wwPDB X-ray Structure Validation Summary Report (i)

Aug 10, 2023 – 07:43 pm BST

PDB ID	:	7P4R
Title	:	Ultra High Resolution X-ray Structure of Orthorhombic Bovine Pancreatic Ribonuclease at 100K
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Deposited on	:	2021-07-12
Resolution	:	0.85 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

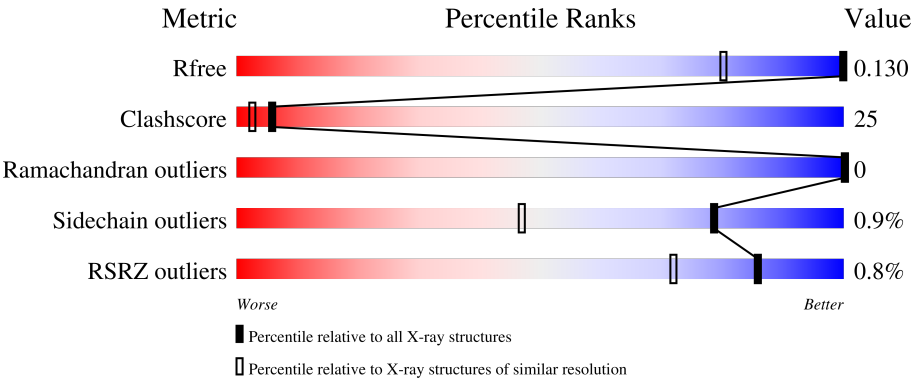
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 0.85 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	1071 (1.04-0.70)
Clashscore	141614	1143 (1.04-0.68)
Ramachandran outliers	138981	1065 (1.04-0.68)
Sidechain outliers	138945	1066 (1.04-0.68)
RSRZ outliers	127900	1038 (1.04-0.70)

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 of 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 <=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	AAA	124	% 74% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EOH	AAA	203	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EOH	AAA	204	-	-	X	-
2	EOH	AAA	208	-	-	X	-
2	EOH	AAA	210	-	-	X	-

2 Entry composition

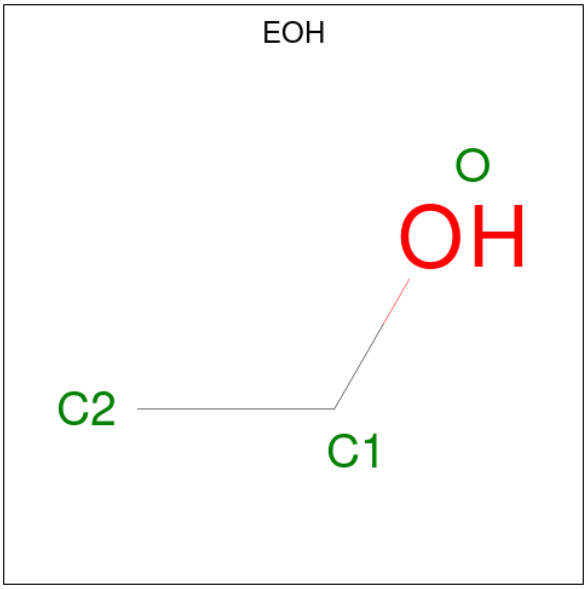
There are 4 unique types of molecules in this entry. The entry contains 2721 atoms, of which 1231 are hydrogens and 0 are deuteriums.

