



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 10:17 AM UTC

PDB ID : 2I3B / pdb_00002i3b
Title : Solution Structure of a Human Cancer-Related Nucleoside Triphosphatase
Authors : Placzek, W.J.; Almeida, M.S.; Wuthrich, K.
Deposited on : 2006-08-17

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

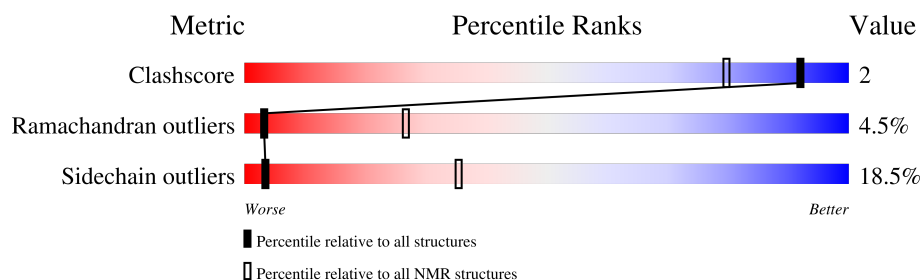
1 Overall quality at a glance

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	189	79% 14% • 6%

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:2-A:97, A:106-A:187 (178)	1.25	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 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2954 atoms, of which 1508 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Human Cancer-Related NTPase.

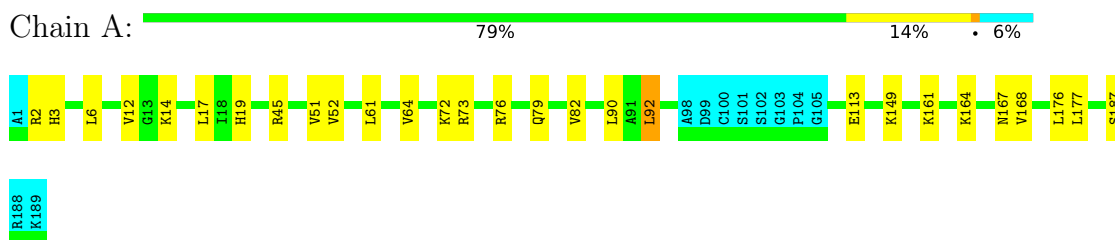
Mol	Chain	Residues	Atoms						Trace
1	A	189	Total	C	H	N	O	S	0
			2954	912	1508	264	265	5	

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: Human Cancer-Related NTPase

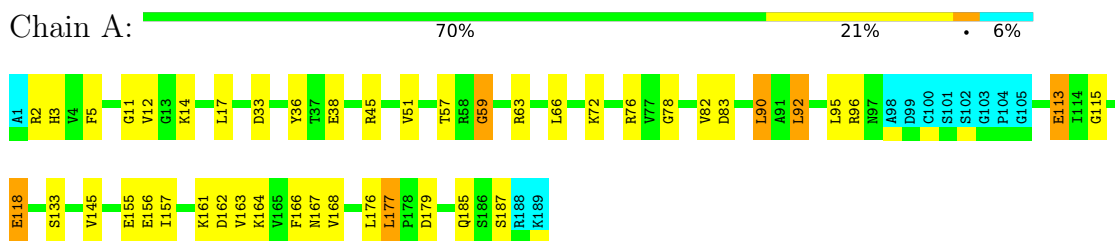


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

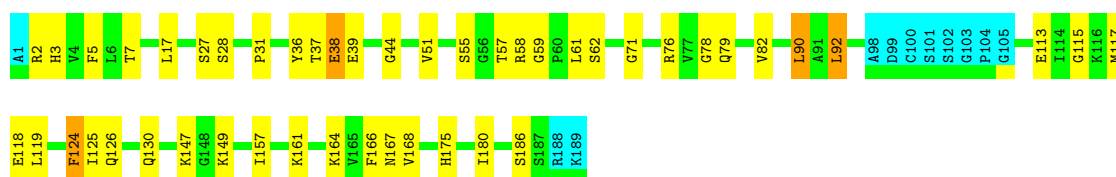
- Molecule 1: Human Cancer-Related NTPase



