Full wwPDB NMR Structure Validation Report (i)

Feb 10, 2022 – 10:51 AM EST

PDB ID	:	1EWS
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.

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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

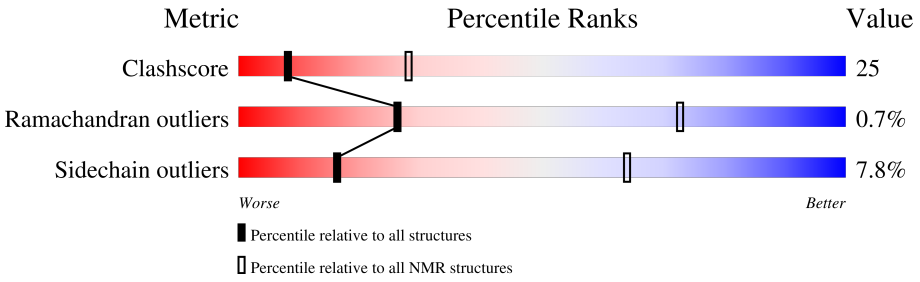
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	32	69% 16% 16%

2 Ensemble composition and analysis (i)

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)	0.22	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
			Total	C	H	N	O	S	
1	A	32	494	159	240	41	47	7	0

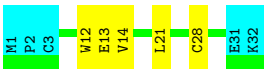
4 Residue-property plots (i)

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: RK-1 DEFENSIN

Chain A:



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

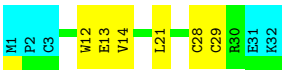
• Molecule 1: RK-1 DEFENSIN

Chain A:

4.2.2 Score per residue for model 2

• Molecule 1: RK-1 DEFENSIN

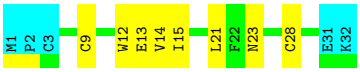
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: RK-1 DEFENSIN

