



wwPDB X-ray Structure Validation Summary Report

Feb 13, 2017 – 06:18 pm GMT

PDB ID : 1JFZ
Title : Crystal Structure of MN(II)-Complex of RNase III Endonuclease Domain from Aquifex Aeolicus at 2.10 Angstrom Resolution
Authors : Blaszczyk, J.; Ji, X.
Deposited on : 2001-06-22
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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

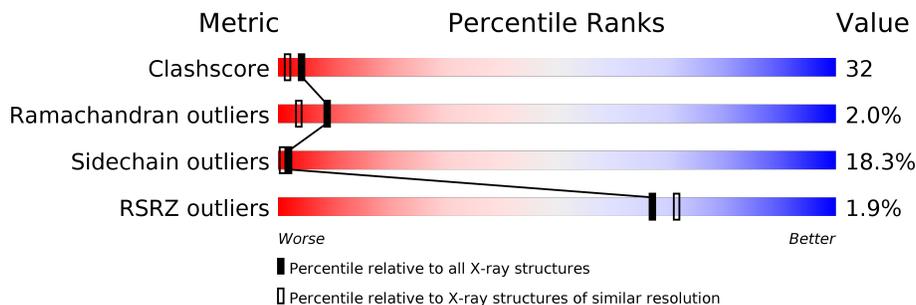
1 Overall quality at a glance

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))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. 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	154	 % 47% 38% 12% .
1	B	154	 3% 44% 34% 18% ..
1	C	154	 % 44% 42% 10% .
1	D	154	 3% 34% 47% 14% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5664 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 RIBONUCLEASE III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	148	1233	809	199	223	2	0	2	0
1	B	149	1247	818	202	225	2	0	3	0
1	C	149	1243	816	202	223	2	0	2	0
1	D	148	1225	805	198	220	2	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	SEE REMARK 999	UNP O67082
A	148	HIS	-	EXPRESSION TAG	UNP O67082
A	149	HIS	-	EXPRESSION TAG	UNP O67082
A	150	HIS	-	EXPRESSION TAG	UNP O67082
A	151	HIS	-	EXPRESSION TAG	UNP O67082
A	152	HIS	-	EXPRESSION TAG	UNP O67082
A	153	HIS	-	EXPRESSION TAG	UNP O67082
B	200	GLY	-	SEE REMARK 999	UNP O67082
B	348	HIS	-	EXPRESSION TAG	UNP O67082
B	349	HIS	-	EXPRESSION TAG	UNP O67082
B	350	HIS	-	EXPRESSION TAG	UNP O67082
B	351	HIS	-	EXPRESSION TAG	UNP O67082
B	352	HIS	-	EXPRESSION TAG	UNP O67082
B	353	HIS	-	EXPRESSION TAG	UNP O67082
C	400	GLY	-	SEE REMARK 999	UNP O67082
C	548	HIS	-	EXPRESSION TAG	UNP O67082
C	549	HIS	-	EXPRESSION TAG	UNP O67082
C	550	HIS	-	EXPRESSION TAG	UNP O67082
C	551	HIS	-	EXPRESSION TAG	UNP O67082
C	552	HIS	-	EXPRESSION TAG	UNP O67082
C	553	HIS	-	EXPRESSION TAG	UNP O67082

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Chain	Residue	Modelled	Actual	Comment	Reference
D	600	GLY	-	SEE REMARK 999	UNP O67082
D	748	HIS	-	EXPRESSION TAG	UNP O67082
D	749	HIS	-	EXPRESSION TAG	UNP O67082
D	750	HIS	-	EXPRESSION TAG	UNP O67082
D	751	HIS	-	EXPRESSION TAG	UNP O67082
D	752	HIS	-	EXPRESSION TAG	UNP O67082
D	753	HIS	-	EXPRESSION TAG	UNP O67082

