



Full wwPDB NMR Structure Validation Report ⓘ

Mar 30, 2026 – 03:00 AM UTC

PDB ID : 8XZ2 / pdb_00008xz2
BMRB ID : 52158
Title : The structural model of a homodimeric D-Ala-D-Ala metallopeptidase, VanX, from vancomycin-resistant bacteria
Authors : Konuma, T.; Takai, T.; Tsuchiya, C.; Nishida, M.; Hashiba, M.; Yamada, Y.; Shirai, H.; Motoda, Y.; Nagadoi, A.; Chikaishi, E.; Akagi, K.; Akashi, S.; Yamazaki, T.; Akutsu, H.; Oe, A.; Ikegami, T.
Deposited on : 2024-01-20

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

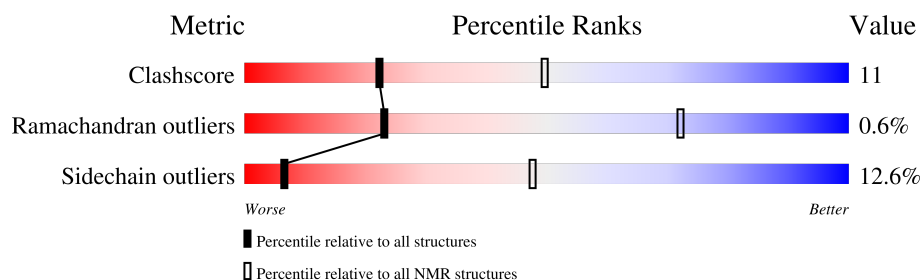
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 17%.

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	B	202	
1	C	202	

2 Ensemble composition and analysis

This entry contains 4 models. Model 4 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	B:1-B:6, B:17-B:32, B:38-B:202 (187)	0.14	4
2	C:1-C:9, C:20-C:202 (192)	0.15	4

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. No single-model clusters were found.

Cluster number	Models
1	3, 4
2	1, 2

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 4048 atoms, of which 746 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called D-alanyl-D-alanine dipeptidase.

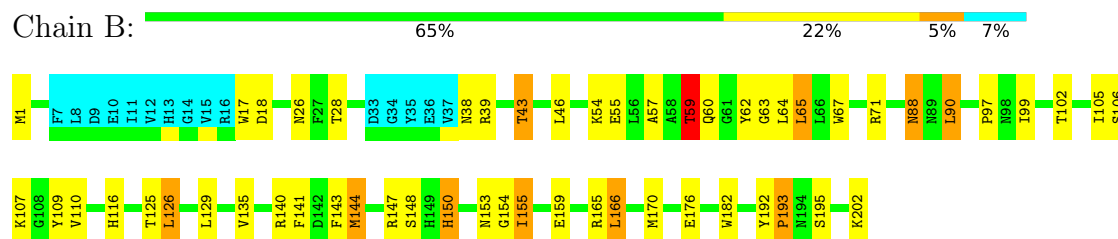
Mol	Chain	Residues	Atoms						Trace
1	B	202	Total	C	H	N	O	S	0
			2024	1048	373	284	311	8	
1	C	202	Total	C	H	N	O	S	0
			2024	1048	373	284	311	8	

4 Residue-property plots

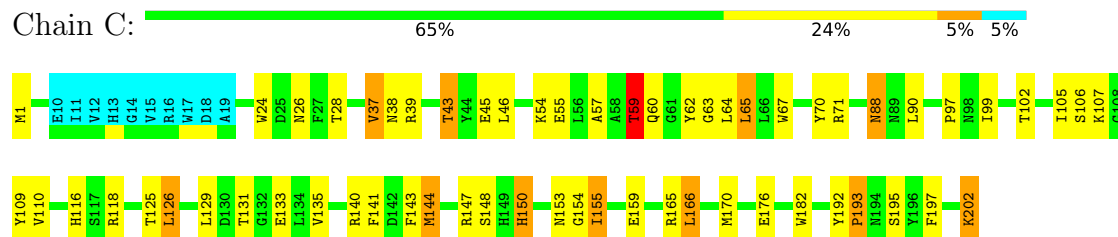
4.1 Average score per residue in the NMR ensemble

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: D-alanyl-D-alanine dipeptidase



- Molecule 1: D-alanyl-D-alanine dipeptidase

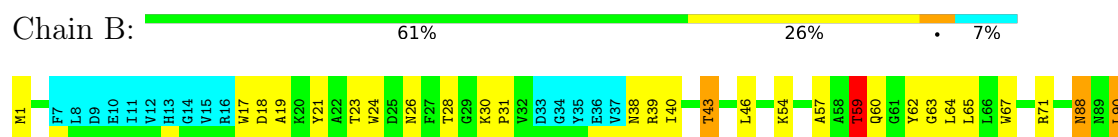


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

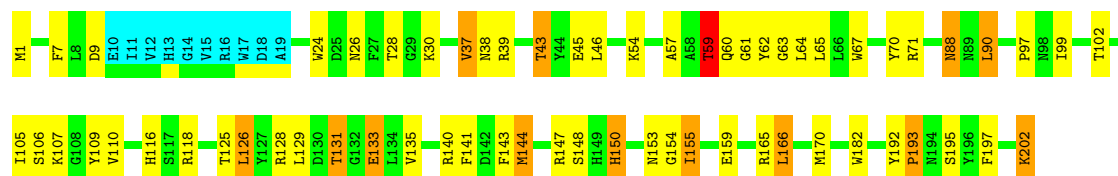
- Molecule 1: D-alanyl-D-alanine dipeptidase





• Molecule 1: D-alanyl-D-alanine dipeptidase

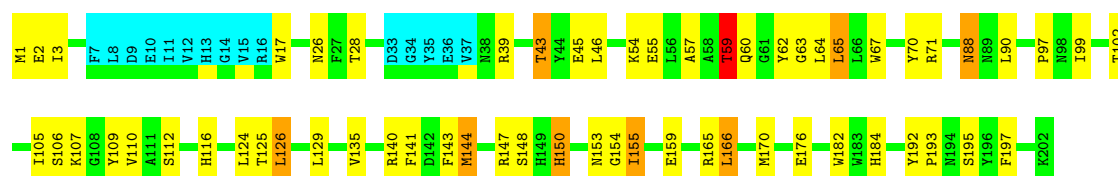
Chain C: 63% 25% 6% 5%



4.2.2 Score per residue for model 2

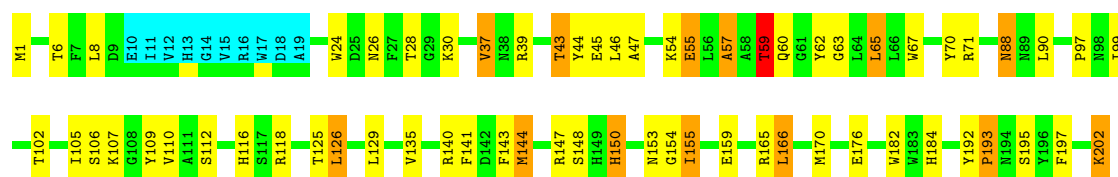
• Molecule 1: D-alanyl-D-alanine dipeptidase