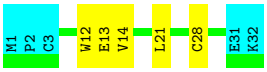
Chain A: 59% 25% 16%



4.2.4 Score per residue for model 4

- Molecule 1: RK-1 DEFENSIN

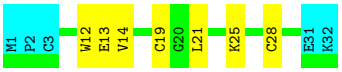
Chain A: 69% 16% 16%



4.2.5 Score per residue for model 5

- Molecule 1: RK-1 DEFENSIN

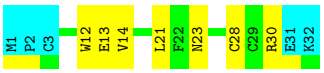
Chain A: 62% 22% 16%



4.2.6 Score per residue for model 6

- Molecule 1: RK-1 DEFENSIN

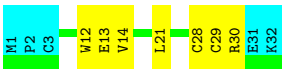
Chain A: 62% 22% 16%



4.2.7 Score per residue for model 7

- Molecule 1: RK-1 DEFENSIN

Chain A: 62% 22% 16%



4.2.8 Score per residue for model 8

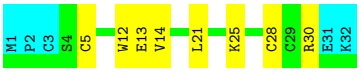
- Molecule 1: RK-1 DEFENSIN

Chain A: 62% 22% 16%

4.2.9 Score per residue for model 9

- Molecule 1: RK-1 DEFENSIN

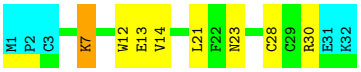
Chain A: 59% 25% 16%



4.2.10 Score per residue for model 10

- Molecule 1: RK-1 DEFENSIN

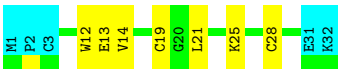
Chain A: 59% 22% • 16%



4.2.11 Score per residue for model 11

- Molecule 1: RK-1 DEFENSIN

Chain A: 62% 22% 16%



4.2.12 Score per residue for model 12

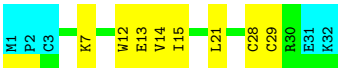
- Molecule 1: RK-1 DEFENSIN

Chain A: 59% 25% 16%

4.2.13 Score per residue for model 13

- Molecule 1: RK-1 DEFENSIN

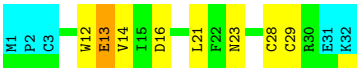
Chain A: 59% 25% 16%



4.2.14 Score per residue for model 14

- Molecule 1: RK-1 DEFENSIN

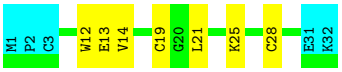
Chain A: 59% 22% • 16%



4.2.15 Score per residue for model 15

- Molecule 1: RK-1 DEFENSIN

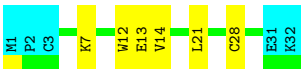
Chain A: 62% 22% 16%



4.2.16 Score per residue for model 16

- Molecule 1: RK-1 DEFENSIN

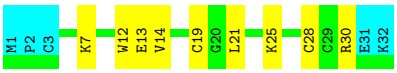
Chain A: 66% 19% 16%



4.2.17 Score per residue for model 17

- Molecule 1: RK-1 DEFENSIN

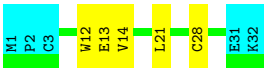
Chain A: 56% 28% 16%



4.2.18 Score per residue for model 18

- Molecule 1: RK-1 DEFENSIN

Chain A: 69% 16% 16%



4.2.19 Score per residue for model 19

- Molecule 1: RK-1 DEFENSIN

Chain A: 59% 25% 16%

4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: RK-1 DEFENSIN

Chain A: 25% 16% 22% 22% 16%

5 Refinement protocol and experimental data overview (i)

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 (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.31±4.92	3±14/220 (1.4± 6.2%)	2.12±3.67	7±15/296 (2.3± 4.9%)
All	All	5.44	63/4400 (1.4%)	4.24	134/5920 (2.3%)

