



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:33 PM UTC

PDB ID : 3S87 / pdb_00003s87
Title : Structure of Yeast Ribonucleotide Reductase 1 with dGTP and ADP
Authors : Ahmad, M.F.; Kaushal, P.S.; Wan, Q.; Wijeratna, S.R.; Huang, M.; Dealwis, C.D.
Deposited on : 2011-05-27
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

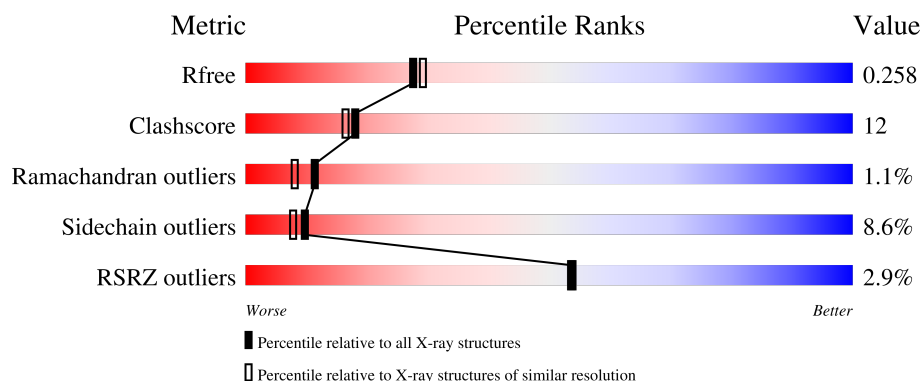
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	888	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5544 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.

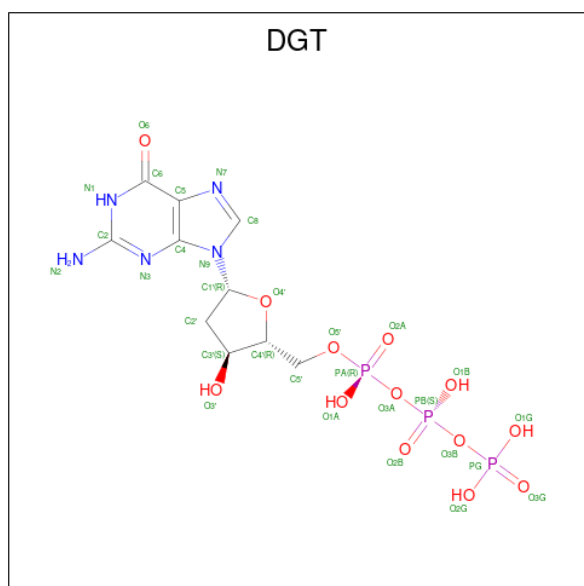
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	664	5283	3362	897	993	31	0	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

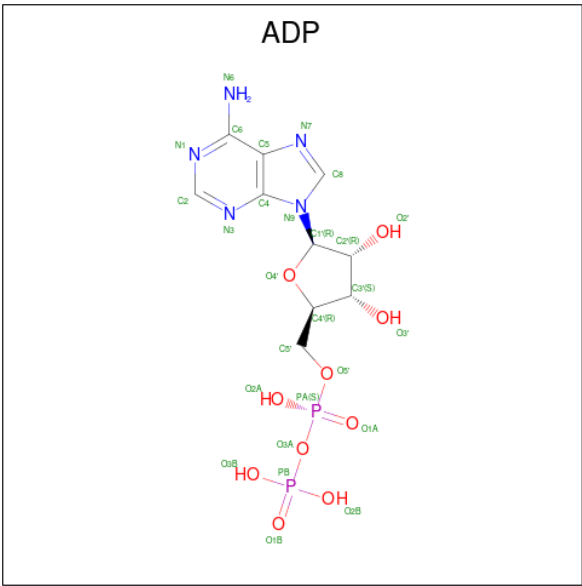
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	202	Total	O	0	0
			202	202		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.62Å 117.19Å 65.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.25) 99.5 (20.00-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.204 , 0.261 0.208 , 0.258	Depositor DCC
R_{free} test set	4022 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5544	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: DGT, MG, ADP

