



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 05:03 PM UTC

PDB ID : 2JMZ / pdb_00002jmz
Title : Solution structure of a KlbA intein precursor from *Methanococcus jannaschii*
Authors : Johnson, M.A.; Southworth, M.W.; Herrmann, T.; Brace, L.; Perler, F.B.;
Wuthrich, K.A.
Deposited on : 2006-12-14

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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

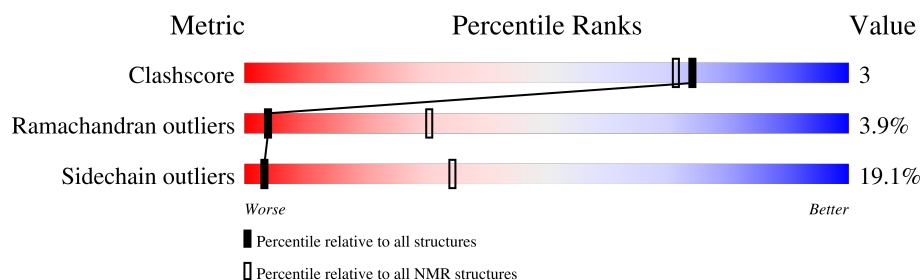
1 Overall quality at a glance

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	186	

2 Ensemble composition and analysis

This entry contains 20 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:8-A:176 (169)	0.66	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 and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3008 atoms, of which 1494 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical protein MJ0781.

Mol	Chain	Residues	Atoms						Trace
1	A	186	Total	C	H	N	O	S	0
			3008	967	1494	260	285	2	

There are 8 discrepancies between the modelled and reference sequences:

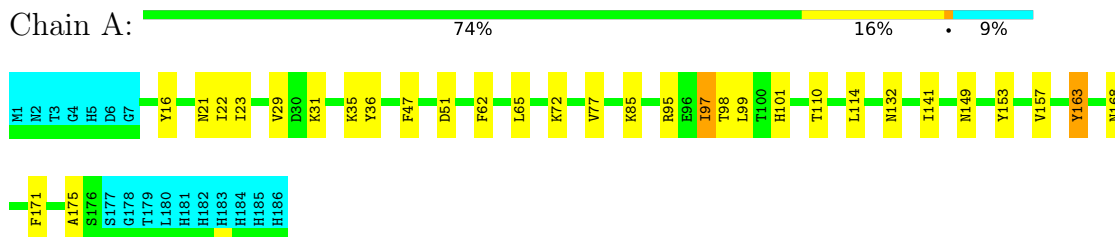
Chain	Residue	Modelled	Actual	Comment	Reference
A	175	ALA	ASN	engineered mutation	UNP Q58191
A	176	SER	CYS	engineered mutation	UNP Q58191
A	181	HIS	-	expression tag	UNP Q58191
A	182	HIS	-	expression tag	UNP Q58191
A	183	HIS	-	expression tag	UNP Q58191
A	184	HIS	-	expression tag	UNP Q58191
A	185	HIS	-	expression tag	UNP Q58191
A	186	HIS	-	expression tag	UNP Q58191

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: Hypothetical protein MJ0781

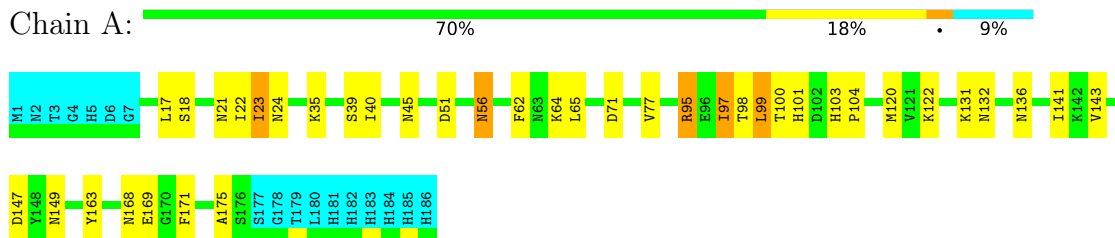


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

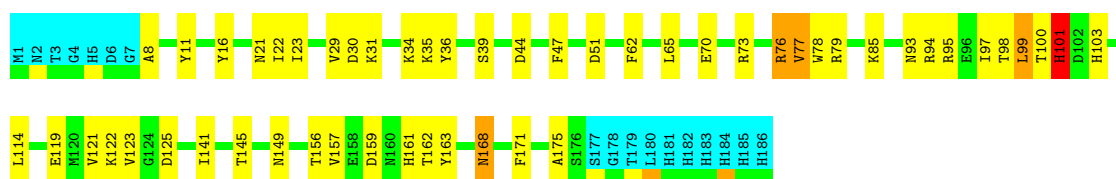
- Molecule 1: Hypothetical protein MJ0781



