



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:26 am BST

PDB ID : 3DHS
Title : Mapping metal-binding sites in the catalytic domain of bacterial RNase P RNA
Authors : Pace, N.R.; Kazantsev, A.V.; Krivenko, A.A.
Deposited on : 2008-06-18
Resolution : 3.60 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

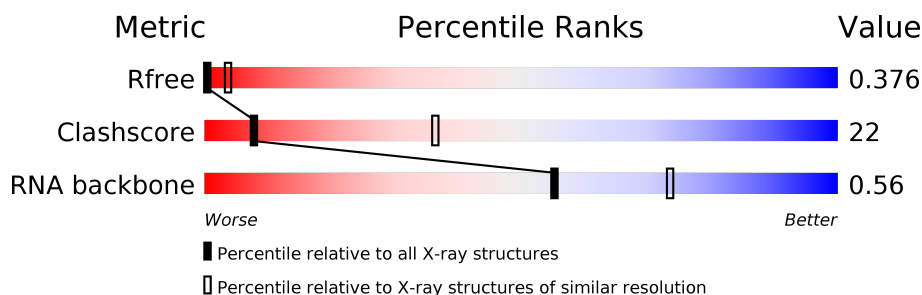
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	268	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4628 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 RNA chain called RNase P RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	P	0	0	0
			4613	2063	863	1476	211			

- Molecule 2 is OSMIUM ION (three-letter code: OS) (formula: Os).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	Os	0	0
			15	15		

- Molecule 1: RNase P RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	147.35Å 160.01Å 133.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.07 – 3.60 42.07 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.1 (42.07-3.60) 97.0 (42.07-3.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.290 , 0.314 0.354 , 0.376	Depositor DCC
R_{free} test set	1260 reflections (6.86%)	wwPDB-VP
Wilson B-factor (Å ²)	147.7	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4628	wwPDB-VP
Average B, all atoms (Å ²)	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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: OS

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	0.23	0/5167	0.71	3/8056 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	390	A	C2'-C3'-O3'	8.34	127.85	109.50
1	A	331	G	N9-C1'-C2'	5.62	121.30	114.00
1	A	389	A	N9-C1'-C2'	5.47	121.11	114.00

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	4613	0	2335	149	0
2	A	15	0	0	0	0
All	All	4628	0	2335	149	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 22.

