



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 01:37 AM UTC

PDB ID : 3IFB / pdb_00003ifb
Title : NMR STUDY OF HUMAN INTESTINAL FATTY ACID BINDING PROTEIN
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Deposited on : 1998-10-16

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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

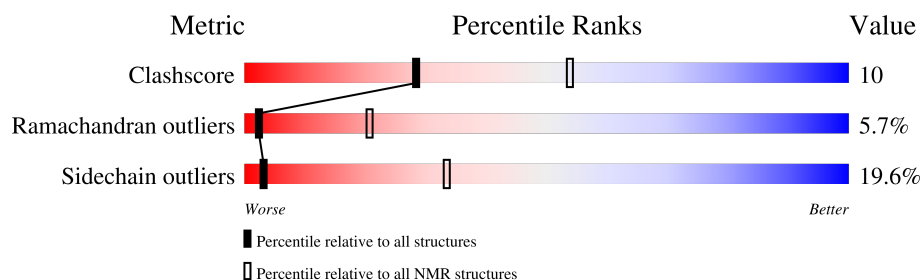
1 Overall quality at a glance

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	131	52% 41% 6% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 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:2-A:131 (130)	1.12	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 8, 9
2	7, 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2126 atoms, of which 1062 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INTESTINAL FATTY ACID BINDING PROTEIN.

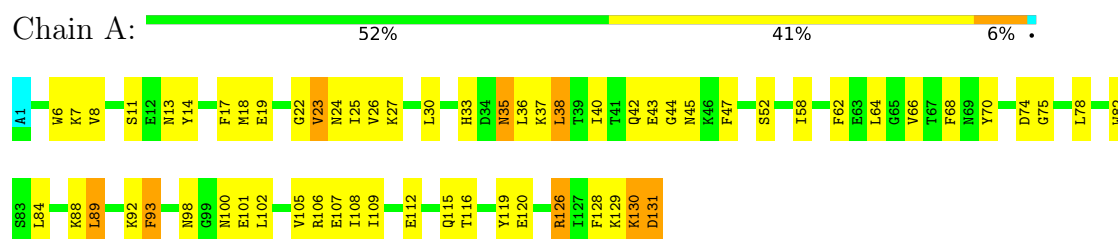
Mol	Chain	Residues	Atoms						Trace
1	A	131	Total	C	H	N	O	S	0
			2126	673	1062	183	206	2	

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: INTESTINAL FATTY ACID BINDING PROTEIN

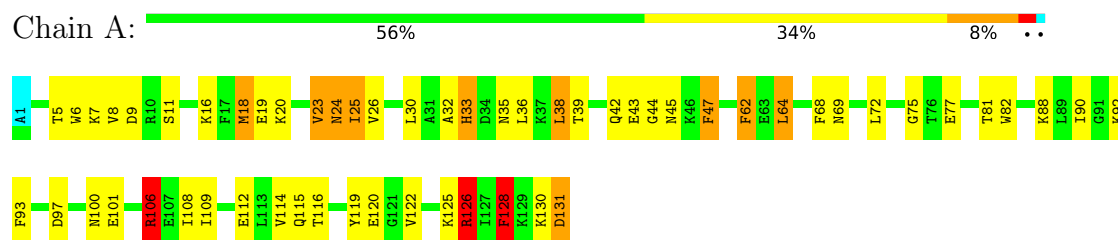


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

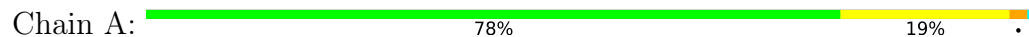
4.2.1 Score per residue for model 1 (medoid)

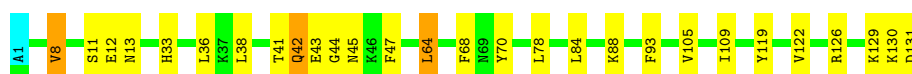
- Molecule 1: INTESTINAL FATTY ACID BINDING PROTEIN



