wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:56 PM 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 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

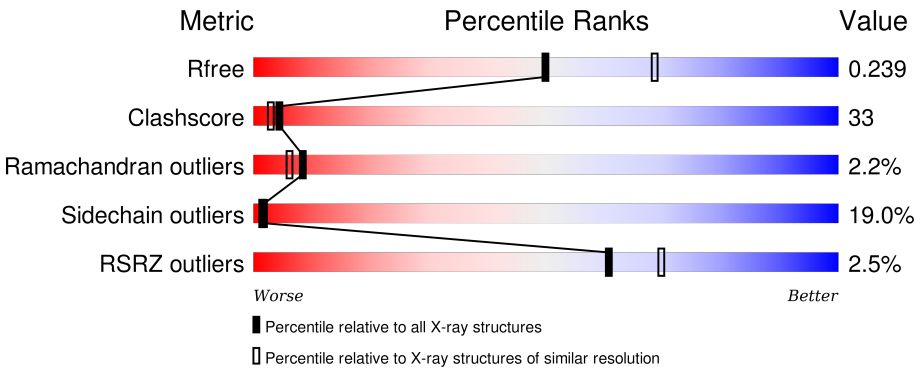
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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 <=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% 40% 9% •
1	B	154	3% 44% 36% 16% • •
1	C	154	2% 39% 46% 11% • •
1	D	154	4% 36% 46% 14% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5608 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	1225	805	198	220	2	0	0	0
			Total	C	N	O	S			
1	B	149	1244	817	202	223	2	0	2	0
			Total	C	N	O	S			
1	C	149	1235	811	201	221	2	0	0	0
			Total	C	N	O	S			
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	-	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.

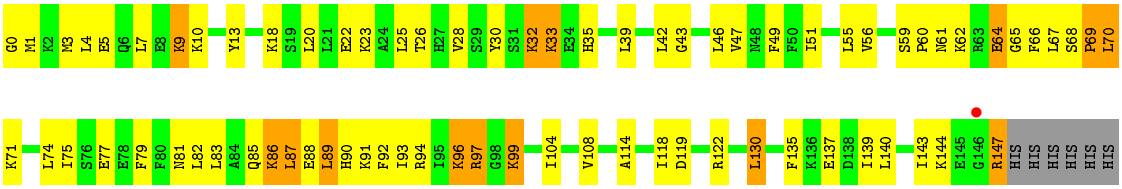
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	213	Total O 213 213	0	0
3	B	144	Total O 144 144	0	0
3	C	172	Total O 172 172	0	0
3	D	146	Total O 146 146	0	0

3 Residue-property plots (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 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:

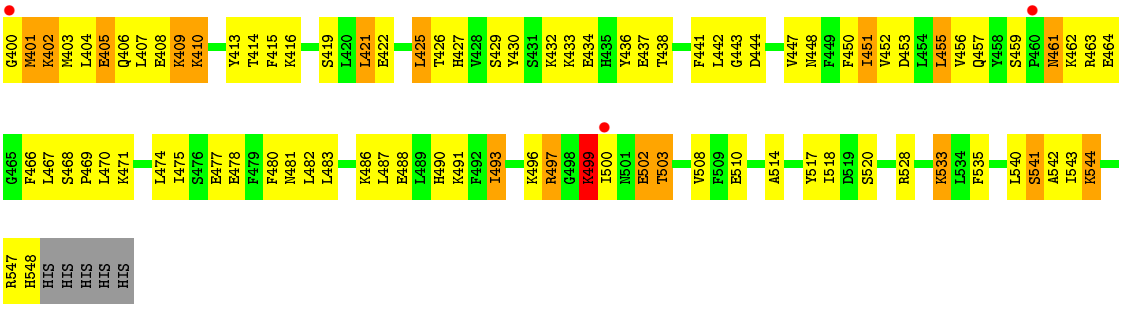


- Molecule 1: Ribonuclease III

Chain B:

