



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:25 PM GMT

PDB ID : 4ERM  
Title : Crystal structure of the dATP inhibited E. coli class Ia ribonucleotide reductase complex at 4 Angstroms resolution  
Authors : Zimanyi, C.M.; Drennan, C.L.  
Deposited on : 2012-04-20  
Resolution : 3.95 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

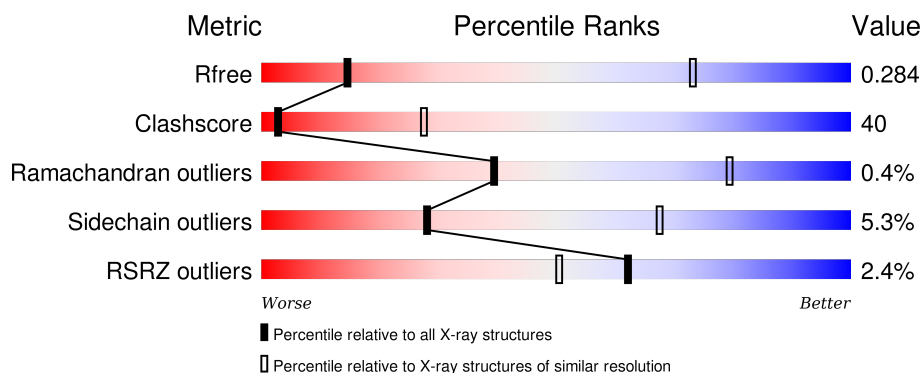
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.95 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	1011 (4.38-3.54)
Clashscore	102246	1025 (4.32-3.60)
Ramachandran outliers	100387	1008 (4.34-3.58)
Sidechain outliers	100360	1027 (4.36-3.56)
RSRZ outliers	91569	1015 (4.38-3.54)

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  $\geq 3$ , 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	761	<div> <div>42%</div> <div>52%</div> <div>• •</div> </div>
1	B	761	<div> <div>44%</div> <div>49%</div> <div>• •</div> </div>
1	C	761	<div> <div>4%</div> <div>45%</div> <div>47%</div> <div>• •</div> </div>
1	D	761	<div> <div>4%</div> <div>46%</div> <div>47%</div> <div>• •</div> </div>
2	E	375	<div> <div>3%</div> <div>44%</div> <div>47%</div> <div>• 6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	375	
2	G	375	
2	H	375	

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
4	DAT	D	802	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35345 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.

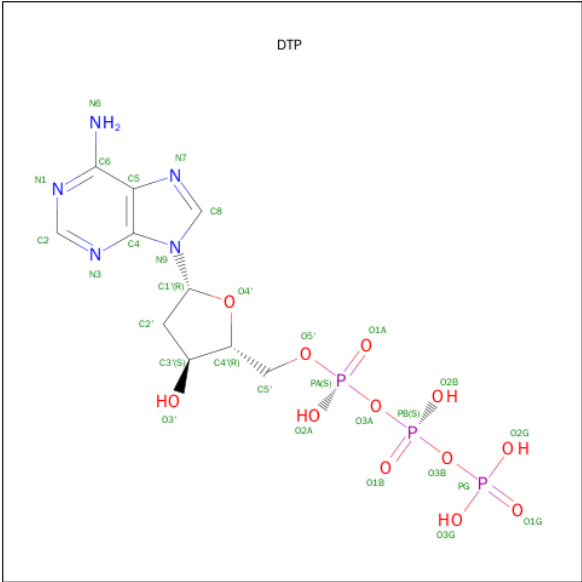
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			5841	3710	1003	1104	24			
1	B	734	Total	C	N	O	S	0	0	0
			5845	3712	1004	1105	24			
1	C	731	Total	C	N	O	S	0	0	0
			5821	3696	1000	1101	24			
1	D	733	Total	C	N	O	S	0	0	0
			5837	3708	1002	1103	24			

- Molecule 2 is a protein called Ribonucleoside-diphosphate reductase 1 subunit beta.