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	8	TYR	CG-CD1	-99.53	0.09	1.39	20	1
1	A	8	TYR	CE2-CZ	-99.14	0.09	1.38	20	1
1	A	24	SER	CB-OG	-82.10	0.35	1.42	20	1
1	A	13	GLU	CD-OE1	-79.45	0.38	1.25	20	1
1	A	30	ARG	CZ-NH1	-78.49	0.31	1.33	20	1
1	A	30	ARG	CZ-NH2	-76.34	0.33	1.33	20	1
1	A	4	SER	CB-OG	-73.75	0.46	1.42	20	1
1	A	8	TYR	CG-CD2	-62.24	0.58	1.39	20	1
1	A	8	TYR	CE1-CZ	-61.95	0.58	1.38	20	1
1	A	30	ARG	CD-NE	-61.33	0.42	1.46	20	1
1	A	30	ARG	NE-CZ	-59.03	0.56	1.33	20	1
1	A	8	TYR	CB-CG	-56.21	0.67	1.51	20	1
1	A	22	PHE	CG-CD1	-56.13	0.54	1.38	20	1
1	A	13	GLU	CD-OE2	-54.09	0.66	1.25	20	1
1	A	8	TYR	CD1-CE1	-52.56	0.60	1.39	20	1
1	A	8	TYR	CD2-CE2	-52.56	0.60	1.39	20	1
1	A	22	PHE	CG-CD2	-52.10	0.60	1.38	20	1
1	A	26	TYR	CG-CD2	-50.42	0.73	1.39	20	1
1	A	26	TYR	CE1-CZ	-50.14	0.73	1.38	20	1
1	A	18	SER	CB-OG	-48.95	0.78	1.42	20	1
1	A	26	TYR	CG-CD1	-47.97	0.76	1.39	20	1
1	A	26	TYR	CE2-CZ	-47.65	0.76	1.38	20	1
1	A	8	TYR	CZ-OH	-45.53	0.60	1.37	20	1
1	A	22	PHE	CE2-CZ	-44.03	0.53	1.37	20	1
1	A	23	ASN	CG-OD1	-42.29	0.30	1.24	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	6	LYS	CE-NZ	-41.31	0.45	1.49	20	1
1	A	14	VAL	CB-CG2	-41.21	0.66	1.52	20	1
1	A	16	ASP	CG-OD2	-40.89	0.31	1.25	20	1
1	A	22	PHE	CE1-CZ	-40.82	0.59	1.37	20	1
1	A	7	LYS	CE-NZ	-38.82	0.52	1.49	20	1
1	A	30	ARG	CB-CG	-34.94	0.58	1.52	20	1
1	A	16	ASP	CG-OD1	-34.07	0.47	1.25	20	1
1	A	6	LYS	CD-CE	-30.12	0.76	1.51	20	1
1	A	10	ASP	CG-OD1	-29.57	0.57	1.25	20	1
1	A	14	VAL	CB-CG1	-29.46	0.91	1.52	20	1
1	A	10	ASP	CG-OD2	-29.27	0.58	1.25	20	1
1	A	25	LYS	CD-CE	-26.90	0.83	1.51	20	1
1	A	29	CYS	CB-SG	-26.71	1.36	1.82	20	1
1	A	23	ASN	CB-CG	-26.14	0.91	1.51	20	1
1	A	7	LYS	CD-CE	-25.97	0.86	1.51	20	1
1	A	7	LYS	CG-CD	-25.40	0.66	1.52	20	1
1	A	25	LYS	CE-NZ	-25.36	0.85	1.49	20	1
1	A	23	ASN	CG-ND2	-24.35	0.71	1.32	20	1
1	A	7	LYS	CB-CG	-23.67	0.88	1.52	20	1
1	A	13	GLU	CG-CD	-22.52	1.18	1.51	20	1
1	A	30	ARG	C-O	-21.08	0.83	1.23	20	1
1	A	16	ASP	CB-CG	-20.94	1.07	1.51	20	1
1	A	6	LYS	CG-CD	-20.11	0.84	1.52	20	1
1	A	30	ARG	C-N	-18.41	0.91	1.34	20	1
1	A	21	LEU	CG-CD1	-18.17	0.84	1.51	20	1
1	A	22	PHE	CB-CG	-17.39	1.21	1.51	20	1
1	A	21	LEU	CG-CD2	-15.60	0.94	1.51	20	1
1	A	22	PHE	CD1-CE1	-14.97	1.09	1.39	20	1
1	A	22	PHE	CD2-CE2	-14.95	1.09	1.39	20	1
1	A	30	ARG	CG-CD	-14.80	1.15	1.51	20	1
1	A	12	TRP	NE1-CE2	-9.48	1.25	1.37	20	1
1	A	12	TRP	CG-CD2	-8.02	1.30	1.43	20	1
1	A	12	TRP	CD1-NE1	-7.57	1.25	1.38	20	1
1	A	25	LYS	CG-CD	-7.30	1.27	1.52	20	1
1	A	12	TRP	CD2-CE2	-6.81	1.33	1.41	20	1
1	A	8	TYR	C-O	-6.22	1.11	1.23	20	1
1	A	13	GLU	CB-CG	-5.33	1.42	1.52	20	1
1	A	12	TRP	CD2-CE3	-5.16	1.32	1.40	20	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	8	TYR	CB-CG-CD2	84.98	171.99	121.00	20	1
1	A	22	PHE	CD1-CG-CD2	-69.32	28.18	118.30	20	1
1	A	26	TYR	CD1-CG-CD2	-68.88	42.13	117.90	20	1
1	A	22	PHE	CB-CG-CD2	65.70	166.79	120.80	20	1
1	A	26	TYR	CB-CG-CD1	63.73	159.24	121.00	20	1
1	A	22	PHE	CB-CG-CD1	63.18	165.02	120.80	20	1
1	A	8	TYR	CG-CD2-CE2	62.80	171.54	121.30	20	1
