



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2025 – 04:05 PM EDT

PDB ID : 9NM2
BMRB ID : 31232
Title : Dimeric Structure of full-length CrgA, a Cell Division Protein from Mycobacterium tuberculosis, in Lipid Bilayers
Authors : Shin, Y.; Prasad, R.; Das, N.; Taylor, J.A.; Qin, H.; Hu, W.; Hu, Y.-Y.; Fu, R.; Zhang, R.; Zhou, H.-X.; Cross, T.A.
Deposited on : 2025-03-03

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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 : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
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) : 2.41.4

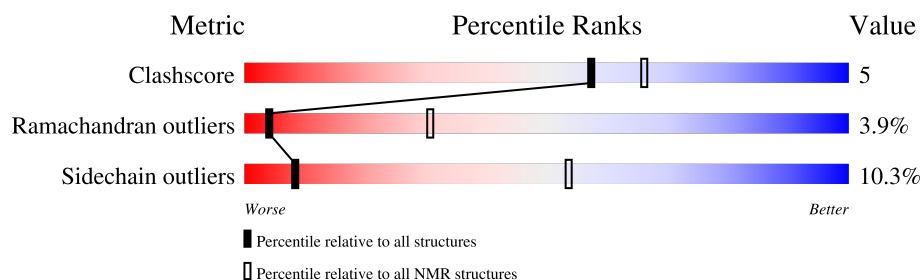
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 3%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	102	
1	B	102	

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:17-A:93, B:17-B:93 (154)	0.25	3

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	1, 2, 3, 4, 5, 6, 7, 8
2	9, 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2478 atoms, of which 1266 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cell division protein CrgA.

Mol	Chain	Residues	Atoms						Trace
1	A	77	Total	C	H	N	O	S	0
			1239	411	633	97	92	6	
1	B	77	Total	C	H	N	O	S	0
			1239	411	633	97	92	6	

There are 18 discrepancies between the modelled and reference sequences:

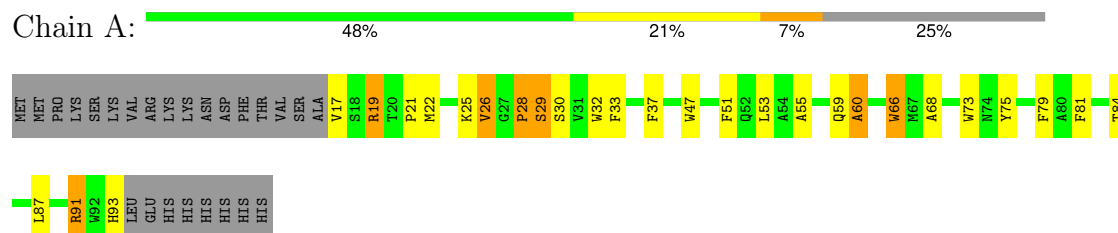
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P9WP57
A	94	LEU	-	expression tag	UNP P9WP57
A	95	GLU	-	expression tag	UNP P9WP57
A	96	HIS	-	expression tag	UNP P9WP57
A	97	HIS	-	expression tag	UNP P9WP57
A	98	HIS	-	expression tag	UNP P9WP57
A	99	HIS	-	expression tag	UNP P9WP57
A	100	HIS	-	expression tag	UNP P9WP57
A	101	HIS	-	expression tag	UNP P9WP57
B	0	MET	-	initiating methionine	UNP P9WP57
B	94	LEU	-	expression tag	UNP P9WP57
B	95	GLU	-	expression tag	UNP P9WP57
B	96	HIS	-	expression tag	UNP P9WP57
B	97	HIS	-	expression tag	UNP P9WP57
B	98	HIS	-	expression tag	UNP P9WP57
B	99	HIS	-	expression tag	UNP P9WP57
B	100	HIS	-	expression tag	UNP P9WP57
B	101	HIS	-	expression tag	UNP P9WP57

4 Residue-property plots

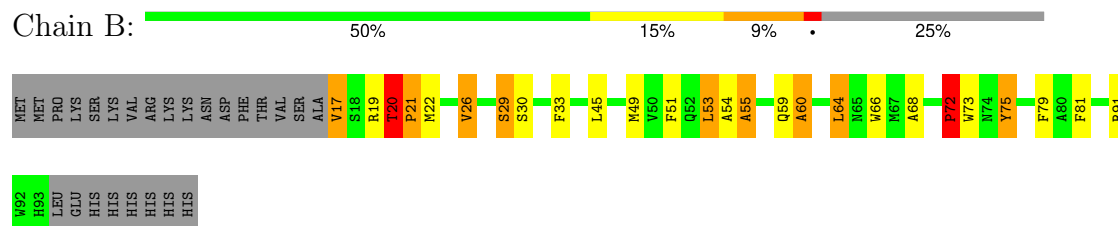
4.1 Average score per residue in the NMR ensemble

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: Cell division protein CrgA



- Molecule 1: Cell division protein CrgA

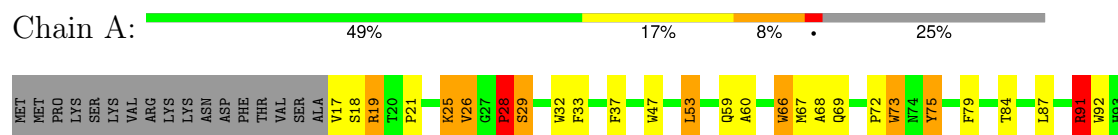


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Cell division protein CrgA



LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Cell division protein CrgA

Chain B:  50% 13% 10% • 25%

MET MET PRO LYS SER LYS VAL ARG LYS LYS ASN ASP PHE THR VAL SER SER ALA V17 V18 S18 R19 T20 P21 M22 V26 V27 G27 P28 S29 S30 V31 V32 F33 L45 M49 L53 A54 A55 Q59 A60 L64 A68 P72 Y75 A78 R91 W92 H93 LEU GLU HIS

HIS
HIS
HIS
HIS
HIS

4.2.2 Score per residue for model 2

- Molecule 1: Cell division protein CrgA

Chain A:  49% 20% 5% • 25%

MET MET PRO LYS SER LYS VAL ARG LYS LYS ASN ASP PHE THR VAL SER SER ALA V17 V18 S18 R19 T20 P21 M22 K25 V26 V27 G27 P28 S29 S30 V31 V32 F33 F37 F51 Q59 A60 P61 W66 W67 A68 Q69 W73 A76 F79 F81 T84 R91 W92 H93

LEU
GLU
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Cell division protein CrgA

Chain B:  37% 25% 9% 5% 25%

MET MET PRO LYS SER LYS VAL ARG LYS LYS ASN ASP PHE THR VAL SER SER ALA V17 V18 S18 R19 T20 P21 M22 K23 V26 V27 G27 P28 S29 S30 V31 V32 S35 I43 G44 L45 M49 V50 F51 Q52 Q53 A54 A55 Q59 A60 L64 W65 W66 W67 A68 Q69 L70 G71 P72 W73

