



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:11 PM UTC

PDB ID : 2KBZ / pdb_00002kbz
Title : NMR structure of protein gp15 of bacteriophage SPP1
Authors : Gallopin, M.; Gilquin, B.; Zinn-Justin, S.
Deposited on : 2008-12-12

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
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

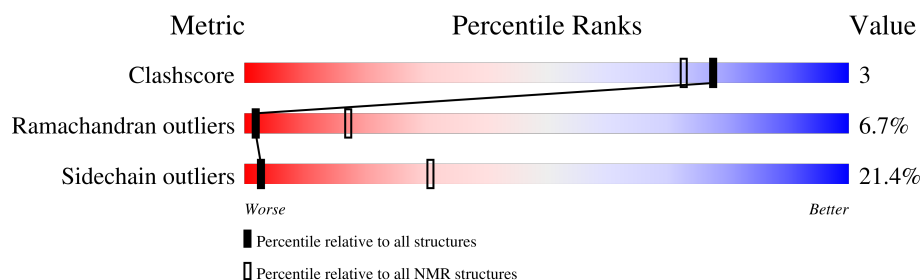
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#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	99	34% 35% 9% • 20%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:42-A:102, A:116-A:133 (79)	1.29	2

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1586 atoms, of which 797 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 15 protein (Bacteriophage SPP1 complete nucleotide sequence).

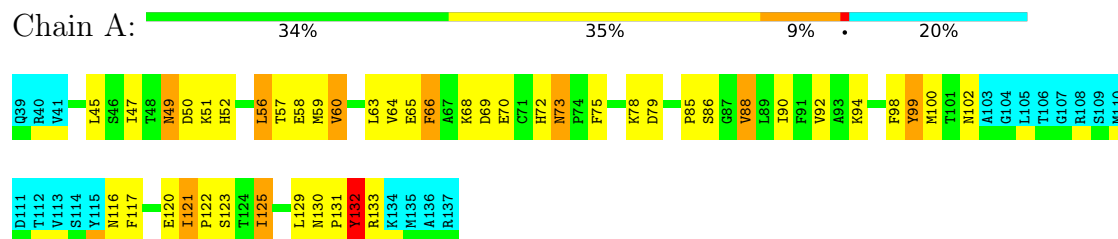
Mol	Chain	Residues	Atoms						Trace
1	A	99	Total	C	H	N	O	S	0
			1586	502	797	134	148	5	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)

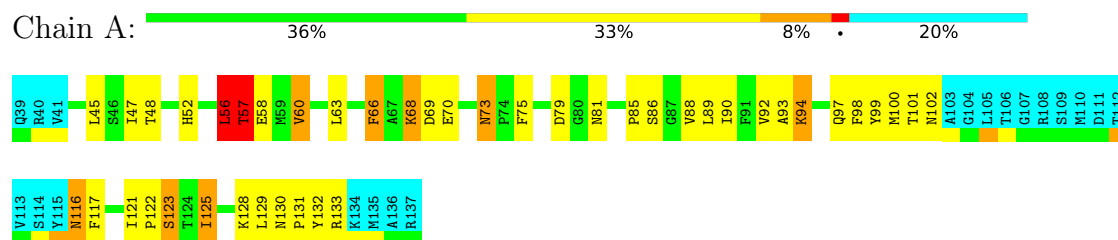


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

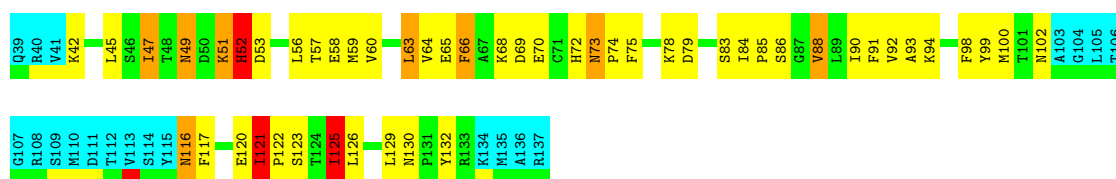
- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)



4.2.2 Score per residue for model 2 (medoid)

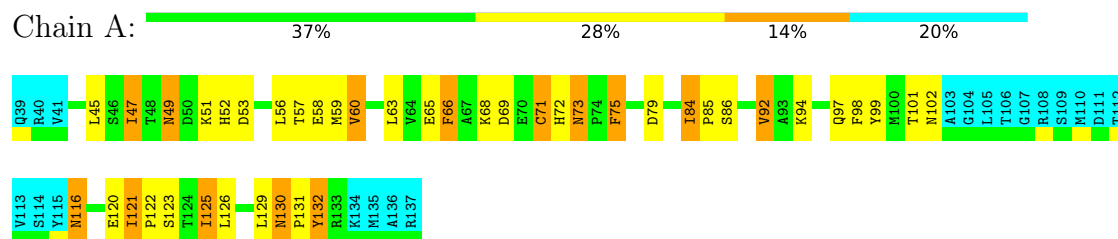
- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)





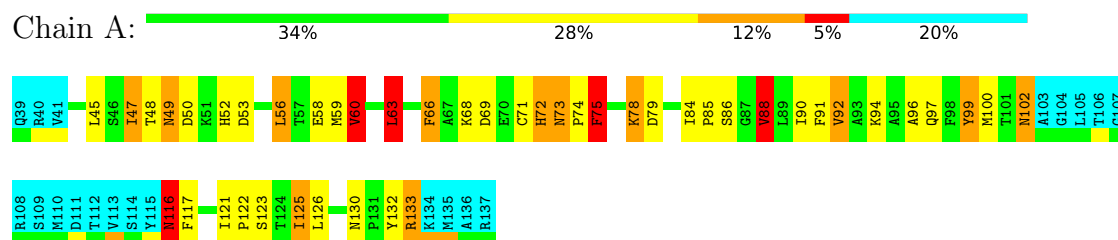
4.2.3 Score per residue for model 3

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)