4.2.2 Score per residue for model 2

- Molecule 1: Hypothetical protein MJ0781

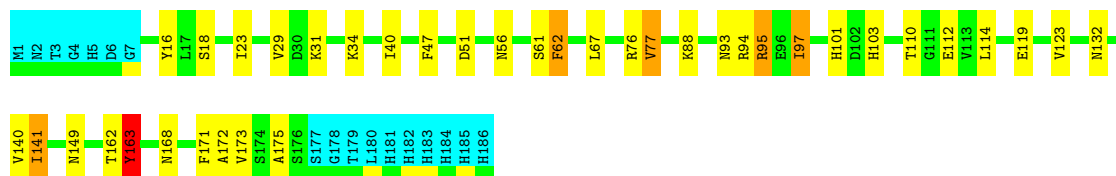




4.2.3 Score per residue for model 3

- Molecule 1: Hypothetical protein MJ0781

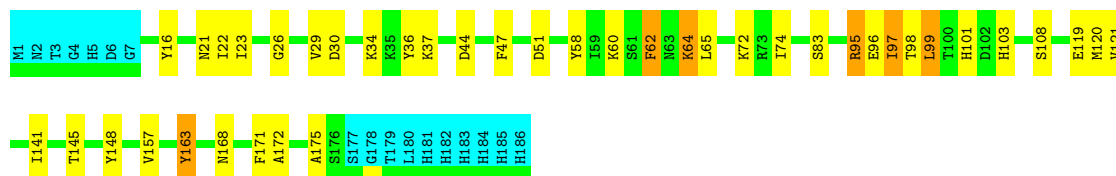
Chain A: 70% 17% 9%



4.2.4 Score per residue for model 4

- Molecule 1: Hypothetical protein MJ0781

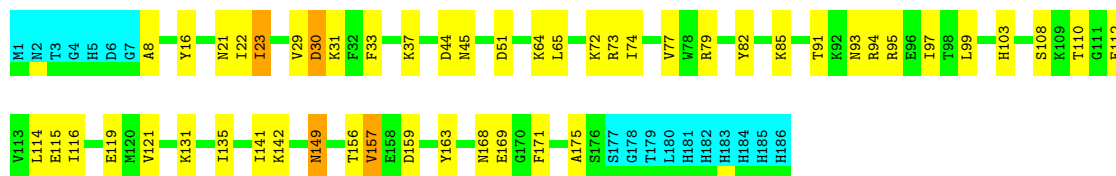
Chain A: 69% 19% 9%



4.2.5 Score per residue for model 5

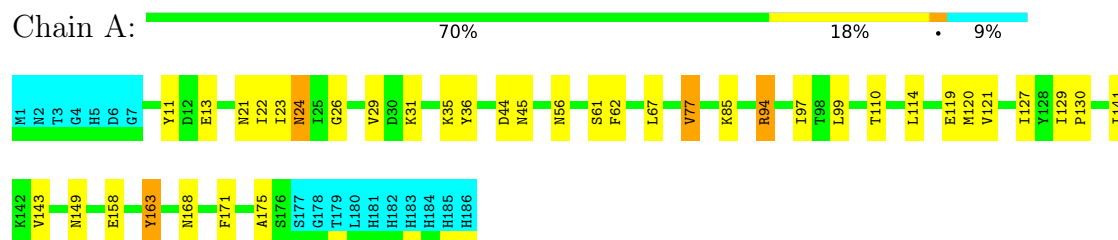
- Molecule 1: Hypothetical protein MJ0781

Chain A: 64% 25% 9%



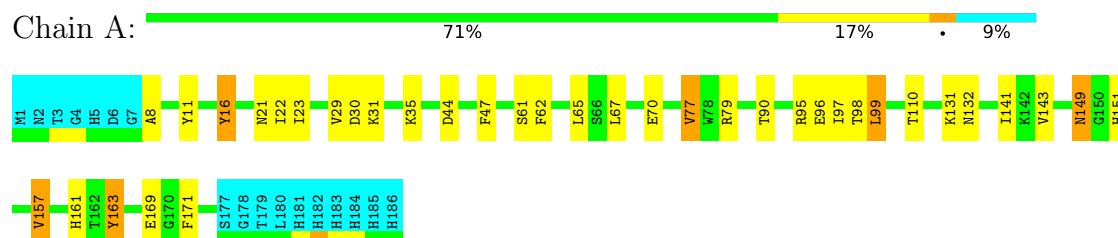
4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical protein MJ0781