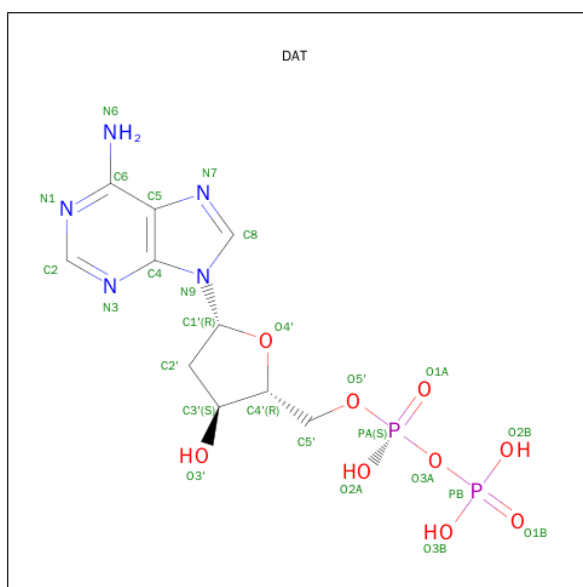
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	352	Total	C	N	O	S	0	0	0
			2885	1841	478	553	13			
2	F	356	Total	C	N	O	S	0	0	0
			2917	1861	483	560	13			
2	G	356	Total	C	N	O	S	0	0	0
			2917	1861	483	560	13			
2	H	356	Total	C	N	O	S	0	0	0
			2914	1859	482	560	13			

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 4 is 2'-DEOXYADENOSINE-5'-DIPHOSPHATE (three-letter code: DAT) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>9</sub>P<sub>2</sub>).

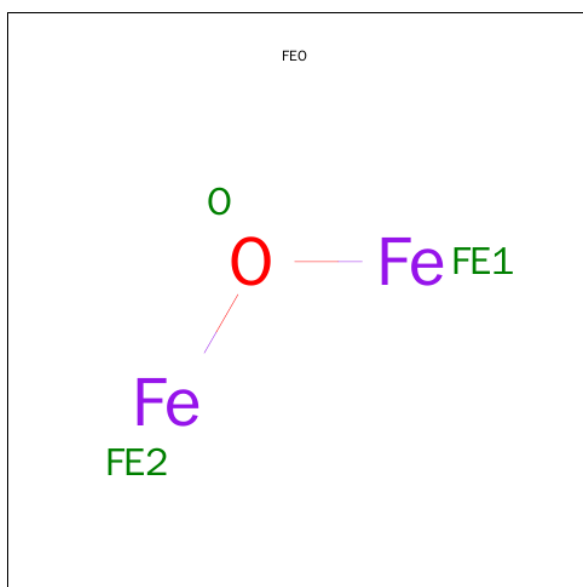


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	B	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	C	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	D	1	Total	C	N	O	P	0	0
			26	10	5	9	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe<sub>2</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	Fe	O	0	0
			3	2	1		
6	F	1	Total	Fe	O	0	0
			3	2	1		
6	G	1	Total	Fe	O	0	0
			3	2	1		
6	H	1	Total	Fe	O	0	0
			3	2	1		

