



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 04:14 AM UTC

PDB ID : 1BWY / pdb_00001bwy
Title : NMR STUDY OF BOVINE HEART FATTY ACID BINDING PROTEIN
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Deposited on : 1998-09-29

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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

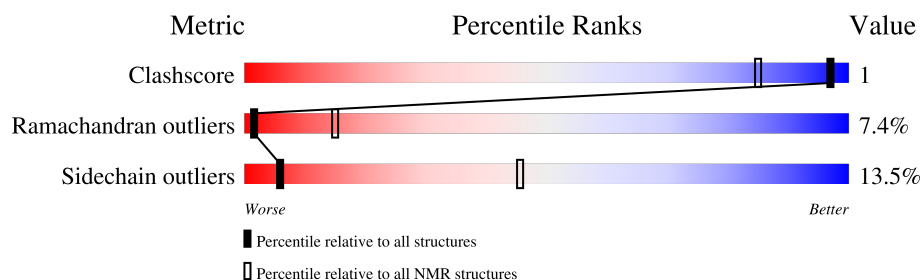
1 Overall quality at a glance

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	132	

2 Ensemble composition and analysis

This entry contains 25 models. Model 5 is the overall representative, medoid model (most similar to other models).

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:1-A:132 (132)	1.39	5

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 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	3, 5, 6, 8, 10, 11, 14, 16, 17, 20
2	1, 15, 18, 21, 22
3	9, 24, 25
4	2, 7, 19
Single-model clusters	4; 12; 13; 23

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2076 atoms, of which 1047 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (HEART FATTY ACID BINDING PROTEIN).

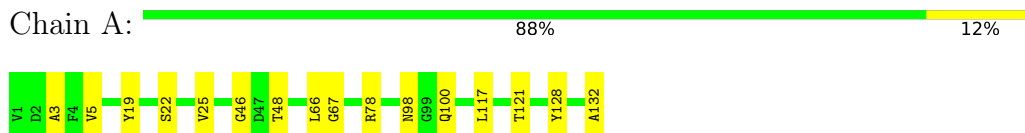
Mol	Chain	Residues	Atoms						Trace
1	A	132	Total	C	H	N	O	S	0
			2076	649	1047	173	203	4	

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: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

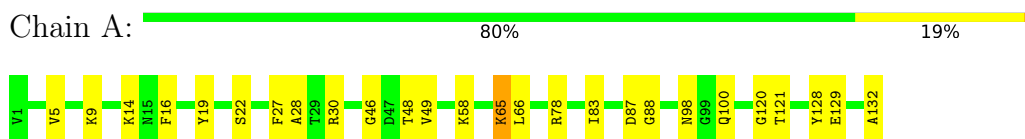


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

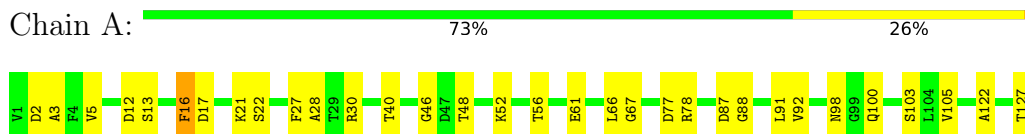
4.2.1 Score per residue for model 1

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)



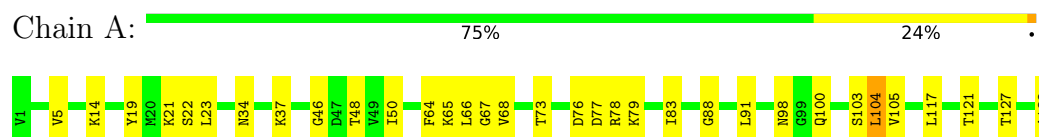
4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)



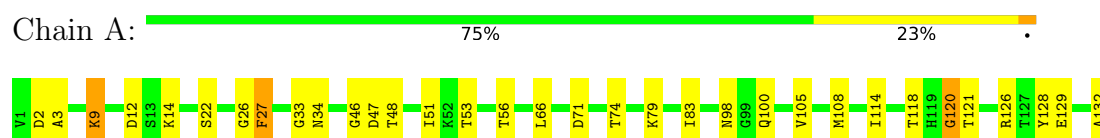
4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)



