



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 02:58 PM GMT

PDB ID : 2CVX  
Title : Structures of Yeast Ribonucleotide Reductase I  
Authors : Xu, H.; Faber, C.; Uchiki, T.; Fairman, J.W.; Racca, J.; Dealwis, C.  
Deposited on : 2005-06-14  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

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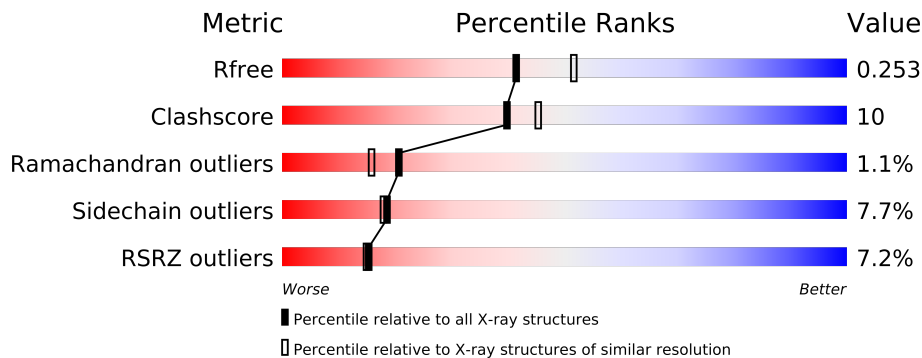
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	888	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	2001	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5580 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