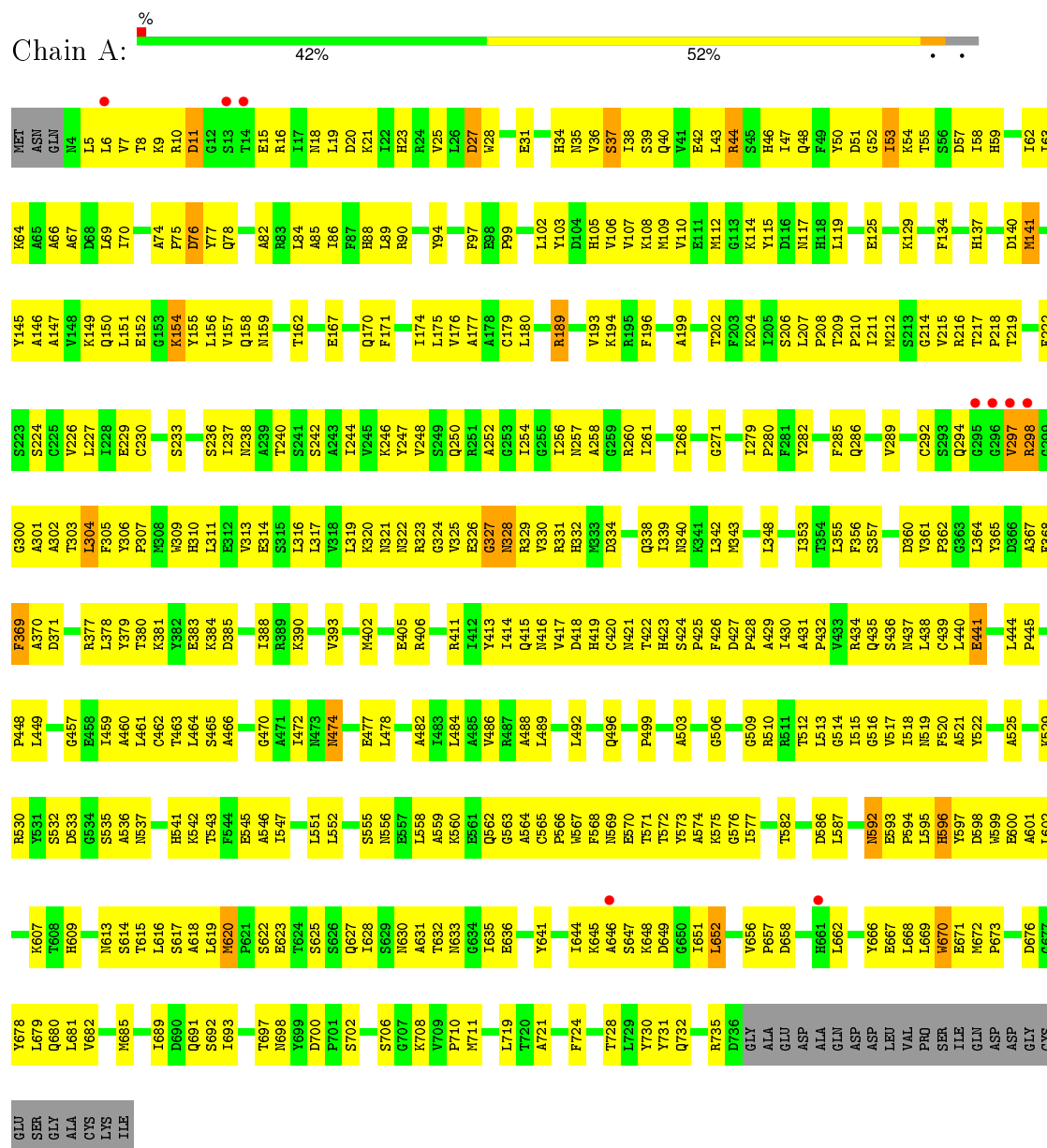
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	2	Total	O	0	0
			2	2		
7	F	2	Total	O	0	0
			2	2		
7	G	2	Total	O	0	0
			2	2		
7	H	2	Total	O	0	0
			2	2		

### 3 Residue-property plots

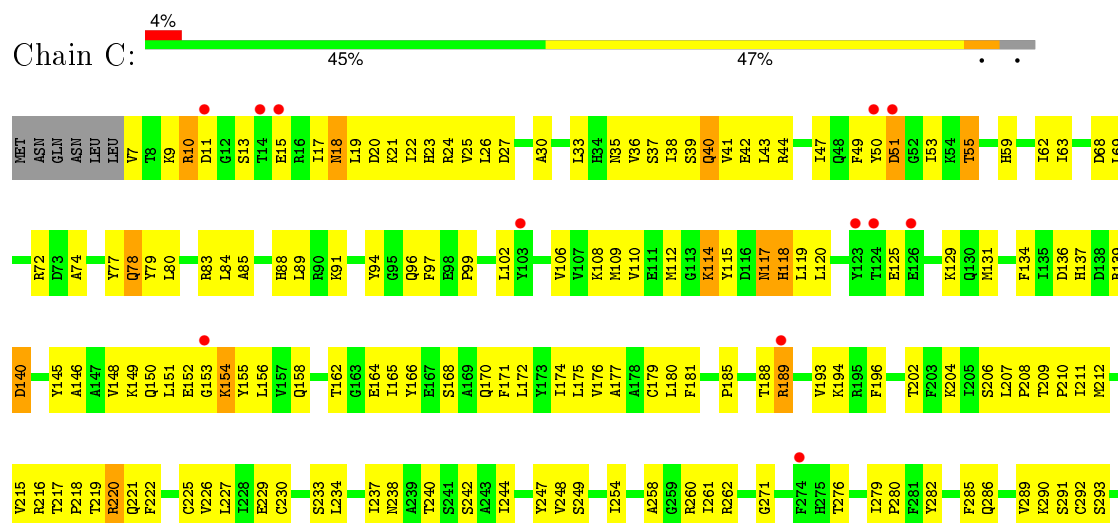
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Ribonucleoside-diphosphate reductase 1 subunit alpha

