Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:23 AM 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)

The following versions of software and data (see references (i)) 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
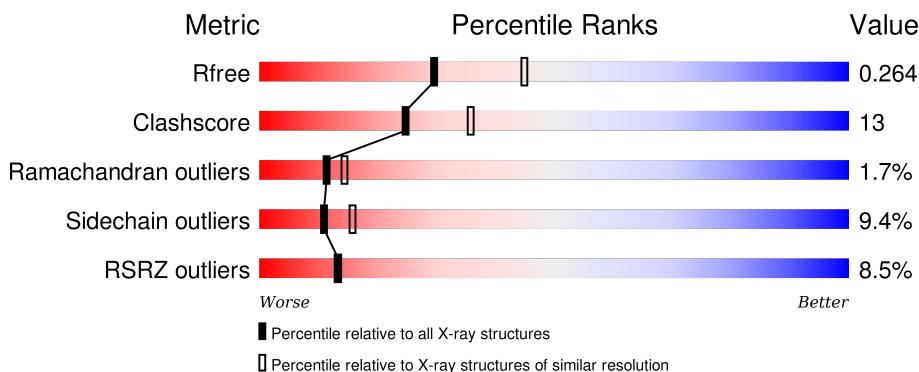
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	Percentile Ranks	Value
Rfree		0.264
Clashscore		13
Ramachandran outliers		1.7%
Sidechain outliers		9.4%
RSRZ outliers		8.5%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 >=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 <=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	888	6% 51% 18% • 27%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5374 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.
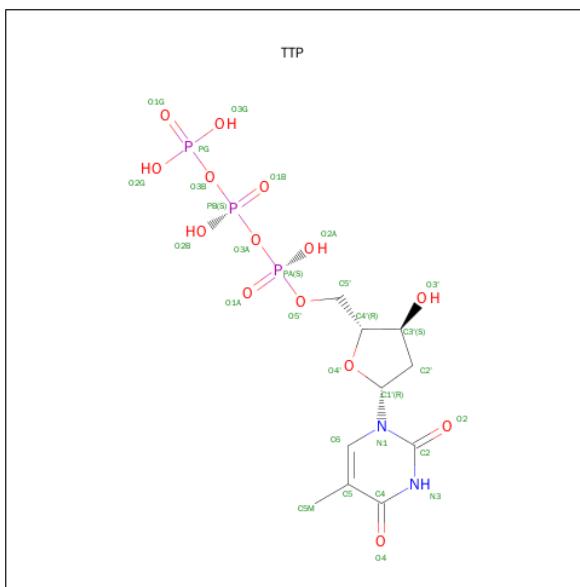
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

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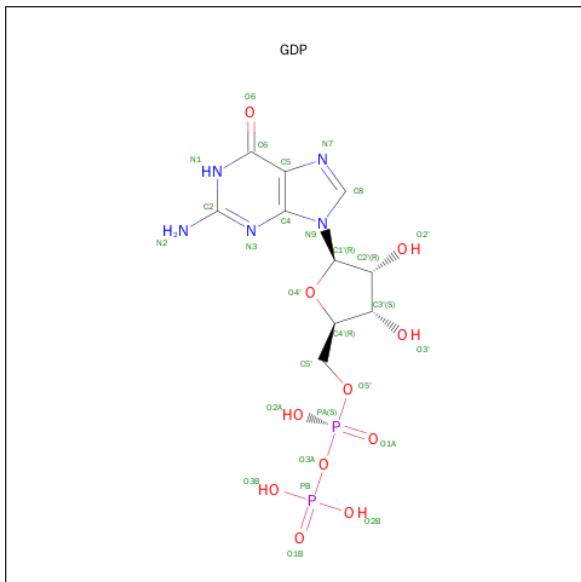
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).

