



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 07:34 AM UTC

PDB ID : 1G7E / pdb_00001g7e
Title : NMR STRUCTURE OF N-DOMAIN OF ERP29 PROTEIN
Authors : Liepinsh, E.; Mkrtchian, S.; Barishev, M.; Sharipo, M.; Ingelman-Sundberg, M.; Otting, G.
Deposited on : 2000-11-10

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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

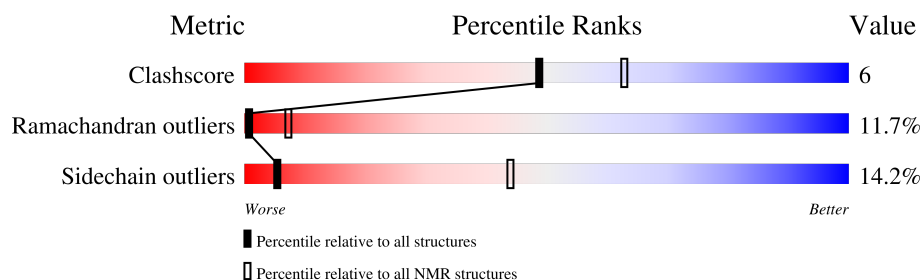
1 Overall quality at a glance

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	122	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models). The authors have identified model 17 as representative, based on the following criterion: *lowest energy. model #1 was best after dyana calculations, model #17 was best after opal refinement.*

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:33-A:152 (120)	1.07	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 5 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1951 atoms, of which 971 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ENDOPLASMIC RETICULUM PROTEIN ERP29.

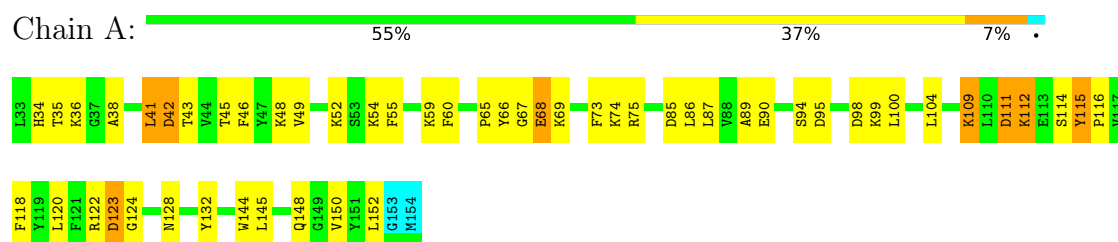
Mol	Chain	Residues	Atoms						Trace
1	A	122	Total	C	H	N	O	S	0
			1951	638	971	154	186	2	

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: ENDOPLASMIC RETICULUM PROTEIN ERP29

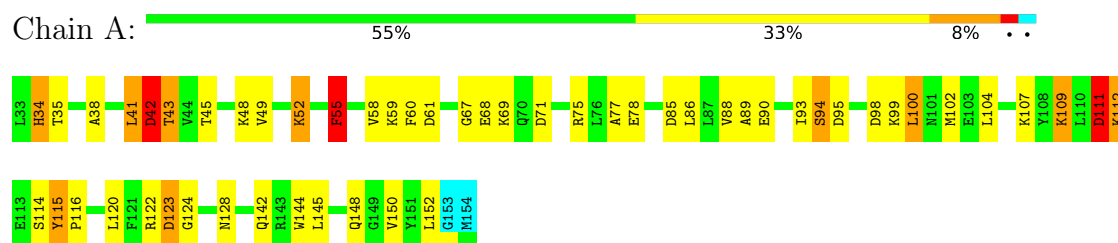


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

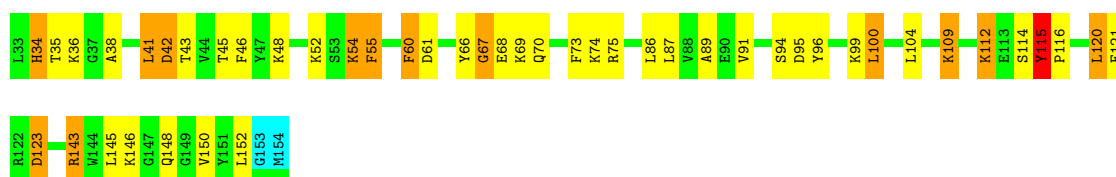
- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



4.2.2 Score per residue for model 2

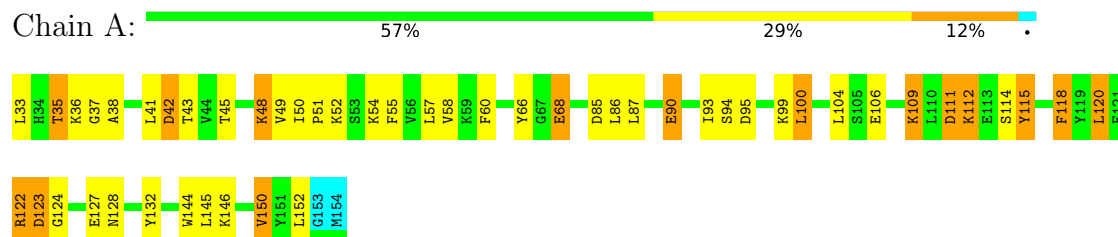
- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29