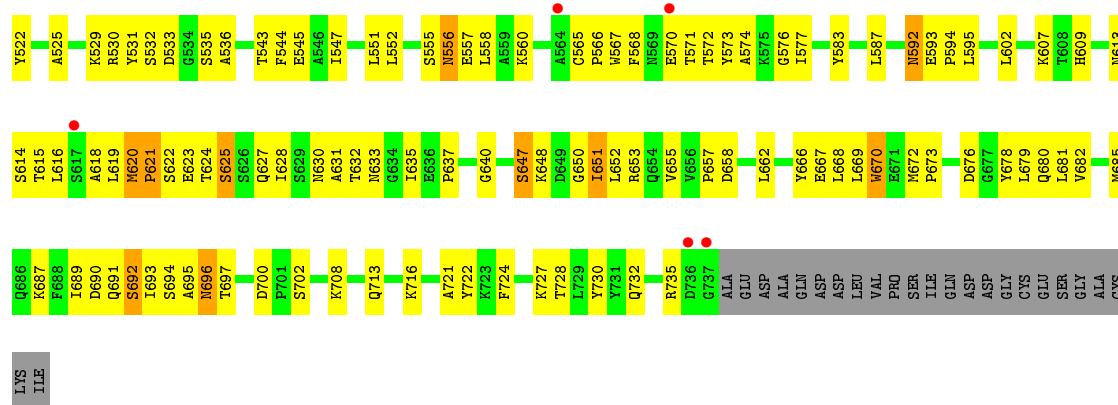


- Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

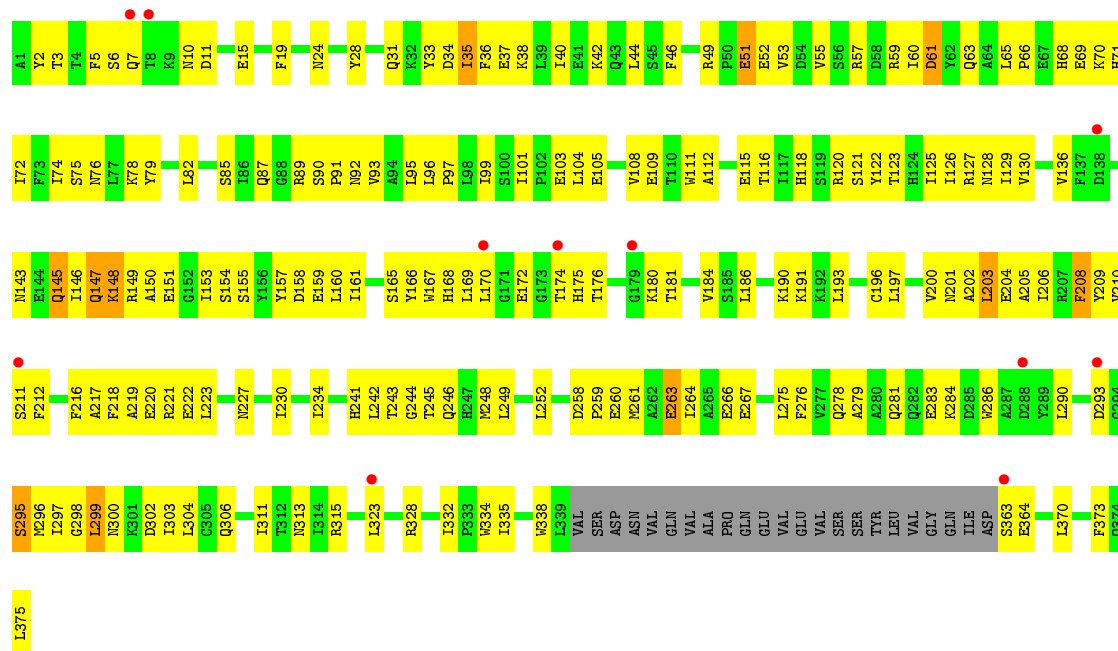




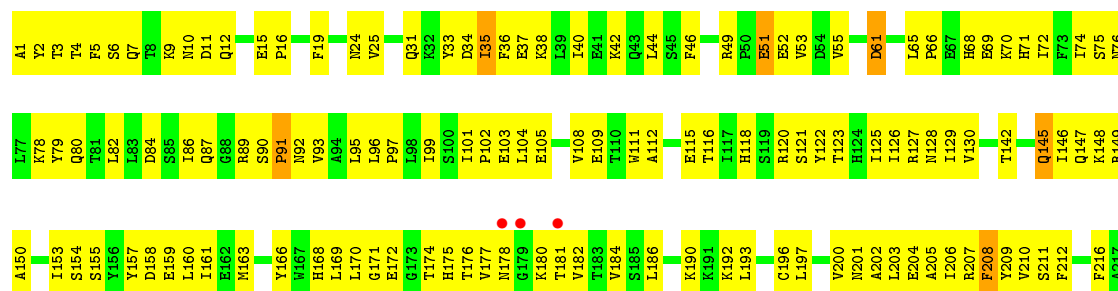
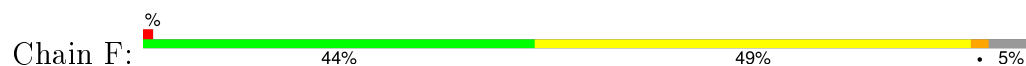