Chain B: 63% 25% 7%



• Molecule 1: D-alanyl-D-alanine dipeptidase

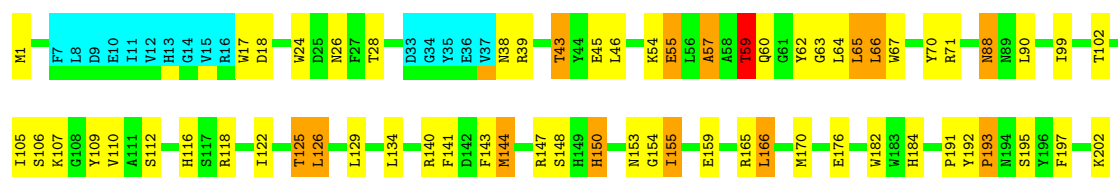
Chain C: 63% 25% 6% 5%



4.2.3 Score per residue for model 3

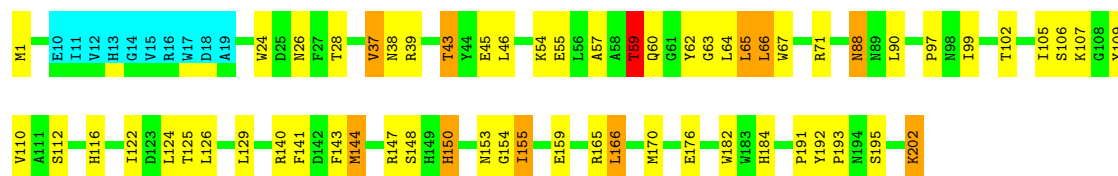
• Molecule 1: D-alanyl-D-alanine dipeptidase

Chain B: 61% 25% 6% 7%



• Molecule 1: D-alanyl-D-alanine dipeptidase

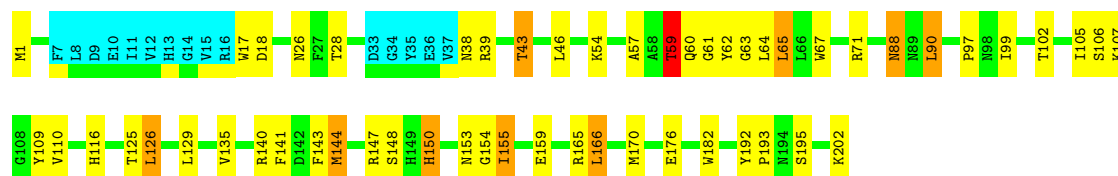
Chain C: 



4.2.4 Score per residue for model 4 (medoid)

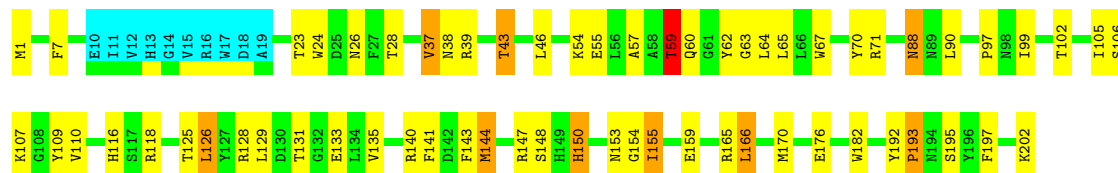
- Molecule 1: D-alanyl-D-alanine dipeptidase

Chain B: 



- Molecule 1: D-alanyl-D-alanine dipeptidase

Chain C: 



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 4 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	2.4

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	1882
Number of shifts mapped to atoms	1882
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	17%

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	
		RMSZ	#Z>5	RMSZ	#Z>5
1	B	0.62±0.03	0±0/1571 (0.0± 0.0%)	1.11±0.02	8±1/2126 (0.4± 0.0%)
1	C	0.62±0.03	0±0/1611 (0.0± 0.0%)	1.10±0.02	9±0/2179 (0.4± 0.0%)
All	All	0.62	0/12728 (0.0%)	1.11	66/17220 (0.4%)

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	C	57	ALA	N-CA-C	-10.79	98.84	113.30	1	4
1	B	57	ALA	N-CA-C	-10.79	98.84	113.30	1	4
1	B	107	LYS	N-CA-C	-7.68	103.89	113.18	4	4
1	C	107	LYS	N-CA-C	-7.67	103.90	113.18	4	4
1	B	193	PRO	N-CA-C	-6.32	101.94	111.41	4	4
1	C	193	PRO	N-CA-C	-6.28	101.99	111.41	4	4
1	C	154	GLY	N-CA-C	-6.06	106.73	115.27	3	4
1	B	154	GLY	N-CA-C	-6.02	106.78	115.27	3	4
1	C	59	THR	CA-C-N	-5.95	113.15	122.08	3	4
1	C	59	THR	C-N-CA	-5.95	113.15	122.08	3	4
1	B	59	THR	CA-C-N	-5.91	113.22	122.08	3	4
1	B	59	THR	C-N-CA	-5.91	113.22	122.08	3	4
1	B	97	PRO	N-CA-C	-5.70	102.91	111.57	4	3
1	C	97	PRO	N-CA-C	-5.66	102.96	111.57	1	4
1	B	55	GLU	N-CA-C	-5.62	106.37	113.18	3	2
1	C	55	GLU	N-CA-C	-5.60	106.40	113.18	3	3
1	C	7	PHE	N-CA-C	-5.30	101.13	109.25	4	2
1	C	184	HIS	N-CA-C	5.17	117.17	109.25	3	2
1	B	184	HIS	N-CA-C	5.16	117.15	109.25	3	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	1528	351	1452	36±3
1	C	1568	356	1488	37±2
All	All	12384	2828	11760	276