4.2.2 Score per residue for model 2

- Molecule 1: Human Cancer-Related NTPase

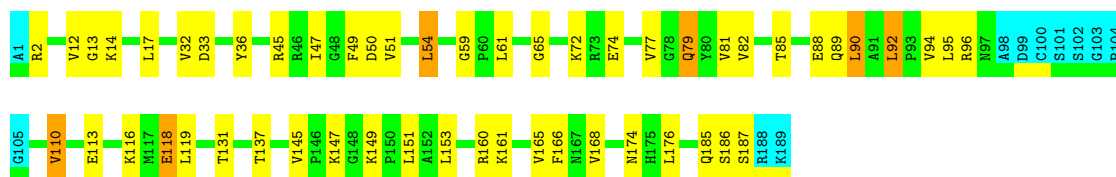




4.2.3 Score per residue for model 3

- Molecule 1: Human Cancer-Related NTPase

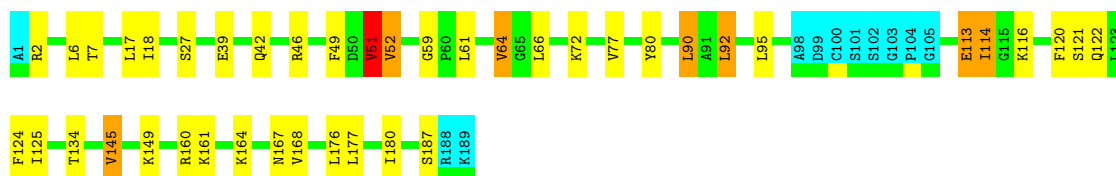
Chain A: 66% 25% 6%



4.2.4 Score per residue for model 4

- Molecule 1: Human Cancer-Related NTPase

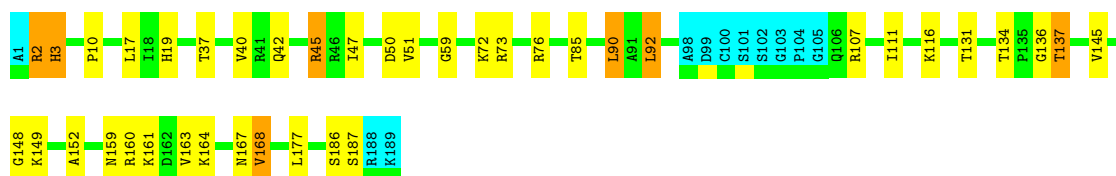
Chain A: 72% 18% 6%



4.2.5 Score per residue for model 5

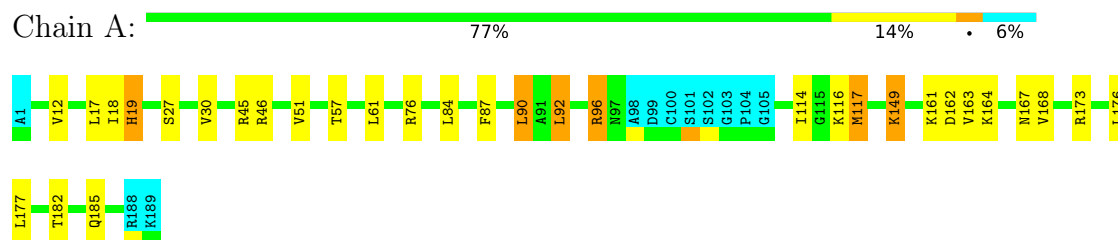
- Molecule 1: Human Cancer-Related NTPase

