



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 02:30 AM UTC

PDB ID : 1EWS / pdb_00001ews
Title : THE THREE-DIMENSIONAL SOLUTION STRUCTURE OF THE RABBIT
KIDNEY DEFENSIN, RK-1
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Deposited on : 2000-04-26

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

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<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

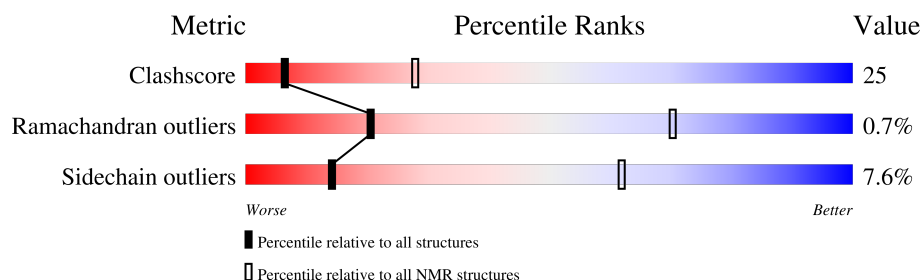
1 Overall quality at a glance

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	32	

2 Ensemble composition and analysis

This entry contains 20 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 9 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:4-A:30 (27)	0.38	20

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 494 atoms, of which 240 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RK-1 DEFENSIN.

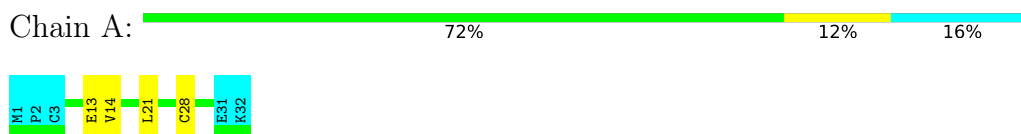
Mol	Chain	Residues	Atoms						Trace
1	A	32	Total	C	H	N	O	S	0
			494	159	240	41	47	7	

