



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 10:49 pm BST

PDB ID : 5THE
Title : Crystal structure of the C-terminal lobe of a budding yeast Argonaute
Authors : Dayeh, D.M.; Nakanishi, K.
Deposited on : 2016-09-29
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

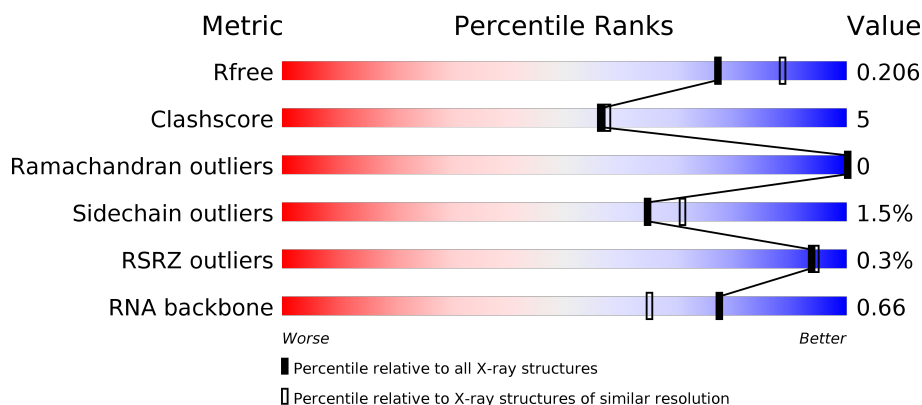
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)
RNA backbone	3102	1000 (2.54-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	
1	C	549	
1	E	549	
1	G	549	

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Mol	Chain	Length	Quality of chain
2	B	8	 63% 25% 13%
2	D	8	 63% 38%
2	F	8	 75% 25%
2	H	8	 63% 38%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18231 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			4032	2562	681	769	20			
1	C	510	Total	C	N	O	S	0	0	0
			4026	2559	680	767	20			
1	E	514	Total	C	N	O	S	0	0	0
			4061	2582	686	773	20			
1	G	514	Total	C	N	O	S	0	0	0
			4061	2582	686	773	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	SER	-	expression tag	UNP A7TMA9
A	725	GLY	-	linker	UNP A7TMA9
A	726	SER	-	linker	UNP A7TMA9
A	727	GLY	-	linker	UNP A7TMA9
C	220	SER	-	expression tag	UNP A7TMA9
C	725	GLY	-	linker	UNP A7TMA9
C	726	SER	-	linker	UNP A7TMA9
C	727	GLY	-	linker	UNP A7TMA9
E	220	SER	-	expression tag	UNP A7TMA9
E	725	GLY	-	linker	UNP A7TMA9
E	726	SER	-	linker	UNP A7TMA9
E	727	GLY	-	linker	UNP A7TMA9
G	220	SER	-	expression tag	UNP A7TMA9
G	725	GLY	-	linker	UNP A7TMA9
G	726	SER	-	linker	UNP A7TMA9
G	727	GLY	-	linker	UNP A7TMA9

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	8	Total 157	C 69	N 32	O 48	P 8	0	0	0
2	D	8	Total 157	C 69	N 32	O 48	P 8	0	0	0
2	F	8	Total 157	C 69	N 32	O 48	P 8	0	0	0
2	H	8	Total 157	C 69	N 32	O 48	P 8	0	0	0

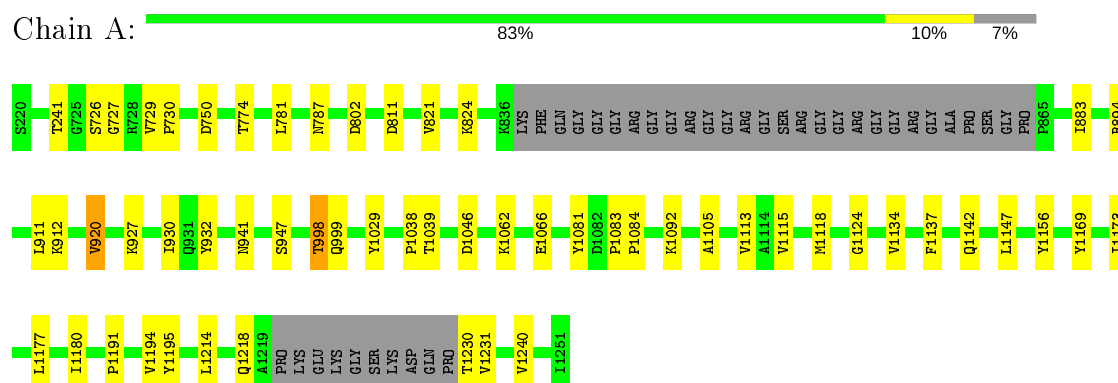
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	344	Total 344	O 344	0	0
3	B	18	Total 18	O 18	0	0
3	C	363	Total 363	O 363	0	0
3	D	12	Total 12	O 12	0	0
3	E	336	Total 336	O 336	0	0
3	F	12	Total 12	O 12	0	0
3	G	329	Total 329	O 329	0	0
3	H	9	Total 9	O 9	0	0

