wwPDB X-ray Structure Validation Summary Report (i)

Sep 19, 2023 – 04:22 AM EDT

PDB ID	:	5D1Y
Title	:	Low resolution crystal structure of human ribonucleotide reductase alpha6 hexamer in complex with dATP
Authors	:	Ando, N.; Li, H.; Brignole, E.J.; Thompson, S.; McLaughlin, M.I.; Page, J.; Asturias, F.; Stubbe, J.; Drennan, C.L.
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 (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:

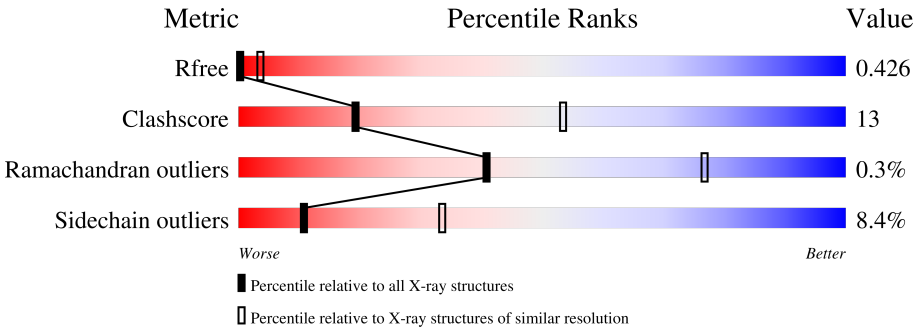
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)

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%

Mol	Chain	Length	Quality of chain
1	A	812	70% 16% • 12%
1	B	812	73% 16% • 9%

2 Entry composition (i)

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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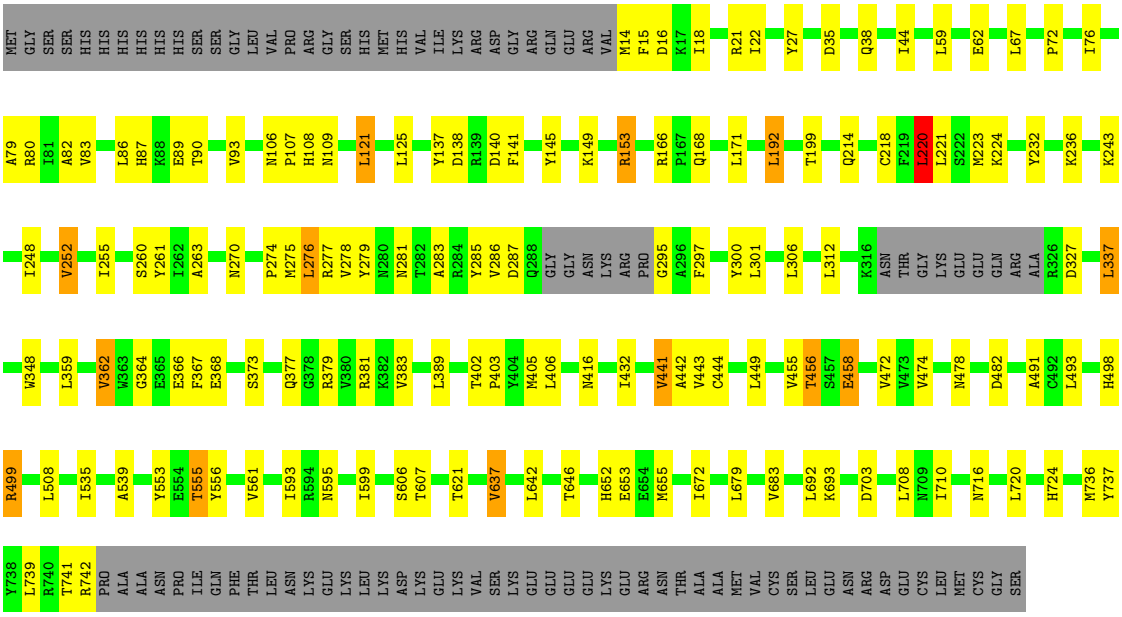
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P23921
B	-13	HIS	-	expression tag	UNP P23921
B	-12	HIS	-	expression tag	UNP P23921
B	-11	HIS	-	expression tag	UNP P23921
B	-10	HIS	-	expression tag	UNP P23921
B	-9	SER	-	expression tag	UNP P23921
B	-8	SER	-	expression tag	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

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. 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.