4.2.2 Score per residue for model 2

- Molecule 1: INTESTINAL FATTY ACID BINDING PROTEIN

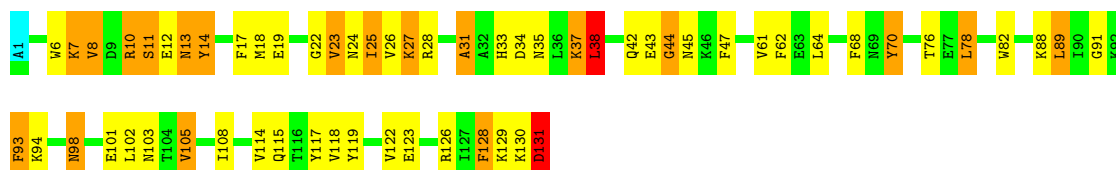




4.2.3 Score per residue for model 3

- Molecule 1: INTESTINAL FATTY ACID BINDING PROTEIN

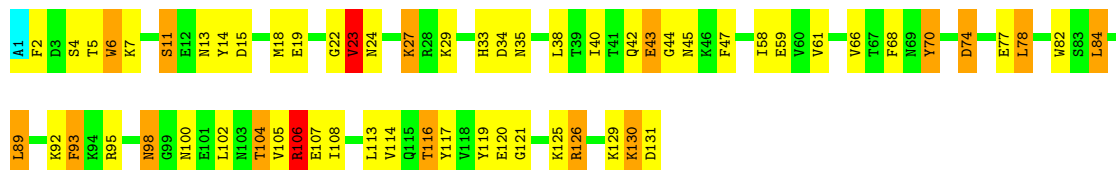
Chain A: 53% 30% 15% ..



4.2.4 Score per residue for model 4

- Molecule 1: INTESTINAL FATTY ACID BINDING PROTEIN

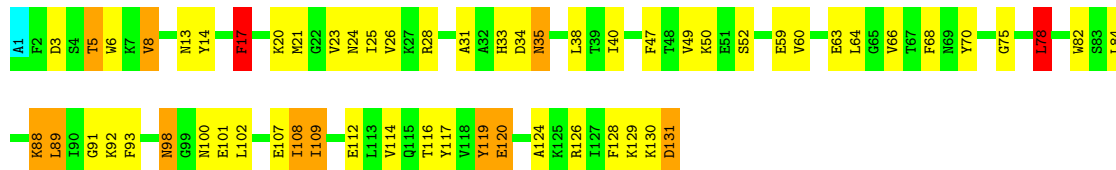
Chain A: 53% 34% 11% ..



4.2.5 Score per residue for model 5

- Molecule 1: INTESTINAL FATTY ACID BINDING PROTEIN

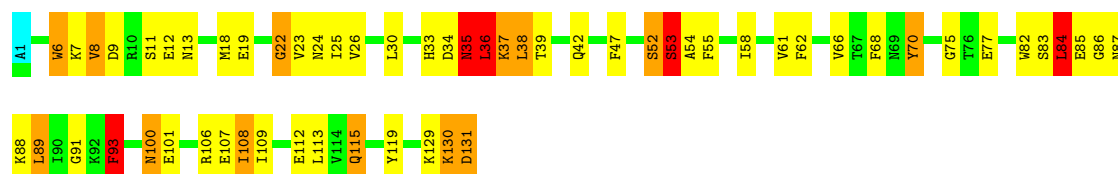
Chain A: 54% 35% 8% ..



4.2.6 Score per residue for model 6

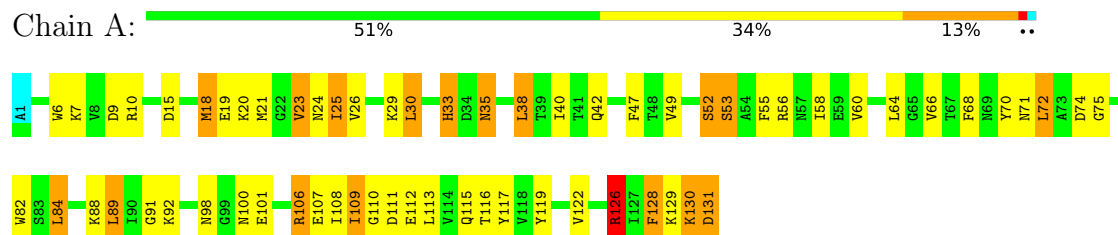
- Molecule 1: INTESTINAL FATTY ACID BINDING PROTEIN

Chain A: 54% 31% 10% ..