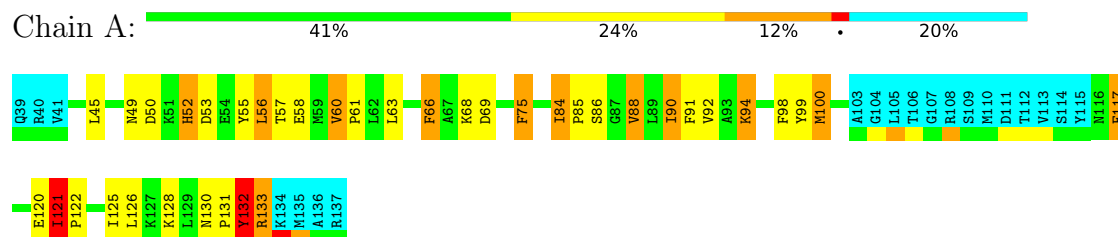
4.2.4 Score per residue for model 4

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)



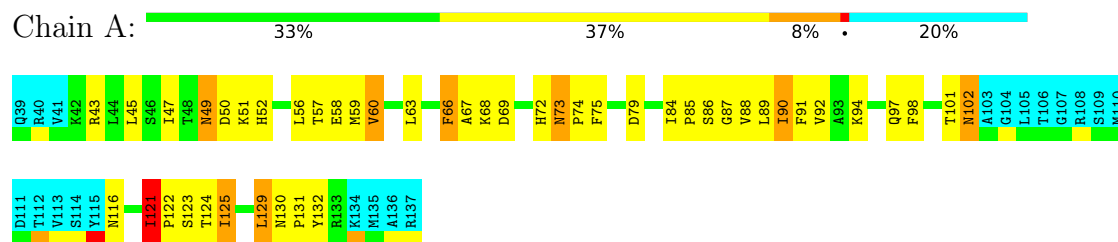
4.2.5 Score per residue for model 5

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)



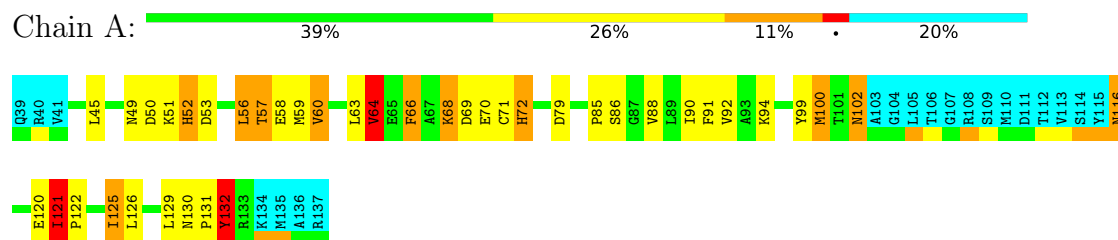
4.2.6 Score per residue for model 6

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)



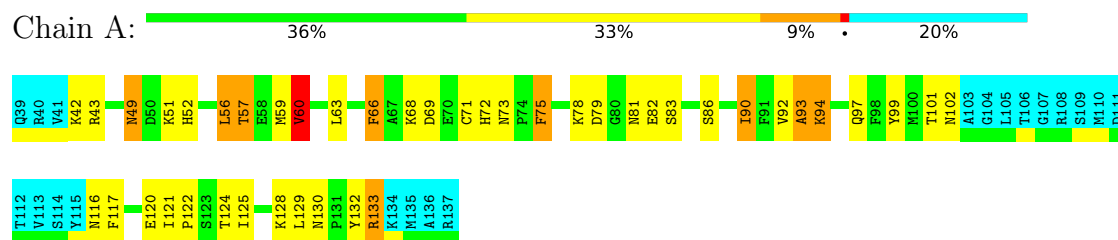
4.2.7 Score per residue for model 7

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)



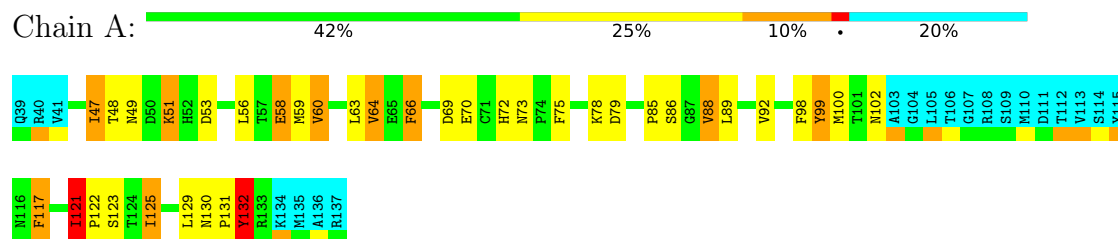
4.2.8 Score per residue for model 8

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)



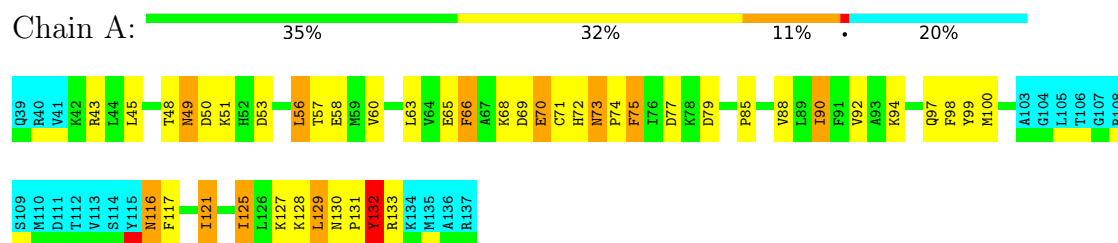
4.2.9 Score per residue for model 9

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)