1	A	26	TYR	CB-CG-CD2	62.71	158.62	121.00	20	1
1	A	30	ARG	NE-CZ-NH2	59.52	150.06	120.30	20	8
1	A	16	ASP	CB-CG-OD1	58.55	170.99	118.30	20	1
1	A	8	TYR	CD1-CE1-CZ	57.46	171.51	119.80	20	1
1	A	30	ARG	NE-CZ-NH1	55.21	147.91	120.30	20	1
1	A	16	ASP	CB-CG-OD2	53.62	166.56	118.30	20	1
1	A	16	ASP	OD1-CG-OD2	-53.08	22.45	123.30	20	1
1	A	30	ARG	NH1-CZ-NH2	-52.15	62.03	119.40	20	1
1	A	22	PHE	CE1-CZ-CE2	-50.75	28.66	120.00	20	1
1	A	26	TYR	CE1-CZ-CE2	-48.51	42.18	119.80	20	1
1	A	26	TYR	CG-CD1-CE1	47.70	159.46	121.30	20	1
1	A	10	ASP	CB-CG-OD1	46.68	160.31	118.30	20	1
1	A	10	ASP	CB-CG-OD2	46.36	160.02	118.30	20	1
1	A	26	TYR	CG-CD2-CE2	46.34	158.37	121.30	20	1
1	A	10	ASP	OD1-CG-OD2	-44.02	39.66	123.30	20	1
1	A	26	TYR	CZ-CE2-CD2	44.02	159.42	119.80	20	1
1	A	26	TYR	CD1-CE1-CZ	42.93	158.44	119.80	20	1
1	A	22	PHE	CG-CD2-CE2	41.72	166.69	120.80	20	1
1	A	8	TYR	CD1-CG-CD2	-41.51	72.24	117.90	20	1
1	A	13	GLU	OE1-CD-OE2	-41.13	73.94	123.30	20	1
1	A	22	PHE	CG-CD1-CE1	40.32	165.15	120.80	20	1
1	A	22	PHE	CD1-CE1-CZ	38.57	166.38	120.10	20	1
1	A	22	PHE	CZ-CE2-CD2	37.37	164.94	120.10	20	1
1	A	21	LEU	CD1-CG-CD2	-34.39	7.34	110.50	20	1
1	A	8	TYR	CE1-CZ-CE2	-28.93	73.51	119.80	20	1
1	A	30	ARG	CG-CD-NE	22.96	160.01	111.80	20	1
1	A	14	VAL	CA-CB-CG2	21.98	143.88	110.90	20	1
1	A	30	ARG	CD-NE-CZ	21.62	153.87	123.60	20	1
1	A	6	LYS	CG-CD-CE	19.58	170.65	111.90	20	1
1	A	30	ARG	CB-CG-CD	19.33	161.86	111.60	20	1
1	A	14	VAL	CG1-CB-CG2	-19.11	80.33	110.90	20	1
1	A	8	TYR	CE1-CZ-OH	19.07	171.59	120.10	20	1
1	A	30	ARG	CA-CB-CG	18.21	153.46	113.40	20	1
1	A	13	GLU	CG-CD-OE2	18.05	154.41	118.30	20	1
1	A	23	ASN	CB-CG-ND2	15.82	154.68	116.70	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	25	LYS	CD-CE-NZ	15.81	148.07	111.70	20	1
1	A	24	SER	CA-CB-OG	15.53	153.12	111.20	20	1
1	A	30	ARG	O-C-N	-14.86	98.92	122.70	20	1
1	A	26	TYR	OH-CZ-CE2	14.60	159.51	120.10	20	1
1	A	26	TYR	CE1-CZ-OH	14.15	158.31	120.10	20	1
1	A	23	ASN	OD1-CG-ND2	-13.72	90.35	121.90	20	1
1	A	8	TYR	CA-CB-CG	13.28	138.63	113.40	20	1
1	A	14	VAL	CA-CB-CG1	12.84	130.16	110.90	20	1
1	A	7	LYS	CB-CG-CD	11.99	142.79	111.60	20	1
1	A	7	LYS	CA-CB-CG	11.27	138.20	113.40	20	1
1	A	21	LEU	CB-CG-CD1	11.15	129.96	111.00	20	1
1	A	4	SER	CA-CB-OG	10.92	140.69	111.20	20	1
1	A	25	LYS	CG-CD-CE	9.86	141.48	111.90	20	1
1	A	7	LYS	CG-CD-CE	9.74	141.12	111.90	20	1
1	A	8	TYR	CB-CG-CD1	-8.71	115.78	121.00	20	1
1	A	12	TRP	CD1-NE1-CE2	8.08	116.28	109.00	9	20
1	A	29	CYS	CA-CB-SG	7.52	127.53	114.00	20	1
1	A	6	LYS	CB-CG-CD	7.26	130.47	111.60	20	1
1	A	21	LEU	CB-CG-CD2	6.92	122.77	111.00	20	1
1	A	13	GLU	CG-CD-OE1	6.67	131.64	118.30	20	1
1	A	8	TYR	CG-CD1-CE1	-6.35	116.22	121.30	20	1
1	A	6	LYS	CD-CE-NZ	6.14	125.81	111.70	20	1
1	A	12	TRP	CG-CD1-NE1	-5.88	104.22	110.10	13	20
1	A	12	TRP	NE1-CE2-CZ2	5.85	136.83	130.40	10	20
1	A	23	ASN	CA-CB-CG	5.61	125.73	113.40	20	1
1	A	30	ARG	CA-C-O	5.61	131.87	120.10	20	1
1	A	30	ARG	CA-C-N	5.45	129.20	117.20	20	1
1	A	8	TYR	CZ-CE2-CD2	-5.37	114.97	119.80	20	1

