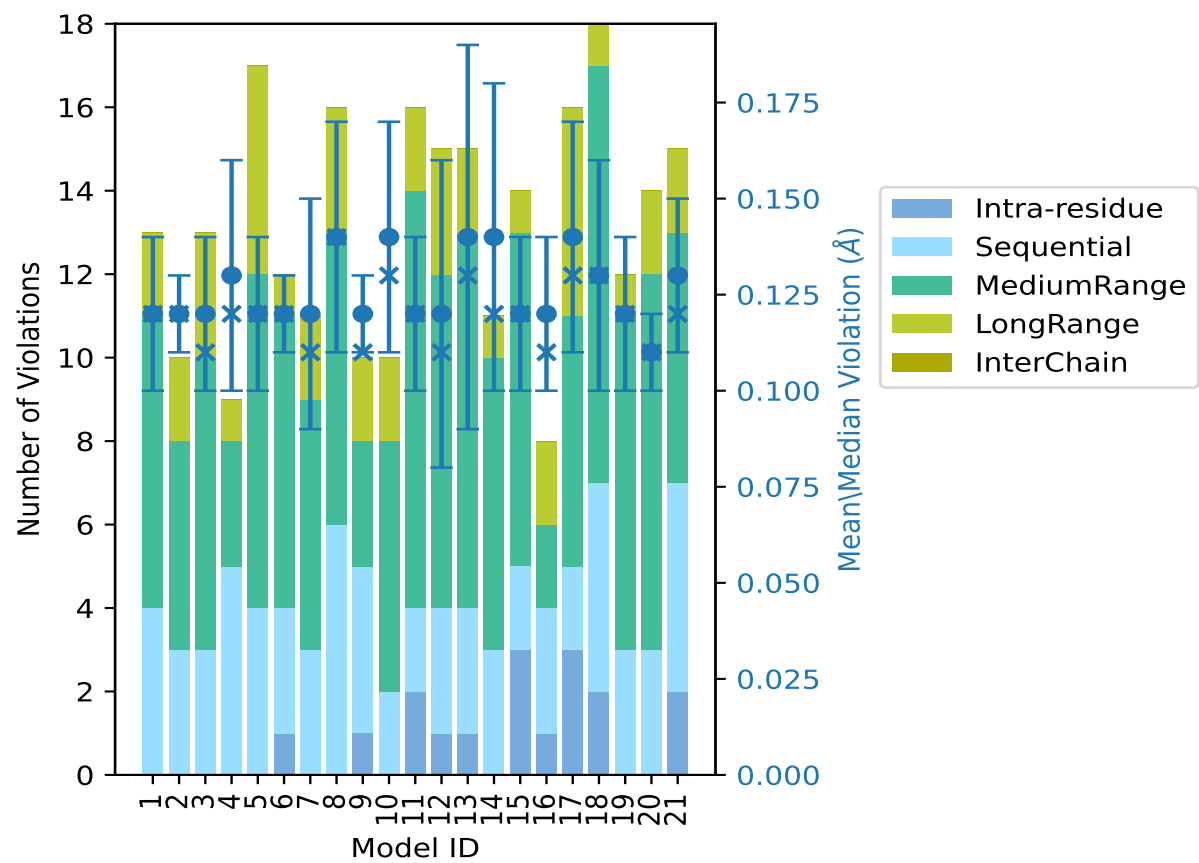
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	2	2	10	2	0	16	0.12	0.19	0.02	0.12
12	1	3	8	3	0	15	0.12	0.25	0.04	0.11
13	1	3	9	2	0	15	0.14	0.32	0.05	0.13
14	0	3	7	1	0	11	0.14	0.27	0.04	0.12
15	3	2	8	1	0	14	0.12	0.16	0.02	0.12
16	1	3	2	2	0	8	0.12	0.15	0.02	0.11
17	3	2	6	5	0	16	0.14	0.24	0.03	0.13
18	2	5	10	1	0	18	0.13	0.24	0.03	0.13
19	0	3	8	1	0	12	0.12	0.16	0.02	0.12
20	0	3	9	2	0	14	0.11	0.13	0.01	0.11
21	2	5	6	2	0	15	0.13	0.19	0.02	0.12

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 ⓘ



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

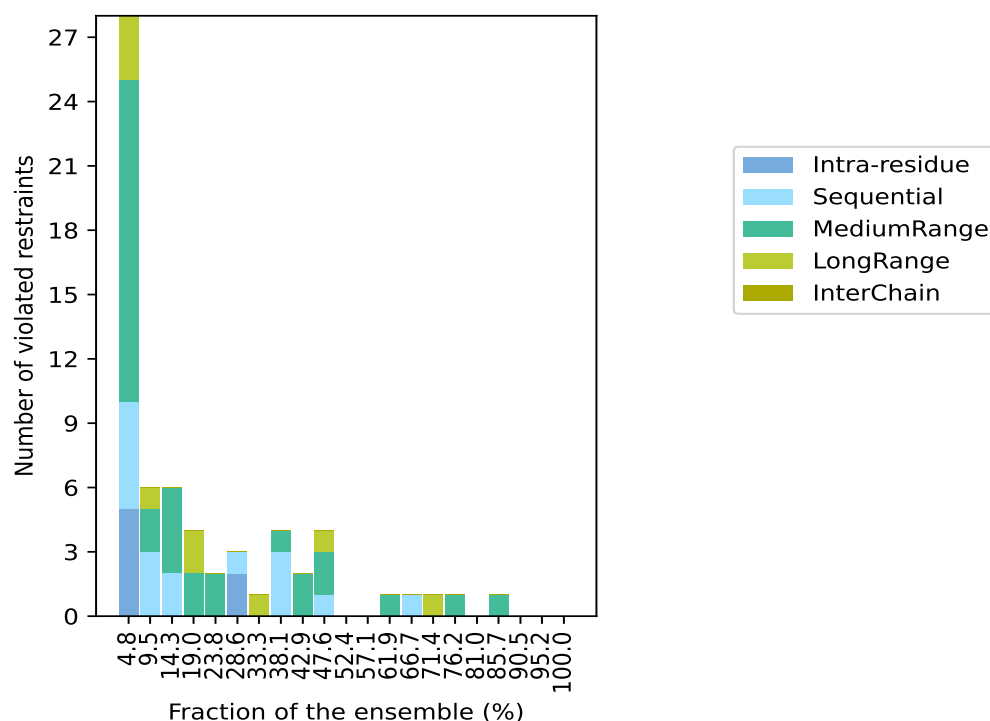
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1348(IR:285, SQ:519, MR:330, LR:214, IC:0) restraints are 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	%
5	5	15	3	0	28	1	4.8
0	3	2	1	0	6	2	9.5
0	2	4	0	0	6	3	14.3
0	0	2	2	0	4	4	19.0
0	0	2	0	0	2	5	23.8
2	1	0	0	0	3	6	28.6
0	0	0	1	0	1	7	33.3
0	3	1	0	0	4	8	38.1
0	0	2	0	0	2	9	42.9
0	1	2	1	0	4	10	47.6
0	0	0	0	0	0	11	52.4
0	0	0	0	0	0	12	57.1
0	0	1	0	0	1	13	61.9
0	1	0	0	0	1	14	66.7
0	0	0	1	0	1	15	71.4
0	0	1	0	0	1	16	76.2
0	0	0	0	0	0	17	81.0
0	0	1	0	0	1	18	85.7
0	0	0	0	0	0	19	90.5
0	0	0	0	0	0	20	95.2
0	0	0	0	0	0	21	100.0

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

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

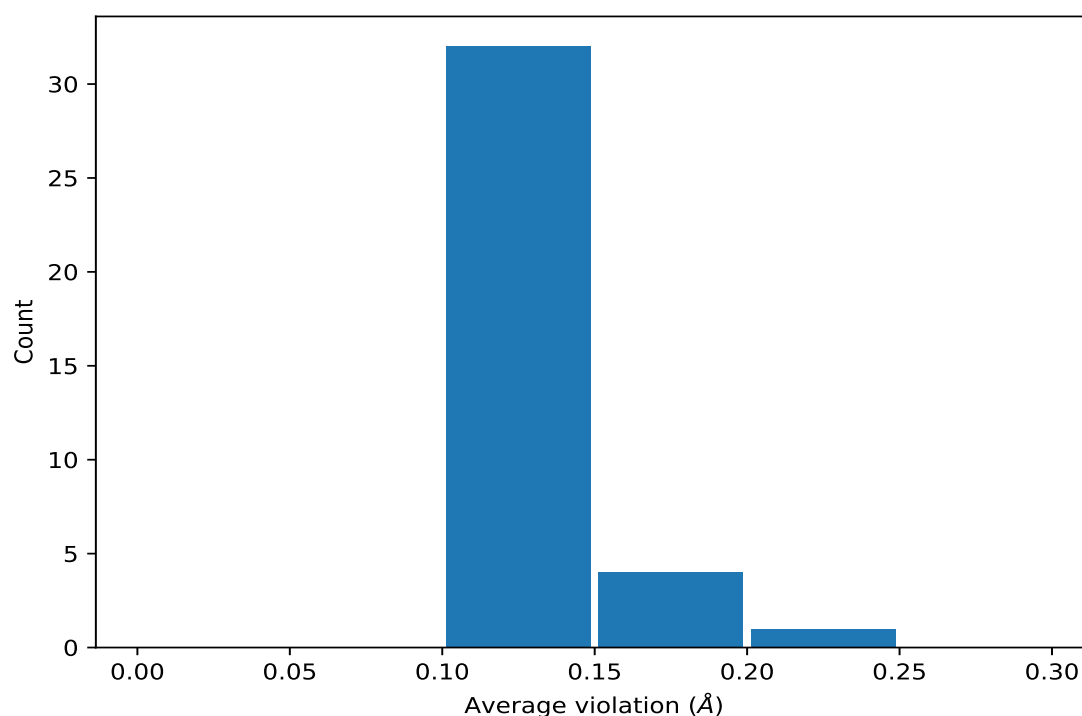
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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)
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	18	0.13	0.02	0.12
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	16	0.13	0.02	0.13
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	15	0.15	0.03	0.15
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	14	0.13	0.04	0.12
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	13	0.11	0.01	0.11
(1,366)	1:57:A:LEU:H	1:67:A:HIS:H	10	0.13	0.04	0.12
(1,483)	1:77:A:SER:H	1:79:A:VAL:H	10	0.12	0.02	0.12
(1,386)	1:60:A:GLY:H	1:61:A:ALA:H	10	0.12	0.01	0.12
(1,457)	1:74:A:ASN:HA	1:76:A:VAL:H	10	0.11	0.01	0.12
(1,1046)	1:155:A:ALA:H	1:157:A:ALA:H	9	0.13	0.02	0.13