Chain A: 73% 17% 6%



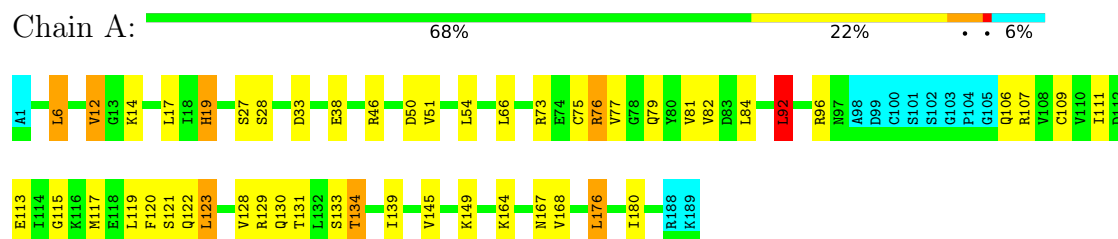
4.2.6 Score per residue for model 6

- Molecule 1: Human Cancer-Related NTPase



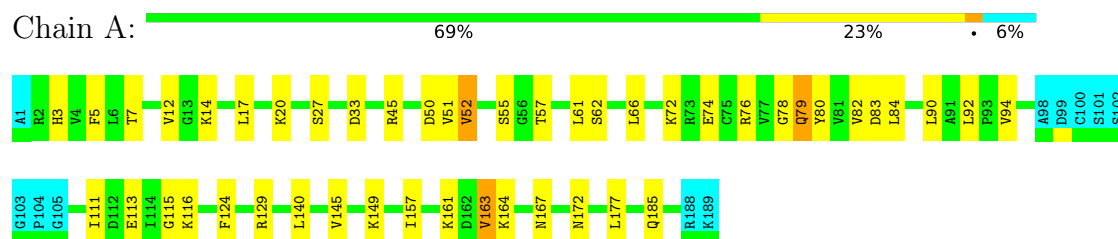
4.2.7 Score per residue for model 7

- Molecule 1: Human Cancer-Related NTPase



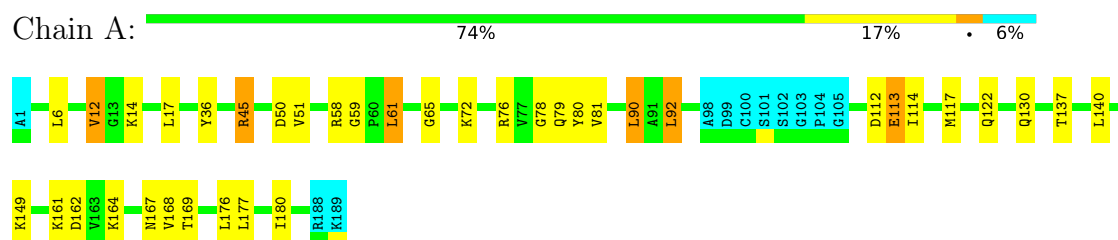
4.2.8 Score per residue for model 8

- Molecule 1: Human Cancer-Related NTPase



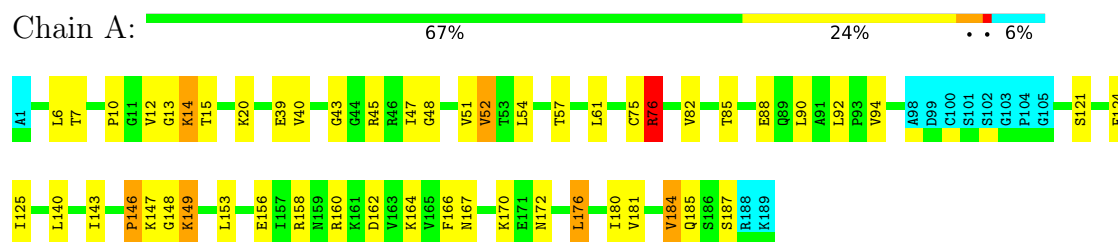
4.2.9 Score per residue for model 9

- Molecule 1: Human Cancer-Related NTPase



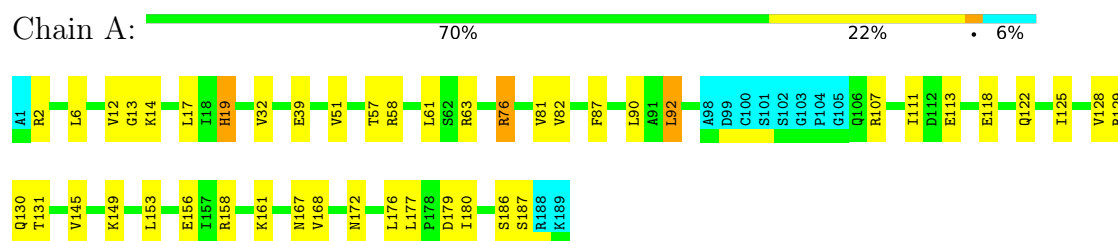
4.2.10 Score per residue for model 10

- Molecule 1: Human Cancer-Related NTPase



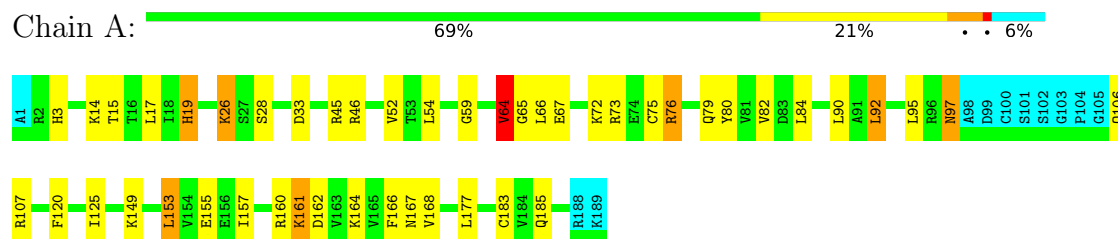
4.2.11 Score per residue for model 11

- Molecule 1: Human Cancer-Related NTPase