W74 Y75 A76 F79 A80 F81 M82 I83 L87 L88 R91 W92 H93 LEU GLU HIS HIS HIS HIS HIS HIS

4.2.3 Score per residue for model 3 (medoid)

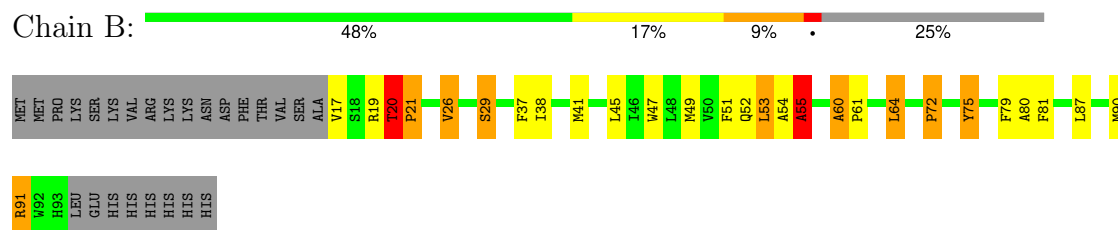
- Molecule 1: Cell division protein CrgA

Chain A:  49% 19% 7% • 25%

MET MET PRO LYS SER LYS VAL ARG LYS LYS ASN ASP PHE THR VAL SER SER ALA V17 V18 S18 R19 T20 P21 K25 V26 V27 G27 P28 S29 S30 V31 V32 F33 F37 L45 L46 W47 F51 Q52 L53 A54 A55 Q59 A60 W66 Q69 Y75 F79 A80 F81 T84

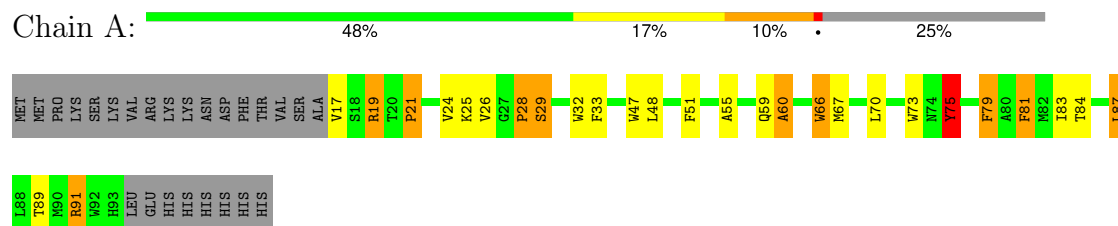
L87 R91 W92 H93 LEU GLU HIS HIS HIS HIS HIS HIS

- Molecule 1: Cell division protein CrgA

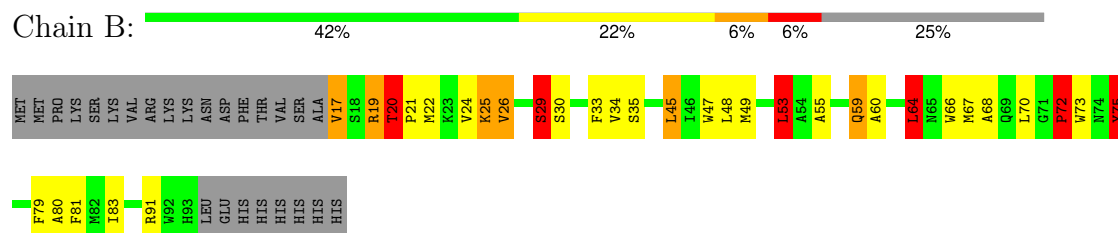


4.2.4 Score per residue for model 4

- Molecule 1: Cell division protein CrgA

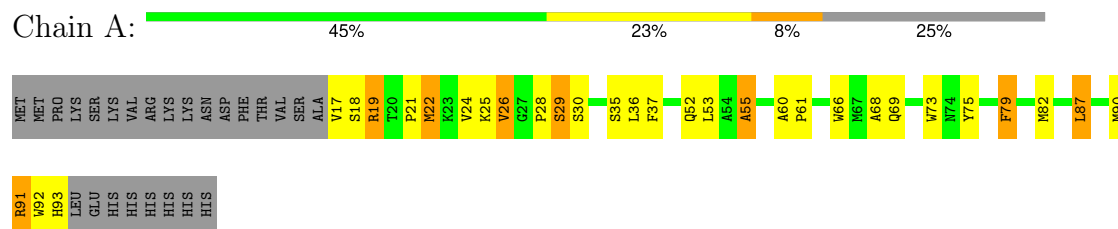


- Molecule 1: Cell division protein CrgA

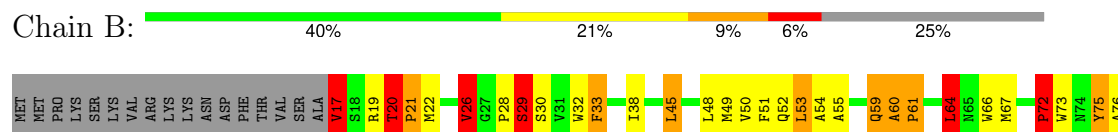


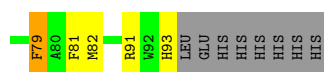
4.2.5 Score per residue for model 5

- Molecule 1: Cell division protein CrgA



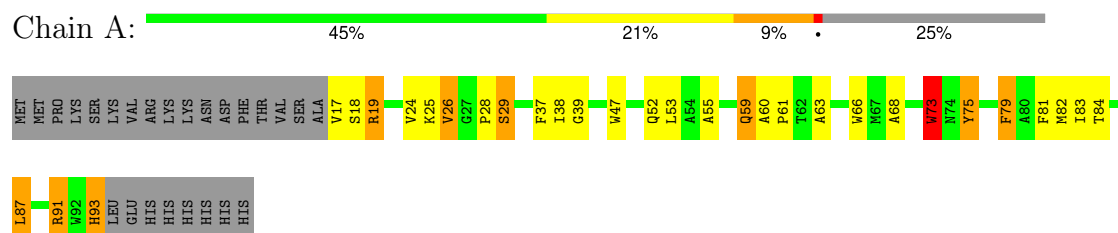
- Molecule 1: Cell division protein CrgA