(1,329)	1:52:A:VAL:HA	1:54:A:LYS:H	9	0.12	0.01	0.12
(1,290)	1:46:A:ASP:H	1:48:A:GLN:H	8	0.14	0.03	0.13
(1,50)	1:9:A:GLY:H	1:10:A:ASP:H	8	0.13	0.02	0.13
(1,932)	1:137:A:ALA:H	1:138:A:ASP:H	8	0.13	0.01	0.13
(1,795)	1:121:A:LEU:H	1:122:A:THR:HB	8	0.11	0.01	0.11
(2,82)	1:37:A:LEU:HG	1:43:A:GLU:H	7	0.13	0.01	0.12

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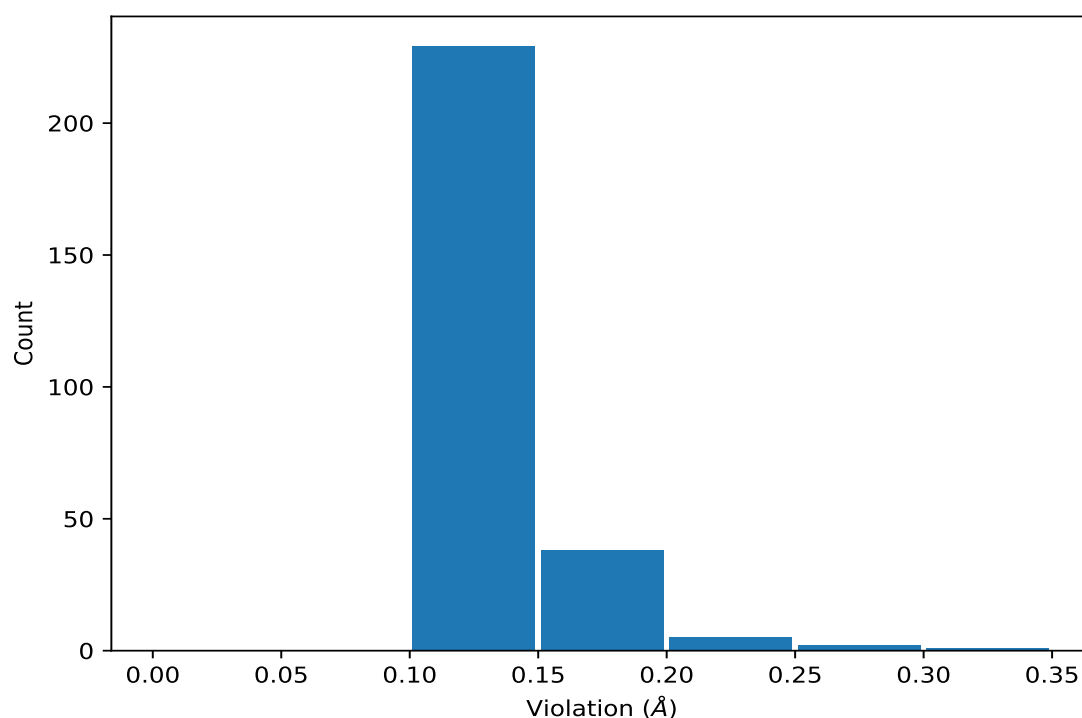
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,740)	1:104:A:VAL:H	1:104:A:VAL:HB	6	0.13	0.01	0.13
(1,980)	1:148:A:TRP:HA	1:148:A:TRP:HD1	6	0.13	0.01	0.13
(1,440)	1:69:A:VAL:H	1:70:A:GLY:H	6	0.12	0.02	0.12
(1,963)	1:146:A:LYS:HA	1:148:A:TRP:H	5	0.12	0.02	0.11
(1,701)	1:97:A:ASN:H	1:99:A:ASN:H	5	0.11	0.0	0.11
(1,446)	1:72:A:ASN:H	1:75:A:LYS:H	4	0.13	0.02	0.12
(1,373)	1:58:A:VAL:H	1:65:A:ILE:HA	4	0.12	0.01	0.12
(1,582)	1:85:A:LEU:HG	1:127:A:HIS:HD2	4	0.11	0.01	0.11
(1,526)	1:81:A:GLY:HA3	1:85:A:LEU:H	4	0.11	0.0	0.11
(1,899)	1:131:A:ALA:HA	1:134:A:THR:HB	3	0.19	0.09	0.13
(1,897)	1:131:A:ALA:HA	1:133:A:ASP:H	3	0.13	0.02	0.15
(1,846)	1:126:A:ASN:H	1:128:A:LEU:H	3	0.11	0.0	0.11
(1,341)	1:54:A:LYS:H	1:55:A:ALA:H	3	0.11	0.01	0.11
(1,89)	1:14:A:ALA:H	1:16:A:GLU:H	3	0.11	0.0	0.11
(1,715)	1:99:A:ASN:HB2	1:100:A:ASN:H	3	0.11	0.0	0.11
(1,790)	1:120:A:ARG:HA	1:121:A:LEU:H	2	0.24	0.03	0.24
(1,954)	1:144:A:ARG:HA	1:146:A:LYS:H	2	0.17	0.01	0.17
(1,3)	1:1:A:ALA:HA	1:136:A:ASP:H	2	0.16	0.04	0.16
(1,986)	1:148:A:TRP:HD1	1:149:A:GLU:H	2	0.12	0.01	0.12
(1,704)	1:97:A:ASN:HA	1:101:A:TYR:H	2	0.12	0.02	0.12
(1,283)	1:45:A:PHE:H	1:46:A:ASP:H	2	0.11	0.0	0.11

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)
(1,899)	1:131:A:ALA:HA	1:134:A:THR:HB	13	0.32
(1,790)	1:120:A:ARG:HA	1:121:A:LEU:H	14	0.27
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	12	0.25
(1,677)	1:95:A:ILE:H	1:95:A:ILE:HB	18	0.24
(1,366)	1:57:A:LEU:H	1:67:A:HIS:H	17	0.24
(1,790)	1:120:A:ARG:HA	1:121:A:LEU:H	4	0.22
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	10	0.22
(1,3)	1:1:A:ALA:HA	1:136:A:ASP:H	8	0.21
(1,797)	1:121:A:LEU:HA	1:121:A:LEU:HG	11	0.19
(1,290)	1:46:A:ASP:H	1:48:A:GLN:H	21	0.19
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	7	0.19
