



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:23 PM UTC

PDB ID : 2CVX / pdb_00002cvx
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 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

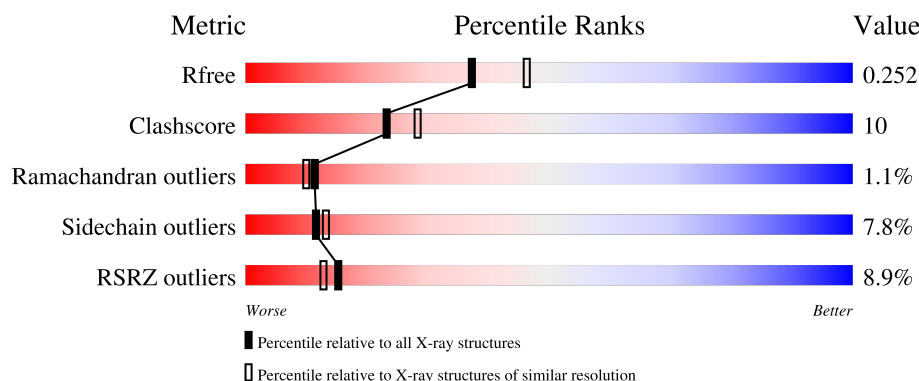
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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 5580 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.

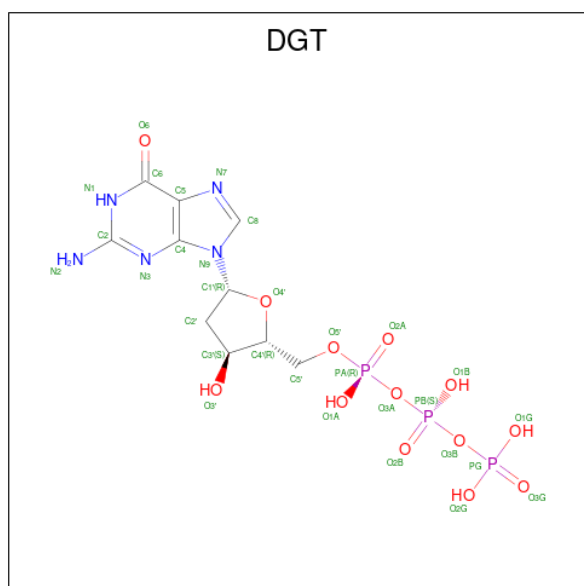
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

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

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

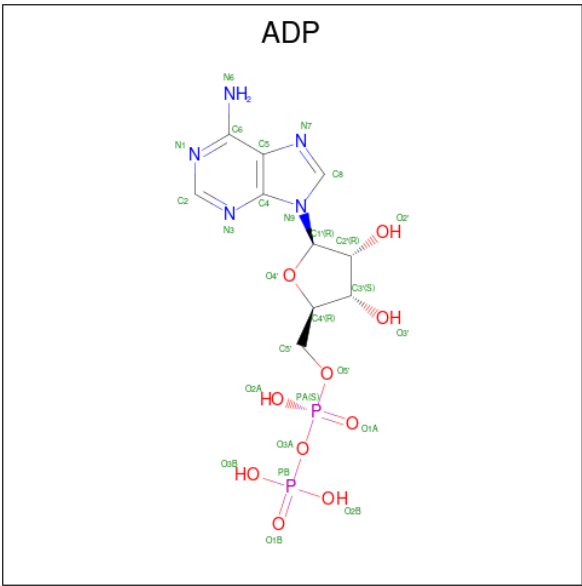
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- 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).



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.69Å 117.28Å 65.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.20) 99.3 (50.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.61 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, R_{free}	0.210 , 0.254 0.209 , 0.252	Depositor DCC
R_{free} test set	4235 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	1.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5580	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.73	0/5428	1.02	5/7348 (0.1%)

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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ILE	N-CA-C	8.74	116.59	107.76
1	A	503	ARG	CB-CA-C	-7.13	104.00	110.71
1	A	482	ASN	CA-CB-CG	-5.97	106.62	112.60
1	A	126	GLU	OE1-CD-OE2	-5.33	110.11	122.90
1	A	206	PHE	CB-CA-C	-5.14	102.11	110.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	GLU	Sidechain

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	5306	0	5245	110	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	4	0
All	All	5580	0	5269	110	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 10.