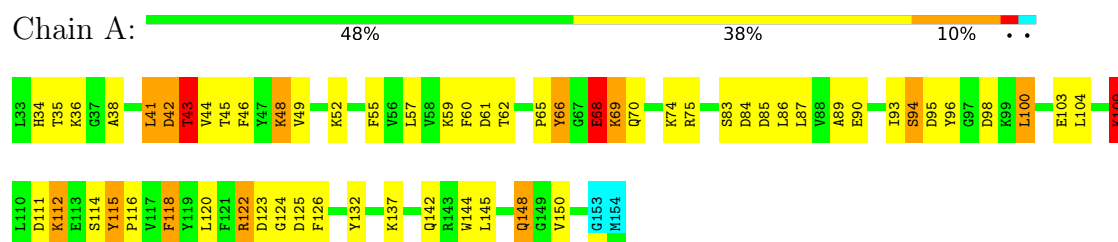
4.2.3 Score per residue for model 3

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



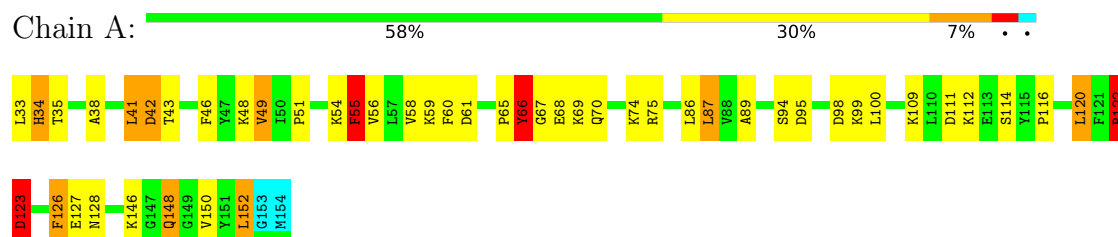
4.2.4 Score per residue for model 4

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



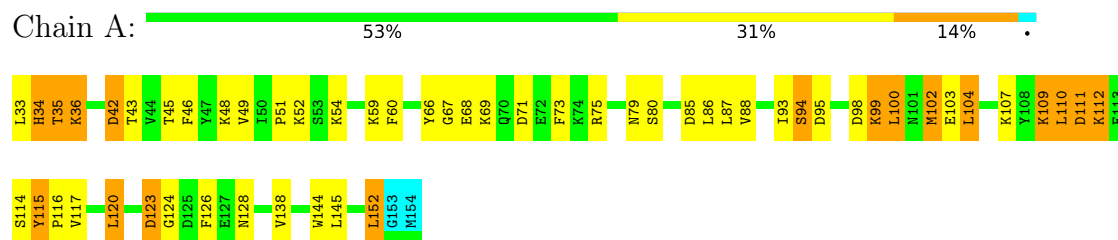
4.2.5 Score per residue for model 5

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



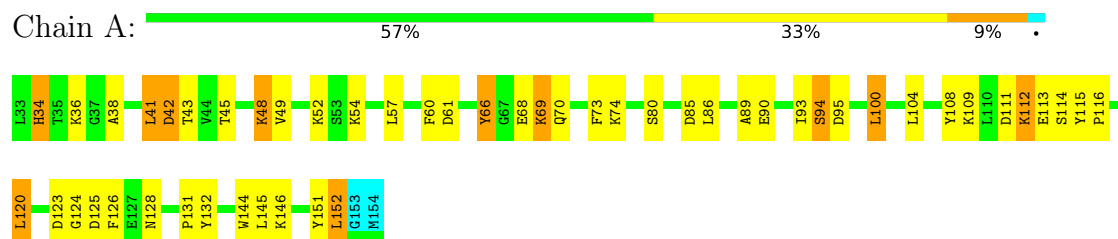
4.2.6 Score per residue for model 6

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



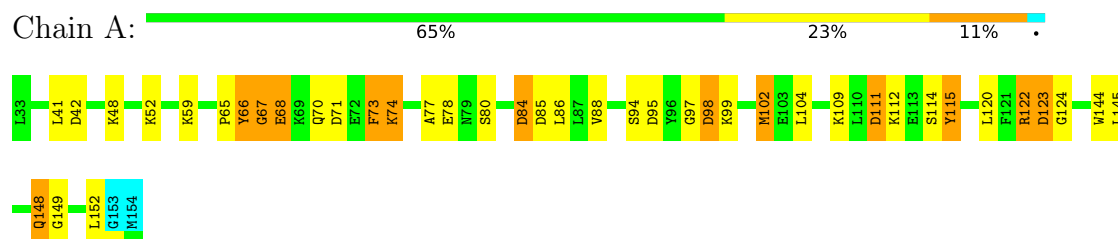
4.2.7 Score per residue for model 7

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



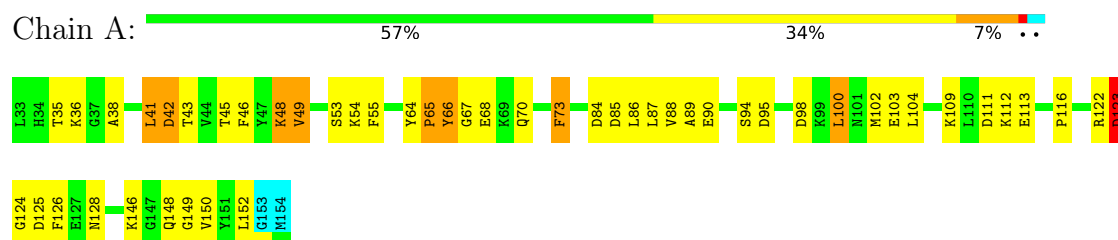
4.2.8 Score per residue for model 8

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



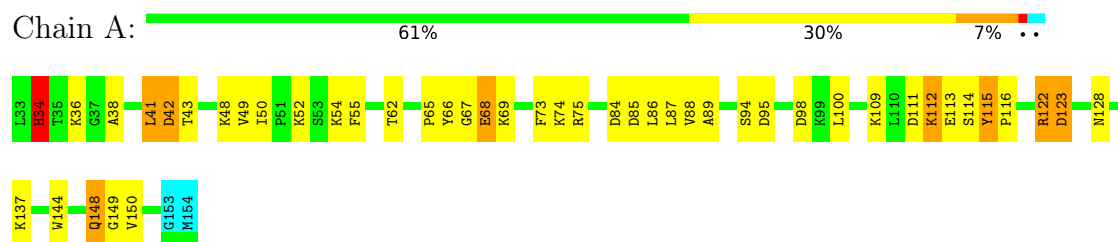
4.2.9 Score per residue for model 9

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



