



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:58 PM GMT

PDB ID : 2CVW  
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 : 2.40 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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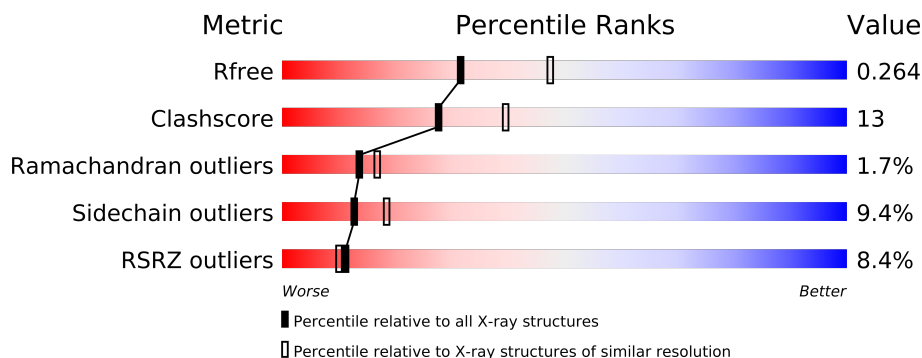
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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  $\geq 3$ , 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	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5374 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.

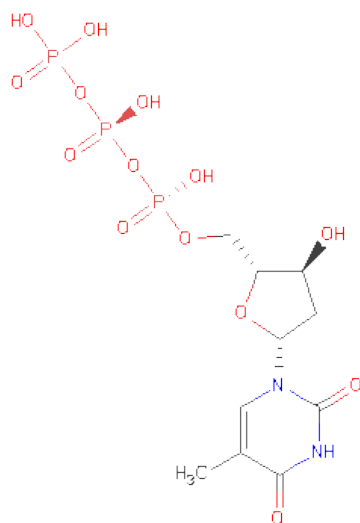
- Molecule 1 is a protein called Ribonucleoside-diphosphatereductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	0
			5192	3308	880	973	31			

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

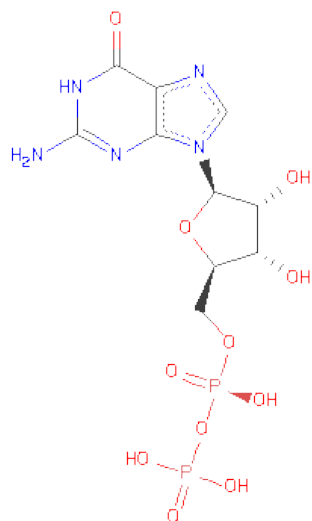
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>2</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	28	10	5	11	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total	O	0	0
			124	124		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.53Å 117.39Å 64.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 48.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.40) 98.2 (48.88-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, $R_{free}$	0.204 , 0.266 0.204 , 0.264	Depositor DCC
$R_{free}$ test set	3244 reflections (11.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 34.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 32263 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: GDP, MG, TTP

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	0.69	0/5313	0.90	18/7192 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	226	ASP	CB-CG-OD2	8.81	126.23	118.30
1	A	586	ASP	CB-CG-OD2	7.47	125.02	118.30
1	A	438	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	138	ASP	CB-CG-OD2	6.43	124.08	118.30
1	A	119	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	287	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	100	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	707	ASP	CB-CG-OD2	5.93	123.63	118.30
1	A	182	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	503	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	365	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	727	MET	CG-SD-CE	5.30	108.68	100.20
1	A	514	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	656	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	651	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	118	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	576	ASP	CB-CG-OD2	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	5192	0	5120	131	0
2	A	1	0	0	0	0
3	A	29	0	13	3	0
4	A	28	0	12	3	0
5	A	124	0	0	6	0
All	All	5374	0	5145	133	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 13.