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	0.86	1/5404 (0.0%)	1.03	13/7320 (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	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	708	GLN	N-CA	-7.85	1.41	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ILE	N-CA-C	10.17	118.03	107.76
1	A	246	GLY	N-CA-C	8.11	122.93	112.54
1	A	319	GLY	N-CA-C	7.84	120.96	112.33
1	A	460	GLY	N-CA-C	-5.99	102.65	111.03
1	A	211	PRO	CA-C-N	-5.54	115.32	123.30
1	A	211	PRO	C-N-CA	-5.54	115.32	123.30
1	A	302	GLU	CA-C-N	5.53	125.24	119.82
1	A	302	GLU	C-N-CA	5.53	125.24	119.82
1	A	432	VAL	CB-CA-C	5.38	117.06	111.09
1	A	245	ALA	N-CA-C	5.22	121.92	110.80
1	A	206	PHE	CB-CA-C	-5.09	102.35	110.79
1	A	673	LEU	CA-C-N	5.08	126.19	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	LEU	C-N-CA	5.08	126.19	119.84

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	HIS	Peptide
1	A	459	ASP	Peptide
1	A	460	GLY	Peptide
1	A	461	LYS	Peptide
1	A	706	ILE	Peptide

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	5283	0	5194	129	0
2	A	1	0	0	0	0
3	A	31	0	12	0	0
4	A	27	0	12	1	0
5	A	202	0	0	16	0
All	All	5544	0	5218	129	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 12.

