



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:30 PM UTC

PDB ID : 1KRS / pdb_00001krs
Title : SOLUTION STRUCTURE OF THE ANTICODON BINDING DOMAIN OF
ESCHERICHIA COLI LYSYL-TRNA SYNTHETASE AND STUDIES OF
ITS INTERACTIONS WITH TRNA-LYS
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Deposited on : 1995-06-09

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

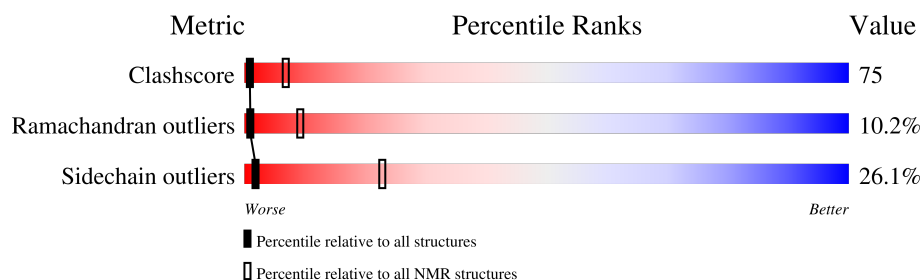
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	120	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1758 atoms, of which 881 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LYSYL-TRNA SYNTHETASE (PRODUCT OF LYSS GENE).

Mol	Chain	Residues	Atoms						Trace
1	A	110	Total	C	H	N	O	S	0
			1758	550	881	157	166	4	

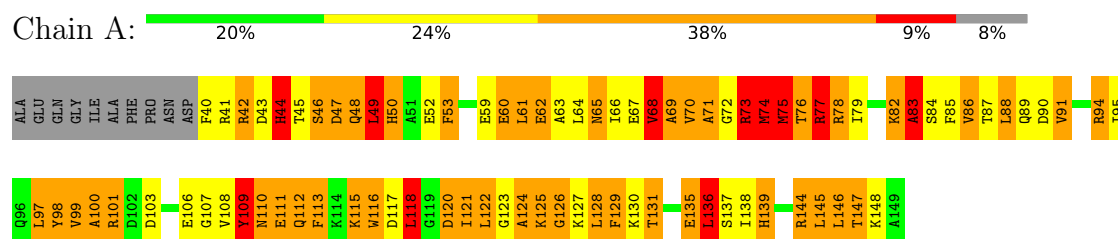
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP P0A8N3
A	?	-	LEU	deletion	UNP P0A8N3
A	?	-	ARG	deletion	UNP P0A8N3

4 Residue-property plots

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: LYSYL-TRNA SYNTHETASE (PRODUCT OF LYSS GENE)



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
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	2.26	30/889 (3.4%)	2.90	90/1189 (7.6%)
All	All	2.26	30/889 (3.4%)	2.90	90/1189 (7.6%)

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	7
All	All	0	7

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	ALA	CA-CB	-17.93	1.26	1.53
1	A	74	MET	CA-CB	-14.33	1.42	1.54
1	A	83	ALA	CA-CB	-10.85	1.35	1.53
1	A	44	HIS	CG-ND1	-9.41	1.27	1.38
1	A	139	HIS	CG-ND1	-8.09	1.29	1.38
1	A	124	ALA	CA-CB	-8.03	1.41	1.53
1	A	146	LEU	CB-CG	7.75	1.69	1.53
1	A	50	HIS	CG-ND1	-7.71	1.29	1.38
1	A	70	VAL	CA-CB	-7.35	1.44	1.54
1	A	69	ALA	CA-C	-7.22	1.43	1.53
1	A	121	ILE	N-CA	6.71	1.54	1.46
1	A	116	TRP	NE1-CE2	-6.70	1.30	1.37
1	A	113	PHE	CA-CB	-6.53	1.43	1.53
1	A	124	ALA	CA-C	-6.45	1.44	1.52
1	A	62	GLU	CA-CB	-6.08	1.43	1.53
1	A	116	TRP	CG-CD2	-5.94	1.33	1.43
1	A	111	GLU	CA-CB	-5.94	1.44	1.53
1	A	44	HIS	ND1-CE1	-5.82	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	VAL	CA-C	-5.82	1.46	1.52
1	A	76	THR	CA-CB	-5.57	1.45	1.53
1	A	108	VAL	CA-CB	-5.53	1.47	1.54
1	A	66	ILE	CA-CB	-5.45	1.47	1.54
1	A	112	GLN	CA-CB	-5.42	1.45	1.53
1	A	139	HIS	CD2-NE2	-5.21	1.32	1.37
1	A	116	TRP	CA-CB	-5.13	1.45	1.53
1	A	135	GLU	C-N	-5.13	1.26	1.33
1	A	50	HIS	CD2-NE2	-5.12	1.32	1.37
1	A	103	ASP	CA-CB	-5.10	1.45	1.53
1	A	44	HIS	CD2-NE2	-5.05	1.32	1.37
1	A	59	GLU	CA-CB	-5.05	1.45	1.53