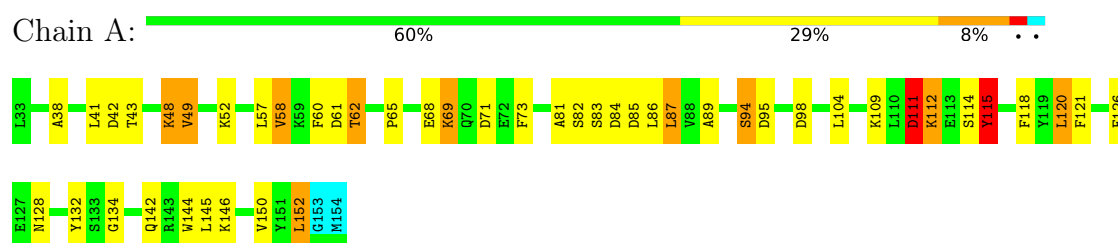
4.2.10 Score per residue for model 10

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



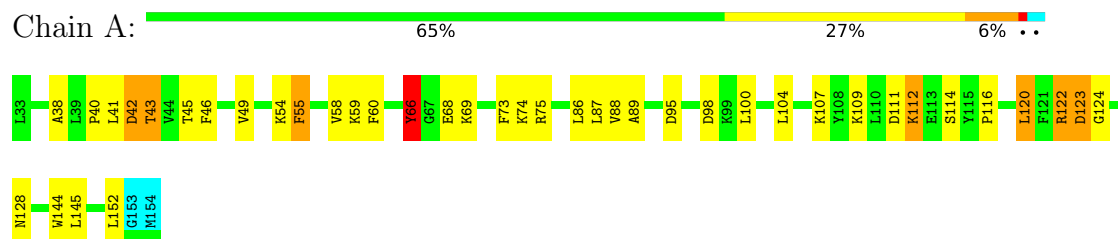
4.2.11 Score per residue for model 11

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



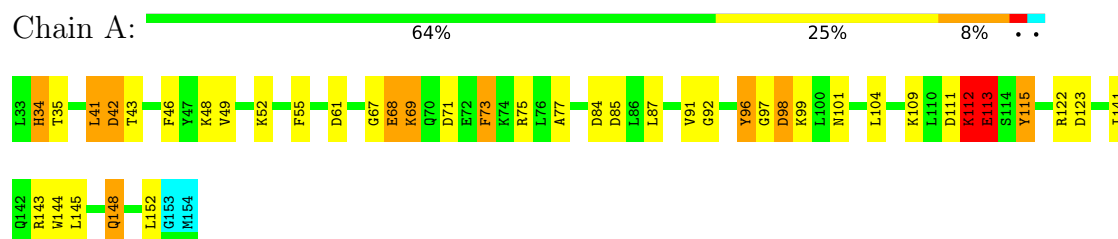
4.2.12 Score per residue for model 12

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



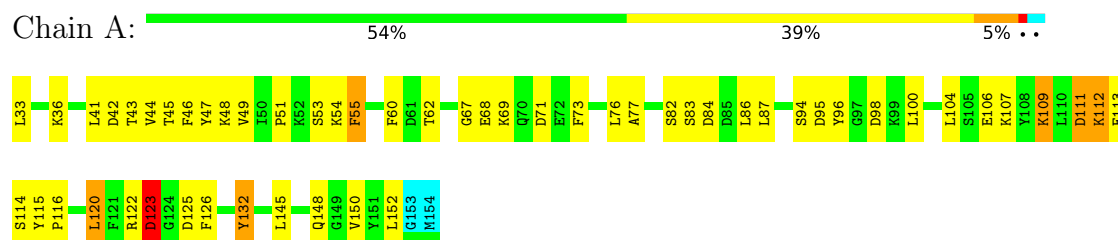
4.2.13 Score per residue for model 13

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



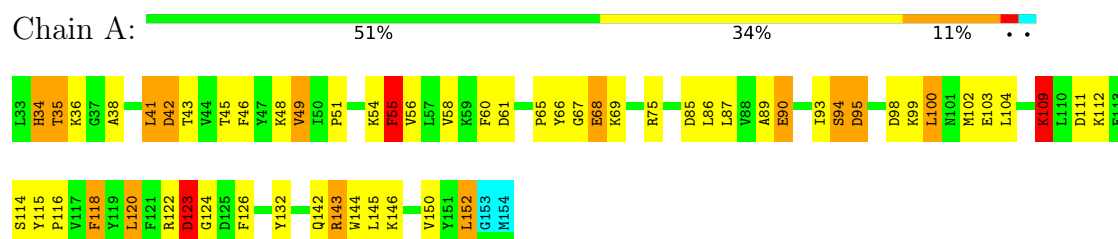
4.2.14 Score per residue for model 14

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



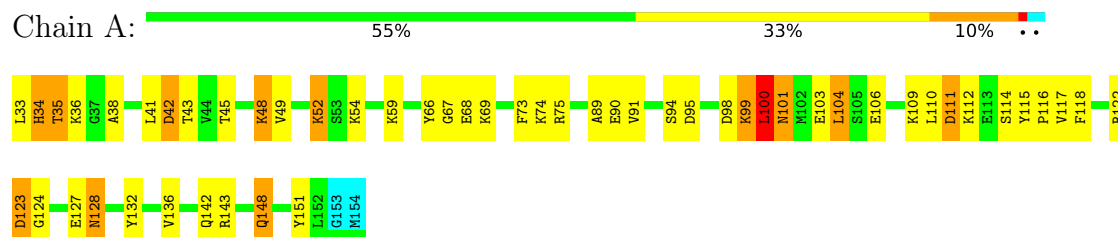
4.2.15 Score per residue for model 15

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



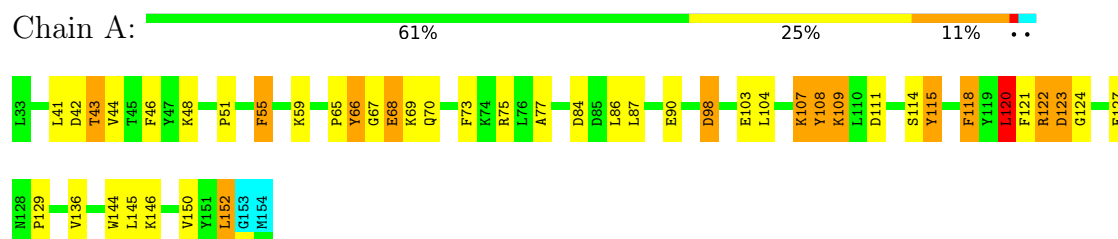
4.2.16 Score per residue for model 16

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