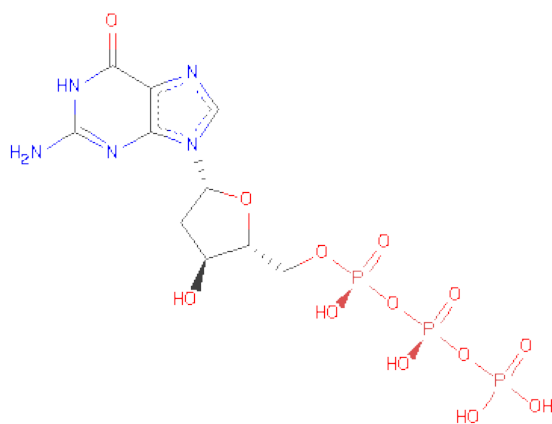
- Molecule 1 is a protein called Ribonucleoside-diphosphatereductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	664	5306	3379	903	993	31	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	5	13	3	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	27	10	5	10	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.69Å 117.28Å 65.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 33.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.20) 99.2 (33.86-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.61 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, $R_{free}$	0.210 , 0.254 0.210 , 0.253	Depositor DCC
$R_{free}$ test set	4235 reflections (11.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	1.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42423 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.59	0/5428	0.84	17/7348 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	GLU	OE1-CD-OE2	-10.99	110.11	123.30
1	A	503	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	A	182	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	707	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	138	ASP	CB-CG-OD2	6.58	124.23	118.30
1	A	327	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	287	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	503	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	438	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	365	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	586	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	100	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	459	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	648	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	170	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	140	ASP	CB-CG-OD2	5.04	122.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	GLU	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5306	0	5245	101	0
2	A	1	0	0	0	0
3	A	31	0	12	1	0
4	A	27	0	12	1	0
5	A	215	0	0	3	0
All	All	5580	0	5269	101	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (101) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:106:ASN:OD1	1:A:109:THR:HG22	1.55	1.06
1:A:534:GLN:O	1:A:538:THR:HG22	1.62	0.97
1:A:522:PRO:HG2	1:A:525:SER:HB3	1.44	0.96
1:A:538:THR:HB	1:A:583:TRP:HE1	1.41	0.83
1:A:538:THR:HB	1:A:583:TRP:NE1	1.96	0.79
1:A:686:THR:HG22	1:A:688:TRP:H	1.52	0.75
1:A:505:ILE:HG22	1:A:602:THR:HA	1.70	0.73
1:A:445:LEU:HD22	1:A:506:ALA:HB3	1.70	0.73
1:A:170:LEU:HD22	1:A:173:ARG:NH2	2.04	0.72
1:A:481:LEU:HB3	1:A:505:ILE:HG13	1.73	0.70
1:A:717:ARG:O	1:A:719:PRO:HD3	1.91	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:457:SER:HB3	1:A:462:THR:HG23	1.74	0.70
1:A:319:GLY:O	1:A:320:LYS:HB2	1.92	0.70
1:A:502:HIS:ND1	1:A:559:THR:HG21	2.09	0.67
1:A:485:ILE:HD11	1:A:505:ILE:HD13	1.77	0.67
1:A:508:GLY:HA3	1:A:606:MET:HE1	1.78	0.65
1:A:214:GLN:HE22	1:A:216:SER:HB2	1.61	0.65
1:A:334:ILE:HD12	1:A:404:VAL:HG13	1.80	0.64
1:A:520:ARG:HH22	1:A:648:ASP:CG	2.01	0.64
1:A:447:SER:HB3	1:A:606:MET:HE3	1.79	0.64
1:A:745:THR:O	1:A:746:GLN:HB2	1.99	0.63
1:A:481:LEU:HB3	1:A:505:ILE:CG1	2.30	0.61
1:A:251:HIS:HD2	5:A:2033:HOH:O	1.84	0.61
1:A:662:TYR:CD1	1:A:662:TYR:O	2.54	0.61
1:A:520:ARG:NH2	1:A:648:ASP:OD2	2.33	0.59