All (133) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:746:GLN:HE21	1:A:746:GLN:HA	1.12	1.11
1:A:522:PRO:HG2	1:A:525:SER:HB3	1.44	1.00
1:A:746:GLN:NE2	1:A:746:GLN:HA	1.84	0.92
1:A:693:LYS:H	1:A:693:LYS:CD	1.86	0.88
1:A:432:VAL:H	1:A:708:GLN:HE21	1.22	0.87
1:A:277:ARG:HD2	1:A:322:GLU:O	1.73	0.87
1:A:693:LYS:H	1:A:693:LYS:HD3	1.41	0.83
1:A:538:THR:HB	1:A:583:TRP:NE1	1.96	0.80
1:A:106:ASN:OD1	1:A:109:THR:HG22	1.85	0.77
1:A:319:GLY:HA2	1:A:324:ARG:NH1	2.01	0.75
1:A:483:ARG:HH22	1:A:487:ARG:HD2	1.52	0.73
1:A:319:GLY:HA2	1:A:324:ARG:HH11	1.53	0.73
1:A:320:LYS:HB3	1:A:323:ILE:HG13	1.72	0.71
1:A:432:VAL:H	1:A:708:GLN:NE2	1.90	0.70
1:A:588:LEU:O	1:A:592:ILE:HG12	1.92	0.69
1:A:140:ASP:OD2	1:A:168:GLN:HG2	1.92	0.69
1:A:383:ILE:HD11	1:A:387:LYS:HD3	1.76	0.68
1:A:401:THR:HB	1:A:402:PRO:HA	1.76	0.68
1:A:606:MET:HE3	1:A:608:THR:HG22	1.77	0.67
1:A:211:PRO:O	1:A:213:PRO:HD3	1.93	0.66
1:A:109:THR:HG23	1:A:111:LYS:HB2	1.77	0.66
1:A:297:PHE:HB2	1:A:328:LEU:HD22	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:746:GLN:CA	1:A:746:GLN:HE21	1.99	0.66
1:A:693:LYS:N	1:A:693:LYS:CD	2.57	0.66
1:A:686:THR:CG2	1:A:688:TRP:HD1	2.09	0.66
1:A:518:LEU:HD21	1:A:644:TYR:CE2	2.32	0.65
1:A:520:ARG:HH22	1:A:648:ASP:CG	2.00	0.65
1:A:534:GLN:O	1:A:538:THR:HG22	1.97	0.65
1:A:214:GLN:HE22	1:A:216:SER:HB2	1.62	0.65
1:A:691:SER:HB3	1:A:694:THR:OG1	1.98	0.62
1:A:481:LEU:HB3	1:A:505:ILE:HD12	1.82	0.61
1:A:483:ARG:NH2	1:A:487:ARG:HD2	2.16	0.61
1:A:538:THR:HB	1:A:583:TRP:HE1	1.62	0.60
1:A:270:ASN:HB3	1:A:274:PRO:HG2	1.83	0.60
1:A:251:HIS:HD2	5:A:2019:HOH:O	1.86	0.58
1:A:475:LYS:O	1:A:479:ARG:HG3	2.03	0.58
1:A:606:MET:HE3	1:A:608:THR:CG2	2.32	0.58
1:A:431:ILE:HG23	1:A:708:GLN:HE22	1.68	0.58
1:A:127:ASN:HB2	1:A:131:LEU:HD22	1.85	0.57
1:A:101:LEU:CB	1:A:116:ILE:HD12	2.36	0.56
1:A:697:ASN:OD1	1:A:734:LYS:NZ	2.24	0.56
1:A:383:ILE:CD1	1:A:387:LYS:HD3	2.36	0.56
1:A:92:LYS:HG3	1:A:166:ARG:NH1	2.20	0.56
1:A:445:LEU:HD23	1:A:606:MET:HG3	1.87	0.56
1:A:534:GLN:O	1:A:538:THR:CG2	2.55	0.55
1:A:428:CYS:SG	4:A:1002:GDP:H3'	2.46	0.55
1:A:101:LEU:HB2	1:A:116:ILE:HD12	1.88	0.54
1:A:293:ARG:N	1:A:294:PRO:HD3	2.22	0.54
1:A:297:PHE:HB2	1:A:328:LEU:CD2	2.38	0.53
1:A:686:THR:CG2	1:A:688:TRP:CD1	2.91	0.53
1:A:717:ARG:O	1:A:719:PRO:HD3	2.08	0.52
1:A:210:THR:HB	1:A:211:PRO:HD2	1.92	0.52
1:A:214:GLN:HE21	1:A:488:ASN:HD21	1.58	0.52
1:A:332:LEU:HD11	1:A:392:ILE:HD12	1.92	0.52
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.44	0.52
1:A:630:SER:HB3	1:A:638:PHE:O	2.10	0.51
1:A:101:LEU:HB2	1:A:116:ILE:CD1	2.41	0.51
1:A:608:THR:N	4:A:1002:GDP:O2A	2.44	0.51
1:A:92:LYS:HG3	1:A:166:ARG:HH12	1.74	0.51
1:A:325:ALA:HB1	1:A:328:LEU:HD12	1.93	0.51
1:A:520:ARG:NH2	1:A:648:ASP:OD1	2.43	0.51
1:A:273:ILE:HB	1:A:274:PRO:HD3	1.92	0.51
1:A:702:ARG:HH11	1:A:710:HIS:CE1	2.30	0.50
1:A:654:ILE:O	1:A:659:MET:HG3	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:589:ARG:O	1:A:593:MET:HG3	2.12	0.49
1:A:256:ARG:HG2	1:A:260:SER:CB	2.43	0.49
1:A:701:ASP:O	1:A:704:VAL:HG22	2.13	0.49
1:A:569:ILE:HG22	1:A:574:MET:HG3	1.94	0.48