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:66:LEU:HB3	1:B:122:ILE:HD11	0.81	1.52	3	1
1:C:66:LEU:HB3	1:C:122:ILE:HD11	0.79	1.54	3	1
1:C:59:THR:HG22	1:C:60:GLN:H	0.78	1.39	4	4
1:B:59:THR:HG22	1:B:60:GLN:H	0.76	1.40	3	4
1:C:63:GLY:O	1:C:126:LEU:HA	0.73	1.84	4	4
1:B:63:GLY:O	1:B:126:LEU:HA	0.72	1.85	4	4
1:B:17:TRP:NE1	1:B:39:ARG:HA	0.70	2.02	4	4
1:C:147:ARG:HG3	1:C:155:ILE:HD11	0.69	1.63	2	4
1:B:147:ARG:HG3	1:B:155:ILE:HD11	0.69	1.63	2	4
1:B:24:TRP:CZ3	1:C:65:LEU:HD22	0.68	2.23	3	1
1:B:109:TYR:CG	1:B:144:MET:HG3	0.66	2.25	2	4
1:C:43:THR:HG22	1:C:46:LEU:H	0.66	1.51	4	4
1:B:59:THR:HG22	1:B:60:GLN:N	0.66	2.05	2	4
1:B:43:THR:HG22	1:B:46:LEU:H	0.65	1.50	3	4
1:C:24:TRP:HA	1:C:30:LYS:HA	0.65	1.69	2	2
1:C:59:THR:HG22	1:C:60:GLN:N	0.65	2.05	2	4
1:B:17:TRP:HE1	1:B:39:ARG:HA	0.65	1.52	1	4
1:B:65:LEU:HD22	1:C:24:TRP:CZ3	0.65	2.27	3	2
1:C:128:ARG:HB2	1:C:131:THR:HG22	0.61	1.72	1	2
1:B:18:ASP:HA	1:C:38:ASN:ND2	0.59	2.13	4	3
1:C:67:TRP:CZ3	1:C:141:PHE:HB2	0.58	2.33	3	4
1:C:26:ASN:HD22	1:C:28:THR:H	0.58	1.42	4	4
1:C:66:LEU:CB	1:C:122:ILE:HD11	0.58	2.28	3	1
1:C:109:TYR:CG	1:C:144:MET:HG3	0.58	2.34	2	4
1:B:26:ASN:HD22	1:B:28:THR:H	0.58	1.41	1	4
1:C:37:VAL:HB	1:C:202:LYS:HA	0.57	1.75	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:62:TYR:HB3	1:B:126:LEU:HB3	0.56	1.77	4	4
1:B:128:ARG:HD2	1:B:135:VAL:HG22	0.56	1.77	1	1
1:C:155:ILE:HG23	1:C:159:GLU:HB2	0.56	1.77	3	4
1:B:147:ARG:HG3	1:B:155:ILE:CD1	0.56	2.31	3	4
1:B:155:ILE:HG23	1:B:159:GLU:HB2	0.55	1.77	3	4
1:C:62:TYR:HB3	1:C:126:LEU:HB3	0.55	1.79	3	4
1:B:109:TYR:CD2	1:B:144:MET:HG3	0.55	2.35	2	3
1:C:147:ARG:HG3	1:C:155:ILE:CD1	0.55	2.31	2	4
1:C:109:TYR:CD2	1:C:144:MET:HG3	0.54	2.37	2	4
1:B:67:TRP:CZ3	1:B:141:PHE:HB2	0.54	2.38	3	4
1:C:128:ARG:CB	1:C:131:THR:HG22	0.54	2.33	1	1
1:B:66:LEU:CB	1:B:122:ILE:HD11	0.52	2.31	3	1
1:B:62:TYR:CD1	1:B:135:VAL:HG21	0.52	2.40	1	3
1:C:62:TYR:CD1	1:C:135:VAL:HG21	0.52	2.40	2	3
1:C:105:ILE:HG22	1:C:110:VAL:O	0.52	2.05	3	4
1:B:43:THR:HG21	1:B:191:PRO:HG3	0.52	1.82	3	1
1:B:105:ILE:HG22	1:B:110:VAL:O	0.52	2.05	3	4
1:C:65:LEU:O	1:C:65:LEU:HG	0.51	2.05	3	1
1:B:64:LEU:HD23	1:B:126:LEU:HD23	0.51	1.81	4	3
1:B:65:LEU:HG	1:B:65:LEU:O	0.51	2.06	3	1
1:B:192:TYR:HB3	1:B:195:SER:HB2	0.50	1.82	3	4
1:C:150:HIS:CE1	1:C:182:TRP:HA	0.50	2.41	3	4
1:B:118:ARG:HD3	1:B:193:PRO:HA	0.49	1.84	3	2
1:B:150:HIS:CE1	1:B:182:TRP:HA	0.49	2.41	3	4
1:C:192:TYR:HB3	1:C:195:SER:HB2	0.49	1.84	4	4
1:C:8:LEU:HD22	1:C:47:ALA:HB2	0.49	1.84	2	1
1:B:64:LEU:CD2	1:B:126:LEU:HD23	0.48	2.39	4	3
1:B:128:ARG:HB3	1:B:130:ASP:OD2	0.48	2.08	1	1
1:C:6:THR:HB	1:C:44:TYR:CZ	0.48	2.43	2	1
1:B:65:LEU:HD13	1:C:24:TRP:HZ3	0.48	1.68	2	3
1:B:17:TRP:CH2	1:C:37:VAL:HG22	0.48	2.44	1	3
1:B:71:ARG:HB3	1:B:116:HIS:HB3	0.48	1.86	4	4
1:B:24:TRP:HA	1:B:30:LYS:HA	0.47	1.86	1	1
1:C:64:LEU:CD2	1:C:126:LEU:HD23	0.47	2.39	4	2
1:C:23:THR:HG22	1:C:24:TRP:H	0.47	1.69	4	1
1:C:71:ARG:HB3	1:C:116:HIS:HB3	0.47	1.86	1	4
1:C:64:LEU:HB3	1:C:124:LEU:HD12	0.47	1.85	3	1
1:C:59:THR:CG2	1:C:60:GLN:N	0.47	2.78	2	4
1:C:70:TYR:CE1	1:C:197:PHE:HB2	0.47	2.44	2	3
1:C:118:ARG:HD3	1:C:193:PRO:HA	0.47	1.86	4	3
1:C:143:PHE:HB3	1:C:148:SER:OG	0.47	2.10	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:59:THR:CG2	1:B:60:GLN:N	0.46	2.78	3	4
1:B:143:PHE:HB3	1:B:148:SER:OG	0.46	2.10	3	4
1:C:60:GLN:HG2	1:C:165:ARG:HH12	0.46	1.71	4	4
1:C:64:LEU:HD23	1:C:126:LEU:HD23	0.46	1.87	1	2
1:C:126:LEU:HD21	1:C:166:LEU:HD23	0.46	1.88	4	3
1:C:62:TYR:CE1	1:C:135:VAL:HG21	0.45	2.46	2	3
1:B:26:ASN:ND2	1:B:28:THR:H	0.45	2.10	3	4
1:B:60:GLN:HG2	1:B:165:ARG:HH12	0.45	1.71	1	4
1:C:26:ASN:ND2	1:C:28:THR:H	0.45	2.10	3	3
1:B:21:TYR:O	1:B:31:PRO:HA	0.44	2.12	1	1
1:B:126:LEU:HD21	1:B:166:LEU:HD23	0.44	1.90	1	1
1:C:43:THR:HG21	1:C:191:PRO:HG3	0.44	1.88	3	1
1:B:70:TYR:CE1	1:B:197:PHE:HB2	0.44	2.48	3	2
1:B:62:TYR:CE1	1:B:135:VAL:HG21	0.43	2.48	2	3
1:C:166:LEU:O	1:C:170:MET:HG2	0.43	2.14	2	4
1:C:88:ASN:HD22	1:C:90:LEU:H	0.42	1.56	4	4
1:C:131:THR:HG23	1:C:133:GLU:H	0.42	1.74	1	1
1:B:166:LEU:O	1:B:170:MET:HG2	0.42	2.13	3	4
1:B:88:ASN:HD22	1:B:90:LEU:H	0.42	1.56	4	4
1:C:202:LYS:HE2	1:C:202:LYS:HB2	0.42	1.77	1	2
1:B:43:THR:HG23	1:B:45:GLU:OE2	0.42	2.15	2	2
1:B:17:TRP:CD1	1:B:40:ILE:HG12	0.41	2.49	1	1
1:B:2:GLU:HG3	1:B:3:ILE:N	0.41	2.30	2	1
1:B:64:LEU:HD22	1:B:124:LEU:HD12	0.41	1.92	2	1
1:B:43:THR:HG21	1:B:191:PRO:CG	0.41	2.45	3	1
1:B:55:GLU:C	1:B:57:ALA:N	0.41	2.79	3	1
1:C:59:THR:O	1:C:61:GLY:N	0.41	2.53	1	1
1:C:55:GLU:C	1:C:57:ALA:N	0.41	2.79	2	1
1:C:43:THR:HG23	1:C:45:GLU:OE2	0.41	2.15	2	3
1:C:118:ARG:HA	1:C:195:SER:O	0.41	2.15	2	1
1:B:125:THR:HG23	1:B:182:TRP:CZ3	0.41	2.50	3	1
1:B:59:THR:O	1:B:61:GLY:N	0.41	2.51	4	1
1:C:60:GLN:HG2	1:C:165:ARG:NH1	0.40	2.31	3	1
1:C:43:THR:HG21	1:C:191:PRO:CG	0.40	2.47	3	1
1:B:17:TRP:CE2	1:C:38:ASN:HB3	0.40	2.51	1	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	B	185/202 (92%)	171±0 (92±0%)	13±0 (7±0%)	1±0 (1±0%)	20	70
1	C	190/202 (94%)	177±0 (93±0%)	12±0 (6±0%)	1±0 (1±0%)	26	74
All	All	1500/1616 (93%)	1391 (93%)	100 (7%)	9 (1%)	23	72