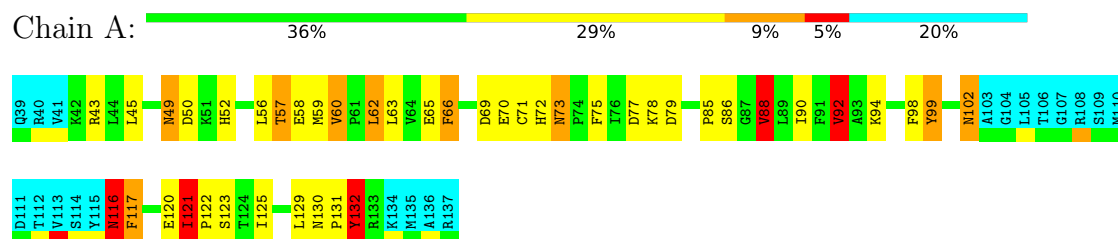
4.2.10 Score per residue for model 10

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)



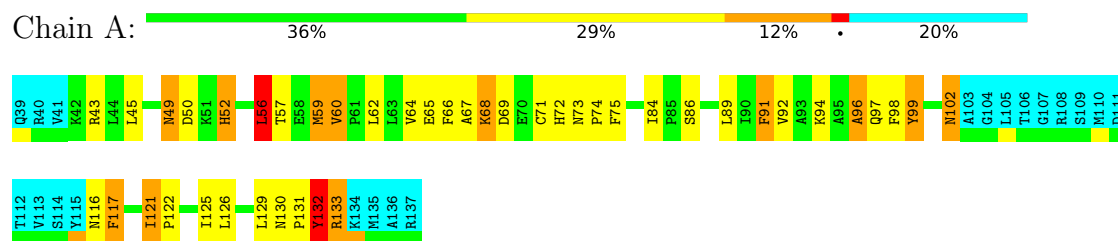
4.2.11 Score per residue for model 11

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)



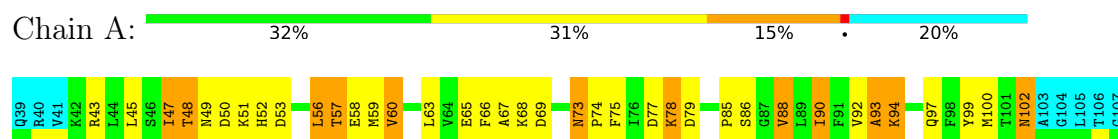
4.2.12 Score per residue for model 12

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)



4.2.13 Score per residue for model 13

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)

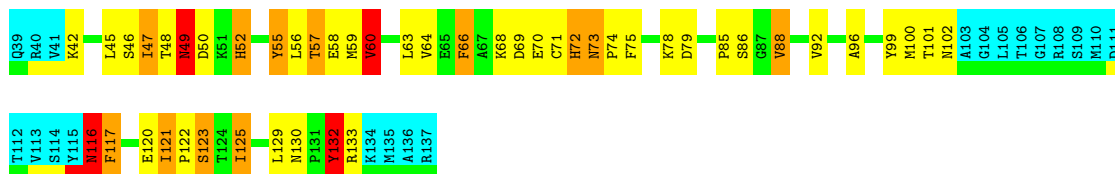




4.2.14 Score per residue for model 14

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)

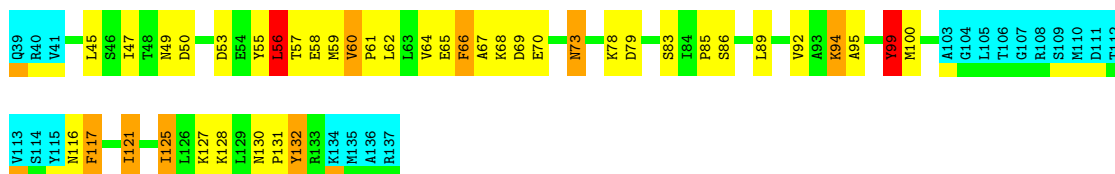
Chain A: 32% 31% 12% • 20%



4.2.15 Score per residue for model 15

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)

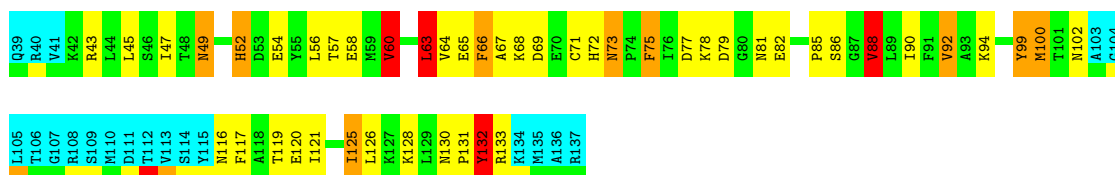
Chain A: 38% 31% 8% • 20%



4.2.16 Score per residue for model 16

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)

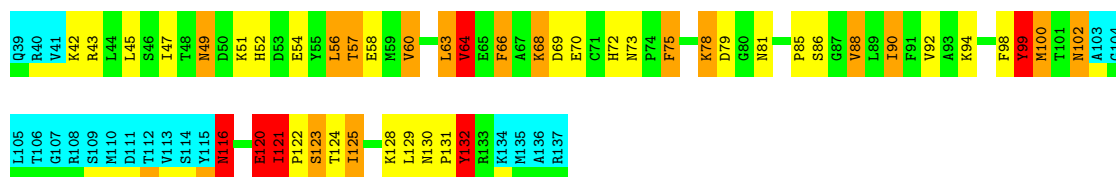
Chain A: 32% 34% 9% • 20%



4.2.17 Score per residue for model 17

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)