1:A:104:TYR:CD1	1:A:159:ILE:HG23	2.48	0.48
1:A:92:LYS:HA	1:A:166:ARG:CZ	2.43	0.48
1:A:480:ASN:O	1:A:484:VAL:HG23	2.14	0.48
1:A:277:ARG:NH1	5:A:2028:HOH:O	2.46	0.48
1:A:264:GLY:O	1:A:265:THR:HB	2.14	0.48
1:A:277:ARG:CD	1:A:322:GLU:O	2.54	0.47
1:A:165:GLU:HG2	1:A:169:HIS:HB2	1.97	0.47
1:A:153:ARG:HH11	1:A:153:ARG:HG3	1.80	0.47
1:A:606:MET:CE	1:A:608:THR:CG2	2.93	0.47
1:A:388:LEU:O	1:A:392:ILE:HG12	2.15	0.47
1:A:256:ARG:HG2	1:A:260:SER:HB2	1.97	0.46
1:A:524:ASP:OD1	1:A:524:ASP:N	2.45	0.46
1:A:665:THR:HG22	1:A:666:GLN:NE2	2.31	0.46
1:A:91:THR:HG21	1:A:96:LYS:HB3	1.97	0.46
1:A:529:ARG:HB2	5:A:2052:HOH:O	2.15	0.46
1:A:116:ILE:HG22	1:A:117:SER:O	2.15	0.46
1:A:219:PHE:HA	1:A:441:ALA:O	2.16	0.46
1:A:486:ASP:CG	1:A:503:ARG:HH22	2.19	0.45
1:A:456:THR:HA	1:A:463:SER:HA	1.97	0.45
1:A:648:ASP:HB3	1:A:680:LEU:HD11	1.99	0.45
1:A:509:VAL:O	1:A:620:CYS:HA	2.16	0.45
1:A:326:ARG:HB2	5:A:2050:HOH:O	2.18	0.44
1:A:506:ALA:HB1	1:A:604:ALA:HB3	1.98	0.44
1:A:551:ALA:HB2	1:A:597:VAL:C	2.38	0.44
1:A:714:LEU:HB2	1:A:740:MET:HE2	1.99	0.44
1:A:686:THR:HG23	1:A:688:TRP:HD1	1.80	0.44
3:A:1001:TTP:O1B	3:A:1001:TTP:O1A	2.35	0.44
1:A:214:GLN:HE22	1:A:216:SER:CB	2.29	0.44
1:A:172:MET:O	1:A:176:LEU:HD22	2.18	0.43
1:A:693:LYS:H	1:A:693:LYS:HD2	1.77	0.43
1:A:530:LEU:O	1:A:534:GLN:HG3	2.18	0.43
1:A:106:ASN:HB3	1:A:109:THR:HG22	2.00	0.43
4:A:1002:GDP:PB	5:A:2053:HOH:O	2.76	0.43
1:A:521:LEU:HA	1:A:522:PRO:HD2	1.92	0.43
1:A:702:ARG:HH11	1:A:710:HIS:HE1	1.66	0.43
1:A:630:SER:HB3	1:A:639:GLN:HA	2.00	0.43
1:A:256:ARG:CZ	3:A:1001:TTP:H5'2	2.48	0.43
1:A:220:LEU:N	1:A:220:LEU:HD23	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:256:ARG:NH1	3:A:1001:TTP:O3G	2.38	0.43
1:A:251:HIS:HB3	1:A:424:SER:HB3	2.01	0.43
1:A:393:LEU:HD22	1:A:724:LEU:HG	2.01	0.43
1:A:447:SER:HB3	1:A:606:MET:HE3	2.01	0.42
1:A:227:SER:O	1:A:231:ILE:HD12	2.19	0.42
1:A:514:ASP:O	1:A:518:LEU:HD23	2.20	0.42
1:A:101:LEU:HB3	1:A:116:ILE:HD12	2.01	0.42
1:A:306:ALA:HA	1:A:350:LEU:HB3	2.01	0.42
1:A:106:ASN:OD1	1:A:109:THR:CG2	2.63	0.42
1:A:447:SER:HB3	1:A:606:MET:CE	2.50	0.42
1:A:608:THR:C	5:A:2053:HOH:O	2.58	0.42
1:A:475:LYS:HB3	1:A:546:ALA:HB2	2.01	0.42
1:A:486:ASP:OD2	1:A:503:ARG:NH2	2.49	0.42
1:A:686:THR:HG21	1:A:688:TRP:HD1	1.84	0.42
1:A:98:VAL:HG13	1:A:116:ILE:HD13	2.01	0.41
1:A:723:LYS:HA	1:A:723:LYS:HD2	1.88	0.41
1:A:220:LEU:HD22	1:A:426:ASN:HB3	2.02	0.41
1:A:240:LEU:O	1:A:243:LYS:HB2	2.21	0.41
1:A:625:THR:HA	1:A:687:VAL:HG12	2.03	0.41
1:A:673:LEU:HA	1:A:674:PRO:HD2	1.90	0.41
1:A:220:LEU:HG	1:A:441:ALA:HB3	2.02	0.41
1:A:641:VAL:O	1:A:642:ASN:C	2.59	0.41
1:A:388:LEU:HD22	1:A:392:ILE:HD11	2.02	0.40
1:A:606:MET:CE	1:A:608:THR:HG23	2.52	0.40
1:A:314:ILE:HG12	1:A:325:ALA:HB3	2.02	0.40
1:A:686:THR:HB	1:A:689:GLU:OE1	2.20	0.40
1:A:196:LYS:HG2	1:A:615:LEU:HD22	2.04	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	645/888 (73%)	594 (92%)	40 (6%)	11 (2%)	14 17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	ASP
1	A	457	SER
1	A	461	LYS
1	A	654	ILE
1	A	707	ASP
1	A	458	GLU
1	A	321	GLU
1	A	674	PRO
1	A	620	CYS
1	A	293	ARG
1	A	629	TYR