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	HIS	CA-CB-CG	20.15	133.95	113.80
1	A	43	ASP	N-CA-C	-17.35	88.32	111.74
1	A	112	GLN	N-CA-C	-16.41	93.08	110.97
1	A	69	ALA	N-CA-C	14.20	132.37	110.36
1	A	136	LEU	N-CA-C	12.49	137.41	110.80
1	A	146	LEU	O-C-N	10.59	135.61	121.74
1	A	85	PHE	CA-CB-CG	-10.17	103.63	113.80
1	A	111	GLU	CA-CB-CG	-10.02	94.06	114.10
1	A	116	TRP	CA-CB-CG	-9.77	95.04	113.60
1	A	121	ILE	N-CA-C	9.58	122.79	108.80
1	A	112	GLN	N-CA-CB	-9.46	96.10	109.91
1	A	116	TRP	CB-CG-CD1	-9.41	112.78	126.90
1	A	146	LEU	CA-C-O	9.09	133.12	121.67
1	A	146	LEU	N-CA-CB	-9.08	97.38	110.45
1	A	116	TRP	N-CA-C	8.73	123.05	109.96
1	A	123	GLY	N-CA-C	-8.61	92.78	113.18
1	A	136	LEU	N-CA-CB	-8.46	96.20	110.49
1	A	69	ALA	N-CA-CB	-8.45	97.56	110.49
1	A	145	LEU	CA-C-N	8.39	135.70	121.86
1	A	145	LEU	C-N-CA	8.39	135.70	121.86
1	A	120	ASP	CA-CB-CG	8.26	120.86	112.60
1	A	129	PHE	CA-CB-CG	-8.07	105.73	113.80
1	A	69	ALA	O-C-N	8.05	132.19	122.20
1	A	85	PHE	N-CA-C	-7.62	96.48	108.90
1	A	68	VAL	CA-C-O	7.42	130.59	121.54
1	A	117	ASP	N-CA-C	7.36	121.59	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	LEU	N-CA-C	7.31	121.20	109.79
1	A	109	TYR	N-CA-CB	-7.20	98.33	110.49
1	A	76	THR	N-CA-C	7.19	121.12	107.75
1	A	68	VAL	O-C-N	7.05	131.26	122.59
1	A	71	ALA	N-CA-C	-6.92	99.72	109.69
1	A	115	LYS	CA-C-N	-6.92	111.27	120.95
1	A	115	LYS	C-N-CA	-6.92	111.27	120.95
1	A	135	GLU	CA-C-N	6.78	134.50	121.54
1	A	135	GLU	C-N-CA	6.78	134.50	121.54
1	A	112	GLN	CB-CA-C	6.60	121.13	110.96
1	A	62	GLU	N-CA-CB	-6.57	100.41	110.13
1	A	47	ASP	N-CA-C	-6.54	103.99	112.68
1	A	86	VAL	N-CA-CB	-6.47	103.45	112.52
1	A	116	TRP	CB-CG-CD2	6.47	135.85	126.80
1	A	106	GLU	N-CA-C	6.44	124.52	110.80
1	A	145	LEU	N-CA-CB	-6.41	100.70	110.45
1	A	136	LEU	CA-C-N	-6.33	112.18	122.81
1	A	136	LEU	C-N-CA	-6.33	112.18	122.81
1	A	64	LEU	N-CA-C	6.27	121.12	112.90