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	59	THR	4
1	C	59	THR	4
1	B	19	ALA	1

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	B	160/173 (92%)	140±1 (88±0%)	20±1 (12±0%)	7	48
1	C	165/173 (95%)	144±1 (87±0%)	21±1 (13±0%)	6	47
All	All	1300/1384 (94%)	1136 (87%)	164 (13%)	6	48

All 49 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	B	1	MET	4
1	B	43	THR	4
1	B	54	LYS	4
1	B	65	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	B	88	ASN	4
1	B	99	ILE	4
1	B	102	THR	4
1	B	106	SER	4
1	B	125	THR	4
1	B	126	LEU	4
1	B	129	LEU	4
1	B	140	ARG	4
1	B	144	MET	4
1	B	150	HIS	4
1	B	153	ASN	4
1	B	155	ILE	4
1	B	166	LEU	4
1	C	1	MET	4
1	C	37	VAL	4
1	C	43	THR	4
1	C	54	LYS	4
1	C	65	LEU	4
1	C	88	ASN	4
1	C	99	ILE	4
1	C	102	THR	4
1	C	106	SER	4
1	C	125	THR	4
1	C	129	LEU	4
1	C	140	ARG	4
1	C	144	MET	4
1	C	150	HIS	4
1	C	153	ASN	4
1	C	155	ILE	4
1	C	166	LEU	4
1	C	126	LEU	3
1	C	202	LYS	3
1	B	176	GLU	3
1	C	176	GLU	3
1	B	90	LEU	2
1	B	202	LYS	2
1	C	133	GLU	2
1	B	112	SER	2
1	C	112	SER	2
1	B	23	THR	1
1	C	90	LEU	1
1	C	131	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	B	66	LEU	1
1	B	134	LEU	1
1	C	66	LEU	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 17% for the well-defined parts and 17% 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	926
Number of shifts mapped to atoms	926
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	194	-0.45 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	174	0.43 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	192	-0.56 ± 0.23	Should be applied
^{15}N	183	0.39 ± 0.24	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 16%, i.e. 852 atoms were assigned a chemical shift out of a possible 5202. 0 out of 46 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	691/1888 (37%)	167/767 (22%)	356/758 (47%)	168/363 (46%)
Sidechain	161/2731 (6%)	0/1763 (0%)	161/842 (19%)	0/126 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/583 (0%)	0/283 (0%)	0/281 (0%)	0/19 (0%)
Overall	852/5202 (16%)	167/2813 (6%)	517/1881 (27%)	168/508 (33%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 17%, i.e. 925 atoms were assigned a chemical shift out of a possible 5552. 0 out of 52 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	751/2016 (37%)	182/820 (22%)	386/808 (48%)	183/388 (47%)
Sidechain	174/2908 (6%)	0/1878 (0%)	174/898 (19%)	0/132 (0%)
Aromatic	0/628 (0%)	0/306 (0%)	0/300 (0%)	0/22 (0%)
Overall	925/5552 (17%)	182/3004 (6%)	560/2006 (28%)	183/542 (34%)

7.1.4 Statistically unusual chemical shifts [i](#)

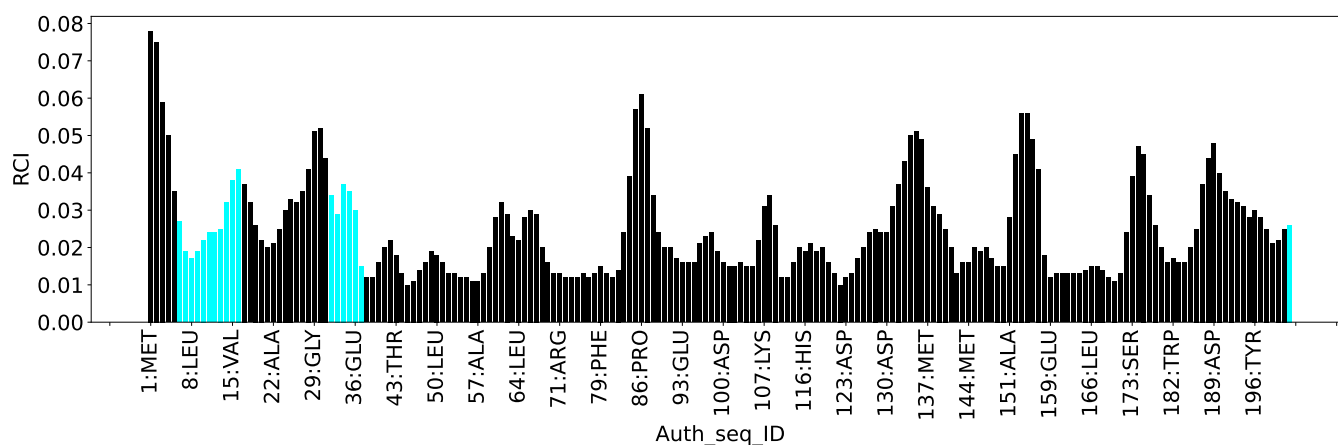
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	142	ASP	H	3.46	5.52 – 11.08	-8.7