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: RK-1 DEFENSIN



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

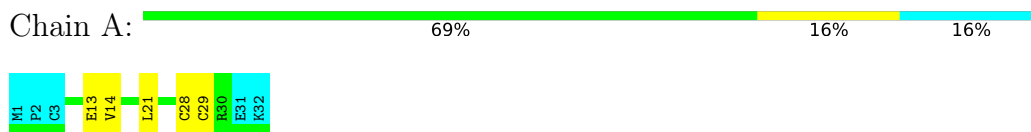
4.2.1 Score per residue for model 1

- Molecule 1: RK-1 DEFENSIN



4.2.2 Score per residue for model 2

- Molecule 1: RK-1 DEFENSIN



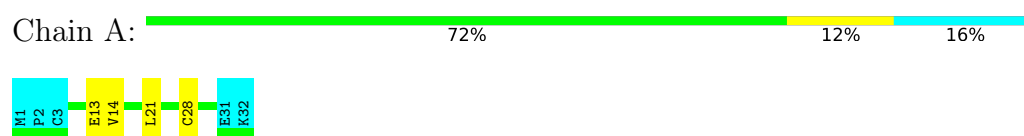
4.2.3 Score per residue for model 3

- Molecule 1: RK-1 DEFENSIN



4.2.4 Score per residue for model 4

- Molecule 1: RK-1 DEFENSIN



4.2.5 Score per residue for model 5

- Molecule 1: RK-1 DEFENSIN



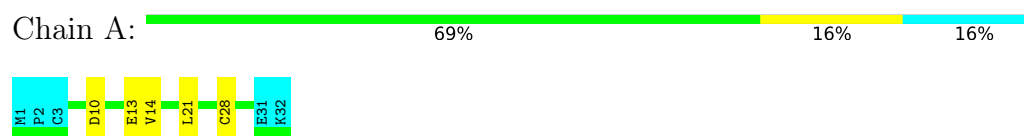
4.2.6 Score per residue for model 6

- Molecule 1: RK-1 DEFENSIN



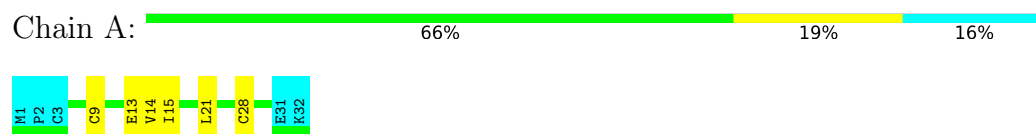
4.2.7 Score per residue for model 7

- Molecule 1: RK-1 DEFENSIN



4.2.8 Score per residue for model 8

- Molecule 1: RK-1 DEFENSIN



4.2.9 Score per residue for model 9

- Molecule 1: RK-1 DEFENSIN



4.2.10 Score per residue for model 10

- Molecule 1: RK-1 DEFENSIN



4.2.11 Score per residue for model 11

- Molecule 1: RK-1 DEFENSIN



4.2.12 Score per residue for model 12

- Molecule 1: RK-1 DEFENSIN



4.2.13 Score per residue for model 13

- Molecule 1: RK-1 DEFENSIN



4.2.14 Score per residue for model 14

- Molecule 1: RK-1 DEFENSIN



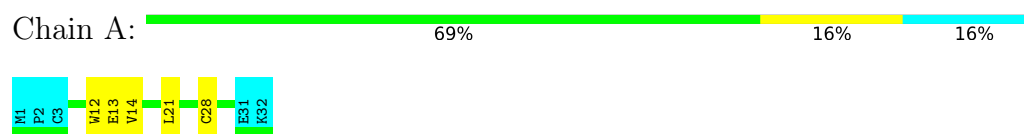
4.2.15 Score per residue for model 15

- Molecule 1: RK-1 DEFENSIN



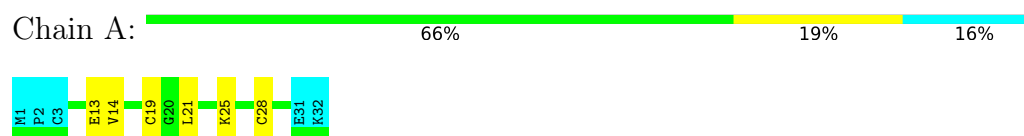
4.2.16 Score per residue for model 16

- Molecule 1: RK-1 DEFENSIN



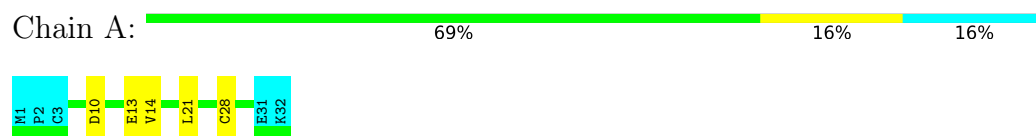
4.2.17 Score per residue for model 17

- Molecule 1: RK-1 DEFENSIN



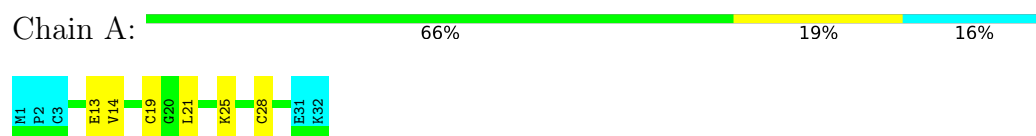
4.2.18 Score per residue for model 18

- Molecule 1: RK-1 DEFENSIN



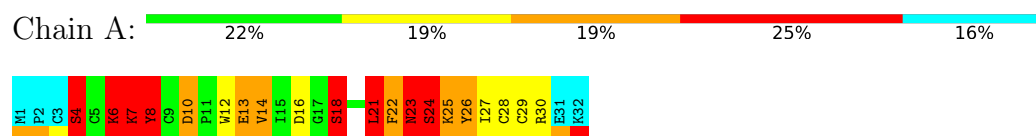
4.2.19 Score per residue for model 19

- Molecule 1: RK-1 DEFENSIN



4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: RK-1 DEFENSIN



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.1
X-PLOR	refinement	3.1

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	2.46±3.70	4±14/220 (1.7± 6.4%)	1.83±2.32	3±14/296 (1.1± 4.7%)
All	All	4.44	75/4400 (1.7%)	2.96	67/5920 (1.1%)