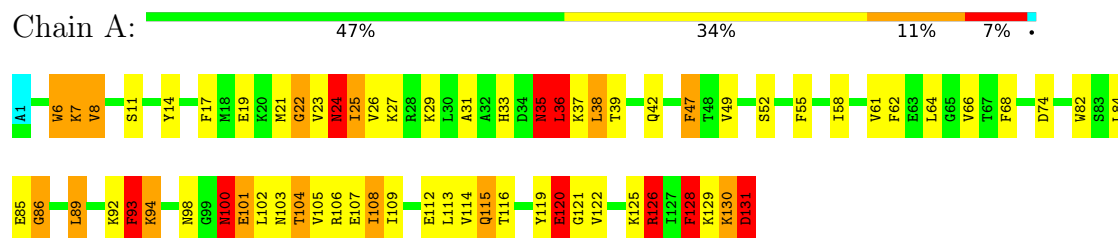
4.2.7 Score per residue for model 7

- Molecule 1: INTESTINAL FATTY ACID BINDING PROTEIN



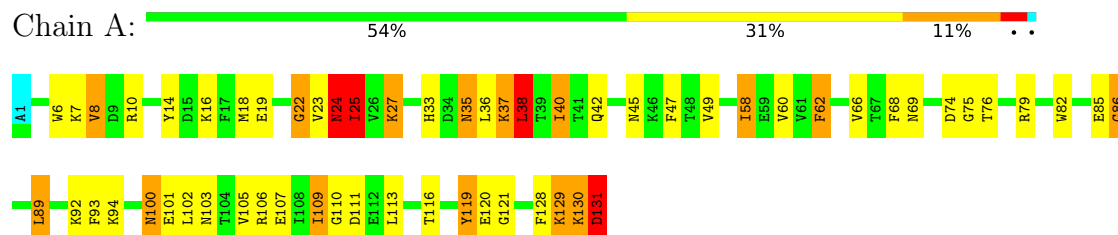
4.2.8 Score per residue for model 8

- Molecule 1: INTESTINAL FATTY ACID BINDING PROTEIN



4.2.9 Score per residue for model 9

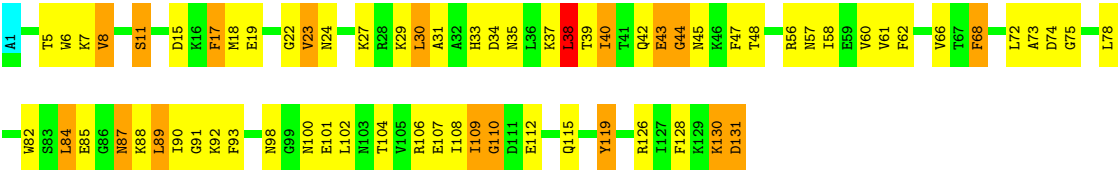
- Molecule 1: INTESTINAL FATTY ACID BINDING PROTEIN



4.2.10 Score per residue for model 10

- Molecule 1: INTESTINAL FATTY ACID BINDING PROTEIN

Chain A: 47% 39% 13% ..



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATED ANNEALING*.

Of the 50 calculated structures, 10 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	6.2
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	1.22±0.01	4±0/1075 (0.4± 0.0%)	1.76±0.15	22±7/1441 (1.5± 0.5%)
All	All	1.22	40/10750 (0.4%)	1.77	221/14410 (1.5%)

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	5.3±1.8
All	All	0	53

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	131	ASP	C-OXT	7.49	1.38	1.23	4	10
1	A	33	HIS	CE1-NE2	-6.76	1.25	1.32	4	10
1	A	33	HIS	CG-ND1	-6.24	1.31	1.38	1	10
1	A	33	HIS	CD2-NE2	6.02	1.44	1.37	10	10