All (149) 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:349:G:H2'	1:A:379:G:H1	1.17	1.04
1:A:8:A:H61	1:A:406:A:H61	1.04	0.95
1:A:275:G:H3'	1:A:276:C:H5'	1.53	0.91
1:A:333:U:H4'	1:A:335:G:H1'	1.55	0.88
1:A:8:A:N6	1:A:406:A:H61	1.74	0.85
1:A:47:G:H4'	1:A:48:A:H4'	1.58	0.84
1:A:257:A:H62	1:A:275:G:H21	1.21	0.84
1:A:399:A:H3'	1:A:400:U:H5''	1.60	0.83
1:A:275:G:H3'	1:A:276:C:C5'	2.09	0.82
1:A:8:A:H61	1:A:406:A:N6	1.78	0.82
1:A:257:A:N6	1:A:275:G:H21	1.78	0.80
1:A:349:G:H2'	1:A:379:G:N1	1.98	0.79
1:A:399:A:C3'	1:A:400:U:H5''	2.12	0.79
1:A:285:G:H22	1:A:299:G:H1'	1.47	0.78
1:A:301:G:H2'	1:A:302:G:H8	1.49	0.75
1:A:5:A:H61	1:A:409:A:N6	1.86	0.73
1:A:47:G:C4'	1:A:48:A:H4'	2.19	0.72
1:A:330:A:H2'	1:A:331:G:O4'	1.91	0.70
1:A:333:U:H4'	1:A:335:G:C1'	2.23	0.69
1:A:34:U:H3'	1:A:35:U:C5'	2.23	0.68
1:A:45:A:H1'	1:A:389:A:C5	2.30	0.67
1:A:42:U:H2'	1:A:43:A:C8	2.30	0.67
1:A:305:A:H2'	1:A:306:G:H8	1.59	0.66
1:A:305:A:H2'	1:A:306:G:C8	2.31	0.66
1:A:59:U:H2'	1:A:60:C:C6	2.29	0.66
1:A:337:U:H5''	1:A:338:G:O4'	1.95	0.66
1:A:257:A:H62	1:A:275:G:N2	1.94	0.66
1:A:34:U:H3'	1:A:35:U:H5''	1.77	0.65
1:A:5:A:N6	1:A:409:A:H61	1.95	0.65
1:A:294:G:H2'	1:A:295:A:C8	2.32	0.65
1:A:40:C:O2'	1:A:41:G:H5'	1.98	0.64
1:A:60:C:H5'	1:A:258:C:O2'	1.97	0.64
1:A:42:U:H2'	1:A:43:A:H8	1.63	0.64
1:A:255:A:H5'	1:A:256:A:OP1	1.99	0.63
1:A:5:A:N6	1:A:409:A:N6	2.49	0.61
1:A:342:A:H2'	1:A:343:C:C6	2.36	0.60
1:A:277:A:O2'	1:A:278:C:H5'	2.02	0.59
1:A:280:U:O2'	1:A:281:U:H5'	2.02	0.58
1:A:16:G:O2'	1:A:17:U:H5'	2.04	0.58
1:A:39:C:H2'	1:A:40:C:C6	2.40	0.57
1:A:41:G:O2'	1:A:42:U:H5'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:C:H2'	1:A:319:A:C8	2.40	0.56
1:A:255:A:H1'	1:A:257:A:C5	2.41	0.56
1:A:388:G:H2'	1:A:389:A:H5''	1.86	0.56
1:A:5:A:H61	1:A:409:A:H61	1.48	0.56
1:A:333:U:C4'	1:A:335:G:H1'	2.34	0.56
1:A:343:C:H2'	1:A:344:C:C6	2.41	0.56
1:A:283:C:H2'	1:A:284:C:C6	2.41	0.55
1:A:81:U:H2'	1:A:250:G:H5''	1.89	0.55
1:A:276:C:O2'	1:A:277:A:OP2	2.24	0.55
1:A:20:U:H2'	1:A:21:C:C6	2.42	0.55
1:A:59:U:H1'	1:A:257:A:C2	2.42	0.55
1:A:24:U:H2'	1:A:25:G:H8	1.73	0.54
1:A:388:G:C2'	1:A:389:A:H5''	2.36	0.54
1:A:318:C:H2'	1:A:319:A:H8	1.72	0.54
1:A:255:A:N6	1:A:391:C:C2	2.76	0.54
1:A:313:C:H2'	1:A:314:G:O4'	2.08	0.54
1:A:338:G:H2'	1:A:339:A:C8	2.44	0.53
1:A:53:C:O2'	1:A:54:C:H5'	2.09	0.53
1:A:399:A:C2'	1:A:400:U:H5''	2.38	0.52
1:A:340:U:H2'	1:A:341:U:C6	2.44	0.52
1:A:62:C:H2'	1:A:63:A:H5''	1.92	0.52
1:A:346:C:O2'	1:A:347:C:H5'	2.12	0.50
1:A:256:A:HO2'	1:A:257:A:P	2.34	0.50
1:A:10:G:H2'	1:A:11:C:C6	2.47	0.50
1:A:293:U:OP2	1:A:294:G:N7	2.45	0.50
1:A:294:G:C6	1:A:295:A:N6	2.80	0.50
1:A:330:A:N1	1:A:331:G:C2	2.80	0.49
1:A:73:G:H22	1:A:291:A:H2'	1.76	0.49
1:A:348:G:H21	1:A:381:A:H62	1.59	0.49
1:A:303:G:O2'	1:A:304:A:H5'	2.12	0.49
1:A:399:A:H2'	1:A:400:U:H5''	1.95	0.49
1:A:285:G:N1	1:A:299:G:N3	2.62	0.48
1:A:60:C:O4'	1:A:258:C:H4'	2.13	0.48
1:A:331:G:OP2	1:A:331:G:H8	1.96	0.48
1:A:385:A:H2'	1:A:386:C:H6	1.79	0.48
1:A:45:A:H2'	1:A:49:A:H2	1.78	0.48
1:A:47:G:N3	1:A:47:G:H5''	2.29	0.48
1:A:387:A:O2'	1:A:388:G:H5'	2.13	0.47
1:A:273:G:N1	1:A:274:G:C5	2.82	0.47
1:A:15:G:H2'	1:A:16:G:H8	1.80	0.47
1:A:350:A:C6	1:A:380:A:H1'	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:U:H2'	1:A:281:U:H6	1.78	0.47
1:A:283:C:H2'	1:A:284:C:H6	1.80	0.47
1:A:338:G:H2'	1:A:339:A:H8	1.79	0.47
1:A:255:A:O2'	1:A:275:G:N2	2.48	0.47