(1,954)	1:144:A:ARG:HA	1:146:A:LYS:H	18	0.18
(1,290)	1:46:A:ASP:H	1:48:A:GLN:H	8	0.18
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	17	0.18
(1,883)	1:129:A:LEU:HA	1:133:A:ASP:H	13	0.17
(1,483)	1:77:A:SER:H	1:79:A:VAL:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	1:45:A:PHE:HA	1:47:A:LEU:H	17	0.17
(2,2)	1:3:A:SER:H	1:138:A:ASP:H	17	0.16
(1,980)	1:148:A:TRP:HA	1:148:A:TRP:HD1	21	0.16
(1,963)	1:146:A:LYS:HA	1:148:A:TRP:H	8	0.16
(1,954)	1:144:A:ARG:HA	1:146:A:LYS:H	15	0.16
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	19	0.16
(1,740)	1:104:A:VAL:H	1:104:A:VAL:HB	13	0.16
(1,446)	1:72:A:ASN:H	1:75:A:LYS:H	5	0.16
(1,440)	1:69:A:VAL:H	1:70:A:GLY:H	8	0.16
(1,366)	1:57:A:LEU:H	1:67:A:HIS:H	5	0.16
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	1	0.16
(1,50)	1:9:A:GLY:H	1:10:A:ASP:H	19	0.16
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	3	0.16
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	12	0.16
(2,82)	1:37:A:LEU:HG	1:43:A:GLU:H	17	0.15
(1,1046)	1:155:A:ALA:H	1:157:A:ALA:H	18	0.15
(1,897)	1:131:A:ALA:HA	1:133:A:ASP:H	11	0.15
(1,897)	1:131:A:ALA:HA	1:133:A:ASP:H	13	0.15
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	1	0.15
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	7	0.15
(1,655)	1:93:A:ALA:H	1:95:A:ILE:H	18	0.15
(1,366)	1:57:A:LEU:H	1:67:A:HIS:H	8	0.15
(1,363)	1:57:A:LEU:H	1:57:A:LEU:HG	15	0.15
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	14	0.15
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	6	0.15
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	13	0.15
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	16	0.15
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	11	0.15
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	18	0.15
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	21	0.15
(2,82)	1:37:A:LEU:HG	1:43:A:GLU:H	16	0.14
(1,1046)	1:155:A:ALA:H	1:157:A:ALA:H	1	0.14
(1,1046)	1:155:A:ALA:H	1:157:A:ALA:H	8	0.14
(1,1046)	1:155:A:ALA:H	1:157:A:ALA:H	17	0.14
(1,980)	1:148:A:TRP:HA	1:148:A:TRP:HD1	11	0.14
(1,980)	1:148:A:TRP:HA	1:148:A:TRP:HD1	15	0.14