All (129) 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:106:ASN:OD1	1:A:109:THR:HG22	1.54	1.08
1:A:706:ILE:HG13	5:A:965:HOH:O	1.59	1.01
1:A:445:LEU:HD22	1:A:506:ALA:HB3	1.54	0.90
1:A:393:LEU:HD22	1:A:724:LEU:HD13	1.55	0.87
1:A:686:THR:HG22	1:A:688:TRP:H	1.41	0.83
1:A:710:HIS:HD2	5:A:1092:HOH:O	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:ILE:CD1	5:A:965:HOH:O	2.28	0.79
1:A:706:ILE:CG1	5:A:965:HOH:O	2.23	0.78
1:A:534:GLN:O	1:A:538:THR:HG22	1.84	0.78
1:A:457:SER:HB3	1:A:462:THR:HG22	1.64	0.78
1:A:723:LYS:HG3	5:A:929:HOH:O	1.84	0.76
1:A:724:LEU:HA	1:A:727:MET:HE3	1.68	0.76
1:A:314:ILE:HG12	1:A:325:ALA:HB3	1.66	0.76
1:A:508:GLY:HA3	1:A:606:MET:HE1	1.68	0.75
1:A:459:ASP:C	1:A:459:ASP:OD2	2.30	0.74
1:A:538:THR:HB	1:A:583:TRP:HE1	1.53	0.73
1:A:106:ASN:OD1	1:A:109:THR:CG2	2.35	0.73
1:A:662:TYR:O	1:A:662:TYR:CD1	2.43	0.71
1:A:538:THR:HB	1:A:583:TRP:NE1	2.06	0.70
1:A:109:THR:HG23	1:A:111:LYS:H	1.56	0.70
1:A:485:ILE:HD11	1:A:505:ILE:CD1	2.22	0.69
1:A:501:ARG:HG2	1:A:501:ARG:HH11	1.58	0.68
1:A:520:ARG:HH22	1:A:648:ASP:CG	2.02	0.68
1:A:740:MET:SD	1:A:743:LEU:HB2	2.33	0.67
1:A:485:ILE:HD11	1:A:505:ILE:HD12	1.77	0.67
1:A:319:GLY:O	1:A:320:LYS:HB2	1.94	0.66
1:A:706:ILE:HD11	5:A:965:HOH:O	1.93	0.65
1:A:557:TYR:CD1	1:A:559:THR:HG22	2.32	0.65
1:A:505:ILE:HG22	1:A:602:THR:HA	1.78	0.64
1:A:502:HIS:ND1	1:A:559:THR:HG21	2.12	0.64
1:A:501:ARG:HG2	1:A:501:ARG:NH1	2.12	0.64
1:A:273:ILE:HB	1:A:274:PRO:HD3	1.80	0.64
1:A:214:GLN:HE22	1:A:216:SER:HB2	1.63	0.63
1:A:745:THR:O	1:A:746:GLN:HB2	1.98	0.63
1:A:168:GLN:HE22	1:A:194:SER:HB2	1.65	0.62
1:A:522:PRO:HB3	1:A:682:ASP:O	2.00	0.62
1:A:606:MET:HE3	1:A:608:THR:CG2	2.29	0.62
1:A:534:GLN:O	1:A:538:THR:CG2	2.48	0.61
1:A:746:GLN:HA	5:A:926:HOH:O	2.00	0.61
1:A:710:HIS:CD2	5:A:1092:HOH:O	2.46	0.61
1:A:332:LEU:HD11	1:A:392:ILE:HD12	1.82	0.60
1:A:606:MET:HE3	1:A:608:THR:HG22	1.82	0.60
1:A:557:TYR:CE1	1:A:559:THR:HG22	2.36	0.60
1:A:444:ASN:C	1:A:445:LEU:HD23	2.28	0.59
1:A:485:ILE:CD1	1:A:505:ILE:CD1	2.81	0.59
1:A:508:GLY:HA3	1:A:606:MET:CE	2.34	0.58
1:A:716:LEU:HG	1:A:727:MET:HE1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD22	1:A:173:ARG:NH2	2.19	0.58
1:A:314:ILE:CG1	1:A:325:ALA:HB3	2.33	0.57
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.05	0.57
1:A:475:LYS:O	1:A:479:ARG:HG3	2.05	0.56
1:A:724:LEU:HA	1:A:727:MET:CE	2.34	0.56
1:A:622:GLU:HG3	5:A:932:HOH:O	2.05	0.56
1:A:483:ARG:HD3	5:A:949:HOH:O	2.06	0.55
1:A:686:THR:HG22	1:A:687:VAL:N	2.22	0.55
1:A:277:ARG:HD2	1:A:322:GLU:O	2.06	0.55
1:A:242:SER:O	1:A:288:GLN:HA	2.07	0.55
1:A:251:HIS:HD2	5:A:1080:HOH:O	1.88	0.54
1:A:457:SER:CB	1:A:462:THR:HG22	2.37	0.54
1:A:458:GLU:O	1:A:459:ASP:HB3	2.08	0.54
1:A:692:GLN:O	1:A:696:ILE:HG12	2.08	0.54
1:A:383:ILE:CG1	1:A:384:LYS:H	2.22	0.53
1:A:428:CYS:SG	4:A:1002:ADP:H3'	2.49	0.53
1:A:170:LEU:C	1:A:170:LEU:CD1	2.82	0.52
1:A:213:PRO:HB2	1:A:215:MET:HE2	1.92	0.52
1:A:683:LEU:HD23	1:A:684:TYR:CZ	2.45	0.52