All (110) 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	1.55	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:417:LYS:HE3	1:A:574:MET:HE1	1.69	0.74
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:457:SER:HB3	1:A:462:THR:HG23	1.74	0.70
1:A:717:ARG:O	1:A:719:PRO:HD3	1.91	0.70
1:A:319:GLY:O	1:A:320:LYS:HB2	1.92	0.70
1:A:520:ARG:HH22	1:A:648:ASP:CG	2.01	0.69
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: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:606:MET:HE3	1:A:608:THR:HG22	1.81	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:HIS:HD2	5:A:2033:HOH:O	1.84	0.61
1:A:662:TYR:O	1:A:662:TYR:CD1	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:606:MET:HE3	1:A:608:THR:CG2	2.33	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:CD2	1:A:145:TYR:N	2.72	0.55
1:A:213:PRO:HB2	1:A:215:MET:HE2	1.88	0.55
1:A:447:SER:HB3	1:A:606:MET:CE	2.37	0.55
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:126:GLU:CD	1:A:181:ARG:HH12	2.18	0.52
1:A:314:ILE:HG12	1:A:325:ALA:HB3	1.91	0.52
1:A:508:GLY:HA3	1:A:606:MET:HE1	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: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:488:ASN:ND2	5:A:2173:HOH:O	2.31	0.50
1:A:504:PRO:O	1:A:505:ILE:HD12	2.12	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:79:ALA:C	1:A:81:ILE:H	2.21	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
1:A:383:ILE:CG1	1:A:384:LYS:H	2.26	0.47
1:A:713:ASN:ND2	1:A:742:TYR:HB2	2.29	0.47
1:A:242:SER:O	1:A:288:GLN:HA	2.15	0.47
1:A:519:LEU:O	1:A:520:ARG:HB2	2.15	0.47
1:A:220:LEU:HD21	1:A:426:ASN:HB3	1.97	0.47
1:A:740:MET:SD	1:A:743:LEU:HB2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:SER:HB3	1:A:606:MET:HE1	1.96	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: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:210:THR:HB	1:A:211:PRO:CD	2.48	0.44
1:A:686:THR:CG2	1:A:688:TRP:HD1	2.31	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:603:MET:HE3	1:A:603:MET:HB3	1.95	0.43
1:A:109:THR:HG23	1:A:111:LYS:H	1.83	0.43
1:A:264:GLY:HA3	3:A:1001:DGT:O2B	2.18	0.43
1:A:719:PRO:HG3	1:A:745:THR:OG1	2.19	0.43
1:A:662:TYR:O	1:A:662:TYR:HD1	2.00	0.43
1:A:455:GLU:CD	1:A:466:ASN:HD22	2.27	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:413:LYS:NZ	1:A:735:GLY:O	2.52	0.42
1:A:432:VAL:CG1	1:A:708:GLN:HA	2.48	0.42
1:A:508:GLY:HA3	1:A:606:MET:CE	2.49	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:126:GLU:OE1	1:A:181:ARG:NH1	2.53	0.42
1:A:383:ILE:CG1	1:A:384:LYS:N	2.83	0.42
1:A:104:TYR:CD1	1:A:159:ILE:HG23	2.55	0.42
1:A:119:ASP:O	1:A:123:ILE:HG13	2.19	0.42
1:A:178:ILE:O	1:A:487:ARG:HD3	2.20	0.41
1:A:524:ASP:HB3	1:A:694:THR:HG21	2.01	0.41
1:A:444:ASN:C	1:A:445:LEU:HD23	2.45	0.41
1:A:160:ASN:C	1:A:162:GLN:H	2.29	0.41
1:A:570:LEU:O	1:A:571:GLN:C	2.64	0.41
1:A:557:TYR:CD1	1:A:559:THR:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:447:SER:HB3	1:A:606:MET:HE3	2.01	0.40
1:A:606:MET:HE2	5:A:2031:HOH:O	2.22	0.40
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 [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%)	624 (94%)	29 (4%)	7 (1%)	11 10

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 [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	575/761 (76%)	530 (92%)	45 (8%)	11	13

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	131	LEU
1	A	145	TYR
1	A	154	SER
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	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	445	LEU
1	A	456	THR
1	A	473	ILE
1	A	505	ILE
1	A	512	LEU
1	A	518	LEU
1	A	530	LEU
1	A	538	THR
1	A	594	LYS
1	A	606	MET
1	A	619	GLU
1	A	628	MET
1	A	639	GLN