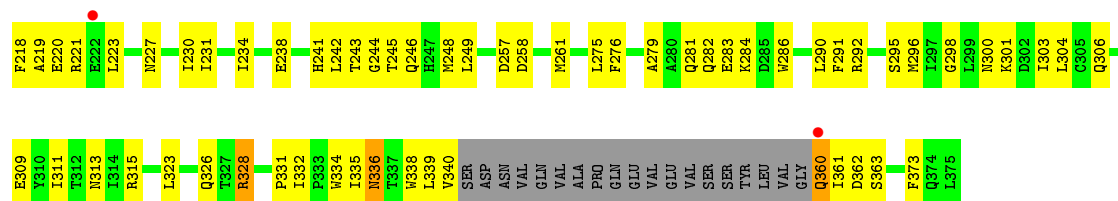


• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

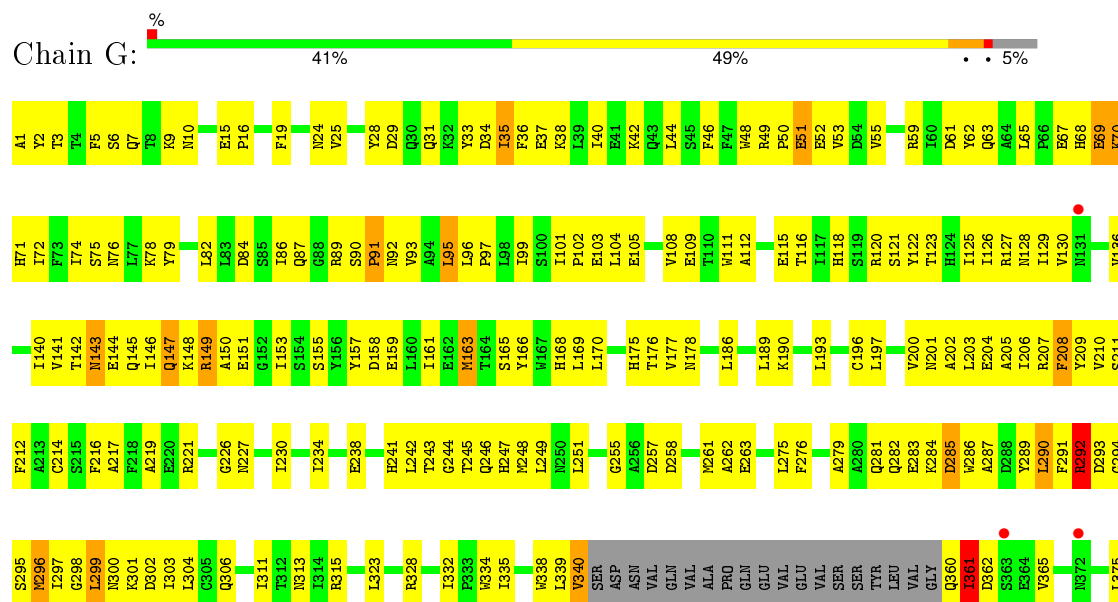


• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

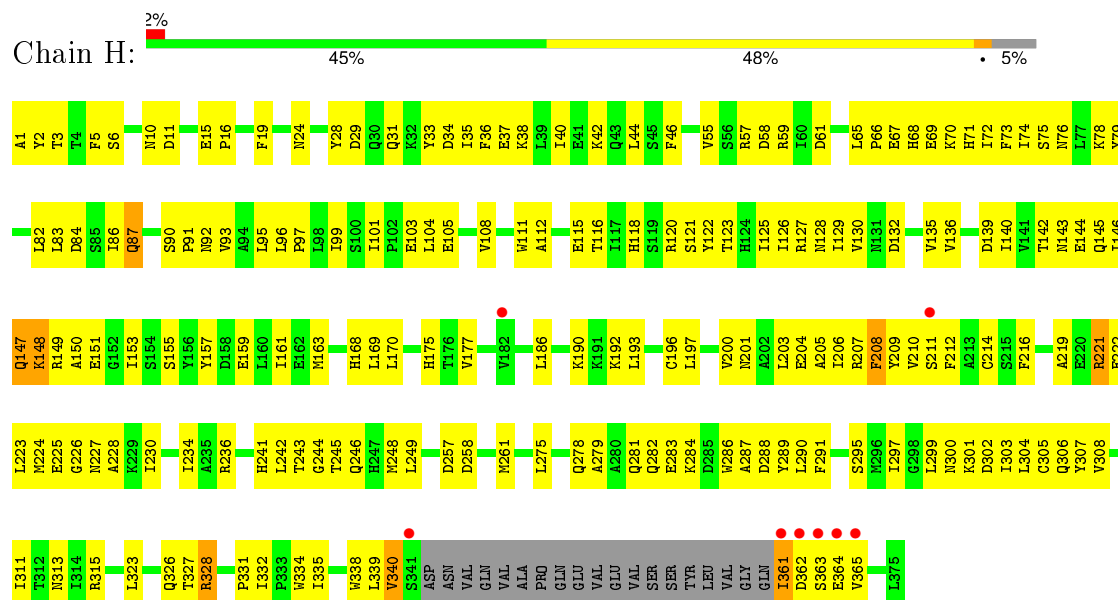




• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta



• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	280.47Å 155.74Å 166.92Å 90.00° 119.07° 90.00°	Depositor
Resolution (Å)	30.00 – 3.95 29.99 – 3.93	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.00-3.95) 95.2 (29.99-3.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 3.98Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.259 , 0.284 0.267 , 0.284	Depositor DCC
$R_{free}$ test set	2515 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	95.3	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 61.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 53173 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	35345	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.26	0/5969	0.46	1/8085 (0.0%)
1	B	0.25	0/5973	0.45	1/8090 (0.0%)
1	C	0.25	0/5949	0.44	0/8057
1	D	0.25	0/5965	0.44	1/8079 (0.0%)
2	E	0.30	1/2949 (0.0%)	0.44	1/3998 (0.0%)
2	F	0.25	0/2981	0.41	0/4042
2	G	0.25	0/2981	0.42	0/4042
2	H	0.25	0/2978	0.43	0/4038