(1,932)	1:137:A:ALA:H	1:138:A:ASP:H	2	0.14
(1,932)	1:137:A:ALA:H	1:138:A:ASP:H	3	0.14
(1,932)	1:137:A:ALA:H	1:138:A:ASP:H	8	0.14
(1,930)	1:136:A:ASP:H	1:137:A:ALA:H	8	0.14
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	14	0.14
(1,740)	1:104:A:VAL:H	1:104:A:VAL:HB	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:104:A:VAL:H	1:104:A:VAL:HB	21	0.14
(1,483)	1:77:A:SER:H	1:79:A:VAL:H	13	0.14
(1,483)	1:77:A:SER:H	1:79:A:VAL:H	14	0.14
(1,386)	1:60:A:GLY:H	1:61:A:ALA:H	8	0.14
(1,290)	1:46:A:ASP:H	1:48:A:GLN:H	12	0.14
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	1	0.14
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	13	0.14
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	9	0.14
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	10	0.14
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	14	0.14
(1,50)	1:9:A:GLY:H	1:10:A:ASP:H	6	0.14
(1,50)	1:9:A:GLY:H	1:10:A:ASP:H	21	0.14
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	19	0.14
(2,82)	1:37:A:LEU:HG	1:43:A:GLU:H	5	0.13
(1,1046)	1:155:A:ALA:H	1:157:A:ALA:H	10	0.13
(1,1046)	1:155:A:ALA:H	1:157:A:ALA:H	19	0.13
(1,986)	1:148:A:TRP:HD1	1:149:A:GLU:H	13	0.13
(1,932)	1:137:A:ALA:H	1:138:A:ASP:H	6	0.13
(1,932)	1:137:A:ALA:H	1:138:A:ASP:H	18	0.13
(1,899)	1:131:A:ALA:HA	1:134:A:THR:HB	6	0.13
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	4	0.13
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	5	0.13
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	10	0.13
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	17	0.13
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	18	0.13
(1,795)	1:121:A:LEU:H	1:122:A:THR:HB	20	0.13
(1,704)	1:97:A:ASN:HA	1:101:A:TYR:H	11	0.13
(1,582)	1:85:A:LEU:HG	1:127:A:HIS:HD2	15	0.13
(1,483)	1:77:A:SER:H	1:79:A:VAL:H	5	0.13
(1,457)	1:74:A:ASN:HA	1:76:A:VAL:H	15	0.13
(1,457)	1:74:A:ASN:HA	1:76:A:VAL:H	17	0.13
(1,446)	1:72:A:ASN:H	1:75:A:LYS:H	2	0.13
(1,440)	1:69:A:VAL:H	1:70:A:GLY:H	19	0.13
(1,386)	1:60:A:GLY:H	1:61:A:ALA:H	1	0.13
(1,386)	1:60:A:GLY:H	1:61:A:ALA:H	18	0.13
(1,329)	1:52:A:VAL:HA	1:54:A:LYS:H	18	0.13
(1,290)	1:46:A:ASP:H	1:48:A:GLN:H	2	0.13
(1,290)	1:46:A:ASP:H	1:48:A:GLN:H	5	0.13
