



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 12:02 PM EDT

PDB ID : 1ZYQ  
Title : T7 DNA polymerase in complex with 8oG and incoming ddATP  
Authors : Brieba, L.G.; Kokoska, R.J.; Bebenek, K.; Kunkel, T.A.; Ellenberger, T.  
Deposited on : 2005-06-10  
Resolution : 2.70 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

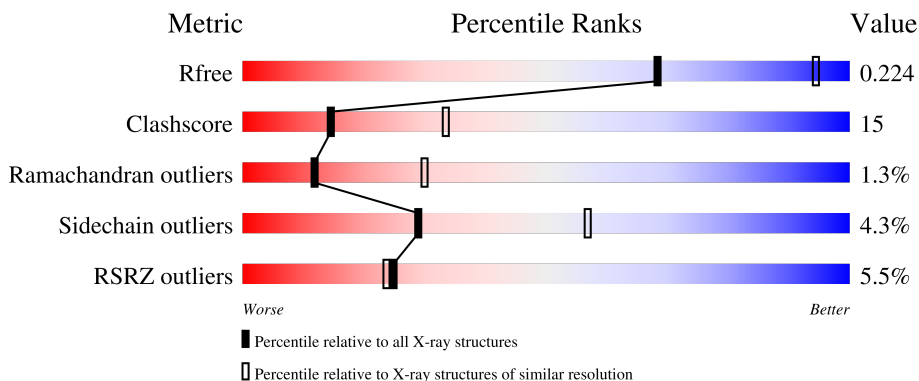
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	P	22	
2	T	26	
3	A	698	
4	B	108	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DAD	A	1024	X	-	-	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7041 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 DNA chain called 5'-D(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*AP\*(DDG))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	P	13	266	125	52	76	13	0	0	0

- Molecule 2 is a DNA chain called 5'-D(\*CP\*CP\*CP\*(8OG)P\*CP\*TP\*GP\*GP\*CP\*AP\*C P\*TP\*GP\*GP\*CP\*CP\*GP\*TP\*CP\*GP\*TP\*TP\*TP\*TP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	15	308	144	57	92	15	0	0	0

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	680	5414	3445	939	1007	23	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P00581
A	?	-	ARG	deletion	UNP P00581
A	?	-	PHE	deletion	UNP P00581
A	?	-	GLY	deletion	UNP P00581
A	?	-	SER	deletion	UNP P00581
A	?	-	HIS	deletion	UNP P00581
A	536	ALA	LYS	engineered mutation	UNP P00581

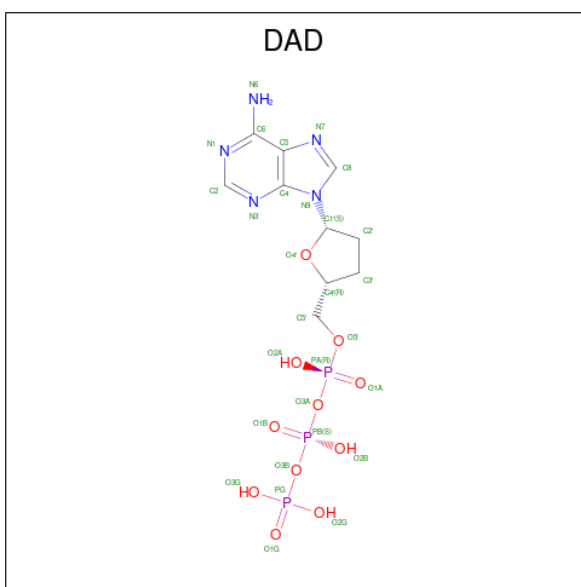
- Molecule 4 is a protein called Thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	105	802	518	129	152	3	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	3	3	3	0	0

- Molecule 6 is 2',3'-DIDEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: DAD) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>11</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	29	10	5	11	3	0	0

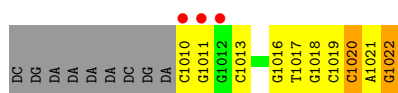
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	P	8	8	8	0	0
7	T	11	11	11	0	0
7	A	179	179	179	0	0
7	B	21	21	21	0	0