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
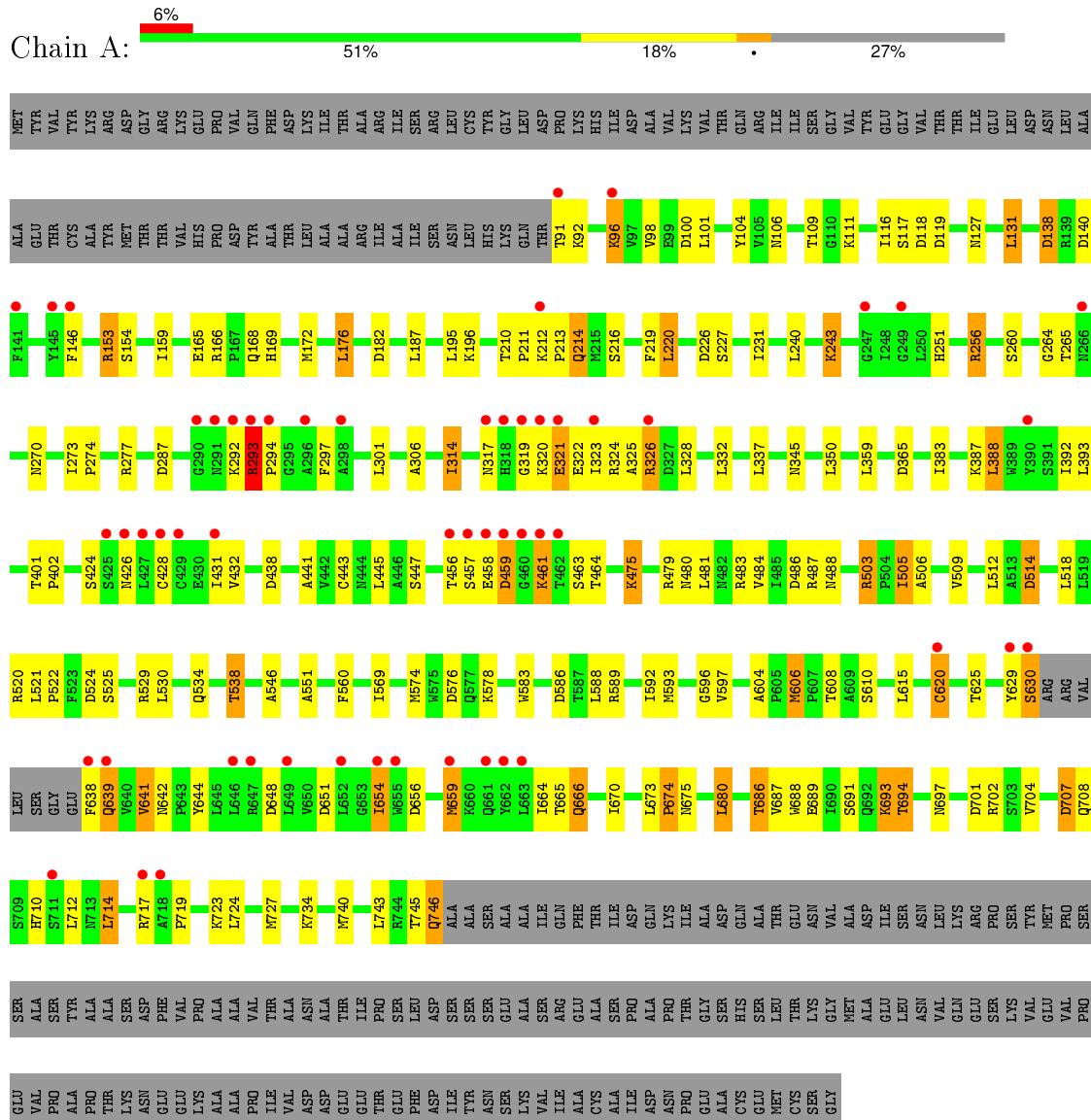
- Molecule 5 is water.

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

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 large chain 1

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	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) 98.1 (48.88-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	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	3242 reflections (11.18%)	DCC
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	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^2)	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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	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

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.