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 B:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_2*

7.2.1 Bookkeeping ⓘ

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

Total number of shifts	956
Number of shifts mapped to atoms	956
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	198	-0.82 ± 0.13	Should be checked
$^{13}\text{C}_\beta$	184	0.41 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	198	-0.37 ± 0.16	None needed (< 0.5 ppm)
^{15}N	189	0.53 ± 0.19	Should be applied

7.2.3 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 17%, i.e. 881 atoms were assigned a chemical shift out of a possible 5202. 0 out of 46 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	709/1888 (38%)	171/767 (22%)	366/758 (48%)	172/363 (47%)
Sidechain	172/2731 (6%)	0/1763 (0%)	172/842 (20%)	0/126 (0%)
Aromatic	0/583 (0%)	0/283 (0%)	0/281 (0%)	0/19 (0%)
Overall	881/5202 (17%)	171/2813 (6%)	538/1881 (29%)	172/508 (34%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 17%, i.e. 953 atoms were assigned a chemical shift out of a possible 5552. 0 out of 52 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	769/2016 (38%)	186/820 (23%)	396/808 (49%)	187/388 (48%)
Sidechain	184/2908 (6%)	0/1878 (0%)	184/898 (20%)	0/132 (0%)
Aromatic	0/628 (0%)	0/306 (0%)	0/300 (0%)	0/22 (0%)
Overall	953/5552 (17%)	186/3004 (6%)	580/2006 (29%)	187/542 (35%)

7.2.4 Statistically unusual chemical shifts [i](#)

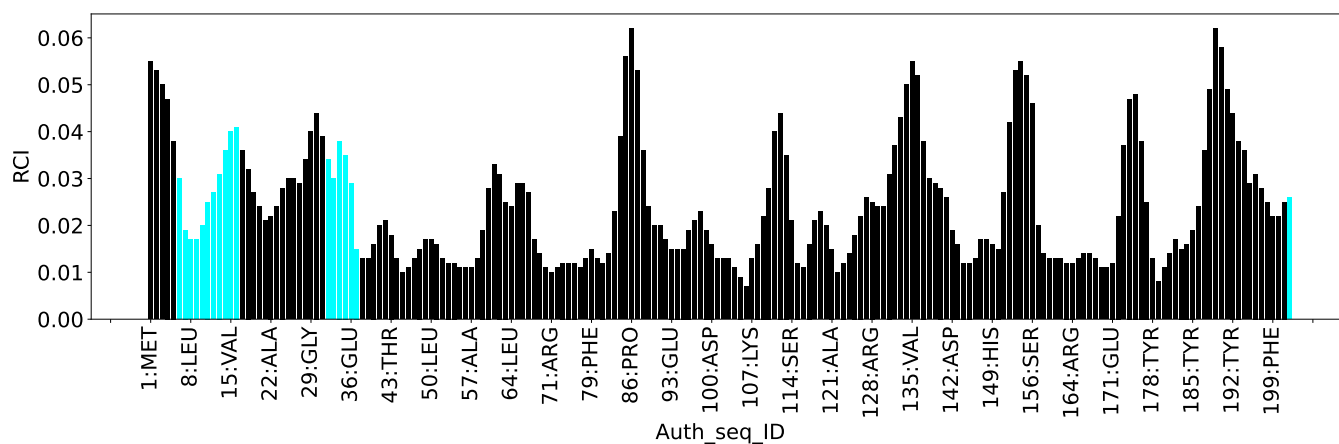
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	106	SER	CA	41.08	48.46 – 68.96	-8.6
2	B	179	SER	CA	41.58	48.46 – 68.96	-8.4
2	B	145	ASP	CB	49.45	32.98 – 48.76	5.4

7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	16
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	16
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.0
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)	None	None
0.2-0.5 (Medium)	None	None
>0.5 (Large)	14.0	4.91

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

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

9 Distance violation analysis ⓘ

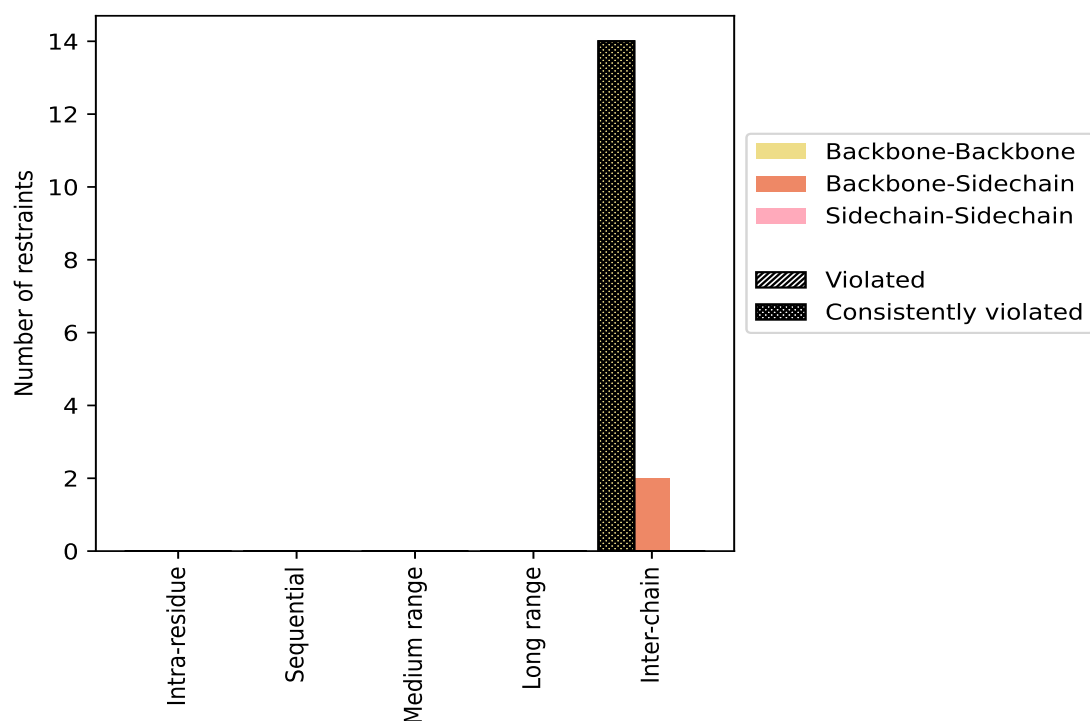
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥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	16	100.0	14	87.5	87.5	14	87.5	87.5
Backbone-Backbone	14	87.5	14	100.0	87.5	14	100.0	87.5
Backbone-Sidechain	2	12.5	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	16	100.0	14	87.5	87.5	14	87.5	87.5
Backbone-Backbone	14	87.5	14	100.0	87.5	14	100.0	87.5
Backbone-Sidechain	2	12.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