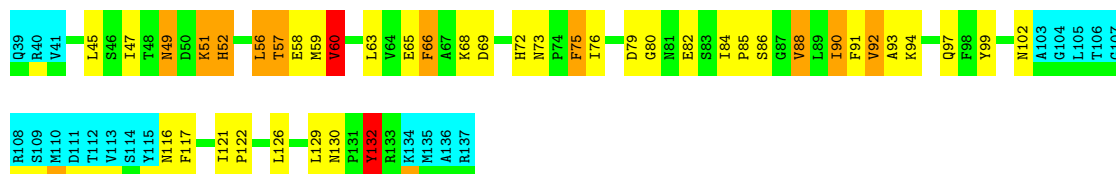
Chain A: 33% 25% 15% 6% 20%



4.2.18 Score per residue for model 18

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)

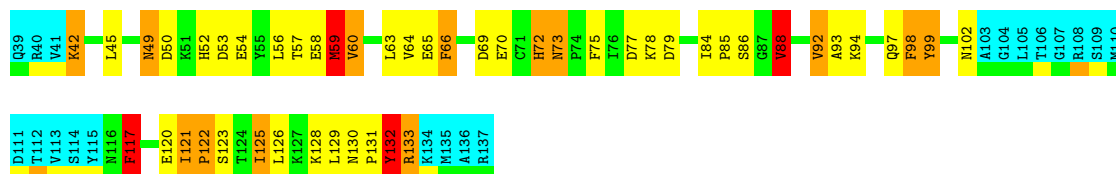
Chain A: 37% 30% 10% • 20%



4.2.19 Score per residue for model 19

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)

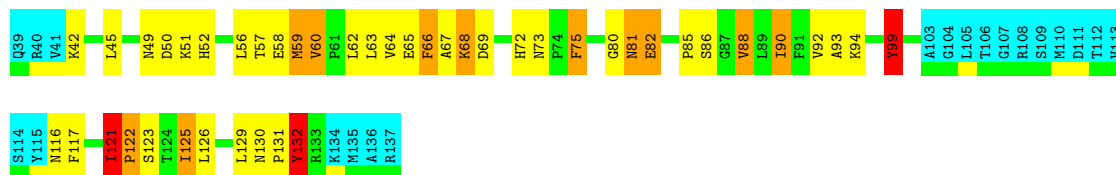
Chain A: 31% 31% 13% • 20%



4.2.20 Score per residue for model 20

- Molecule 1: 15 protein (Bacteriophage SPP1 complete nucleotide sequence)

Chain A: 35% 30% 11% • 20%



5 Refinement protocol and experimental data overview ⓘ

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

Of the 500 calculated structures, 20 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
INCA	refinement	1.0

No chemical shift data was provided.

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	1.43±0.03	0±1/651 (0.1± 0.1%)	2.49±0.06	57±6/883 (6.5± 0.7%)
All	All	1.43	9/13020 (0.1%)	2.49	1149/17660 (6.5%)