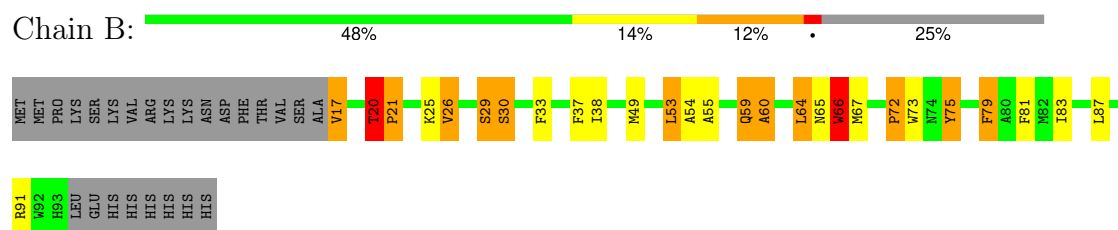


4.2.6 Score per residue for model 6

- Molecule 1: Cell division protein CrgA

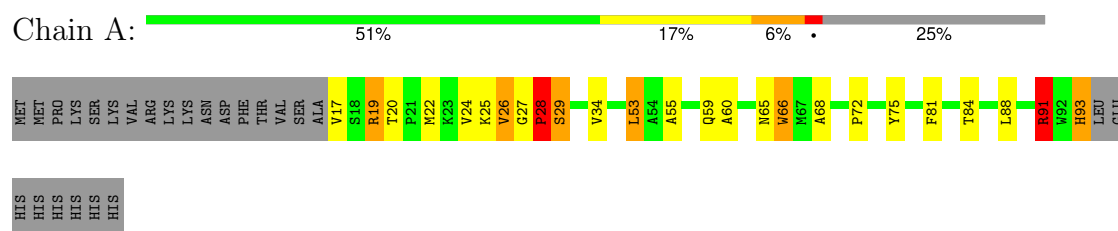


- Molecule 1: Cell division protein CrgA

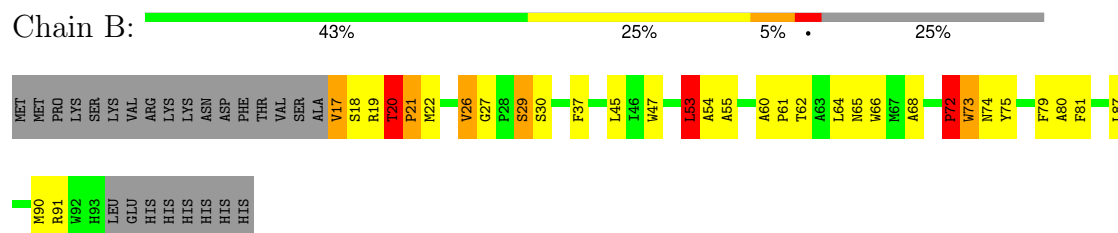


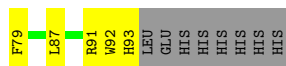
4.2.7 Score per residue for model 7

- Molecule 1: Cell division protein CrgA

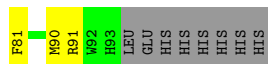


- Molecule 1: Cell division protein CrgA





- Molecule 1: Cell division protein CrgA



5 Refinement protocol and experimental data overview

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

Of the 13 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
NAMD	refinement	2.13
X-PLOR NIH	structure calculation	3.4

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	1
Total number of shifts	69
Number of shifts mapped to atoms	69
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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	1.62±0.04	3±2/626 (0.5± 0.2%)	2.19±0.10	25±3/854 (2.9± 0.4%)
1	B	1.67±0.07	5±2/626 (0.8± 0.3%)	2.32±0.08	26±4/854 (3.0± 0.4%)
All	All	1.65	76/12520 (0.6%)	2.25	505/17080 (3.0%)

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	6.9±1.4
1	B	1.0±0.0	6.6±1.0
All	All	10	135

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	20	THR	CA-CB	8.29	1.75	1.53	2	10
1	B	18	SER	CA-CB	8.04	1.65	1.52	7	2
1	A	51	PHE	CG-CD2	7.47	1.50	1.38	4	1
1	A	75	TYR	CE1-CZ	7.20	1.48	1.38	3	1
1	B	91	ARG	CD-NE	6.86	1.58	1.46	3	1
1	A	26	VAL	C-N	6.83	1.45	1.33	8	1
1	A	92	TRP	NE1-CE2	-6.77	1.28	1.37	5	1
1	B	30	SER	CB-OG	6.72	1.50	1.42	2	1
1	A	47	TRP	CG-CD1	6.69	1.46	1.36	8	1
1	B	75	TYR	CB-CG	-6.45	1.42	1.51	10	3
1	A	37	PHE	CG-CD2	6.33	1.48	1.38	1	1
1	A	37	PHE	CG-CD1	6.33	1.48	1.38	6	1
1	B	27	GLY	CA-C	-6.33	1.41	1.51	7	1
1	B	66	TRP	NE1-CE2	-6.16	1.29	1.37	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	35	SER	CA-CB	6.15	1.62	1.52	9	3
1	A	92	TRP	CD2-CE3	-6.09	1.31	1.40	1	1
1	B	32	TRP	CD2-CE2	6.04	1.48	1.41	5	1
1	B	32	TRP	NE1-CE2	-5.97	1.29	1.37	5	1
1	B	73	TRP	CD2-CE2	5.93	1.48	1.41	10	3
1	B	33	PHE	CG-CD2	5.90	1.47	1.38	5	2
1	A	61	PRO	CA-CB	5.88	1.65	1.53	2	2
1	A	75	TYR	CB-CG	-5.84	1.42	1.51	9	1
1	A	84	THR	C-N	5.82	1.43	1.33	6	1
1	A	93	HIS	CB-CG	5.79	1.60	1.50	7	1
1	B	92	TRP	CD1-NE1	5.78	1.47	1.38	8	1
1	B	26	VAL	C-N	5.71	1.43	1.33	6	1
1	B	51	PHE	CG-CD2	5.71	1.47	1.38	5	2
1	A	92	TRP	CZ3-CH2	5.71	1.49	1.40	1	1
1	B	23	LYS	CA-CB	5.70	1.66	1.53	2	1
1	B	33	PHE	CA-CB	5.65	1.66	1.53	1	1
1	A	92	TRP	CG-CD1	5.63	1.44	1.36	10	1
1	B	75	TYR	CE2-CZ	5.59	1.45	1.38	3	1
1	A	66	TRP	CD2-CE3	-5.48	1.32	1.40	7	1
1	A	33	PHE	CB-CG	5.46	1.60	1.51	3	1
1	A	81	PHE	CG-CD2	5.46	1.47	1.38	6	2
1	A	67	MET	CA-CB	5.42	1.65	1.53	1	1
1	A	51	PHE	CG-CD1	5.37	1.46	1.38	9	1
1	A	69	GLN	CA-CB	5.32	1.65	1.53	2	1
1	A	18	SER	CA-CB	5.32	1.60	1.52	5	2
1	B	70	LEU	C-N	5.29	1.42	1.33	4	1
1	A	66	TRP	CD2-CE2	5.28	1.47	1.41	4	1
1	B	91	ARG	NE-CZ	-5.27	1.26	1.33	3	1
1	B	26	VAL	CB-CG2	5.18	1.63	1.52	10	1
1	B	27	GLY	N-CA	5.18	1.53	1.46	2	1
1	A	47	TRP	CE3-CZ3	5.17	1.47	1.38	8	1
1	B	66	TRP	CD2-CE3	5.15	1.48	1.40	6	1
1	B	50	VAL	CB-CG2	5.11	1.63	1.52	5	1
1	B	65	ASN	CB-CG	5.11	1.62	1.51	6	1
1	B	73	TRP	CZ2-CH2	5.09	1.47	1.37	7	1
1	A	79	PHE	CG-CD1	5.09	1.46	1.38	1	1
1	A	32	TRP	N-CA	-5.05	1.36	1.46	1	1
1	B	29	SER	CB-OG	5.01	1.48	1.42	10	1
1	A	32	TRP	CB-CG	5.01	1.59	1.50	2	1
1	B	81	PHE	CG-CD2	5.01	1.46	1.38	2	1
1	B	55	ALA	CA-CB	5.01	1.62	1.52	3	1