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

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



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

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

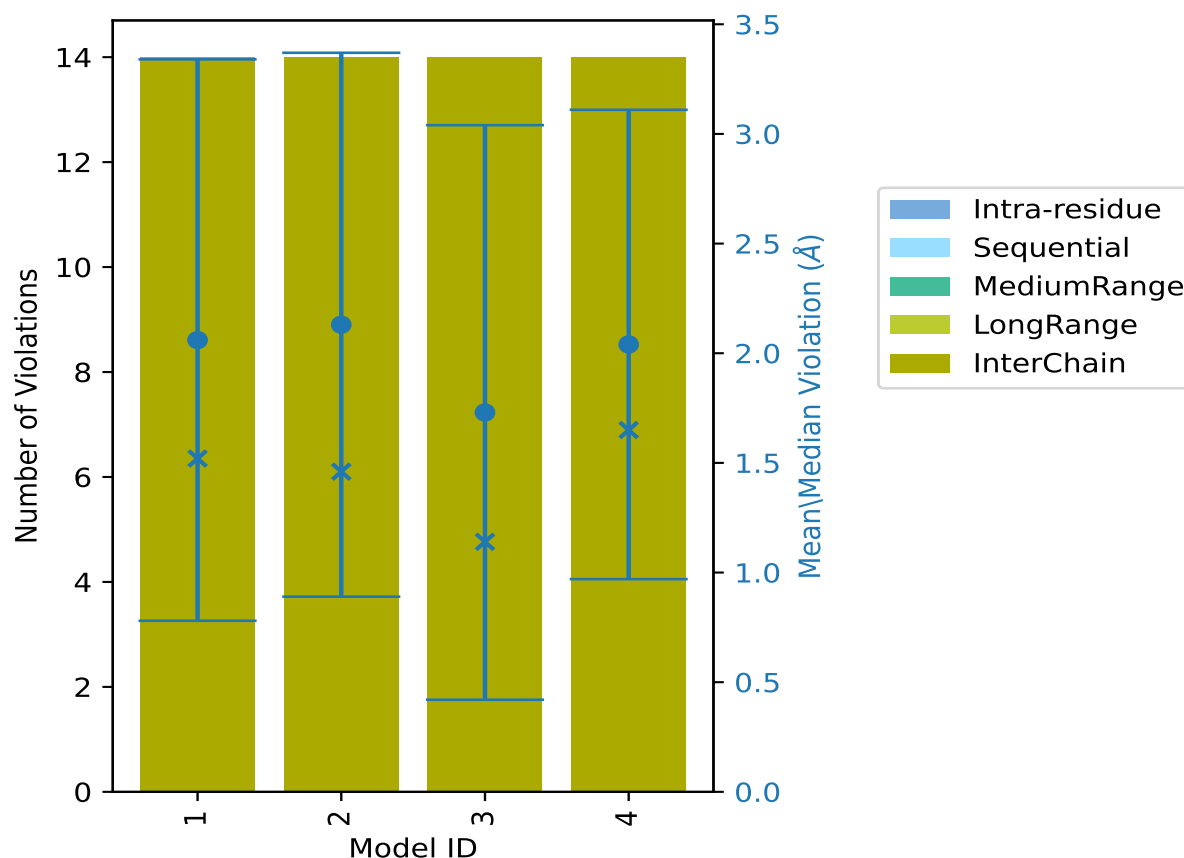
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	0	14	14	2.06	4.76	1.28	1.52
2	0	0	0	0	14	14	2.13	4.87	1.24	1.46
3	0	0	0	0	14	14	1.73	4.91	1.31	1.14
4	0	0	0	0	14	14	2.04	4.7	1.07	1.65

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](#)

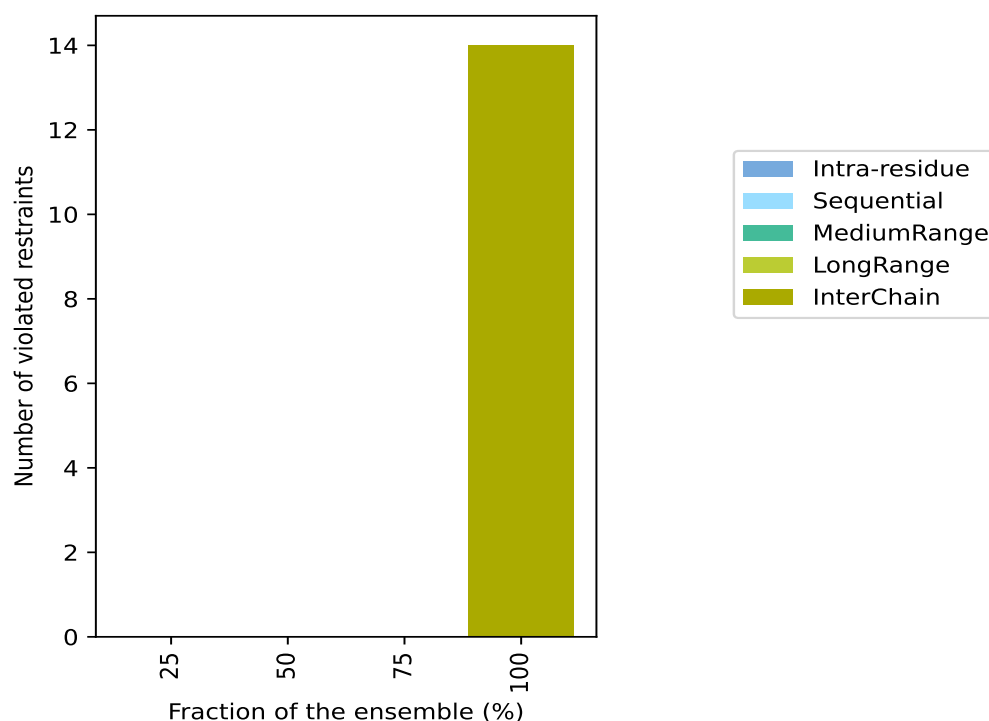
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2(IR:0, SQ:0, MR:0, LR:0, IC:2) restraints are not violated 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	0	0	1	25.0
0	0	0	0	0	0	2	50.0
0	0	0	0	0	0	3	75.0
0	0	0	0	14	14	4	100.0