All	All	0.26	1/35745 (0.0%)	0.44	4/48431 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	203	LEU	C-N	5.68	1.47	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	48	GLN	O-C-N	5.88	132.10	122.70
1	A	48	GLN	O-C-N	5.86	132.08	122.70
1	B	48	GLN	O-C-N	5.85	132.07	122.70
2	E	203	LEU	C-N-CA	-5.43	108.12	121.70

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	5841	0	5767	494	0
1	B	5845	0	5770	497	0
1	C	5821	0	5742	483	0
1	D	5837	0	5764	459	0
2	E	2885	0	2813	211	0
2	F	2917	0	2845	240	0
2	G	2917	0	2845	285	0
2	H	2914	0	2842	232	0
3	A	60	0	22	1	0
3	B	60	0	22	8	0
3	C	60	0	22	10	0
3	D	60	0	22	9	0
4	A	26	0	12	3	0
4	B	26	0	12	1	0
4	C	26	0	12	5	0
4	D	26	0	12	9	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	3	0	0	0	0
6	G	3	0	0	0	0
6	H	3	0	0	0	0
7	E	2	0	0	1	0
7	F	2	0	0	1	0
7	G	2	0	0	0	0
7	H	2	0	0	1	0
All	All	35345	0	34524	2786	0

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 40.

The worst 5 of 2786 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:354:THR:HG21	1:B:356:PHE:CZ	1.44	1.52
1:A:646:ALA:HB2	1:A:651:ILE:CG2	1.40	1.52
1:A:646:ALA:CB	1:A:651:ILE:HG22	1.41	1.46
1:A:297:VAL:CG1	1:A:298:ARG:HG2	1.50	1.41
1:A:53:ILE:HD11	1:A:58:ILE:CD1	1.50	1.40

There are no symmetry-related clashes.