(1,290)	1:46:A:ASP:H	1:48:A:GLN:H	18	0.13
(1,108)	1:16:A:GLU:HA	1:18:A:VAL:H	5	0.13
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	4	0.13
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	11	0.13
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	17	0.13
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	18	0.13
(1,50)	1:9:A:GLY:H	1:10:A:ASP:H	10	0.13
(1,50)	1:9:A:GLY:H	1:10:A:ASP:H	15	0.13
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	2	0.13
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	6	0.13
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	8	0.13
(2,82)	1:37:A:LEU:HG	1:43:A:GLU:H	3	0.12
(2,82)	1:37:A:LEU:HG	1:43:A:GLU:H	9	0.12
(2,82)	1:37:A:LEU:HG	1:43:A:GLU:H	11	0.12
(1,1046)	1:155:A:ALA:H	1:157:A:ALA:H	3	0.12
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	8	0.12
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	9	0.12
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	14	0.12
(1,980)	1:148:A:TRP:HA	1:148:A:TRP:HD1	9	0.12
(1,980)	1:148:A:TRP:HA	1:148:A:TRP:HD1	17	0.12
(1,980)	1:148:A:TRP:HA	1:148:A:TRP:HD1	18	0.12
(1,963)	1:146:A:LYS:HA	1:148:A:TRP:H	11	0.12
(1,932)	1:137:A:ALA:H	1:138:A:ASP:H	4	0.12
(1,870)	1:128:A:LEU:H	1:131:A:ALA:H	6	0.12
(1,846)	1:126:A:ASN:H	1:128:A:LEU:H	6	0.12
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	2	0.12
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	6	0.12
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	20	0.12
(1,798)	1:121:A:LEU:HA	1:123:A:GLN:H	14	0.12
(1,740)	1:104:A:VAL:H	1:104:A:VAL:HB	12	0.12
(1,740)	1:104:A:VAL:H	1:104:A:VAL:HB	15	0.12
(1,740)	1:104:A:VAL:H	1:104:A:VAL:HB	17	0.12
(1,483)	1:77:A:SER:H	1:79:A:VAL:H	2	0.12
(1,457)	1:74:A:ASN:HA	1:76:A:VAL:H	3	0.12
(1,457)	1:74:A:ASN:HA	1:76:A:VAL:H	8	0.12
(1,457)	1:74:A:ASN:HA	1:76:A:VAL:H	20	0.12
(1,446)	1:72:A:ASN:H	1:75:A:LYS:H	19	0.12
(1,440)	1:69:A:VAL:H	1:70:A:GLY:H	5	0.12
(1,386)	1:60:A:GLY:H	1:61:A:ALA:H	5	0.12
(1,386)	1:60:A:GLY:H	1:61:A:ALA:H	12	0.12
(1,386)	1:60:A:GLY:H	1:61:A:ALA:H	21	0.12
(1,373)	1:58:A:VAL:H	1:65:A:ILE:HA	12	0.12
(1,373)	1:58:A:VAL:H	1:65:A:ILE:HA	17	0.12
