



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 01:40 AM GMT

PDB ID : 1RC5
Title : CRYSTAL STRUCTURE OF MG(II)-COMPLEX OF RNASE III ENDONUCLEASE DOMAIN FROM AQUIFEX AEOLICUS AT 2.30 ANGSTROM RESOLUTION
Authors : Blaszczyk, J.; Gan, J.; Ji, X.
Deposited on : 2003-11-03
Resolution : 2.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

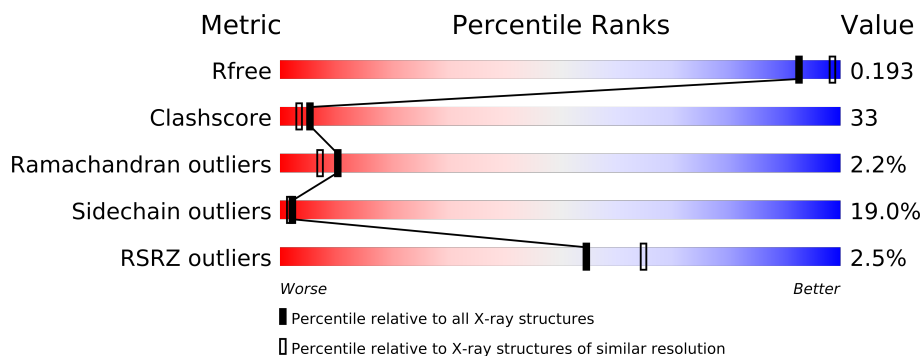
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	154	
1	B	154	
1	C	154	
1	D	154	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	761	-	X
2	MG	C	763	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5608 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	148	Total	C	N	O	S	0	0	0
			1225	805	198	220	2			
1	B	149	Total	C	N	O	S	0	2	0
			1244	817	202	223	2			
1	C	149	Total	C	N	O	S	0	0	0
			1235	811	201	221	2			
1	D	148	Total	C	N	O	S	0	0	0
			1225	805	198	220	2			

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	-	SEE REMARK 999	UNP O67082
A	149	HIS	-	SEE REMARK 999	UNP O67082
A	150	HIS	-	SEE REMARK 999	UNP O67082
A	151	HIS	-	SEE REMARK 999	UNP O67082
A	152	HIS	-	SEE REMARK 999	UNP O67082
A	153	HIS	-	SEE REMARK 999	UNP O67082
B	200	GLY	-	SEE REMARK 999	UNP O67082
B	348	HIS	-	SEE REMARK 999	UNP O67082
B	349	HIS	-	SEE REMARK 999	UNP O67082
B	350	HIS	-	SEE REMARK 999	UNP O67082
B	351	HIS	-	SEE REMARK 999	UNP O67082
B	352	HIS	-	SEE REMARK 999	UNP O67082
B	353	HIS	-	SEE REMARK 999	UNP O67082
C	400	GLY	-	SEE REMARK 999	UNP O67082
C	548	HIS	-	SEE REMARK 999	UNP O67082
C	549	HIS	-	SEE REMARK 999	UNP O67082
C	550	HIS	-	SEE REMARK 999	UNP O67082
C	551	HIS	-	SEE REMARK 999	UNP O67082
C	552	HIS	-	SEE REMARK 999	UNP O67082
C	553	HIS	-	SEE REMARK 999	UNP O67082

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

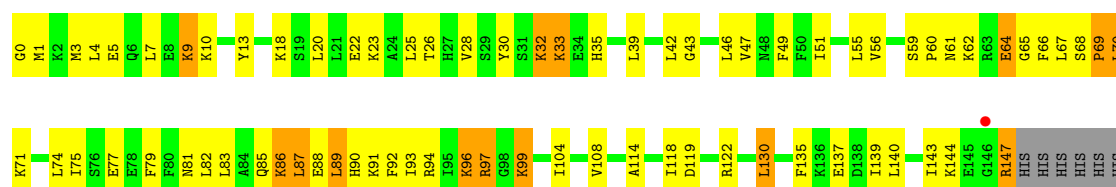
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	213	Total O 213 213	0	0
3	B	144	Total O 144 144	0	0
3	C	172	Total O 172 172	0	0
3	D	146	Total O 146 146	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