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Mol	Chain	Res	Type
1	A	641	VAL
1	A	663	LEU
1	A	673	LEU
1	A	679	GLU
1	A	696	ILE
1	A	712	LEU
1	A	724	LEU
1	A	743	LEU
1	A	745	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	168	GLN
1	A	214	GLN
1	A	251	HIS
1	A	266	ASN
1	A	270	ASN
1	A	281	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 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
3	DGT	A	1001	2	32,33,33	1.08	3 (9%)	48,52,52	1.60	9 (18%)
4	ADP	A	1002	-	28,29,29	1.58	6 (21%)	43,45,45	1.82	9 (20%)

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

All (9) 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
4	A	1002	ADP	PA-O3A	3.57	1.63	1.59
4	A	1002	ADP	C5-C6	3.02	1.49	1.41
3	A	1001	DGT	C2-N3	2.60	1.39	1.33
4	A	1002	ADP	C8-N7	2.53	1.36	1.31
4	A	1002	ADP	C4-N9	-2.42	1.32	1.37
3	A	1001	DGT	PB-O3A	2.41	1.62	1.59
3	A	1001	DGT	PA-O3A	2.31	1.62	1.59
4	A	1002	ADP	C5-N7	-2.26	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ADP	C5-C4-N3	-5.43	119.24	126.72
3	A	1001	DGT	C5-C4-N3	-4.97	120.48	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	DGT	C2-N3-C4	4.57	120.17	112.30
4	A	1002	ADP	C2-N3-C4	3.95	121.48	111.83
4	A	1002	ADP	C4-C5-N7	-3.79	106.25	110.58
4	A	1002	ADP	N3-C4-N9	3.64	133.35	127.17
4	A	1002	ADP	N3-C2-N1	-3.59	123.14	128.58
3	A	1001	DGT	N9-C4-N3	3.52	133.00	125.95
3	A	1001	DGT	O1B-PB-O3A	3.15	115.79	107.27
3	A	1001	DGT	C2-N1-C6	-3.01	119.65	125.11
4	A	1002	ADP	C6-C5-N7	2.86	137.61	132.09
3	A	1001	DGT	C5-C6-N1	2.76	120.28	113.25
3	A	1001	DGT	O6-C6-C5	-2.65	119.53	126.53
4	A	1002	ADP	C5-N7-C8	2.48	107.35	103.45
3	A	1001	DGT	O2G-PG-O3B	2.27	112.24	104.64
4	A	1002	ADP	O2A-PA-O3A	2.20	113.23	107.27
3	A	1001	DGT	N9-C8-N7	-2.12	109.48	113.40
4	A	1002	ADP	C2'-C1'-N9	-2.00	108.33	113.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