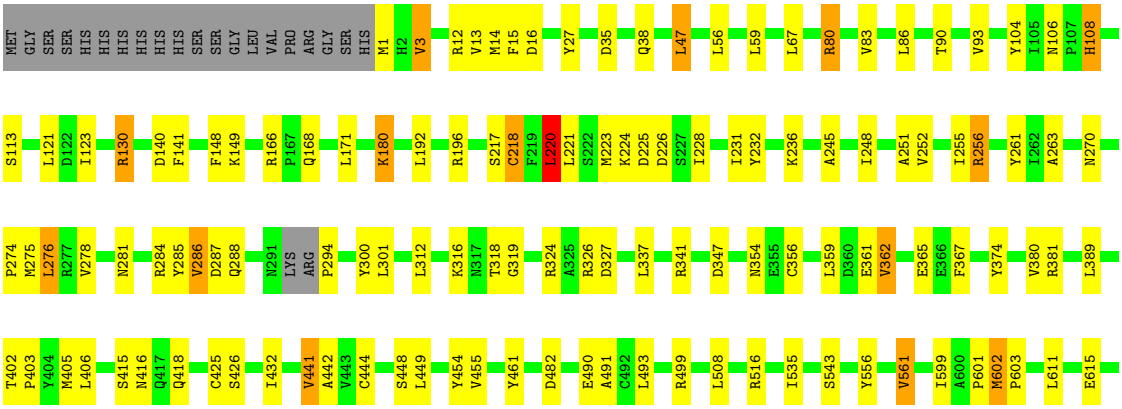
• Molecule 1: Ribonucleoside-diphosphate reductase large subunit

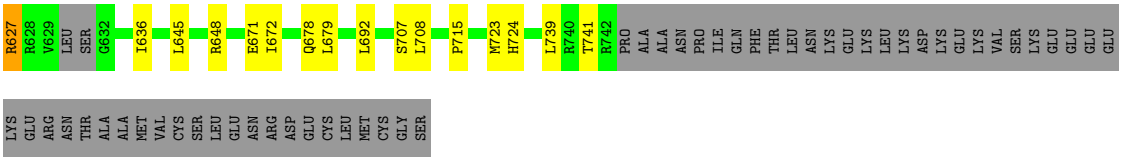
Chain A:



• Molecule 1: Ribonucleoside-diphosphate reductase large subunit

Chain B:




R627 R628 V629 LEU SER G632 I636 L645 R648 E671 I672 Q678 L679 L692 S707 L708 P715 M723 H724 L739 R740 T741 R742 PRO ALA ALA ASN PRO ILE GLN PHE THR LEU ASN LYS GLU LYS LEU LYS ASP LYS GLU LYS VAL SER LYS GLU GLU GLU
LYS GLU ARG ASN THR ALA ALA MET VAL CYS SER LEU GLU ASN ARG ASP GLU CYS LEU MET CYS GLY SER

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	0.93 (at 8.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.405 , 0.426 0.406 , 0.426	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)	0.62 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	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 7.90% 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

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(^{o})	Ideal(^{o})
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

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%)	41	77
1	B	730/812 (90%)	700 (96%)	28 (4%)	2 (0%)	41	77
All	All	1436/1624 (88%)	1383 (96%)	49 (3%)	4 (0%)	41	77

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 (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	592/710 (83%)	545 (92%)	47 (8%)	12 35
1	B	607/710 (86%)	553 (91%)	54 (9%)	9 30
All	All	1199/1420 (84%)	1098 (92%)	101 (8%)	11 33

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

Mol	Chain	Res	Type
1	B	130	ARG
1	B	312	LEU
1	B	723	MET
1	B	171	LEU
1	B	225	ASP

Sometimes 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	108	HIS
1	B	281	ASN
1	B	270	ASN
1	A	160	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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

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.