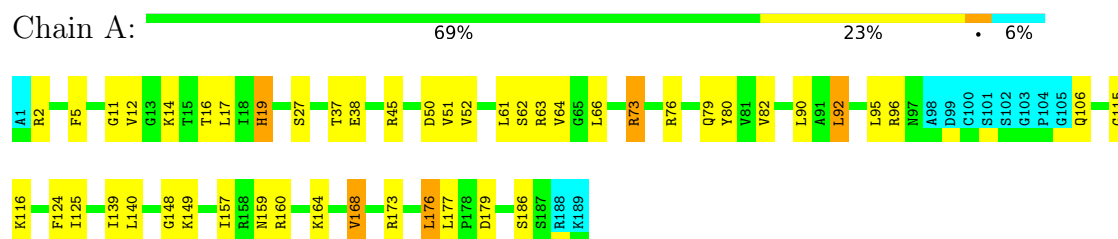
4.2.12 Score per residue for model 12

- Molecule 1: Human Cancer-Related NTPase



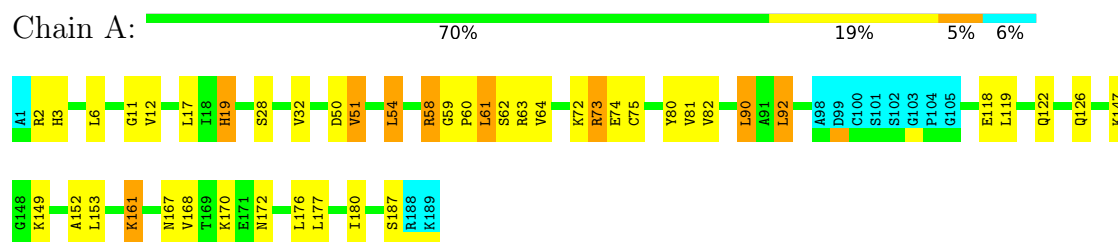
4.2.13 Score per residue for model 13

- Molecule 1: Human Cancer-Related NTPase



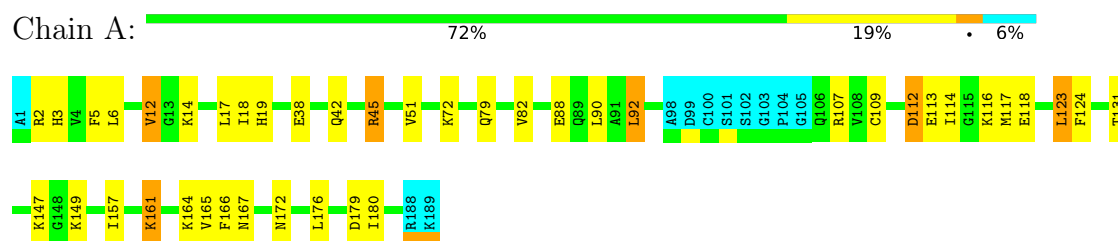
4.2.14 Score per residue for model 14

- Molecule 1: Human Cancer-Related NTPase



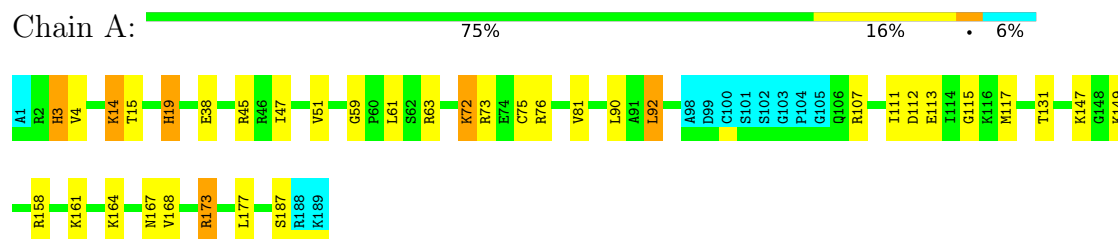
4.2.15 Score per residue for model 15

- Molecule 1: Human Cancer-Related NTPase



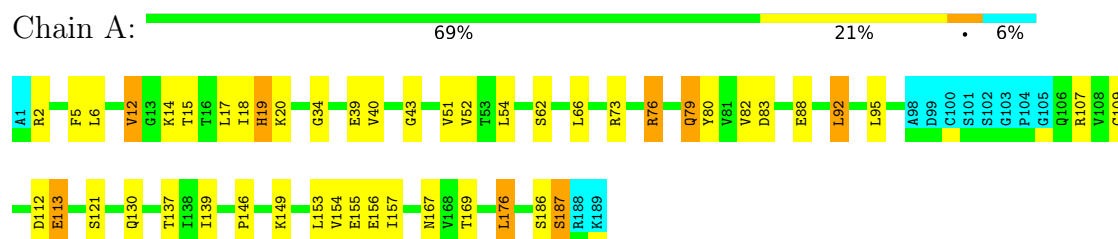
4.2.16 Score per residue for model 16

- Molecule 1: Human Cancer-Related NTPase



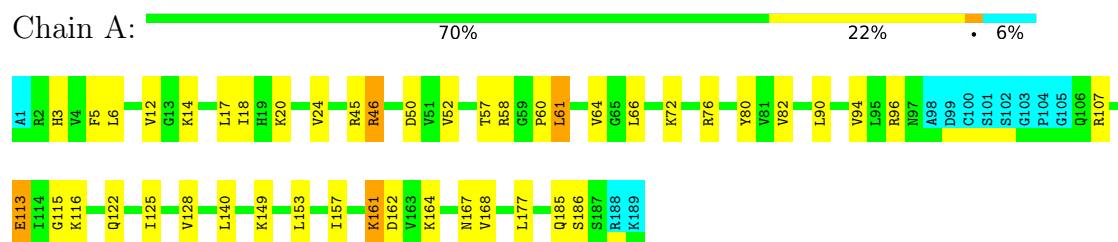
4.2.17 Score per residue for model 17

- Molecule 1: Human Cancer-Related NTPase



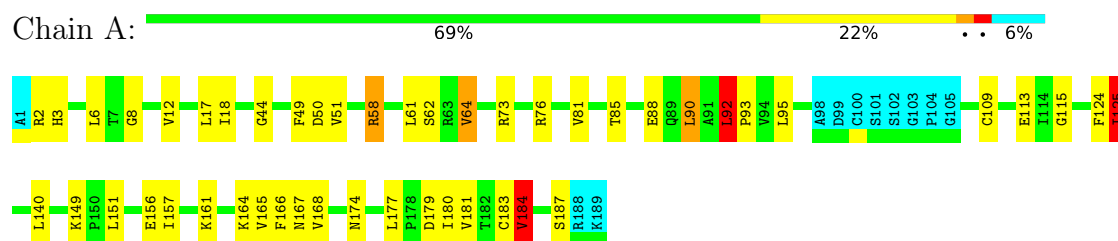
