



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:22 PM GMT

PDB ID : 5C0Y
Title : Crystal structure of the Rrp6 catalytic domain bound to poly(U) RNA
Authors : Schuch, B.; Conti, E.
Deposited on : 2015-06-12
Resolution : 2.10 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

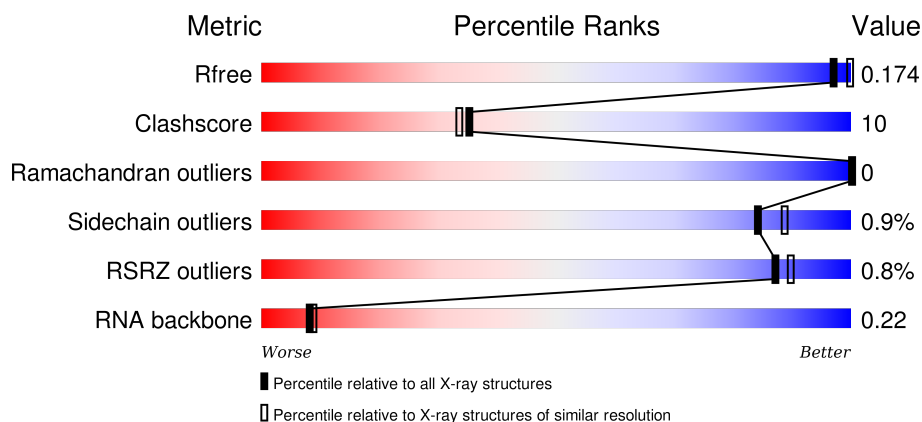
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)
RNA backbone	2183	1118 (2.80-1.40)

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	402	 77% 19% .
1	B	402	 76% 20% .
2	C	15	 27% 7% 67%
2	D	15	 20% 27% 13% 40%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7106 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 Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3163	2030	543	583	7			
1	B	388	Total	C	N	O	S	0	0	0
			3178	2039	545	587	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLY	-	expression tag	UNP Q12149
A	118	PRO	-	expression tag	UNP Q12149
A	119	ASP	-	expression tag	UNP Q12149
A	120	SER	-	expression tag	UNP Q12149
A	121	MET	-	expression tag	UNP Q12149
A	296	ASN	ASP	engineered mutation	UNP Q12149
B	117	GLY	-	expression tag	UNP Q12149
B	118	PRO	-	expression tag	UNP Q12149
B	119	ASP	-	expression tag	UNP Q12149
B	120	SER	-	expression tag	UNP Q12149
B	121	MET	-	expression tag	UNP Q12149
B	296	ASN	ASP	engineered mutation	UNP Q12149

- Molecule 2 is a RNA chain called poly U RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	9	Total	C	N	O	P	0	0	1
			128	54	12	54	8			
2	C	5	Total	C	N	O	P	0	0	1
			48	18	4	22	4			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0

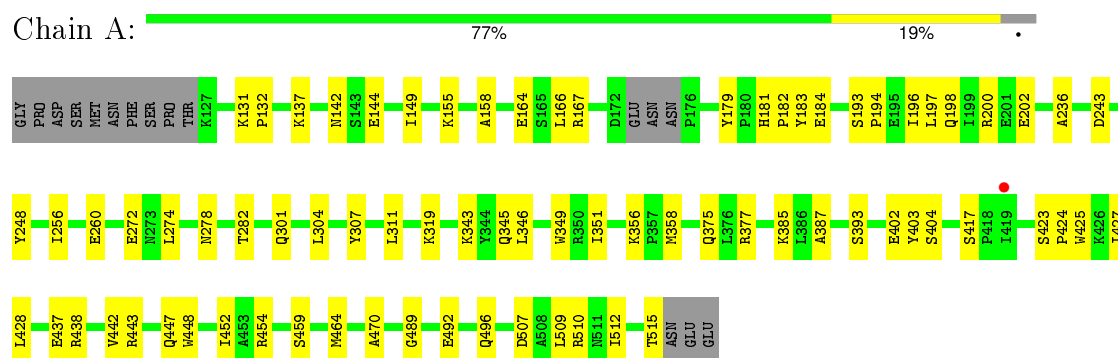
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	292	Total 292	O 292	0	0
4	B	273	Total 273	O 273	0	0
4	D	18	Total 18	O 18	0	0
4	C	5	Total 5	O 5	0	0

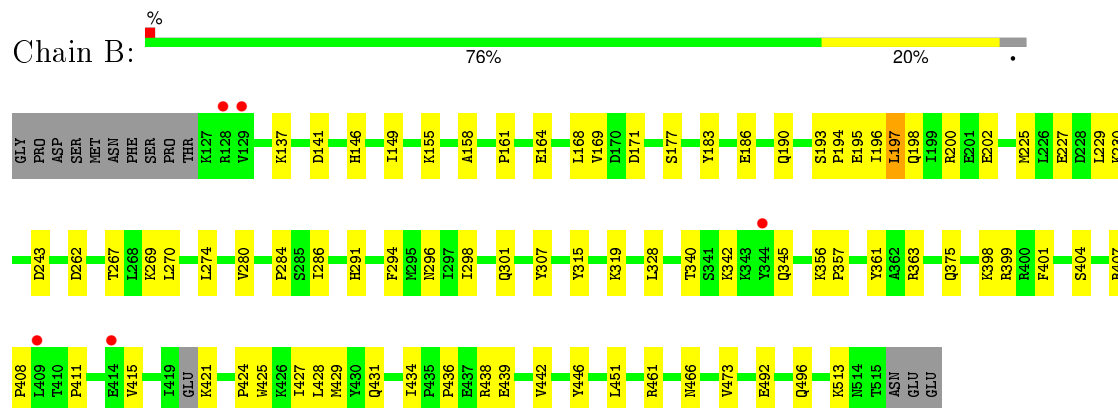
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