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	2.2±0.9
All	All	0	44

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	A	83	SER	C-N	5.86	1.38	1.33	2	1
1	A	119	THR	C-N	5.55	1.37	1.33	16	1
1	A	121	ILE	C-N	5.47	1.39	1.33	16	2
1	A	65	GLU	C-N	5.35	1.40	1.33	10	2
1	A	120	GLU	C-N	5.28	1.39	1.33	8	1
1	A	102	ASN	CA-CB	5.21	1.57	1.53	7	1
1	A	49	ASN	CA-CB	5.17	1.58	1.53	7	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	A	69	ASP	CA-C-N	12.79	137.07	120.44	1	19
1	A	69	ASP	C-N-CA	12.79	137.07	120.44	1	19
1	A	99	TYR	N-CA-C	12.41	124.55	111.14	9	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	73	ASN	CA-CB-CG	9.89	122.49	112.60	3	12
1	A	98	PHE	CA-CB-CG	9.85	123.65	113.80	19	7
1	A	73	ASN	N-CA-CB	-9.84	98.13	110.03	15	2
1	A	100	MET	CA-C-N	9.67	133.63	120.38	5	8
1	A	100	MET	C-N-CA	9.67	133.63	120.38	5	8
1	A	133	ARG	CA-C-N	9.62	139.92	121.54	5	2
1	A	133	ARG	C-N-CA	9.62	139.92	121.54	5	2
1	A	60	VAL	CA-C-O	-9.57	107.13	119.95	18	19
1	A	53	ASP	CA-C-N	9.49	133.34	120.44	7	9
1	A	53	ASP	C-N-CA	9.49	133.34	120.44	7	9
1	A	132	TYR	N-CA-C	9.46	121.53	111.03	1	6
1	A	102	ASN	CA-CB-CG	9.34	121.94	112.60	13	4
1	A	66	PHE	CA-CB-CG	9.34	123.14	113.80	9	20
1	A	58	GLU	CA-C-N	9.32	133.15	120.38	11	17
1	A	58	GLU	C-N-CA	9.32	133.15	120.38	11	17
1	A	56	LEU	CA-C-N	9.30	133.95	120.38	15	3
1	A	56	LEU	C-N-CA	9.30	133.95	120.38	15	3
1	A	51	LYS	CA-C-N	9.27	133.63	120.28	18	6
1	A	51	LYS	C-N-CA	9.27	133.63	120.28	18	6
1	A	60	VAL	O-C-N	-9.20	110.61	121.10	12	16
1	A	90	ILE	N-CA-CB	9.13	122.96	110.54	5	8
1	A	122	PRO	CA-C-N	9.12	132.88	120.38	11	11
1	A	122	PRO	C-N-CA	9.12	132.88	120.38	11	11
1	A	66	PHE	CA-C-N	9.07	133.17	120.29	14	16
1	A	66	PHE	C-N-CA	9.07	133.17	120.29	14	16
1	A	116	ASN	CA-C-N	9.04	138.81	121.54	20	3
1	A	116	ASN	C-N-CA	9.04	138.81	121.54	20	3
1	A	82	GLU	N-CA-C	8.96	122.90	110.35	18	3
1	A	80	GLY	CA-C-N	8.88	133.75	121.05	20	2
1	A	80	GLY	C-N-CA	8.88	133.75	121.05	20	2
1	A	63	LEU	CA-C-N	8.76	131.60	120.56	8	13
1	A	63	LEU	C-N-CA	8.76	131.60	120.56	8	13
1	A	117	PHE	CA-C-N	8.66	132.76	120.28	14	4
1	A	117	PHE	C-N-CA	8.66	132.76	120.28	14	4
1	A	129	LEU	CA-C-N	8.61	130.85	120.09	10	1
1	A	129	LEU	C-N-CA	8.61	130.85	120.09	10	1
1	A	130	ASN	CA-C-N	8.60	130.59	119.84	19	15
1	A	130	ASN	C-N-CA	8.60	130.59	119.84	19	15
1	A	117	PHE	N-CA-C	8.55	123.13	112.87	4	4
1	A	57	THR	CA-C-O	-8.51	111.88	120.82	13	8
1	A	88	VAL	CA-C-N	8.45	132.29	120.29	6	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	88	VAL	C-N-CA	8.45	132.29	120.29	6	15
1	A	117	PHE	CA-CB-CG	-8.43	105.37	113.80	19	6
1	A	72	HIS	CA-CB-CG	8.41	122.21	113.80	7	1
1	A	86	SER	N-CA-C	8.37	121.45	111.33	7	19
1	A	52	HIS	CA-C-N	8.23	131.31	120.28	19	14
1	A	52	HIS	C-N-CA	8.23	131.31	120.28	19	14
1	A	116	ASN	CA-CB-CG	8.10	120.70	112.60	1	6
1	A	63	LEU	N-CA-C	8.03	121.20	111.40	16	13
1	A	59	MET	CA-C-O	7.98	129.25	120.63	11	12
1	A	58	GLU	N-CA-C	7.96	120.86	111.71	16	13
1	A	121	ILE	O-C-N	-7.91	112.08	121.10	6	3
1	A	125	ILE	CA-CB-CG1	7.90	123.83	110.40	6	5
1	A	51	LYS	N-CA-C	7.88	122.57	113.19	20	6
1	A	85	PRO	CA-C-N	7.85	131.14	120.38	20	18
1	A	85	PRO	C-N-CA	7.85	131.14	120.38	20	18
1	A	120	GLU	CA-C-N	7.48	135.97	122.13	17	9
1	A	120	GLU	C-N-CA	7.48	135.97	122.13	17	9
1	A	69	ASP	CA-CB-CG	7.48	120.08	112.60	17	1
1	A	47	ILE	N-CA-CB	7.45	117.75	111.64	3	2
1	A	92	VAL	N-CA-CB	7.35	118.34	110.62	3	10
1	A	72	HIS	N-CA-C	7.31	121.50	112.58	7	2