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	100	ASN	CA-CB-CG	-12.38	100.22	112.60	8	2
1	A	38	LEU	N-CA-CB	-11.55	93.50	110.37	8	6
1	A	128	PHE	CA-CB-CG	10.30	124.10	113.80	8	5
1	A	33	HIS	CA-CB-CG	10.27	124.07	113.80	10	6
1	A	24	ASN	CA-CB-CG	10.17	122.77	112.60	9	2
1	A	126	ARG	CB-CA-C	9.70	131.09	109.56	8	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	108	ILE	N-CA-CB	9.59	121.69	110.95	5	2
1	A	62	PHE	CA-CB-CG	9.58	123.38	113.80	9	1
1	A	93	PHE	CA-CB-CG	9.18	122.98	113.80	6	4
1	A	40	ILE	N-CA-C	-8.94	97.06	109.21	9	2
1	A	23	VAL	CB-CA-C	8.83	122.47	110.99	8	4
1	A	84	LEU	CB-CA-C	8.22	122.60	110.26	7	5
1	A	23	VAL	N-CA-CB	-8.19	102.24	112.15	6	6
1	A	8	VAL	N-CA-CB	8.11	119.37	110.53	3	4
1	A	126	ARG	N-CA-CB	-7.99	96.67	111.53	8	4
1	A	33	HIS	CG-CD2-NE2	-7.93	99.27	107.20	1	10
1	A	38	LEU	CB-CA-C	7.84	126.53	111.17	4	1
1	A	118	VAL	CB-CA-C	7.75	120.66	110.12	3	1
1	A	36	LEU	N-CA-CB	7.63	123.39	110.49	6	2
1	A	89	LEU	N-CA-CB	7.60	121.26	109.48	5	2
1	A	6	TRP	CB-CG-CD2	-7.53	116.26	126.80	7	9
1	A	64	LEU	N-CA-CB	7.40	122.99	110.49	1	1
1	A	106	ARG	N-CA-CB	7.26	124.26	111.13	4	1
1	A	78	LEU	N-CA-CB	7.23	124.53	111.37	4	2
1	A	17	PHE	CA-CB-CG	-7.11	106.69	113.80	5	1
1	A	39	THR	N-CA-CB	7.03	121.19	109.94	8	4
1	A	40	ILE	N-CA-CB	6.97	119.81	110.26	9	1
1	A	130	LYS	N-CA-C	6.97	120.38	110.14	10	1
1	A	68	PHE	CA-CB-CG	-6.87	106.93	113.80	3	8
1	A	113	LEU	CB-CA-C	6.87	122.15	110.81	7	4
1	A	42	GLN	N-CA-CB	6.83	120.00	110.17	9	1
1	A	101	GLU	N-CA-C	6.78	119.48	110.53	6	2
1	A	89	LEU	CB-CA-C	-6.72	98.18	109.48	6	3
1	A	101	GLU	N-CA-CB	-6.72	99.85	111.55	9	1
1	A	6	TRP	CE2-CD2-CE3	6.68	125.48	118.80	7	5
1	A	23	VAL	N-CA-C	-6.62	98.71	108.97	7	3
1	A	74	ASP	N-CA-C	-6.53	104.16	111.28	4	3
1	A	37	LYS	CB-CA-C	-6.51	98.50	111.91	3	1
1	A	115	GLN	CA-C-O	-6.50	113.70	120.99	3	2
1	A	68	PHE	N-CA-CB	-6.45	101.57	111.56	10	1
1	A	48	THR	N-CA-CB	6.42	119.89	109.95	10	1
1	A	8	VAL	N-CA-C	6.38	117.32	108.89	8	1
1	A	31	ALA	N-CA-CB	6.33	119.37	109.94	3	3
1	A	105	VAL	CA-C-O	-6.31	114.69	121.19	4	2
1	A	62	PHE	N-CA-CB	-6.28	101.79	111.46	8	2
1	A	33	HIS	N-CA-CB	-6.21	101.97	111.66	1	1
1	A	107	GLU	CA-C-O	-6.20	114.59	121.23	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	131	ASP	CA-CB-CG	6.19	118.79	112.60	5	1
1	A	100	ASN	CB-CA-C	-6.12	100.94	111.23	7	1
1	A	10	ARG	N-CA-CB	-6.12	102.04	111.46	7	2
1	A	131	ASP	N-CA-CB	-6.05	100.22	110.50	5	4
1	A	120	GLU	N-CA-C	6.04	123.67	110.80	8	2
1	A	30	LEU	N-CA-CB	6.04	119.29	110.47	1	3
1	A	129	LYS	N-CA-CB	6.03	120.97	111.20	4	1
1	A	52	SER	N-CA-CB	-5.97	102.30	111.56	7	2
1	A	38	LEU	N-CA-C	5.92	117.79	107.49	8	3
1	A	9	ASP	N-CA-C	-5.87	103.69	111.96	1	3