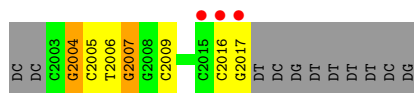
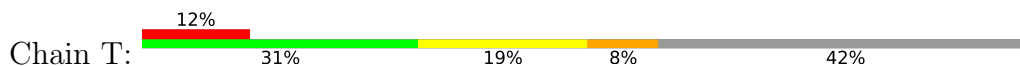
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

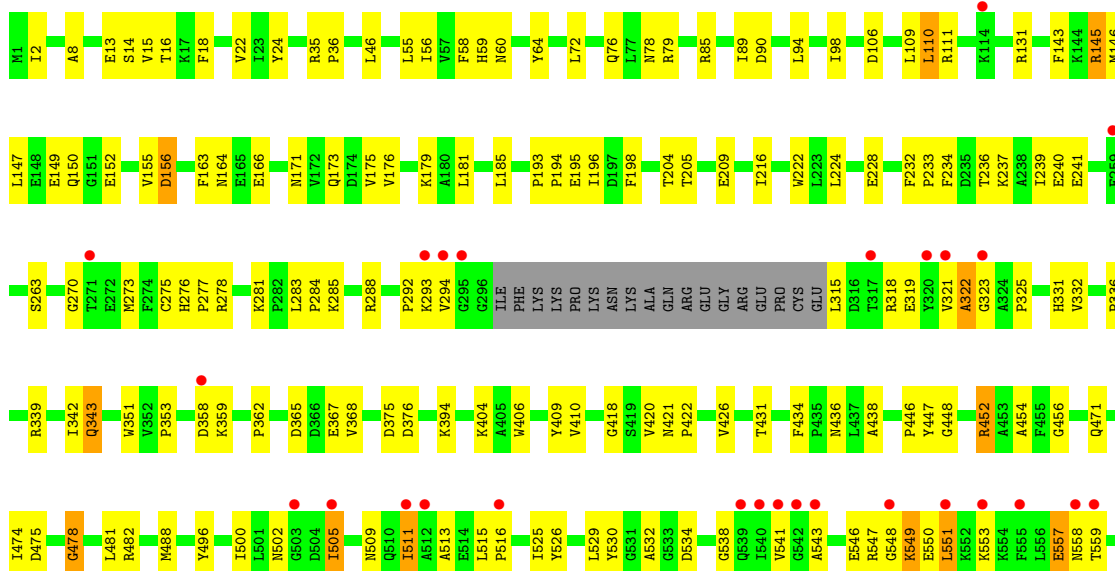
- Molecule 1: 5'-D(\*CP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*AP\*CP\*GP\*GP\*CP\*CP\*AP\*GP\*TP\*GP\*CP\*CP\*AP\*(DDG))-3'

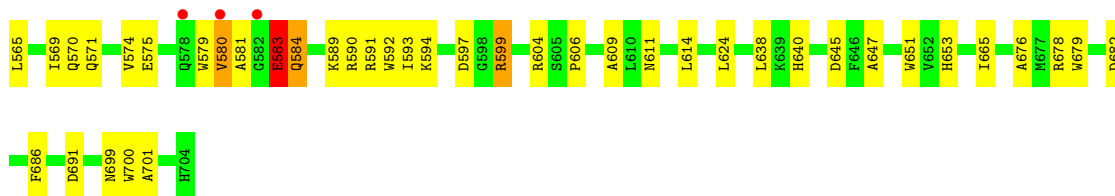


- Molecule 2: 5'-D(\*CP\*CP\*CP\*(8OG)P\*CP\*TP\*GP\*GP\*CP\*AP\*CP\*TP\*GP\*GP\*CP\*CP\*GP\*TP\*CP\*GP\*TP\*TP\*TP\*CP\*G)-3'