(1,373)	1:58:A:VAL:H	1:65:A:ILE:HA	21	0.12
(1,366)	1:57:A:LEU:H	1:67:A:HIS:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:57:A:LEU:H	1:67:A:HIS:H	13	0.12
(1,366)	1:57:A:LEU:H	1:67:A:HIS:H	16	0.12
(1,341)	1:54:A:LYS:H	1:55:A:ALA:H	20	0.12
(1,329)	1:52:A:VAL:HA	1:54:A:LYS:H	4	0.12
(1,329)	1:52:A:VAL:HA	1:54:A:LYS:H	10	0.12
(1,329)	1:52:A:VAL:HA	1:54:A:LYS:H	11	0.12
(1,329)	1:52:A:VAL:HA	1:54:A:LYS:H	13	0.12
(1,329)	1:52:A:VAL:HA	1:54:A:LYS:H	19	0.12
(1,290)	1:46:A:ASP:H	1:48:A:GLN:H	1	0.12
(1,215)	1:33:A:VAL:HA	1:37:A:LEU:H	20	0.12
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	15	0.12
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	5	0.12
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	7	0.12
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	15	0.12
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	21	0.12
(1,69)	1:11:A:ILE:HA	1:13:A:THR:H	12	0.12
(1,50)	1:9:A:GLY:H	1:10:A:ASP:H	2	0.12
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	1	0.12
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	13	0.12
(1,3)	1:1:A:ALA:HA	1:136:A:ASP:H	2	0.12
(2,82)	1:37:A:LEU:HG	1:43:A:GLU:H	14	0.11
(1,1046)	1:155:A:ALA:H	1:157:A:ALA:H	20	0.11
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	11	0.11
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	15	0.11
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	17	0.11
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	19	0.11
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	20	0.11
(1,986)	1:148:A:TRP:HD1	1:149:A:GLU:H	5	0.11
(1,963)	1:146:A:LYS:HA	1:148:A:TRP:H	20	0.11
(1,939)	1:139:A:VAL:H	1:139:A:VAL:HB	16	0.11
(1,932)	1:137:A:ALA:H	1:138:A:ASP:H	9	0.11
(1,932)	1:137:A:ALA:H	1:138:A:ASP:H	14	0.11
(1,927)	1:135:A:THR:HB	1:136:A:ASP:H	12	0.11
(1,899)	1:131:A:ALA:HA	1:134:A:THR:HB	18	0.11
(1,871)	1:128:A:LEU:HA	1:130:A:THR:H	18	0.11
(1,846)	1:126:A:ASN:H	1:128:A:LEU:H	10	0.11
(1,846)	1:126:A:ASN:H	1:128:A:LEU:H	18	0.11
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	3	0.11
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	12	0.11
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	15	0.11