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0

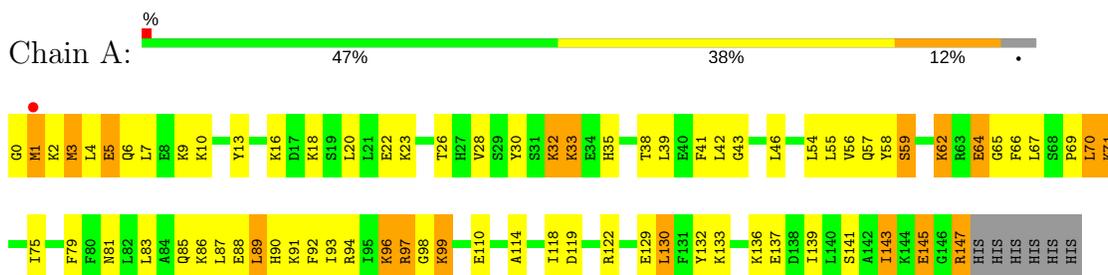
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	201	Total 201	O 201	0	0
3	B	166	Total 166	O 166	0	0
3	C	175	Total 175	O 175	0	0
3	D	170	Total 170	O 170	0	0

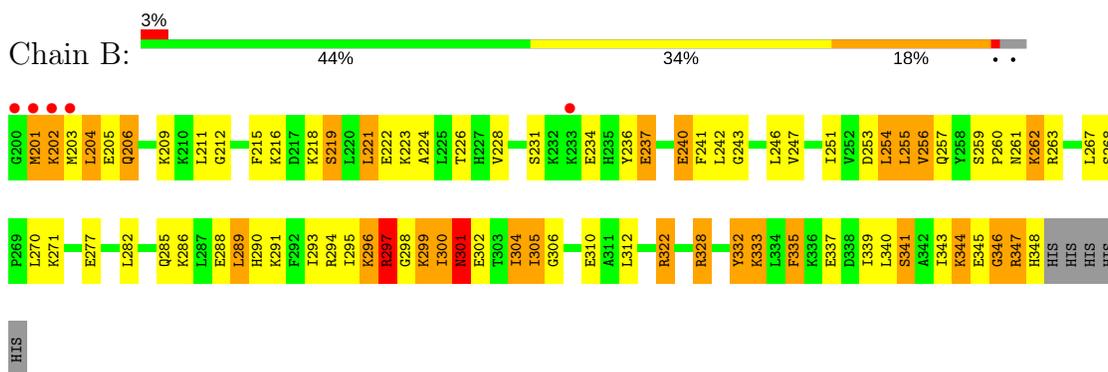
3 Residue-property plots [i](#)

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.