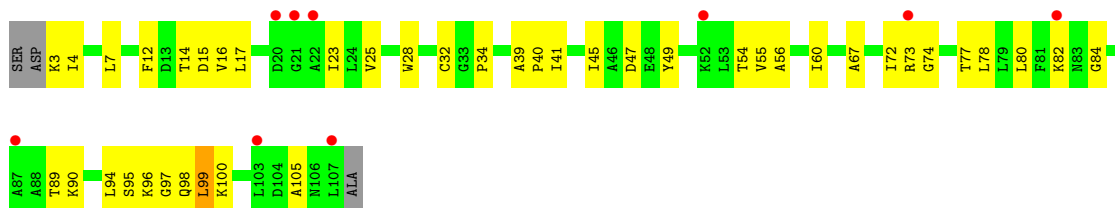


- Molecule 3: DNA polymerase





• Molecule 4: Thioredoxin 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.15Å 213.01Å 52.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 2.70 47.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (47.60-2.70) 91.5 (47.60-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.272 0.221 , 0.224	Depositor DCC
$R_{free}$ test set	1958 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtrriage
Anisotropy	0.246	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7041	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DAD, MG, 8OG, DDG

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	P	0.43	0/274	0.82	0/420
2	T	0.48	0/317	0.85	0/484
3	A	0.38	0/5545	0.59	0/7503
4	B	0.36	0/817	0.64	0/1108
All	All	0.39	0/6953	0.62	0/9515

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	P	0	2
2	T	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	1020	DC	Sidechain
1	P	1021	DA	Sidechain
2	T	2007	DG	Sidechain

## 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	P	266	0	145	14	0
2	T	308	0	168	10	0
3	A	5414	0	5291	160	0
4	B	802	0	816	31	0
5	A	3	0	0	0	0
6	A	29	0	12	2	0
7	A	179	0	0	17	0
7	B	21	0	0	15	0
7	P	8	0	0	0	0
7	T	11	0	0	0	0
All	All	7041	0	6432	204	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 15.