1	A	121	ILE	N-CA-CB	-6.19	103.85	112.52
1	A	129	PHE	O-C-N	6.11	130.22	123.25
1	A	120	ASP	N-CA-CB	-6.09	100.01	109.69
1	A	75	MET	CA-C-N	-6.04	114.45	122.85
1	A	75	MET	C-N-CA	-6.04	114.45	122.85
1	A	69	ALA	CA-C-O	6.04	129.12	121.82
1	A	100	ALA	N-CA-CB	-6.03	101.24	110.65
1	A	106	GLU	N-CA-CB	-6.02	100.32	110.49
1	A	98	TYR	N-CA-CB	-5.95	101.17	110.87
1	A	49	LEU	N-CA-CB	-5.95	100.43	110.49
1	A	70	VAL	CA-C-O	5.75	127.97	120.78
1	A	99	VAL	N-CA-CB	-5.69	106.54	112.06
1	A	127	LYS	CA-C-N	-5.66	114.22	122.19
1	A	127	LYS	C-N-CA	-5.66	114.22	122.19
1	A	117	ASP	O-C-N	5.57	130.11	122.59
1	A	84	SER	N-CA-CB	-5.54	102.50	110.87
1	A	131	THR	CA-CB-OG1	-5.50	101.34	109.60
1	A	79	ILE	N-CA-C	5.46	120.69	109.34
1	A	146	LEU	CA-C-N	5.45	133.56	123.32
1	A	146	LEU	C-N-CA	5.45	133.56	123.32
1	A	50	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
1	A	121	ILE	O-C-N	-5.41	117.04	123.00
1	A	63	ALA	N-CA-C	-5.41	104.62	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ASP	CB-CA-C	5.41	118.40	109.70
1	A	126	GLY	CA-C-N	-5.38	111.21	122.03
1	A	126	GLY	C-N-CA	-5.38	111.21	122.03
1	A	116	TRP	O-C-N	5.36	129.53	122.93
1	A	59	GLU	O-C-N	5.35	129.71	122.59
1	A	68	VAL	CA-CB-CG1	-5.33	101.34	110.40
1	A	146	LEU	CA-CB-CG	-5.33	97.65	116.30
1	A	66	ILE	O-C-N	5.30	128.91	123.18
1	A	139	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	A	59	GLU	CA-C-O	5.27	128.04	120.51
1	A	76	THR	CA-CB-CG2	-5.24	101.59	110.50
1	A	147	THR	N-CA-C	-5.21	102.19	109.69
1	A	116	TRP	CA-C-O	5.19	126.78	120.81
1	A	73	ARG	N-CA-C	5.16	116.92	108.76
1	A	59	GLU	CA-C-N	5.15	127.64	120.63
1	A	59	GLU	C-N-CA	5.15	127.64	120.63
1	A	118	LEU	N-CA-CB	-5.14	101.80	110.49
1	A	66	ILE	N-CA-CB	-5.13	102.46	111.39
1	A	48	GLN	N-CA-CB	-5.06	102.47	110.06
1	A	135	GLU	N-CA-CB	-5.06	101.94	110.49
1	A	74	MET	N-CA-C	5.06	114.31	108.49
1	A	60	GLU	N-CA-CB	-5.01	102.71	109.98