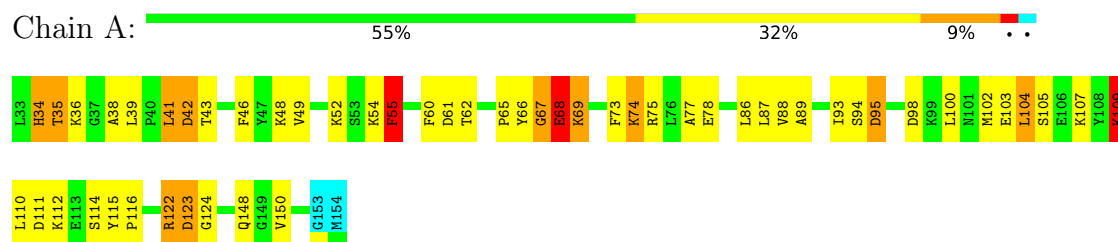
4.2.17 Score per residue for model 17

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



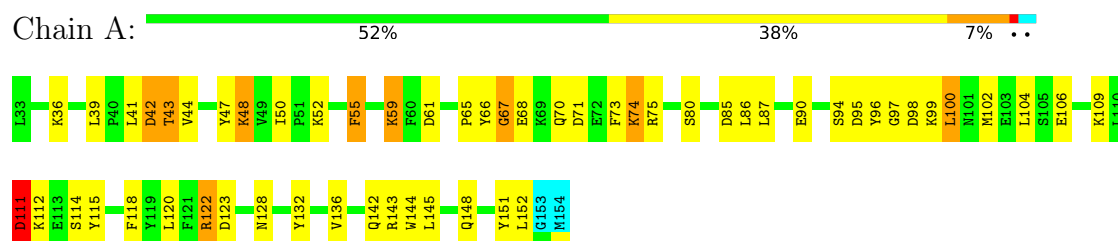
4.2.18 Score per residue for model 18

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



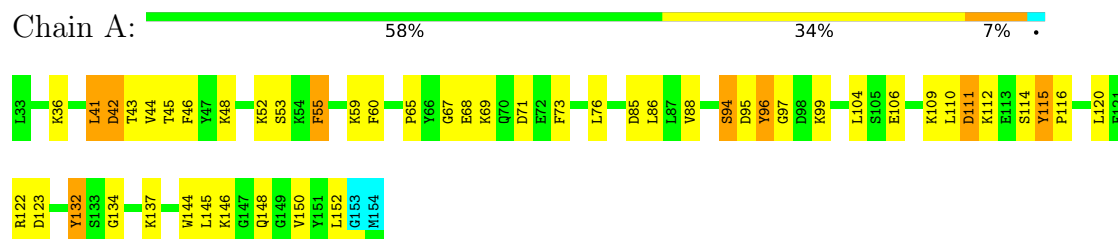
4.2.19 Score per residue for model 19

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



4.2.20 Score per residue for model 20

- Molecule 1: ENDOPLASMIC RETICULUM PROTEIN ERP29



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy, target function*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
OPAL	refinement	2.6

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	0.77±0.02	0±0/993 (0.0± 0.0%)	1.85±0.07	25±6/1343 (1.9± 0.4%)
All	All	0.77	0/19860 (0.0%)	1.85	506/26860 (1.9%)

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	4.8±1.4
All	All	0	95

There are no bond-length outliers.