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	B	91	ARG	NE-CZ-NH1	24.44	132.52	120.30	9	7
1	A	91	ARG	NE-CZ-NH1	22.16	131.38	120.30	2	7
1	A	91	ARG	NE-CZ-NH2	-20.90	109.85	120.30	6	5
1	B	20	THR	N-CA-C	18.31	160.44	111.00	8	10
1	A	19	ARG	NE-CZ-NH1	17.52	129.06	120.30	6	6
1	B	19	ARG	NE-CZ-NH1	17.14	128.87	120.30	2	7
1	B	19	ARG	NE-CZ-NH2	-15.64	112.48	120.30	1	5
1	A	19	ARG	NE-CZ-NH2	-14.95	112.83	120.30	3	6
1	B	20	THR	N-CA-CB	-14.83	82.11	110.30	2	10
1	B	91	ARG	NE-CZ-NH2	-14.44	113.08	120.30	2	8
1	A	79	PHE	CB-CG-CD2	12.92	129.84	120.80	6	4
1	B	20	THR	CA-CB-CG2	12.59	130.03	112.40	4	10
1	A	51	PHE	CB-CG-CD1	-12.40	112.12	120.80	2	2
1	B	51	PHE	CB-CG-CD1	12.11	129.28	120.80	8	3
1	A	81	PHE	CB-CG-CD2	11.65	128.96	120.80	6	4
1	A	75	TYR	CB-CG-CD2	-11.48	114.11	121.00	4	5
1	B	20	THR	CB-CA-C	-11.41	80.80	111.60	5	10
1	A	51	PHE	CB-CG-CD2	11.28	128.69	120.80	2	2
1	B	54	ALA	N-CA-CB	-10.92	94.81	110.10	5	1
1	B	51	PHE	CB-CG-CD2	-10.52	113.44	120.80	8	2
1	B	91	ARG	NH1-CZ-NH2	-10.37	107.99	119.40	6	7
1	B	75	TYR	CB-CG-CD2	-10.33	114.80	121.00	1	4
1	A	33	PHE	CB-CG-CD1	-9.97	113.82	120.80	1	1
1	B	37	PHE	CB-CG-CD2	9.92	127.74	120.80	7	2
1	A	79	PHE	CB-CG-CD1	-9.78	113.95	120.80	10	3
1	A	82	MET	CG-SD-CE	-9.74	84.61	100.20	8	3
1	A	29	SER	N-CA-C	9.44	136.50	111.00	1	10
1	B	29	SER	N-CA-C	9.31	136.13	111.00	8	10
1	A	81	PHE	CB-CG-CD1	9.08	127.16	120.80	3	4
1	B	19	ARG	NH1-CZ-NH2	-9.08	109.41	119.40	2	2
1	A	33	PHE	CB-CG-CD2	-9.08	114.45	120.80	9	5
1	B	26	VAL	CA-C-N	9.05	134.30	116.20	1	3
1	A	37	PHE	CB-CG-CD1	-9.02	114.49	120.80	2	5
1	B	75	TYR	CG-CD2-CE2	-8.93	114.15	121.30	1	2
1	A	19	ARG	O-C-N	-8.90	108.46	122.70	1	8
1	B	33	PHE	CB-CG-CD1	-8.88	114.58	120.80	10	3
1	B	75	TYR	CB-CG-CD1	8.81	126.29	121.00	5	1
1	A	37	PHE	CB-CG-CD2	8.81	126.97	120.80	2	2
1	B	81	PHE	CB-CG-CD2	-8.78	114.66	120.80	5	4
1	A	29	SER	N-CA-CB	-8.76	97.37	110.50	4	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	75	TYR	CG-CD2-CE2	-8.45	114.54	121.30	4	2
1	A	21	PRO	N-CA-CB	-8.22	93.44	103.30	8	2
1	B	37	PHE	CB-CG-CD1	-8.07	115.15	120.80	7	2
1	B	55	ALA	N-CA-C	8.07	132.78	111.00	9	9
1	B	33	PHE	CB-CG-CD2	7.92	126.34	120.80	10	2
1	B	47	TRP	CE2-CD2-CG	-7.62	101.20	107.30	7	3
1	A	52	GLN	N-CA-CB	7.60	124.28	110.60	3	1
1	B	20	THR	CA-CB-OG1	7.51	124.77	109.00	7	5
1	A	75	TYR	CZ-CE2-CD2	-7.46	113.08	119.80	6	2
1	B	50	VAL	CG1-CB-CG2	-7.40	99.06	110.90	8	1
1	B	68	ALA	N-CA-CB	7.38	120.43	110.10	9	1
1	A	75	TYR	CB-CA-C	7.38	125.15	110.40	9	2
1	B	53	LEU	C-N-CA	-7.35	103.32	121.70	7	5
1	B	79	PHE	CB-CG-CD2	-7.34	115.66	120.80	6	3
1	A	84	THR	CA-CB-CG2	-7.34	102.13	112.40	7	3
1	A	93	HIS	N-CA-CB	-7.33	97.41	110.60	9	3
1	A	60	ALA	CB-CA-C	7.33	121.09	110.10	8	2
1	A	75	TYR	CB-CG-CD1	7.32	125.39	121.00	8	3
1	B	68	ALA	CB-CA-C	-7.32	99.13	110.10	1	1
1	B	72	PRO	N-CA-CB	-7.30	94.54	103.30	9	4
1	B	26	VAL	N-CA-C	-7.21	91.53	111.00	1	4
1	B	81	PHE	CB-CG-CD1	7.18	125.83	120.80	10	3
1	A	47	TRP	CE3-CZ3-CH2	7.18	129.09	121.20	10	1
1	A	67	MET	O-C-N	-7.15	111.26	122.70	1	1
1	A	47	TRP	CB-CG-CD1	-7.15	117.71	127.00	6	3
1	A	53	LEU	CB-CG-CD1	7.12	123.11	111.00	8	4
1	A	26	VAL	N-CA-C	-7.11	91.82	111.00	5	4
1	A	66	TRP	CA-CB-CG	6.97	126.95	113.70	7	1
1	A	32	TRP	CH2-CZ2-CE2	6.96	124.36	117.40	2	3
1	A	34	VAL	CA-CB-CG2	-6.95	100.48	110.90	7	1
1	B	32	TRP	CH2-CZ2-CE2	6.94	124.34	117.40	2	2
1	B	47	TRP	NE1-CE2-CD2	6.88	114.18	107.30	3	1
1	B	93	HIS	CA-CB-CG	6.88	125.30	113.60	8	1
1	A	33	PHE	CG-CD1-CE1	-6.88	113.23	120.80	9	1
1	B	60	ALA	CB-CA-C	6.86	120.39	110.10	6	2
1	B	53	LEU	CB-CA-C	6.83	123.18	110.20	8	2
1	A	32	TRP	CB-CG-CD1	-6.79	118.17	127.00	8	1
1	B	75	TYR	CZ-CE2-CD2	6.77	125.89	119.80	1	1
1	A	66	TRP	CB-CG-CD1	-6.76	118.21	127.00	10	3
1	A	26	VAL	C-N-CA	-6.74	108.14	122.30	8	6
1	B	41	MET	CG-SD-CE	-6.70	89.48	100.20	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	73	TRP	CD1-CG-CD2	-6.70	100.94	106.30	6	1
1	B	88	LEU	CB-CA-C	6.68	122.90	110.20	9	1
1	A	87	LEU	CB-CG-CD2	6.64	122.29	111.00	4	3
1	B	19	ARG	N-CA-CB	6.63	122.53	110.60	5	2
1	A	67	MET	CG-SD-CE	-6.62	89.60	100.20	1	3
1	B	49	MET	CG-SD-CE	6.62	110.80	100.20	9	1
1	B	54	ALA	N-CA-C	6.60	128.82	111.00	6	6
1	B	64	LEU	CB-CG-CD2	6.56	122.15	111.00	3	2
1	A	22	MET	CG-SD-CE	-6.50	89.80	100.20	5	1
1	A	19	ARG	NH1-CZ-NH2	6.50	126.55	119.40	3	2
1	A	35	SER	N-CA-CB	6.48	120.23	110.50	5	1
1	B	67	MET	N-CA-CB	6.45	122.22	110.60	5	1
1	A	37	PHE	CB-CA-C	6.44	123.28	110.40	5	1
1	B	17	VAL	CG1-CB-CG2	6.43	121.19	110.90	5	1
1	A	41	MET	CG-SD-CE	6.39	110.42	100.20	10	1
1	B	29	SER	CB-CA-C	-6.36	98.02	110.10	9	3
1	A	58	SER	O-C-N	-6.35	112.54	122.70	9	1
1	B	19	ARG	CG-CD-NE	-6.35	98.47	111.80	9	1
1	B	26	VAL	C-N-CA	-6.33	109.02	122.30	10	7
1	A	31	VAL	CA-CB-CG2	6.31	120.37	110.90	2	1
1	B	75	TYR	CB-CA-C	6.30	123.01	110.40	10	2
1	A	45	LEU	CB-CG-CD1	-6.28	100.33	111.00	3	1
1	A	91	ARG	CB-CA-C	6.25	122.89	110.40	8	1
1	B	53	LEU	O-C-N	-6.23	112.74	122.70	3	2
1	A	32	TRP	CE2-CD2-CG	-6.21	102.33	107.30	4	1
1	A	41	MET	CA-CB-CG	6.21	123.86	113.30	9	1
1	A	19	ARG	N-CA-CB	6.20	121.76	110.60	7	5
1	A	19	ARG	CG-CD-NE	-6.17	98.83	111.80	8	1
1	A	18	SER	N-CA-CB	6.16	119.74	110.50	1	1
1	A	75	TYR	CG-CD1-CE1	-6.16	116.38	121.30	5	1
1	A	47	TRP	CD1-CG-CD2	6.15	111.22	106.30	6	3
1	B	70	LEU	CB-CG-CD2	6.11	121.38	111.00	2	1
1	B	53	LEU	CB-CG-CD1	6.09	121.36	111.00	7	2