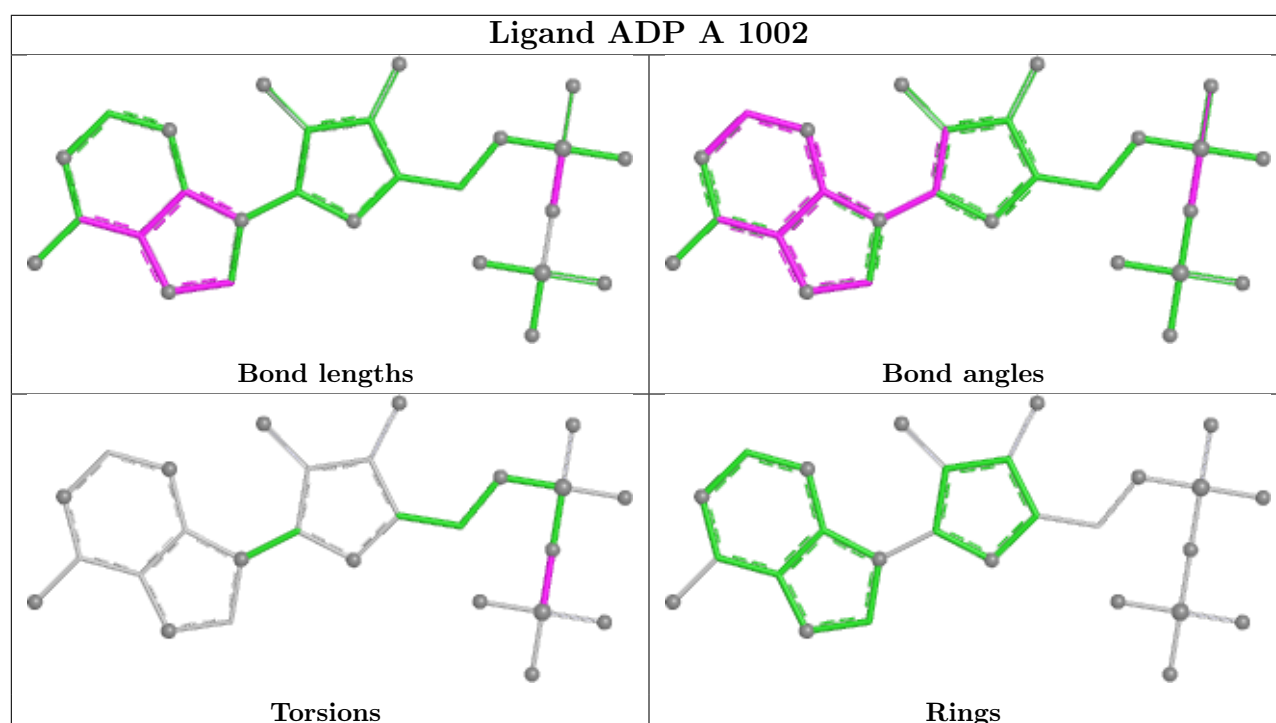
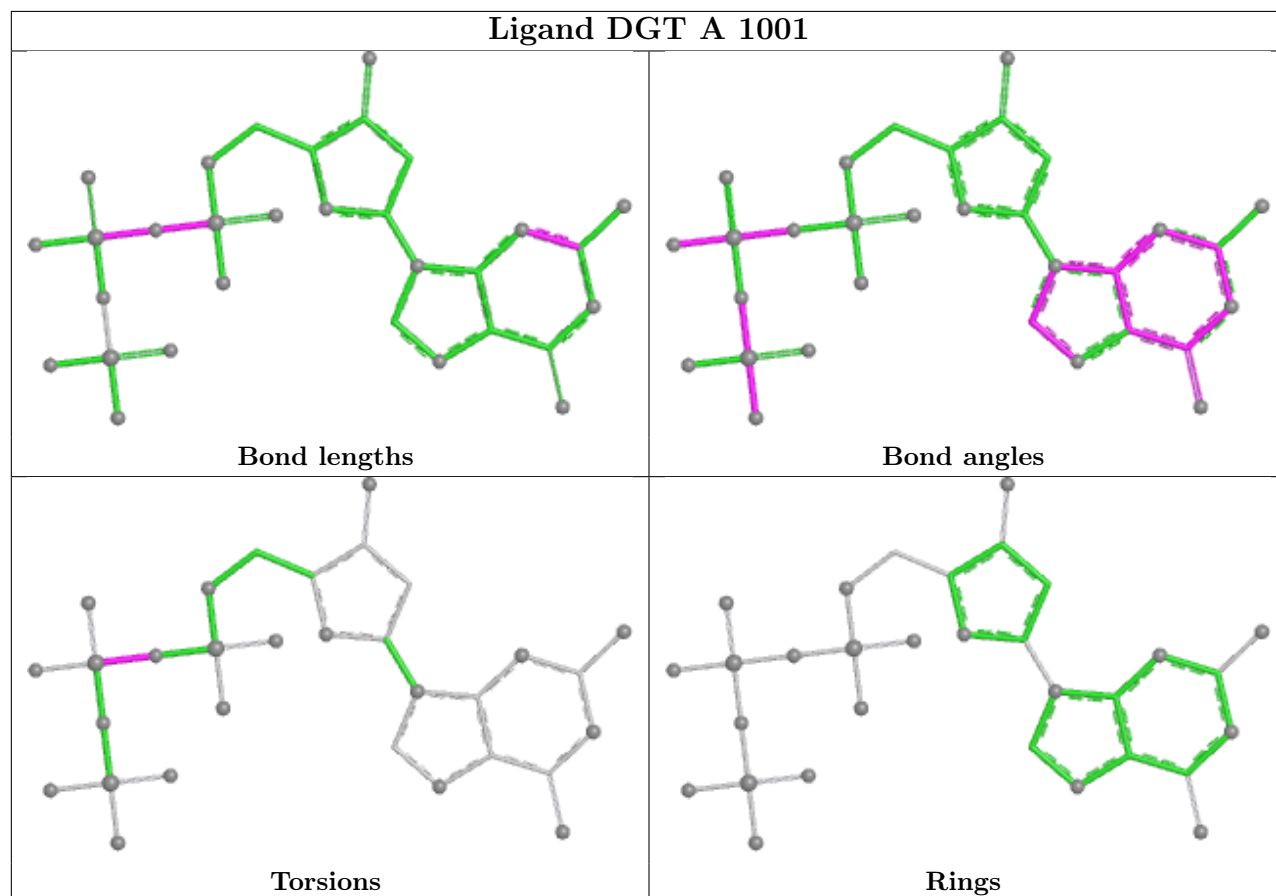
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	DGT	1	0
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%)	0.46	59 (8%) 15 13	22, 38, 76, 98	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	THR	5.6
1	A	665	THR	5.4
1	A	146	PHE	5.2
1	A	662	TYR	5.0
1	A	145	TYR	4.7
1	A	390	TYR	4.4
1	A	664	ILE	4.3
1	A	159	ILE	4.1
1	A	383	ILE	4.0
1	A	666	GLN	3.9
1	A	458	GLU	3.9
1	A	460	GLY	3.9
1	A	638	PHE	3.7
1	A	628	MET	3.7
1	A	629	TYR	3.7
1	A	647	ARG	3.5
1	A	78	ALA	3.5
1	A	456	THR	3.3
1	A	160	ASN	3.2
1	A	654	ILE	3.1
1	A	82	ALA	3.1
1	A	77	LEU	3.1
1	A	489	TYR	3.0
1	A	675	ASN	2.9
1	A	727	MET	2.9
1	A	641	VAL	2.9
1	A	663	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	683	LEU	2.8
1	A	646	LEU	2.7
1	A	669	SER	2.6
1	A	457	SER	2.6
1	A	691	SER	2.6
1	A	655	TRP	2.6
1	A	718	ALA	2.6
1	A	141	PHE	2.6
1	A	645	LEU	2.5
1	A	528	ALA	2.5
1	A	89	GLN	2.5
1	A	726	SER	2.4
1	A	658	GLY	2.4
1	A	656	ASP	2.3
1	A	365	ASP	2.3
1	A	459	ASP	2.3
1	A	81	ILE	2.3
1	A	673	LEU	2.3
1	A	659	MET	2.3
1	A	79	ALA	2.3
1	A	676	VAL	2.3
1	A	91	THR	2.2
1	A	136	VAL	2.2
1	A	649	LEU	2.1
1	A	724	LEU	2.1
1	A	322	GLU	2.1
1	A	650	VAL	2.1
1	A	462	THR	2.1
1	A	85	ASN	2.1
1	A	725	THR	2.0
1	A	109	THR	2.0
1	A	679	GLU	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 ⓘ