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	68	GLU	CA-C-N	14.11	139.22	122.44	4	4
1	A	68	GLU	C-N-CA	14.11	139.22	122.44	4	4
1	A	118	PHE	CA-CB-CG	11.04	124.84	113.80	17	4
1	A	67	GLY	CA-C-N	10.81	142.18	121.54	15	14
1	A	67	GLY	C-N-CA	10.81	142.18	121.54	15	14
1	A	98	ASP	CA-CB-CG	10.31	122.91	112.60	8	3
1	A	122	ARG	CA-C-N	9.93	140.50	121.54	5	11
1	A	122	ARG	C-N-CA	9.93	140.50	121.54	5	11
1	A	69	LYS	N-CA-C	-9.89	100.96	113.43	18	1
1	A	65	PRO	CA-C-N	9.58	139.84	121.54	5	11
1	A	65	PRO	C-N-CA	9.58	139.84	121.54	5	11
1	A	123	ASP	CA-CB-CG	-9.23	103.37	112.60	10	11
1	A	152	LEU	CA-C-N	9.16	139.37	121.41	9	1
1	A	152	LEU	C-N-CA	9.16	139.37	121.41	9	1
1	A	84	ASP	CA-CB-CG	-8.96	103.64	112.60	9	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	149	GLY	CA-C-N	8.75	130.72	121.97	9	3
1	A	149	GLY	C-N-CA	8.75	130.72	121.97	9	3
1	A	46	PHE	CA-CB-CG	8.62	122.42	113.80	14	10
1	A	100	LEU	N-CA-C	-8.56	101.53	111.03	3	9
1	A	100	LEU	CA-C-N	8.49	132.02	120.38	14	5
1	A	100	LEU	C-N-CA	8.49	132.02	120.38	14	5
1	A	113	GLU	N-CA-C	8.44	123.35	112.89	9	2
1	A	99	LYS	CA-C-N	8.37	132.02	120.63	3	6
1	A	99	LYS	C-N-CA	8.37	132.02	120.63	3	6
1	A	98	ASP	N-CA-C	8.34	120.25	110.41	18	5
1	A	61	ASP	CA-CB-CG	8.30	120.90	112.60	13	9
1	A	77	ALA	CA-C-N	8.26	132.17	120.28	8	6
1	A	77	ALA	C-N-CA	8.26	132.17	120.28	8	6
1	A	126	PHE	CA-CB-CG	8.09	121.89	113.80	15	4
1	A	34	HIS	CA-CB-CG	8.09	121.89	113.80	10	7
1	A	49	VAL	CB-CA-C	8.00	121.81	111.81	9	7
1	A	99	LYS	N-CA-C	7.93	120.78	108.96	3	3
1	A	74	LYS	N-CA-C	-7.91	102.34	110.97	8	4
1	A	84	ASP	CA-C-N	7.85	136.53	121.54	4	3
1	A	84	ASP	C-N-CA	7.85	136.53	121.54	4	3
1	A	101	ASN	CA-CB-CG	7.66	120.26	112.60	16	1
1	A	129	PRO	CA-C-N	7.52	127.71	122.60	17	1
1	A	129	PRO	C-N-CA	7.52	127.71	122.60	17	1
1	A	71	ASP	CA-CB-CG	-7.44	105.16	112.60	11	6
1	A	98	ASP	N-CA-CB	-7.44	102.86	111.79	10	7
1	A	34	HIS	CB-CG-CD2	-7.33	121.68	131.20	10	10
1	A	94	SER	CA-C-N	7.31	135.51	121.54	2	15
1	A	94	SER	C-N-CA	7.31	135.51	121.54	2	15
1	A	48	LYS	N-CA-C	-7.25	103.28	112.93	19	4
1	A	55	PHE	N-CA-CB	-7.11	98.30	111.52	5	8
1	A	35	THR	CA-C-N	7.03	131.83	122.06	15	3
1	A	35	THR	C-N-CA	7.03	131.83	122.06	15	3
1	A	123	ASP	N-CA-CB	-7.02	98.63	110.49	5	7
1	A	125	ASP	N-CA-C	6.99	120.36	110.23	7	1
1	A	55	PHE	CA-CB-CG	6.84	120.64	113.80	5	2
1	A	73	PHE	N-CA-C	-6.81	103.94	111.36	9	3
1	A	85	ASP	CA-CB-CG	6.78	119.38	112.60	11	4
1	A	85	ASP	N-CA-C	-6.74	103.96	112.93	9	5
1	A	50	ILE	CB-CA-C	6.64	122.70	114.00	3	2
1	A	88	VAL	CA-CB-CG2	6.64	121.69	110.40	8	7
1	A	98	ASP	CA-C-N	6.58	134.10	121.54	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	98	ASP	C-N-CA	6.58	134.10	121.54	13	2
1	A	101	ASN	CA-C-N	6.53	129.32	120.44	16	1
1	A	101	ASN	C-N-CA	6.53	129.32	120.44	16	1
1	A	151	TYR	N-CA-CB	6.49	120.70	110.84	16	1
1	A	127	GLU	CA-C-N	6.48	137.62	121.80	16	1
1	A	127	GLU	C-N-CA	6.48	137.62	121.80	16	1
1	A	110	LEU	CA-C-N	6.45	133.87	121.54	18	2
1	A	110	LEU	C-N-CA	6.45	133.87	121.54	18	2
1	A	45	THR	CA-C-N	6.28	129.02	120.54	4	11
1	A	45	THR	C-N-CA	6.28	129.02	120.54	4	11
1	A	120	LEU	N-CA-C	-6.27	99.66	109.25	17	1
1	A	143	ARG	CD-NE-CZ	6.25	133.14	124.40	16	1
1	A	122	ARG	CB-CA-C	6.21	122.60	110.30	20	1
1	A	106	GLU	N-CA-C	6.20	117.84	111.14	14	1
1	A	102	MET	CA-C-N	6.19	129.42	120.38	8	3
1	A	102	MET	C-N-CA	6.19	129.42	120.38	8	3
1	A	69	LYS	CA-C-N	6.18	131.84	122.56	13	1
1	A	69	LYS	C-N-CA	6.18	131.84	122.56	13	1
1	A	53	SER	CA-C-N	6.14	129.01	120.29	14	2
1	A	53	SER	C-N-CA	6.14	129.01	120.29	14	2
1	A	103	GLU	N-CA-C	-6.11	104.73	111.82	4	3
1	A	78	GLU	CA-CB-CG	6.09	126.28	114.10	18	3
1	A	106	GLU	N-CA-CB	-6.09	101.15	110.16	3	5
1	A	90	GLU	CB-CG-CD	6.09	122.95	112.60	15	1
1	A	123	ASP	N-CA-C	6.08	123.75	110.80	16	5
1	A	68	GLU	CB-CA-C	-6.06	98.36	110.42	17	1
1	A	122	ARG	CA-CB-CG	6.04	126.18	114.10	17	2
1	A	66	TYR	N-CA-C	6.02	123.63	110.80	5	1
1	A	108	TYR	CA-C-N	6.00	133.00	121.54	17	2