1	A	17	VAL	CA-CB-CG2	6.08	120.02	110.90	9	1
1	A	34	VAL	CA-CB-CG1	6.05	119.97	110.90	7	1
1	A	70	LEU	CB-CA-C	6.02	121.64	110.20	4	1
1	A	79	PHE	N-CA-CB	6.01	121.43	110.60	4	1
1	B	26	VAL	O-C-N	-6.01	112.98	123.20	4	5
1	B	52	GLN	N-CA-CB	5.98	121.36	110.60	5	1
1	A	73	TRP	CG-CD2-CE3	5.96	139.26	133.90	9	1
1	A	73	TRP	N-CA-C	5.94	127.05	111.00	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	55	ALA	N-CA-C	5.93	127.02	111.00	7	2
1	A	52	GLN	O-C-N	-5.93	113.21	122.70	6	1
1	A	55	ALA	N-CA-CB	5.92	118.39	110.10	10	1
1	B	80	ALA	N-CA-CB	-5.89	101.85	110.10	7	2
1	B	64	LEU	CA-CB-CG	5.88	128.83	115.30	1	1
1	A	24	VAL	CG1-CB-CG2	-5.88	101.49	110.90	7	1
1	A	24	VAL	CA-CB-CG1	-5.88	102.08	110.90	5	1
1	A	73	TRP	CE2-CD2-CG	-5.86	102.61	107.30	9	1
1	A	87	LEU	CB-CG-CD1	-5.82	101.10	111.00	6	1
1	B	54	ALA	C-N-CA	5.82	136.25	121.70	9	3
1	B	30	SER	N-CA-CB	-5.80	101.79	110.50	9	2
1	A	55	ALA	O-C-N	-5.79	113.43	122.70	3	1
1	A	84	THR	N-CA-CB	5.76	121.24	110.30	1	4
1	B	19	ARG	O-C-N	-5.76	113.48	122.70	3	1
1	A	69	GLN	CB-CA-C	5.75	121.91	110.40	5	1
1	B	73	TRP	CB-CG-CD2	5.75	134.08	126.60	4	2
1	B	32	TRP	CE2-CD2-CG	-5.74	102.71	107.30	2	1
1	A	81	PHE	CD1-CG-CD2	-5.74	110.84	118.30	6	1
1	B	67	MET	CG-SD-CE	-5.73	91.04	100.20	10	3
1	A	92	TRP	NE1-CE2-CD2	5.73	113.03	107.30	5	1
1	B	49	MET	CB-CA-C	5.71	121.82	110.40	1	1
1	B	92	TRP	CE2-CD2-CG	-5.71	102.73	107.30	1	1
1	A	26	VAL	CA-CB-CG2	-5.66	102.41	110.90	6	1
1	A	22	MET	CA-CB-CG	5.64	122.89	113.30	8	1
1	B	60	ALA	CA-C-N	5.63	132.88	117.10	2	1
1	A	91	ARG	NH1-CZ-NH2	-5.61	113.23	119.40	2	2
1	A	92	TRP	CB-CG-CD1	5.59	134.27	127.00	1	1
1	B	38	ILE	CB-CA-C	-5.57	100.46	111.60	6	1
1	A	43	ILE	CB-CA-C	5.57	122.74	111.60	9	1
1	B	21	PRO	N-CA-C	5.57	126.57	112.10	1	3
1	A	83	ILE	CB-CA-C	5.55	122.70	111.60	4	1
1	A	69	GLN	O-C-N	-5.54	113.83	122.70	3	2
1	A	26	VAL	CA-CB-CG1	5.54	119.20	110.90	1	1
1	A	26	VAL	N-CA-CB	5.53	123.67	111.50	5	1
1	B	90	MET	O-C-N	-5.53	113.86	122.70	10	2
1	A	91	ARG	N-CA-CB	5.51	120.52	110.60	4	1
1	A	34	VAL	CG1-CB-CG2	5.51	119.71	110.90	10	1
1	B	92	TRP	CE3-CZ3-CH2	5.50	127.25	121.20	2	1
1	B	30	SER	N-CA-C	5.49	125.82	111.00	6	1
1	A	32	TRP	O-C-N	-5.44	114.00	122.70	3	1
1	A	26	VAL	O-C-N	-5.44	113.95	123.20	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	90	MET	C-N-CA	5.44	135.29	121.70	5	1
1	A	79	PHE	CB-CA-C	5.42	121.25	110.40	1	1
1	B	64	LEU	N-CA-CB	5.42	121.24	110.40	5	1
1	A	73	TRP	CD1-NE1-CE2	5.40	113.86	109.00	1	2
1	A	90	MET	CG-SD-CE	-5.39	91.57	100.20	5	2
1	B	22	MET	CA-CB-CG	5.38	122.44	113.30	1	1
1	B	31	VAL	CA-CB-CG1	-5.37	102.84	110.90	2	1
1	B	80	ALA	CB-CA-C	5.37	118.16	110.10	3	1
1	A	92	TRP	CG-CD1-NE1	5.37	115.47	110.10	1	1
1	A	53	LEU	CB-CA-C	5.36	120.39	110.20	6	2
1	A	83	ILE	CA-CB-CG2	-5.33	100.24	110.90	4	1
1	B	19	ARG	CD-NE-CZ	5.32	131.04	123.60	1	1
1	A	48	LEU	N-CA-CB	5.32	121.03	110.40	10	1
1	A	50	VAL	CA-CB-CG2	-5.31	102.93	110.90	9	1
1	A	75	TYR	CD1-CE1-CZ	-5.31	115.02	119.80	3	1
1	A	79	PHE	CG-CD2-CE2	-5.29	114.98	120.80	5	1
1	A	32	TRP	CD2-CE2-CZ2	-5.29	115.95	122.30	4	1
1	B	22	MET	CB-CA-C	-5.29	99.83	110.40	8	1
1	B	28	PRO	N-CA-CB	5.27	109.62	103.30	5	1
1	B	83	ILE	CB-CA-C	-5.27	101.07	111.60	2	2
1	B	45	LEU	O-C-N	-5.26	114.28	122.70	1	1
1	A	37	PHE	CZ-CE2-CD2	-5.26	113.79	120.10	5	1
1	B	53	LEU	N-CA-CB	5.25	120.90	110.40	8	1
1	A	30	SER	N-CA-CB	5.25	118.37	110.50	10	1
1	B	43	ILE	CG1-CB-CG2	5.25	122.94	111.40	2	1
1	A	37	PHE	CG-CD1-CE1	-5.24	115.04	120.80	10	1
1	A	66	TRP	O-C-N	-5.23	114.34	122.70	7	1
1	A	25	LYS	O-C-N	-5.22	114.34	122.70	2	2
1	B	45	LEU	CA-CB-CG	5.22	127.31	115.30	4	1
1	B	25	LYS	O-C-N	-5.22	114.35	122.70	4	2
1	A	89	THR	CA-CB-CG2	-5.21	105.10	112.40	4	1
1	A	36	LEU	CB-CG-CD2	5.21	119.85	111.00	5	1
1	A	32	TRP	CZ3-CH2-CZ2	-5.19	115.37	121.60	2	1
1	A	63	ALA	N-CA-CB	-5.19	102.83	110.10	6	1
1	A	65	ASN	CB-CA-C	-5.18	100.03	110.40	7	1
1	B	53	LEU	N-CA-C	5.18	124.97	111.00	2	1
1	B	59	GLN	N-CA-CB	5.18	119.92	110.60	5	1
1	A	47	TRP	CE2-CD2-CG	-5.17	103.16	107.30	6	1
1	B	90	MET	CG-SD-CE	-5.17	91.92	100.20	10	2
1	B	65	ASN	O-C-N	-5.17	114.43	122.70	7	1
1	A	47	TRP	CG-CD1-NE1	-5.17	104.93	110.10	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	93	HIS	N-CA-CB	5.16	119.89	110.60	1	1
1	A	88	LEU	CB-CG-CD2	-5.16	102.24	111.00	7	1
1	A	75	TYR	CD1-CG-CD2	5.14	123.55	117.90	4	1
1	A	45	LEU	CB-CG-CD2	5.13	119.72	111.00	9	1
1	B	82	MET	O-C-N	-5.13	114.50	122.70	2	1
1	A	79	PHE	CA-CB-CG	-5.12	101.61	113.90	3	1
1	A	66	TRP	N-CA-CB	5.12	119.82	110.60	2	1
1	B	28	PRO	O-C-N	-5.10	114.54	122.70	1	1
1	B	78	ALA	CB-CA-C	5.10	117.75	110.10	1	1
1	B	88	LEU	O-C-N	-5.09	114.55	122.70	2	1
1	A	60	ALA	O-C-N	-5.09	111.42	121.10	4	1
1	A	51	PHE	CG-CD1-CE1	5.09	126.40	120.80	8	1
1	A	39	GLY	O-C-N	-5.09	114.56	122.70	6	1
1	B	32	TRP	O-C-N	-5.08	114.58	122.70	1	1
1	A	76	ALA	N-CA-CB	5.07	117.20	110.10	2	1
1	A	49	MET	CG-SD-CE	5.07	108.31	100.20	10	1
1	B	17	VAL	CA-CB-CG1	-5.05	103.33	110.90	2	1
1	B	57	GLY	O-C-N	-5.05	114.62	122.70	9	1
1	B	58	SER	N-CA-CB	5.04	118.06	110.50	9	1
1	B	75	TYR	CG-CD1-CE1	-5.03	117.28	121.30	4	1
1	A	48	LEU	CB-CG-CD2	5.03	119.55	111.00	9	1
1	B	35	SER	CB-CA-C	-5.02	100.57	110.10	4	1
1	A	91	ARG	CB-CG-CD	5.01	124.62	111.60	5	1
1	A	26	VAL	CG1-CB-CG2	-5.00	102.89	110.90	7	1
1	A	47	TRP	CZ3-CH2-CZ2	-5.00	115.59	121.60	10	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	B	20	THR	CA	10

