



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5D1Y
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
<http://wwpdb.org/validation/2016/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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
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)	:	rb-20026982

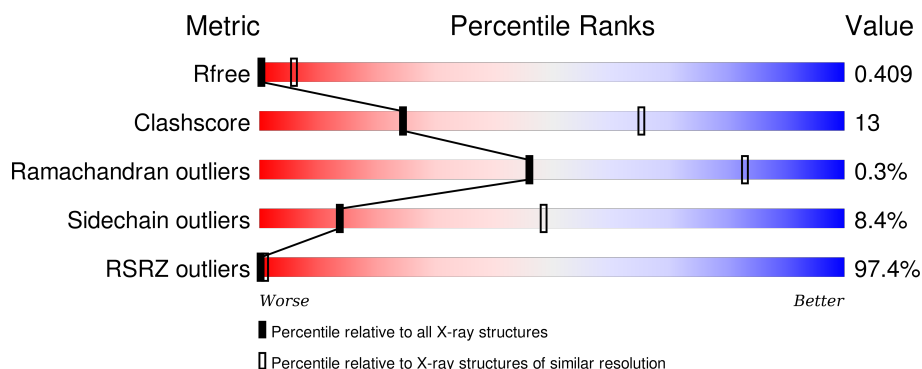
1 Overall quality at a glance

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}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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 $\leq 5\%$. 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	<div> <div>85%</div> <div>70% 16% • 12%</div> </div>
1	B	812	<div> <div>89%</div> <div>73% 16% • 9%</div> </div>

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



GLU	W581	I641	F701	GLU
LYS	K582	I642	I702	LYS
VAL	V583	R643	D703	VAL
SER	L584	D644	Q704	SER
LYS	K585	L645	S705	LYS
GLU	E586	T646	Q706	GLU
GLU	K587	E647	S707	GLU
GLU	I588	R648	L708	GLU
LYS	K590	L650	N709	GLU
GLU	Y591	W651	I710	LYS
ARG	G592	H652	H711	ARG
ASN	I593	E653	I712	ASN
THR	R594	E654	A713	THR
ALA	N595	E655	E714	ALA
ALA	S596	R656	P715	ALA
MET	L597	N657	N716	MET
VAL	L598	Q658	Y717	VAL
CYS	I599	I659	K718	CYS
SER	A600	I660	K719	SER
LEU	P601	A661	L720	LEU
GLU	M602	G662	T721	GLU
ASN	P603	N663	S722	ASN
ARG	T604	G664	M723	ARG
ASP	A605	S665	H724	ASP
GLU	S606	I666	F725	GLU
CYS	T607	Q667	Y726	CYS
LEU	A608	S668	G727	LEU
MET	Q609	I669	W728	MET
CYS	I610	P670	K729	CYS
GLY	L611	E671	Q730	GLY
SER	G612	L672	G731	SER
LYS	N613	P673	L732	LYS
GLU	M614	D674	K733	GLU
GLU	E615	D675	I734	GLU
GLU	S616	L676	G735	GLU
LYS	I617	K677	M736	LYS
LYS	E618	Q677	Y737	LYS
LYS	P619	Q678	Y738	LYS
LYS	Y620	L679	L739	LYS
LYS	T621	K681	R740	LYS
LYS	S622	T682	T741	LYS
LYS	N623	V683	R742	LYS
LYS	I624	W684	PRO	LYS
LYS	Y625	E685	ALA	LYS
LYS	T626	I686	ALA	LYS
LYS	R627	S687	ASN	LYS
LYS	R628	Q688	PRO	LYS
LYS	V629	K689	ILE	LYS
LYS	LEU	T690	GLN	LYS
LYS	SER	W691	PHE	LYS
LYS	G632	L692	THR	LYS
LYS	E633	K693	LEU	LYS
LYS	F634	N694	ASN	LYS
LYS	Q635	A695	LYS	LYS
LYS	I636	A696	GLU	LYS
LYS	V637	E697	LYS	LYS
LYS	M638	H698	LEU	LYS
LYS	P639	G699	LYS	LYS
LYS	H640	A700	ASP	LYS
LYS			LYS	LYS

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 – 8.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.90-9.01) 85.6 (75.90-8.55)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 8.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.405 , 0.426 0.388 , 0.409	Depositor DCC
R_{free} test set	535 reflections (9.97%)	DCC
Wilson B-factor (Å ²)	386.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.62 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 7071 reflections	Xtriage
F_o, F_c correlation	0.83	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 7.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.52	0/5699	0.63	3/7751 (0.0%)
1	B	0.45	0/5876	0.60	1/7986 (0.0%)
All	All	0.49	0/11575	0.61	4/15737 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	LEU	CA-CB-CG	7.02	131.46	115.30
1	A	499	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	220	LEU	CA-CB-CG	5.90	128.86	115.30
1	A	508	LEU	CA-CB-CG	5.29	127.48	115.30

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	5577	0	5412	199	28
1	B	5751	0	5584	185	14
All	All	11328	0	10996	288	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 288 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:B:86:LEU:HD13	1:B:148:PHE:CE1	1.39	1.54
1:A:281:ASN:CG	1:B:281:ASN:HB3	1.23	1.53
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%)	46	83
1	B	730/812 (90%)	700 (96%)	28 (4%)	2 (0%)	46	83
All	All	1436/1624 (88%)	1383 (96%)	49 (3%)	4 (0%)	46	83

All (4) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	545 (92%)	47 (8%)	15	51
1	B	607/710 (86%)	553 (91%)	54 (9%)	12	44
All	All	1199/1420 (84%)	1098 (92%)	101 (8%)	14	48

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	741	THR
1	B	121	LEU
1	B	648	ARG
1	B	3	VAL
1	B	59	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	B	281	ASN
1	B	108	HIS
1	A	106	ASN
1	B	270	ASN

5.3.3 RNA ⓘ

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](#)

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	B	1
1	A	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%)	15.87	691 (96%) 0 1	631, 631, 660, 660	0
1	B	738/812 (90%)	17.88	723 (97%) 0 1	631, 631, 642, 642	0
All	All	1452/1624 (89%)	16.89	1414 (97%) 0 1	631, 631, 660, 660	0

The worst 5 of 1414 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	682	THR	75.2
1	B	495	ASN	63.1
1	A	677	LYS	61.0
1	B	359	LEU	60.7
1	B	335	PRO	59.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.