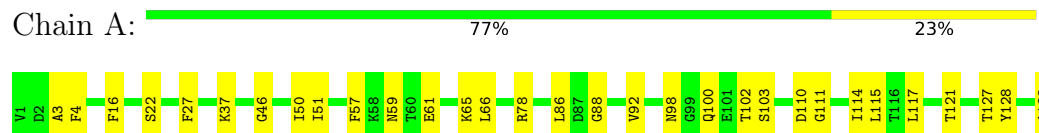
4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)



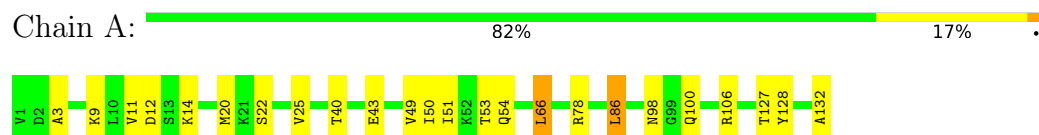
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)



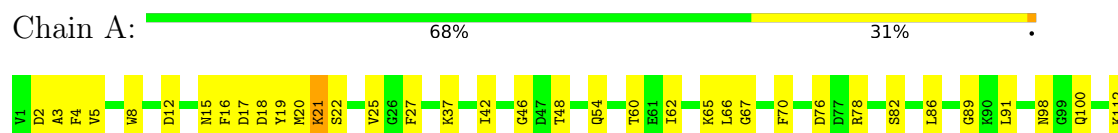
4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)



4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

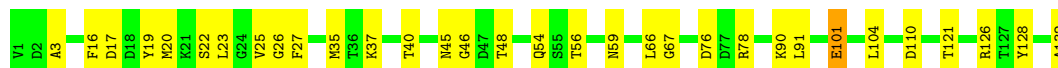




4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

Chain A: 76% 23%



4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

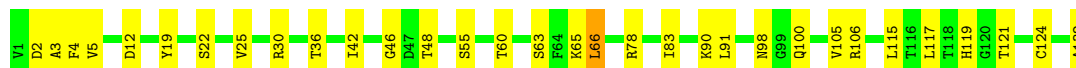
Chain A: 78% 20%



4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

Chain A: 76% 23%



4.2.11 Score per residue for model 11

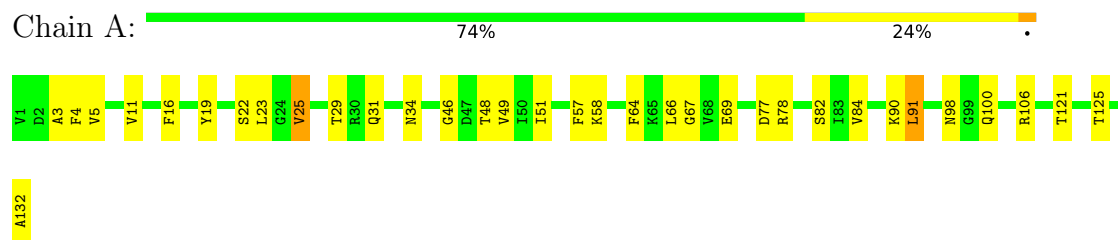
- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

Chain A: 75% 25%



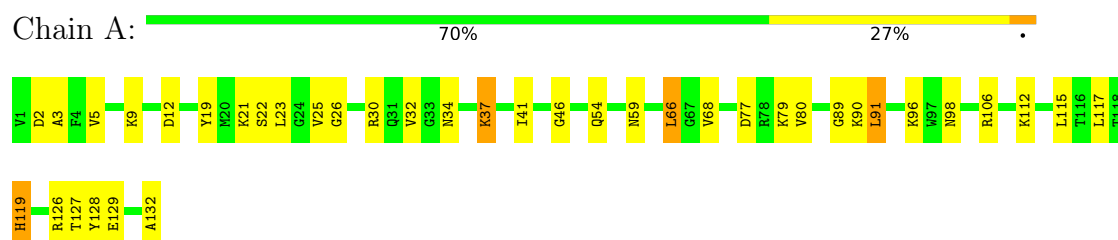
4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)



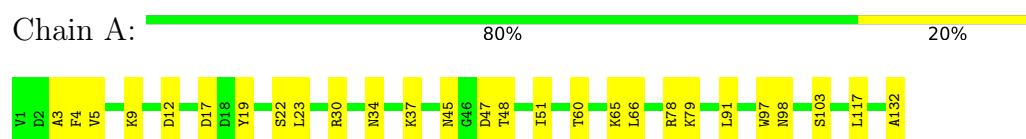
4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)