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	19	ARG	Sidechain,Peptide,Mainchain	10
1	A	26	VAL	Peptide	10
1	B	20	THR	Peptide	10
1	B	29	SER	Peptide	10
1	B	72	PRO	Peptide	10
1	A	28	PRO	Peptide	9

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Mol	Chain	Res	Type	Group	Models (Total)
1	B	26	VAL	Peptide	9
1	A	25	LYS	Peptide	8
1	B	75	TYR	Sidechain	8
1	B	53	LEU	Peptide	7
1	A	68	ALA	Peptide	6
1	A	55	ALA	Peptide	6
1	A	79	PHE	Sidechain	5
1	A	75	TYR	Sidechain	3
1	B	79	PHE	Sidechain	3
1	A	91	ARG	Sidechain	2
1	A	93	HIS	Sidechain	2
1	B	55	ALA	Peptide	2
1	B	68	ALA	Peptide	2
1	B	33	PHE	Sidechain	2
1	B	51	PHE	Sidechain	1
1	B	91	ARG	Sidechain	1
1	A	81	PHE	Sidechain	1
1	B	19	ARG	Sidechain	1
1	A	73	TRP	Peptide	1
1	A	51	PHE	Sidechain	1
1	A	92	TRP	Peptide	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	606	633	632	4±1
1	B	606	633	632	8±4
All	All	12120	12660	12640	114