## 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	731/761 (96%)	687 (94%)	40 (6%)	4 (0%)	34	76
1	B	732/761 (96%)	693 (95%)	37 (5%)	2 (0%)	46	82
1	C	729/761 (96%)	690 (95%)	36 (5%)	3 (0%)	39	79
1	D	731/761 (96%)	694 (95%)	33 (4%)	4 (0%)	34	76
2	E	348/375 (93%)	336 (97%)	12 (3%)	0	100	100
2	F	352/375 (94%)	338 (96%)	13 (4%)	1 (0%)	46	82
2	G	352/375 (94%)	336 (96%)	13 (4%)	3 (1%)	21	66
2	H	352/375 (94%)	339 (96%)	13 (4%)	0	100	100
All	All	4327/4544 (95%)	4113 (95%)	197 (5%)	17 (0%)	39	79

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	GLY
1	A	300	GLY
1	B	300	GLY
1	C	299	GLY
1	C	300	GLY



### 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	629/651 (97%)	593 (94%)	36 (6%)	25	65
1	B	629/651 (97%)	594 (94%)	35 (6%)	26	65
1	C	626/651 (96%)	591 (94%)	35 (6%)	26	65
1	D	628/651 (96%)	592 (94%)	36 (6%)	25	65
2	E	319/340 (94%)	305 (96%)	14 (4%)	35	72
2	F	323/340 (95%)	311 (96%)	12 (4%)	41	75
2	G	323/340 (95%)	299 (93%)	24 (7%)	17	56
2	H	323/340 (95%)	312 (97%)	11 (3%)	44	77
All	All	3800/3964 (96%)	3597 (95%)	203 (5%)	28	67

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	435	GLN
1	D	68	ASP
2	G	299	LEU
1	C	474	ASN
1	C	692	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	686	GLN
1	D	474	ASN
2	G	336	ASN
1	C	691	GLN
1	D	23	HIS

### 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](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

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$
3	DTP	A	801	-	24,32,32	1.66	6 (25%)	32,50,50	1.95	7 (21%)
4	DAT	A	802	-	22,28,28	1.59	6 (27%)	28,43,43	2.66	5 (17%)
3	DTP	A	803	5	24,32,32	1.61	5 (20%)	32,50,50	1.95	7 (21%)
3	DTP	B	801	-	24,32,32	1.66	6 (25%)	32,50,50	2.04	7 (21%)
4	DAT	B	802	-	22,28,28	1.59	6 (27%)	28,43,43	2.39	5 (17%)
3	DTP	B	803	5	24,32,32	1.62	5 (20%)	32,50,50	1.99	7 (21%)
3	DTP	C	801	-	24,32,32	1.66	6 (25%)	32,50,50	1.95	7 (21%)
4	DAT	C	802	-	22,28,28	1.68	7 (31%)	28,43,43	2.34	5 (17%)
3	DTP	C	803	5	24,32,32	1.62	5 (20%)	32,50,50	1.96	7 (21%)
3	DTP	D	801	-	24,32,32	1.65	6 (25%)	32,50,50	1.95	7 (21%)
4	DAT	D	802	-	22,28,28	1.60	6 (27%)	28,43,43	2.27	5 (17%)
3	DTP	D	803	5	24,32,32	1.63	5 (20%)	32,50,50	1.97	7 (21%)
6	FEO	E	501	2,7	0,2,2	0.00	-	0,1,1	0.00	-
6	FEO	F	501	2,7	0,2,2	0.00	-	0,1,1	0.00	-
6	FEO	G	501	2,7	0,2,2	0.00	-	0,1,1	0.00	-
6	FEO	H	501	2,7	0,2,2	0.00	-	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTP	A	801	-	-	0/18/34/34	0/3/3/3
4	DAT	A	802	-	-	0/12/28/28	0/3/3/3
3	DTP	A	803	5	-	0/18/34/34	0/3/3/3
3	DTP	B	801	-	-	0/18/34/34	0/3/3/3
4	DAT	B	802	-	-	0/12/28/28	0/3/3/3
3	DTP	B	803	5	-	0/18/34/34	0/3/3/3
3	DTP	C	801	-	-	0/18/34/34	0/3/3/3
4	DAT	C	802	-	-	0/12/28/28	0/3/3/3
3	DTP	C	803	5	-	0/18/34/34	0/3/3/3
3	DTP	D	801	-	-	0/18/34/34	0/3/3/3
4	DAT	D	802	-	-	0/12/28/28	0/3/3/3
3	DTP	D	803	5	-	0/18/34/34	0/3/3/3
6	FEO	E	501	2,7	-	0/0/0/0	0/0/0/0
6	FEO	F	501	2,7	-	0/0/0/0	0/0/0/0
6	FEO	G	501	2,7	-	0/0/0/0	0/0/0/0
6	FEO	H	501	2,7	-	0/0/0/0	0/0/0/0