4.2.18 Score per residue for model 18

- Molecule 1: Human Cancer-Related NTPase



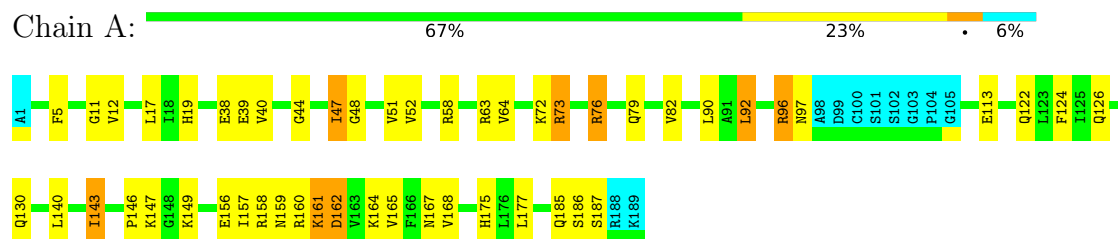
4.2.19 Score per residue for model 19

- Molecule 1: Human Cancer-Related NTPase



4.2.20 Score per residue for model 20

- Molecule 1: Human Cancer-Related NTPase



5 Refinement protocol and experimental data overview ⓘ

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

Of the 80 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
CYANA	structure solution	version 1.0.3
CYANA	refinement	

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±0/1400 (0.0± 0.0%)	1.46±0.03	7±3/1899 (0.4± 0.2%)
All	All	0.67	0/28000 (0.0%)	1.46	145/37980 (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	2.5±1.2
All	All	0	50