1	A	108	TYR	C-N-CA	6.00	133.00	121.54	17	2
1	A	82	SER	CA-C-N	5.94	132.88	121.54	11	2
1	A	82	SER	C-N-CA	5.94	132.88	121.54	11	2
1	A	115	TYR	N-CA-CB	-5.90	103.77	111.09	17	1
1	A	122	ARG	N-CA-CB	-5.88	100.89	110.59	17	1
1	A	103	GLU	CA-C-N	5.87	128.96	120.38	17	1
1	A	103	GLU	C-N-CA	5.87	128.96	120.38	17	1
1	A	45	THR	CB-CA-C	5.86	119.49	109.24	15	1
1	A	93	ILE	CA-C-N	5.83	132.68	121.54	1	6
1	A	93	ILE	C-N-CA	5.83	132.68	121.54	1	6
1	A	111	ASP	CA-CB-CG	5.81	118.41	112.60	11	3
1	A	48	LYS	CA-C-N	5.81	127.96	120.70	4	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	48	LYS	C-N-CA	5.81	127.96	120.70	4	4
1	A	41	LEU	CB-CA-C	5.78	121.93	110.42	13	7
1	A	95	ASP	CA-CB-CG	5.73	118.33	112.60	15	1
1	A	34	HIS	CA-C-N	5.69	132.41	121.54	4	2
1	A	34	HIS	C-N-CA	5.69	132.41	121.54	4	2
1	A	62	THR	CA-C-N	5.68	128.15	120.65	11	1
1	A	62	THR	C-N-CA	5.68	128.15	120.65	11	1
1	A	103	GLU	CA-CB-CG	5.66	125.42	114.10	9	1
1	A	83	SER	CA-C-N	5.64	132.31	121.54	4	1
1	A	83	SER	C-N-CA	5.64	132.31	121.54	4	1
1	A	49	VAL	CA-C-O	-5.63	115.55	121.41	7	1
1	A	110	LEU	N-CA-CB	5.62	116.65	110.35	20	1
1	A	152	LEU	N-CA-C	-5.59	99.69	108.63	9	1
1	A	53	SER	N-CA-C	-5.59	98.90	110.80	20	1
1	A	40	PRO	CA-C-N	5.57	132.18	121.54	12	1
1	A	40	PRO	C-N-CA	5.57	132.18	121.54	12	1
1	A	52	LYS	CA-C-N	5.52	131.03	121.64	16	2
1	A	52	LYS	C-N-CA	5.52	131.03	121.64	16	2
1	A	99	LYS	CA-C-O	-5.51	115.34	121.51	8	2
1	A	141	ILE	CA-C-N	5.46	127.91	120.54	13	1
1	A	141	ILE	C-N-CA	5.46	127.91	120.54	13	1
1	A	59	LYS	N-CA-CB	-5.44	101.67	110.71	19	1
1	A	109	LYS	N-CA-CB	5.42	119.65	110.49	4	3
1	A	144	TRP	CA-C-N	5.41	127.80	120.38	10	1
1	A	144	TRP	C-N-CA	5.41	127.80	120.38	10	1
1	A	81	ALA	CA-C-N	5.41	128.07	120.28	11	1
1	A	81	ALA	C-N-CA	5.41	128.07	120.28	11	1
1	A	122	ARG	CD-NE-CZ	5.40	131.97	124.40	19	1
1	A	123	ASP	CA-C-N	5.30	131.81	121.41	17	1
1	A	123	ASP	C-N-CA	5.30	131.81	121.41	17	1
1	A	50	ILE	N-CA-C	-5.30	105.99	112.35	3	1
1	A	91	VAL	CB-CA-C	5.29	118.64	110.91	2	1
1	A	120	LEU	CA-C-N	5.29	132.00	122.64	5	1
1	A	120	LEU	C-N-CA	5.29	132.00	122.64	5	1
1	A	113	GLU	CA-C-N	5.27	131.61	121.54	7	2
1	A	113	GLU	C-N-CA	5.27	131.61	121.54	7	2
1	A	46	PHE	N-CA-C	-5.24	105.26	110.97	17	2
1	A	134	GLY	CA-C-N	5.23	128.20	120.82	11	2
1	A	134	GLY	C-N-CA	5.23	128.20	120.82	11	2
1	A	124	GLY	CA-C-N	5.20	128.73	121.24	15	2
1	A	124	GLY	C-N-CA	5.20	128.73	121.24	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	68	GLU	N-CA-C	5.17	121.82	110.80	17	1
1	A	102	MET	CA-CB-CG	-5.17	103.77	114.10	15	1
1	A	150	VAL	CB-CA-C	5.15	119.74	111.29	5	2
1	A	73	PHE	CA-CB-CG	-5.14	108.66	113.80	10	2
1	A	115	TYR	N-CA-C	5.13	118.09	110.39	2	1
1	A	74	LYS	N-CA-CB	5.13	117.40	109.91	8	1
1	A	128	ASN	N-CA-CB	5.13	119.50	110.37	16	1
1	A	128	ASN	CA-C-N	5.12	125.12	120.21	19	1
1	A	128	ASN	C-N-CA	5.12	125.12	120.21	19	1
1	A	50	ILE	CA-C-N	5.09	126.20	119.84	3	1
1	A	50	ILE	C-N-CA	5.09	126.20	119.84	3	1
1	A	88	VAL	CG1-CB-CG2	-5.08	99.62	110.80	10	1
1	A	45	THR	N-CA-C	5.06	119.61	113.38	12	1
1	A	58	VAL	CB-CA-C	5.05	118.78	110.69	11	1
1	A	68	GLU	O-C-N	5.03	129.27	122.59	4	1
1	A	111	ASP	CA-C-N	5.02	131.13	121.54	3	1
1	A	111	ASP	C-N-CA	5.02	131.13	121.54	3	1
1	A	43	THR	CB-CA-C	5.01	120.39	110.42	4	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	115	TYR	Sidechain	13
1	A	73	PHE	Sidechain	13
1	A	75	ARG	Sidechain	12
1	A	66	TYR	Sidechain	11
1	A	132	TYR	Sidechain	9
1	A	55	PHE	Sidechain	6
1	A	96	TYR	Sidechain	6
1	A	122	ARG	Sidechain	4
1	A	123	ASP	Sidechain	4
1	A	143	ARG	Sidechain	3
1	A	42	ASP	Mainchain	2
1	A	126	PHE	Sidechain	2
1	A	151	TYR	Sidechain	2
1	A	118	PHE	Sidechain	2
1	A	121	PHE	Sidechain	2
1	A	60	PHE	Sidechain	1
1	A	64	TYR	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	34	HIS	Sidechain	1
1	A	47	TYR	Sidechain	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	968	959	957	11±3
All	All	19360	19180	19140	223

