



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 11, 2018 – 04:38 pm GMT

PDB ID : 5RSA
Title : COMPARISON OF TWO INDEPENDENTLY REFINED MODELS OF
RIBONUCLEASE-A
Authors : Wlodawer, A.
Deposited on : 1985-04-29
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

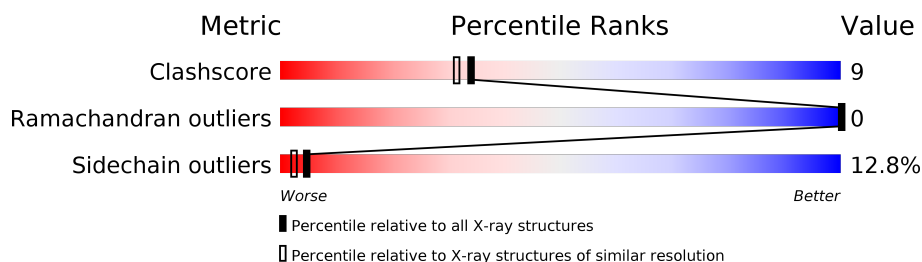
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION, NEUTRON DIFFRACTION

The reported resolution of this entry is 2.00 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	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	124	 61% 28% 6% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2249 atoms, of which 693 are hydrogens and 472 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 A.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	124	Total	C	D	H	N	O	S		0	0	0
			1860	575	216	693	171	193	12				

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	128	Total	D	O	0	0
			384	256	128		

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. 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. 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 A

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	30.18Å 38.40Å 53.32Å 90.00° 105.85° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 9.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 96.2 (9.91-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.9	EDS
L-test for twinning ¹	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2249	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, DOD

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	1.23	4/967 (0.4%)	2.61	52/1304 (4.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	GLU	CD-OE1	-7.65	1.17	1.25
1	A	86	GLU	CD-OE2	-6.85	1.18	1.25
1	A	49	GLU	CD-OE1	-5.22	1.20	1.25
1	A	50	SER	CB-OG	-5.06	1.35	1.42

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ARG	NE-CZ-NH1	35.22	137.91	120.30
1	A	10	ARG	NE-CZ-NH2	-21.01	109.80	120.30
1	A	33	ARG	NE-CZ-NH1	20.70	130.65	120.30
1	A	83	ASP	CB-CG-OD2	-12.66	106.90	118.30
1	A	73	TYR	CB-CG-CD1	11.58	127.95	121.00
1	A	118	VAL	CG1-CB-CG2	10.60	127.86	110.90
1	A	9	GLU	OE1-CD-OE2	10.59	136.01	123.30
1	A	70	THR	CA-CB-CG2	10.32	126.84	112.40
1	A	33	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	73	TYR	CB-CG-CD2	-9.61	115.24	121.00
1	A	118	VAL	N-CA-CB	-9.54	90.51	111.50
1	A	39	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	A	17	THR	N-CA-CB	-8.94	93.31	110.30
1	A	85	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	86	GLU	OE1-CD-OE2	8.09	133.00	123.30
1	A	34	ASN	CB-CG-OD1	-7.85	105.89	121.60
1	A	10	ARG	CD-NE-CZ	7.71	134.39	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	THR	N-CA-CB	-7.67	95.72	110.30
1	A	87	THR	N-CA-CB	-7.30	96.43	110.30
1	A	83	ASP	OD1-CG-OD2	7.09	136.77	123.30
1	A	70	THR	CA-CB-OG1	-6.75	94.82	109.00
1	A	118	VAL	CB-CA-C	6.70	124.13	111.40
1	A	10	ARG	NH1-CZ-NH2	-6.51	112.24	119.40
1	A	85	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	17	THR	OG1-CB-CG2	6.45	124.83	110.00
1	A	20	ALA	N-CA-CB	-6.39	101.16	110.10
1	A	111	GLU	OE1-CD-OE2	6.29	130.85	123.30
1	A	12	HIS	CA-C-O	-6.27	106.92	120.10
1	A	75	SER	N-CA-CB	6.14	119.71	110.50
1	A	116	VAL	CA-CB-CG1	6.14	120.11	110.90
1	A	87	THR	CA-CB-OG1	-5.99	96.42	109.00
1	A	76	TYR	CZ-CE2-CD2	-5.99	114.41	119.80
1	A	61	LYS	O-C-N	5.88	132.10	122.70
1	A	11	GLN	O-C-N	5.83	132.03	122.70
1	A	111	GLU	CG-CD-OE2	-5.69	106.92	118.30
1	A	37	LYS	CD-CE-NZ	5.64	124.67	111.70
1	A	73	TYR	O-C-N	5.61	131.67	122.70
1	A	73	TYR	CG-CD2-CE2	5.58	125.76	121.30
1	A	53	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	85	ARG	CB-CG-CD	-5.41	97.53	111.60
1	A	119	HIS	CA-CB-CG	5.37	122.72	113.60
1	A	34	ASN	OD1-CG-ND2	5.35	134.21	121.90
1	A	43	VAL	CA-CB-CG2	-5.35	102.88	110.90
1	A	51	LEU	CB-CA-C	5.33	120.32	110.20
1	A	104	LYS	CB-CA-C	-5.31	99.78	110.40
1	A	25	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	A	25	TYR	CG-CD2-CE2	-5.20	117.14	121.30
1	A	90	SER	O-C-N	5.14	130.93	122.70
1	A	73	TYR	CZ-CE2-CD2	-5.14	115.17	119.80
1	A	101	GLN	CG-CD-OE1	-5.06	111.48	121.60
1	A	34	ASN	N-CA-CB	-5.01	101.58	110.60
1	A	78	THR	N-CA-CB	5.01	119.81	110.30