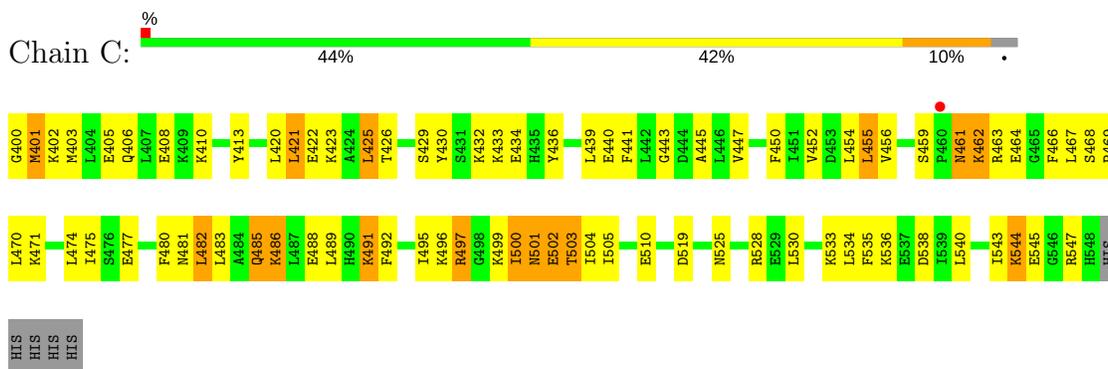
- Molecule 1: RIBONUCLEASE III



- Molecule 1: RIBONUCLEASE III

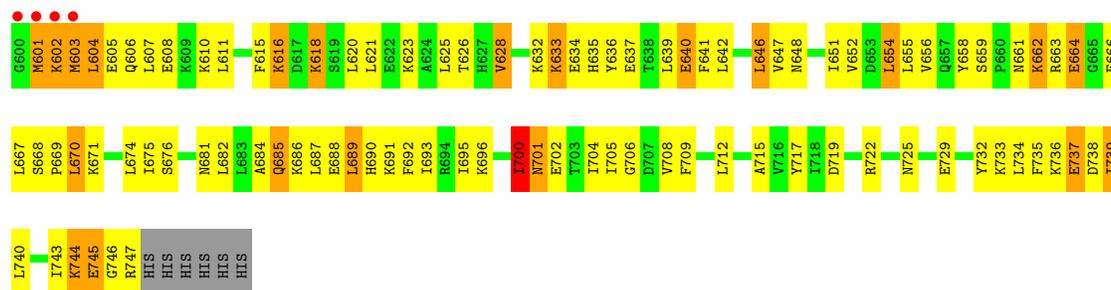


- Molecule 1: RIBONUCLEASE III



- Molecule 1: RIBONUCLEASE III





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.74Å 140.55Å 49.76Å 90.00° 117.42° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 27.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.2 (30.00-2.10) 82.8 (27.50-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.195 , 0.286 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.065 for -h-l,k,h 0.065 for l,k,-h-l 0.074 for h,-k,-h-l 0.076 for -h-l,-k,l 0.437 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5664	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.34	0/1268	0.85	0/1699
1	B	0.33	0/1288	0.87	3/1725 (0.2%)
1	C	0.31	0/1279	0.80	1/1713 (0.1%)
1	D	0.34	0/1250	0.86	0/1675
All	All	0.33	0/5085	0.85	4/6812 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	436	TYR	CB-CG-CD1	5.86	124.51	121.00
1	B	328	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	332	TYR	CB-CG-CD1	5.28	124.17	121.00
1	B	332	TYR	CB-CG-CD2	-5.14	117.92	121.00

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	1233	0	1263	78	0
1	B	1247	0	1274	90	0
1	C	1243	0	1272	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1225	0	1254	96	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	201	0	0	17	0
3	B	166	0	0	15	0
3	C	175	0	0	16	0
3	D	170	0	0	16	0
All	All	5664	0	5063	325	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 32.

The worst 5 of 325 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:205[B]:GLU:HG2	1:B:206:GLN:H	1.07	1.12
1:C:430:TYR:HA	1:C:496:LYS:HD3	1.41	1.01
1:B:205[B]:GLU:HG2	1:B:206:GLN:N	1.83	0.94
1:A:96:LYS:HG2	1:A:97:ARG:HD2	1.55	0.89
1:A:71:LYS:HE2	1:A:75:ILE:HD13	1.56	0.85

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	148/154 (96%)	134 (90%)	10 (7%)	4 (3%)	6 2
1	B	150/154 (97%)	136 (91%)	10 (7%)	4 (3%)	6 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	149/154 (97%)	143 (96%)	6 (4%)	0	100	100
1	D	146/154 (95%)	129 (88%)	13 (9%)	4 (3%)	6	2
All	All	593/616 (96%)	542 (91%)	39 (7%)	12 (2%)	9	4

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	B	206	GLN
1	D	602	LYS
1	D	700	ILE
1	D	701	ASN

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	133/137 (97%)	110 (83%)	23 (17%)	2	1
1	B	135/137 (98%)	103 (76%)	32 (24%)	1	0
1	C	134/137 (98%)	113 (84%)	21 (16%)	3	1
1	D	131/137 (96%)	109 (83%)	22 (17%)	2	1
All	All	533/548 (97%)	435 (82%)	98 (18%)	2	1

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	299[B]	LYS
1	B	347	ARG
1	D	670	LEU
1	B	300	ILE
1	B	322	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	235	HIS
1	B	285	GLN
1	C	485	GLN
1	B	206	GLN
1	C	435	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	148/154 (96%)	-0.68	1 (0%) 87 89	8, 23, 51, 86	0
1	B	149/154 (96%)	-0.41	5 (3%) 46 53	12, 30, 61, 106	0
1	C	149/154 (96%)	-0.65	1 (0%) 87 89	8, 23, 60, 93	0
1	D	148/154 (96%)	-0.41	4 (2%) 55 61	13, 30, 61, 84	0
All	All	594/616 (96%)	-0.54	11 (1%) 67 71	8, 27, 61, 106	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	602	LYS	4.8
1	B	201	MET	4.5
1	B	200	GLY	4.0
1	D	600	GLY	3.9
1	D	601	MET	3.6

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	C	763	1/1	0.99	0.07	-	29,29,29,29	0
2	MN	A	761	1/1	1.00	0.04	-	24,24,24,24	0
2	MN	D	764	1/1	0.99	0.06	-	31,31,31,31	0
2	MN	B	762	1/1	0.96	0.07	-	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.