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:THR:CB	1:B:20:THR:CA	1.59	1.74	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:THR:CB	1:B:20:THR:C	1.16	2.13	10	3
1:B:20:THR:CB	1:B:20:THR:N	1.09	2.15	2	3
1:B:20:THR:N	1:B:20:THR:HB	0.96	1.74	9	3
1:B:20:THR:CA	1:B:20:THR:HB	0.89	1.97	9	3
1:B:19:ARG:C	1:B:20:THR:HB	0.72	2.05	9	3
1:B:20:THR:CB	1:B:21:PRO:N	0.65	2.59	10	1
1:A:17:VAL:N	1:A:29:SER:HG	0.65	1.89	3	10
1:B:17:VAL:N	1:B:30:SER:HG	0.63	1.91	6	7
1:A:17:VAL:N	1:A:30:SER:HG	0.62	1.92	5	5
1:B:22:MET:SD	1:B:93:HIS:HB3	0.62	2.35	5	1
1:B:45:LEU:HD13	1:B:76:ALA:HA	0.59	1.75	5	2
1:A:26:VAL:HG12	1:A:33:PHE:HB2	0.55	1.77	3	3
1:B:64:LEU:HD23	1:B:66:TRP:CH2	0.55	2.37	6	5
1:B:60:ALA:HB1	1:B:61:PRO:CD	0.54	2.32	3	2
1:B:38:ILE:HD11	1:B:87:LEU:CD1	0.54	2.32	3	1
1:A:22:MET:CG	1:A:93:HIS:HB3	0.53	2.33	8	2
1:A:68:ALA:HB2	1:B:62:THR:HG23	0.52	1.80	7	1
1:B:20:THR:HG23	1:B:21:PRO:N	0.52	2.20	5	10
1:A:26:VAL:O	1:A:29:SER:HA	0.51	2.05	9	1
1:A:91:ARG:HA	1:A:91:ARG:HE	0.50	1.66	8	3
1:B:52:GLN:HA	1:B:55:ALA:HB3	0.50	1.83	3	1
1:B:73:TRP:CG	1:B:74:ASN:N	0.48	2.81	7	1
1:B:79:PHE:O	1:B:83:ILE:HG13	0.48	2.09	4	1
1:B:26:VAL:H	1:B:29:SER:HB3	0.47	1.70	5	1
1:A:73:TRP:CE2	1:B:59:GLN:HB3	0.46	2.45	1	4
1:B:49:MET:O	1:B:53:LEU:HB2	0.46	2.11	10	2
1:B:53:LEU:HD23	1:B:68:ALA:HB2	0.46	1.86	10	2
1:B:53:LEU:HB3	1:B:68:ALA:HB2	0.46	1.85	1	2
1:A:48:LEU:HD23	1:A:75:TYR:CZ	0.46	2.45	4	1
1:B:20:THR:CG2	1:B:21:PRO:N	0.45	2.79	3	3
1:A:22:MET:SD	1:B:26:VAL:HB	0.45	2.51	2	1
1:A:60:ALA:HB1	1:A:61:PRO:CD	0.45	2.42	9	2
1:B:45:LEU:CD1	1:B:76:ALA:HA	0.45	2.41	5	1
1:B:48:LEU:HD23	1:B:75:TYR:CE2	0.45	2.47	4	1
1:B:22:MET:HB3	1:B:93:HIS:HB3	0.44	1.90	2	1
1:A:22:MET:SD	1:A:93:HIS:HB3	0.44	2.52	7	2
1:B:53:LEU:HD23	1:B:68:ALA:CB	0.43	2.44	4	1
1:B:75:TYR:CE1	1:B:79:PHE:CD1	0.42	3.07	2	2
1:A:24:VAL:HG23	1:B:24:VAL:HG22	0.42	1.91	4	1
1:A:60:ALA:HB1	1:A:61:PRO:HD2	0.41	1.90	9	1
1:A:22:MET:HB3	1:A:93:HIS:HB3	0.41	1.92	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:GLY:HA2	1:A:28:PRO:C	0.41	2.35	7	2
1:B:19:ARG:O	1:B:20:THR:HB	0.41	2.04	4	1
1:A:59:GLN:HB3	1:B:73:TRP:CE2	0.41	2.51	6	1
1:A:20:THR:HA	1:A:22:MET:H	0.41	1.76	8	1
1:A:52:GLN:HA	1:A:55:ALA:HB3	0.40	1.94	5	1
1:A:38:ILE:HD13	1:A:83:ILE:HG22	0.40	1.94	6	1
1:B:25:LYS:HA	1:B:29:SER:HB3	0.40	1.93	4	1
1:B:48:LEU:HD23	1:B:75:TYR:CZ	0.40	2.52	5	1
1:B:35:SER:HA	1:B:38:ILE:HD12	0.40	1.92	10	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	75/102 (74%)	68±1 (90±1%)	5±1 (6±1%)	3±1 (4±1%)	4	31
1	B	75/102 (74%)	68±1 (91±1%)	4±1 (5±2%)	3±1 (4±1%)	4	30
All	All	1500/2040 (74%)	1360 (91%)	81 (5%)	59 (4%)	4	31

All 11 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	60	ALA	10
1	B	60	ALA	10
1	B	72	PRO	10
1	A	28	PRO	8
1	A	21	PRO	7
1	B	21	PRO	5
1	B	55	ALA	4
1	A	71	GLY	2
1	A	61	PRO	1
1	B	61	PRO	1
1	A	72	PRO	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	63/87 (72%)	58±2 (92±3%)	5±2 (8±3%)	12	60
1	B	63/87 (72%)	55±2 (88±3%)	8±2 (12±3%)	6	48
All	All	1260/1740 (72%)	1130 (90%)	130 (10%)	8	53

All 33 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	66	TRP	10
1	A	91	ARG	10
1	B	17	VAL	10
1	B	64	LEU	10
1	A	59	GLN	9
1	B	45	LEU	9
1	B	49	MET	9
1	A	87	LEU	7
1	B	20	THR	6
1	B	59	GLN	6
1	B	72	PRO	6
1	B	66	TRP	5
1	A	28	PRO	3
1	A	53	LEU	3
1	B	22	MET	3
1	B	87	LEU	3
1	A	72	PRO	2
1	A	75	TYR	2
1	B	88	LEU	2
1	B	61	PRO	2
1	B	26	VAL	1
1	B	34	VAL	1
1	B	38	ILE	1
1	B	82	MET	1
1	A	24	VAL	1
1	A	20	THR	1
1	A	22	MET	1
1	A	31	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	69	GLN	1
1	B	67	MET	1
1	B	83	ILE	1
1	A	83	ILE	1
1	B	79	PHE	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 3% for the well-defined parts and 3% 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	69
Number of shifts mapped to atoms	69
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	65

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
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	69	-7.01 ± 8.19	None needed (imprecise)