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	803	DTP	O3'-C3'	-3.82	1.34	1.43
3	B	801	DTP	O3'-C3'	-3.79	1.34	1.43
3	D	803	DTP	O3'-C3'	-3.78	1.34	1.43
3	B	803	DTP	O3'-C3'	-3.74	1.35	1.43
3	A	801	DTP	O3'-C3'	-3.69	1.35	1.43

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	DAT	N3-C2-N1	-9.56	121.57	128.89
4	C	802	DAT	N3-C2-N1	-9.51	121.61	128.89
4	B	802	DAT	N3-C2-N1	-9.43	121.68	128.89
4	D	802	DAT	N3-C2-N1	-9.26	121.81	128.89
3	D	801	DTP	N3-C2-N1	-7.13	123.44	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	802	DAT	3	0
3	A	803	DTP	1	0
3	B	801	DTP	5	0
4	B	802	DAT	1	0
3	B	803	DTP	3	0
3	C	801	DTP	7	0
4	C	802	DAT	5	0
3	C	803	DTP	3	0
3	D	801	DTP	5	0
4	D	802	DAT	9	0
3	D	803	DTP	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	733/761 (96%)	-0.07	9 (1%) 81 72	56, 95, 121, 142	0
1	B	734/761 (96%)	-0.01	9 (1%) 81 72	59, 101, 127, 151	0
1	C	731/761 (96%)	0.21	29 (3%) 42 31	101, 130, 150, 160	0
1	D	733/761 (96%)	0.25	31 (4%) 40 29	89, 128, 151, 163	0
2	E	352/375 (93%)	0.06	11 (3%) 52 40	72, 117, 154, 176	0
2	F	356/375 (94%)	-0.11	5 (1%) 78 68	55, 91, 131, 158	0
2	G	356/375 (94%)	-0.07	3 (0%) 87 82	59, 97, 145, 192	0
2	H	356/375 (94%)	-0.04	8 (2%) 65 54	65, 98, 145, 174	0
All	All	4351/4544 (95%)	0.05	105 (2%) 62 50	55, 110, 146, 192	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	737	GLY	6.1
2	H	363	SER	4.5
1	D	298	ARG	3.9
1	D	297	VAL	3.4
1	D	617	SER	3.4

### 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 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	DAT	D	802	26/26	0.72	0.34	1.27	156,156,156,156	0
4	DAT	B	802	26/26	0.79	0.36	1.24	149,149,149,149	0
4	DAT	A	802	26/26	0.83	0.29	0.57	126,126,126,126	0
4	DAT	C	802	26/26	0.82	0.27	0.15	156,156,156,156	0
3	DTP	C	801	30/30	0.76	0.35	-0.22	175,175,175,175	0
3	DTP	D	801	30/30	0.82	0.36	-0.29	140,140,140,140	0
3	DTP	B	801	30/30	0.90	0.31	-0.32	111,111,111,111	0
3	DTP	A	801	30/30	0.91	0.22	-0.68	124,124,124,124	0
3	DTP	B	803	30/30	0.93	0.16	-0.94	94,94,94,94	0
3	DTP	C	803	30/30	0.93	0.16	-0.97	123,123,123,123	0
3	DTP	A	803	30/30	0.95	0.15	-1.07	94,94,94,94	0
3	DTP	D	803	30/30	0.94	0.15	-1.18	118,118,118,118	0
6	FEO	E	501	3/3	0.99	0.15	-1.42	89,89,89,89	0
6	FEO	G	501	3/3	0.96	0.18	-1.43	78,78,78,78	0
6	FEO	F	501	3/3	0.98	0.15	-1.47	61,61,61,61	0
6	FEO	H	501	3/3	0.97	0.14	-2.39	69,69,69,69	0
5	MG	D	804	1/1	0.92	0.28	-	118,118,118,118	0
5	MG	B	804	1/1	0.92	0.18	-	94,94,94,94	0
5	MG	C	804	1/1	0.97	0.13	-	123,123,123,123	0
5	MG	A	804	1/1	0.95	0.12	-	94,94,94,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.