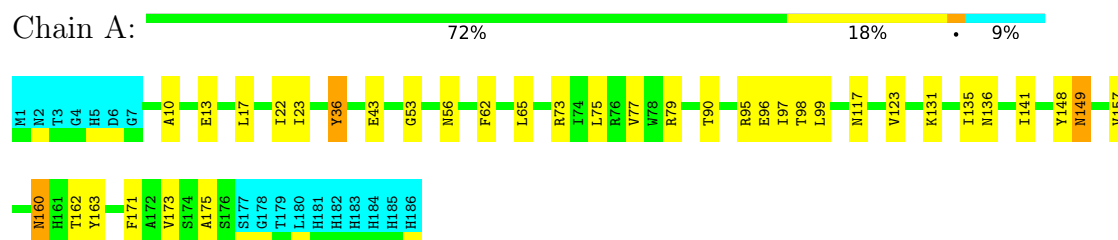
4.2.7 Score per residue for model 7

- Molecule 1: Hypothetical protein MJ0781



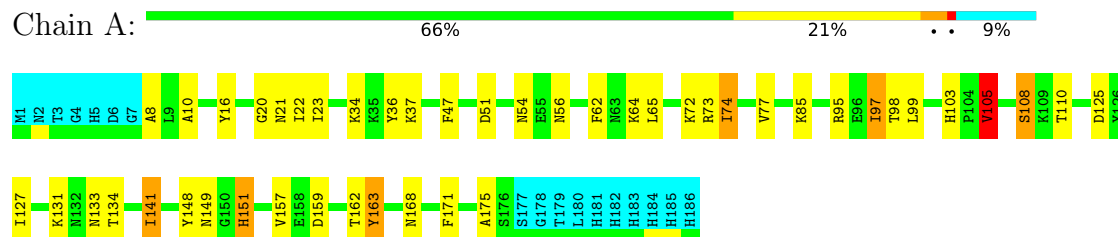
4.2.8 Score per residue for model 8

- Molecule 1: Hypothetical protein MJ0781



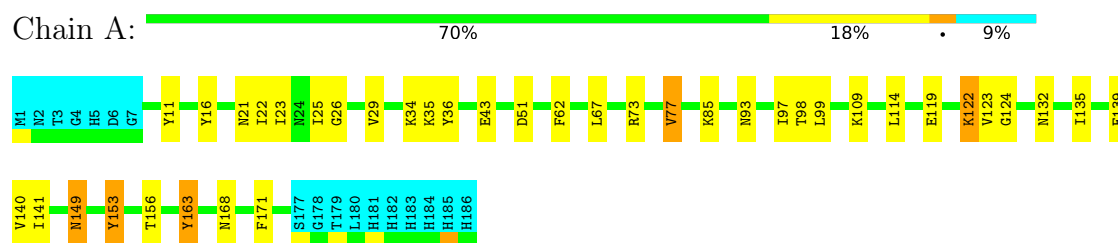
4.2.9 Score per residue for model 9

- Molecule 1: Hypothetical protein MJ0781



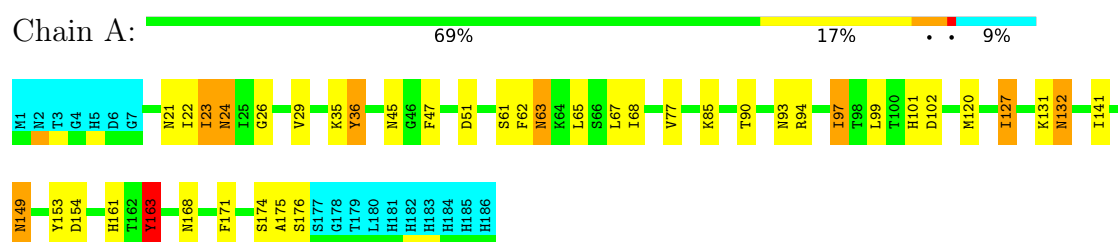
4.2.10 Score per residue for model 10

- Molecule 1: Hypothetical protein MJ0781



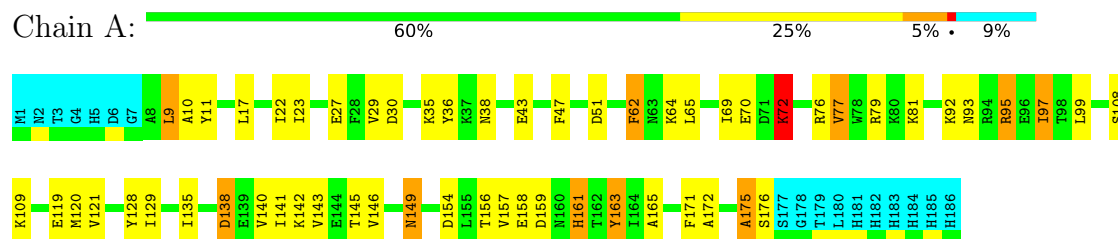
4.2.11 Score per residue for model 11

- Molecule 1: Hypothetical protein MJ0781



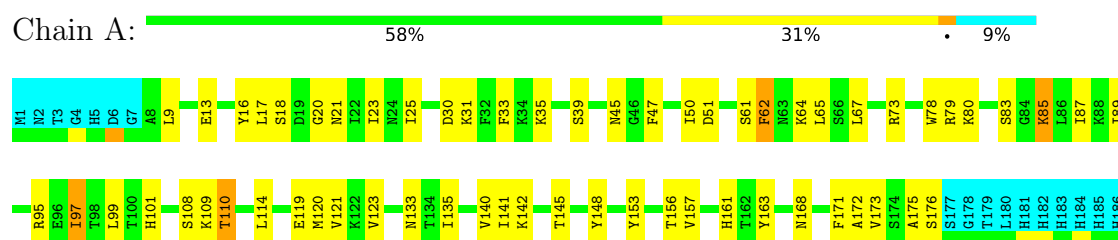