(1,835)	1:125:A:LEU:HA	1:127:A:HIS:H	21	0.11
(1,826)	1:124:A:SER:HA	1:126:A:ASN:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:121:A:LEU:H	1:123:A:GLN:H	12	0.11
(1,795)	1:121:A:LEU:H	1:122:A:THR:HB	1	0.11
(1,795)	1:121:A:LEU:H	1:122:A:THR:HB	3	0.11
(1,795)	1:121:A:LEU:H	1:122:A:THR:HB	4	0.11
(1,795)	1:121:A:LEU:H	1:122:A:THR:HB	7	0.11
(1,795)	1:121:A:LEU:H	1:122:A:THR:HB	10	0.11
(1,715)	1:99:A:ASN:HB2	1:100:A:ASN:H	2	0.11
(1,715)	1:99:A:ASN:HB2	1:100:A:ASN:H	8	0.11
(1,701)	1:97:A:ASN:H	1:99:A:ASN:H	11	0.11
(1,701)	1:97:A:ASN:H	1:99:A:ASN:H	14	0.11
(1,701)	1:97:A:ASN:H	1:99:A:ASN:H	19	0.11
(1,701)	1:97:A:ASN:H	1:99:A:ASN:H	20	0.11
(1,695)	1:96:A:VAL:H	1:98:A:ASP:H	11	0.11
(1,582)	1:85:A:LEU:HG	1:127:A:HIS:HD2	7	0.11
(1,582)	1:85:A:LEU:HG	1:127:A:HIS:HD2	10	0.11
(1,526)	1:81:A:GLY:HA3	1:85:A:LEU:H	5	0.11
(1,526)	1:81:A:GLY:HA3	1:85:A:LEU:H	15	0.11
(1,526)	1:81:A:GLY:HA3	1:85:A:LEU:H	20	0.11
(1,483)	1:77:A:SER:H	1:79:A:VAL:H	15	0.11
(1,483)	1:77:A:SER:H	1:79:A:VAL:H	21	0.11
(1,457)	1:74:A:ASN:HA	1:76:A:VAL:H	7	0.11
(1,457)	1:74:A:ASN:HA	1:76:A:VAL:H	19	0.11
(1,446)	1:72:A:ASN:H	1:75:A:LYS:H	3	0.11
(1,440)	1:69:A:VAL:H	1:70:A:GLY:H	9	0.11
(1,438)	1:69:A:VAL:H	1:69:A:VAL:HB	17	0.11
(1,386)	1:60:A:GLY:H	1:61:A:ALA:H	9	0.11
(1,386)	1:60:A:GLY:H	1:61:A:ALA:H	16	0.11
(1,386)	1:60:A:GLY:H	1:61:A:ALA:H	17	0.11
(1,366)	1:57:A:LEU:H	1:67:A:HIS:H	9	0.11
(1,366)	1:57:A:LEU:H	1:67:A:HIS:H	12	0.11
(1,341)	1:54:A:LYS:H	1:55:A:ALA:H	4	0.11
(1,329)	1:52:A:VAL:HA	1:54:A:LYS:H	3	0.11
(1,329)	1:52:A:VAL:HA	1:54:A:LYS:H	15	0.11
(1,283)	1:45:A:PHE:H	1:46:A:ASP:H	13	0.11
(1,283)	1:45:A:PHE:H	1:46:A:ASP:H	18	0.11
(1,110)	1:16:A:GLU:HB2	1:18:A:VAL:H	21	0.11
(1,89)	1:14:A:ALA:H	1:16:A:GLU:H	6	0.11
(1,89)	1:14:A:ALA:H	1:16:A:GLU:H	21	0.11
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	3	0.11
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	5	0.11
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	9	0.11
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	17	0.11
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	2	0.11
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	8	0.11