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:THR:HG21	1:A:38:ALA:HB3	0.80	1.51	3	2
1:A:38:ALA:HB1	1:A:89:ALA:HA	0.69	1.65	7	12
1:A:120:LEU:HD22	1:A:145:LEU:HD23	0.68	1.64	2	5
1:A:41:LEU:HD12	1:A:42:ASP:H	0.68	1.47	9	13
1:A:55:PHE:CD2	1:A:150:VAL:HG11	0.65	2.26	1	5
1:A:86:LEU:HD13	1:A:152:LEU:CD1	0.65	2.21	6	6
1:A:99:LYS:HE2	1:A:102:MET:SD	0.59	2.37	6	1
1:A:86:LEU:O	1:A:87:LEU:HD12	0.58	1.98	14	8
1:A:120:LEU:HD22	1:A:145:LEU:CD2	0.57	2.29	17	12
1:A:100:LEU:CD1	1:A:104:LEU:HD21	0.57	2.30	16	1
1:A:60:PHE:CE2	1:A:104:LEU:HD12	0.56	2.36	18	1
1:A:144:TRP:CZ3	1:A:145:LEU:HD21	0.56	2.36	20	9
1:A:35:THR:CG2	1:A:38:ALA:HB3	0.56	2.29	15	1
1:A:80:SER:CB	1:A:86:LEU:HD11	0.56	2.31	19	2
1:A:60:PHE:CZ	1:A:104:LEU:HD12	0.55	2.36	6	1
1:A:69:LYS:HE2	1:A:69:LYS:H	0.55	1.62	11	1
1:A:35:THR:OG1	1:A:38:ALA:HB3	0.54	2.02	18	3
1:A:49:VAL:HG13	1:A:87:LEU:CD2	0.54	2.32	9	6
1:A:55:PHE:CE2	1:A:150:VAL:HG11	0.53	2.37	18	2
1:A:118:PHE:CZ	1:A:136:VAL:HG22	0.53	2.38	16	1
1:A:86:LEU:C	1:A:87:LEU:HD12	0.52	2.29	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:VAL:HG13	1:A:87:LEU:HD22	0.52	1.81	10	3
1:A:86:LEU:HD12	1:A:86:LEU:C	0.52	2.28	8	9
1:A:68:GLU:CD	1:A:68:GLU:H	0.52	2.13	15	2
1:A:80:SER:HA	1:A:86:LEU:HD11	0.51	1.81	6	2
1:A:91:VAL:HG12	1:A:92:GLY:H	0.51	1.64	13	1
1:A:80:SER:HB2	1:A:86:LEU:HD11	0.50	1.84	8	2
1:A:69:LYS:H	1:A:69:LYS:CD	0.50	2.20	4	1
1:A:35:THR:HG21	1:A:38:ALA:CB	0.49	2.32	3	2
1:A:36:LYS:HE3	1:A:36:LYS:H	0.49	1.66	6	1
1:A:59:LYS:HZ2	1:A:136:VAL:HG13	0.48	1.67	17	1
1:A:55:PHE:CE1	1:A:145:LEU:HD22	0.48	2.43	17	2
1:A:120:LEU:HD21	1:A:148:GLN:OE1	0.47	2.08	2	2
1:A:86:LEU:HB3	1:A:150:VAL:CG2	0.47	2.39	14	7
1:A:41:LEU:HD12	1:A:42:ASP:N	0.47	2.24	4	6
1:A:148:GLN:NE2	1:A:148:GLN:H	0.47	2.06	16	3
1:A:96:TYR:CG	1:A:97:GLY:N	0.47	2.82	13	2
1:A:96:TYR:CG	1:A:101:ASN:HB2	0.47	2.44	13	1
1:A:148:GLN:N	1:A:148:GLN:HE21	0.47	2.07	8	3
1:A:58:VAL:HG12	1:A:60:PHE:CE2	0.46	2.45	1	5
1:A:110:LEU:HD13	1:A:117:VAL:HG21	0.46	1.87	6	2
1:A:39:LEU:HD11	1:A:87:LEU:HD12	0.46	1.88	19	1
1:A:86:LEU:HD13	1:A:152:LEU:HD13	0.46	1.87	20	1
1:A:59:LYS:HE2	1:A:118:PHE:CD2	0.46	2.45	4	1
1:A:110:LEU:HD22	1:A:117:VAL:HG11	0.46	1.88	16	1
1:A:60:PHE:CE2	1:A:104:LEU:HD23	0.45	2.46	2	1
1:A:122:ARG:HG3	1:A:123:ASP:H	0.45	1.71	5	1
1:A:39:LEU:CD1	1:A:87:LEU:HD12	0.45	2.41	19	1
1:A:56:VAL:HG22	1:A:87:LEU:HD22	0.45	1.87	15	2
1:A:75:ARG:HB2	1:A:138:VAL:HG21	0.45	1.87	6	1
1:A:112:LYS:HZ3	1:A:113:GLU:CD	0.45	2.19	13	1
1:A:60:PHE:CE2	1:A:104:LEU:CD2	0.45	2.99	3	9
1:A:120:LEU:HB2	1:A:144:TRP:CH2	0.45	2.45	17	3
1:A:55:PHE:CE2	1:A:120:LEU:HD21	0.45	2.47	5	1
1:A:125:ASP:CG	1:A:126:PHE:H	0.45	2.20	9	2
1:A:59:LYS:HE2	1:A:136:VAL:HG13	0.45	1.88	19	1
1:A:55:PHE:CZ	1:A:145:LEU:HD22	0.44	2.46	3	3
1:A:59:LYS:HE3	1:A:118:PHE:CD1	0.44	2.47	19	1
1:A:61:ASP:CG	1:A:69:LYS:HZ3	0.44	2.20	7	1
1:A:55:PHE:C	1:A:55:PHE:CD1	0.43	2.96	1	1
1:A:91:VAL:HG12	1:A:92:GLY:N	0.43	2.28	13	1
1:A:58:VAL:HG12	1:A:60:PHE:CZ	0.43	2.48	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:VAL:HG12	1:A:87:LEU:CD2	0.42	2.44	5	2
1:A:43:THR:HG23	1:A:44:VAL:H	0.42	1.73	17	1
1:A:49:VAL:HG13	1:A:87:LEU:HD23	0.42	1.91	11	1
1:A:107:LYS:HE3	1:A:108:TYR:CZ	0.42	2.49	17	1
1:A:54:LYS:O	1:A:54:LYS:HE3	0.42	2.14	2	1
1:A:38:ALA:HB2	1:A:90:GLU:CD	0.42	2.39	3	1
1:A:42:ASP:O	1:A:43:THR:C	0.42	2.61	4	2
1:A:49:VAL:CG1	1:A:87:LEU:CD2	0.42	2.97	14	2
1:A:93:ILE:HD12	1:A:105:SER:HB3	0.42	1.91	18	1
1:A:46:PHE:CE2	1:A:126:PHE:CD1	0.42	3.08	9	1
1:A:79:ASN:HD22	1:A:79:ASN:C	0.42	2.23	6	1
1:A:73:PHE:CE2	1:A:90:GLU:HB3	0.42	2.49	17	1
1:A:47:TYR:HA	1:A:126:PHE:CE1	0.41	2.50	14	1
1:A:76:LEU:HD11	1:A:88:VAL:HG11	0.41	1.91	20	1
1:A:125:ASP:CG	1:A:126:PHE:N	0.41	2.78	9	3
1:A:86:LEU:HD12	1:A:87:LEU:N	0.41	2.31	19	1
1:A:115:TYR:CD1	1:A:115:TYR:N	0.41	2.88	8	1
1:A:115:TYR:N	1:A:115:TYR:CD1	0.41	2.87	11	1
1:A:76:LEU:HD11	1:A:88:VAL:CG1	0.41	2.45	20	1
1:A:60:PHE:CE1	1:A:104:LEU:HD12	0.41	2.51	6	1
1:A:91:VAL:HG11	1:A:101:ASN:HD22	0.41	1.76	13	1
1:A:95:ASP:HB3	1:A:102:MET:HE2	0.41	1.92	18	1
1:A:144:TRP:CZ3	1:A:145:LEU:CD2	0.40	3.04	13	3
1:A:55:PHE:CD1	1:A:150:VAL:HG11	0.40	2.50	15	1
1:A:120:LEU:HD12	1:A:121:PHE:N	0.40	2.32	2	1
1:A:146:LYS:HD3	1:A:146:LYS:C	0.40	2.42	3	1
1:A:55:PHE:CE1	1:A:120:LEU:HD13	0.40	2.51	19	1
1:A:86:LEU:C	1:A:86:LEU:HD12	0.40	2.41	5	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	119/122 (98%)	80±4 (67±3%)	25±4 (21±3%)	14±2 (12±1%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2380/2440 (98%)	1599 (67%)	502 (21%)	279 (12%)	1 7