4.2.12 Score per residue for model 12

- Molecule 1: Hypothetical protein MJ0781



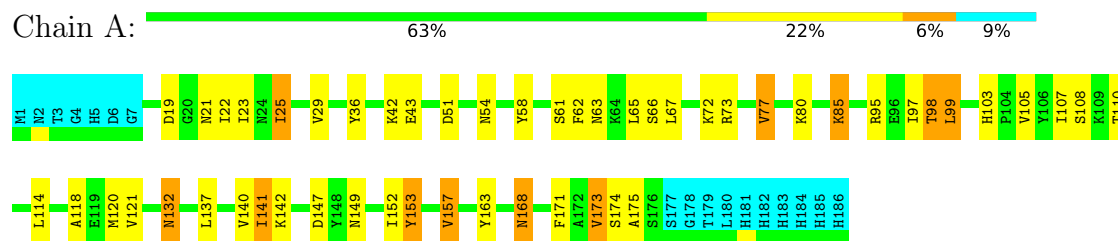
4.2.13 Score per residue for model 13

- Molecule 1: Hypothetical protein MJ0781



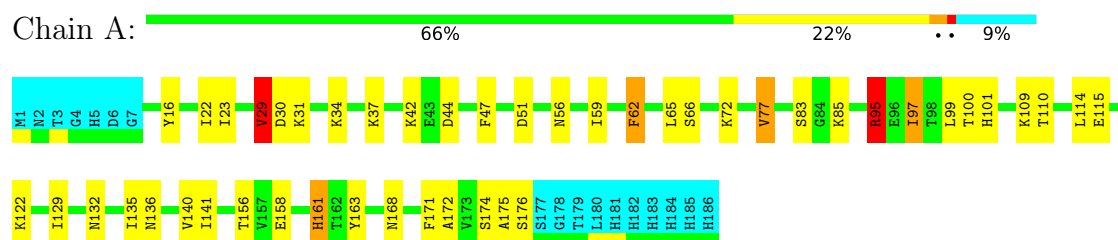
4.2.14 Score per residue for model 14

- Molecule 1: Hypothetical protein MJ0781



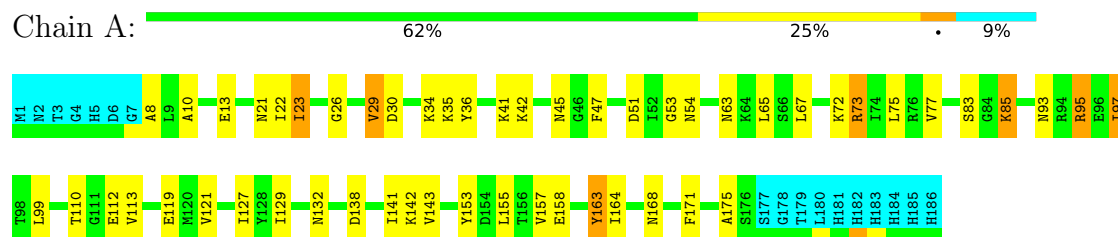
4.2.15 Score per residue for model 15

- Molecule 1: Hypothetical protein MJ0781



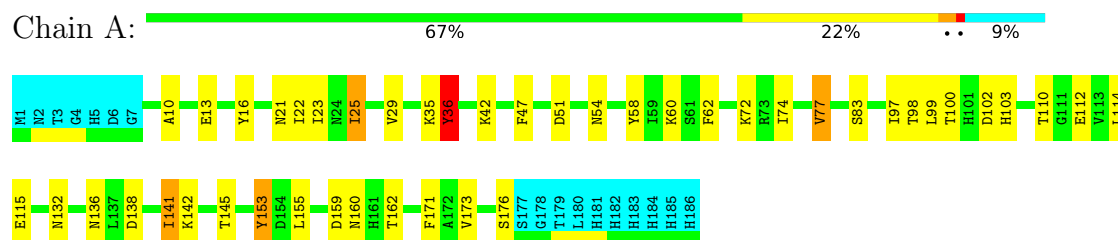
4.2.16 Score per residue for model 16

- Molecule 1: Hypothetical protein MJ0781



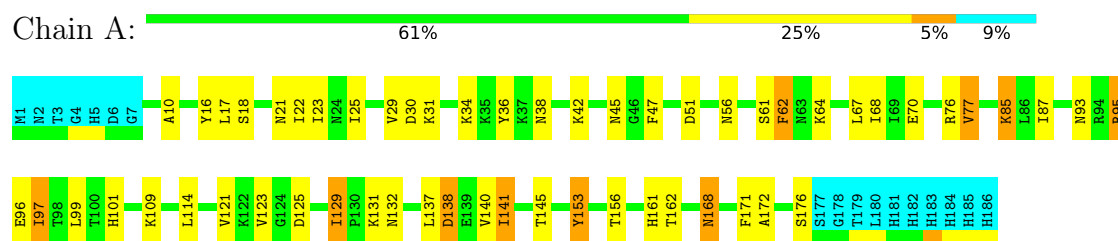
4.2.17 Score per residue for model 17