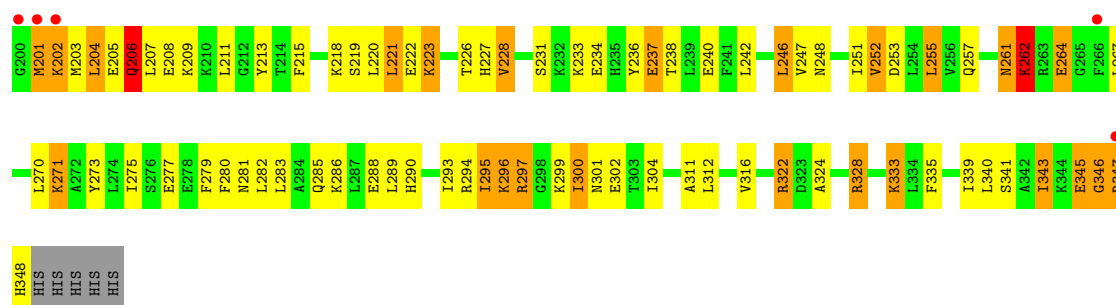
• Molecule 1: Ribonuclease III

Chain A: 



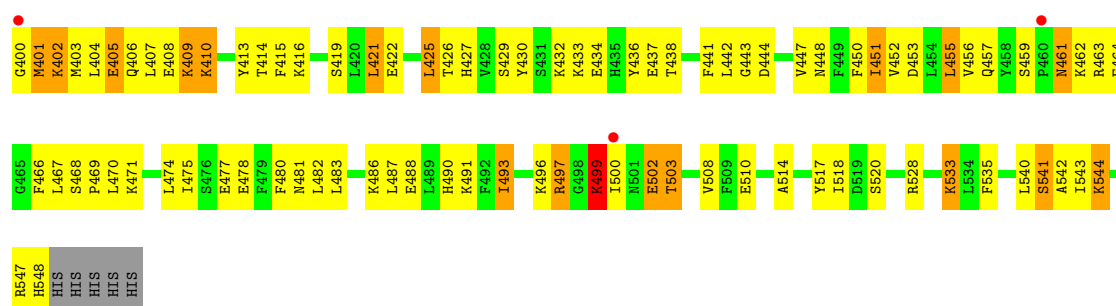
• Molecule 1: Ribonuclease III

Chain B: 



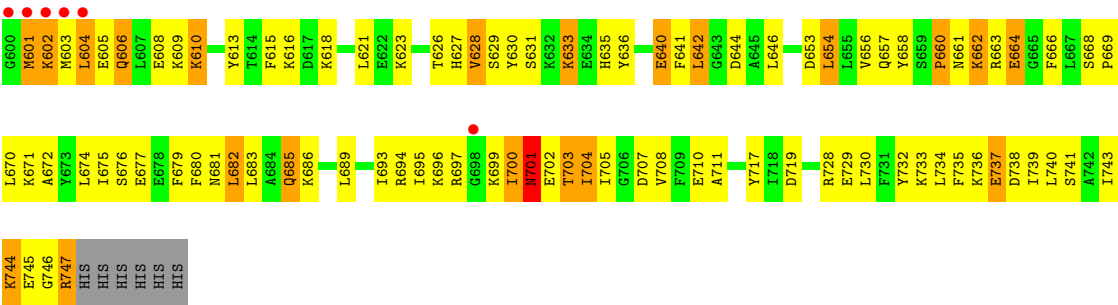
• Molecule 1: Ribonuclease III

Chain C: 