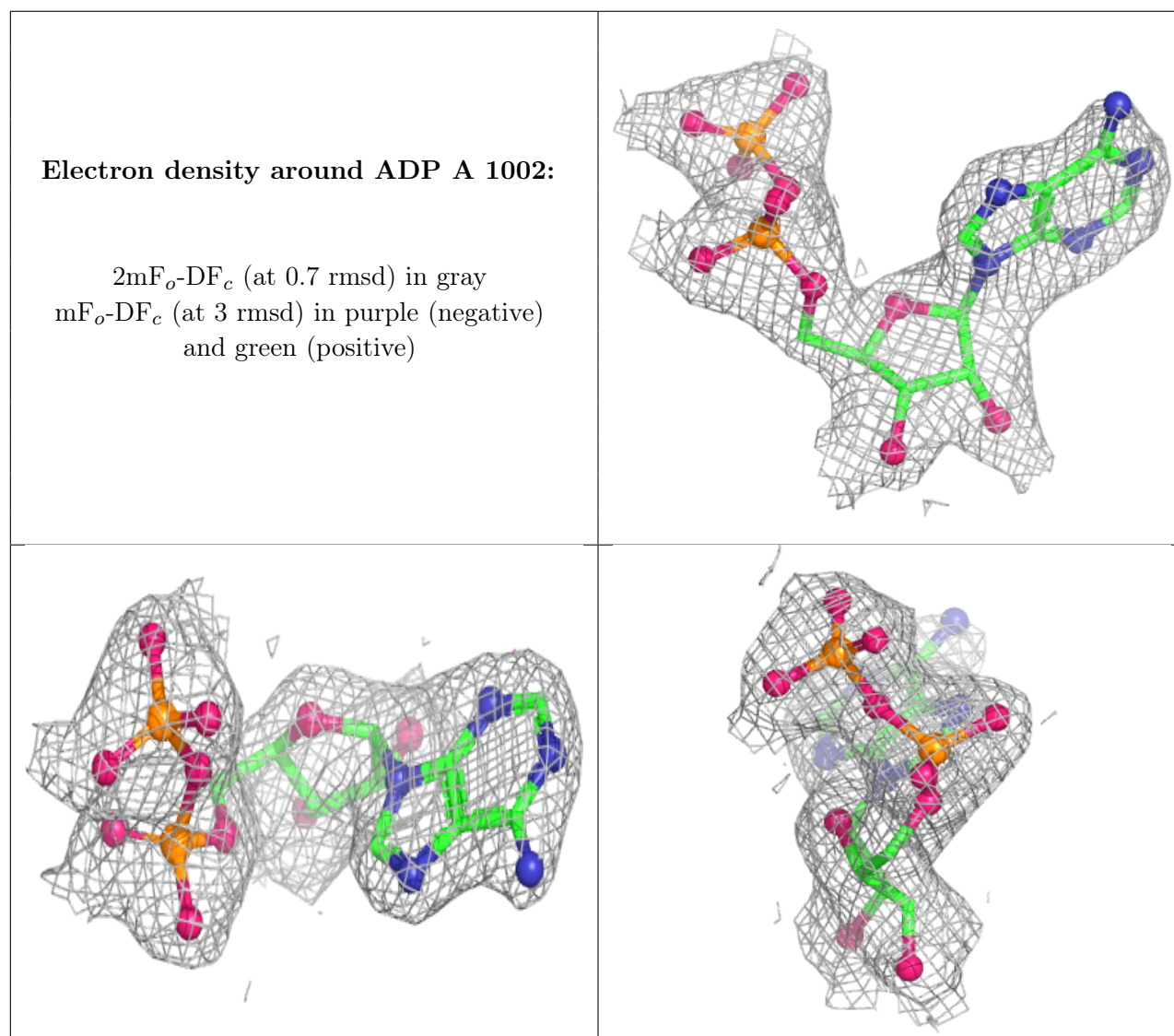
There are no oligosaccharides in this entry.