All (133) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ILE:O	1:A:659:MET:HG3	2.11	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	645/888 (73%)	594 (92%)	40 (6%)	11 (2%)	11 14

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 (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	563/761 (74%)	510 (91%)	53 (9%)	11 16

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

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Mol	Chain	Res	Type
1	A	214	GLN
1	A	220	LEU
1	A	243	LYS
1	A	256	ARG
1	A	292	LYS
1	A	293	ARG
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

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Mol	Chain	Res	Type
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
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 (i)

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 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	21,30,30	0.75	0	31,47,47	2.39	5 (16%)
4	GDP	A	1002	-	23,30,30	1.30	2 (8%)	30,47,47	2.02	8 (26%)

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	-	0/18/34/34	0/2/2/2
4	GDP	A	1002	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	GDP	C5-C4	3.36	1.48	1.40
4	A	1002	GDP	C6-C5	3.61	1.48	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	TTP	C5-C4-N3	-6.36	118.06	125.14
3	A	1001	TTP	PB-O3A-PA	-6.18	115.37	132.73
4	A	1002	GDP	C2'-C1'-N9	-5.97	105.17	114.29
3	A	1001	TTP	PB-O3B-PG	-3.81	119.88	132.67
4	A	1002	GDP	C5-C6-N1	-3.76	118.45	123.59
4	A	1002	GDP	C6-C5-C4	-3.24	117.03	120.90
4	A	1002	GDP	N3-C2-N1	-3.11	122.70	127.44
4	A	1002	GDP	C1'-N9-C4	-2.50	123.18	126.94
4	A	1002	GDP	C4-C5-N7	-2.39	107.28	109.48
4	A	1002	GDP	O4'-C1'-N9	2.08	112.45	108.10
3	A	1001	TTP	O3G-PG-O3B	2.40	115.98	105.09
4	A	1002	GDP	C6-N1-C2	4.01	121.51	115.94
3	A	1001	TTP	C4-N3-C2	7.44	121.67	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	TTP	3	0
4	A	1002	GDP	3	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 (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	649/888 (73%)	0.29	55 (8%)	13	13	25, 40, 75, 89	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	ILE	7.4
1	A	457	SER	7.1
1	A	458	GLU	6.5
1	A	638	PHE	6.5
1	A	629	TYR	6.4
1	A	290	GLY	5.8
1	A	294	PRO	5.5
1	A	320	LYS	5.5
1	A	460	GLY	5.0
1	A	321	GLU	4.9
1	A	319	GLY	4.8
1	A	266	ASN	4.6
1	A	145	TYR	4.5
1	A	292	LYS	4.5
1	A	318	HIS	4.3
1	A	390	TYR	4.1
1	A	146	PHE	4.1
1	A	630	SER	4.0
1	A	654	ILE	4.0
1	A	291	ASN	3.8
1	A	141	PHE	3.8
1	A	461	LYS	3.7
1	A	655	TRP	3.7
1	A	91	THR	3.6
1	A	659	MET	3.6
1	A	459	ASP	3.5
1	A	639	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	427	LEU	3.1
1	A	317	ASN	3.0
1	A	652	LEU	3.0
1	A	326	ARG	3.0
1	A	428	CYS	2.9
1	A	298	ALA	2.9
1	A	429	CYS	2.8
1	A	456	THR	2.7
1	A	662	TYR	2.7
1	A	431	ILE	2.6
1	A	663	LEU	2.6
1	A	661	GLN	2.6
1	A	647	ARG	2.6
1	A	426	ASN	2.6
1	A	649	LEU	2.5
1	A	249	GLY	2.5
1	A	620	CYS	2.5
1	A	96	LYS	2.4
1	A	462	THR	2.4
1	A	646	LEU	2.3
1	A	212	LYS	2.3
1	A	425	SER	2.2
1	A	247	GLY	2.1
1	A	711	SER	2.1
1	A	293	ARG	2.1
1	A	717	ARG	2.0
1	A	718	ALA	2.0
1	A	296	ALA	2.0

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($Å^2$)	Q<0.9
4	GDP	A	1002	28/28	0.96	0.18	-0.68	36,46,48,48	0
3	TTP	A	1001	29/29	0.93	0.13	-0.94	30,40,58,59	0
2	MG	A	2001	1/1	0.96	0.10	-	54,54,54,54	0

6.5　Other polymers (i)

There are no such residues in this entry.