1	A	131	PRO	N-CA-C	7.27	123.36	113.98	15	4
1	A	99	TYR	N-CA-CB	7.27	120.92	110.16	15	3
1	A	84	ILE	CA-C-N	7.24	127.41	120.31	6	7
1	A	84	ILE	C-N-CA	7.24	127.41	120.31	6	7
1	A	49	ASN	CA-CB-CG	7.19	119.79	112.60	14	1
1	A	57	THR	N-CA-C	7.16	118.73	111.07	13	12
1	A	94	LYS	CA-C-N	7.16	129.75	120.44	2	16
1	A	94	LYS	C-N-CA	7.16	129.75	120.44	2	16
1	A	48	THR	CA-C-N	7.14	135.18	121.54	13	2
1	A	48	THR	C-N-CA	7.14	135.18	121.54	13	2
1	A	99	TYR	CA-C-N	7.13	130.54	120.28	3	8
1	A	99	TYR	C-N-CA	7.13	130.54	120.28	3	8
1	A	130	ASN	O-C-N	-7.11	113.14	121.32	2	8
1	A	62	LEU	N-CA-CB	7.10	120.67	110.16	11	1
1	A	92	VAL	CA-C-N	7.10	130.66	120.79	11	7
1	A	92	VAL	C-N-CA	7.10	130.66	120.79	11	7
1	A	98	PHE	CA-C-N	7.07	130.05	120.44	5	4
1	A	98	PHE	C-N-CA	7.07	130.05	120.44	5	4
1	A	93	ALA	N-CA-C	7.03	118.94	111.28	18	7
1	A	121	ILE	CB-CA-C	7.00	124.11	111.36	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	133	ARG	N-CA-C	6.99	119.75	111.71	13	3
1	A	67	ALA	N-CA-C	6.97	118.95	111.36	6	6
1	A	71	CYS	N-CA-C	6.96	119.89	111.82	16	4
1	A	130	ASN	CA-CB-CG	-6.95	105.65	112.60	10	1
1	A	123	SER	CA-C-N	6.93	129.79	120.65	19	7
1	A	123	SER	C-N-CA	6.93	129.79	120.65	19	7
1	A	131	PRO	CA-C-N	6.93	134.77	121.54	17	9
1	A	131	PRO	C-N-CA	6.93	134.77	121.54	17	9
1	A	132	TYR	CA-C-N	6.90	134.72	121.54	19	3
1	A	132	TYR	C-N-CA	6.90	134.72	121.54	19	3
1	A	92	VAL	N-CA-C	6.89	117.39	110.23	14	9
1	A	101	THR	CA-C-N	6.88	134.68	121.54	14	1
1	A	101	THR	C-N-CA	6.88	134.68	121.54	14	1
1	A	74	PRO	CA-C-N	6.87	132.14	122.46	13	7
1	A	74	PRO	C-N-CA	6.87	132.14	122.46	13	7
1	A	57	THR	CA-C-N	6.84	129.77	120.54	10	3
1	A	57	THR	C-N-CA	6.84	129.77	120.54	10	3
1	A	121	ILE	N-CA-C	6.84	123.65	108.88	11	3
1	A	90	ILE	CA-C-N	6.83	129.32	120.44	6	4
1	A	90	ILE	C-N-CA	6.83	129.32	120.44	6	4
1	A	116	ASN	N-CA-C	6.82	121.06	112.87	7	3
1	A	125	ILE	CA-C-N	6.81	130.33	120.38	1	13
1	A	125	ILE	C-N-CA	6.81	130.33	120.38	1	13
1	A	68	LYS	CA-C-N	6.78	131.44	120.60	15	5
1	A	68	LYS	C-N-CA	6.78	131.44	120.60	15	5
1	A	81	ASN	CA-C-N	6.62	132.37	121.39	16	5
1	A	81	ASN	C-N-CA	6.62	132.37	121.39	16	5
1	A	43	ARG	CA-C-N	6.61	130.36	120.31	16	7
1	A	43	ARG	C-N-CA	6.61	130.36	120.31	16	7
1	A	132	TYR	CA-CB-CG	6.61	125.80	113.90	19	1
1	A	95	ALA	CB-CA-C	-6.61	100.51	110.88	15	1
1	A	98	PHE	CB-CA-C	-6.60	100.72	110.95	10	2
1	A	71	CYS	CA-C-N	6.57	131.45	122.19	3	2
1	A	71	CYS	C-N-CA	6.57	131.45	122.19	3	2
1	A	121	ILE	CA-C-N	6.56	126.59	119.90	2	5
1	A	121	ILE	C-N-CA	6.56	126.59	119.90	2	5
1	A	75	PHE	CA-C-N	6.56	132.51	122.68	3	6
1	A	75	PHE	C-N-CA	6.56	132.51	122.68	3	6
1	A	128	LYS	CA-C-N	6.55	129.06	120.28	1	7
1	A	128	LYS	C-N-CA	6.55	129.06	120.28	1	7
1	A	130	ASN	N-CA-C	6.51	124.20	109.81	1	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	72	HIS	N-CA-CB	6.45	121.39	110.49	14	3
1	A	62	LEU	CA-C-N	6.40	128.76	120.44	15	2
1	A	62	LEU	C-N-CA	6.40	128.76	120.44	15	2
1	A	91	PHE	CA-C-N	6.40	129.16	120.77	18	4
1	A	91	PHE	C-N-CA	6.40	129.16	120.77	18	4
1	A	64	VAL	N-CA-CB	6.36	120.12	110.58	9	4
1	A	78	LYS	N-CA-C	6.36	120.61	112.34	11	9
1	A	65	GLU	CB-CA-C	6.35	123.33	110.38	2	6
1	A	56	LEU	CB-CA-C	6.34	120.93	110.90	12	3
1	A	102	ASN	N-CA-CB	6.33	121.19	110.49	12	3
1	A	60	VAL	CA-C-N	6.31	127.73	119.84	4	7
1	A	60	VAL	C-N-CA	6.31	127.73	119.84	4	7
1	A	70	GLU	N-CA-CB	-6.29	100.54	110.22	9	4
1	A	49	ASN	N-CA-CB	6.29	121.11	110.49	4	12
1	A	43	ARG	N-CA-C	6.29	119.80	111.75	13	1