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	1167	693	905	17	1
2	A	5	0	0	1	0
3	A	384	0	0	4	1
All	All	1556	693	905	17	2

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 9.

All (17) 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:A:87:THR:HG23	1:A:89:SER:H	1.37	0.80
1:A:119:HIS:HB2	3:A:205:DOD:O	1.87	0.70
1:A:40:CYS:O	3:A:260:DOD:O	2.12	0.67
1:A:17:THR:HG22	1:A:48:HIS:ND1	2.08	0.62
1:A:58:CYS:O	3:A:185:DOD:O	2.19	0.60
1:A:94:ASN:ND2	3:A:191:DOD:O	2.24	0.59
1:A:119:HIS:ND1	2:A:125:PO4:O1	2.36	0.56
1:A:42:PRO:O	1:A:43:VAL:HG23	2.06	0.51
1:A:17:THR:CG2	1:A:48:HIS:CE1	2.93	0.51
1:A:87:THR:CG2	1:A:89:SER:H	2.14	0.50
1:A:42:PRO:C	1:A:43:VAL:HG23	2.27	0.50
1:A:43:VAL:HG22	1:A:85:ARG:HD3	1.84	0.49
1:A:34:ASN:CG	1:A:37:LYS:HD3	2.29	0.48
1:A:17:THR:CG2	1:A:48:HIS:ND1	2.77	0.47
1:A:11:GLN:HG2	1:A:35:LEU:HD21	1.91	0.43
1:A:74:GLN:HG2	1:A:75:SER:N	2.29	0.43
1:A:87:THR:HG23	1:A:89:SER:N	2.19	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:188:DOD:O	3:A:306:DOD:O[1_655]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:OD2	1:A:70:THR:CG2[2_745]	2.14	0.06

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	122/124 (98%)	118 (97%)	4 (3%)	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	109/109 (100%)	95 (87%)	14 (13%)	5	2

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	17	THR
1	A	28	GLN
1	A	31	LYS
1	A	34	ASN
1	A	37	LYS
1	A	61	LYS

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Mol	Chain	Res	Type
1	A	66	LYS
1	A	70	THR
1	A	77	SER
1	A	83	ASP
1	A	87	THR
1	A	118	VAL
1	A	124	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	125	-	4,4,4	1.04	0	6,6,6	1.01	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	125	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	125	PO4	O3-P-O1	-2.02	102.30	110.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	125	PO4	1	0

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.