1	A	15	ASP	N-CA-C	-5.82	105.07	111.82	7	3
1	A	106	ARG	N-CA-C	-5.75	98.91	108.34	10	1
1	A	101	GLU	CB-CA-C	-5.72	99.72	109.51	1	2
1	A	6	TRP	N-CA-CB	5.68	118.01	110.29	9	1
1	A	116	THR	CB-CA-C	5.66	118.89	110.62	4	1
1	A	18	MET	CB-CA-C	5.64	120.43	110.85	7	1
1	A	104	THR	N-CA-CB	5.63	119.34	110.56	10	1
1	A	122	VAL	N-CA-CB	-5.62	104.59	110.72	8	3
1	A	125	LYS	CA-C-O	-5.61	114.72	120.89	4	1
1	A	119	TYR	CB-CA-C	-5.61	101.56	110.81	9	1
1	A	52	SER	CA-C-O	-5.58	115.06	121.47	6	1
1	A	2	PHE	CA-CB-CG	-5.56	108.24	113.80	4	1
1	A	7	LYS	N-CA-CB	-5.50	101.63	110.77	7	2
1	A	106	ARG	CA-CB-CG	5.46	125.03	114.10	8	2
1	A	6	TRP	CB-CG-CD1	5.46	135.09	126.90	1	4
1	A	50	LYS	CA-C-O	-5.44	114.96	121.11	5	1
1	A	115	GLN	CB-CG-CD	5.42	121.82	112.60	8	2
1	A	27	LYS	N-CA-C	-5.41	105.28	111.07	4	1
1	A	72	LEU	CB-CA-C	5.40	121.17	110.42	7	1
1	A	100	ASN	N-CA-CB	5.40	119.59	110.69	7	2
1	A	94	LYS	N-CA-CB	5.39	119.80	111.24	8	1
1	A	33	HIS	ND1-CG-CD2	5.36	111.46	106.10	1	1
1	A	42	GLN	N-CA-C	-5.36	102.94	110.50	9	1
1	A	40	ILE	CA-CB-CG1	5.36	119.50	110.40	9	1
1	A	97	ASP	CB-CA-C	5.33	121.03	110.42	1	1
1	A	78	LEU	CB-CA-C	-5.33	100.88	110.36	3	1
1	A	72	LEU	N-CA-CB	5.31	118.53	110.45	1	1
1	A	43	GLU	CA-C-O	-5.30	115.76	121.38	10	2
1	A	35	ASN	CA-CB-CG	-5.29	107.31	112.60	5	1
1	A	106	ARG	CA-C-O	-5.29	114.65	120.36	8	1
1	A	27	LYS	CB-CA-C	5.28	121.77	110.21	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	90	ILE	CB-CA-C	5.27	117.54	110.42	1	1
1	A	130	LYS	N-CA-CB	-5.27	101.59	110.49	5	1
1	A	66	VAL	CA-C-O	-5.26	115.18	121.28	5	1
1	A	7	LYS	CB-CA-C	5.25	118.73	109.80	9	1
1	A	129	LYS	CB-CA-C	-5.25	100.38	110.24	8	1
1	A	29	LYS	N-CA-C	-5.23	105.58	111.28	7	1
1	A	43	GLU	N-CA-CB	-5.22	103.42	111.46	10	1
1	A	98	ASN	CA-CB-CG	5.22	117.82	112.60	3	1
1	A	31	ALA	N-CA-C	-5.21	105.78	111.82	10	1
1	A	5	THR	N-CA-C	-5.15	101.31	109.96	5	2
1	A	58	ILE	N-CA-C	-5.15	100.23	107.75	9	1
1	A	7	LYS	CA-C-O	-5.14	115.09	121.06	3	1
1	A	122	VAL	CA-C-O	-5.11	116.47	121.58	2	1
1	A	125	LYS	CB-CA-C	-5.07	100.89	110.16	8	1
1	A	34	ASP	CB-CA-C	-5.01	101.53	110.70	5	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	93	PHE	Sidechain	7
1	A	119	TYR	Sidechain	5
1	A	14	TYR	Sidechain	5
1	A	130	LYS	Peptide	4
1	A	22	GLY	Peptide	4
1	A	47	PHE	Sidechain	3
1	A	128	PHE	Sidechain	3
1	A	17	PHE	Sidechain	3
1	A	70	TYR	Sidechain	3
1	A	117	TYR	Sidechain	3
1	A	55	PHE	Sidechain	3
1	A	68	PHE	Sidechain	2
1	A	100	ASN	Peptide	2
1	A	38	LEU	Peptide	1
1	A	62	PHE	Sidechain	1
1	A	88	LYS	Peptide	1
1	A	106	ARG	Peptide	1
1	A	28	ARG	Sidechain	1
1	A	35	ASN	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	1059	1055	1054	20±7
All	All	10590	10550	10540	201