All (204) 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:P:1013:DC:H3'	3:A:111:ARG:HH22	1.08	1.07
3:A:293:LYS:HA	3:A:294:VAL:N	1.78	0.98
4:B:60:ILE:HG23	7:B:5048:HOH:O	1.67	0.94
3:A:293:LYS:HD3	3:A:294:VAL:N	1.90	0.87
3:A:500:ILE:HD13	3:A:505:ILE:HG13	1.59	0.83
3:A:359:LYS:HA	3:A:359:LYS:HE2	1.60	0.82
1:P:1013:DC:H3'	3:A:111:ARG:NH2	1.91	0.80
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.63	0.80
2:T:2006:DT:H6	2:T:2006:DT:H5'	1.46	0.80
3:A:145:ARG:HB2	3:A:145:ARG:NH1	1.98	0.79
3:A:270:GLY:HA3	3:A:288:ARG:HB2	1.64	0.78
4:B:12:PHE:HA	7:B:5007:HOH:O	1.84	0.78
3:A:553:LYS:HG3	3:A:557:GLU:OE2	1.86	0.75
3:A:529:LEU:HB3	7:A:5055:HOH:O	1.87	0.75
3:A:410:VAL:HG13	7:A:5200:HOH:O	1.86	0.73
3:A:292:PRO:O	3:A:293:LYS:HG2	1.90	0.72
4:B:41:ILE:HD12	4:B:96:LYS:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:78:LEU:HD12	7:B:5114:HOH:O	1.90	0.70
3:A:530:TYR:HE1	3:A:614:LEU:HD12	1.57	0.69
1:P:1013:DC:C3'	3:A:111:ARG:HH22	1.97	0.69
3:A:275:CYS:HA	7:A:5181:HOH:O	1.92	0.69
3:A:315:LEU:HD21	4:B:105:ALA:HB1	1.75	0.68
3:A:558:ASN:O	3:A:559:THR:HG23	1.94	0.68
4:B:100:LYS:N	7:B:5020:HOH:O	2.27	0.68
3:A:530:TYR:CE1	3:A:614:LEU:HD12	2.29	0.68
4:B:32:CYS:SG	4:B:34:PRO:HD2	2.34	0.67
4:B:16:VAL:HG23	7:B:5007:HOH:O	1.94	0.66
3:A:515:LEU:HB3	7:A:5102:HOH:O	1.95	0.66
3:A:46:LEU:HD22	3:A:56:ILE:HD13	1.78	0.66
1:P:1016:DG:H2''	1:P:1017:DT:C5'	2.26	0.65
3:A:570:GLN:HE22	3:A:606:PRO:HB3	1.62	0.65
3:A:321:VAL:HG21	4:B:94:LEU:HD22	1.78	0.65
3:A:481:LEU:HD21	3:A:525:ILE:HG21	1.79	0.64
3:A:343:GLN:HG3	3:A:362:PRO:CG	2.26	0.64
3:A:513:ALA:HB3	3:A:515:LEU:HG	1.77	0.64
3:A:426:VAL:HG21	3:A:604:ARG:CZ	2.28	0.64
3:A:15:VAL:HG22	3:A:72:LEU:HD21	1.81	0.63
3:A:18:PHE:H	3:A:76:GLN:HE22	1.44	0.63
4:B:7:LEU:HD22	7:B:5007:HOH:O	1.97	0.63
3:A:294:VAL:HG12	3:A:318:ARG:HH12	1.63	0.63
4:B:95:SER:OG	4:B:98:GLN:HG3	1.98	0.63
4:B:39:ALA:HB3	4:B:40:PRO:HD3	1.80	0.63
4:B:49:TYR:OH	4:B:100:LYS:HG3	1.98	0.62
3:A:234:PHE:HB3	7:A:5200:HOH:O	2.00	0.61
3:A:575:GLU:OE1	3:A:589:LYS:HE2	2.00	0.61
3:A:59:HIS:O	3:A:60:ASN:HB3	2.00	0.61
3:A:85:ARG:HG3	3:A:222:TRP:CG	2.35	0.61
3:A:55:LEU:HD13	3:A:89:ILE:HD11	1.84	0.60
3:A:509:ASN:HD22	3:A:525:ILE:HG13	1.67	0.60
3:A:343:GLN:HG3	3:A:362:PRO:HG2	1.84	0.60
4:B:55:VAL:HG12	7:B:5012:HOH:O	2.00	0.60
4:B:23:ILE:HD13	4:B:54:THR:HB	1.84	0.59
1:P:1016:DG:H2''	1:P:1017:DT:H5'	1.84	0.59
2:T:2005:DC:H2''	2:T:2006:DT:H5'	1.85	0.59
2:T:2007:DG:OP1	3:A:426:VAL:HG23	2.03	0.59
4:B:80:LEU:HG	7:B:5054:HOH:O	2.03	0.59
2:T:2004:8OG:H5''	3:A:532:ALA:HA	1.85	0.58
4:B:82:LYS:HB3	7:B:5025:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:194:PRO:HG2	3:A:195:GLU:OE2	2.03	0.58
3:A:145:ARG:HB2	3:A:145:ARG:HH11	1.69	0.58
3:A:530:TYR:CE1	3:A:611:ASN:HA	2.39	0.57
4:B:97:GLY:C	7:B:5020:HOH:O	2.42	0.57
1:P:1020:DC:H5'	3:A:394:LYS:HE2	1.86	0.57
3:A:526:TYR:HA	7:A:5055:HOH:O	2.03	0.57
3:A:511:ILE:HD13	3:A:511:ILE:O	2.05	0.57
3:A:233:PRO:HB2	3:A:456:GLY:O	2.05	0.56
3:A:234:PHE:CZ	3:A:239:ILE:HG13	2.40	0.56
3:A:79:ARG:HD3	7:A:5083:HOH:O	2.06	0.56
2:T:2004:8OG:H2'	2:T:2005:DC:H6	1.71	0.56