1:A:214:GLN:NE2	5:A:2173:HOH:O	2.31	0.59
1:A:428:CYS:SG	4:A:1002:ADP:H3'	2.44	0.57
1:A:686:THR:HG21	1:A:688:TRP:HD1	1.69	0.56
1:A:506:ALA:HB1	1:A:604:ALA:HB3	1.87	0.56
1:A:692:GLN:HB2	1:A:727:MET:SD	2.47	0.55
1:A:401:THR:HB	1:A:402:PRO:HA	1.89	0.55
1:A:589:ARG:O	1:A:593:MET:HG3	2.06	0.55
1:A:145:TYR:N	1:A:145:TYR:CD2	2.72	0.55
1:A:447:SER:HB3	1:A:606:MET:CE	2.37	0.54
1:A:683:LEU:HD23	1:A:684:TYR:CZ	2.43	0.53
1:A:383:ILE:HG13	1:A:384:LYS:H	1.75	0.52
1:A:109:THR:HG23	1:A:111:LYS:HB2	1.89	0.52
1:A:314:ILE:HG12	1:A:325:ALA:HB3	1.91	0.52
1:A:320:LYS:O	1:A:323:ILE:HG22	2.10	0.52
1:A:485:ILE:HD11	1:A:505:ILE:CD1	2.38	0.51
1:A:82:ALA:HA	1:A:85:ASN:HD22	1.75	0.51
1:A:606:MET:HE3	1:A:608:THR:HG22	1.92	0.51
1:A:332:LEU:HD11	1:A:392:ILE:HD12	1.91	0.51
1:A:610:SER:O	1:A:613:GLN:HB3	2.11	0.50
1:A:504:PRO:O	1:A:505:ILE:HD12	2.12	0.50
1:A:488:ASN:ND2	5:A:2173:HOH:O	2.31	0.50
1:A:388:LEU:HD22	1:A:392:ILE:HD11	1.93	0.50
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.47	0.49
1:A:356:ALA:HB1	1:A:374:TYR:CD1	2.47	0.49
1:A:86:LEU:HD22	1:A:148:PHE:HE1	1.78	0.48
1:A:388:LEU:O	1:A:392:ILE:HG12	2.12	0.48
1:A:393:LEU:HD22	1:A:724:LEU:HB3	1.95	0.48
1:A:251:HIS:HB3	1:A:424:SER:HB3	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:383:ILE:CG1	1:A:384:LYS:H	2.26	0.47
1:A:714:LEU:HD22	1:A:740:MET:HE3	1.96	0.47
1:A:126:GLU:CD	1:A:181:ARG:HH12	2.18	0.47
1:A:713:ASN:ND2	1:A:742:TYR:HB2	2.29	0.47
1:A:519:LEU:O	1:A:520:ARG:HB2	2.15	0.47
1:A:242:SER:O	1:A:288:GLN:HA	2.15	0.47
1:A:740:MET:SD	1:A:743:LEU:HB2	2.54	0.47
1:A:220:LEU:HD21	1:A:426:ASN:HB3	1.97	0.47
1:A:297:PHE:HB2	1:A:328:LEU:HD22	1.96	0.47
1:A:106:ASN:OD1	1:A:109:THR:CG2	2.44	0.46
1:A:606:MET:HE3	1:A:608:THR:CG2	2.46	0.45
1:A:220:LEU:CD2	1:A:426:ASN:HB3	2.47	0.45
1:A:86:LEU:HD22	1:A:148:PHE:CE1	2.51	0.45
1:A:594:LYS:O	1:A:594:LYS:HE3	2.17	0.45
1:A:383:ILE:HG13	1:A:384:LYS:N	2.32	0.45
1:A:475:LYS:O	1:A:479:ARG:HG3	2.16	0.45
1:A:179:HIS:ND1	1:A:483:ARG:NH1	2.65	0.45
1:A:692:GLN:NE2	1:A:715:PHE:H	2.15	0.44
1:A:273:ILE:HG21	1:A:323:ILE:HA	1.99	0.44
1:A:686:THR:CG2	1:A:688:TRP:HD1	2.31	0.44
1:A:210:THR:HB	1:A:211:PRO:CD	2.48	0.44
1:A:273:ILE:HB	1:A:274:PRO:HD3	2.00	0.44
1:A:338:PHE:O	1:A:342:VAL:HG23	2.17	0.43
1:A:79:ALA:C	1:A:81:ILE:H	2.21	0.43
1:A:109:THR:HG23	1:A:111:LYS:H	1.83	0.43
1:A:719:PRO:HG3	1:A:745:THR:OG1	2.19	0.43
1:A:264:GLY:HA3	3:A:1001:DGT:O2B	2.18	0.43
1:A:662:TYR:O	1:A:662:TYR:HD1	2.00	0.43
1:A:288:GLN:HG3	1:A:293:ARG:O	2.19	0.43
1:A:76:THR:HG23	1:A:77:LEU:H	1.83	0.42
1:A:432:VAL:CG1	1:A:708:GLN:HA	2.48	0.42
1:A:413:LYS:NZ	1:A:735:GLY:O	2.52	0.42
1:A:248:ILE:HD12	1:A:297:PHE:CE2	2.54	0.42
1:A:436:ALA:HB1	1:A:437:PRO:HD2	2.01	0.42
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.20	0.42
1:A:413:LYS:HE2	1:A:575:TRP:CE2	2.55	0.42
1:A:715:PHE:CE2	1:A:744:ARG:HG3	2.55	0.42
1:A:383:ILE:CG1	1:A:384:LYS:N	2.83	0.42
1:A:126:GLU:OE1	1:A:181:ARG:NH1	2.53	0.42
1:A:119:ASP:O	1:A:123:ILE:HG13	2.19	0.42
1:A:104:TYR:CD1	1:A:159:ILE:HG23	2.55	0.42
1:A:524:ASP:HB3	1:A:694:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:178:ILE:O	1:A:487:ARG:HD3	2.20	0.41
1:A:557:TYR:CD1	1:A:559:THR:HG22	2.56	0.41
1:A:714:LEU:HD22	1:A:740:MET:CE	2.51	0.41
1:A:450:LEU:N	1:A:451:PRO:CD	2.84	0.41
1:A:120:VAL:O	1:A:124:VAL:HG23	2.21	0.40
1:A:128:LYS:O	1:A:132:ASN:HB2	2.21	0.40