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:THR:HG22	1:A:131:ASP:OXT	0.98	1.57	5	1
1:A:82:TRP:CE3	1:A:89:LEU:HD22	0.86	2.05	7	2
1:A:5:THR:CG2	1:A:131:ASP:OXT	0.82	2.27	5	1
1:A:5:THR:HB	1:A:131:ASP:OXT	0.81	1.74	10	1
1:A:82:TRP:CE3	1:A:89:LEU:HD23	0.80	2.11	8	3
1:A:82:TRP:CH2	1:A:104:THR:CG2	0.72	2.71	4	1
1:A:11:SER:OG	1:A:126:ARG:NE	0.72	2.23	4	1
1:A:17:PHE:CZ	1:A:119:TYR:CZ	0.71	2.78	10	1
1:A:126:ARG:CZ	1:A:128:PHE:CD1	0.71	2.74	1	2
1:A:126:ARG:CZ	1:A:128:PHE:CE1	0.67	2.78	1	2
1:A:131:ASP:OXT	1:A:131:ASP:OD1	0.66	2.13	3	2
1:A:42:GLN:NE2	1:A:47:PHE:CE2	0.66	2.64	10	7
1:A:47:PHE:CG	1:A:62:PHE:CE1	0.65	2.84	3	2
1:A:131:ASP:OD1	1:A:131:ASP:OXT	0.65	2.15	9	1
1:A:17:PHE:CE1	1:A:119:TYR:CG	0.64	2.86	10	1
1:A:126:ARG:NH1	1:A:128:PHE:CZ	0.64	2.66	1	3
1:A:47:PHE:CD2	1:A:84:LEU:HD13	0.64	2.28	7	1
1:A:82:TRP:CD2	1:A:89:LEU:HD23	0.64	2.27	8	2
1:A:17:PHE:CE1	1:A:119:TYR:CD1	0.63	2.86	10	1
1:A:23:VAL:HG13	1:A:27:LYS:HB3	0.63	1.68	3	1
1:A:62:PHE:CE2	1:A:82:TRP:CD1	0.62	2.88	1	1
1:A:102:LEU:HD23	1:A:103:ASN:N	0.59	2.12	9	3
1:A:17:PHE:CZ	1:A:119:TYR:CE1	0.58	2.92	10	2
1:A:102:LEU:HD13	1:A:119:TYR:CD1	0.57	2.34	5	1
1:A:47:PHE:CE2	1:A:84:LEU:HD13	0.57	2.34	7	2
1:A:102:LEU:HD22	1:A:119:TYR:CE2	0.57	2.34	10	1
1:A:21:MET:HE1	1:A:119:TYR:CD2	0.57	2.34	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:TYR:O	1:A:121:GLY:N	0.57	2.37	8	3
1:A:92:LYS:C	1:A:93:PHE:CD1	0.56	2.82	4	1
1:A:82:TRP:CZ3	1:A:91:GLY:N	0.56	2.73	3	3
1:A:126:ARG:NH1	1:A:128:PHE:CE2	0.56	2.74	8	1
1:A:11:SER:OG	1:A:126:ARG:NH2	0.55	2.40	10	2
1:A:8:VAL:HG21	1:A:126:ARG:CZ	0.55	2.32	3	2
1:A:78:LEU:N	1:A:78:LEU:HD13	0.54	2.15	5	1
1:A:126:ARG:NH2	1:A:128:PHE:CD1	0.54	2.75	1	2
1:A:6:TRP:CH2	1:A:108:ILE:HD11	0.53	2.38	8	2
1:A:130:LYS:O	1:A:131:ASP:C	0.53	2.51	7	1
1:A:126:ARG:NH1	1:A:128:PHE:CE1	0.53	2.76	1	1
1:A:24:ASN:O	1:A:25:ILE:C	0.52	2.52	3	7
1:A:88:LYS:O	1:A:89:LEU:C	0.52	2.53	5	1
1:A:62:PHE:CZ	1:A:82:TRP:NE1	0.51	2.78	9	1
1:A:85:GLU:O	1:A:86:GLY:C	0.51	2.53	9	2
1:A:23:VAL:HG13	1:A:24:ASN:N	0.50	2.21	4	1
1:A:123:GLU:CD	1:A:123:GLU:C	0.50	2.80	3	1
1:A:17:PHE:CD1	1:A:124:ALA:HB2	0.50	2.42	5	1
1:A:20:LYS:O	1:A:119:TYR:CE2	0.49	2.65	1	1
1:A:21:MET:SD	1:A:119:TYR:CD1	0.49	3.05	7	1
1:A:35:ASN:O	1:A:36:LEU:HG	0.49	2.08	6	1
1:A:82:TRP:CH2	1:A:106:ARG:HG3	0.49	2.43	7	3
1:A:42:GLN:NE2	1:A:47:PHE:CE1	0.49	2.81	2	1
1:A:18:MET:O	1:A:19:GLU:C	0.48	2.56	4	7
1:A:109:ILE:O	1:A:111:ASP:N	0.48	2.47	7	2
1:A:59:GLU:CD	1:A:59:GLU:C	0.48	2.82	5	1
1:A:17:PHE:CE1	1:A:119:TYR:CE1	0.48	3.02	10	1
1:A:17:PHE:CD1	1:A:119:TYR:CD1	0.48	3.01	10	1
1:A:83:SER:O	1:A:85:GLU:N	0.48	2.47	6	1
1:A:107:GLU:O	1:A:108:ILE:C	0.48	2.57	4	1
1:A:22:GLY:O	1:A:23:VAL:C	0.48	2.57	3	1
1:A:38:LEU:HD12	1:A:128:PHE:CE2	0.47	2.44	3	1
1:A:5:THR:CG2	1:A:131:ASP:C	0.47	2.87	5	1
1:A:17:PHE:CZ	1:A:119:TYR:CD1	0.47	3.02	5	1
1:A:37:LYS:CG	1:A:38:LEU:N	0.47	2.77	9	4
1:A:113:LEU:HD21	1:A:115:GLN:OE1	0.47	2.09	8	1
1:A:70:TYR:CD1	1:A:71:ASN:O	0.47	2.67	7	1
1:A:37:LYS:HG2	1:A:52:SER:HB3	0.47	1.87	8	1
1:A:6:TRP:CZ2	1:A:108:ILE:HD11	0.47	2.43	6	1
1:A:85:GLU:O	1:A:87:ASN:N	0.47	2.48	10	2
1:A:108:ILE:HD13	1:A:112:GLU:O	0.47	2.08	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ASN:O	1:A:45:ASN:ND2	0.47	2.48	3	2