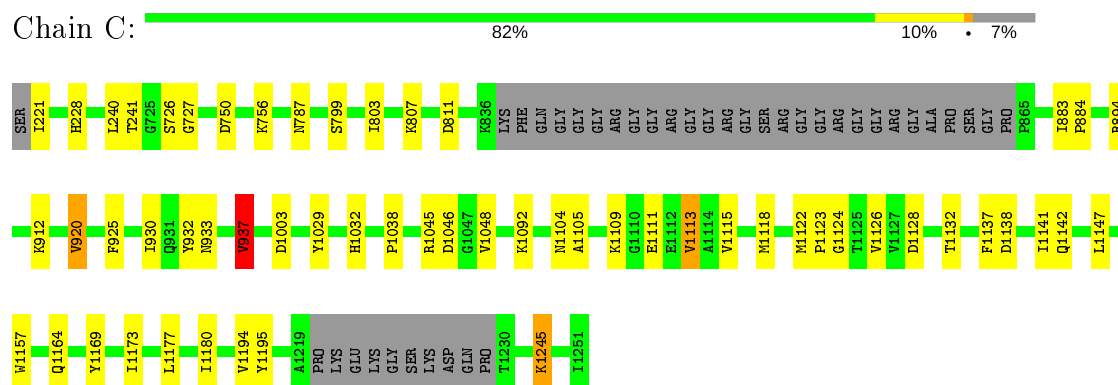
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

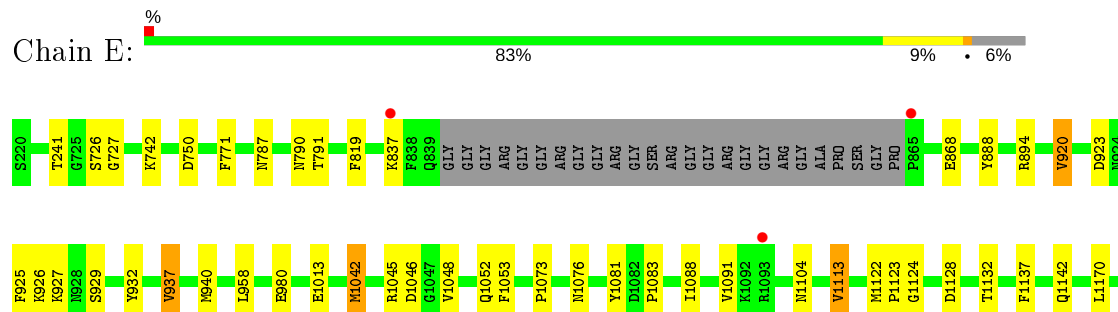
- Molecule 1: Uncharacterized protein

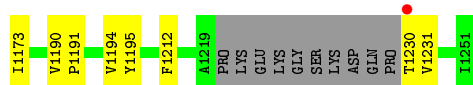


- Molecule 1: Uncharacterized protein

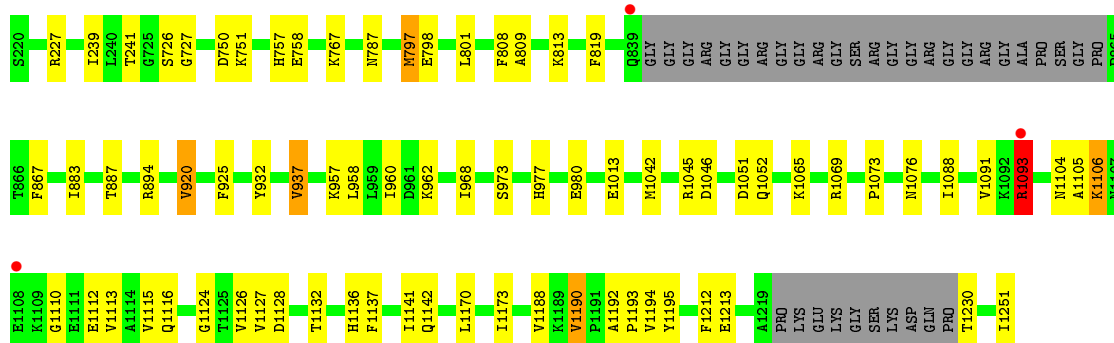
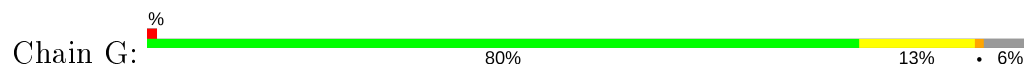


- Molecule 1: Uncharacterized protein





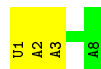
- Molecule 1: Uncharacterized protein



- Molecule 2: RNA (5'-R(P*UP*AP*AP*AP*AP*AP*A)-3')



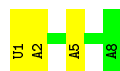
- Molecule 2: RNA (5'-R(P*UP*AP*AP*AP*AP*AP*A)-3')



- Molecule 2: RNA (5'-R(P*UP*AP*AP*AP*AP*AP*A)-3')