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

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

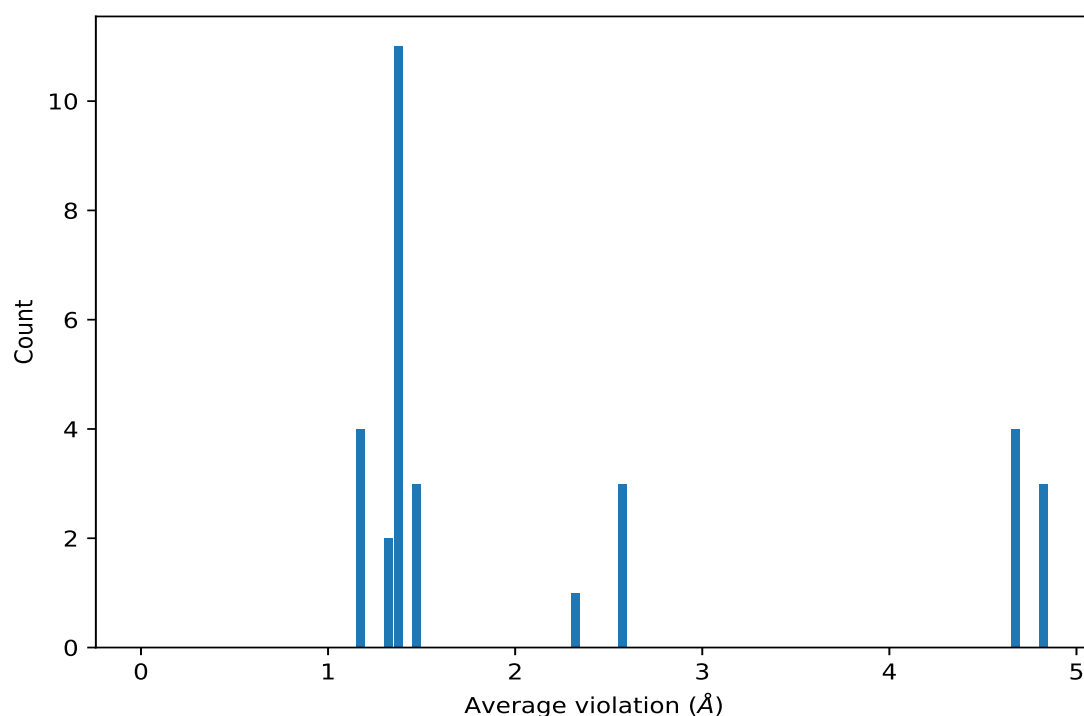
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,7)	1:66:C:LEU:H	1:24:B:TRP:CZ3	4	4.8	0.09	4.79
(2,7)	1:66:C:LEU:H	1:24:B:TRP:CH2	4	4.8	0.09	4.79
(2,7)	1:66:C:LEU:N	1:24:B:TRP:CZ3	4	4.8	0.09	4.79
(2,14)	1:66:B:LEU:H	1:24:C:TRP:CZ3	4	4.66	0.17	4.63
(2,14)	1:66:B:LEU:H	1:24:C:TRP:CH2	4	4.66	0.17	4.63
(2,14)	1:66:B:LEU:N	1:24:C:TRP:CH2	4	4.66	0.17	4.63
(2,14)	1:66:B:LEU:N	1:24:C:TRP:CZ3	4	4.66	0.17	4.63
(2,11)	1:19:B:ALA:H	1:18:C:ASP:OD1	4	2.59	1.05	2.72
(2,11)	1:19:B:ALA:O	1:17:C:TRP:O	4	2.59	1.05	2.72
(2,11)	1:19:B:ALA:O	1:18:C:ASP:OD1	4	2.59	1.05	2.72
(2,4)	1:19:C:ALA:O	1:18:B:ASP:OD1	4	2.31	0.5	2.37
(2,8)	1:16:B:ARG:O	1:24:C:TRP:CZ3	4	1.48	0.12	1.48
(2,8)	1:16:B:ARG:HH21	1:34:C:GLY:H	4	1.48	0.12	1.48
(2,6)	1:65:C:LEU:CD2	1:24:B:TRP:CZ3	4	1.47	0.22	1.52
(2,9)	1:17:B:TRP:CZ3	1:37:C:VAL:CG2	4	1.38	0.05	1.36
(2,9)	1:17:B:TRP:CH2	1:37:C:VAL:CG2	4	1.38	0.05	1.36

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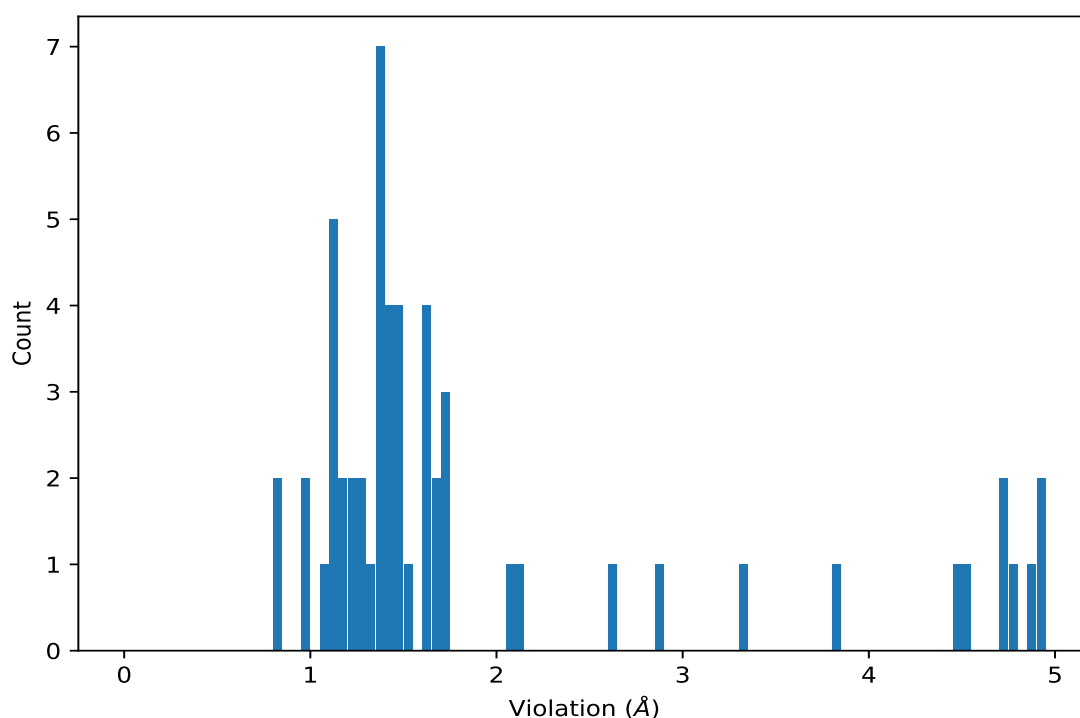
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,5)	1:39:C:ARG:HH12	1:39:B:ARG:HH22	4	1.38	0.23	1.34
(2,5)	1:39:C:ARG:HH22	1:39:B:ARG:HH12	4	1.38	0.23	1.34
(2,12)	1:39:B:ARG:HH22	1:39:C:ARG:HH12	4	1.38	0.23	1.34
(2,12)	1:39:B:ARG:HH12	1:39:C:ARG:HH22	4	1.38	0.23	1.34
(2,2)	1:17:C:TRP:CH2	1:37:B:VAL:CG1	4	1.38	0.07	1.39
(2,2)	1:17:C:TRP:CH2	1:37:B:VAL:CG2	4	1.38	0.07	1.39
(2,2)	1:17:C:TRP:CZ3	1:37:B:VAL:CG2	4	1.38	0.07	1.39
(2,13)	1:65:B:LEU:CD2	1:24:C:TRP:CZ3	4	1.36	0.2	1.31
(2,13)	1:65:B:LEU:CD1	1:24:C:TRP:CZ3	4	1.36	0.2	1.31
(2,1)	1:16:C:ARG:O	1:24:B:TRP:CZ3	4	1.33	0.16	1.38
(2,1)	1:16:C:ARG:HH21	1:34:B:GLY:H	4	1.33	0.16	1.38
(2,3)	1:18:C:ASP:OD1	1:18:B:ASP:OD1	4	1.17	0.31	1.08
(2,3)	1:18:C:ASP:OD2	1:18:B:ASP:OD1	4	1.17	0.31	1.08
(2,10)	1:18:B:ASP:OD1	1:18:C:ASP:OD1	4	1.17	0.31	1.08
(2,10)	1:18:B:ASP:OD1	1:18:C:ASP:OD2	4	1.17	0.31	1.08