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 3%, i.e. 69 atoms were assigned a chemical shift out of a possible 2198. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	69/766 (9%)	0/312 (0%)	0/308 (0%)	69/146 (47%)
Sidechain	0/1180 (0%)	0/798 (0%)	0/356 (0%)	0/26 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/252 (0%)	0/126 (0%)	0/114 (0%)	0/12 (0%)
Overall	69/2198 (3%)	0/1236 (0%)	0/778 (0%)	69/184 (38%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 69 atoms were assigned a chemical shift out of a possible 2198. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	69/766 (9%)	0/312 (0%)	0/308 (0%)	69/146 (47%)
Sidechain	0/1180 (0%)	0/798 (0%)	0/356 (0%)	0/26 (0%)
Aromatic	0/252 (0%)	0/126 (0%)	0/114 (0%)	0/12 (0%)
Overall	69/2198 (3%)	0/1236 (0%)	0/778 (0%)	69/184 (38%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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	35	SER	N	228.00	99.14 – 133.45	32.6
1	A	30	SER	N	225.00	99.14 – 133.45	31.7
1	A	39	GLY	N	220.00	91.59 – 127.52	30.7
1	A	80	ALA	N	229.00	106.13 – 140.55	30.7
1	A	49	MET	N	222.00	102.99 – 137.21	29.8
1	A	87	LEU	N	230.00	102.77 – 140.89	28.4
1	A	76	ALA	N	221.00	106.13 – 140.55	28.4
1	A	42	LEU	N	226.00	102.77 – 140.89	27.3
1	A	45	LEU	N	225.00	102.77 – 140.89	27.1
1	A	73	TRP	N	225.00	101.51 – 141.60	25.8
1	A	51	PHE	N	225.00	99.93 – 140.82	25.6
1	A	88	LEU	N	219.00	102.77 – 140.89	25.5
1	A	85	GLY	N	201.00	91.59 – 127.52	25.4
1	A	90	MET	N	207.00	102.99 – 137.21	25.4
1	A	46	ILE	N	227.00	100.55 – 142.30	25.3
1	A	48	LEU	N	216.00	102.77 – 140.89	24.7

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	41	MET	N	203.00	102.99 – 137.21	24.2
1	A	79	PHE	N	219.00	99.93 – 140.82	24.1
1	A	38	ILE	N	222.00	100.55 – 142.30	24.1
1	A	84	THR	N	227.00	91.89 – 138.78	23.8
1	A	77	ILE	N	220.00	100.55 – 142.30	23.6
1	A	83	ILE	N	219.00	100.55 – 142.30	23.4
1	A	74	ASN	N	209.00	99.66 – 138.23	23.4
1	A	44	GLY	N	193.00	91.59 – 127.52	23.2
1	A	31	VAL	N	221.00	99.23 – 142.92	22.9
1	A	32	TRP	N	213.00	101.51 – 141.60	22.8
1	A	92	TRP	N	213.00	101.51 – 141.60	22.8
1	A	78	ALA	N	201.00	106.13 – 140.55	22.6
1	A	36	LEU	N	207.00	102.77 – 140.89	22.3
1	A	37	PHE	N	209.00	99.93 – 140.82	21.7
1	A	81	PHE	N	209.00	99.93 – 140.82	21.7
1	A	82	MET	N	194.00	102.99 – 137.21	21.6
1	A	86	LEU	N	204.00	102.77 – 140.89	21.6
1	A	89	THR	N	216.00	91.89 – 138.78	21.5
1	A	43	ILE	N	209.00	100.55 – 142.30	21.0
1	A	34	VAL	N	211.00	99.23 – 142.92	20.6
1	A	33	PHE	N	204.00	99.93 – 140.82	20.4
1	A	40	LEU	N	198.00	102.77 – 140.89	20.0
1	A	29	SER	N	179.00	99.14 – 133.45	18.3
1	A	75	TYR	N	190.00	100.12 – 140.79	17.1
1	A	47	TRP	N	188.00	101.51 – 141.60	16.6
1	A	91	ARG	N	177.00	102.91 – 138.82	15.6
1	A	54	ALA	N	173.00	106.13 – 140.55	14.4
1	A	53	LEU	N	175.00	102.77 – 140.89	13.9
1	A	19	ARG	N	73.00	102.91 – 138.82	-13.3
1	A	63	ALA	N	78.00	106.13 – 140.55	-13.2
1	A	64	LEU	N	74.00	102.77 – 140.89	-12.6
1	A	55	ALA	N	166.00	106.13 – 140.55	12.4
1	A	17	VAL	N	175.00	99.23 – 142.92	12.3
1	A	23	LYS	N	77.00	102.74 – 139.42	-12.0
1	A	25	LYS	N	77.00	102.74 – 139.42	-12.0
1	A	18	SER	N	77.00	99.14 – 133.45	-11.4
1	A	58	SER	N	77.00	99.14 – 133.45	-11.4
1	A	50	VAL	N	171.00	99.23 – 142.92	11.4
1	A	62	THR	N	62.00	91.89 – 138.78	-11.4
1	A	24	VAL	N	72.00	99.23 – 142.92	-11.2
1	A	65	ASN	N	77.00	99.66 – 138.23	-10.9
1	A	26	VAL	N	74.00	99.23 – 142.92	-10.8

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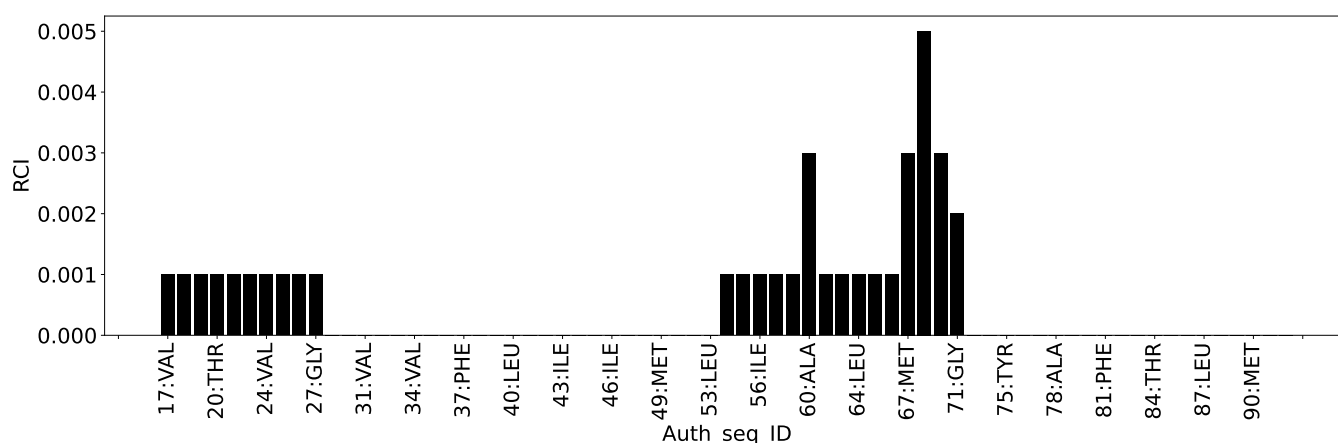
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	56	ILE	N	78.00	100.55 – 142.30	-10.4
1	A	57	GLY	N	74.00	91.59 – 127.52	-9.9
1	A	66	TRP	N	85.00	101.51 – 141.60	-9.1
1	A	22	MET	N	89.00	102.99 – 137.21	-9.1
1	A	20	THR	N	74.00	91.89 – 138.78	-8.8
1	A	27	GLY	N	78.00	91.59 – 127.52	-8.8
1	A	70	LEU	N	97.00	102.77 – 140.89	-6.5

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

No restraints data found

9 Distance violation analysis ⓘ

No distance restraints data found

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found