1:A:21:MET:SD	1:A:119:TYR:CG	0.47	3.08	7	1
1:A:84:LEU:HD23	1:A:84:LEU:C	0.47	2.35	7	1
1:A:64:LEU:HD22	1:A:64:LEU:C	0.46	2.35	2	1
1:A:43:GLU:O	1:A:44:GLY:C	0.46	2.58	10	2
1:A:82:TRP:CH2	1:A:106:ARG:CG	0.46	2.99	4	2
1:A:131:ASP:OXT	1:A:131:ASP:CG	0.46	2.58	6	1
1:A:24:ASN:O	1:A:27:LYS:N	0.46	2.48	9	2
1:A:109:ILE:O	1:A:110:GLY:C	0.46	2.58	10	1
1:A:82:TRP:CE3	1:A:91:GLY:HA3	0.46	2.46	10	2
1:A:38:LEU:HD11	1:A:49:VAL:HG13	0.46	1.88	8	1
1:A:17:PHE:CE2	1:A:119:TYR:CE1	0.46	3.04	10	1
1:A:34:ASP:OD1	1:A:34:ASP:C	0.45	2.59	3	1
1:A:82:TRP:CE3	1:A:89:LEU:CD2	0.45	2.94	8	1
1:A:4:SER:HB2	1:A:6:TRP:CE2	0.45	2.47	4	1
1:A:30:LEU:O	1:A:33:HIS:C	0.45	2.58	7	1
1:A:38:LEU:HD12	1:A:40:ILE:N	0.45	2.27	9	2
1:A:17:PHE:CE1	1:A:21:MET:HG2	0.45	2.46	8	1
1:A:62:PHE:CZ	1:A:82:TRP:CG	0.45	3.05	1	1
1:A:62:PHE:CE1	1:A:89:LEU:HD21	0.44	2.47	3	1
1:A:47:PHE:CD1	1:A:47:PHE:N	0.44	2.84	5	1
1:A:115:GLN:OE1	1:A:128:PHE:CE1	0.44	2.70	10	1
1:A:92:LYS:C	1:A:92:LYS:CD	0.44	2.90	4	1
1:A:43:GLU:O	1:A:45:ASN:N	0.44	2.51	1	3
1:A:100:ASN:C	1:A:101:GLU:O	0.44	2.61	8	1
1:A:82:TRP:CE3	1:A:89:LEU:HB3	0.44	2.48	4	2
1:A:59:GLU:C	1:A:59:GLU:CD	0.44	2.86	4	1
1:A:82:TRP:CZ3	1:A:89:LEU:HB3	0.44	2.48	4	1
1:A:37:LYS:HG3	1:A:38:LEU:N	0.44	2.28	8	2
1:A:7:LYS:HD3	1:A:7:LYS:C	0.43	2.38	8	1
1:A:21:MET:SD	1:A:119:TYR:CD2	0.43	3.11	5	1
1:A:22:GLY:C	1:A:23:VAL:O	0.43	2.58	4	1
1:A:52:SER:O	1:A:53:SER:CB	0.43	2.66	6	2
1:A:47:PHE:CB	1:A:62:PHE:CE1	0.43	3.02	10	1
1:A:17:PHE:CD1	1:A:17:PHE:C	0.43	2.94	10	1
1:A:70:TYR:C	1:A:70:TYR:CD1	0.42	2.97	3	3
1:A:102:LEU:C	1:A:102:LEU:HD23	0.42	2.40	8	1
1:A:62:PHE:CZ	1:A:89:LEU:HD11	0.42	2.49	10	1
1:A:11:SER:OG	1:A:126:ARG:CD	0.42	2.67	4	1
1:A:30:LEU:O	1:A:34:ASP:N	0.42	2.53	10	1
1:A:12:GLU:O	1:A:13:ASN:C	0.42	2.63	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:LEU:HD12	1:A:89:LEU:CD1	0.42	2.44	4	1
1:A:12:GLU:O	1:A:14:TYR:N	0.42	2.53	3	1
1:A:30:LEU:O	1:A:34:ASP:CG	0.42	2.62	6	1
1:A:129:LYS:O	1:A:131:ASP:N	0.42	2.52	9	1
1:A:82:TRP:CE3	1:A:91:GLY:CA	0.42	3.03	5	1
1:A:34:ASP:C	1:A:35:ASN:CG	0.42	2.88	6	1
1:A:84:LEU:HD12	1:A:89:LEU:HD11	0.41	1.92	6	1
1:A:18:MET:SD	1:A:31:ALA:CB	0.41	3.08	3	1
1:A:82:TRP:CZ2	1:A:104:THR:CG2	0.41	3.03	4	1
1:A:95:ARG:NE	1:A:98:ASN:OD1	0.41	2.53	4	1
1:A:119:TYR:C	1:A:121:GLY:N	0.41	2.78	4	1
1:A:131:ASP:OD1	1:A:131:ASP:C	0.41	2.64	3	1
1:A:92:LYS:O	1:A:93:PHE:CD1	0.41	2.73	4	1
1:A:70:TYR:CD1	1:A:70:TYR:C	0.41	2.99	6	1
1:A:93:PHE:CD2	1:A:104:THR:CG2	0.41	3.03	8	1
1:A:85:GLU:N	1:A:88:LYS:O	0.41	2.53	6	1
1:A:109:ILE:N	1:A:112:GLU:O	0.41	2.54	5	1
1:A:35:ASN:N	1:A:35:ASN:ND2	0.41	2.69	8	1
1:A:17:PHE:CE2	1:A:119:TYR:CZ	0.41	3.09	10	1
1:A:20:LYS:C	1:A:21:MET:HE2	0.40	2.41	7	1
1:A:17:PHE:CZ	1:A:119:TYR:CE2	0.40	3.08	10	1
1:A:62:PHE:CZ	1:A:82:TRP:CD1	0.40	3.10	1	1
1:A:47:PHE:CE1	1:A:63:GLU:O	0.40	2.74	5	1
1:A:11:SER:HB2	1:A:126:ARG:CZ	0.40	2.46	4	1
1:A:47:PHE:CZ	1:A:84:LEU:HB3	0.40	2.52	7	1
1:A:82:TRP:CH2	1:A:104:THR:HG23	0.40	2.51	4	1
1:A:108:ILE:HD12	1:A:112:GLU:O	0.40	2.16	5	1
1:A:45:ASN:ND2	1:A:45:ASN:O	0.40	2.54	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	129/131 (98%)	106±3 (82±2%)	15±2 (12±1%)	7±2 (6±2%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1290/1310 (98%)	1063 (82%)	154 (12%)	73 (6%)	2 21