- Molecule 1: Hypothetical protein MJ0781



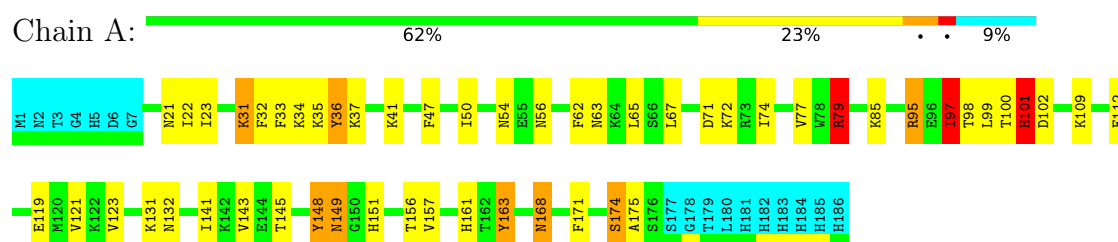
4.2.18 Score per residue for model 18

- Molecule 1: Hypothetical protein MJ0781



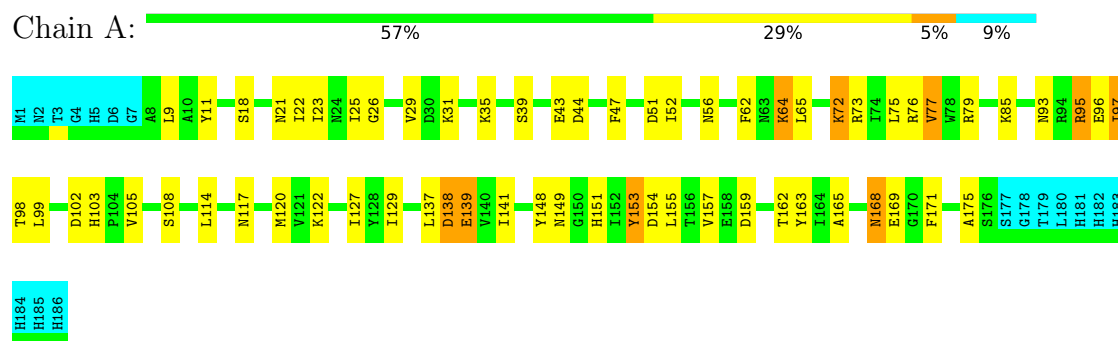
4.2.19 Score per residue for model 19

- Molecule 1: Hypothetical protein MJ0781



4.2.20 Score per residue for model 20

- Molecule 1: Hypothetical protein MJ0781



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
ATNOS/CANDID	structure solution	1.2
CYANA	structure solution	1.0.3
OPAL	refinement	1.2

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	0.67±0.01	0±0/1408 (0.0± 0.0%)	1.44±0.04	7±4/1902 (0.4± 0.2%)
All	All	0.67	0/28160 (0.0%)	1.44	137/38040 (0.4%)