- Molecule 2: RNA (5'-R(P*UP*AP*AP*AP*AP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.61Å 85.56Å 127.86Å 90.00° 89.81° 90.00°	Depositor
Resolution (Å)	47.12 – 2.10 49.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.12-2.10) 95.8 (49.02-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10.1-2155)	Depositor
R, R_{free}	0.158 , 0.206 0.158 , 0.206	Depositor DCC
R_{free} test set	2005 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18231	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 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 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	0.40	0/4115	0.56	0/5566
1	C	0.40	0/4109	0.57	1/5558 (0.0%)
1	E	0.42	0/4145	0.57	1/5605 (0.0%)
1	G	0.44	2/4145 (0.0%)	0.59	0/5605
2	B	1.04	1/176 (0.6%)	1.32	1/271 (0.4%)
2	D	1.01	1/176 (0.6%)	1.24	0/271
2	F	0.95	1/176 (0.6%)	1.19	1/271 (0.4%)
2	H	1.03	1/176 (0.6%)	1.41	3/271 (1.1%)
All	All	0.46	6/17218 (0.0%)	0.63	7/23418 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.95	1.48	1.61
2	H	1	U	OP3-P	-10.37	1.48	1.61
2	D	1	U	OP3-P	-10.04	1.49	1.61
2	F	1	U	OP3-P	-9.56	1.49	1.61
1	G	1093	ARG	CZ-NH2	-5.51	1.25	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	A	N1-C6-N6	8.03	123.42	118.60
2	H	2	A	C5-C6-N6	-6.05	118.86	123.70
1	C	937	VAL	CB-CA-C	-5.39	101.16	111.40
2	F	2	A	N1-C6-N6	5.33	121.80	118.60
1	E	937	VAL	CG1-CB-CG2	5.30	119.39	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4032	0	4017	37	0
1	C	4026	0	4012	39	0
1	E	4061	0	4047	35	0
1	G	4061	0	4047	59	0
2	B	157	0	76	1	0
2	D	157	0	76	1	0
2	F	157	0	76	0	0
2	H	157	0	76	0	0
3	A	344	0	0	1	0
3	B	18	0	0	0	0
3	C	363	0	0	5	0
3	D	12	0	0	0	0
3	E	336	0	0	0	0
3	F	12	0	0	0	0
3	G	329	0	0	2	0
3	H	9	0	0	0	0
All	All	18231	0	16427	167	0

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 5.

The worst 5 of 167 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:813:LYS:HZ2	1:G:819:PHE:N	1.59	1.00
1:E:750:ASP:HB3	1:E:1113:VAL:HG21	1.49	0.95
1:G:787:ASN:HD21	1:G:894:ARG:HH11	1.17	0.91
1:A:1118:MET:HE2	1:A:1147:LEU:HA	1.52	0.90
1:G:813:LYS:NZ	1:G:819:PHE:H	1.70	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	505/549 (92%)	498 (99%)	7 (1%)	0	100	100
1	C	504/549 (92%)	495 (98%)	9 (2%)	0	100	100
1	E	508/549 (92%)	494 (97%)	14 (3%)	0	100	100
1	G	508/549 (92%)	493 (97%)	15 (3%)	0	100	100
All	All	2025/2196 (92%)	1980 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	457/479 (95%)	452 (99%)	5 (1%)	73	79
1	C	456/479 (95%)	449 (98%)	7 (2%)	65	71
1	E	460/479 (96%)	452 (98%)	8 (2%)	60	67
1	G	460/479 (96%)	452 (98%)	8 (2%)	60	67
All	All	1833/1916 (96%)	1805 (98%)	28 (2%)	65	71

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	920	VAL
1	E	1042	MET
1	G	1137	PHE

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Mol	Chain	Res	Type
1	E	929	SER
1	E	937	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	787	ASN
1	G	878	ASN
1	E	882	ASN
1	A	1145	GLN
1	E	829	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	6/8 (75%)	0	0
2	D	6/8 (75%)	0	0
2	F	6/8 (75%)	0	0
2	H	6/8 (75%)	0	0
All	All	24/32 (75%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	511/549 (93%)	-0.18	0 100 100	21, 29, 49, 87	0
1	C	510/549 (92%)	-0.18	0 100 100	20, 29, 49, 87	0
1	E	514/549 (93%)	-0.13	4 (0%) 86 88	21, 30, 52, 99	0
1	G	514/549 (93%)	-0.17	3 (0%) 89 91	21, 30, 53, 99	0
2	B	8/8 (100%)	-0.55	0 100 100	27, 33, 81, 103	0
2	D	8/8 (100%)	-0.47	0 100 100	27, 33, 85, 116	0
2	F	8/8 (100%)	-0.55	0 100 100	26, 34, 90, 122	0
2	H	8/8 (100%)	-0.72	0 100 100	27, 34, 92, 120	0
All	All	2081/2228 (93%)	-0.17	7 (0%) 94 94	20, 30, 52, 122	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	839	GLN	3.5
1	G	1108	GLU	3.3
1	E	1230	THR	3.2
1	E	1093	ARG	2.9
1	E	865	PRO	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.