1:A:25:G:O2'	1:A:26:C:H5'	2.15	0.47
1:A:30:C:H2'	1:A:31:G:H8	1.80	0.47
1:A:77:C:O4'	1:A:296:A:C2	2.69	0.46
1:A:69:C:H2'	1:A:70:U:C6	2.51	0.46
1:A:285:G:HO2'	1:A:286:A:C5'	2.28	0.46
1:A:336:A:H3'	1:A:337:U:C6	2.50	0.46
1:A:24:U:H2'	1:A:25:G:C8	2.50	0.46
1:A:285:G:N2	1:A:299:G:H1'	2.25	0.46
1:A:385:A:O2'	1:A:386:C:H5'	2.16	0.46
1:A:20:U:H2'	1:A:21:C:H6	1.78	0.45
1:A:279:C:H2'	1:A:280:U:C6	2.51	0.45
1:A:20:U:O2'	1:A:21:C:H5'	2.16	0.45
1:A:308:A:H2'	1:A:309:C:C6	2.50	0.45
1:A:323:A:H2'	1:A:324:G:O4'	2.16	0.45
1:A:49:A:N1	1:A:388:G:N3	2.65	0.45
1:A:294:G:H2'	1:A:295:A:H8	1.80	0.45
1:A:286:A:H61	1:A:299:G:H4'	1.81	0.45
1:A:386:C:N4	1:A:387:A:C2	2.85	0.45
1:A:255:A:HO2'	1:A:275:G:N2	2.15	0.45
1:A:45:A:H1'	1:A:389:A:N7	2.31	0.45
1:A:385:A:H2'	1:A:386:C:C6	2.51	0.45
1:A:397:U:H2'	1:A:398:U:C6	2.52	0.44
1:A:302:G:N2	1:A:303:G:C4	2.85	0.44
1:A:50:A:H5'	1:A:388:G:H5''	1.98	0.44
1:A:298:G:C2'	1:A:299:G:H5'	2.48	0.44
1:A:332:A:H2'	1:A:333:U:H5'	2.00	0.44
1:A:295:A:O2'	1:A:296:A:H5'	2.18	0.44
1:A:275:G:O6	1:A:276:C:N4	2.50	0.43
1:A:255:A:N7	1:A:391:C:C5	2.86	0.43
1:A:349:G:C2'	1:A:379:G:H22	2.30	0.43
1:A:79:C:H2'	1:A:80:G:O4'	2.17	0.43
1:A:384:U:H4'	1:A:385:A:H5'	2.00	0.43
1:A:279:C:H2'	1:A:280:U:H6	1.83	0.43
1:A:317:G:O2'	1:A:318:C:H5'	2.18	0.43
1:A:277:A:O2'	1:A:278:C:C5'	2.66	0.42
1:A:298:G:H2'	1:A:299:G:H5'	2.00	0.42
1:A:297:C:H2'	1:A:298:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:C:H2'	1:A:55:A:H8	1.85	0.42
1:A:256:A:O2'	1:A:257:A:OP1	2.31	0.42
1:A:310:A:O2'	1:A:311:G:H5'	2.19	0.42
1:A:306:G:O2'	1:A:307:G:H5'	2.19	0.41
1:A:307:G:H2'	1:A:308:A:H8	1.85	0.41
1:A:307:G:O2'	1:A:308:A:H5'	2.20	0.41
1:A:32:G:C2'	1:A:33:U:H5''	2.50	0.41
1:A:77:C:H2'	1:A:78:C:C6	2.56	0.41
1:A:403:A:H2'	1:A:404:G:H8	1.86	0.41
1:A:277:A:C5	1:A:331:G:C5	3.09	0.41
1:A:308:A:H2'	1:A:309:C:H6	1.86	0.41
1:A:323:A:C2	1:A:324:G:H1'	2.56	0.41
1:A:49:A:C2	1:A:388:G:N3	2.89	0.41
1:A:54:C:H2'	1:A:55:A:C8	2.55	0.41
1:A:396:C:H2'	1:A:397:U:C6	2.55	0.41
1:A:51:G:C6	1:A:53:C:N4	2.89	0.41
1:A:258:C:O2'	1:A:259:C:H5'	2.21	0.41
1:A:282:C:C2	1:A:283:C:C5	3.09	0.41
1:A:70:U:O2	1:A:295:A:C2	2.74	0.41
1:A:77:C:H2'	1:A:78:C:O4'	2.20	0.41
1:A:255:A:N3	1:A:257:A:C6	2.89	0.41
1:A:325:C:H2'	1:A:326:C:C6	2.56	0.41
1:A:80:G:H2'	1:A:81:U:C6	2.56	0.40
1:A:327:U:H2'	1:A:328:G:O4'	2.21	0.40
1:A:77:C:H2'	1:A:78:C:H6	1.85	0.40
1:A:39:C:H2'	1:A:40:C:H6	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	211/268 (78%)	36 (17%)	10 (4%)

All (36) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	15	G
1	A	33	U
1	A	35	U
1	A	36	C
1	A	38	G
1	A	45	A
1	A	46	G
1	A	48	A
1	A	50	A
1	A	52	U
1	A	53	C
1	A	63	A
1	A	67	U
1	A	68	G
1	A	74	A
1	A	75	U
1	A	254	G
1	A	255	A
1	A	256	A
1	A	257	A
1	A	262	A
1	A	276	C
1	A	278	C
1	A	292	A
1	A	300	A
1	A	315	G
1	A	317	G
1	A	330	A
1	A	335	G
1	A	336	A
1	A	349	G
1	A	384	U
1	A	385	A
1	A	389	A
1	A	391	C
1	A	400	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	47	G
1	A	74	A
1	A	75	U
1	A	254	G
1	A	256	A
1	A	299	G
1	A	329	U
1	A	333	U
1	A	384	U
1	A	390	A

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 15 ligands modelled in this entry, 15 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 ⓘ

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 ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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