There are no chirality outliers.

There are no planarity outliers.

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	214	199	198	10±29
All	All	4280	3980	3979	204

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: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:23:ASN:CG	1:A:23:ASN:CA	1.09	2.20	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:23:ASN:CG	1:A:23:ASN:HB2	1.04	1.50	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:HB3	1.01	1.50	20	1
1:A:21:LEU:CG	1:A:21:LEU:HD22	1.00	1.56	20	1
1:A:23:ASN:CG	1:A:23:ASN:CB	1.00	0.90	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: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: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: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: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: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:13:GLU:OE2	1:A:13:GLU:CD	0.82	0.66	20	1
1:A:25:LYS:CD	1:A:25:LYS:HE2	0.81	1.38	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
1:A:8:TYR:HD1	1:A:8:TYR:C	0.78	1.81	20	1
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:23:ASN:CG	1:A:23:ASN:HD21	0.76	1.37	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ASP:OD1	1:A:10:ASP:CG	0.76	0.57	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:10:ASP:OD2	1:A:10:ASP:CG	0.75	0.58	20	1
1:A:6:LYS:HE2	1:A:6:LYS:HD3	0.75	1.07	20	1
1:A:23:ASN:CG	1:A:23:ASN:HD22	0.74	1.37	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: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: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:23:ASN:CG	1:A:23:ASN:ND2	0.66	0.72	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:13:GLU:OE2	1:A:13:GLU:OE1	0.65	0.66	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:6:LYS:HD3	1:A:6:LYS:CE	0.61	1.26	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
1:A:6:LYS:HD2	1:A:6:LYS:CE	0.60	1.26	20	1
1:A:14:VAL:C	1:A:28:CYS:SG	0.57	2.83	19	18
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:23:ASN:CG	1:A:23:ASN:N	0.51	2.65	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:4:SER:CA	1:A:4:SER:HG	0.49	1.97	20	1
1:A:7:LYS:CD	1:A:7:LYS:CE	0.49	0.86	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:8:TYR:CD1	1:A:8:TYR:C	0.44	2.72	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:6:LYS:CE	1:A:6:LYS:HZ1	0.42	1.13	20	1
1:A:6:LYS:NZ	1:A:6:LYS:CE	0.42	0.45	20	1
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 (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	27/32 (84%)	23±1 (85±5%)	4±1 (14±5%)	0±0 (1±1%)	26	73
All	All	540/640 (84%)	461 (85%)	75 (14%)	4 (1%)	26	73

All 1 unique Ramachandran outliers are listed below.

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

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	25/30 (83%)	23±1 (92±6%)	2±1 (8±6%)	16	64
All	All	500/600 (83%)	461 (92%)	39 (8%)	16	64

All 13 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	6
1	A	29	CYS	3
1	A	25	LYS	1
1	A	30	ARG	1
1	A	11	PRO	1
1	A	15	ILE	1
1	A	13	GLU	1
1	A	4	SER	1
1	A	6	LYS	1
1	A	8	TYR	1
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 monosaccharides 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 (i)

No chemical shift data were provided