1	A	84	ILE	N-CA-C	6.19	114.28	108.15	2	1
1	A	90	ILE	CA-CB-CG1	6.08	120.73	110.40	5	2
1	A	120	GLU	N-CA-C	6.08	113.76	108.78	16	1
1	A	57	THR	N-CA-CB	6.04	119.53	110.22	8	2
1	A	121	ILE	CA-CB-CG1	6.03	120.66	110.40	20	1
1	A	59	MET	CG-SD-CE	-6.02	87.66	100.90	19	1
1	A	77	ASP	CA-C-N	6.01	130.30	120.63	19	5
1	A	77	ASP	C-N-CA	6.01	130.30	120.63	19	5
1	A	102	ASN	CA-C-N	5.97	132.95	121.54	16	2
1	A	102	ASN	C-N-CA	5.97	132.95	121.54	16	2
1	A	70	GLU	N-CA-C	5.92	117.40	111.07	7	1
1	A	79	ASP	CA-C-N	5.91	129.65	121.26	1	16
1	A	79	ASP	C-N-CA	5.91	129.65	121.26	1	16
1	A	54	GLU	CA-C-N	5.88	128.09	120.44	19	3
1	A	54	GLU	C-N-CA	5.88	128.09	120.44	19	3
1	A	73	ASN	CB-CA-C	5.88	117.32	108.86	15	2
1	A	70	GLU	CA-C-N	5.87	129.23	120.31	19	1
1	A	70	GLU	C-N-CA	5.87	129.23	120.31	19	1
1	A	86	SER	CA-C-N	5.86	126.44	120.00	15	1
1	A	86	SER	C-N-CA	5.86	126.44	120.00	15	1
1	A	122	PRO	N-CA-C	5.85	120.04	111.03	1	4
1	A	65	GLU	N-CA-CB	5.84	118.90	110.20	12	5
1	A	126	LEU	CA-C-N	5.81	130.43	120.72	18	2
1	A	126	LEU	C-N-CA	5.81	130.43	120.72	18	2
1	A	94	LYS	N-CA-CB	5.77	118.80	110.20	17	2
1	A	74	PRO	CA-C-O	-5.75	116.95	121.38	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	79	ASP	N-CA-CB	5.74	120.46	110.98	18	1
1	A	123	SER	N-CA-C	5.73	118.27	111.33	11	3
1	A	53	ASP	CA-CB-CG	5.73	118.33	112.60	3	1
1	A	70	GLU	CA-CB-CG	5.70	125.51	114.10	10	2
1	A	130	ASN	CA-C-O	-5.69	112.36	120.16	7	5
1	A	73	ASN	N-CA-C	5.69	114.68	108.14	19	1
1	A	73	ASN	O-C-N	-5.58	114.79	121.31	3	1
1	A	52	HIS	N-CA-C	5.57	117.57	110.61	1	1
1	A	46	SER	CA-C-N	5.55	131.96	121.97	14	1
1	A	46	SER	C-N-CA	5.55	131.96	121.97	14	1
1	A	42	LYS	N-CA-CB	5.48	118.77	110.28	19	1
1	A	68	LYS	N-CA-C	5.44	119.64	112.89	3	1
1	A	101	THR	N-CA-C	5.43	117.28	111.36	3	1
1	A	100	MET	CG-SD-CE	-5.42	88.97	100.90	15	1
1	A	133	ARG	N-CA-CB	5.39	119.60	110.49	8	1
1	A	96	ALA	CA-C-N	5.39	128.04	120.28	14	1
1	A	96	ALA	C-N-CA	5.39	128.04	120.28	14	1
1	A	47	ILE	CA-C-N	5.38	131.82	121.54	13	2
1	A	47	ILE	C-N-CA	5.38	131.82	121.54	13	2
1	A	121	ILE	CA-C-O	-5.38	112.75	119.95	6	1
1	A	124	THR	CA-C-N	5.36	129.09	120.30	8	1
1	A	124	THR	C-N-CA	5.36	129.09	120.30	8	1
1	A	91	PHE	CA-CB-CG	5.34	119.14	113.80	2	1
1	A	101	THR	N-CA-CB	5.32	117.78	110.07	6	1
1	A	66	PHE	N-CA-CB	5.29	117.69	110.01	8	1
1	A	94	LYS	N-CA-C	5.25	117.08	111.36	10	1
1	A	75	PHE	N-CA-C	5.22	118.54	111.17	2	2
1	A	87	GLY	CA-C-N	5.22	128.72	120.47	6	1
1	A	87	GLY	C-N-CA	5.22	128.72	120.47	6	1
1	A	56	LEU	N-CA-CB	5.20	117.61	110.07	18	1
1	A	60	VAL	CB-CA-C	5.18	120.79	111.36	20	6
1	A	68	LYS	CB-CA-C	5.18	120.81	109.99	1	1
1	A	116	ASN	N-CA-CB	-5.16	101.76	110.49	11	1
1	A	55	TYR	N-CA-C	5.16	116.71	111.14	14	1
1	A	96	ALA	N-CA-CB	-5.12	102.56	110.20	12	1
1	A	97	GLN	CA-C-N	5.11	127.39	120.44	6	1
1	A	97	GLN	C-N-CA	5.11	127.39	120.44	6	1
1	A	125	ILE	N-CA-CB	5.10	120.00	110.77	6	1
1	A	100	MET	N-CA-CB	5.08	118.15	110.28	14	1
1	A	68	LYS	N-CA-CB	5.06	118.65	110.40	3	1
1	A	120	GLU	N-CA-CB	5.05	115.17	108.96	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	61	PRO	N-CA-CB	5.04	108.55	103.25	5	1
1	A	127	LYS	CA-C-N	5.04	131.41	121.58	10	1
1	A	127	LYS	C-N-CA	5.04	131.41	121.58	10	1
1	A	52	HIS	N-CA-CB	-5.04	104.60	111.65	7	1
1	A	56	LEU	N-CA-C	5.03	116.57	111.14	10	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	75	PHE	Sidechain	17
1	A	132	TYR	Sidechain	15
1	A	99	TYR	Sidechain	8
1	A	117	PHE	Sidechain	2
1	A	55	TYR	Sidechain	2