All 28 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	75	GLY	6
1	A	98	ASN	6
1	A	130	LYS	6
1	A	44	GLY	5
1	A	120	GLU	5
1	A	35	ASN	5
1	A	23	VAL	4
1	A	101	GLU	3
1	A	22	GLY	3
1	A	86	GLY	3
1	A	110	GLY	3
1	A	8	VAL	2
1	A	13	ASN	2
1	A	36	LEU	2
1	A	53	SER	2
1	A	56	ARG	2
1	A	74	ASP	2
1	A	25	ILE	2
1	A	32	ALA	1
1	A	64	LEU	1
1	A	3	ASP	1
1	A	88	LYS	1
1	A	54	ALA	1
1	A	84	LEU	1
1	A	107	GLU	1
1	A	57	ASN	1
1	A	73	ALA	1
1	A	87	ASN	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	115/115 (100%)	92±4 (80±4%)	22±4 (20±4%)	3	33
All	All	1150/1150 (100%)	925 (80%)	225 (20%)	3	33

All 72 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	38	LEU	8
1	A	109	ILE	8
1	A	11	SER	7
1	A	35	ASN	7
1	A	26	VAL	6
1	A	92	LYS	6
1	A	100	ASN	6
1	A	116	THR	6
1	A	8	VAL	6
1	A	129	LYS	6
1	A	58	ILE	6
1	A	66	VAL	6
1	A	7	LYS	5
1	A	108	ILE	5
1	A	114	VAL	5
1	A	126	ARG	5
1	A	64	LEU	5
1	A	78	LEU	5
1	A	61	VAL	5
1	A	89	LEU	5
1	A	24	ASN	4
1	A	25	ILE	4
1	A	36	LEU	4
1	A	88	LYS	4
1	A	106	ARG	4
1	A	131	ASP	4
1	A	105	VAL	4
1	A	60	VAL	4
1	A	77	GLU	3
1	A	112	GLU	3
1	A	115	GLN	3
1	A	130	LYS	3
1	A	27	LYS	3
1	A	37	LYS	3
1	A	94	LYS	3
1	A	29	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	40	ILE	3
1	A	49	VAL	3
1	A	107	GLU	3
1	A	16	LYS	2
1	A	69	ASN	2
1	A	84	LEU	2
1	A	10	ARG	2
1	A	76	THR	2
1	A	104	THR	2
1	A	93	PHE	2
1	A	23	VAL	2
1	A	72	LEU	2
1	A	5	THR	1
1	A	18	MET	1
1	A	33	HIS	1
1	A	81	THR	1
1	A	125	LYS	1
1	A	41	THR	1
1	A	42	GLN	1
1	A	28	ARG	1
1	A	70	TYR	1
1	A	117	TYR	1
1	A	122	VAL	1
1	A	13	ASN	1
1	A	34	ASP	1
1	A	74	ASP	1
1	A	102	LEU	1
1	A	20	LYS	1
1	A	98	ASN	1
1	A	53	SER	1
1	A	19	GLU	1
1	A	120	GLU	1
1	A	128	PHE	1
1	A	45	ASN	1
1	A	79	ARG	1
1	A	90	ILE	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