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)
(2,7)	1:66:C:LEU:N	1:24:B:TRP:CZ3	3	4.91
(2,14)	1:66:B:LEU:N	1:24:C:TRP:CH2	3	4.9
(2,7)	1:66:C:LEU:H	1:24:B:TRP:CH2	2	4.87
(2,14)	1:66:B:LEU:H	1:24:C:TRP:CZ3	1	4.76
(2,7)	1:66:C:LEU:H	1:24:B:TRP:CZ3	1	4.71
(2,7)	1:66:C:LEU:N	1:24:B:TRP:CZ3	4	4.7
(2,14)	1:66:B:LEU:N	1:24:C:TRP:CZ3	4	4.5
(2,14)	1:66:B:LEU:H	1:24:C:TRP:CH2	2	4.49
(2,11)	1:19:B:ALA:O	1:17:C:TRP:O	2	3.81
(2,11)	1:19:B:ALA:H	1:18:C:ASP:OD1	1	3.32
(2,4)	1:19:C:ALA:O	1:18:B:ASP:OD1	1	2.89
(2,4)	1:19:C:ALA:O	1:18:B:ASP:OD1	2	2.64
(2,11)	1:19:B:ALA:O	1:18:C:ASP:OD1	4	2.12
(2,4)	1:19:C:ALA:O	1:18:B:ASP:OD1	4	2.09
(2,12)	1:39:B:ARG:HH12	1:39:C:ARG:HH22	4	1.72
(2,5)	1:39:C:ARG:HH22	1:39:B:ARG:HH12	4	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6)	1:65:C:LEU:CD2	1:24:B:TRP:CZ3	1	1.71
(2,13)	1:65:B:LEU:CD2	1:24:C:TRP:CZ3	1	1.68
(2,8)	1:16:B:ARG:O	1:24:C:TRP:CZ3	1	1.66
(2,10)	1:18:B:ASP:OD1	1:18:C:ASP:OD1	4	1.65
(2,3)	1:18:C:ASP:OD1	1:18:B:ASP:OD1	4	1.65
(2,6)	1:65:C:LEU:CD2	1:24:B:TRP:CZ3	2	1.62
(2,4)	1:19:C:ALA:O	1:18:B:ASP:OD1	3	1.61
(2,1)	1:16:C:ARG:O	1:24:B:TRP:CZ3	2	1.51
(2,8)	1:16:B:ARG:HH21	1:34:C:GLY:H	4	1.49
(2,9)	1:17:B:TRP:CH2	1:37:C:VAL:CG2	4	1.47
(2,8)	1:16:B:ARG:O	1:24:C:TRP:CZ3	2	1.46
(2,2)	1:17:C:TRP:CH2	1:37:B:VAL:CG2	4	1.46
(2,12)	1:39:B:ARG:HH22	1:39:C:ARG:HH12	2	1.45
(2,5)	1:39:C:ARG:HH12	1:39:B:ARG:HH22	2	1.45
(2,6)	1:65:C:LEU:CD2	1:24:B:TRP:CZ3	4	1.42
(2,2)	1:17:C:TRP:CZ3	1:37:B:VAL:CG2	3	1.42
(2,1)	1:16:C:ARG:HH21	1:34:B:GLY:H	4	1.38
(2,1)	1:16:C:ARG:O	1:24:B:TRP:CZ3	1	1.37
(2,13)	1:65:B:LEU:CD1	1:24:C:TRP:CZ3	2	1.36
(2,9)	1:17:B:TRP:CZ3	1:37:C:VAL:CG2	2	1.36
(2,9)	1:17:B:TRP:CZ3	1:37:C:VAL:CG2	3	1.36
(2,2)	1:17:C:TRP:CH2	1:37:B:VAL:CG2	2	1.36
(2,9)	1:17:B:TRP:CZ3	1:37:C:VAL:CG2	1	1.35
(2,8)	1:16:B:ARG:HH21	1:34:C:GLY:H	3	1.32
(2,2)	1:17:C:TRP:CH2	1:37:B:VAL:CG1	1	1.27
(2,13)	1:65:B:LEU:CD2	1:24:C:TRP:CZ3	4	1.25
(2,12)	1:39:B:ARG:HH22	1:39:C:ARG:HH12	1	1.23
(2,5)	1:39:C:ARG:HH12	1:39:B:ARG:HH22	1	1.23
(2,10)	1:18:B:ASP:OD1	1:18:C:ASP:OD1	2	1.2
(2,3)	1:18:C:ASP:OD1	1:18:B:ASP:OD1	2	1.2
(2,13)	1:65:B:LEU:CD2	1:24:C:TRP:CZ3	3	1.15
(2,6)	1:65:C:LEU:CD2	1:24:B:TRP:CZ3	3	1.14
(2,12)	1:39:B:ARG:HH22	1:39:C:ARG:HH12	3	1.12
(2,5)	1:39:C:ARG:HH12	1:39:B:ARG:HH22	3	1.12
(2,11)	1:19:B:ALA:O	1:18:C:ASP:OD1	3	1.11
(2,1)	1:16:C:ARG:HH21	1:34:B:GLY:H	3	1.07
(2,10)	1:18:B:ASP:OD1	1:18:C:ASP:OD2	3	0.97
(2,3)	1:18:C:ASP:OD2	1:18:B:ASP:OD1	3	0.97
(2,10)	1:18:B:ASP:OD1	1:18:C:ASP:OD1	1	0.85
(2,3)	1:18:C:ASP:OD1	1:18:B:ASP:OD1	1	0.85

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found