1:A:170:LEU:C	1:A:170:LEU:HD13	2.35	0.51
1:A:401:THR:HB	1:A:402:PRO:HA	1.92	0.51
1:A:686:THR:CG2	1:A:687:VAL:N	2.73	0.51
1:A:481:LEU:HB3	1:A:505:ILE:CG1	2.40	0.51
1:A:662:TYR:O	1:A:662:TYR:HD1	1.94	0.51
1:A:686:THR:HG22	1:A:688:TRP:N	2.20	0.51
1:A:570:LEU:O	1:A:571:GLN:C	2.55	0.50
1:A:79:ALA:C	1:A:81:ILE:H	2.19	0.49
1:A:459:ASP:OD2	1:A:459:ASP:O	2.30	0.49
1:A:692:GLN:NE2	1:A:715:PHE:H	2.10	0.48
1:A:530:LEU:O	1:A:534:GLN:HG2	2.13	0.48
1:A:481:LEU:HB3	1:A:505:ILE:HG13	1.95	0.48
1:A:504:PRO:O	1:A:505:ILE:HD12	2.13	0.48
1:A:724:LEU:HD21	1:A:740:MET:HE1	1.96	0.48
1:A:127:ASN:HB2	1:A:131:LEU:HD22	1.96	0.47
1:A:257:SER:OG	1:A:352:SER:HB2	2.15	0.47
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.50	0.47
1:A:606:MET:HE2	1:A:606:MET:H	1.79	0.47
1:A:501:ARG:HH11	1:A:501:ARG:CG	2.27	0.46
1:A:557:TYR:HD1	1:A:559:THR:HG22	1.79	0.46
1:A:393:LEU:CD2	1:A:724:LEU:HD13	2.38	0.46
1:A:388:LEU:O	1:A:392:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLN:HE21	1:A:488:ASN:HD21	1.63	0.46
1:A:606:MET:HE2	5:A:890:HOH:O	2.15	0.46
1:A:288:GLN:HG3	1:A:293:ARG:O	2.16	0.45
1:A:649:LEU:HB3	1:A:655:TRP:HB2	1.98	0.45
1:A:744:ARG:NH1	5:A:977:HOH:O	2.50	0.45
1:A:322:GLU:HG2	5:A:935:HOH:O	2.16	0.45
1:A:503:ARG:N	1:A:504:PRO:CD	2.79	0.45
1:A:544:MET:HB2	1:A:588:LEU:HD21	1.98	0.45
1:A:734:LYS:HA	1:A:734:LYS:HD2	1.82	0.45
1:A:519:LEU:O	1:A:520:ARG:HB2	2.17	0.45
1:A:686:THR:HG21	1:A:688:TRP:HD1	1.82	0.45
1:A:332:LEU:CD1	1:A:392:ILE:HD12	2.46	0.45
1:A:383:ILE:HD12	1:A:384:LYS:H	1.80	0.45
1:A:276:ILE:HD12	1:A:299:LEU:HD13	1.99	0.44
1:A:383:ILE:CG1	1:A:384:LYS:N	2.80	0.44
1:A:664:ILE:HG13	5:A:1044:HOH:O	2.17	0.44
1:A:383:ILE:CD1	1:A:384:LYS:H	2.30	0.44
1:A:661:GLN:HG2	5:A:1044:HOH:O	2.17	0.43
1:A:696:ILE:HD11	1:A:714:LEU:HD11	1.99	0.43
1:A:671:GLN:C	1:A:673:LEU:H	2.25	0.43
1:A:485:ILE:CD1	1:A:505:ILE:HD11	2.49	0.43
1:A:716:LEU:HG	1:A:727:MET:CE	2.49	0.43
1:A:661:GLN:C	1:A:663:LEU:H	2.27	0.43
1:A:128:LYS:O	1:A:132:ASN:HB2	2.19	0.43
1:A:683:LEU:HD23	1:A:684:TYR:CE1	2.54	0.43
1:A:724:LEU:HD22	1:A:728:HIS:NE2	2.34	0.42
1:A:251:HIS:HE1	1:A:435:SER:OG	2.03	0.42
1:A:334:ILE:HD12	1:A:404:VAL:HG13	2.02	0.42
1:A:334:ILE:HG22	1:A:335:PRO:O	2.20	0.41
1:A:481:LEU:CB	1:A:505:ILE:HG12	2.50	0.41
1:A:383:ILE:HG13	1:A:384:LYS:H	1.85	0.41
1:A:481:LEU:HB3	1:A:505:ILE:HG12	2.02	0.41
1:A:120:VAL:O	1:A:124:VAL:HG23	2.20	0.41
1:A:686:THR:HG21	1:A:688:TRP:CD1	2.56	0.41
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.94	0.41
1:A:261:TYR:HE2	1:A:266:ASN:HD22	1.67	0.41
1:A:87:HIS:HE1	1:A:140:ASP:OD1	2.05	0.41
1:A:557:TYR:HE1	1:A:559:THR:CG2	2.34	0.40
1:A:628:MET:SD	1:A:664:ILE:HG23	2.62	0.40
1:A:172:MET:HG3	1:A:176:LEU:HD22	2.04	0.40
1:A:506:ALA:HB1	1:A:604:ALA:HB3	2.03	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	660/888 (74%)	620 (94%)	33 (5%)	7 (1%)	11 8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	LYS
1	A	459	ASP
1	A	662	TYR
1	A	674	PRO
1	A	707	ASP
1	A	245	ALA
1	A	717	ARG