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 pancreatic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	124	Total	C	H	N	O	S	46	28	0
			2294	705	1165	193	218	13			

- Molecule 2 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	0	0
			9	2	6	1		
2	AAA	1	Total	C	H	O	0	0
			9	2	6	1		
2	AAA	1	Total	C	H	O	0	0
			9	2	6	1		
2	AAA	1	Total	C	H	O	0	0
			9	2	6	1		
2	AAA	1	Total	C	H	O	0	0
			9	2	6	1		

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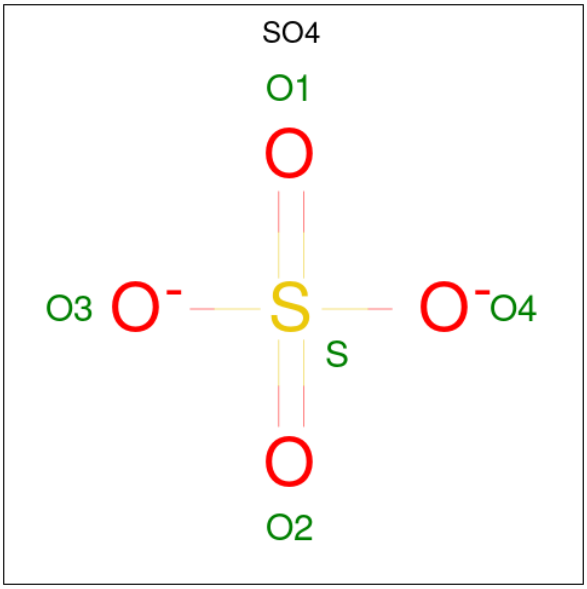
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C H O 9 2 6 1	0	0
2	AAA	1	Total C H O 9 2 6 1	0	0
2	AAA	1	Total C H O 9 2 6 1	0	0
2	AAA	1	Total C H O 9 2 6 1	0	0
2	AAA	1	Total C H O 9 2 6 1	0	0
2	AAA	1	Total C H O 9 2 6 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total O S 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	1
3	AAA	1	Total O S 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total O S 5 4 1	0	1
3	AAA	1	Total O S 5 4 1	0	1

- Molecule 4 is water.

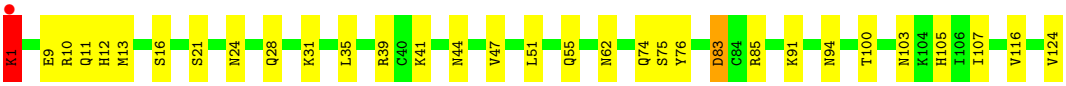
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	293	Total O 293 293	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 pancreatic

Chain AAA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.00Å 45.70Å 51.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.29 – 0.85 34.29 – 0.85	Depositor EDS
% Data completeness (in resolution range)	92.2 (34.29-0.85) 92.2 (34.29-0.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 0.85Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.112 , 0.129 0.113 , 0.130	Depositor DCC
R_{free} test set	4279 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	4.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	2721	wwPDB-VP
Average B, all atoms (Å^2)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.21% 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, 0.333 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: EOH, SO4

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	AAA	0.81	2/1232 (0.2%)	1.21	25/1651 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	9[A]	GLU	CD-OE1	-7.12	1.17	1.25
1	AAA	9[B]	GLU	CD-OE1	-7.12	1.17	1.25

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	85	ARG	NE-CZ-NH1	11.87	126.24	120.30
1	AAA	85	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	AAA	76[A]	TYR	CB-CG-CD1	6.86	125.12	121.00
1	AAA	76[B]	TYR	CB-CG-CD1	6.86	125.12	121.00
1	AAA	1[A]	LYS	C-N-CA	6.11	136.98	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	1[A]	LYS	Mainchain

CLOSE-CONTACTS INFOmissingINFO

5.2 Torsion angles (i)

5.2.1 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	AAA	150/124 (121%)	143 (95%)	7 (5%)	0	100 100

There are no Ramachandran outliers to report.

5.2.2 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	AAA	141/109 (129%)	137 (97%)	4 (3%)	43 11

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	1[A]	LYS
1	AAA	1[B]	LYS
1	AAA	1[C]	LYS
1	AAA	1[D]	LYS

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

5.2.3 RNA

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains

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

5.4 Carbohydrates

There are no monosaccharides in this entry.