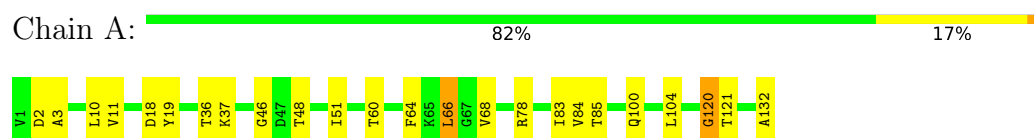
4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)



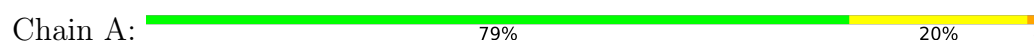
4.2.15 Score per residue for model 15

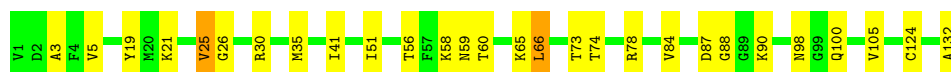
- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)



4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)





4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

Chain A: 77% 23%



4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

Chain A: 78% 20%



4.2.19 Score per residue for model 19

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

Chain A: 75% 25%



4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

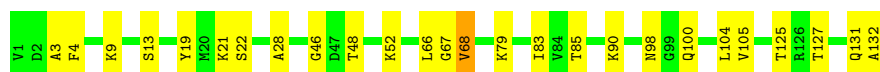
Chain A: 80% 19%



4.2.21 Score per residue for model 21

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

Chain A:  80% 19% .



4.2.22 Score per residue for model 22

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

Chain A:  77% 20% .



4.2.23 Score per residue for model 23

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

Chain A:  81% 18% .



4.2.24 Score per residue for model 24

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

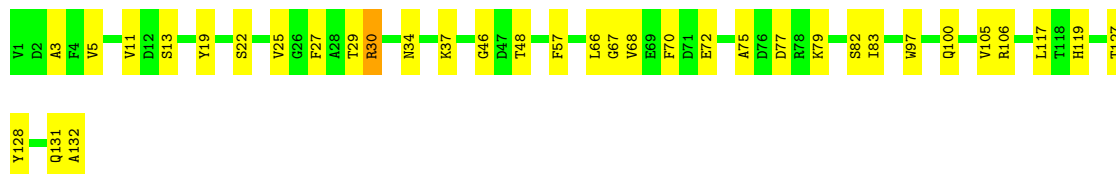
Chain A:  79% 20% .



4.2.25 Score per residue for model 25

- Molecule 1: PROTEIN (HEART FATTY ACID BINDING PROTEIN)

Chain A:  73% 26% .



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, ENERGY MINIMIZATION*.

Of the 100 calculated structures, 25 were deposited, based on the following criterion: *LOWEST VIOLATION OF EXPERIMENTAL DISTANCE CONSTRAINTS*.

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

Software name	Classification	Version
SYBYL	refinement	6.0
DIANA	structure solution	
SYBYL	structure solution	

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	0.63±0.01	1±0/1043 (0.1± 0.0%)	1.22±0.03	1±1/1407 (0.1± 0.1%)
All	All	0.63	25/26075 (0.1%)	1.22	35/35175 (0.1%)

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	2.9±1.3
All	All	0	72

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	132	ALA	C-OXT	7.46	1.38	1.23	13	25