### 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	563/761 (74%)	510 (91%)	53 (9%)	13	18

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	131	LEU
1	A	138	ASP
1	A	146	PHE
1	A	153	ARG
1	A	154	SER
1	A	176	LEU
1	A	187	LEU
1	A	195	LEU
1	A	212	LYS
1	A	214	GLN
1	A	220	LEU
1	A	243	LYS
1	A	256	ARG
1	A	292	LYS
1	A	293	ARG

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Mol	Chain	Res	Type
1	A	301	LEU
1	A	314	ILE
1	A	317	ASN
1	A	321	GLU
1	A	326	ARG
1	A	337	LEU
1	A	345	ASN
1	A	359	LEU
1	A	388	LEU
1	A	443	CYS
1	A	459	ASP
1	A	461	LYS
1	A	464	THR
1	A	475	LYS
1	A	505	ILE
1	A	512	LEU
1	A	538	THR
1	A	578	LYS
1	A	606	MET
1	A	610	SER
1	A	630	SER
1	A	639	GLN
1	A	641	VAL
1	A	659	MET
1	A	664	ILE
1	A	666	GLN
1	A	670	ILE
1	A	675	ASN
1	A	680	LEU
1	A	686	THR
1	A	693	LYS
1	A	694	THR
1	A	712	LEU
1	A	714	LEU
1	A	743	LEU
1	A	745	THR
1	A	746	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN

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Mol	Chain	Res	Type
1	A	127	ASN
1	A	168	GLN
1	A	214	GLN
1	A	251	HIS
1	A	345	ASN
1	A	661	GLN
1	A	666	GLN
1	A	692	GLN
1	A	708	GLN
1	A	710	HIS
1	A	713	ASN
1	A	746	GLN

### 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	TTP	A	1001	2	30,30,30	1.25	3 (10%)	42,47,47	1.84	6 (14%)
4	GDP	A	1002	-	30,30,30	1.44	5 (16%)	44,47,47	2.54	12 (27%)

