



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3DLB / pdb_00003dlb
Title : Crystal structure of the guide-strand-containing Argonaute protein silencing complex
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Deposited on : 2008-06-26
Resolution : 2.70 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 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

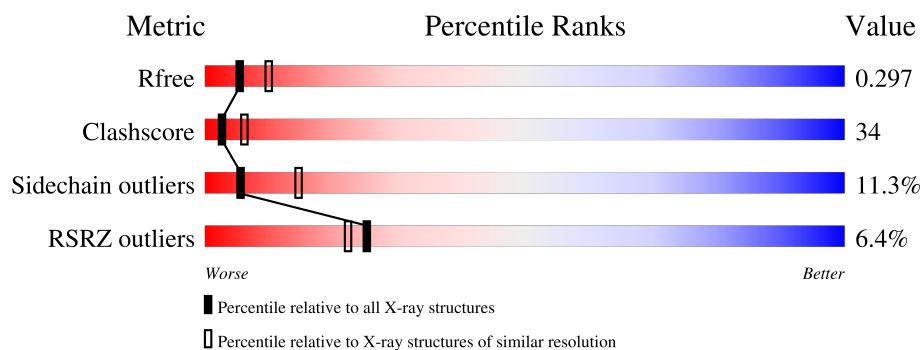
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 of 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	685	5% 51% 34% 8% 7%
1	B	685	7% 43% 38% 8% 10%
2	X	10	20% 20% 10% 50%
2	Y	10	10% 40% 10% 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9793 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 argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	9	0	0
			4891	3125	913	846	7			
1	B	614	Total	C	N	O	S	34	0	0
			4668	2983	873	806	6			

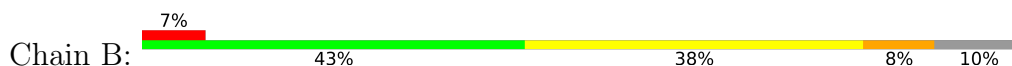
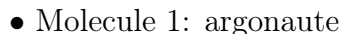
- Molecule 2 is a DNA chain called DNA (5'-D(*DTP*DGP*DAP*DGP*DGP*DTP*DAP*DGP*DTP*DA)-3').

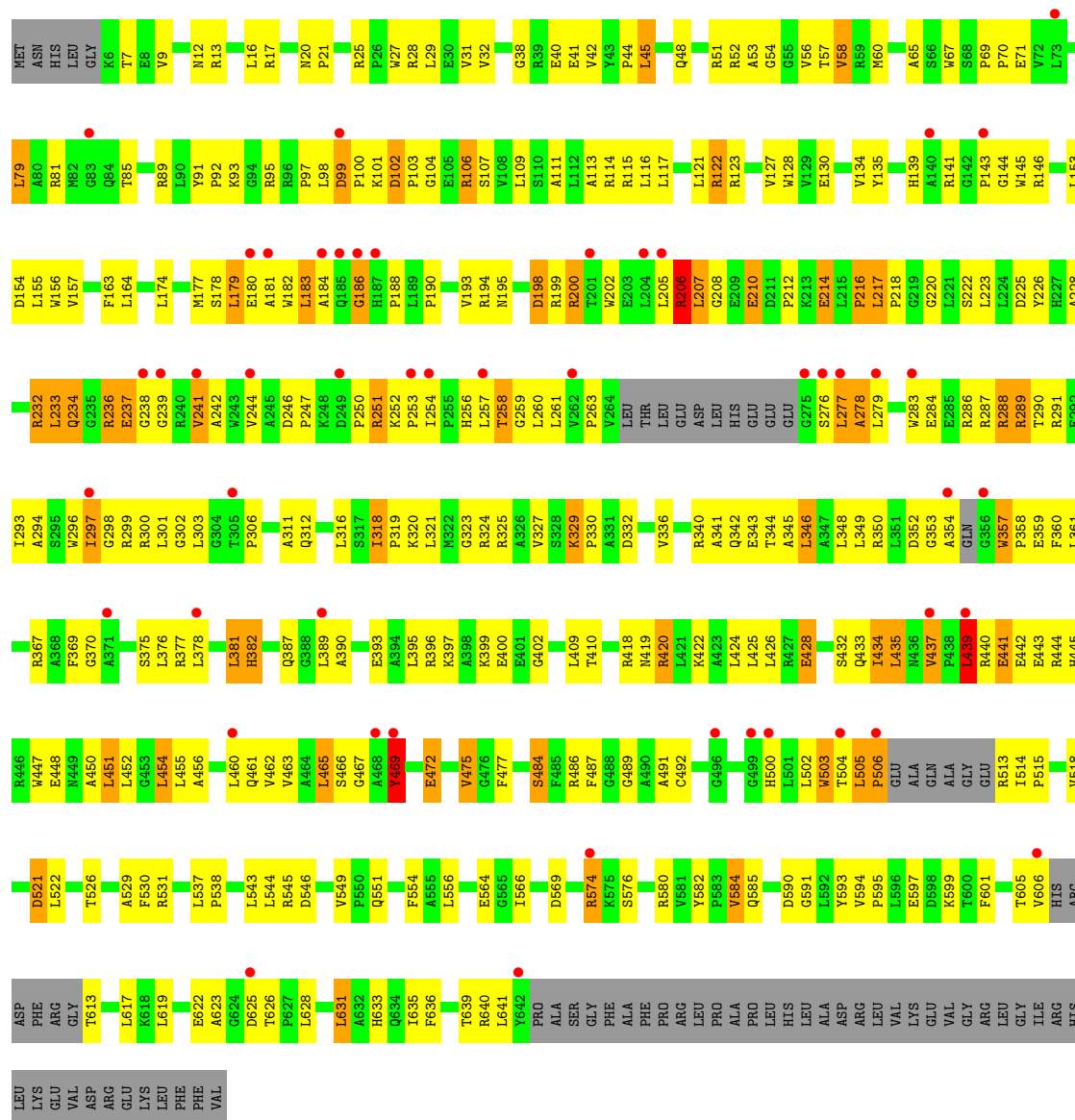
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	5	Total	C	N	O	P	0	0	0
			101	50	19	28	4			
2	Y	5	Total	C	N	O	P	0	0	1
			85	40	17	24	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	19	Total	O	0	0
			19	19		
3	X	3	Total	O	0	0
			3	3		
3	Y	1	Total	O	0	0
			1	1		