5.5 Ligand geometry

18 ligands are 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	EOH	AAA	204	-	2,2,2	0.10	0	1,1,1	0.08	0
3	SO4	AAA	217[B]	-	4,4,4	0.75	0	6,6,6	1.14	0
3	SO4	AAA	213[A]	-	4,4,4	0.96	0	6,6,6	0.93	0
2	EOH	AAA	210	-	2,2,2	0.66	0	1,1,1	0.35	0
2	EOH	AAA	207	-	2,2,2	0.21	0	1,1,1	0.88	0
2	EOH	AAA	208	-	2,2,2	0.23	0	1,1,1	0.30	0
2	EOH	AAA	209	-	2,2,2	0.45	0	1,1,1	0.08	0
2	EOH	AAA	211	-	2,2,2	0.22	0	1,1,1	0.34	0
3	SO4	AAA	214	-	4,4,4	1.05	0	6,6,6	0.91	0
2	EOH	AAA	205	-	2,2,2	0.23	0	1,1,1	0.03	0
2	EOH	AAA	203	-	2,2,2	0.32	0	1,1,1	0.58	0
3	SO4	AAA	216[B]	-	4,4,4	0.69	0	6,6,6	0.44	0
3	SO4	AAA	218[A]	-	4,4,4	0.97	0	6,6,6	0.55	0
2	EOH	AAA	202	-	2,2,2	0.27	0	1,1,1	0.15	0
2	EOH	AAA	206	-	2,2,2	0.22	0	1,1,1	0.66	0
3	SO4	AAA	215	-	4,4,4	0.45	0	6,6,6	0.47	0
3	SO4	AAA	212	-	4,4,4	0.83	0	6,6,6	0.59	0
2	EOH	AAA	201	-	2,2,2	0.22	0	1,1,1	0.02	0

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.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	204	EOH	1	2
3	AAA	213[A]	SO4	1	0
2	AAA	210	EOH	2	0
2	AAA	207	EOH	1	0
2	AAA	208	EOH	2	0
3	AAA	214	SO4	1	0
2	AAA	203	EOH	3	0
3	AAA	218[A]	SO4	1	0
2	AAA	202	EOH	1	0
2	AAA	206	EOH	1	0

5.6 Other polymers (i)

There are no such residues in this entry.

5.7 Polymer linkage issues (i)

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, 95^{th} 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	AAA	124/124 (100%)	-0.73	1 (0%) 86 72	3, 4, 8, 12	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	1[A]	LYS	5.6

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	EOH	AAA	203	3/3	0.85	0.15	17,21,23,23	0
2	EOH	AAA	211	3/3	0.88	0.12	20,22,29,30	0
2	EOH	AAA	209	3/3	0.91	0.27	16,22,25,27	0
2	EOH	AAA	202	3/3	0.91	0.15	11,11,12,12	0
2	EOH	AAA	206	3/3	0.92	0.26	16,17,19,20	0
2	EOH	AAA	207	3/3	0.92	0.30	17,25,28,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	AAA	214	5/5	0.92	0.20	5,7,19,21	0
3	SO4	AAA	215	5/5	0.92	0.20	11,16,22,30	0
2	EOH	AAA	204	3/3	0.93	0.26	11,16,23,23	0
2	EOH	AAA	208	3/3	0.93	0.16	9,10,15,16	0
2	EOH	AAA	210	3/3	0.95	0.27	13,14,16,19	0
2	EOH	AAA	205	3/3	0.97	0.17	11,13,15,16	0
3	SO4	AAA	212	5/5	0.97	0.12	10,14,16,17	0
3	SO4	AAA	216[B]	5/5	0.98	0.12	7,8,10,11	5
2	EOH	AAA	201	3/3	0.99	0.07	4,5,6,6	0
3	SO4	AAA	217[B]	5/5	0.99	0.06	3,5,7,9	5
3	SO4	AAA	218[A]	5/5	0.99	0.10	7,9,11,13	5
3	SO4	AAA	213[A]	5/5	1.00	0.06	4,8,8,11	5

6.5 Other polymers (i)

There are no such residues in this entry.