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	50	ASP	CA-CB-CG	10.36	122.96	112.60	9	6
1	A	112	ASP	CA-CB-CG	9.64	122.24	112.60	15	3
1	A	19	HIS	CB-CG-CD2	-9.31	119.10	131.20	6	10
1	A	12	VAL	CB-CA-C	8.29	118.91	110.70	9	2
1	A	49	PHE	CA-CB-CG	6.82	120.62	113.80	19	2
1	A	97	ASN	CA-CB-CG	6.77	119.37	112.60	12	2
1	A	134	THR	CA-CB-CG2	6.71	121.90	110.50	7	1
1	A	64	VAL	CB-CA-C	6.52	121.99	111.29	12	2
1	A	51	VAL	CA-CB-CG2	6.50	121.45	110.40	3	3
1	A	168	VAL	CA-CB-CG2	6.44	121.35	110.40	5	1
1	A	19	HIS	CB-CG-ND1	6.38	132.27	122.70	6	5
1	A	75	CYS	CA-C-N	6.37	133.70	121.54	16	3
1	A	75	CYS	C-N-CA	6.37	133.70	121.54	16	3
1	A	112	ASP	CA-C-N	6.31	133.59	121.54	16	1
1	A	112	ASP	C-N-CA	6.31	133.59	121.54	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	LYS	CA-C-N	6.27	129.00	120.54	1	2
1	A	14	LYS	C-N-CA	6.27	129.00	120.54	1	2
1	A	186	SER	CA-C-N	6.15	133.28	121.54	17	1
1	A	186	SER	C-N-CA	6.15	133.28	121.54	17	1
1	A	161	LYS	CA-C-N	6.14	129.64	120.31	4	3
1	A	161	LYS	C-N-CA	6.14	129.64	120.31	4	3
1	A	81	VAL	CB-CA-C	6.11	119.00	111.25	9	2
1	A	51	VAL	CA-CB-CG1	5.99	120.58	110.40	20	7
1	A	162	ASP	CA-CB-CG	5.92	118.52	112.60	9	2
1	A	149	LYS	CB-CA-C	5.89	121.78	110.17	10	1
1	A	130	GLN	CA-C-N	5.86	128.13	120.28	2	1
1	A	130	GLN	C-N-CA	5.86	128.13	120.28	2	1
1	A	15	THR	CA-C-N	5.85	128.12	120.28	16	2
1	A	15	THR	C-N-CA	5.85	128.12	120.28	16	2
1	A	145	VAL	CB-CA-C	5.85	116.38	110.94	4	2
1	A	3	HIS	CB-CG-CD2	-5.85	123.60	131.20	2	6
1	A	72	LYS	CB-CA-C	5.83	119.87	111.82	16	1
1	A	19	HIS	CA-CB-CG	5.72	119.52	113.80	7	3
1	A	87	PHE	CA-CB-CG	5.71	119.51	113.80	11	1
1	A	168	VAL	CA-C-N	5.67	131.86	122.33	9	1
1	A	168	VAL	C-N-CA	5.67	131.86	122.33	9	1
1	A	38	GLU	CA-C-N	5.66	132.35	121.54	2	1
1	A	38	GLU	C-N-CA	5.66	132.35	121.54	2	1
1	A	110	VAL	CA-CB-CG1	5.55	119.84	110.40	3	1
1	A	88	GLU	CA-C-N	5.54	128.02	120.54	15	1
1	A	88	GLU	C-N-CA	5.54	128.02	120.54	15	1
1	A	54	LEU	CA-C-N	5.48	127.56	120.44	10	1
1	A	54	LEU	C-N-CA	5.48	127.56	120.44	10	1
1	A	113	GLU	CA-C-N	5.48	131.83	121.97	4	1
1	A	113	GLU	C-N-CA	5.48	131.83	121.97	4	1
1	A	162	ASP	CA-C-N	5.44	130.50	123.10	6	1
1	A	162	ASP	C-N-CA	5.44	130.50	123.10	6	1
1	A	154	VAL	CA-C-N	5.44	127.56	120.28	17	1
1	A	154	VAL	C-N-CA	5.44	127.56	120.28	17	1
1	A	184	VAL	CA-CB-CG2	5.39	119.56	110.40	19	1
1	A	165	VAL	CA-CB-CG2	5.38	119.55	110.40	19	2
1	A	146	PRO	CA-C-N	5.37	131.80	121.54	10	1
1	A	146	PRO	C-N-CA	5.37	131.80	121.54	10	1
1	A	175	HIS	CB-CG-CD2	-5.37	124.22	131.20	20	2
1	A	149	LYS	CA-C-N	5.36	125.34	120.03	10	1
1	A	149	LYS	C-N-CA	5.36	125.34	120.03	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	PRO	N-CA-CB	5.35	106.29	102.65	2	1
1	A	52	VAL	CB-CA-C	5.32	117.91	110.99	8	2
1	A	51	VAL	CB-CA-C	5.31	117.75	111.59	2	3
1	A	120	PHE	CA-C-N	5.30	129.21	121.31	4	1
1	A	120	PHE	C-N-CA	5.30	129.21	121.31	4	1
1	A	52	VAL	CA-CB-CG1	5.29	119.40	110.40	10	2
1	A	8	GLY	CA-C-N	5.25	123.44	119.66	19	1
1	A	8	GLY	C-N-CA	5.25	123.44	119.66	19	1
1	A	59	GLY	CA-C-N	5.22	126.37	119.84	3	2
1	A	59	GLY	C-N-CA	5.22	126.37	119.84	3	2
1	A	60	PRO	CA-C-N	5.17	131.41	121.54	18	2
1	A	60	PRO	C-N-CA	5.17	131.41	121.54	18	2
1	A	179	ASP	CA-CB-CG	5.15	117.75	112.60	15	2
1	A	167	ASN	CA-CB-CG	-5.13	107.47	112.60	17	1
1	A	166	PHE	CA-CB-CG	5.09	118.89	113.80	3	1
1	A	128	VAL	CA-CB-CG1	5.07	119.02	110.40	18	1
1	A	134	THR	CA-C-N	5.07	126.17	119.84	5	1
1	A	134	THR	C-N-CA	5.07	126.17	119.84	5	1
1	A	26	LYS	CA-C-N	5.07	127.38	120.54	12	1
1	A	26	LYS	C-N-CA	5.07	127.38	120.54	12	1
1	A	120	PHE	CA-CB-CG	5.06	118.86	113.80	7	1
1	A	77	VAL	CB-CA-C	5.05	116.08	110.62	7	1
1	A	71	GLY	CA-C-N	5.02	130.39	122.36	2	1
1	A	71	GLY	C-N-CA	5.02	130.39	122.36	2	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	76	ARG	Sidechain	6
1	A	80	TYR	Sidechain	5
1	A	45	ARG	Sidechain	4
1	A	2	ARG	Sidechain,Peptide	3
1	A	36	TYR	Sidechain	3
1	A	59	GLY	Peptide	3
1	A	63	ARG	Sidechain	3
1	A	58	ARG	Sidechain	3
1	A	107	ARG	Sidechain	3
1	A	160	ARG	Sidechain	2
1	A	173	ARG	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	73	ARG	Sidechain	2
1	A	46	ARG	Sidechain	1
1	A	136	GLY	Peptide	1
1	A	30	VAL	Peptide	1
1	A	133	SER	Peptide	1
1	A	129	ARG	Sidechain	1
1	A	32	VAL	Peptide	1
1	A	112	ASP	Peptide	1
1	A	131	THR	Peptide	1
1	A	158	ARG	Sidechain	1
1	A	139	ILE	Peptide	1
1	A	96	ARG	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	1375	1440	1440	4±2
All	All	27500	28800	28800	85

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD21	1:A:180:ILE:HD11	0.81	1.51	9	2
1:A:6:LEU:HD21	1:A:18:ILE:HD11	0.71	1.62	17	1
1:A:6:LEU:HD11	1:A:180:ILE:HD11	0.69	1.64	4	4
1:A:92:LEU:HD21	1:A:123:LEU:HD11	0.68	1.64	7	1
1:A:64:VAL:HG12	1:A:65:GLY:H	0.62	1.55	12	1
1:A:6:LEU:HD23	1:A:18:ILE:HD11	0.62	1.71	15	2
1:A:123:LEU:HD12	1:A:123:LEU:C	0.57	2.24	15	1
1:A:17:LEU:HD13	1:A:176:LEU:CB	0.56	2.30	13	1
1:A:6:LEU:CD2	1:A:18:ILE:HD11	0.53	2.32	17	3
1:A:36:TYR:CE1	1:A:38:GLU:HG3	0.53	2.39	2	1
1:A:17:LEU:HD13	1:A:176:LEU:HB3	0.53	1.80	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:ASN:HD21	1:A:176:LEU:HD12	0.53	1.63	10	1
1:A:12:VAL:HG12	1:A:14:LYS:H	0.53	1.64	17	1
1:A:111:ILE:HD13	1:A:128:VAL:HG23	0.52	1.81	11	1
1:A:54:LEU:H	1:A:54:LEU:HD22	0.51	1.66	14	1
1:A:58:ARG:C	1:A:90:LEU:HD21	0.51	2.30	19	1
1:A:40:VAL:HG12	1:A:48:GLY:C	0.51	2.30	20	2
1:A:5:PHE:CZ	1:A:157:ILE:HG21	0.51	2.40	13	2
1:A:59:GLY:HA3	1:A:90:LEU:HD11	0.50	1.83	5	4
1:A:40:VAL:HG13	1:A:47:ILE:HG13	0.50	1.81	20	1
1:A:61:LEU:HD21	1:A:87:PHE:CE2	0.50	2.42	6	1
1:A:168:VAL:HG23	1:A:176:LEU:HD12	0.49	1.83	13	1
1:A:14:LYS:H	1:A:14:LYS:HE3	0.49	1.66	16	1
1:A:64:VAL:CG1	1:A:65:GLY:H	0.48	2.21	12	1
1:A:49:PHE:CZ	1:A:116:LYS:HE2	0.47	2.44	4	1
1:A:5:PHE:CE1	1:A:157:ILE:HG21	0.47	2.44	20	5
1:A:59:GLY:HA3	1:A:90:LEU:HD21	0.47	1.86	9	1
1:A:164:LYS:HE2	1:A:166:PHE:CE1	0.46	2.45	15	3
1:A:3:HIS:HB2	1:A:163:VAL:HG12	0.46	1.86	1	2
1:A:92:LEU:H	1:A:93:PRO:HD2	0.46	1.70	19	1
1:A:153:LEU:C	1:A:153:LEU:HD13	0.46	2.36	12	1
1:A:34:GLY:C	1:A:54:LEU:HD23	0.46	2.36	17	1
1:A:109:CYS:SG	1:A:139:ILE:HD13	0.45	2.51	7	1
1:A:166:PHE:CD2	1:A:180:ILE:HG12	0.45	2.46	2	1
1:A:54:LEU:HD22	1:A:54:LEU:N	0.45	2.26	3	3
1:A:131:THR:CG2	1:A:137:THR:HG21	0.44	2.42	3	1
1:A:172:ASN:ND2	1:A:176:LEU:HD12	0.44	2.27	10	1
1:A:89:GLN:HB2	1:A:90:LEU:HD23	0.44	1.89	3	1
1:A:160:ARG:C	1:A:162:ASP:H	0.44	2.20	20	1
1:A:166:PHE:CE2	1:A:180:ILE:HA	0.44	2.48	19	1
1:A:109:CYS:HB2	1:A:137:THR:CG2	0.43	2.43	17	1
1:A:20:LYS:O	1:A:24:VAL:HG23	0.43	2.13	18	1
1:A:125:ILE:HD12	1:A:125:ILE:H	0.42	1.73	10	1
1:A:181:VAL:HA	1:A:184:VAL:HG23	0.42	1.91	10	2
1:A:164:LYS:HE3	1:A:166:PHE:CE1	0.42	2.49	1	1
1:A:26:LYS:HE2	1:A:54:LEU:HD12	0.42	1.90	12	1
1:A:5:PHE:CD2	1:A:143:ILE:HG23	0.42	2.49	20	1
1:A:36:TYR:CE1	1:A:38:GLU:CG	0.42	3.02	2	1
1:A:5:PHE:CE2	1:A:157:ILE:HG21	0.42	2.50	15	1
1:A:180:ILE:O	1:A:184:VAL:HG22	0.42	2.14	19	1
1:A:42:GLN:HB2	1:A:47:ILE:HD13	0.42	1.90	5	1
1:A:111:ILE:HD13	1:A:128:VAL:CG2	0.42	2.45	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:LEU:HD23	1:A:180:ILE:HD11	0.41	1.92	14	1
1:A:168:VAL:HG22	1:A:173:ARG:HA	0.41	1.92	13	1
1:A:17:LEU:CD1	1:A:176:LEU:H	0.41	2.28	17	1
1:A:153:LEU:HD13	1:A:153:LEU:O	0.41	2.16	3	1
1:A:51:VAL:HG13	1:A:90:LEU:HD11	0.41	1.92	4	1
1:A:125:ILE:H	1:A:125:ILE:HD12	0.41	1.75	19	1
1:A:177:LEU:C	1:A:177:LEU:HD22	0.41	2.41	1	1
1:A:40:VAL:HG22	1:A:47:ILE:HD11	0.40	1.93	5	1
1:A:117:MET:SD	1:A:117:MET:N	0.40	2.94	6	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	178/189 (94%)	142±5 (80±3%)	28±5 (16±3%)	8±2 (4±1%)	3	27
All	All	3560/3780 (94%)	2837 (80%)	563 (16%)	160 (4%)	3	27

All 44 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	92	LEU	18
1	A	12	VAL	13
1	A	115	GLY	8
1	A	113	GLU	7
1	A	79	GLN	7
1	A	187	SER	7
1	A	125	ILE	6
1	A	161	LYS	6
1	A	64	VAL	6
1	A	39	GLU	5
1	A	61	LEU	5
1	A	11	GLY	4
1	A	78	GLY	4

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Mol	Chain	Res	Type	Models (Total)
1	A	114	ILE	4
1	A	76	ARG	4
1	A	147	LYS	4
1	A	118	GLU	3
1	A	44	GLY	3
1	A	124	PHE	3
1	A	13	GLY	3
1	A	148	GLY	3
1	A	96	ARG	3
1	A	106	GLN	3
1	A	146	PRO	3
1	A	65	GLY	2
1	A	3	HIS	2
1	A	10	PRO	2
1	A	111	ILE	2
1	A	137	THR	2
1	A	152	ALA	2
1	A	46	ARG	2
1	A	43	GLY	2
1	A	77	VAL	1
1	A	90	LEU	1
1	A	149	LYS	1
1	A	170	LYS	1
1	A	28	SER	1
1	A	75	CYS	1
1	A	162	ASP	1
1	A	73	ARG	1
1	A	47	ILE	1
1	A	121	SER	1
1	A	66	LEU	1
1	A	186	SER	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	157/164 (96%)	128±5 (81±3%)	29±5 (19±3%)	3 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3140/3280 (96%)	2558 (81%)	582 (19%)	3 35

All 116 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	149	LYS	19
1	A	90	LEU	18
1	A	92	LEU	18
1	A	167	ASN	17
1	A	17	LEU	15
1	A	168	VAL	15
1	A	82	VAL	14
1	A	177	LEU	14
1	A	76	ARG	13
1	A	72	LYS	12
1	A	161	LYS	12
1	A	164	LYS	12
1	A	45	ARG	11
1	A	113	GLU	11
1	A	176	LEU	11
1	A	14	LYS	11
1	A	61	LEU	10
1	A	2	ARG	9
1	A	73	ARG	9
1	A	185	GLN	8
1	A	19	HIS	8
1	A	51	VAL	7
1	A	57	THR	7
1	A	66	LEU	7
1	A	95	LEU	7
1	A	116	LYS	7
1	A	52	VAL	7
1	A	122	GLN	7
1	A	140	LEU	7
1	A	38	GLU	6
1	A	145	VAL	6
1	A	156	GLU	6
1	A	27	SER	6
1	A	62	SER	6
1	A	117	MET	6
1	A	124	PHE	6

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Mol	Chain	Res	Type	Models (Total)
1	A	186	SER	6
1	A	79	GLN	6
1	A	153	LEU	6
1	A	33	ASP	5
1	A	96	ARG	5
1	A	118	GLU	5
1	A	187	SER	5
1	A	58	ARG	5
1	A	81	VAL	5
1	A	107	ARG	5
1	A	130	GLN	5
1	A	7	THR	4
1	A	119	LEU	4
1	A	85	THR	4
1	A	88	GLU	4
1	A	94	VAL	4
1	A	160	ARG	4
1	A	131	THR	4
1	A	84	LEU	4
1	A	172	ASN	4
1	A	83	ASP	3
1	A	155	GLU	3
1	A	179	ASP	3
1	A	28	SER	3
1	A	37	THR	3
1	A	126	GLN	3
1	A	147	LYS	3
1	A	47	ILE	3
1	A	50	ASP	3
1	A	74	GLU	3
1	A	80	TYR	3
1	A	121	SER	3
1	A	159	ASN	3
1	A	163	VAL	3
1	A	46	ARG	3
1	A	6	LEU	3
1	A	12	VAL	3
1	A	20	LYS	3
1	A	158	ARG	3
1	A	162	ASP	3
1	A	63	ARG	3
1	A	55	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	32	VAL	2
1	A	54	LEU	2
1	A	151	LEU	2
1	A	174	ASN	2
1	A	42	GLN	2
1	A	64	VAL	2
1	A	134	THR	2
1	A	18	ILE	2
1	A	123	LEU	2
1	A	129	ARG	2
1	A	169	THR	2
1	A	15	THR	2
1	A	143	ILE	2
1	A	184	VAL	2
1	A	125	ILE	2
1	A	3	HIS	2
1	A	157	ILE	2
1	A	183	CYS	2
1	A	109	CYS	2
1	A	165	VAL	2
1	A	133	SER	1
1	A	77	VAL	1
1	A	110	VAL	1
1	A	114	ILE	1
1	A	137	THR	1
1	A	182	THR	1
1	A	111	ILE	1
1	A	67	GLU	1
1	A	97	ASN	1
1	A	120	PHE	1
1	A	16	THR	1
1	A	139	ILE	1
1	A	75	CYS	1
1	A	170	LYS	1
1	A	4	VAL	1
1	A	173	ARG	1
1	A	39	GLU	1
1	A	40	VAL	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