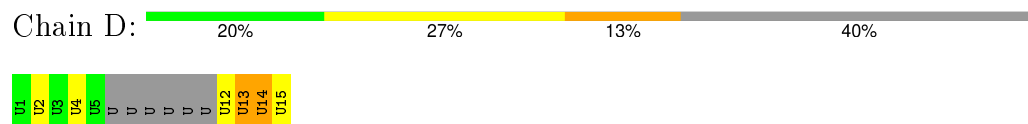
- Molecule 1: Exosome complex exonuclease RRP6



- Molecule 1: Exosome complex exonuclease RRP6



- Molecule 2: poly U RNA



- Molecule 2: poly U RNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	110.19 Å 110.19 Å 78.88 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.71 – 2.10 47.71 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.71-2.10) 100.0 (47.71-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.10 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.148 , 0.180 0.146 , 0.174	Depositor DCC
R_{free} test set	3003 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.3	EDS
Estimated twinning fraction	0.500 for h,-h-k,-l 0.023 for -h,-k,l 0.489 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for h,-h-k,-l	Depositor
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 62547 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7106	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.41	0/3243	0.60	1/4411 (0.0%)
1	B	0.41	0/3258	0.61	0/4433
2	C	1.19	1/49 (2.0%)	1.23	1/71 (1.4%)
2	D	0.86	1/136 (0.7%)	1.15	1/203 (0.5%)
All	All	0.44	2/6686 (0.0%)	0.63	3/9118 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	U	P-O5'	-7.67	1.52	1.59
2	C	4	U	P-O5'	-7.59	1.52	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	U	OP1-P-OP2	-6.86	109.32	119.60
1	A	489	GLY	N-CA-C	-5.94	98.24	113.10
2	D	4	U	OP1-P-OP2	-5.74	110.98	119.60

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	3163	0	3129	49	0
1	B	3178	0	3141	74	0
2	C	48	0	20	0	0
2	D	128	0	61	11	0
3	B	1	0	0	0	0
4	A	292	0	0	9	3
4	B	273	0	0	17	3
4	C	5	0	0	0	0
4	D	18	0	0	2	0
All	All	7106	0	6351	126	3

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 10.

The worst 5 of 126 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:B:428:LEU:HB2	1:B:446:TYR:OH	1.79	0.81
1:A:155:LYS:NZ	1:A:182:PRO:O	2.14	0.81
1:B:408:PRO:HG2	1:B:415:VAL:HG21	1.62	0.80
1:B:227:GLU:OE1	4:B:701:HOH:O	2.03	0.77
1:B:461:ARG:HE	2:D:2:U:H1'	1.50	0.74

All (3) 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)
4:A:930:HOH:O	4:B:888:HOH:O[3_565]	2.10	0.10
4:A:865:HOH:O	4:B:946:HOH:O[3_565]	2.13	0.07
4:A:897:HOH:O	4:B:777:HOH:O[3_665]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	382/402 (95%)	371 (97%)	11 (3%)	0	100	100
1	B	384/402 (96%)	377 (98%)	7 (2%)	0	100	100
All	All	766/804 (95%)	748 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	349/373 (94%)	347 (99%)	2 (1%)	90	94
1	B	351/373 (94%)	347 (99%)	4 (1%)	80	85
All	All	700/746 (94%)	694 (99%)	6 (1%)	84	89

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	197	LEU
1	B	451	LEU
1	B	294	PHE
1	A	515	THR
1	B	340	THR

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	1/15 (6%)	0	0
2	D	4/15 (26%)	3 (75%)	0
All	All	5/30 (16%)	3 (60%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	13	U
2	D	14	U
2	D	15	U

There are no RNA pucker outliers to report.

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 1 ligands modelled in this entry, 1 is 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 [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	386/402 (96%)	-0.58	1 (0%) 94 95	30, 50, 94, 147	0
1	B	388/402 (96%)	-0.58	5 (1%) 79 84	30, 49, 98, 145	1 (0%)
2	C	5/15 (33%)	-0.91	0 100 100	57, 58, 66, 70	5 (100%)
2	D	9/15 (60%)	-0.46	0 100 100	62, 73, 77, 77	9 (100%)
All	All	788/834 (94%)	-0.58	6 (0%) 87 90	30, 50, 96, 147	15 (1%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	ILE	5.0
1	B	344	TYR	3.4
1	B	409	LEU	3.2
1	B	414	GLU	3.1
1	B	128	ARG	3.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	B	601	1/1	0.75	0.09	-0.49	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.