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	42	ARG	Sidechain
1	A	73	ARG	Sidechain
1	A	77	ARG	Sidechain
1	A	78	ARG	Sidechain
1	A	94	ARG	Sidechain
1	A	101	ARG	Sidechain
1	A	144	ARG	Sidechain

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	877	881	881	131
All	All	877	881	881	131

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 75.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:53:PHE:CE1	1:A:61:LEU:HD12	0.88	2.03
1:A:121:ILE:O	1:A:146:LEU:HB3	0.86	1.69
1:A:44:HIS:CD2	1:A:69:ALA:CB	0.79	2.66
1:A:40:PHE:CE1	1:A:44:HIS:CE1	0.76	2.73
1:A:44:HIS:CD2	1:A:69:ALA:HB3	0.73	2.18
1:A:121:ILE:N	1:A:146:LEU:HD12	0.71	2.00
1:A:146:LEU:N	1:A:146:LEU:CD2	0.67	2.57
1:A:109:TYR:CG	1:A:110:ASN:N	0.66	2.64
1:A:53:PHE:CD2	1:A:128:LEU:HD21	0.65	2.27
1:A:53:PHE:CD1	1:A:61:LEU:CD1	0.65	2.80
1:A:53:PHE:CE2	1:A:128:LEU:HG	0.65	2.27
1:A:53:PHE:CE1	1:A:61:LEU:CD1	0.64	2.80
1:A:74:MET:CB	1:A:88:LEU:HA	0.64	2.23
1:A:53:PHE:CG	1:A:128:LEU:HD21	0.64	2.28
1:A:44:HIS:CE1	1:A:68:VAL:HA	0.63	2.28
1:A:107:GLY:C	1:A:109:TYR:N	0.63	2.56
1:A:98:TYR:CE1	1:A:100:ALA:HB2	0.62	2.29
1:A:121:ILE:N	1:A:146:LEU:CD1	0.62	2.61
1:A:69:ALA:CB	1:A:124:ALA:O	0.61	2.48
1:A:109:TYR:CE1	1:A:110:ASN:HB3	0.61	2.31
1:A:122:LEU:CD1	1:A:122:LEU:N	0.60	2.64
1:A:136:LEU:C	1:A:136:LEU:HD12	0.60	2.22
1:A:112:GLN:O	1:A:116:TRP:NE1	0.60	2.34
1:A:146:LEU:CD2	1:A:146:LEU:H	0.60	2.10
1:A:69:ALA:HB2	1:A:124:ALA:O	0.59	1.95
1:A:107:GLY:C	1:A:109:TYR:H	0.59	2.04
1:A:70:VAL:CG2	1:A:124:ALA:HB3	0.59	2.28
1:A:44:HIS:CD2	1:A:69:ALA:HB2	0.59	2.31
1:A:113:PHE:HA	1:A:116:TRP:CD1	0.58	2.33
1:A:40:PHE:CE2	1:A:44:HIS:NE2	0.58	2.71
1:A:136:LEU:C	1:A:136:LEU:CD1	0.58	2.76
1:A:44:HIS:CE1	1:A:67:GLU:O	0.58	2.56
1:A:49:LEU:C	1:A:49:LEU:CD1	0.58	2.77
1:A:53:PHE:CE2	1:A:128:LEU:CG	0.58	2.87
1:A:71:ALA:HA	1:A:122:LEU:C	0.57	2.25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:121:ILE:O	1:A:146:LEU:CB	0.57	2.50
1:A:118:LEU:H	1:A:118:LEU:CD1	0.57	2.13
1:A:49:LEU:HD11	1:A:128:LEU:CD2	0.56	2.31
1:A:53:PHE:CD1	1:A:61:LEU:HD12	0.56	2.34
1:A:74:MET:SD	1:A:75:MET:N	0.56	2.79
1:A:40:PHE:CZ	1:A:44:HIS:CE1	0.56	2.94
1:A:40:PHE:CZ	1:A:44:HIS:NE2	0.55	2.74
1:A:41:ARG:O	1:A:69:ALA:HB3	0.55	2.02
1:A:98:TYR:CD2	1:A:139:HIS:CD2	0.54	2.96
1:A:46:SER:HB3	1:A:49:LEU:CB	0.54	2.33
1:A:49:LEU:C	1:A:49:LEU:HD13	0.54	2.28
1:A:116:TRP:CZ2	1:A:145:LEU:HG	0.54	2.38
1:A:109:TYR:CD1	1:A:110:ASN:N	0.53	2.77
1:A:112:GLN:C	1:A:116:TRP:NE1	0.52	2.67
1:A:69:ALA:C	1:A:70:VAL:HG13	0.52	2.28
1:A:53:PHE:CZ	1:A:128:LEU:CD2	0.52	2.93
1:A:97:LEU:HD23	1:A:97:LEU:N	0.52	2.18
1:A:40:PHE:CE2	1:A:125:LYS:HB2	0.50	2.41
1:A:82:LYS:O	1:A:83:ALA:C	0.50	2.54
1:A:46:SER:HB3	1:A:49:LEU:HB2	0.50	1.82