3:A:321:VAL:HG12	3:A:322:ALA:N	2.20	0.56
3:A:448:GLY:O	3:A:452:ARG:HB2	2.06	0.56
3:A:278:ARG:HD2	7:A:5045:HOH:O	2.06	0.55
3:A:481:LEU:HD12	3:A:505:ILE:HG21	1.88	0.55
3:A:236:THR:O	3:A:240:GLU:HG3	2.06	0.55
3:A:343:GLN:HG3	3:A:362:PRO:HG3	1.89	0.55
3:A:276:HIS:CD2	3:A:278:ARG:H	2.26	0.54
3:A:593:ILE:HG22	3:A:594:LYS:N	2.21	0.54
3:A:143:PHE:O	3:A:147:LEU:HB2	2.07	0.54
4:B:4:ILE:HG23	7:B:5012:HOH:O	2.07	0.54
3:A:565:LEU:O	3:A:569:ILE:HG12	2.07	0.54
4:B:100:LYS:NZ	4:B:100:LYS:HB3	2.23	0.54
3:A:145:ARG:HB2	3:A:145:ARG:CZ	2.39	0.53
3:A:456:GLY:HA2	3:A:471:GLN:OE1	2.09	0.53
2:T:2004:8OG:H2'	2:T:2005:DC:C6	2.44	0.53
3:A:315:LEU:HD11	4:B:105:ALA:O	2.09	0.53
3:A:8:ALA:HB3	3:A:64:TYR:OH	2.09	0.52
3:A:546:GLU:O	3:A:550:GLU:HG3	2.09	0.52
3:A:421:ASN:HB3	3:A:431:THR:OG1	2.09	0.52
3:A:146:MET:O	3:A:150:GLN:HG2	2.09	0.52
2:T:2006:DT:H5'	2:T:2006:DT:C6	2.35	0.52
3:A:196:ILE:HB	3:A:198:PHE:CE1	2.45	0.52
3:A:276:HIS:HD2	3:A:277:PRO:HD2	1.75	0.52
3:A:543:ALA:HB3	3:A:547:ARG:CB	2.39	0.52
3:A:351:TRP:CZ3	3:A:353:PRO:HG3	2.46	0.51
3:A:534:ASP:CG	3:A:549:LYS:HG2	2.31	0.51
3:A:18:PHE:H	3:A:76:GLN:NE2	2.08	0.51
3:A:173:GLN:HA	3:A:176:VAL:CG1	2.41	0.51
3:A:590:ARG:HD2	3:A:592:TRP:CZ2	2.45	0.51
3:A:509:ASN:ND2	3:A:525:ILE:HG13	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:580:VAL:O	3:A:581:ALA:HB3	2.11	0.51
1:P:1010:DC:H2''	1:P:1011:DG:C8	2.46	0.50
3:A:228:GLU:HG2	3:A:418:GLY:O	2.12	0.50
4:B:67:ALA:HB1	4:B:72:ILE:HG13	1.93	0.50
1:P:1016:DG:H2''	1:P:1017:DT:H5''	1.93	0.50
3:A:224:LEU:HD11	3:A:651:TRP:CZ3	2.46	0.50
3:A:59:HIS:O	3:A:60:ASN:CB	2.60	0.50
3:A:283:LEU:HG	7:A:5181:HOH:O	2.12	0.49
3:A:35:ARG:HB3	3:A:36:PRO:HD2	1.94	0.49
3:A:205:THR:HG23	3:A:209:GLU:HG3	1.94	0.49
4:B:45:ILE:HG13	4:B:99:LEU:HD13	1.93	0.49
2:T:2016:DC:H2''	2:T:2017:DG:C8	2.48	0.49
1:P:1022:DDG:H2'	6:A:1024:DAD:H5'1	1.95	0.49
3:A:404:LYS:HA	3:A:409:TYR:HE2	1.77	0.49
3:A:13:GLU:H	3:A:13:GLU:CD	2.16	0.48
3:A:145:ARG:O	3:A:149:GLU:HG3	2.12	0.48
3:A:195:GLU:H	3:A:195:GLU:CD	2.17	0.48
3:A:420:VAL:O	3:A:422:PRO:HD3	2.13	0.48
4:B:28:TRP:N	7:B:5048:HOH:O	2.47	0.48
3:A:35:ARG:HB3	3:A:36:PRO:CD	2.44	0.48
4:B:17:LEU:HA	4:B:84:GLY:HA2	1.96	0.48
3:A:541:VAL:HG23	3:A:541:VAL:O	2.14	0.48
3:A:569:ILE:HG21	3:A:609:ALA:HB1	1.95	0.48
3:A:678:ARG:NH1	3:A:691:ASP:OD1	2.47	0.48
3:A:173:GLN:O	3:A:176:VAL:HG13	2.14	0.47
3:A:98:ILE:HG22	3:A:98:ILE:O	2.15	0.47
1:P:1022:DDG:H5'	7:A:5193:HOH:O	2.14	0.47
3:A:173:GLN:HA	3:A:176:VAL:HG12	1.96	0.47
3:A:110:LEU:HD11	3:A:434:PHE:HZ	1.80	0.47
3:A:597:ASP:OD1	3:A:599:ARG:HD2	2.15	0.47
3:A:478:GLY:O	3:A:482:ARG:HG3	2.15	0.46
3:A:574:VAL:O	3:A:589:LYS:HE3	2.14	0.46
4:B:15:ASP:HB2	7:B:5007:HOH:O	2.15	0.46
3:A:682:ASP:C	3:A:682:ASP:OD2	2.54	0.46
3:A:163:PHE:CG	3:A:164:ASN:N	2.84	0.46
1:P:1022:DDG:C3'	6:A:1024:DAD:H5'1	2.45	0.46
3:A:2:ILE:HD11	3:A:56:ILE:HG12	1.98	0.46
1:P:1018:DG:H2''	1:P:1019:DC:OP2	2.15	0.46
3:A:164:ASN:OD1	3:A:166:GLU:HB3	2.15	0.46
3:A:590:ARG:NH1	3:A:592:TRP:O	2.49	0.46
3:A:699:ASN:OD1	3:A:701:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:288:ARG:HG2	3:A:288:ARG:HH11	1.82	0.45