• Molecule 1: Ribonuclease III

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.74Å 140.86Å 49.75Å 90.00° 117.29° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 27.54 – 2.30	Depositor EDS
% Data completeness (in resolution range)	85.1 (30.00-2.30) 87.7 (27.54-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.31Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.197 , 0.255 0.158 , 0.193	Depositor DCC
R_{free} test set	1177 reflections (5.55%)	DCC
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.0	EDS
Estimated twinning fraction	0.056 for -h-l,k,h 0.056 for l,k,-h-l 0.077 for h,-k,-h-l 0.059 for -h-l,-k,l 0.460 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 24190 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5608	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.29	0/1250	0.79	0/1675
1	B	0.29	0/1279	0.76	1/1713 (0.1%)
1	C	0.30	0/1261	0.78	1/1690 (0.1%)
1	D	0.31	0/1250	0.75	0/1675
All	All	0.30	0/5040	0.77	2/6753 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	499	LYS	O-C-N	-5.14	114.47	122.70
1	B	328	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1225	0	1257	77	0
1	B	1244	0	1272	71	0
1	C	1235	0	1261	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1225	0	1254	103	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	213	0	0	13	0
3	B	144	0	0	13	0
3	C	172	0	0	7	0
3	D	146	0	0	11	0
All	All	5608	0	5044	326	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

The worst 5 of 326 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:345:GLU:HA	1:B:345:GLU:OE1	1.41	1.13
1:D:700:ILE:HG22	1:D:701:ASN:H	1.11	1.07
1:D:700:ILE:HG22	1:D:701:ASN:N	1.80	0.95
1:C:430:TYR:HA	1:C:496:LYS:HD3	1.47	0.93
1:B:202:LYS:HG3	1:B:206:GLN:HB2	1.50	0.93

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	146/154 (95%)	134 (92%)	9 (6%)	3 (2%)	11	8
1	B	149/154 (97%)	132 (89%)	14 (9%)	3 (2%)	11	8
1	C	147/154 (96%)	136 (92%)	11 (8%)	0	100	100
1	D	146/154 (95%)	123 (84%)	16 (11%)	7 (5%)	4	1
All	All	588/616 (96%)	525 (89%)	50 (8%)	13 (2%)	10	7

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	B	206	GLN
1	D	700	ILE
1	D	701	ASN
1	A	3	MET

5.3.2 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 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	131/137 (96%)	114 (87%)	17 (13%)	6	6
1	B	134/137 (98%)	99 (74%)	35 (26%)	1	0
1	C	132/137 (96%)	108 (82%)	24 (18%)	2	2
1	D	131/137 (96%)	105 (80%)	26 (20%)	2	1
All	All	528/548 (96%)	426 (81%)	102 (19%)	2	2

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	335	PHE
1	C	421	LEU
1	D	701	ASN
1	B	339	ILE
1	B	347	ARG

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	C	485	GLN
1	D	701	ASN
1	D	635	HIS
1	B	261	ASN
1	D	606	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.39	1 (0%) 84 91	15, 25, 55, 88	0
1	B	149/154 (96%)	-0.07	5 (3%) 43 53	14, 32, 73, 118	0
1	C	149/154 (96%)	-0.40	3 (2%) 62 72	13, 26, 64, 79	0
1	D	148/154 (96%)	-0.13	6 (4%) 35 46	17, 32, 68, 92	0
All	All	594/616 (96%)	-0.25	15 (2%) 54 65	13, 28, 67, 118	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	MET	8.9
1	D	603	MET	5.5
1	D	600	GLY	5.2
1	B	202	LYS	4.7
1	C	400	GLY	4.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	C	763	1/1	0.18	14.99	15,15,15,15	0
2	MG	A	761	1/1	0.17	3.99	19,19,19,19	0
2	MG	D	764	1/1	0.12	1.51	24,24,24,24	0
2	MG	B	762	1/1	0.12	0.44	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.