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	569/761 (75%)	520 (91%)	49 (9%)	10 8

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU

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Mol	Chain	Res	Type
1	A	119	ASP
1	A	131	LEU
1	A	154	SER
1	A	159	ILE
1	A	170	LEU
1	A	176	LEU
1	A	183	ILE
1	A	187	LEU
1	A	220	LEU
1	A	268	THR
1	A	301	LEU
1	A	314	ILE
1	A	317	ASN
1	A	320	LYS
1	A	324	ARG
1	A	337	LEU
1	A	359	LEU
1	A	383	ILE
1	A	388	LEU
1	A	390	TYR
1	A	432	VAL
1	A	443	CYS
1	A	445	LEU
1	A	459	ASP
1	A	462	THR
1	A	463	SER
1	A	473	ILE
1	A	505	ILE
1	A	512	LEU
1	A	518	LEU
1	A	530	LEU
1	A	534	GLN
1	A	538	THR
1	A	559	THR
1	A	606	MET
1	A	619	GLU
1	A	628	MET
1	A	639	GLN
1	A	641	VAL
1	A	661	GLN
1	A	664	ILE
1	A	712	LEU

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Mol	Chain	Res	Type
1	A	714	LEU
1	A	716	LEU
1	A	724	LEU
1	A	743	LEU
1	A	745	THR
1	A	746	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	87	HIS
1	A	127	ASN
1	A	168	GLN
1	A	191	ASN
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	567	GLN
1	A	613	GLN
1	A	692	GLN
1	A	710	HIS
1	A	713	ASN
1	A	746	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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
4	ADP	A	1002	-	28,29,29	1.50	6 (21%)	43,45,45	1.82	12 (27%)
3	DGT	A	1001	2	32,33,33	1.62	6 (18%)	48,52,52	1.74	7 (14%)

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
4	ADP	A	1002	-	-	2/16/32/32	0/3/3/3
3	DGT	A	1001	2	-	1/22/34/34	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	ADP	C5-C4	4.87	1.47	1.39
3	A	1001	DGT	PB-O3A	4.59	1.64	1.59
3	A	1001	DGT	PA-O3A	3.49	1.63	1.59
3	A	1001	DGT	C5-C4	3.10	1.47	1.38
3	A	1001	DGT	C6-N1	-2.84	1.33	1.38
4	A	1002	ADP	PA-O3A	2.75	1.62	1.59
4	A	1002	ADP	C4-N9	-2.60	1.32	1.37
4	A	1002	ADP	C5-C6	2.60	1.48	1.41
4	A	1002	ADP	C8-N7	2.45	1.36	1.31
3	A	1001	DGT	C5-N7	-2.28	1.34	1.39
4	A	1002	ADP	C5-N7	-2.17	1.35	1.39
3	A	1001	DGT	C4-N9	-2.03	1.32	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	DGT	C5-C4-N3	-6.07	118.72	128.39
3	A	1001	DGT	N9-C4-N3	5.24	136.43	125.95
4	A	1002	ADP	C5-C4-N3	-4.43	120.61	126.72
3	A	1001	DGT	C2-N3-C4	4.37	119.83	112.30
4	A	1002	ADP	N3-C2-N1	-4.08	122.40	128.58
4	A	1002	ADP	N3-C4-N9	3.61	133.31	127.17
4	A	1002	ADP	C2-N3-C4	3.55	120.51	111.83
4	A	1002	ADP	C2'-C1'-N9	-3.37	104.92	113.30
3	A	1001	DGT	O6-C6-C5	-3.19	118.11	126.53
4	A	1002	ADP	C4-N9-C8	2.91	108.80	105.74
4	A	1002	ADP	C2-N1-C6	2.71	123.19	118.73
4	A	1002	ADP	C4-C5-N7	-2.56	107.66	110.58
3	A	1001	DGT	O1B-PB-O3A	2.49	114.01	107.27
3	A	1001	DGT	C5-C6-N1	2.39	119.35	113.25
4	A	1002	ADP	C6-C5-N7	2.33	136.58	132.09
4	A	1002	ADP	O2A-PA-O3A	2.33	113.56	107.27
4	A	1002	ADP	N9-C8-N7	-2.24	110.75	113.94
3	A	1001	DGT	O3A-PB-O2B	-2.21	104.06	110.70
4	A	1002	ADP	C5-N7-C8	2.07	106.71	103.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	ADP	PA-O3A-PB-O3B
3	A	1001	DGT	PA-O3A-PB-O1B
4	A	1002	ADP	PA-O3A-PB-O2B