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	30	ARG	CZ-NH2	-76.65	0.33	1.33	20	1
1	A	30	ARG	CD-NE	-74.33	0.42	1.46	20	1
1	A	30	ARG	CZ-NH1	-72.67	0.31	1.32	20	1
1	A	30	ARG	NE-CZ	-69.77	0.56	1.33	20	1
1	A	8	TYR	CG-CD1	-61.71	0.09	1.39	20	1
1	A	8	TYR	CE2-CZ	-53.57	0.09	1.38	20	1
1	A	24	SER	CB-OG	-53.31	0.35	1.42	20	1
1	A	16	ASP	CG-OD2	-49.50	0.31	1.25	20	1
1	A	23	ASN	CG-OD1	-48.76	0.30	1.23	20	1
1	A	4	SER	CB-OG	-47.89	0.46	1.42	20	1
1	A	13	GLU	CD-OE1	-45.84	0.38	1.25	20	1
1	A	16	ASP	CG-OD1	-41.25	0.47	1.25	20	1
1	A	22	PHE	CG-CD1	-40.14	0.54	1.38	20	1
1	A	8	TYR	CG-CD2	-38.63	0.58	1.39	20	1
1	A	8	TYR	CB-CG	-38.32	0.67	1.51	20	1
1	A	22	PHE	CG-CD2	-37.27	0.60	1.38	20	1
1	A	8	TYR	CZ-OH	-36.95	0.60	1.38	20	1
1	A	10	ASP	CG-OD1	-35.80	0.57	1.25	20	1
1	A	10	ASP	CG-OD2	-35.43	0.58	1.25	20	1
1	A	6	LYS	CE-NZ	-34.52	0.45	1.49	20	1
1	A	8	TYR	CE1-CZ	-33.43	0.58	1.38	20	1
1	A	30	ARG	C-O	-33.42	0.83	1.23	20	1
1	A	30	ARG	C-N	-32.66	0.91	1.33	20	1
1	A	7	LYS	CE-NZ	-32.45	0.52	1.49	20	1
1	A	18	SER	CB-OG	-31.77	0.78	1.42	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	30	ARG	CB-CG	-31.41	0.58	1.52	20	1
1	A	26	TYR	CG-CD2	-31.31	0.73	1.39	20	1
1	A	13	GLU	CD-OE2	-31.16	0.66	1.25	20	1
1	A	26	TYR	CG-CD1	-29.79	0.76	1.39	20	1
1	A	23	ASN	CG-ND2	-29.18	0.71	1.33	20	1
1	A	7	LYS	CG-CD	-28.79	0.66	1.52	20	1
1	A	22	PHE	CE2-CZ	-28.32	0.53	1.38	20	1
1	A	26	TYR	CE1-CZ	-27.03	0.73	1.38	20	1
1	A	22	PHE	CE1-CZ	-26.29	0.59	1.38	20	1
1	A	14	VAL	CB-CG2	-26.13	0.66	1.52	20	1
1	A	8	TYR	CD1-CE1	-26.05	0.60	1.38	20	1
1	A	8	TYR	CD2-CE2	-26.05	0.60	1.38	20	1
1	A	26	TYR	CE2-CZ	-25.68	0.76	1.38	20	1
1	A	6	LYS	CD-CE	-25.50	0.76	1.52	20	1
1	A	23	ASN	CB-CG	-24.45	0.91	1.52	20	1
1	A	25	LYS	CD-CE	-22.82	0.83	1.52	20	1
1	A	6	LYS	CG-CD	-22.79	0.84	1.52	20	1
1	A	7	LYS	CD-CE	-22.04	0.86	1.52	20	1
1	A	7	LYS	CB-CG	-21.27	0.88	1.52	20	1
1	A	25	LYS	CE-NZ	-21.23	0.85	1.49	20	1
1	A	21	LEU	CG-CD1	-20.58	0.84	1.52	20	1
1	A	14	VAL	CB-CG1	-18.66	0.91	1.52	20	1
1	A	21	LEU	CG-CD2	-17.71	0.94	1.52	20	1
