



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5D1Y / pdb_00005d1y
Title : Low resolution crystal structure of human ribonucleotide reductase alpha6 hexamer in complex with dATP
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Deposited on : 2015-08-04
Resolution : 9.01 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

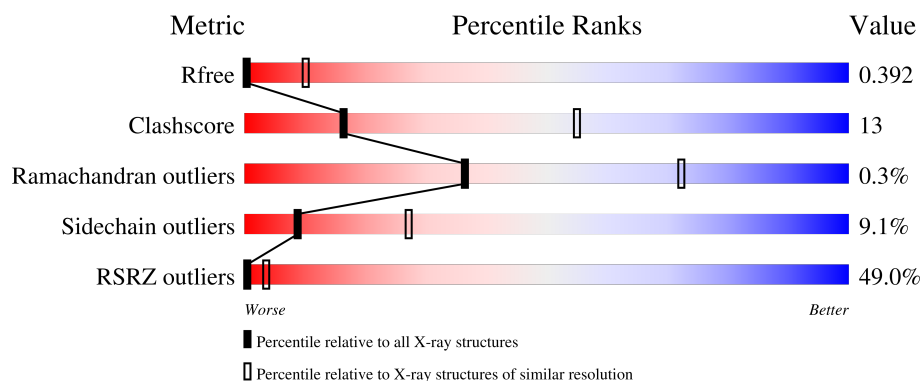
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 9.01 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}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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 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 $\leq 5\%$. 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	812	43% 69% 16% • 12%
1	B	812	44% 73% 16% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11328 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 Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	0	0	0
			5577	3567	926	1052	32			
1	B	738	Total	C	N	O	S	0	0	0
			5751	3669	968	1080	34			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P23921
A	-18	GLY	-	expression tag	UNP P23921
A	-17	SER	-	expression tag	UNP P23921
A	-16	SER	-	expression tag	UNP P23921
A	-15	HIS	-	expression tag	UNP P23921
A	-14	HIS	-	expression tag	UNP P23921
A	-13	HIS	-	expression tag	UNP P23921
A	-12	HIS	-	expression tag	UNP P23921
A	-11	HIS	-	expression tag	UNP P23921
A	-10	HIS	-	expression tag	UNP P23921
A	-9	SER	-	expression tag	UNP P23921
A	-8	SER	-	expression tag	UNP P23921
A	-7	GLY	-	expression tag	UNP P23921
A	-6	LEU	-	expression tag	UNP P23921
A	-5	VAL	-	expression tag	UNP P23921
A	-4	PRO	-	expression tag	UNP P23921
A	-3	ARG	-	expression tag	UNP P23921
A	-2	GLY	-	expression tag	UNP P23921
A	-1	SER	-	expression tag	UNP P23921
A	0	HIS	-	expression tag	UNP P23921
B	-19	MET	-	initiating methionine	UNP P23921
B	-18	GLY	-	expression tag	UNP P23921
B	-17	SER	-	expression tag	UNP P23921
B	-16	SER	-	expression tag	UNP P23921
B	-15	HIS	-	expression tag	UNP P23921

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P23921
B	-13	HIS	-	expression tag	UNP P23921
B	-12	HIS	-	expression tag	UNP P23921
B	-11	HIS	-	expression tag	UNP P23921
B	-10	HIS	-	expression tag	UNP P23921
B	-9	SER	-	expression tag	UNP P23921
B	-8	SER	-	expression tag	UNP P23921
B	-7	GLY	-	expression tag	UNP P23921
B	-6	LEU	-	expression tag	UNP P23921
B	-5	VAL	-	expression tag	UNP P23921
B	-4	PRO	-	expression tag	UNP P23921
B	-3	ARG	-	expression tag	UNP P23921
B	-2	GLY	-	expression tag	UNP P23921
B	-1	SER	-	expression tag	UNP P23921
B	0	HIS	-	expression tag	UNP P23921

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	356.01Å 356.01Å 356.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.90 – 9.01 75.90 – 9.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.90-9.01) 87.9 (75.90-9.01)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 8.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.405 , 0.426 0.388 , 0.392	Depositor DCC
R_{free} test set	707 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	407.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.03 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	11328	wwPDB-VP
Average B, all atoms (Å ²)	633.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.90% 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](#)

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	0.67	3/5699 (0.1%)	0.91	7/7751 (0.1%)
1	B	0.58	0/5876	0.88	3/7986 (0.0%)
All	All	0.63	3/11575 (0.0%)	0.89	10/15737 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	VAL	C-O	-6.39	1.17	1.24
1	A	286	VAL	CA-CB	5.33	1.60	1.53
1	A	442	ALA	CA-CB	-5.10	1.45	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	ILE	N-CA-C	6.52	115.07	107.77
1	A	334	ILE	N-CA-C	6.37	114.90	107.77
1	B	446	LEU	N-CA-C	6.08	119.11	109.50
1	A	443	VAL	CA-C-N	-5.95	112.81	122.81
1	A	443	VAL	C-N-CA	-5.95	112.81	122.81

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	5577	0	5412	201	28
1	B	5751	0	5584	184	14
All	All	11328	0	10996	290	28

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 13.

The worst 5 of 290 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:261:TYR:HB2	1:B:108:HIS:CE1	1.10	1.62
1:B:83:VAL:CG1	1:B:141:PHE:HD1	1.16	1.59
1:A:281:ASN:CG	1:B:281:ASN:HB3	1.23	1.58
1:B:86:LEU:HD13	1:B:148:PHE:CE1	1.39	1.54
1:B:90:THR:CG2	1:B:140:ASP:OD1	1.63	1.43

The worst 5 of 28 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)
1:A:27:TYR:CD1	1:A:27:TYR:CD1[22_554]	0.73	1.47
1:A:27:TYR:CG	1:A:27:TYR:CE1[22_554]	0.90	1.30
1:A:27:TYR:CE2	1:A:27:TYR:CZ[22_554]	1.07	1.13
1:A:27:TYR:CD2	1:A:27:TYR:CZ[22_554]	1.15	1.05
1:A:27:TYR:CD2	1:A:27:TYR:CE1[22_554]	1.27	0.93

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	706/812 (87%)	683 (97%)	21 (3%)	2 (0%)	36 72
1	B	730/812 (90%)	700 (96%)	28 (4%)	2 (0%)	36 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1436/1624 (88%)	1383 (96%)	49 (3%)	4 (0%)	36 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	B	224	LYS
1	A	737	TYR
1	B	601	PRO

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	592/710 (83%)	539 (91%)	53 (9%)	9 27
1	B	607/710 (86%)	551 (91%)	56 (9%)	8 27
All	All	1199/1420 (84%)	1090 (91%)	109 (9%)	9 27

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	VAL
1	B	225	ASP
1	B	615	GLU
1	B	59	LEU
1	B	149	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	346	GLN
1	B	711	HIS
1	A	550	GLN
1	A	667	GLN

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Mol	Chain	Res	Type
1	B	108	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	90:THR	C	91:LYS	N	11.08
1	B	90:THR	C	91:LYS	N	5.88

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	714/812 (87%)	2.65	352 (49%) 0 3	631, 631, 660, 660	0
1	B	738/812 (90%)	2.64	360 (48%) 0 3	631, 631, 642, 642	0
All	All	1452/1624 (89%)	2.64	712 (49%) 0 3	631, 631, 660, 660	0

The worst 5 of 712 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	THR	21.7
1	A	288	GLN	21.4
1	A	264	GLY	20.6
1	B	265	THR	20.2
1	A	47	LEU	17.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.