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	2.8±1.8
All	All	0	55

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	138	ASP	CA-CB-CG	15.67	128.27	112.60	18	3
1	A	63	ASN	CA-CB-CG	11.88	124.48	112.60	11	1
1	A	100	THR	CA-C-N	9.03	138.79	121.54	2	2
1	A	100	THR	C-N-CA	9.03	138.79	121.54	2	2
1	A	95	ARG	CD-NE-CZ	8.91	136.87	124.40	16	6
1	A	173	VAL	N-CA-CB	-8.62	102.41	112.32	17	1
1	A	154	ASP	CA-CB-CG	8.07	120.67	112.60	20	2
1	A	159	ASP	CA-CB-CG	7.65	120.25	112.60	5	1
1	A	149	ASN	CA-CB-CG	7.25	119.85	112.60	7	9
1	A	29	VAL	CA-CB-CG2	6.68	121.76	110.40	15	2
1	A	101	HIS	CA-CB-CG	6.65	120.45	113.80	3	5
1	A	98	THR	CA-CB-OG1	6.54	119.41	109.60	14	1
1	A	161	HIS	CA-CB-CG	6.51	120.31	113.80	12	5
1	A	138	ASP	CA-C-N	6.49	129.93	120.71	17	1
1	A	138	ASP	C-N-CA	6.49	129.93	120.71	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	136	ASN	CA-CB-CG	6.46	119.06	112.60	1	2
1	A	105	VAL	CA-CB-CG1	6.28	121.08	110.40	9	1
1	A	13	GLU	CB-CA-C	6.16	118.36	110.16	16	2
1	A	56	ASN	CA-CB-CG	6.16	118.76	112.60	1	1
1	A	154	ASP	CA-C-N	6.14	133.27	121.54	20	1
1	A	154	ASP	C-N-CA	6.14	133.27	121.54	20	1
1	A	140	VAL	CA-C-N	6.14	133.02	121.97	18	2
1	A	140	VAL	C-N-CA	6.14	133.02	121.97	18	2
1	A	24	ASN	CA-CB-CG	5.95	118.55	112.60	11	3
1	A	103	HIS	CB-CG-CD2	-5.88	123.55	131.20	2	6
1	A	9	LEU	CA-C-N	5.88	132.78	121.54	12	1
1	A	9	LEU	C-N-CA	5.88	132.78	121.54	12	1
1	A	102	ASP	CA-CB-CG	5.87	118.47	112.60	20	1
1	A	175	ALA	CA-C-N	5.80	132.62	121.54	12	1
1	A	175	ALA	C-N-CA	5.80	132.62	121.54	12	1
1	A	101	HIS	CB-CG-CD2	-5.80	123.66	131.20	1	3
1	A	64	LYS	CA-C-N	5.74	128.76	120.38	18	3
1	A	64	LYS	C-N-CA	5.74	128.76	120.38	18	3
1	A	158	GLU	CA-C-N	5.74	128.44	120.63	6	2
1	A	158	GLU	C-N-CA	5.74	128.44	120.63	6	2
1	A	98	THR	CB-CA-C	5.74	118.94	111.42	14	1
1	A	43	GLU	CA-C-N	5.73	128.28	120.54	12	1
1	A	43	GLU	C-N-CA	5.73	128.28	120.54	12	1
1	A	56	ASN	CA-C-N	5.72	128.38	120.49	1	3
1	A	56	ASN	C-N-CA	5.72	128.38	120.49	1	3
1	A	140	VAL	CB-CA-C	5.62	118.17	111.20	3	2
1	A	72	LYS	CG-CD-CE	5.60	124.18	111.30	12	1
1	A	93	ASN	CA-CB-CG	5.59	118.19	112.60	3	1
1	A	36	TYR	CA-C-N	5.58	128.07	120.54	11	2
1	A	36	TYR	C-N-CA	5.58	128.07	120.54	11	2
1	A	139	GLU	CA-C-N	5.56	130.07	121.34	20	1
1	A	139	GLU	C-N-CA	5.56	130.07	121.34	20	1
1	A	30	ASP	CA-CB-CG	5.51	118.11	112.60	5	1
1	A	113	VAL	CB-CA-C	5.50	118.68	111.53	16	1
1	A	132	ASN	CA-CB-CG	5.46	118.06	112.60	11	1
1	A	102	ASP	N-CA-CB	-5.44	104.03	111.65	20	1
1	A	141	ILE	CA-C-N	5.44	131.47	122.33	14	1
1	A	141	ILE	C-N-CA	5.44	131.47	122.33	14	1
1	A	117	ASN	CA-C-N	5.39	127.82	120.54	20	1
1	A	117	ASN	C-N-CA	5.39	127.82	120.54	20	1
1	A	52	ILE	CA-C-N	5.35	126.88	120.13	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	52	ILE	C-N-CA	5.35	126.88	120.13	20	1
1	A	173	VAL	CA-C-N	5.35	128.47	120.87	13	1
1	A	173	VAL	C-N-CA	5.35	128.47	120.87	13	1
1	A	87	ILE	CB-CA-C	5.35	117.47	111.59	13	1
1	A	127	ILE	CB-CA-C	5.34	118.09	111.15	11	1
1	A	22	ILE	CB-CA-C	5.34	120.05	111.29	2	1
1	A	143	VAL	CB-CA-C	5.31	118.08	110.33	7	1
1	A	20	GLY	CA-C-N	5.31	127.70	120.54	9	1
1	A	20	GLY	C-N-CA	5.31	127.70	120.54	9	1
1	A	151	HIS	CB-CG-CD2	-5.28	124.33	131.20	9	2
1	A	160	ASN	CA-CB-CG	-5.27	107.33	112.60	8	1
1	A	23	ILE	CA-C-N	5.24	128.21	120.82	1	3
1	A	23	ILE	C-N-CA	5.24	128.21	120.82	1	3
1	A	23	ILE	N-CA-CB	-5.17	106.44	112.34	5	1
1	A	129	ILE	CA-CB-CG1	5.17	119.20	110.40	18	1
1	A	141	ILE	N-CA-C	5.16	120.06	109.34	18	1
1	A	117	ASN	CA-CB-CG	5.08	117.68	112.60	8	1
1	A	9	LEU	N-CA-CB	-5.06	103.09	110.53	13	1
1	A	10	ALA	CA-C-N	5.02	127.26	120.38	18	1
1	A	10	ALA	C-N-CA	5.02	127.26	120.38	18	1
1	A	104	PRO	N-CA-CB	5.01	107.31	103.30	1	1
1	A	96	GLU	CA-C-N	5.00	129.83	123.03	4	1
1	A	96	GLU	C-N-CA	5.00	129.83	123.03	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	16	TYR	Sidechain	10
1	A	36	TYR	Sidechain	6
1	A	73	ARG	Sidechain	6
1	A	163	TYR	Sidechain	6
1	A	94	ARG	Sidechain	3
1	A	58	TYR	Sidechain	3
1	A	148	TYR	Sidechain	3
1	A	71	ASP	Peptide	2
1	A	11	TYR	Sidechain	2
1	A	79	ARG	Sidechain	2
1	A	99	LEU	Peptide	1
1	A	88	LYS	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	82	TYR	Peptide	1
1	A	130	PRO	Peptide	1
1	A	108	SER	Peptide	1
1	A	133	ASN	Peptide	1
1	A	154	ASP	Peptide	1
1	A	101	HIS	Peptide	1
1	A	164	ILE	Peptide	1
1	A	95	ARG	Sidechain	1
1	A	174	SER	Peptide	1
1	A	175	ALA	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	1380	1387	1387	9±4
All	All	27600	27740	27740	175