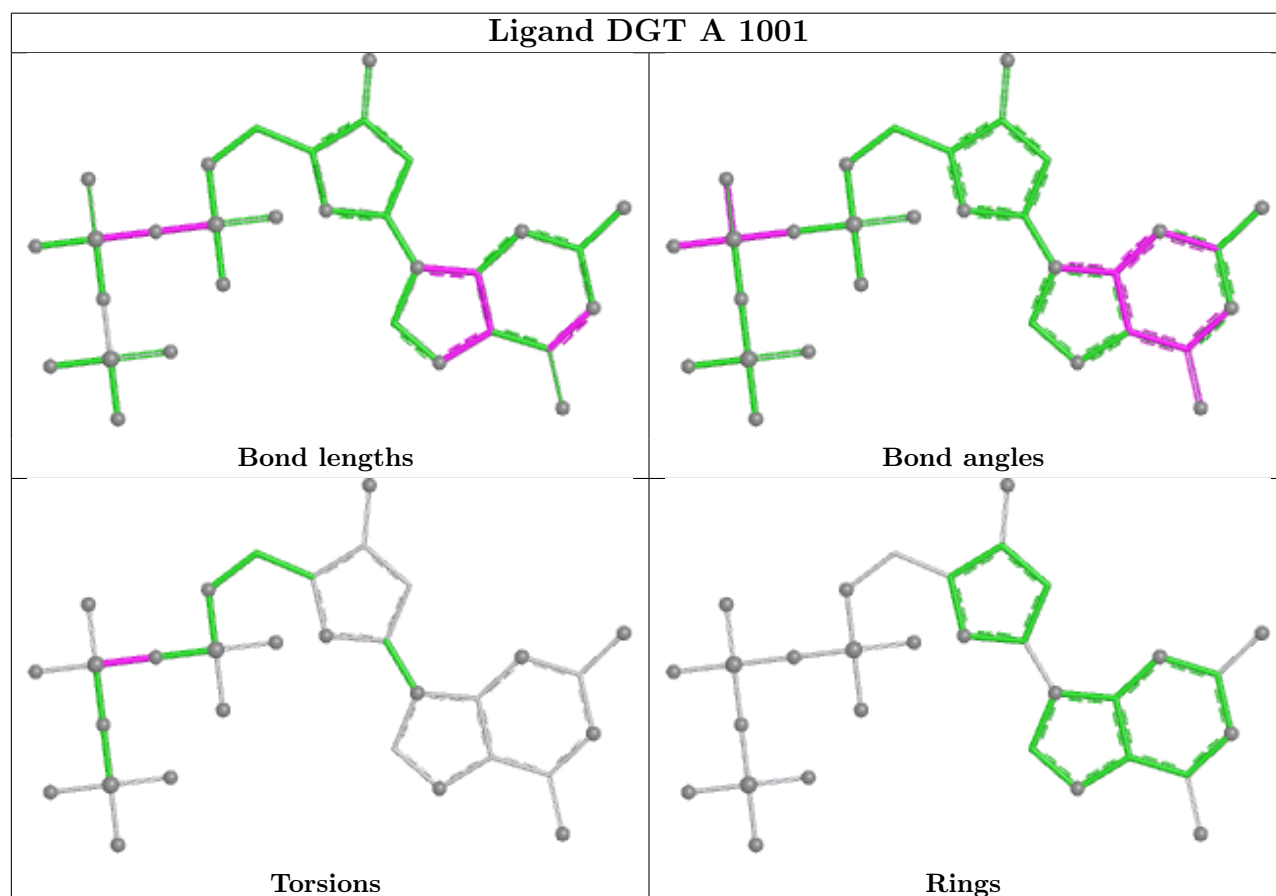
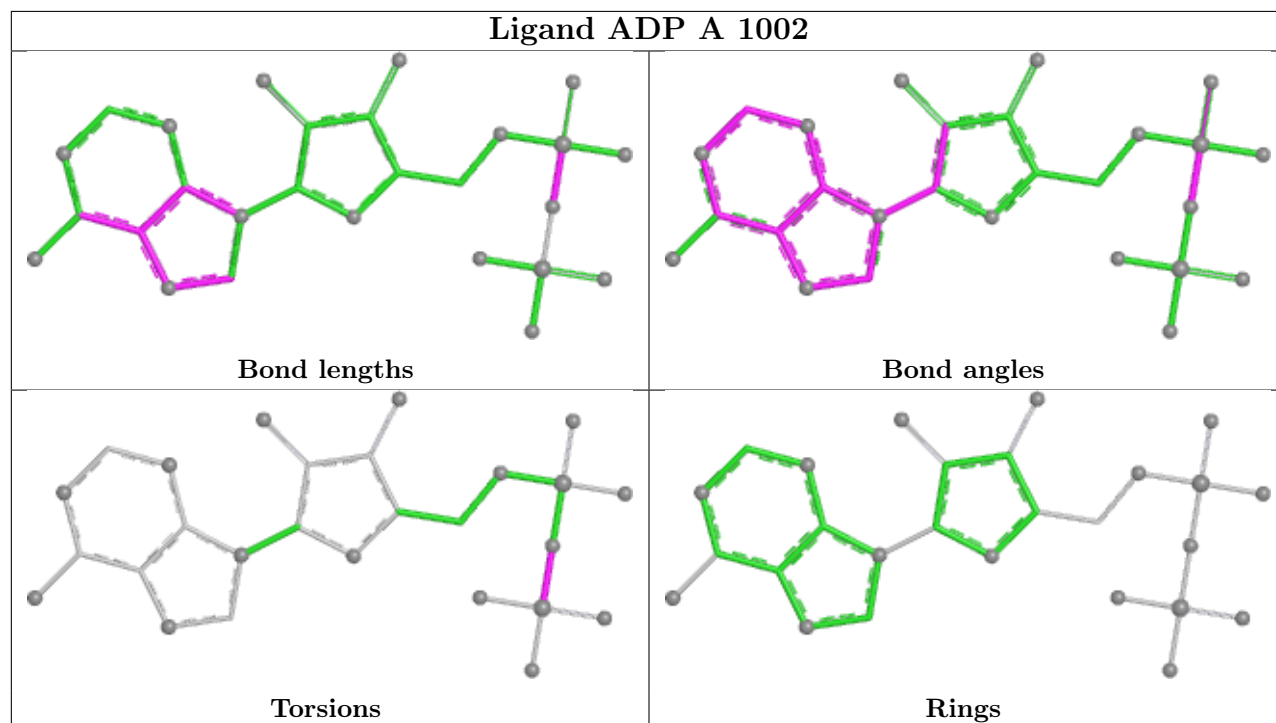
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 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	664/888 (74%)	0.00	19 (2%) 53 54	27, 41, 79, 96	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	629	TYR	4.3
1	A	281	ASN	3.5
1	A	675	ASN	3.2
1	A	638	PHE	3.1
1	A	76	THR	2.9
1	A	662	TYR	2.8
1	A	390	TYR	2.7
1	A	383	ILE	2.6
1	A	78	ALA	2.5
1	A	489	TYR	2.4
1	A	457	SER	2.3
1	A	673	LEU	2.3
1	A	665	THR	2.3
1	A	246	GLY	2.2
1	A	630	SER	2.2
1	A	77	LEU	2.1
1	A	654	ILE	2.1
1	A	664	ILE	2.1
1	A	659	MET	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 [i](#)