1	A	16	ASP	CB-CG	-17.71	1.07	1.52	20	1
1	A	13	GLU	CG-CD	-13.55	1.18	1.52	20	1
1	A	29	CYS	CB-SG	-13.46	1.36	1.81	20	1
1	A	22	PHE	CB-CG	-12.55	1.21	1.50	20	1
1	A	30	ARG	CG-CD	-12.50	1.15	1.52	20	1
1	A	12	TRP	NE1-CE2	-11.12	1.25	1.37	20	8
1	A	8	TYR	C-O	-9.82	1.11	1.23	20	1
1	A	22	PHE	CD1-CE1	-9.78	1.09	1.38	20	1
1	A	22	PHE	CD2-CE2	-9.77	1.09	1.38	20	1
1	A	25	LYS	CG-CD	-8.28	1.27	1.52	20	1
1	A	12	TRP	CG-CD2	-7.63	1.30	1.43	20	1
1	A	16	ASP	C-O	-7.36	1.16	1.24	20	1
1	A	18	SER	C-O	-6.80	1.15	1.23	20	1
1	A	8	TYR	C-N	-6.74	1.23	1.33	20	1
1	A	10	ASP	N-CA	6.10	1.50	1.46	18	2
1	A	12	TRP	CD1-NE1	-6.08	1.25	1.37	20	1
1	A	27	ILE	CG1-CD1	-6.04	1.28	1.51	20	1
1	A	18	SER	C-N	-5.88	1.26	1.33	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	8	TYR	N-CA	5.14	1.49	1.46	5	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	22	PHE	CD1-CG-CD2	-60.28	28.18	118.60	20	1
1	A	22	PHE	CE1-CZ-CE2	-50.75	28.66	120.00	20	1
1	A	26	TYR	CD1-CG-CD2	-50.64	42.13	118.10	20	1
1	A	21	LEU	CD1-CG-CD2	-47.03	7.34	110.80	20	1
1	A	30	ARG	NH1-CZ-NH2	-44.05	62.03	119.30	20	1
1	A	16	ASP	OD1-CG-OD2	-41.85	22.45	122.90	20	1
1	A	26	TYR	CE1-CZ-CE2	-39.06	42.18	120.30	20	1
1	A	10	ASP	OD1-CG-OD2	-34.68	39.66	122.90	20	1
1	A	30	ARG	NE-CZ-NH2	34.29	150.06	119.20	20	1
1	A	8	TYR	CB-CG-CD2	34.12	171.99	120.80	20	1
1	A	8	TYR	CG-CD2-CE2	33.56	171.54	121.20	20	1
1	A	23	ASN	OD1-CG-ND2	-32.25	90.35	122.60	20	1
1	A	8	TYR	CD1-CG-CD2	-30.57	72.24	118.10	20	1
1	A	8	TYR	CD1-CE1-CZ	28.84	171.51	119.60	20	1
1	A	22	PHE	CB-CG-CD2	27.11	166.79	120.70	20	1
1	A	22	PHE	CG-CD2-CE2	27.05	166.69	120.70	20	1
1	A	30	ARG	NE-CZ-NH1	26.41	147.91	121.50	20	1
1	A	22	PHE	CG-CD1-CE1	26.15	165.15	120.70	20	1
1	A	22	PHE	CB-CG-CD1	26.07	165.02	120.70	20	1
1	A	6	LYS	CG-CD-CE	25.80	170.65	111.30	20	1
1	A	22	PHE	CD1-CE1-CZ	25.77	166.38	120.00	20	1
1	A	26	TYR	CB-CG-CD1	25.63	159.24	120.80	20	1
1	A	23	ASN	CB-CG-ND2	25.52	154.68	116.40	20	1
1	A	26	TYR	CG-CD1-CE1	25.51	159.46	121.20	20	1