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	636	637	637	4±2
All	All	12720	12740	12740	74

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:ILE:HG22	1:A:122:PRO:HD2	0.67	1.65	19	1
1:A:121:ILE:HG22	1:A:122:PRO:CD	0.63	2.22	19	1
1:A:88:VAL:O	1:A:92:VAL:HG13	0.59	1.97	11	2
1:A:88:VAL:O	1:A:92:VAL:HG23	0.53	2.02	4	1
1:A:57:THR:HG22	1:A:92:VAL:HG12	0.53	1.81	18	1
1:A:56:LEU:HD13	1:A:57:THR:H	0.52	1.63	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:HD22	1:A:121:ILE:HD12	0.51	1.82	17	1
1:A:56:LEU:HD21	1:A:93:ALA:HA	0.51	1.82	13	2
1:A:47:ILE:HG23	1:A:48:THR:H	0.51	1.65	9	1
1:A:132:TYR:CG	1:A:133:ARG:N	0.51	2.78	14	2
1:A:60:VAL:CG1	1:A:92:VAL:HG12	0.50	2.36	11	2
1:A:60:VAL:HG13	1:A:63:LEU:HD23	0.50	1.81	4	1
1:A:88:VAL:HG11	1:A:132:TYR:CG	0.50	2.42	19	1
1:A:121:ILE:HD13	1:A:121:ILE:H	0.49	1.67	9	1
1:A:121:ILE:HB	1:A:122:PRO:HD2	0.49	1.83	20	6
1:A:56:LEU:HB2	1:A:96:ALA:HB1	0.49	1.83	12	2
1:A:89:LEU:HA	1:A:92:VAL:HG22	0.49	1.83	1	1
1:A:125:ILE:HD12	1:A:125:ILE:H	0.48	1.68	2	1
1:A:60:VAL:HG11	1:A:92:VAL:HA	0.48	1.84	16	1
1:A:64:VAL:HG12	1:A:91:PHE:CE2	0.48	2.43	7	1
1:A:56:LEU:HD23	1:A:57:THR:HG23	0.48	1.86	17	2
1:A:60:VAL:HG13	1:A:61:PRO:HD3	0.48	1.85	15	1
1:A:60:VAL:HG11	1:A:92:VAL:HG12	0.48	1.86	11	1
1:A:68:LYS:HG2	1:A:132:TYR:CE2	0.47	2.45	20	1
1:A:56:LEU:O	1:A:60:VAL:HG12	0.47	2.10	15	1
1:A:60:VAL:HB	1:A:92:VAL:HG12	0.46	1.86	8	1
1:A:63:LEU:HD22	1:A:117:PHE:CB	0.46	2.41	16	1
1:A:68:LYS:HD3	1:A:132:TYR:CE2	0.46	2.46	7	1
1:A:57:THR:HG22	1:A:92:VAL:HG23	0.45	1.88	3	2
1:A:62:LEU:HD12	1:A:117:PHE:CE2	0.45	2.46	11	1
1:A:60:VAL:HG21	1:A:92:VAL:HA	0.45	1.89	11	1
1:A:99:TYR:CE1	1:A:121:ILE:HG23	0.44	2.47	19	1
1:A:52:HIS:CE1	1:A:55:TYR:CD2	0.44	3.05	5	1
1:A:60:VAL:HG21	1:A:92:VAL:O	0.44	2.12	8	1
1:A:122:PRO:HG2	1:A:125:ILE:HD11	0.44	1.89	8	2
1:A:99:TYR:CD1	1:A:121:ILE:HG23	0.44	2.47	19	1
1:A:99:TYR:CE1	1:A:120:GLU:HB2	0.44	2.47	17	1
1:A:117:PHE:CD1	1:A:117:PHE:N	0.43	2.85	9	1
1:A:63:LEU:HD22	1:A:121:ILE:HB	0.43	1.89	2	1
1:A:59:MET:HE3	1:A:99:TYR:CE2	0.43	2.47	20	1
1:A:64:VAL:HG21	1:A:88:VAL:HG13	0.43	1.91	2	1
1:A:59:MET:HB3	1:A:117:PHE:CZ	0.43	2.49	8	1
1:A:121:ILE:H	1:A:121:ILE:CD1	0.42	2.26	9	1
1:A:59:MET:HE2	1:A:117:PHE:CD1	0.42	2.49	12	1
1:A:68:LYS:HG2	1:A:132:TYR:CD2	0.42	2.50	13	1
1:A:64:VAL:O	1:A:68:LYS:HB2	0.42	2.15	17	1
1:A:88:VAL:HG21	1:A:132:TYR:HA	0.42	1.91	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:TYR:CD2	1:A:133:ARG:N	0.42	2.88	12	1
1:A:99:TYR:CE1	1:A:121:ILE:CG2	0.41	3.03	15	1
1:A:91:PHE:CD2	1:A:129:LEU:HB2	0.41	2.50	6	1
1:A:63:LEU:HD22	1:A:117:PHE:HB3	0.41	1.92	16	1
1:A:60:VAL:CG1	1:A:92:VAL:HG22	0.41	2.45	18	1
1:A:94:LYS:HA	1:A:97:GLN:HG2	0.41	1.91	13	3
1:A:47:ILE:HG22	1:A:52:HIS:HB3	0.41	1.93	14	1
1:A:129:LEU:O	1:A:132:TYR:CD2	0.41	2.73	17	1
1:A:52:HIS:CE1	1:A:100:MET:SD	0.41	3.13	2	1
1:A:59:MET:HE2	1:A:117:PHE:CE1	0.40	2.50	19	1
1:A:91:PHE:CE2	1:A:129:LEU:HD23	0.40	2.51	12	1
1:A:60:VAL:HG12	1:A:64:VAL:HG23	0.40	1.93	14	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	79/99 (80%)	67±2 (85±2%)	7±2 (8±2%)	5±2 (7±2%)	2	17
All	All	1580/1980 (80%)	1342 (85%)	132 (8%)	106 (7%)	2	17

All 20 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	49	ASN	18
1	A	72	HIS	14
1	A	132	TYR	13
1	A	50	ASP	12
1	A	121	ILE	11
1	A	116	ASN	6
1	A	102	ASN	6
1	A	78	LYS	4
1	A	133	ARG	4
1	A	123	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	75	PHE	3
1	A	47	ILE	2
1	A	51	LYS	2
1	A	131	PRO	2
1	A	71	CYS	1
1	A	48	THR	1
1	A	52	HIS	1
1	A	117	PHE	1
1	A	120	GLU	1
1	A	82	GLU	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	72/88 (82%)	57±3 (79±4%)	15±3 (21±4%)	3	31
All	All	1440/1760 (82%)	1132 (79%)	308 (21%)	3	31

All 53 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	56	LEU	20
1	A	45	LEU	18
1	A	66	PHE	18
1	A	125	ILE	17
1	A	73	ASN	16
1	A	60	VAL	15
1	A	121	ILE	14
1	A	116	ASN	13
1	A	129	LEU	13
1	A	90	ILE	12
1	A	88	VAL	12
1	A	68	LYS	11
1	A	132	TYR	11
1	A	47	ILE	10
1	A	102	ASN	9

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Mol	Chain	Res	Type	Models (Total)
1	A	126	LEU	8
1	A	64	VAL	7
1	A	42	LYS	6
1	A	52	HIS	6
1	A	97	GLN	6
1	A	100	MET	6
1	A	57	THR	5
1	A	89	LEU	4
1	A	70	GLU	4
1	A	71	CYS	3
1	A	84	ILE	3
1	A	48	THR	3
1	A	133	ARG	3
1	A	94	LYS	3
1	A	117	PHE	3
1	A	101	THR	2
1	A	63	LEU	2
1	A	124	THR	2
1	A	83	SER	2
1	A	59	MET	2
1	A	127	LYS	2
1	A	130	ASN	1
1	A	72	HIS	1
1	A	51	LYS	1
1	A	58	GLU	1
1	A	92	VAL	1
1	A	49	ASN	1
1	A	78	LYS	1
1	A	120	GLU	1
1	A	123	SER	1
1	A	82	GLU	1
1	A	65	GLU	1
1	A	75	PHE	1
1	A	76	ILE	1
1	A	98	PHE	1
1	A	128	LYS	1
1	A	62	LEU	1
1	A	81	ASN	1

6.3.3 RNA ⓘ

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

No chemical shift data were provided