1:A:86:VAL:CG1	1:A:87:THR:N	0.50	2.74
1:A:49:LEU:HD12	1:A:50:HIS:CD2	0.50	2.41
1:A:44:HIS:CG	1:A:68:VAL:HG12	0.49	2.40
1:A:118:LEU:CD1	1:A:118:LEU:N	0.49	2.75
1:A:68:VAL:N	1:A:126:GLY:O	0.49	2.44
1:A:109:TYR:C	1:A:111:GLU:N	0.49	2.70
1:A:42:ARG:HB3	1:A:71:ALA:H	0.49	1.68
1:A:69:ALA:C	1:A:70:VAL:CG1	0.48	2.87
1:A:71:ALA:HA	1:A:122:LEU:O	0.48	2.08
1:A:74:MET:HB2	1:A:88:LEU:HA	0.48	1.83
1:A:118:LEU:H	1:A:118:LEU:HD13	0.48	1.67
1:A:112:GLN:O	1:A:116:TRP:CE2	0.48	2.67
1:A:53:PHE:CE2	1:A:128:LEU:CD2	0.48	2.97
1:A:122:LEU:HG	1:A:145:LEU:HD11	0.48	1.85
1:A:128:LEU:HD12	1:A:135:GLU:O	0.47	2.08
1:A:136:LEU:HD12	1:A:137:SER:N	0.47	2.24
1:A:146:LEU:HG	1:A:147:THR:N	0.47	2.20
1:A:120:ASP:C	1:A:146:LEU:HD12	0.47	2.34
1:A:129:PHE:CD1	1:A:139:HIS:HB2	0.47	2.43
1:A:116:TRP:CD2	1:A:116:TRP:N	0.47	2.71
1:A:53:PHE:CD1	1:A:61:LEU:HD11	0.47	2.44
1:A:112:GLN:C	1:A:116:TRP:HE1	0.47	2.18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:99:VAL:HG12	1:A:109:TYR:CD2	0.46	2.45
1:A:125:LYS:CD	1:A:125:LYS:C	0.46	2.88
1:A:116:TRP:CD1	1:A:116:TRP:H	0.46	2.27
1:A:45:THR:O	1:A:46:SER:CB	0.46	2.63
1:A:109:TYR:O	1:A:111:GLU:N	0.46	2.48
1:A:53:PHE:CE1	1:A:128:LEU:CD2	0.45	2.99
1:A:89:GLN:HG2	1:A:94:ARG:HG3	0.45	1.88
1:A:40:PHE:HA	1:A:44:HIS:CG	0.45	2.47
1:A:98:TYR:CE1	1:A:100:ALA:CB	0.45	3.00
1:A:40:PHE:CD1	1:A:44:HIS:CE1	0.45	3.05
1:A:53:PHE:CD1	1:A:128:LEU:HD21	0.45	2.46
1:A:116:TRP:CD2	1:A:145:LEU:CD1	0.44	3.00
1:A:112:GLN:O	1:A:115:LYS:N	0.44	2.51
1:A:70:VAL:HG22	1:A:124:ALA:HB3	0.44	1.89
1:A:121:ILE:CG2	1:A:122:LEU:N	0.44	2.80
1:A:122:LEU:HG	1:A:145:LEU:CD1	0.43	2.43
1:A:77:ARG:HD2	1:A:77:ARG:C	0.43	2.38
1:A:86:VAL:HG11	1:A:113:PHE:CE2	0.43	2.48
1:A:74:MET:HG3	1:A:88:LEU:HA	0.43	1.89
1:A:41:ARG:H	1:A:44:HIS:HB3	0.43	1.74
1:A:67:GLU:HB3	1:A:125:LYS:CG	0.43	2.44
1:A:53:PHE:CE2	1:A:128:LEU:HD21	0.42	2.50
1:A:99:VAL:CG1	1:A:109:TYR:CD2	0.42	3.03
1:A:116:TRP:CB	1:A:122:LEU:HD11	0.42	2.44
1:A:74:MET:CG	1:A:88:LEU:HA	0.42	2.43
1:A:53:PHE:CE1	1:A:128:LEU:HD23	0.42	2.49
1:A:62:GLU:HA	1:A:65:ASN:HB3	0.42	1.92
1:A:42:ARG:C	1:A:44:HIS:N	0.42	2.63
1:A:122:LEU:CD1	1:A:145:LEU:CD1	0.42	2.97
1:A:122:LEU:N	1:A:122:LEU:HD12	0.42	2.26
1:A:129:PHE:O	1:A:135:GLU:O	0.42	2.37
1:A:60:GLU:C	1:A:62:GLU:N	0.42	2.75
1:A:53:PHE:CZ	1:A:128:LEU:HG	0.42	2.49
1:A:116:TRP:CE2	1:A:145:LEU:HG	0.42	2.50
1:A:146:LEU:N	1:A:146:LEU:HD23	0.42	2.30
1:A:44:HIS:HD2	1:A:69:ALA:CB	0.41	2.21
1:A:49:LEU:O	1:A:52:GLU:N	0.41	2.53
1:A:70:VAL:HG23	1:A:124:ALA:HB3	0.41	1.91
1:A:72:GLY:O	1:A:122:LEU:HD13	0.41	2.14
1:A:137:SER:OG	1:A:138:ILE:N	0.41	2.53
1:A:71:ALA:HB1	1:A:122:LEU:O	0.41	2.16
1:A:89:GLN:HG2	1:A:94:ARG:CG	0.41	2.46