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:PHE:CD2	1:A:172:ALA:HB1	0.73	2.18	4	2
1:A:163:TYR:CD2	1:A:175:ALA:HB2	0.67	2.25	20	11
1:A:105:VAL:HG21	1:A:121:VAL:HG21	0.64	1.68	14	1
1:A:26:GLY:HA2	1:A:29:VAL:HG22	0.64	1.70	16	3
1:A:29:VAL:HG21	1:A:153:TYR:CE2	0.63	2.29	14	5
1:A:29:VAL:HG21	1:A:153:TYR:CZ	0.61	2.30	17	5
1:A:97:ILE:HG23	1:A:171:PHE:CE1	0.59	2.31	12	19
1:A:62:PHE:CD1	1:A:172:ALA:HB1	0.58	2.34	13	2
1:A:98:THR:C	1:A:99:LEU:HD23	0.57	2.25	7	2
1:A:103:HIS:ND1	1:A:118:ALA:HB2	0.56	2.15	14	1
1:A:29:VAL:HG22	1:A:77:VAL:HG21	0.54	1.78	6	9
1:A:29:VAL:HG21	1:A:153:TYR:CD2	0.54	2.38	11	2
1:A:105:VAL:HG21	1:A:121:VAL:CG2	0.53	2.33	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:TYR:C	1:A:149:ASN:HD22	0.53	2.12	20	3
1:A:85:LYS:HE3	1:A:85:LYS:H	0.53	1.64	18	2
1:A:129:ILE:HG12	1:A:138:ASP:CG	0.52	2.29	18	2
1:A:122:LYS:HG3	1:A:124:GLY:H	0.52	1.65	10	1
1:A:72:LYS:HZ3	1:A:157:VAL:HG13	0.52	1.64	20	1
1:A:78:TRP:HE1	1:A:156:THR:HG22	0.52	1.65	2	1
1:A:85:LYS:HE2	1:A:85:LYS:H	0.52	1.65	14	1
1:A:97:ILE:CG2	1:A:171:PHE:CD1	0.51	2.93	13	20
1:A:79:ARG:HD3	1:A:151:HIS:CD2	0.51	2.41	19	2
1:A:76:ARG:CB	1:A:156:THR:HG21	0.50	2.37	2	2
1:A:72:LYS:NZ	1:A:157:VAL:HG13	0.50	2.21	20	1
1:A:95:ARG:HD2	1:A:171:PHE:CE1	0.50	2.42	18	2
1:A:121:VAL:O	1:A:140:VAL:HG11	0.49	2.06	12	1
1:A:120:MET:HA	1:A:120:MET:HE2	0.49	1.83	12	1
1:A:109:LYS:HE3	1:A:114:LEU:HD13	0.49	1.85	10	1
1:A:80:LYS:HE3	1:A:152:ILE:HD11	0.48	1.85	14	1
1:A:33:PHE:CD1	1:A:50:ILE:HD12	0.48	2.43	19	2
1:A:29:VAL:HG22	1:A:77:VAL:CG2	0.48	2.37	3	2
1:A:11:TYR:CD2	1:A:26:GLY:HA3	0.47	2.45	10	2
1:A:25:ILE:HG12	1:A:153:TYR:CE2	0.47	2.45	14	2
1:A:99:LEU:N	1:A:99:LEU:HD23	0.47	2.24	4	1
1:A:127:ILE:HG23	1:A:138:ASP:OD1	0.46	2.10	16	2
1:A:97:ILE:CG2	1:A:171:PHE:CE1	0.45	2.99	14	8
1:A:74:ILE:HG21	1:A:155:LEU:HD11	0.45	1.88	17	1
1:A:101:HIS:CD2	1:A:102:ASP:H	0.45	2.30	19	1
1:A:31:LYS:HE2	1:A:32:PHE:CE1	0.45	2.45	19	1
1:A:78:TRP:HE1	1:A:156:THR:CG2	0.45	2.25	13	1
1:A:163:TYR:CD1	1:A:175:ALA:HB2	0.44	2.47	3	2
1:A:95:ARG:CD	1:A:171:PHE:CE1	0.44	3.00	12	2
1:A:127:ILE:HG23	1:A:138:ASP:CG	0.44	2.37	16	1
1:A:85:LYS:H	1:A:85:LYS:CE	0.44	2.26	18	2
1:A:99:LEU:HD22	1:A:103:HIS:CG	0.44	2.48	14	1
1:A:163:TYR:CE2	1:A:175:ALA:HB2	0.43	2.48	12	1
1:A:97:ILE:HG13	1:A:99:LEU:HD21	0.43	1.91	4	1
1:A:76:ARG:HB3	1:A:156:THR:HG21	0.43	1.88	2	1
1:A:16:TYR:CZ	1:A:169:GLU:C	0.43	2.96	7	1
1:A:99:LEU:HD22	1:A:103:HIS:CD2	0.43	2.49	1	1
1:A:62:PHE:CE1	1:A:172:ALA:HB1	0.43	2.49	3	1
1:A:62:PHE:CE2	1:A:172:ALA:HB1	0.43	2.49	18	2
1:A:29:VAL:CG2	1:A:153:TYR:CE2	0.43	3.00	14	1
1:A:72:LYS:CE	1:A:72:LYS:HA	0.42	2.44	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:LYS:HA	1:A:72:LYS:HE3	0.42	1.89	12	1
1:A:47:PHE:CD1	1:A:80:LYS:HE3	0.42	2.50	13	1
1:A:35:LYS:HB3	1:A:36:TYR:CD1	0.42	2.50	11	1
1:A:161:HIS:C	1:A:175:ALA:HB3	0.42	2.39	12	1
1:A:9:LEU:HD21	1:A:165:ALA:HB1	0.42	1.89	12	1
1:A:89:ILE:HG23	1:A:140:VAL:HG13	0.42	1.91	13	1
1:A:85:LYS:N	1:A:85:LYS:HE2	0.42	2.28	16	1
1:A:163:TYR:CE1	1:A:173:VAL:CG2	0.42	3.03	8	1
1:A:163:TYR:CD2	1:A:175:ALA:CB	0.42	3.03	4	1
1:A:10:ALA:HB1	1:A:148:TYR:CZ	0.42	2.49	9	1
1:A:76:ARG:HB2	1:A:156:THR:HG21	0.42	1.91	18	1
1:A:29:VAL:CG1	1:A:77:VAL:HG21	0.41	2.45	15	1
1:A:29:VAL:CG1	1:A:33:PHE:CE1	0.41	3.03	5	1
1:A:36:TYR:N	1:A:36:TYR:CD1	0.41	2.87	19	1
1:A:163:TYR:CG	1:A:175:ALA:HB2	0.41	2.50	6	3
1:A:121:VAL:HG12	1:A:140:VAL:HG21	0.41	1.92	12	2
1:A:73:ARG:HH11	1:A:75:LEU:CD2	0.41	2.29	16	1
1:A:79:ARG:CD	1:A:151:HIS:CD2	0.41	3.04	19	1
1:A:163:TYR:CE1	1:A:173:VAL:HG23	0.41	2.50	3	1
1:A:74:ILE:H	1:A:74:ILE:HD12	0.41	1.76	9	1
1:A:129:ILE:HG22	1:A:171:PHE:CD2	0.41	2.50	6	1
1:A:163:TYR:CE1	1:A:173:VAL:HG12	0.41	2.51	14	1
1:A:34:LYS:O	1:A:37:LYS:HE3	0.41	2.16	19	1
1:A:95:ARG:HH11	1:A:95:ARG:CG	0.40	2.29	15	1
1:A:11:TYR:CD1	1:A:26:GLY:HA3	0.40	2.51	6	1
1:A:9:LEU:CD2	1:A:165:ALA:HB1	0.40	2.47	20	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	169/186 (91%)	142±4 (84±2%)	20±3 (12±2%)	7±2 (4±1%)	4	30
All	All	3380/3720 (91%)	2841 (84%)	408 (12%)	131 (4%)	4	30