3:A:273:MET:CE	3:A:284:PRO:HG3	2.47	0.45
4:B:3:LYS:CD	4:B:47:ASP:HA	2.47	0.45
3:A:14:SER:O	3:A:16:THR:HG23	2.16	0.45
3:A:193:PRO:HD3	7:A:5192:HOH:O	2.17	0.45
3:A:551:LEU:HD12	3:A:551:LEU:HA	1.81	0.45
1:P:1016:DG:C2'	1:P:1017:DT:H5''	2.47	0.45
3:A:150:GLN:CB	3:A:152:GLU:OE2	2.65	0.45
3:A:436:ASN:OD1	3:A:438:ALA:HB3	2.17	0.45
3:A:593:ILE:CG2	3:A:594:LYS:N	2.80	0.45
3:A:323:GLY:O	3:A:325:PRO:HD3	2.17	0.44
3:A:292:PRO:HG3	7:B:5058:HOH:O	2.15	0.44
3:A:216:ILE:HB	7:A:5112:HOH:O	2.17	0.44
3:A:94:LEU:HB3	3:A:185:LEU:HD13	1.98	0.44
3:A:638:LEU:HD12	3:A:638:LEU:N	2.32	0.44
3:A:85:ARG:HG3	3:A:222:TRP:CD2	2.53	0.44
3:A:375:ASP:O	3:A:376:ASP:C	2.57	0.44
3:A:583:GLU:OE1	3:A:583:GLU:C	2.56	0.44
4:B:90:LYS:HB3	7:B:5114:HOH:O	2.17	0.44
3:A:281:LYS:HD3	7:A:5091:HOH:O	2.18	0.43
3:A:288:ARG:HG2	3:A:288:ARG:NH1	2.33	0.43
3:A:474:ILE:HD12	3:A:474:ILE:N	2.33	0.43
3:A:204:THR:HB	7:A:5220:HOH:O	2.19	0.43
3:A:583:GLU:CD	3:A:584:GLN:N	2.72	0.43
3:A:22:VAL:HB	3:A:175:VAL:HG21	1.99	0.43
3:A:488:MET:HE1	3:A:496:TYR:CD1	2.53	0.43
4:B:74:GLY:O	4:B:77:THR:OG1	2.36	0.43
3:A:640:HIS:CD2	3:A:647:ALA:HA	2.53	0.43
4:B:23:ILE:CD1	4:B:54:THR:HB	2.46	0.43
3:A:557:GLU:N	3:A:557:GLU:OE1	2.51	0.43
3:A:276:HIS:CD2	3:A:277:PRO:HD2	2.54	0.43
2:T:2009:DC:P	3:A:404:LYS:HZ3	2.42	0.43
3:A:591:ARG:HA	7:A:5127:HOH:O	2.19	0.43
3:A:58:PHE:O	3:A:90:ASP:HA	2.18	0.43
3:A:237:LYS:O	3:A:241:GLU:HG3	2.19	0.42
3:A:481:LEU:HD21	3:A:525:ILE:CG2	2.48	0.42
3:A:538:GLY:N	3:A:548:GLY:HA3	2.35	0.42
3:A:155:VAL:HG12	3:A:156:ASP:N	2.33	0.42
3:A:406:TRP:O	3:A:410:VAL:HG23	2.19	0.42
3:A:35:ARG:HH11	3:A:35:ARG:HG3	1.84	0.42
3:A:263:SER:HG	3:A:331:HIS:CE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:422:PRO:HB2	7:A:5031:HOH:O	2.18	0.42
1:P:1018:DG:H4'	3:A:339:ARG:NH2	2.35	0.42
3:A:481:LEU:HD12	3:A:505:ILE:CG2	2.49	0.42
3:A:336:PRO:O	3:A:342:ILE:HD11	2.19	0.42
3:A:98:ILE:O	3:A:98:ILE:CG2	2.67	0.42
4:B:25:VAL:HA	4:B:56:ALA:O	2.20	0.42
3:A:273:MET:HA	3:A:288:ARG:NH2	2.35	0.41
3:A:359:LYS:HE2	3:A:359:LYS:CA	2.42	0.41
3:A:446:PRO:O	3:A:447:TYR:HB2	2.20	0.41
3:A:106:ASP:OD2	3:A:109:LEU:HD12	2.21	0.41
2:T:2005:DC:H2''	2:T:2006:DT:C5'	2.49	0.41
3:A:24:TYR:CZ	3:A:179:LYS:HE3	2.56	0.41
3:A:193:PRO:HB2	3:A:195:GLU:OE1	2.21	0.41
3:A:502:ASN:HB3	7:A:5071:HOH:O	2.20	0.41
3:A:273:MET:HB2	3:A:288:ARG:HH21	1.85	0.40
3:A:293:LYS:HA	3:A:293:LYS:HD3	1.89	0.40
3:A:365:ASP:OD1	3:A:367:GLU:HB3	2.20	0.40
3:A:569:ILE:CG2	3:A:609:ALA:HB1	2.50	0.40
3:A:276:HIS:HD2	3:A:277:PRO:CD	2.34	0.40
3:A:638:LEU:N	3:A:638:LEU:CD1	2.85	0.40
3:A:676:ALA:O	3:A:679:TRP:HB3	2.21	0.40
3:A:319:GLU:O	3:A:319:GLU:HG3	2.22	0.40
3:A:239:ILE:HD11	3:A:454:ALA:CB	2.52	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
3	A	672/698 (96%)	618 (92%)	44 (6%)	10 (2%)	10 26
4	B	103/108 (95%)	94 (91%)	9 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	775/806 (96%)	712 (92%)	53 (7%)	10 (1%)	12	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	516	PRO
3	A	549	LYS
3	A	579	TRP
3	A	583	GLU
3	A	653	HIS
3	A	322	ALA
3	A	584	GLN
3	A	580	VAL
3	A	478	GLY