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:111:GLU:O	1:A:112:GLN:C	0.41	2.63
1:A:46:SER:O	1:A:50:HIS:CD2	0.41	2.73
1:A:131:THR:OG1	1:A:137:SER:HB3	0.41	2.15
1:A:128:LEU:CD1	1:A:135:GLU:C	0.41	2.94
1:A:74:MET:CB	1:A:88:LEU:HG	0.41	2.46
1:A:109:TYR:C	1:A:111:GLU:H	0.41	2.24
1:A:47:ASP:C	1:A:49:LEU:N	0.40	2.75
1:A:107:GLY:O	1:A:109:TYR:N	0.40	2.54
1:A:121:ILE:C	1:A:122:LEU:HD12	0.40	2.41
1:A:116:TRP:CD2	1:A:145:LEU:HD12	0.40	2.52
1:A:49:LEU:CD1	1:A:50:HIS:N	0.40	2.84
1:A:90:ASP:O	1:A:91:VAL:C	0.40	2.63

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	108/120 (90%)	70 (65%)	27 (25%)	11 (10%)	1	9
All	All	108/120 (90%)	70 (65%)	27 (25%)	11 (10%)	1	9

All 11 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	44	HIS
1	A	46	SER
1	A	65	ASN
1	A	75	MET
1	A	83	ALA
1	A	91	VAL
1	A	109	TYR
1	A	110	ASN
1	A	118	LEU
1	A	130	LYS
1	A	136	LEU

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	92/99 (93%)	68 (74%)	24 (26%)	2	23
All	All	92/99 (93%)	68 (74%)	24 (26%)	2	23

All 24 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	44	HIS
1	A	48	GLN
1	A	49	LEU
1	A	53	PHE
1	A	61	LEU
1	A	68	VAL
1	A	73	ARG
1	A	74	MET
1	A	76	THR
1	A	77	ARG
1	A	78	ARG
1	A	82	LYS
1	A	88	LEU
1	A	95	ILE
1	A	97	LEU
1	A	101	ARG
1	A	109	TYR
1	A	118	LEU
1	A	122	LEU
1	A	125	LYS
1	A	128	LEU
1	A	136	LEU
1	A	144	ARG
1	A	148	LYS

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