(2,62)	1:24:A:ASN:H	1:30:A:GLY:H	5	0.1
(1,1046)	1:155:A:ALA:H	1:157:A:ALA:H	11	0.1
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	5	0.1
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	6	0.1
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	7	0.1
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	12	0.1
(1,1007)	1:151:A:THR:HA	1:153:A:LYS:H	13	0.1
(1,981)	1:148:A:TRP:HA	1:150:A:MET:H	7	0.1
(1,963)	1:146:A:LYS:HA	1:148:A:TRP:H	13	0.1
(1,963)	1:146:A:LYS:HA	1:148:A:TRP:H	14	0.1
(1,897)	1:131:A:ALA:HA	1:133:A:ASP:H	8	0.1
(1,890)	1:130:A:THR:H	1:132:A:LEU:H	11	0.1
(1,852)	1:126:A:ASN:HB2	1:127:A:HIS:HD2	7	0.1
(1,795)	1:121:A:LEU:H	1:122:A:THR:HB	18	0.1
(1,795)	1:121:A:LEU:H	1:122:A:THR:HB	21	0.1
(1,715)	1:99:A:ASN:HB2	1:100:A:ASN:H	19	0.1
(1,704)	1:97:A:ASN:HA	1:101:A:TYR:H	12	0.1
(1,701)	1:97:A:ASN:H	1:99:A:ASN:H	16	0.1
(1,681)	1:95:A:ILE:H	1:96:A:VAL:HB	8	0.1
(1,582)	1:85:A:LEU:HG	1:127:A:HIS:HD2	5	0.1
(1,526)	1:81:A:GLY:HA3	1:85:A:LEU:H	1	0.1
(1,483)	1:77:A:SER:H	1:79:A:VAL:H	1	0.1
(1,483)	1:77:A:SER:H	1:79:A:VAL:H	3	0.1
(1,483)	1:77:A:SER:H	1:79:A:VAL:H	20	0.1
(1,457)	1:74:A:ASN:HA	1:76:A:VAL:H	1	0.1
(1,457)	1:74:A:ASN:HA	1:76:A:VAL:H	9	0.1
(1,457)	1:74:A:ASN:HA	1:76:A:VAL:H	12	0.1
(1,450)	1:72:A:ASN:HA	1:114:A:PHE:HA	5	0.1
(1,440)	1:69:A:VAL:H	1:70:A:GLY:H	16	0.1
(1,440)	1:69:A:VAL:H	1:70:A:GLY:H	21	0.1
(1,425)	1:66:A:ILE:HB	1:67:A:HIS:H	21	0.1
(1,386)	1:60:A:GLY:H	1:61:A:ALA:H	6	0.1
(1,373)	1:58:A:VAL:H	1:65:A:ILE:HA	4	0.1
(1,366)	1:57:A:LEU:H	1:67:A:HIS:H	1	0.1
(1,366)	1:57:A:LEU:H	1:67:A:HIS:H	20	0.1
(1,341)	1:54:A:LYS:H	1:55:A:ALA:H	11	0.1
(1,329)	1:52:A:VAL:HA	1:54:A:LYS:H	12	0.1
(1,290)	1:46:A:ASP:H	1:48:A:GLN:H	7	0.1
(1,89)	1:14:A:ALA:H	1:16:A:GLU:H	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:14:A:ALA:H	1:15:A:THR:H	18	0.1
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	3	0.1
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	11	0.1
(1,76)	1:12:A:ALA:H	1:14:A:ALA:H	19	0.1
(1,50)	1:9:A:GLY:H	1:10:A:ASP:H	1	0.1
(1,50)	1:9:A:GLY:H	1:10:A:ASP:H	20	0.1
(1,39)	1:7:A:VAL:H	1:142:A:TYR:H	20	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found