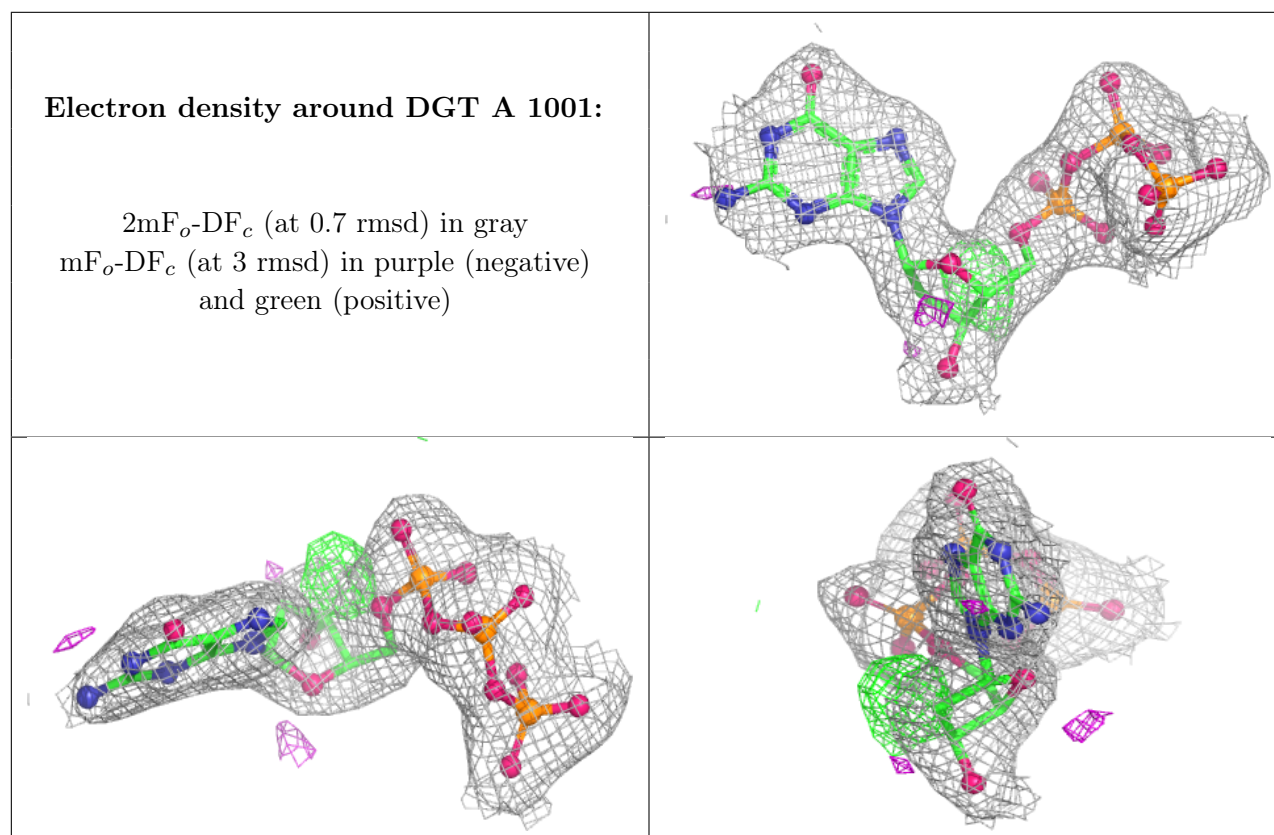
There are no oligosaccharides in this entry.