All 24 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	141	ILE	20
1	A	22	ILE	17
1	A	168	ASN	16
1	A	47	PHE	12
1	A	132	ASN	11
1	A	157	VAL	10
1	A	121	VAL	8
1	A	123	VAL	6
1	A	8	ALA	5
1	A	10	ALA	4
1	A	74	ILE	3
1	A	176	SER	3
1	A	40	ILE	2
1	A	101	HIS	2
1	A	53	GLY	2
1	A	161	HIS	2
1	A	16	TYR	1
1	A	149	ASN	1
1	A	105	VAL	1
1	A	151	HIS	1
1	A	20	GLY	1
1	A	110	THR	1
1	A	97	ILE	1
1	A	155	LEU	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	152/166 (92%)	123±6 (81±4%)	29±6 (19±4%)	3	34
All	All	3040/3320 (92%)	2459 (81%)	581 (19%)	3	34

All 112 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	23	ILE	20
1	A	99	LEU	19
1	A	62	PHE	18
1	A	77	VAL	18
1	A	21	ASN	16
1	A	51	ASP	16
1	A	65	LEU	15
1	A	95	ARG	15
1	A	85	LYS	13
1	A	97	ILE	12
1	A	35	LYS	11
1	A	31	LYS	10
1	A	114	LEU	10
1	A	119	GLU	10
1	A	67	LEU	10
1	A	110	THR	10
1	A	72	LYS	10
1	A	98	THR	9
1	A	30	ASP	9
1	A	163	TYR	9
1	A	131	LYS	8
1	A	34	LYS	8
1	A	93	ASN	8
1	A	149	ASN	8
1	A	36	TYR	8
1	A	45	ASN	7
1	A	56	ASN	7
1	A	64	LYS	7
1	A	120	MET	7
1	A	44	ASP	7
1	A	145	THR	7
1	A	162	THR	7
1	A	61	SER	7
1	A	108	SER	7
1	A	79	ARG	6
1	A	135	ILE	6
1	A	142	LYS	6
1	A	25	ILE	6
1	A	153	TYR	6
1	A	17	LEU	5
1	A	18	SER	5
1	A	122	LYS	5
1	A	143	VAL	5

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Mol	Chain	Res	Type	Models (Total)
1	A	159	ASP	5
1	A	168	ASN	5
1	A	112	GLU	5
1	A	83	SER	5
1	A	54	ASN	5
1	A	109	LYS	5
1	A	42	LYS	5
1	A	39	SER	4
1	A	70	GLU	4
1	A	37	LYS	4
1	A	156	THR	4
1	A	157	VAL	4
1	A	96	GLU	4
1	A	43	GLU	4
1	A	63	ASN	4
1	A	174	SER	4
1	A	100	THR	3
1	A	169	GLU	3
1	A	76	ARG	3
1	A	125	ASP	3
1	A	141	ILE	3
1	A	94	ARG	3
1	A	115	GLU	3
1	A	13	GLU	3
1	A	127	ILE	3
1	A	90	THR	3
1	A	73	ARG	3
1	A	176	SER	3
1	A	137	LEU	3
1	A	129	ILE	3
1	A	147	ASP	2
1	A	101	HIS	2
1	A	161	HIS	2
1	A	60	LYS	2
1	A	24	ASN	2
1	A	75	LEU	2
1	A	136	ASN	2
1	A	160	ASN	2
1	A	105	VAL	2
1	A	139	GLU	2
1	A	68	ILE	2
1	A	102	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	38	ASN	2
1	A	66	SER	2
1	A	158	GLU	2
1	A	41	LYS	2
1	A	123	VAL	1
1	A	91	THR	1
1	A	116	ILE	1
1	A	74	ILE	1
1	A	103	HIS	1
1	A	134	THR	1
1	A	11	TYR	1
1	A	27	GLU	1
1	A	69	ILE	1
1	A	81	LYS	1
1	A	92	LYS	1
1	A	128	TYR	1
1	A	146	VAL	1
1	A	133	ASN	1
1	A	19	ASP	1
1	A	107	ILE	1
1	A	132	ASN	1
1	A	173	VAL	1
1	A	29	VAL	1
1	A	59	ILE	1
1	A	155	LEU	1
1	A	47	PHE	1
1	A	87	ILE	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 ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

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