All 32 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	42	ASP	20
1	A	68	GLU	20
1	A	109	LYS	20
1	A	43	THR	19
1	A	111	ASP	19
1	A	112	LYS	19
1	A	123	ASP	19
1	A	95	ASP	18
1	A	114	SER	18
1	A	116	PRO	14
1	A	66	TYR	11
1	A	124	GLY	10
1	A	128	ASN	10
1	A	94	SER	9
1	A	98	ASP	9
1	A	35	THR	8
1	A	51	PRO	6
1	A	67	GLY	5
1	A	44	VAL	4
1	A	85	ASP	4
1	A	152	LEU	2
1	A	127	GLU	2
1	A	97	GLY	2
1	A	62	THR	2
1	A	83	SER	2
1	A	37	GLY	1
1	A	131	PRO	1
1	A	84	ASP	1
1	A	65	PRO	1
1	A	99	LYS	1
1	A	49	VAL	1
1	A	91	VAL	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	105/106 (99%)	90±3 (86±3%)	15±3 (14±3%)	5 44
All	All	2100/2120 (99%)	1801 (86%)	299 (14%)	5 44

All 46 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	48	LYS	19
1	A	69	LYS	16
1	A	52	LYS	14
1	A	100	LEU	14
1	A	115	TYR	13
1	A	36	LYS	13
1	A	54	LYS	12
1	A	152	LEU	12
1	A	112	LYS	11
1	A	148	GLN	11
1	A	34	HIS	10
1	A	109	LYS	9
1	A	74	LYS	9
1	A	120	LEU	9
1	A	41	LEU	8
1	A	90	GLU	8
1	A	111	ASP	8
1	A	70	GLN	8
1	A	146	LYS	8
1	A	122	ARG	8
1	A	104	LEU	8
1	A	59	LYS	7
1	A	107	LYS	6
1	A	142	GLN	6
1	A	33	LEU	5
1	A	57	LEU	4
1	A	43	THR	3
1	A	55	PHE	3
1	A	102	MET	3

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Mol	Chain	Res	Type	Models (Total)
1	A	99	LYS	3
1	A	143	ARG	3
1	A	68	GLU	3
1	A	62	THR	3
1	A	137	LYS	3
1	A	87	LEU	3
1	A	118	PHE	2
1	A	103	GLU	2
1	A	113	GLU	2
1	A	71	ASP	2
1	A	132	TYR	2
1	A	66	TYR	1
1	A	76	LEU	1
1	A	101	ASN	1
1	A	127	GLU	1
1	A	39	LEU	1
1	A	50	ILE	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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided