



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 06:09 AM UTC

PDB ID : 1P4S / pdb_00001p4s
Title : Solution structure of Mycobacterium tuberculosis adenylate kinase
Authors : Miron, S.; Munier-Lehmann, H.; Craescu, C.T.
Deposited on : 2003-04-24

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

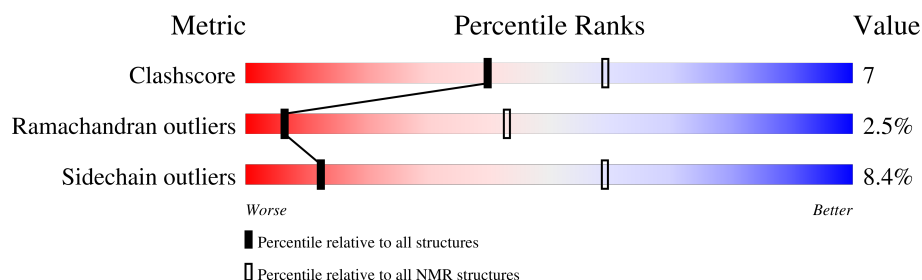
1 Overall quality at a glance

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	181	

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 12 as representative, based on the following criterion: *closest to the average*.

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:1-A:8, A:13-A:73, A:80-A:115, A:139-A:165, A:169-A:181 (145)	0.81	4

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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2850 atoms, of which 1436 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Adenylate kinase.

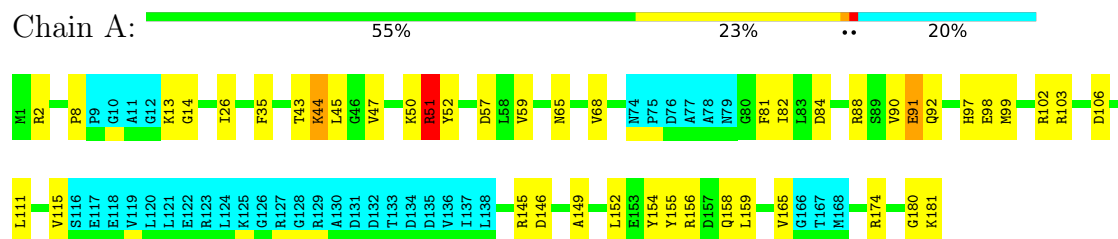
Mol	Chain	Residues	Atoms						Trace
1	A	181	Total	C	H	N	O	S	0
			2850	880	1436	254	276	4	

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: Adenylate kinase

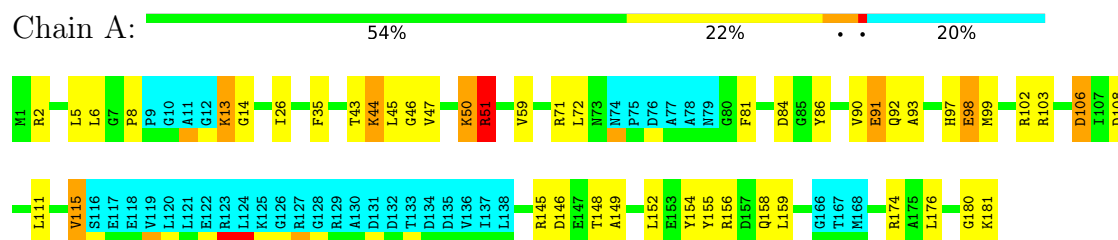


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

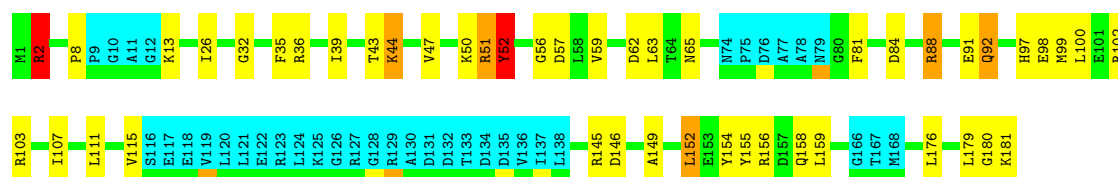
- Molecule 1: Adenylate kinase



4.2.2 Score per residue for model 2

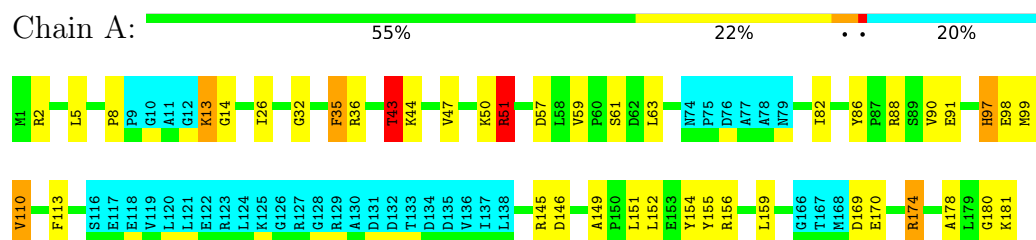
- Molecule 1: Adenylate kinase





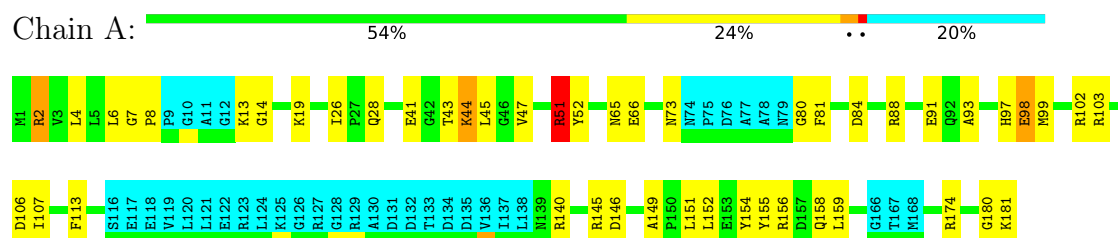
4.2.3 Score per residue for model 3

- Molecule 1: Adenylate kinase



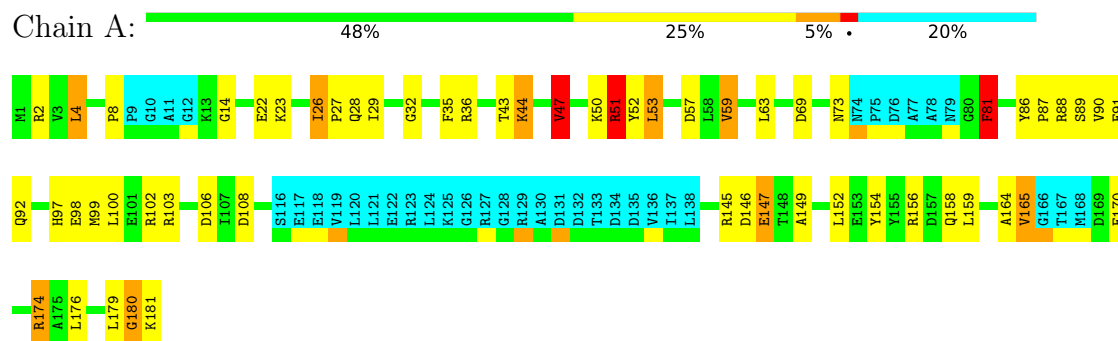
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Adenylate kinase



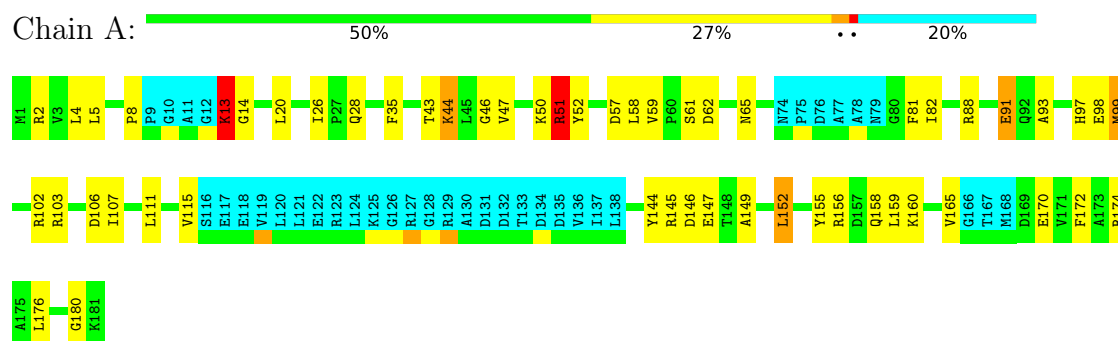
4.2.5 Score per residue for model 5

- Molecule 1: Adenylate kinase



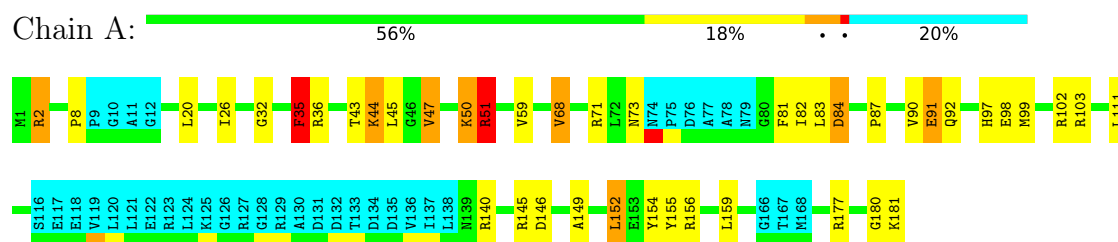
4.2.6 Score per residue for model 6

- Molecule 1: Adenylate kinase



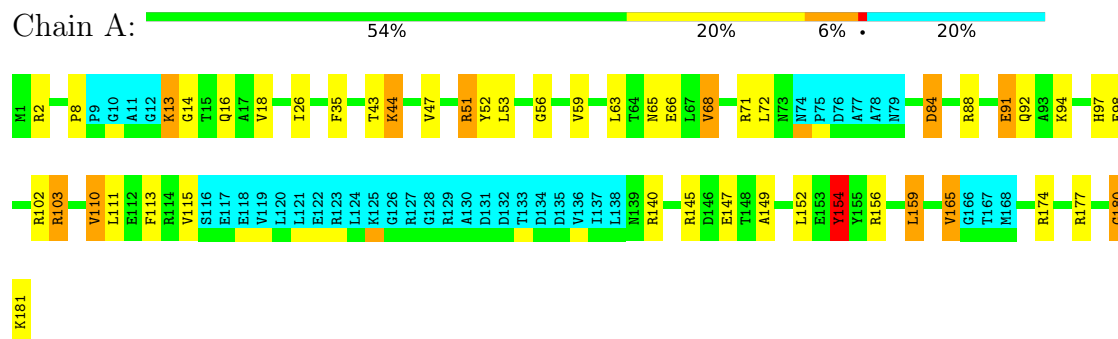
4.2.7 Score per residue for model 7

- Molecule 1: Adenylate kinase



4.2.8 Score per residue for model 8

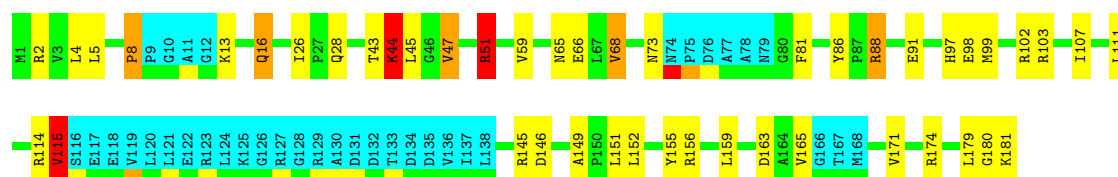
- Molecule 1: Adenylate kinase



4.2.9 Score per residue for model 9

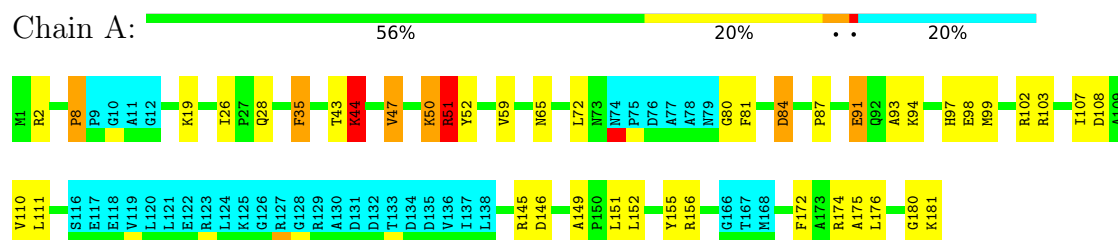
- Molecule 1: Adenylate kinase





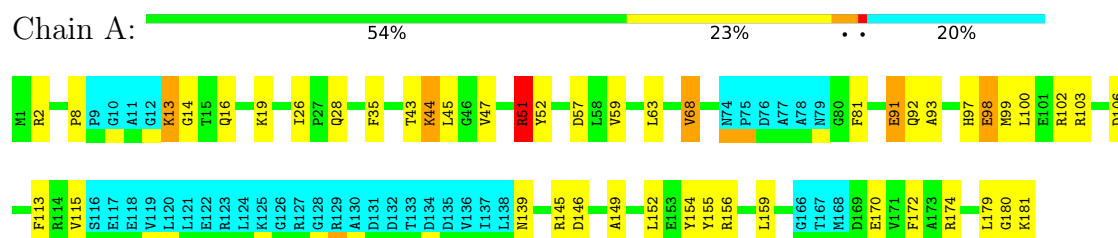
4.2.10 Score per residue for model 10

- Molecule 1: Adenylate kinase



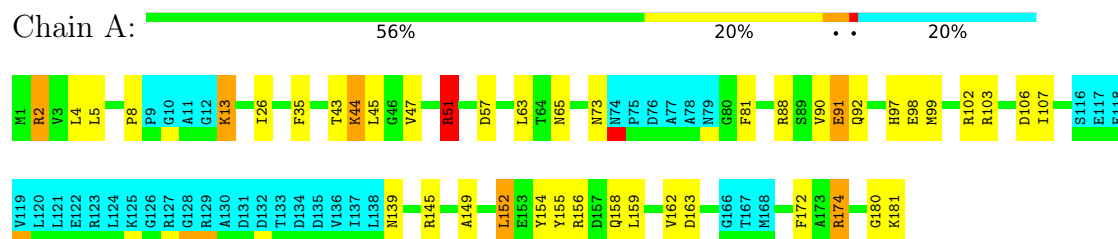
4.2.11 Score per residue for model 11

- Molecule 1: Adenylate kinase



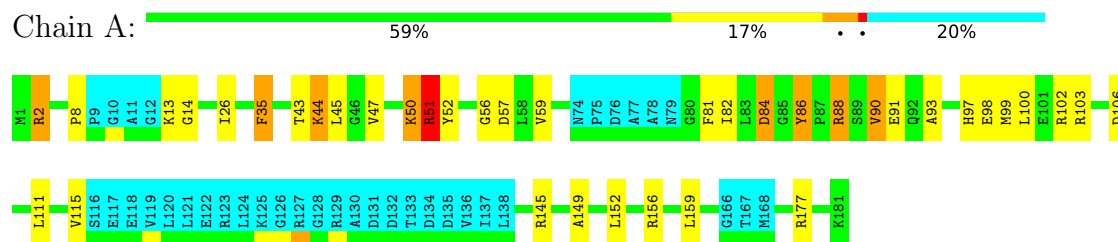
4.2.12 Score per residue for model 12

- Molecule 1: Adenylate kinase



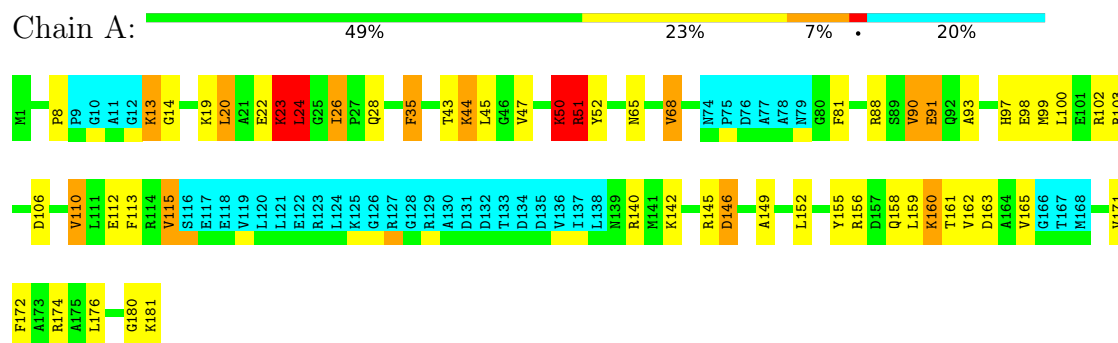
4.2.13 Score per residue for model 13

- Molecule 1: Adenylate kinase



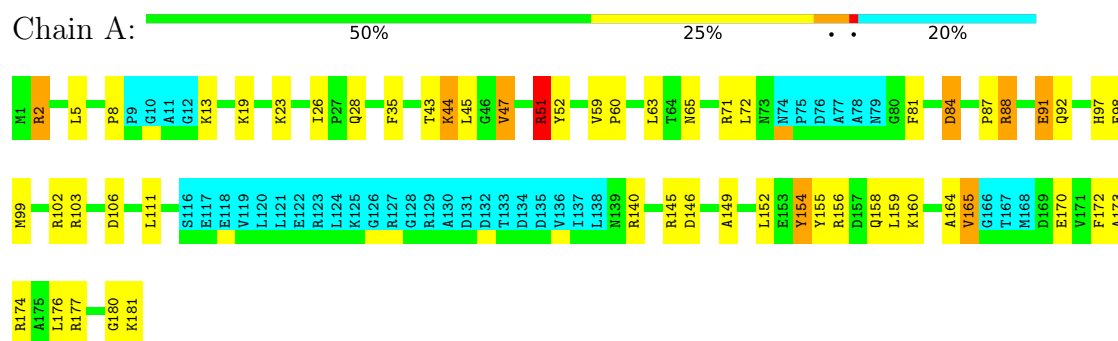
4.2.14 Score per residue for model 14

- Molecule 1: Adenylate kinase



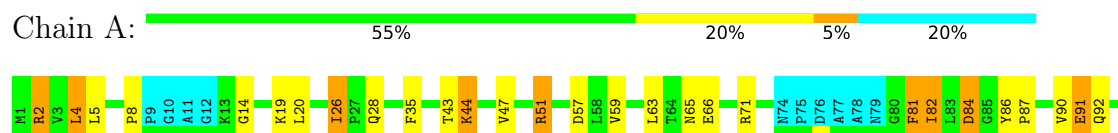
4.2.15 Score per residue for model 15

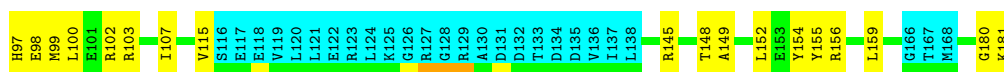
- Molecule 1: Adenylate kinase



4.2.16 Score per residue for model 16

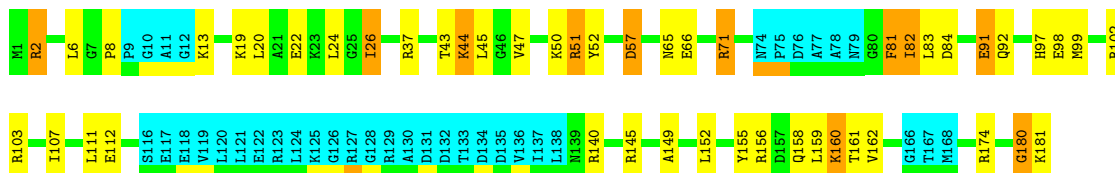
- Molecule 1: Adenylate kinase





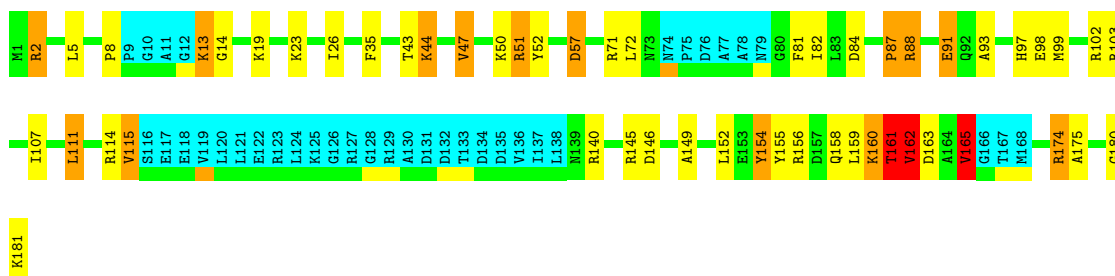
4.2.17 Score per residue for model 17

- Molecule 1: Adenylate kinase



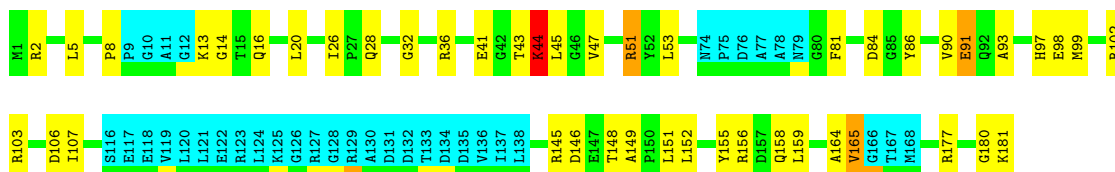
4.2.18 Score per residue for model 18

- Molecule 1: Adenylate kinase



4.2.19 Score per residue for model 19

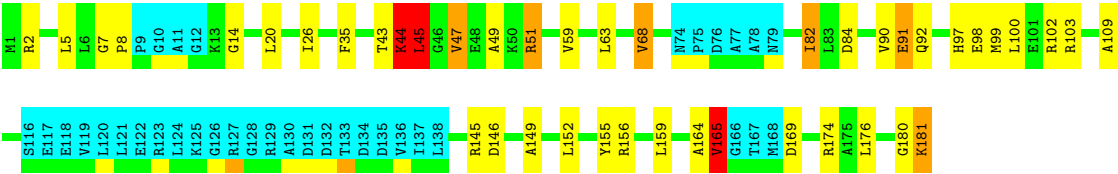
- Molecule 1: Adenylate kinase



4.2.20 Score per residue for model 20

- Molecule 1: Adenylate kinase

Chain A:  56% 19% • • 20%



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing protocol*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest restraint violations and lowest energy*.

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

Software name	Classification	Version
Insight II	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.72±0.02	6±1/1167 (0.5± 0.1%)	2.08±0.07	30±6/1571 (1.9± 0.4%)
All	All	1.72	124/23340 (0.5%)	2.08	606/31420 (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	0.1±0.3	4.3±1.4
All	All	2	86

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	8	PRO	CA-C	10.85	1.57	1.51	4	20
1	A	57	ASP	CA-C	7.64	1.57	1.53	16	4
1	A	59	VAL	CA-C	7.33	1.57	1.52	11	12
1	A	161	THR	CA-C	7.24	1.62	1.52	18	1
1	A	51	ARG	CA-C	6.46	1.61	1.52	8	15
1	A	161	THR	CA-CB	6.27	1.64	1.53	18	1
1	A	165	VAL	CA-C	6.21	1.60	1.52	5	2
1	A	162	VAL	CA-CB	6.13	1.62	1.54	18	1
1	A	112	GLU	N-CA	6.03	1.54	1.46	14	1
1	A	112	GLU	CA-C	6.01	1.60	1.52	14	1
1	A	26	ILE	CA-C	5.90	1.57	1.52	1	1
1	A	149	ALA	CA-C	5.79	1.58	1.52	12	20
1	A	107	ILE	CA-CB	5.74	1.59	1.53	12	8
1	A	27	PRO	CA-C	5.72	1.57	1.52	5	1
1	A	22	GLU	CA-C	5.68	1.60	1.52	14	1
1	A	97	HIS	ND1-CE1	5.54	1.38	1.32	3	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	92	GLN	CA-C	5.44	1.59	1.52	17	10
1	A	20	LEU	CA-C	5.31	1.59	1.52	14	1
1	A	144	TYR	CA-C	5.11	1.59	1.52	6	1
1	A	97	HIS	CG-CD2	5.11	1.41	1.35	3	1
1	A	52	TYR	CA-C	5.10	1.59	1.53	8	1
1	A	52	TYR	N-CA	5.01	1.52	1.46	2	1

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	51	ARG	CA-C-O	-35.39	84.25	120.70	10	20
1	A	24	LEU	N-CA-C	18.29	134.89	112.58	14	1
1	A	23	LYS	CA-C-N	15.36	144.85	122.74	14	1
1	A	23	LYS	C-N-CA	15.36	144.85	122.74	14	1
1	A	51	ARG	O-C-N	-13.54	105.79	122.17	5	20
1	A	97	HIS	ND1-CE1-NE2	12.00	120.40	108.40	6	20
1	A	162	VAL	N-CA-CB	-11.79	91.78	111.23	18	3
1	A	165	VAL	CB-CA-C	10.65	128.76	111.29	5	5
1	A	164	ALA	N-CA-C	10.43	126.34	112.88	19	4
1	A	81	PHE	CA-CB-CG	9.82	123.62	113.80	5	17
1	A	161	THR	CA-C-N	9.58	139.22	121.97	18	1
1	A	161	THR	C-N-CA	9.58	139.22	121.97	18	1
1	A	159	LEU	N-CA-C	9.56	123.74	110.35	13	19
1	A	97	HIS	CE1-NE2-CD2	-9.56	99.44	109.00	13	20
1	A	161	THR	CB-CA-C	8.93	128.19	110.42	14	3
1	A	165	VAL	CA-C-O	-8.86	109.70	120.78	5	3
1	A	91	GLU	N-CA-C	8.84	120.52	111.07	16	20
1	A	161	THR	CA-CB-CG2	8.84	125.52	110.50	18	3
1	A	65	ASN	CA-CB-CG	8.58	121.18	112.60	8	5
1	A	47	VAL	CA-CB-CG1	8.47	124.79	110.40	19	20
1	A	8	PRO	CB-CA-C	8.38	121.15	110.92	9	1
1	A	88	ARG	N-CA-CB	-8.31	97.86	110.16	4	3
1	A	164	ALA	N-CA-CB	-8.25	99.30	111.51	5	3
1	A	84	ASP	CA-CB-CG	8.16	120.77	112.60	10	12
1	A	162	VAL	CA-CB-CG1	8.16	124.28	110.40	18	3
1	A	146	ASP	CA-CB-CG	8.15	120.75	112.60	20	7
1	A	161	THR	N-CA-C	8.10	128.04	110.80	18	1
1	A	52	TYR	N-CA-C	-8.07	100.42	112.04	8	7
1	A	106	ASP	CA-CB-CG	8.06	120.67	112.60	1	10
1	A	111	LEU	N-CA-CB	-7.99	97.18	110.37	18	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	59	VAL	CA-CB-CG1	7.96	123.94	110.40	5	5
1	A	26	ILE	N-CA-CB	-7.66	106.55	111.83	1	2
1	A	72	LEU	N-CA-CB	-7.59	100.41	110.88	8	2
1	A	160	LYS	O-C-N	-7.58	114.84	123.40	14	2
1	A	2	ARG	N-CA-C	7.57	119.65	108.60	13	14
1	A	145	ARG	N-CA-C	7.57	119.53	111.28	4	20
1	A	51	ARG	N-CA-C	7.47	119.42	111.28	8	19
1	A	160	LYS	CB-CA-C	-7.45	101.66	111.42	17	1
1	A	97	HIS	CB-CG-CD2	-7.28	121.74	131.20	12	18
1	A	112	GLU	N-CA-C	7.24	120.57	108.20	14	2
1	A	113	PHE	CA-CB-CG	7.21	121.00	113.80	3	5
1	A	2	ARG	N-CA-CB	-7.20	98.11	111.13	11	3
1	A	161	THR	N-CA-CB	7.09	122.47	110.49	14	3
1	A	165	VAL	N-CA-C	6.96	123.81	109.34	8	1
1	A	47	VAL	N-CA-C	6.77	116.90	110.53	7	15
1	A	97	HIS	CA-CB-CG	6.77	120.57	113.80	3	1
1	A	35	PHE	CA-CB-CG	6.65	120.45	113.80	7	1
1	A	14	GLY	N-CA-C	6.65	120.94	112.83	11	12
1	A	147	GLU	CA-CB-CG	6.63	127.36	114.10	6	2
1	A	93	ALA	N-CA-C	6.62	118.49	111.28	1	9
1	A	81	PHE	N-CA-CB	6.54	121.54	110.49	5	2
1	A	8	PRO	N-CA-C	6.52	116.72	110.47	20	4
1	A	57	ASP	CA-CB-CG	6.50	119.10	112.60	3	3
1	A	110	VAL	N-CA-CB	6.43	118.34	111.00	14	1
1	A	71	ARG	N-CA-C	6.37	120.67	113.02	18	6
1	A	162	VAL	N-CA-C	6.37	122.59	109.34	18	1
1	A	43	THR	N-CA-C	6.36	124.34	110.80	3	1
1	A	35	PHE	N-CA-CB	-6.34	100.80	110.12	14	15
1	A	97	HIS	CG-ND1-CE1	-6.33	98.54	109.30	19	20
1	A	73	ASN	CA-CB-CG	6.33	118.92	112.60	9	3
1	A	68	VAL	CA-CB-CG1	6.26	121.05	110.40	9	6
1	A	82	ILE	CA-CB-CG1	6.26	121.04	110.40	16	7
1	A	22	GLU	CA-C-N	6.24	133.45	121.54	14	1
1	A	22	GLU	C-N-CA	6.24	133.45	121.54	14	1
1	A	158	GLN	N-CA-C	6.23	119.35	111.69	15	11
1	A	90	VAL	CA-CB-CG1	6.21	120.95	110.40	12	3
1	A	148	THR	N-CA-C	6.05	118.65	111.33	19	3
1	A	174	ARG	N-CA-C	6.05	117.87	111.28	1	11
1	A	63	LEU	N-CA-C	6.05	117.54	111.07	20	7
1	A	115	VAL	CB-CA-C	6.03	118.56	110.42	18	1
1	A	111	LEU	N-CA-C	5.99	118.45	108.20	18	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	172	PHE	CA-CB-CG	5.99	119.79	113.80	12	2
1	A	110	VAL	CA-CB-CG2	5.97	120.55	110.40	8	2
1	A	169	ASP	CA-CB-CG	5.97	118.57	112.60	3	1
1	A	60	PRO	N-CA-C	5.92	119.79	111.33	15	1
1	A	61	SER	N-CA-C	5.88	117.49	111.14	3	2
1	A	26	ILE	CA-CB-CG1	5.76	120.20	110.40	20	18
1	A	2	ARG	CB-CA-C	-5.76	99.41	110.24	3	3
1	A	115	VAL	CA-CB-CG1	5.74	120.16	110.40	14	4
1	A	52	TYR	CA-CB-CG	5.70	124.17	113.90	2	1
1	A	110	VAL	N-CA-C	-5.69	98.85	107.73	10	3
1	A	4	LEU	CB-CA-C	5.67	118.88	110.14	5	1
1	A	146	ASP	N-CA-C	5.66	119.00	111.75	19	5
1	A	108	ASP	CA-CB-CG	5.63	118.23	112.60	1	2
1	A	62	ASP	N-CA-C	5.63	117.41	111.28	2	2
1	A	174	ARG	CB-CA-C	-5.58	102.05	110.92	12	1
1	A	80	GLY	N-CA-C	5.57	118.87	110.18	10	1
1	A	23	LYS	CA-C-O	-5.57	112.54	120.51	14	1
1	A	165	VAL	O-C-N	-5.55	115.63	122.57	5	2
1	A	72	LEU	N-CA-C	-5.54	105.16	111.14	18	3
1	A	44	LYS	CA-CB-CG	-5.53	103.03	114.10	19	2
1	A	165	VAL	CA-CB-CG1	5.50	119.74	110.40	18	2
1	A	109	ALA	N-CA-C	5.49	117.56	108.13	20	1
1	A	165	VAL	CA-CB-CG2	5.46	119.69	110.40	5	3
1	A	23	LYS	N-CA-C	5.46	122.42	110.80	14	2
1	A	50	LYS	CB-CA-C	5.46	121.39	109.99	5	1
1	A	169	ASP	N-CA-C	5.42	117.95	111.71	20	1
1	A	177	ARG	N-CA-C	5.42	117.88	111.33	8	4
1	A	53	LEU	N-CA-CB	-5.41	101.34	110.49	5	2
1	A	50	LYS	CA-CB-CG	5.41	124.92	114.10	7	2
1	A	154	TYR	CA-CB-CG	5.40	123.62	113.90	8	1
1	A	19	LYS	N-CA-C	5.36	116.81	111.07	17	4
1	A	111	LEU	CA-C-O	-5.33	114.80	120.40	17	1
1	A	149	ALA	N-CA-CB	-5.33	105.33	110.39	5	1
1	A	26	ILE	N-CA-C	5.32	113.75	107.84	1	1
1	A	90	VAL	CA-CB-CG2	5.32	119.45	110.40	14	2
1	A	7	GLY	CA-C-N	5.28	123.51	119.66	4	2
1	A	7	GLY	C-N-CA	5.28	123.51	119.66	4	2
1	A	154	TYR	N-CA-CB	-5.23	102.42	110.01	18	2
1	A	69	ASP	N-CA-C	5.22	116.98	111.28	5	1
1	A	178	ALA	N-CA-C	5.22	116.66	111.07	3	1
1	A	147	GLU	N-CA-C	5.22	120.30	113.88	6	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	139	ASN	CA-CB-CG	5.22	117.82	112.60	11	2
1	A	82	ILE	CB-CG1-CD1	5.20	124.73	113.80	20	1
1	A	16	GLN	CB-CG-CD	5.19	121.42	112.60	9	1
1	A	97	HIS	ND1-CG-CD2	5.19	111.29	106.10	19	1
1	A	87	PRO	N-CA-C	5.18	123.14	112.47	18	1
1	A	45	LEU	CA-C-N	5.17	125.67	119.94	20	1
1	A	45	LEU	C-N-CA	5.17	125.67	119.94	20	1
1	A	163	ASP	N-CA-C	-5.16	100.32	108.73	9	1
1	A	175	ALA	N-CA-C	5.15	116.58	111.07	10	2
1	A	68	VAL	N-CA-C	5.13	115.85	110.62	20	1
1	A	91	GLU	CA-C-O	-5.12	115.13	120.55	10	1
1	A	142	LYS	N-CA-C	5.10	116.52	111.07	14	1
1	A	86	TYR	CA-C-O	-5.08	113.20	120.16	13	1
1	A	92	GLN	CA-C-N	5.05	127.05	120.28	1	1
1	A	92	GLN	C-N-CA	5.05	127.05	120.28	1	1
1	A	57	ASP	CB-CA-C	5.04	120.44	110.42	17	1
1	A	50	LYS	N-CA-CB	-5.04	102.48	110.28	1	1
1	A	41	GLU	N-CA-C	5.03	116.84	111.36	19	2
1	A	108	ASP	N-CA-CB	5.03	117.98	110.14	5	1
1	A	88	ARG	N-CA-C	5.02	117.48	111.71	13	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	161	THR	CA	2

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	51	ARG	Peptide,Mainchain	20
1	A	155	TYR	Sidechain	17
1	A	154	TYR	Sidechain	12
1	A	160	LYS	Peptide,Mainchain	3
1	A	52	TYR	Sidechain	2
1	A	86	TYR	Sidechain	2
1	A	2	ARG	Sidechain	1
1	A	43	THR	Peptide	1
1	A	35	PHE	Sidechain	1
1	A	88	ARG	Sidechain	1
1	A	73	ASN	Peptide	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	23	LYS	Mainchain	1
1	A	163	ASP	Peptide	1
1	A	161	THR	Peptide,Mainchain	1
1	A	165	VAL	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	1153	1184	1184	17±5
All	All	23060	23680	23680	334

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:ARG:CG	1:A:140:ARG:HH12	1.34	1.35	18	1
1:A:152:LEU:O	1:A:156:ARG:HB2	1.30	1.13	13	20
1:A:99:MET:O	1:A:103:ARG:HB2	1.29	1.26	11	13
1:A:98:GLU:O	1:A:102:ARG:HB2	1.29	1.20	20	12
1:A:99:MET:O	1:A:103:ARG:HB3	1.29	1.27	15	12
1:A:88:ARG:HG3	1:A:140:ARG:NH1	1.26	1.41	18	1
1:A:98:GLU:O	1:A:102:ARG:HB3	1.24	1.32	1	11
1:A:88:ARG:CD	1:A:140:ARG:HH12	1.23	1.47	18	1
1:A:88:ARG:NH2	1:A:140:ARG:HH12	1.14	1.39	15	1
1:A:88:ARG:CG	1:A:140:ARG:NH1	1.11	2.06	18	1
1:A:99:MET:O	1:A:103:ARG:CB	1.09	1.99	9	18
1:A:88:ARG:HG3	1:A:140:ARG:CZ	1.06	1.81	18	1
1:A:180:GLY:O	1:A:181:LYS:HB2	1.03	1.48	20	18
1:A:152:LEU:O	1:A:156:ARG:CB	1.00	2.08	13	20
1:A:47:VAL:O	1:A:51:ARG:HB2	0.99	1.58	5	2
1:A:88:ARG:CD	1:A:140:ARG:NH1	0.96	2.25	18	1
1:A:98:GLU:O	1:A:102:ARG:CB	0.96	2.14	14	14
1:A:20:LEU:HA	1:A:23:LYS:HB3	0.94	1.35	14	1
1:A:162:VAL:HG13	1:A:174:ARG:HB3	0.93	1.35	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:ARG:NH2	1:A:140:ARG:NH1	0.91	2.18	15	1
1:A:5:LEU:HD21	1:A:13:LYS:HB3	0.91	1.41	12	2
1:A:43:THR:O	1:A:44:LYS:HB2	0.90	1.67	19	15
1:A:88:ARG:HH21	1:A:140:ARG:HH12	0.88	0.95	15	1
1:A:88:ARG:HD2	1:A:140:ARG:NH1	0.87	1.84	18	1
1:A:180:GLY:O	1:A:181:LYS:CB	0.87	2.22	5	16
1:A:88:ARG:HG3	1:A:140:ARG:NH2	0.83	1.88	18	1
1:A:111:LEU:HD12	1:A:160:LYS:HB3	0.82	1.50	18	1
1:A:88:ARG:HH21	1:A:140:ARG:NH1	0.81	1.70	15	1
1:A:56:GLY:HA2	1:A:88:ARG:HH12	0.79	1.35	13	1
1:A:111:LEU:HD12	1:A:160:LYS:CB	0.78	2.07	18	1
1:A:170:GLU:HB3	1:A:174:ARG:HH21	0.76	1.39	15	2
1:A:170:GLU:HB3	1:A:174:ARG:NH2	0.73	1.99	3	5
1:A:13:LYS:HB3	1:A:84:ASP:OD1	0.70	1.87	19	1
1:A:32:GLY:O	1:A:36:ARG:HB2	0.69	1.87	5	5
1:A:20:LEU:HA	1:A:23:LYS:CB	0.68	2.16	14	1
1:A:162:VAL:HG13	1:A:174:ARG:CB	0.68	2.15	12	1
1:A:162:VAL:CG1	1:A:174:ARG:HB3	0.67	2.19	12	1
1:A:5:LEU:HD11	1:A:13:LYS:CB	0.66	2.20	9	1
1:A:56:GLY:HA2	1:A:88:ARG:HH22	0.65	1.50	8	1
1:A:19:LYS:HB3	1:A:172:PHE:CE1	0.64	2.28	15	4
1:A:5:LEU:CD1	1:A:13:LYS:HB2	0.63	2.24	9	1
1:A:35:PHE:HB3	1:A:50:LYS:HB2	0.63	1.71	14	1
1:A:43:THR:O	1:A:44:LYS:CB	0.63	2.46	20	19
1:A:5:LEU:CD2	1:A:13:LYS:HB3	0.62	2.23	12	2
1:A:51:ARG:O	1:A:51:ARG:CG	0.60	2.49	9	7
1:A:46:GLY:O	1:A:50:LYS:HB3	0.60	1.96	1	1
1:A:51:ARG:CG	1:A:51:ARG:O	0.59	2.50	12	6
1:A:162:VAL:CG1	1:A:174:ARG:CB	0.58	2.82	12	1
1:A:162:VAL:HG21	1:A:174:ARG:HB3	0.58	1.74	18	1
1:A:51:ARG:O	1:A:51:ARG:HG2	0.57	2.00	9	13
1:A:152:LEU:O	1:A:156:ARG:HB3	0.56	2.01	2	3
1:A:35:PHE:HB3	1:A:50:LYS:CB	0.55	2.30	14	4
1:A:2:ARG:HH21	1:A:4:LEU:HD21	0.55	1.62	16	1
1:A:43:THR:O	1:A:44:LYS:HG3	0.54	2.01	3	1
1:A:2:ARG:HB3	1:A:80:GLY:HA2	0.54	1.78	4	1
1:A:5:LEU:HD11	1:A:13:LYS:HB2	0.53	1.77	9	1
1:A:24:LEU:HD13	1:A:26:ILE:HD11	0.52	1.82	14	1
1:A:114:ARG:HB2	1:A:162:VAL:O	0.52	2.04	18	1
1:A:111:LEU:HD23	1:A:160:LYS:HB2	0.50	1.84	6	2
1:A:111:LEU:HA	1:A:160:LYS:HB2	0.50	1.83	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:PHE:CD1	1:A:50:LYS:HB2	0.49	2.43	14	1
1:A:88:ARG:HG3	1:A:140:ARG:HH22	0.49	1.61	18	1
1:A:174:ARG:HA	1:A:177:ARG:HB2	0.48	1.86	15	1
1:A:102:ARG:O	1:A:103:ARG:HB2	0.48	2.08	8	1
1:A:43:THR:O	1:A:44:LYS:CG	0.47	2.62	9	5
1:A:32:GLY:O	1:A:36:ARG:CB	0.47	2.61	5	1
1:A:56:GLY:HA2	1:A:88:ARG:NH2	0.47	2.21	8	1
1:A:5:LEU:CD1	1:A:13:LYS:CB	0.47	2.90	9	1
1:A:43:THR:O	1:A:44:LYS:HG2	0.47	2.10	9	3
1:A:111:LEU:CD1	1:A:160:LYS:HB3	0.47	2.35	18	1
1:A:35:PHE:HB3	1:A:50:LYS:CG	0.47	2.40	10	2
1:A:114:ARG:CB	1:A:162:VAL:O	0.47	2.63	18	1
1:A:43:THR:O	1:A:44:LYS:HB3	0.47	2.10	6	4
1:A:56:GLY:HA2	1:A:88:ARG:HH11	0.47	1.70	2	1
1:A:35:PHE:CB	1:A:50:LYS:HB2	0.46	2.38	14	1
1:A:47:VAL:O	1:A:51:ARG:CB	0.46	2.49	5	1
1:A:114:ARG:HB3	1:A:163:ASP:HA	0.46	1.88	18	1
1:A:163:ASP:O	1:A:174:ARG:HG3	0.45	2.12	12	1
1:A:39:ILE:HD11	1:A:50:LYS:HB3	0.44	1.88	2	1
1:A:173:ALA:O	1:A:177:ARG:HB2	0.44	2.12	15	1
1:A:94:LYS:O	1:A:98:GLU:HB2	0.44	2.13	10	1
1:A:26:ILE:CD1	1:A:81:PHE:HA	0.43	2.43	5	2
1:A:174:ARG:HA	1:A:177:ARG:CB	0.43	2.43	15	1
1:A:2:ARG:HH22	1:A:4:LEU:HD12	0.43	1.73	4	1
1:A:99:MET:HE3	1:A:103:ARG:HG2	0.43	1.90	16	1
1:A:45:LEU:O	1:A:49:ALA:HB3	0.43	2.14	20	1
1:A:161:THR:HG23	1:A:162:VAL:HB	0.42	1.90	18	1
1:A:35:PHE:CG	1:A:50:LYS:HB2	0.42	2.49	14	1
1:A:99:MET:HG3	1:A:103:ARG:HB2	0.42	1.91	16	1
1:A:57:ASP:O	1:A:88:ARG:NH1	0.42	2.53	18	1
1:A:111:LEU:HD12	1:A:160:LYS:HB2	0.42	1.88	18	1
1:A:26:ILE:CG2	1:A:81:PHE:HA	0.42	2.44	16	1
1:A:58:LEU:HA	1:A:88:ARG:NH2	0.42	2.30	6	1
1:A:114:ARG:O	1:A:115:VAL:HG23	0.42	2.14	9	1
1:A:46:GLY:O	1:A:50:LYS:CB	0.42	2.68	6	1
1:A:88:ARG:CG	1:A:140:ARG:HH22	0.41	2.26	18	1
1:A:13:LYS:CB	1:A:84:ASP:OD2	0.41	2.68	8	1
1:A:100:LEU:HD11	1:A:107:ILE:HB	0.41	1.92	16	1
1:A:100:LEU:HD21	1:A:107:ILE:HD13	0.41	1.92	2	1
1:A:58:LEU:HA	1:A:88:ARG:HH22	0.40	1.76	6	1
1:A:71:ARG:HH22	1:A:83:LEU:HG	0.40	1.76	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:THR:C	1:A:44:LYS:HG3	0.40	2.41	3	1
1:A:99:MET:CG	1:A:103:ARG:HB2	0.40	2.47	18	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	143/181 (79%)	126±2 (88±2%)	14±2 (9±1%)	4±2 (3±1%)	6	43
All	All	2860/3620 (79%)	2518 (88%)	270 (9%)	72 (3%)	6	43

All 20 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	44	LYS	19
1	A	13	LYS	10
1	A	165	VAL	9
1	A	87	PRO	6
1	A	86	TYR	5
1	A	180	GLY	4
1	A	57	ASP	3
1	A	52	TYR	3
1	A	8	PRO	2
1	A	43	THR	1
1	A	81	PHE	1
1	A	88	ARG	1
1	A	89	SER	1
1	A	73	ASN	1
1	A	103	ARG	1
1	A	159	LEU	1
1	A	115	VAL	1
1	A	23	LYS	1
1	A	14	GLY	1
1	A	161	THR	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	122/149 (82%)	112±2 (92±2%)	10±2 (8±2%)	12	59
All	All	2440/2980 (82%)	2234 (92%)	206 (8%)	12	59

All 55 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	91	GLU	14
1	A	45	LEU	12
1	A	115	VAL	10
1	A	2	ARG	10
1	A	28	GLN	10
1	A	176	LEU	8
1	A	5	LEU	7
1	A	90	VAL	7
1	A	65	ASN	6
1	A	100	LEU	6
1	A	47	VAL	6
1	A	20	LEU	6
1	A	68	VAL	6
1	A	88	ARG	5
1	A	151	LEU	5
1	A	66	GLU	5
1	A	4	LEU	5
1	A	146	ASP	5
1	A	84	ASP	5
1	A	152	LEU	4
1	A	179	LEU	4
1	A	16	GLN	4
1	A	50	LYS	4
1	A	6	LEU	3
1	A	98	GLU	3
1	A	110	VAL	3
1	A	13	LYS	3
1	A	82	ILE	3
1	A	52	TYR	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	92	GLN	2
1	A	22	GLU	2
1	A	26	ILE	2
1	A	53	LEU	2
1	A	44	LYS	2
1	A	171	VAL	2
1	A	24	LEU	2
1	A	23	LYS	2
1	A	63	LEU	2
1	A	106	ASP	1
1	A	97	HIS	1
1	A	29	ILE	1
1	A	59	VAL	1
1	A	147	GLU	1
1	A	99	MET	1
1	A	83	LEU	1
1	A	18	VAL	1
1	A	94	LYS	1
1	A	154	TYR	1
1	A	174	ARG	1
1	A	37	ARG	1
1	A	71	ARG	1
1	A	161	THR	1
1	A	162	VAL	1
1	A	165	VAL	1
1	A	181	LYS	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