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	TTP	A	1001	2	-	0/19/34/34	0/2/2/2
4	GDP	A	1002	-	-	0/16/32/32	0/1/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	GDP	C6-C5	4.44	1.48	1.41
3	A	1001	TTP	C2-N1	3.58	1.42	1.38
4	A	1002	GDP	C5-C4	3.36	1.48	1.40
3	A	1001	TTP	C4-C5	3.22	1.49	1.42
3	A	1001	TTP	PB-O3B	2.76	1.64	1.59
4	A	1002	GDP	C4-N9	-2.59	1.34	1.37
4	A	1002	GDP	C2-N3	2.55	1.36	1.33
4	A	1002	GDP	C2-N2	2.28	1.35	1.32

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	GDP	C6-C5-N7	11.49	135.69	134.14
3	A	1001	TTP	PB-O3A-PA	-5.56	115.37	131.68
3	A	1001	TTP	N3-C2-N1	5.48	120.55	115.97
4	A	1002	GDP	N3-C4-N9	5.31	134.70	126.91
3	A	1001	TTP	C6-N1-C2	-5.25	120.91	122.41
4	A	1002	GDP	C5-C4-N3	-4.47	119.47	125.94
4	A	1002	GDP	O4'-C1'-N9	4.31	112.45	108.44
4	A	1002	GDP	C2-N3-C4	4.09	120.84	115.09
3	A	1001	TTP	PB-O3B-PG	-4.02	119.88	131.68
4	A	1002	GDP	C2'-C1'-N9	-3.15	105.17	113.27
4	A	1002	GDP	C8-N9-C4	2.71	108.97	106.90
4	A	1002	GDP	C4-C5-N7	-2.62	107.28	109.52
4	A	1002	GDP	N2-C2-N3	-2.44	117.00	120.30
3	A	1001	TTP	O3G-PG-O3B	2.28	115.98	105.14
4	A	1002	GDP	N2-C2-N1	2.22	120.30	117.86
4	A	1002	GDP	C3'-C2'-C1'	2.11	104.20	100.91
3	A	1001	TTP	O3B-PB-O3A	-2.06	97.48	101.66
4	A	1002	GDP	C1'-N9-C4	-2.00	123.18	126.64

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	649/888 (73%)	0.40	55 (8%) 11 10	25, 40, 75, 89	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	ILE	8.6
1	A	638	PHE	7.5
1	A	457	SER	6.4
1	A	320	LYS	6.4
1	A	266	ASN	6.2
1	A	294	PRO	6.2
1	A	458	GLU	6.2
1	A	460	GLY	6.0
1	A	629	TYR	5.9
1	A	461	LYS	5.8
1	A	145	TYR	5.4
1	A	290	GLY	5.3
1	A	319	GLY	5.3
1	A	292	LYS	5.1
1	A	390	TYR	5.0
1	A	655	TRP	4.7
1	A	141	PHE	4.6
1	A	630	SER	4.5
1	A	321	GLU	4.3
1	A	146	PHE	4.2
1	A	91	THR	4.2
1	A	639	GLN	4.1
1	A	318	HIS	4.0
1	A	654	ILE	3.9
1	A	291	ASN	3.7
1	A	659	MET	3.7
1	A	96	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	459	ASP	3.4
1	A	429	CYS	3.3
1	A	428	CYS	3.3
1	A	456	THR	3.3
1	A	326	ARG	3.1
1	A	427	LEU	3.1
1	A	462	THR	3.0
1	A	646	LEU	3.0
1	A	647	ARG	3.0
1	A	746	GLN	3.0
1	A	317	ASN	2.9
1	A	649	LEU	2.8
1	A	426	ASN	2.7
1	A	718	ALA	2.7
1	A	298	ALA	2.7
1	A	652	LEU	2.7
1	A	431	ILE	2.7
1	A	663	LEU	2.7
1	A	620	CYS	2.6
1	A	662	TYR	2.6
1	A	661	GLN	2.3
1	A	249	GLY	2.3
1	A	711	SER	2.2
1	A	296	ALA	2.2
1	A	425	SER	2.2
1	A	322	GLU	2.2
1	A	717	ARG	2.2
1	A	247	GLY	2.0

## 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	0.12	-0.41	54,54,54,54	0
4	GDP	A	1002	28/28	0.19	-0.56	36,46,48,48	0
3	TTP	A	1001	29/29	0.13	-0.90	30,40,58,59	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.