1	A	26	TYR	CB-CG-CD2	25.22	158.62	120.80	20	1
1	A	22	PHE	CZ-CE2-CD2	24.97	164.94	120.00	20	1
1	A	26	TYR	CG-CD2-CE2	24.78	158.37	121.20	20	1
1	A	8	TYR	CE1-CZ-CE2	-23.39	73.51	120.30	20	1
1	A	16	ASP	CB-CG-OD1	22.87	170.99	118.40	20	1
1	A	26	TYR	CZ-CE2-CD2	22.12	159.42	119.60	20	1
1	A	30	ARG	CB-CG-CD	21.98	161.86	111.30	20	1
1	A	30	ARG	CG-CD-NE	21.82	160.01	112.00	20	1
1	A	26	TYR	CD1-CE1-CZ	21.57	158.44	119.60	20	1
1	A	30	ARG	CD-NE-CZ	21.05	153.87	124.40	20	1
1	A	24	SER	CA-CB-OG	21.01	153.12	111.10	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	16	ASP	CB-CG-OD2	20.94	166.56	118.40	20	1
1	A	13	GLU	OE1-CD-OE2	-20.40	73.94	122.90	20	1
1	A	14	VAL	CA-CB-CG2	19.69	143.88	110.40	20	1
1	A	30	ARG	CA-CB-CG	19.68	153.46	114.10	20	1
1	A	10	ASP	CB-CG-OD1	18.22	160.31	118.40	20	1
1	A	10	ASP	CB-CG-OD2	18.10	160.02	118.40	20	1
1	A	30	ARG	O-C-N	-17.32	98.92	122.48	20	1
1	A	8	TYR	CE1-CZ-OH	17.23	171.59	119.90	20	1
1	A	13	GLU	CG-CD-OE2	15.65	154.41	118.40	20	1
1	A	4	SER	CA-CB-OG	14.80	140.69	111.10	20	1
1	A	14	VAL	CG1-CB-CG2	-13.85	80.33	110.80	20	1
1	A	8	TYR	CA-CB-CG	13.74	138.63	113.90	20	1
1	A	7	LYS	CB-CG-CD	13.69	142.79	111.30	20	1
1	A	26	TYR	OH-CZ-CE2	13.20	159.51	119.90	20	1
1	A	23	ASN	CA-CB-CG	13.13	125.73	112.60	20	1
1	A	25	LYS	CG-CD-CE	13.12	141.48	111.30	20	1
1	A	7	LYS	CG-CD-CE	12.97	141.12	111.30	20	1
1	A	26	TYR	CE1-CZ-OH	12.80	158.31	119.90	20	1
1	A	7	LYS	CA-CB-CG	12.05	138.20	114.10	20	1
1	A	14	VAL	CA-CB-CG1	11.62	130.16	110.40	20	1
1	A	25	LYS	CD-CE-NZ	11.30	148.07	111.90	20	1
1	A	30	ARG	CA-C-O	9.44	131.87	121.02	20	1
1	A	16	ASP	CA-CB-CG	8.72	121.32	112.60	20	1
1	A	6	LYS	CB-CG-CD	8.34	130.47	111.30	20	1
1	A	30	ARG	CA-C-N	7.58	133.53	122.16	20	1
1	A	30	ARG	C-N-CA	7.58	133.53	122.16	20	1
1	A	21	LEU	CB-CG-CD1	6.42	129.96	110.70	20	1
1	A	13	GLU	CG-CD-OE1	5.76	131.64	118.40	20	1
1	A	29	CYS	CA-CB-SG	5.71	127.53	114.40	20	1
1	A	22	PHE	CA-CB-CG	-5.02	108.78	113.80	6	1
1	A	8	TYR	N-CA-CB	-5.02	106.92	111.59	5	1
1	A	11	PRO	N-CA-C	-5.01	107.87	114.03	12	1

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	A	214	199	198	10±29
All	All	4280	3980	3979	209

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:TYR:CZ	1:A:26:TYR:CD1	1.42	2.07	20	1
1:A:26:TYR:CG	1:A:26:TYR:CE2	1.42	2.07	20	1
1:A:26:TYR:CG	1:A:26:TYR:CE1	1.39	2.10	20	1
1:A:25:LYS:CE	1:A:25:LYS:CG	1.38	1.99	20	1
1:A:26:TYR:CZ	1:A:26:TYR:CD2	1.38	2.10	20	1
1:A:8:TYR:CD1	1:A:8:TYR:CA	1.33	2.08	20	1
1:A:8:TYR:CA	1:A:8:TYR:CG	1.33	2.09	20	1
1:A:13:GLU:OE2	1:A:13:GLU:CG	1.30	1.79	20	1
1:A:14:VAL:CG2	1:A:14:VAL:CA	1.28	2.11	20	1
1:A:21:LEU:CD2	1:A:21:LEU:CB	1.22	2.18	20	1
1:A:21:LEU:CB	1:A:21:LEU:CD1	1.22	2.16	20	1
1:A:24:SER:OG	1:A:24:SER:CA	1.22	1.85	20	1
1:A:26:TYR:CD2	1:A:26:TYR:CB	1.21	2.23	20	1
1:A:6:LYS:CD	1:A:6:LYS:CB	1.20	2.18	20	1
1:A:4:SER:OG	1:A:4:SER:CA	1.20	1.89	20	1
1:A:8:TYR:CA	1:A:8:TYR:HD1	1.18	1.41	20	1
1:A:26:TYR:CD1	1:A:26:TYR:CB	1.14	2.26	20	1
1:A:23:ASN:CG	1:A:23:ASN:CA	1.14	2.20	20	1
1:A:7:LYS:CG	1:A:7:LYS:CA	1.13	2.26	20	1
1:A:14:VAL:CA	1:A:14:VAL:CG1	1.12	2.24	20	1
1:A:21:LEU:CD1	1:A:21:LEU:HG	1.11	1.74	20	1
1:A:18:SER:OG	1:A:18:SER:CA	1.09	1.99	20	1
1:A:18:SER:OG	1:A:18:SER:CB	1.08	0.78	20	1
1:A:26:TYR:CE1	1:A:26:TYR:OH	1.07	2.07	20	1
1:A:18:SER:OG	1:A:18:SER:HB3	1.05	1.43	20	1
1:A:18:SER:OG	1:A:18:SER:HB2	1.03	1.43	20	1
1:A:10:ASP:OD1	1:A:10:ASP:CB	1.02	2.07	20	1
1:A:21:LEU:CG	1:A:21:LEU:HD23	1.01	1.56	20	1
1:A:21:LEU:CD2	1:A:21:LEU:HG	1.01	1.86	20	1
1:A:10:ASP:CB	1:A:10:ASP:OD2	1.01	2.07	20	1
1:A:23:ASN:CG	1:A:23:ASN:HB2	1.00	1.50	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:CG	1:A:21:LEU:HD22	1.00	1.56	20	1
1:A:21:LEU:CG	1:A:21:LEU:HD21	0.99	1.56	20	1
1:A:14:VAL:CB	1:A:14:VAL:HG13	0.99	1.53	20	1
1:A:23:ASN:CG	1:A:23:ASN:HB3	0.98	1.50	20	1
1:A:26:TYR:CE2	1:A:26:TYR:OH	0.98	2.10	20	1
1:A:14:VAL:CB	1:A:14:VAL:HG12	0.97	1.53	20	1
1:A:14:VAL:CB	1:A:14:VAL:HG11	0.97	1.53	20	1
1:A:23:ASN:CG	1:A:23:ASN:CB	0.95	0.90	20	1
1:A:21:LEU:CG	1:A:21:LEU:HD11	0.94	1.48	20	1
1:A:21:LEU:CD2	1:A:21:LEU:CG	0.93	0.94	20	1
1:A:4:SER:OG	1:A:4:SER:HB3	0.92	1.15	20	1
1:A:4:SER:OG	1:A:4:SER:HB2	0.91	1.15	20	1
1:A:21:LEU:CG	1:A:21:LEU:HD12	0.90	1.48	20	1
1:A:14:VAL:CG2	1:A:14:VAL:HB	0.90	1.44	20	1
1:A:14:VAL:CG1	1:A:14:VAL:CB	0.90	0.91	20	1
1:A:6:LYS:CD	1:A:6:LYS:HG2	0.90	1.43	20	1
1:A:7:LYS:CG	1:A:7:LYS:HB3	0.90	1.44	20	1
1:A:21:LEU:CG	1:A:21:LEU:HD13	0.89	1.48	20	1
1:A:7:LYS:CG	1:A:7:LYS:HB2	0.89	1.44	20	1
1:A:6:LYS:CD	1:A:6:LYS:HG3	0.88	1.43	20	1
1:A:7:LYS:CG	1:A:7:LYS:CB	0.88	0.88	20	1
1:A:13:GLU:OE2	1:A:13:GLU:CD	0.87	0.66	20	1
1:A:25:LYS:CE	1:A:25:LYS:HD3	0.87	1.40	20	1
1:A:25:LYS:CE	1:A:25:LYS:HD2	0.86	1.40	20	1
1:A:21:LEU:CD1	1:A:21:LEU:CG	0.84	0.84	20	1
1:A:24:SER:OG	1:A:24:SER:HB2	0.84	1.08	20	1
1:A:7:LYS:NZ	1:A:7:LYS:HE3	0.83	1.22	20	1
1:A:24:SER:OG	1:A:24:SER:HB3	0.83	1.08	20	1
1:A:6:LYS:CD	1:A:6:LYS:CG	0.83	0.84	20	1
1:A:8:TYR:HD1	1:A:8:TYR:C	0.83	1.81	20	1
1:A:13:GLU:HG2	1:A:28:CYS:SG	0.83	2.14	20	11
1:A:25:LYS:CE	1:A:25:LYS:CD	0.83	0.84	20	1
1:A:10:ASP:OD2	1:A:10:ASP:CG	0.82	0.58	20	1
1:A:25:LYS:CD	1:A:25:LYS:HE2	0.81	1.38	20	1
1:A:10:ASP:OD1	1:A:10:ASP:CG	0.81	0.57	20	1
1:A:25:LYS:CD	1:A:25:LYS:HE3	0.80	1.38	20	1
1:A:7:LYS:NZ	1:A:7:LYS:HE2	0.80	1.22	20	1
1:A:14:VAL:CB	1:A:14:VAL:HG23	0.80	1.34	20	1
1:A:7:LYS:HE2	1:A:7:LYS:CD	0.79	1.47	20	1
1:A:25:LYS:HE2	1:A:25:LYS:NZ	0.79	1.39	20	1
1:A:14:VAL:CB	1:A:14:VAL:HG22	0.79	1.34	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LYS:HE3	1:A:25:LYS:NZ	0.78	1.39	20	1
1:A:6:LYS:CD	1:A:6:LYS:HE2	0.78	1.38	20	1
1:A:7:LYS:HE3	1:A:7:LYS:CD	0.77	1.47	20	1
1:A:6:LYS:NZ	1:A:6:LYS:HE3	0.77	1.18	20	1
1:A:14:VAL:CB	1:A:14:VAL:HG21	0.76	1.34	20	1
1:A:6:LYS:HG2	1:A:6:LYS:HD2	0.76	1.14	20	1
1:A:4:SER:OG	1:A:4:SER:CB	0.76	0.46	20	1
1:A:6:LYS:HE2	1:A:6:LYS:HD3	0.75	1.07	20	1
1:A:7:LYS:CG	1:A:7:LYS:HD3	0.73	1.27	20	1
1:A:6:LYS:CD	1:A:6:LYS:HE3	0.73	1.38	20	1
1:A:7:LYS:CB	1:A:7:LYS:HG2	0.73	1.43	20	1
1:A:7:LYS:CG	1:A:7:LYS:HD2	0.72	1.27	20	1
1:A:7:LYS:CD	1:A:7:LYS:HG2	0.72	1.27	20	1
1:A:25:LYS:CE	1:A:25:LYS:HZ3	0.72	1.42	20	1
1:A:23:ASN:CG	1:A:23:ASN:HD21	0.71	1.37	20	1
1:A:6:LYS:HE2	1:A:6:LYS:NZ	0.71	1.18	20	1
1:A:8:TYR:CG	1:A:8:TYR:HB2	0.71	1.29	20	1
1:A:26:TYR:CD1	1:A:26:TYR:CG	0.71	0.76	20	1
1:A:25:LYS:CE	1:A:25:LYS:HZ2	0.70	1.42	20	1
1:A:7:LYS:CD	1:A:7:LYS:HG3	0.70	1.27	20	1
1:A:25:LYS:CE	1:A:25:LYS:NZ	0.70	0.85	20	1
1:A:8:TYR:CG	1:A:8:TYR:HB3	0.70	1.29	20	1
1:A:23:ASN:CG	1:A:23:ASN:HD22	0.70	1.37	20	1
1:A:25:LYS:CE	1:A:25:LYS:HZ1	0.69	1.42	20	1
1:A:26:TYR:CZ	1:A:26:TYR:CE2	0.69	0.76	20	1
1:A:7:LYS:CB	1:A:7:LYS:HG3	0.67	1.43	20	1
1:A:26:TYR:CG	1:A:26:TYR:CD2	0.67	0.73	20	1
1:A:6:LYS:HG3	1:A:6:LYS:HD3	0.67	1.13	20	1
1:A:7:LYS:HD2	1:A:7:LYS:CE	0.66	1.42	20	1
1:A:14:VAL:CG2	1:A:14:VAL:CB	0.66	0.66	20	1
1:A:26:TYR:CZ	1:A:26:TYR:CE1	0.66	0.73	20	1
1:A:6:LYS:CG	1:A:6:LYS:HD2	0.65	1.31	20	1
1:A:7:LYS:HD3	1:A:7:LYS:CE	0.64	1.42	20	1
1:A:24:SER:OG	1:A:24:SER:CB	0.63	0.35	20	1
1:A:13:GLU:OE2	1:A:13:GLU:OE1	0.63	0.66	20	1
1:A:14:VAL:C	1:A:28:CYS:SG	0.62	2.83	19	19
1:A:6:LYS:HD3	1:A:6:LYS:CE	0.61	1.26	20	1
1:A:23:ASN:CG	1:A:23:ASN:ND2	0.61	0.72	20	1
1:A:18:SER:CB	1:A:18:SER:HG	0.61	1.32	20	1
1:A:8:TYR:CG	1:A:8:TYR:CB	0.60	0.67	20	1
1:A:6:LYS:CG	1:A:6:LYS:HD3	0.60	1.31	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LYS:HD2	1:A:6:LYS:CE	0.60	1.26	20	1
1:A:13:GLU:CG	1:A:28:CYS:SG	0.56	2.93	11	9
1:A:13:GLU:HG3	1:A:28:CYS:SG	0.55	2.41	18	8
1:A:23:ASN:CG	1:A:23:ASN:N	0.55	2.65	20	1
1:A:26:TYR:CG	1:A:26:TYR:HD1	0.55	1.30	20	1
1:A:26:TYR:CZ	1:A:26:TYR:HE2	0.55	1.30	20	1
1:A:14:VAL:N	1:A:28:CYS:SG	0.53	2.82	14	5
1:A:26:TYR:CZ	1:A:26:TYR:HE1	0.53	1.29	20	1
1:A:26:TYR:CG	1:A:26:TYR:HD2	0.53	1.29	20	1
1:A:19:CYS:SG	1:A:25:LYS:CB	0.50	2.99	11	5
1:A:5:CYS:SG	1:A:25:LYS:HG2	0.50	2.46	9	1
1:A:7:LYS:NZ	1:A:7:LYS:CE	0.49	0.52	20	1
1:A:7:LYS:CD	1:A:7:LYS:CE	0.49	0.86	20	1
1:A:8:TYR:CD1	1:A:8:TYR:C	0.48	2.72	20	1
1:A:9:CYS:SG	1:A:15:ILE:N	0.47	2.87	12	2
1:A:7:LYS:HE3	1:A:7:LYS:HZ1	0.47	1.11	20	1
1:A:7:LYS:CE	1:A:7:LYS:HZ1	0.46	1.17	20	1
1:A:7:LYS:CE	1:A:7:LYS:HZ2	0.46	1.17	20	1
1:A:7:LYS:CE	1:A:7:LYS:HZ3	0.45	1.17	20	1
1:A:7:LYS:CD	1:A:7:LYS:H	0.45	2.24	10	1
1:A:16:ASP:CB	1:A:29:CYS:SG	0.44	3.06	14	1
1:A:8:TYR:OH	1:A:8:TYR:HE2	0.44	0.88	20	1
1:A:7:LYS:H	1:A:7:LYS:HD2	0.43	1.73	10	1
1:A:19:CYS:SG	1:A:25:LYS:HB3	0.43	2.53	1	2
1:A:13:GLU:HB3	1:A:28:CYS:SG	0.43	2.53	14	1
1:A:9:CYS:SG	1:A:15:ILE:HG23	0.43	2.53	8	2
1:A:25:LYS:N	1:A:25:LYS:CD	0.43	2.82	1	1
1:A:19:CYS:SG	1:A:25:LYS:HB2	0.43	2.54	15	2
1:A:21:LEU:HG	1:A:22:PHE:N	0.42	2.28	20	1
1:A:6:LYS:CE	1:A:6:LYS:HZ3	0.42	1.13	20	1
1:A:6:LYS:CE	1:A:6:LYS:HZ2	0.42	1.13	20	1
1:A:14:VAL:CG1	1:A:14:VAL:C	0.42	2.88	20	1
1:A:6:LYS:CE	1:A:6:LYS:HZ1	0.42	1.13	20	1
1:A:13:GLU:CD	1:A:28:CYS:SG	0.42	3.02	8	1
1:A:6:LYS:NZ	1:A:6:LYS:CE	0.42	0.45	20	1
1:A:22:PHE:C	1:A:23:ASN:HD22	0.42	2.23	20	1
1:A:9:CYS:SG	1:A:14:VAL:C	0.41	3.04	12	2
1:A:7:LYS:CA	1:A:7:LYS:HG2	0.41	2.23	20	1
1:A:8:TYR:HE2	1:A:8:TYR:CD2	0.41	1.35	20	1
1:A:7:LYS:HD2	1:A:7:LYS:N	0.40	2.31	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	27/32 (84%)	23±1 (85±5%)	4±1 (14±5%)	0±0 (1±1%)	20	70
All	All	540/640 (84%)	461 (85%)	75 (14%)	4 (1%)	20	70

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	23	ASN	4

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	25/30 (83%)	23±2 (92±7%)	2±2 (8±7%)	14	62
All	All	500/600 (83%)	462 (92%)	38 (8%)	14	62

All 12 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	21	LEU	20
1	A	7	LYS	5
1	A	29	CYS	2
1	A	13	GLU	2
1	A	6	LYS	2
1	A	25	LYS	1
1	A	15	ILE	1
1	A	4	SER	1
1	A	8	TYR	1
1	A	18	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	23	ASN	1
1	A	24	SER	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	20-A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
20	A	2:PRO	C	3:CYS	N	1.18
20	A	30:ARG	C	31:GLU	N	0.91
20	A	31:GLU	C	32:LYS	N	0.55
20	A	1:MET	C	2:PRO	N	0.21

7 Chemical shift validation

No chemical shift data were provided