- Molecule 1: argonaute





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.85Å 123.40Å 84.91Å 90.00° 95.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.70) 94.2 (30.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.293 (Not available) , 0.297	Depositor DCC
R_{free} test set	2154 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9793	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 [i](#)

5.1 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 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	0.74	9/5009 (0.2%)	1.22	56/6817 (0.8%)
1	B	0.67	6/4780 (0.1%)	1.24	54/6509 (0.8%)
2	X	0.48	0/113	1.17	1/173 (0.6%)
2	Y	0.35	0/95	1.11	1/146 (0.7%)
All	All	0.70	15/9997 (0.2%)	1.23	112/13645 (0.8%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	529	ALA	C-N	-7.89	1.22	1.33
1	A	128	TRP	CB-CG	-7.86	1.25	1.50
1	A	503	TRP	CB-CG	-6.43	1.30	1.50
1	A	503	TRP	CA-C	-6.26	1.45	1.52
1	A	128	TRP	N-CA	-6.24	1.38	1.46

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	LEU	N-CA-C	15.05	139.69	108.53
1	A	356	GLY	N-CA-C	14.08	132.73	112.60
1	A	609	ASP	N-CA-C	11.44	125.21	109.54
1	A	608	ARG	N-CA-C	-11.43	86.45	110.80
1	B	250	PRO	N-CA-C	11.28	127.90	114.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4891	0	4892	298	0
1	B	4668	0	4624	357	0
2	X	101	0	59	7	0
2	Y	85	0	46	1	0
3	A	25	0	0	0	0
3	B	19	0	0	0	0
3	X	3	0	0	0	0
3	Y	1	0	0	0	0
All	All	9793	0	9621	650	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 34.

The worst 5 of 650 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:B:506:PRO:HD3	1:B:522:LEU:HD21	1.28	1.12
1:A:175:CYS:HB2	1:A:265:LEU:HD11	1.28	1.08
1:B:237:GLU:O	1:B:237:GLU:HG3	1.51	1.08
1:B:349:LEU:HB2	1:B:381:LEU:HD12	1.38	1.05
1:B:440:ARG:HD3	1:B:441:GLU:N	1.71	1.03

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	475/549 (86%)	429 (90%)	46 (10%)	8	20
1	B	447/549 (81%)	389 (87%)	58 (13%)	4	10
All	All	922/1098 (84%)	818 (89%)	104 (11%)	5	14

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	139	HIS
1	B	258	THR
1	B	574	ARG
1	B	146	ARG
1	B	217	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	382	HIS
1	B	633	HIS
1	B	449	ASN
1	A	585	GLN
1	B	256	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	637/685 (92%)	0.48	31 (4%)	35 31	43, 73, 102, 115	3 (0%)
1	B	614/685 (89%)	0.60	49 (7%)	18 15	41, 78, 116, 126	14 (2%)
2	X	5/10 (50%)	-0.03	0	100 100	57, 68, 87, 117	0
2	Y	5/10 (50%)	0.07	1 (20%)	3 2	68, 72, 76, 93	0
All	All	1261/1390 (90%)	0.53	81 (6%)	25 22	41, 75, 110, 126	17 (1%)

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	THR	7.0
1	A	386	SER	6.0
1	B	187	HIS	5.6
1	B	625	ASP	5.1
1	B	181	ALA	5.1

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 oligosaccharides 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.