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. 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.

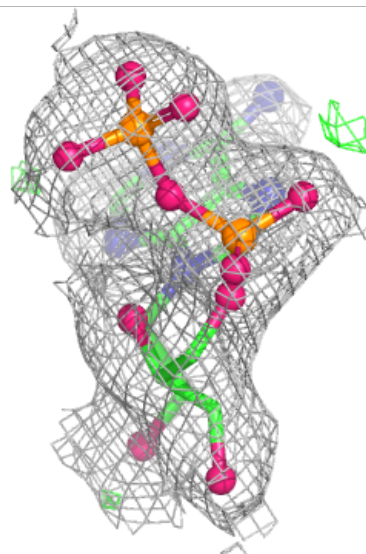
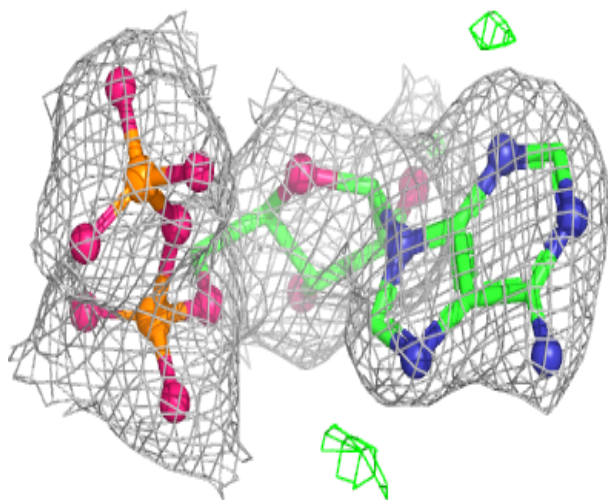
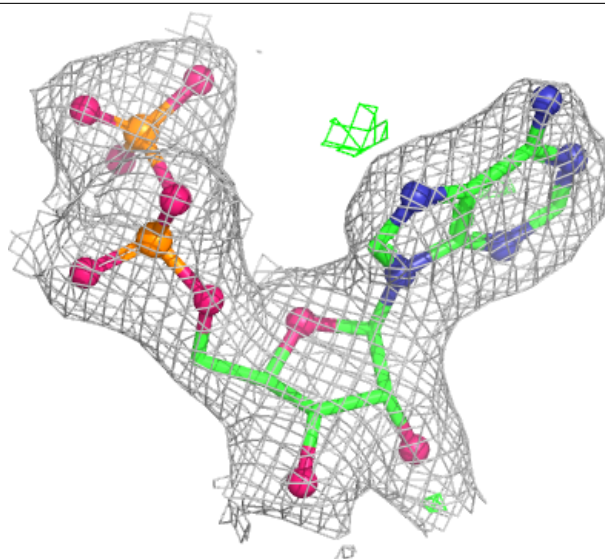
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DGT	A	1001	31/31	0.96	0.06	29,32,37,39	0
4	ADP	A	1002	27/27	0.96	0.06	35,39,41,43	0
2	MG	A	2001	1/1	0.98	0.04	34,34,34,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around ADP A 1002:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.