- Molecule 1: Ribonuclease III

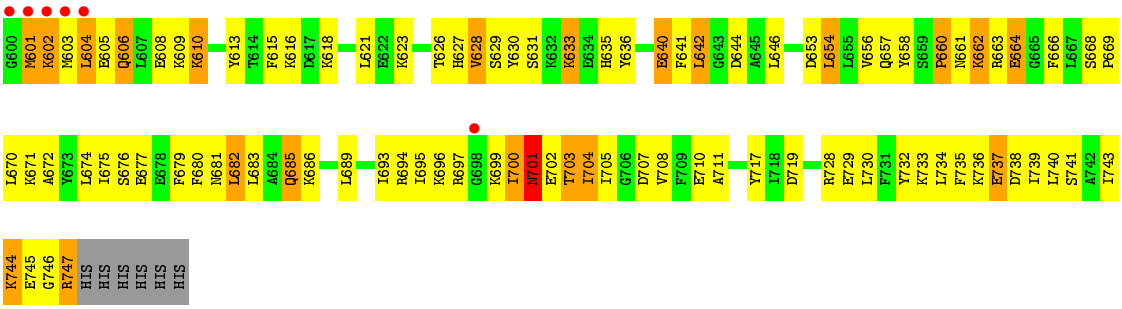
Chain C:



- Molecule 1: Ribonuclease III

Chain D:

4%
36%
46%
14%


G600 M601 K602 M603 L604 E605 Q606 L607 E608 K609 K610 Y613 T614 F615 K616 D617 K618 L621 E622 K623 T626 H627 V628 S629 Y630 S631 K632 K633 E634 H635 Y636 E640 F641 L642 G643 D644 A645 L646 D653 L654 L655 V656 Q657 Y658 S659 P660 N661 K662 R663 E664 G665 F666 L667 S668 P669
L670 K671 A672 Y673 L674 I675 S676 E677 E678 F679 F680 N681 L682 L683 A684 Q685 K686 L689 I693 R694 I695 K696 R697 G698 K699 I700 N701 E702 T703 I704 I705 G706 D707 V708 F709 E710 A711 Y717 I718 D719 R728 E729 L730 F731 Y732 K733 L734 F735 K736 E737 D738 I739 L740 S741 A742 I743
K744 E745 G746 R747 HIS HIS HIS HIS HIS HIS

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 140.86Å 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
$< I/\sigma(I) >$ [1]	3.82 (at 2.31Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.197 , 0.255 0.199 , 0.239	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)	0.28 , 66.6	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[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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(^{o})	Ideal(^{o})
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 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	1225	0	1257	77	0
1	B	1244	0	1272	71	0
1	C	1235	0	1261	87	0
1	D	1225	0	1254	103	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 33.

The worst 5 of 326 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: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 (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	146/154 (95%)	134 (92%)	9 (6%)	3 (2%)	9 7
1	B	149/154 (97%)	132 (89%)	14 (9%)	3 (2%)	9 7
1	C	147/154 (96%)	136 (92%)	11 (8%)	0	100 100
1	D	146/154 (95%)	123 (84%)	16 (11%)	7 (5%)	3 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	588/616 (96%)	525 (89%)	50 (8%)	13 (2%)	8 6

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 (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	131/137 (96%)	114 (87%)	17 (13%)	5 5
1	B	134/137 (98%)	99 (74%)	35 (26%)	0 0
1	C	132/137 (96%)	108 (82%)	24 (18%)	2 2
1	D	131/137 (96%)	105 (80%)	26 (20%)	1 1
All	All	528/548 (96%)	426 (81%)	102 (19%)	2 1

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 (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%)	-0.48	1 (0%)	89	92	15, 25, 55, 88	0
1	B	149/154 (96%)	-0.14	5 (3%)	49	58	14, 32, 73, 118	0
1	C	149/154 (96%)	-0.49	3 (2%)	68	75	13, 26, 64, 79	0
1	D	148/154 (96%)	-0.21	6 (4%)	41	50	17, 32, 68, 92	0
All	All	594/616 (96%)	-0.33	15 (2%)	61	70	13, 28, 67, 118	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	MET	9.0
1	D	603	MET	5.3
1	D	600	GLY	5.1
1	B	202	LYS	4.6
1	C	400	GLY	4.1

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 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(Å^2)	Q<0.9
2	MG	A	761	1/1	0.97	0.18	-	19,19,19,19	0
2	MG	B	762	1/1	0.92	0.12	-	19,19,19,19	0
2	MG	C	763	1/1	0.99	0.20	-	15,15,15,15	0
2	MG	D	764	1/1	0.94	0.12	-	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.