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	660/888 (74%)	624 (94%)	29 (4%)	7 (1%)	21	16

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	LYS
1	A	458	GLU
1	A	459	ASP
1	A	80	ARG
1	A	674	PRO
1	A	741	TYR
1	A	620	CYS

### 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	575/761 (76%)	531 (92%)	44 (8%)	18	18

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	TYR
1	A	154	SER
1	A	170	LEU
1	A	176	LEU
1	A	187	LEU
1	A	214	GLN
1	A	220	LEU
1	A	268	THR
1	A	277	ARG
1	A	293	ARG
1	A	301	LEU
1	A	314	ILE
1	A	317	ASN
1	A	318	HIS
1	A	320	LYS
1	A	323	ILE
1	A	324	ARG
1	A	337	LEU
1	A	359	LEU
1	A	388	LEU
1	A	390	TYR
1	A	443	CYS
1	A	456	THR
1	A	473	ILE
1	A	503	ARG
1	A	505	ILE
1	A	512	LEU
1	A	514	ASP
1	A	518	LEU
1	A	520	ARG
1	A	530	LEU
1	A	538	THR
1	A	594	LYS
1	A	606	MET
1	A	628	MET
1	A	639	GLN
1	A	641	VAL
1	A	673	LEU

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Mol	Chain	Res	Type
1	A	679	GLU
1	A	696	ILE
1	A	712	LEU
1	A	724	LEU
1	A	743	LEU
1	A	745	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	89	GLN
1	A	127	ASN
1	A	168	GLN
1	A	214	GLN
1	A	251	HIS
1	A	266	ASN
1	A	270	ASN
1	A	317	ASN
1	A	534	GLN
1	A	561	GLN
1	A	613	GLN
1	A	692	GLN
1	A	710	HIS
1	A	713	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	DGT	A	1001	2	33,33,33	1.14	1 (3%)	49,52,52	2.94	5 (10%)
4	ADP	A	1002	-	29,29,29	1.23	2 (6%)	45,45,45	1.74	6 (13%)

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	DGT	A	1001	2	-	0/20/34/34	0/1/3/3
4	ADP	A	1002	-	-	0/16/32/32	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	DGT	C2-N3	4.75	1.39	1.33
4	A	1002	ADP	C4-N9	-3.48	1.32	1.37
4	A	1002	ADP	C5-C4	3.22	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	DGT	C6-C5-N7	-18.63	131.63	134.14
4	A	1002	ADP	N3-C2-N1	-6.66	123.14	128.71
4	A	1002	ADP	N3-C4-N9	4.39	133.35	125.43
3	A	1001	DGT	N3-C4-N9	4.15	133.00	126.91
4	A	1002	ADP	C4-C5-N7	-3.82	106.25	109.52
3	A	1001	DGT	C5-C4-N3	-3.77	120.48	125.94
3	A	1001	DGT	C2-N3-C4	3.62	120.17	115.09
4	A	1002	ADP	C5-C4-N3	-2.97	119.24	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ADP	C2-N3-C4	2.62	121.48	114.01
4	A	1002	ADP	C3'-C2'-C1'	2.36	104.61	100.91
3	A	1001	DGT	O1B-PB-O3A	2.25	115.79	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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	664/888 (74%)	0.36	48 (7%) 15 15	22, 38, 76, 98	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	458	GLU	7.0
1	A	145	TYR	6.9
1	A	665	THR	5.8
1	A	457	SER	5.4
1	A	459	ASP	5.4
1	A	638	PHE	5.4
1	A	77	LEU	5.3
1	A	76	THR	5.2
1	A	664	ILE	5.2
1	A	146	PHE	4.7
1	A	390	TYR	4.5
1	A	630	SER	4.5
1	A	81	ILE	4.4
1	A	78	ALA	4.4
1	A	461	LYS	4.4
1	A	80	ARG	4.1
1	A	628	MET	4.0
1	A	456	THR	3.8
1	A	639	GLN	3.8
1	A	79	ALA	3.6
1	A	746	GLN	3.6
1	A	159	ILE	3.5
1	A	319	GLY	3.5
1	A	462	THR	3.4
1	A	647	ARG	3.3
1	A	89	GLN	3.3
1	A	656	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	662	TYR	3.2
1	A	717	ARG	3.2
1	A	489	TYR	3.2
1	A	654	ILE	3.0
1	A	718	ALA	2.8
1	A	667	ASN	2.8
1	A	629	TYR	2.7
1	A	658	GLY	2.7
1	A	153	ARG	2.6
1	A	88	LYS	2.4
1	A	446	ALA	2.4
1	A	652	LEU	2.4
1	A	655	TRP	2.4
1	A	201	ALA	2.3
1	A	723	LYS	2.3
1	A	657	GLU	2.2
1	A	745	THR	2.2
1	A	604	ALA	2.2
1	A	675	ASN	2.1
1	A	82	ALA	2.1
1	A	318	HIS	2.1

## 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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	2001	1/1	0.29	4.24	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ADP	A	1002	27/27	0.11	-0.77	36,40,41,43	0
3	DGT	A	1001	31/31	0.08	-0.98	21,27,30,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.