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	119	HIS	CA-CB-CG	6.73	120.53	113.80	13	2
1	A	93	HIS	CA-CB-CG	6.66	120.45	113.80	23	2
1	A	27	PHE	CA-CB-CG	6.55	120.36	113.80	4	2
1	A	119	HIS	CB-CG-CD2	-6.10	123.27	131.20	19	3
1	A	17	ASP	CA-CB-CG	-5.88	106.72	112.60	14	1
1	A	77	ASP	CA-C-N	5.77	132.55	121.54	23	2
1	A	77	ASP	C-N-CA	5.77	132.55	121.54	23	2
1	A	76	ASP	CA-CB-CG	5.58	118.19	112.60	20	1
1	A	34	ASN	CA-CB-CG	5.52	118.12	112.60	20	2
1	A	32	VAL	CA-C-N	5.49	127.04	120.13	24	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	32	VAL	C-N-CA	5.49	127.04	120.13	24	1
1	A	20	MET	CA-C-N	5.45	128.12	120.28	23	1
1	A	20	MET	C-N-CA	5.45	128.12	120.28	23	1
1	A	91	LEU	CB-CA-C	5.29	118.46	109.84	12	1
1	A	120	GLY	CA-C-N	5.28	131.63	121.54	4	3
1	A	120	GLY	C-N-CA	5.28	131.63	121.54	4	3
1	A	11	VAL	CB-CA-C	5.27	115.74	111.05	19	1
1	A	18	ASP	CA-CB-CG	-5.27	107.33	112.60	15	1
1	A	16	PHE	CA-C-N	5.19	127.18	120.44	5	1
1	A	16	PHE	C-N-CA	5.19	127.18	120.44	5	1
1	A	64	PHE	CA-CB-CG	5.16	118.95	113.80	3	2
1	A	16	PHE	CA-CB-CG	5.14	118.94	113.80	24	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	19	TYR	Sidechain	17
1	A	128	TYR	Sidechain	14
1	A	4	PHE	Sidechain	9
1	A	16	PHE	Sidechain,Peptide	7
1	A	30	ARG	Sidechain	7
1	A	70	PHE	Sidechain	4
1	A	78	ARG	Sidechain	4
1	A	77	ASP	Peptide	3
1	A	126	ARG	Sidechain	2
1	A	101	GLU	Peptide	1
1	A	121	THR	Peptide	1
1	A	27	PHE	Sidechain	1
1	A	62	ILE	Peptide	1
1	A	125	THR	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	1029	1047	1045	1±1
All	All	25725	26175	26125	37

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ASP:OD2	1:A:124:CYS:SG	0.49	2.71	20	3
1:A:10:LEU:HD23	1:A:11:VAL:N	0.49	2.23	15	1
1:A:113:LEU:C	1:A:113:LEU:HD12	0.47	2.35	24	1
1:A:31:GLN:NE2	1:A:32:VAL:HG23	0.47	2.25	19	1
1:A:91:LEU:C	1:A:91:LEU:HD22	0.46	2.35	13	1
1:A:106:ARG:CG	1:A:115:LEU:HD23	0.45	2.41	10	1
1:A:8:TRP:CD2	1:A:42:ILE:HD13	0.45	2.46	7	1
1:A:19:TYR:CD1	1:A:124:CYS:SG	0.45	3.09	9	1
1:A:86:LEU:HD12	1:A:86:LEU:C	0.45	2.37	6	2
1:A:91:LEU:C	1:A:91:LEU:HD23	0.45	2.37	7	3
1:A:12:ASP:HB3	1:A:127:THR:HG22	0.44	1.88	13	1
1:A:9:LYS:NZ	1:A:129:GLU:OE2	0.44	2.51	4	1
1:A:9:LYS:NZ	1:A:129:GLU:OE1	0.44	2.48	1	1
1:A:64:PHE:CD2	1:A:84:VAL:HG11	0.43	2.48	12	1
1:A:113:LEU:HD23	1:A:113:LEU:C	0.43	2.38	19	1
1:A:103:SER:C	1:A:104:LEU:HD23	0.43	2.39	3	1
1:A:8:TRP:CG	1:A:42:ILE:HD13	0.43	2.49	7	1
1:A:19:TYR:CE2	1:A:117:LEU:HD12	0.43	2.49	17	1
1:A:112:LYS:NZ	1:A:129:GLU:OE2	0.42	2.51	13	1
1:A:18:ASP:OD1	1:A:21:LYS:NZ	0.42	2.52	7	2
1:A:12:ASP:OD2	1:A:14:LYS:NZ	0.42	2.52	4	1
1:A:65:LYS:C	1:A:65:LYS:CD	0.41	2.93	1	1
1:A:71:ASP:OD2	1:A:79:LYS:NZ	0.41	2.54	4	1
1:A:12:ASP:OD2	1:A:112:LYS:NZ	0.41	2.50	7	1
1:A:90:LYS:NZ	1:A:107:GLU:OE1	0.41	2.54	18	1
1:A:8:TRP:CZ3	1:A:113:LEU:HB2	0.41	2.51	19	1
1:A:86:LEU:C	1:A:86:LEU:HD12	0.41	2.41	11	1
1:A:19:TYR:CE2	1:A:117:LEU:HD21	0.41	2.51	22	1
1:A:115:LEU:C	1:A:115:LEU:HD23	0.41	2.41	24	1
1:A:91:LEU:HD23	1:A:91:LEU:C	0.40	2.40	3	1
1:A:47:ASP:OD2	1:A:65:LYS:NZ	0.40	2.54	9	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	130/132 (98%)	97±7 (75±6%)	22±5 (17±4%)	10±3 (7±2%)	1	15
All	All	3203/3300 (97%)	2422 (76%)	543 (17%)	238 (7%)	1	15