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. 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.

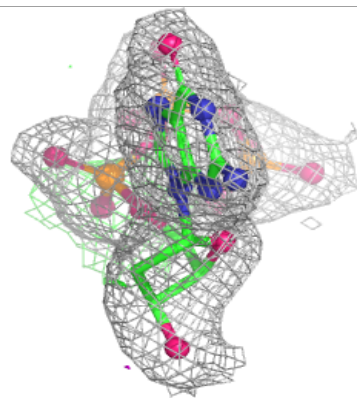
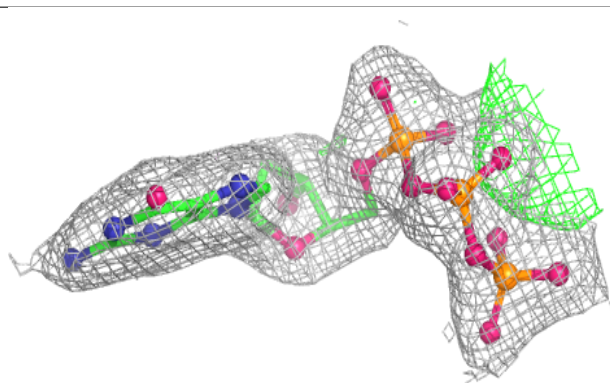
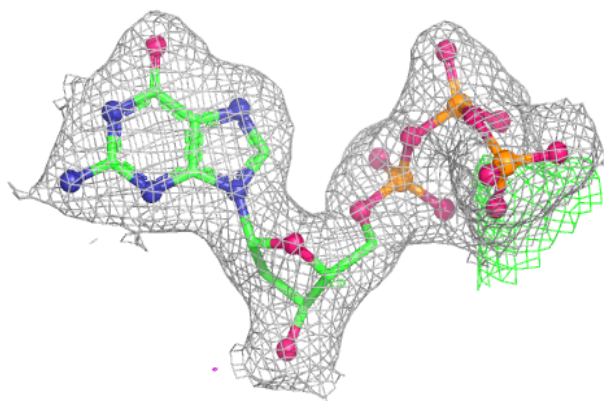
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	2001	1/1	0.86	0.31	43,43,43,43	0
4	ADP	A	1002	27/27	0.96	0.06	36,40,41,43	0
3	DGT	A	1001	31/31	0.97	0.06	21,27,30,33	0

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 DGT A 1001:

$2mF_o-DF_c$ (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.