All 41 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	22	SER	22
1	A	46	GLY	18
1	A	3	ALA	16
1	A	98	ASN	15
1	A	78	ARG	14
1	A	5	VAL	13
1	A	67	GLY	13
1	A	88	GLY	11
1	A	25	VAL	11
1	A	56	THR	7
1	A	34	ASN	7
1	A	66	LEU	7
1	A	121	THR	7
1	A	2	ASP	6
1	A	13	SER	6
1	A	26	GLY	6
1	A	120	GLY	5
1	A	76	ASP	5
1	A	37	LYS	5
1	A	28	ALA	4
1	A	27	PHE	4
1	A	57	PHE	4
1	A	17	ASP	4
1	A	11	VAL	3
1	A	36	THR	3
1	A	90	LYS	3
1	A	110	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	89	GLY	2
1	A	45	ASN	2
1	A	29	THR	2
1	A	122	ALA	1
1	A	73	THR	1
1	A	33	GLY	1
1	A	111	GLY	1
1	A	54	GLN	1
1	A	59	ASN	1
1	A	55	SER	1
1	A	12	ASP	1
1	A	68	VAL	1
1	A	23	LEU	1
1	A	75	ALA	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	93/116 (80%)	99±8 (106±8%)	15±2 (17±3%)	4	39
All	All	2849/2900 (98%)	2464 (86%)	385 (14%)	6	45

All 85 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	LEU	24
1	A	48	THR	20
1	A	100	GLN	18
1	A	83	ILE	11
1	A	127	THR	11
1	A	117	LEU	11
1	A	21	LYS	9
1	A	68	VAL	9
1	A	9	LYS	9
1	A	60	THR	9
1	A	65	LYS	8

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Mol	Chain	Res	Type	Models (Total)
1	A	51	ILE	8
1	A	105	VAL	7
1	A	58	LYS	6
1	A	91	LEU	6
1	A	131	GLN	6
1	A	23	LEU	6
1	A	37	LYS	6
1	A	79	LYS	6
1	A	53	THR	6
1	A	20	MET	6
1	A	90	LYS	6
1	A	87	ASP	5
1	A	121	THR	5
1	A	12	ASP	5
1	A	103	SER	5
1	A	50	ILE	5
1	A	104	LEU	5
1	A	25	VAL	5
1	A	35	MET	5
1	A	14	LYS	4
1	A	27	PHE	4
1	A	49	VAL	4
1	A	52	LYS	4
1	A	92	VAL	4
1	A	47	ASP	4
1	A	59	ASN	4
1	A	115	LEU	4
1	A	106	ARG	4
1	A	54	GLN	4
1	A	82	SER	4
1	A	30	ARG	4
1	A	41	ILE	4
1	A	39	THR	4
1	A	16	PHE	3
1	A	40	THR	3
1	A	61	GLU	3
1	A	77	ASP	3
1	A	74	THR	3
1	A	98	ASN	3
1	A	102	THR	3
1	A	119	HIS	3
1	A	124	CYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	101	GLU	3
1	A	18	ASP	3
1	A	69	GLU	3
1	A	113	LEU	3
1	A	32	VAL	3
1	A	85	THR	3
1	A	108	MET	2
1	A	114	ILE	2
1	A	118	THR	2
1	A	86	LEU	2
1	A	126	ARG	2
1	A	31	GLN	2
1	A	125	THR	2
1	A	97	TRP	2
1	A	84	VAL	2
1	A	34	ASN	2
1	A	17	ASP	1
1	A	43	GLU	1
1	A	15	ASN	1
1	A	62	ILE	1
1	A	42	ILE	1
1	A	63	SER	1
1	A	56	THR	1
1	A	57	PHE	1
1	A	80	VAL	1
1	A	96	LYS	1
1	A	36	THR	1
1	A	73	THR	1
1	A	81	LYS	1
1	A	7	THR	1
1	A	29	THR	1
1	A	72	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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