### 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	
3	A	561/578 (97%)	537 (96%)	24 (4%)	29	57
4	B	85/87 (98%)	81 (95%)	4 (5%)	26	54
All	All	646/665 (97%)	618 (96%)	28 (4%)	29	57

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	78	ASN
3	A	110	LEU
3	A	131	ARG
3	A	145	ARG
3	A	171	ASN
3	A	181	LEU
3	A	232	PHE
3	A	285	LYS

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Mol	Chain	Res	Type
3	A	332	VAL
3	A	343	GLN
3	A	358	ASP
3	A	368	VAL
3	A	452	ARG
3	A	475	ASP
3	A	505	ILE
3	A	511	ILE
3	A	551	LEU
3	A	557	GLU
3	A	571	GLN
3	A	583	GLU
3	A	599	ARG
3	A	624	LEU
3	A	686	PHE
3	A	700	TRP
4	B	14	THR
4	B	73	ARG
4	B	89	THR
4	B	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	76	GLN
3	A	227	GLN
3	A	266	GLN
3	A	276	HIS
3	A	398	GLN
3	A	570	GLN
3	A	667	GLN
4	B	50	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	DDG	P	1022	2,1	17,23,24	1.17	2 (11%)	15,33,36	3.04	5 (33%)
2	8OG	T	2004	2	18,25,26	1.23	2 (11%)	21,37,40	2.85	6 (28%)

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
1	DDG	P	1022	2,1	-	0/3/18/19	0/3/3/3
2	8OG	T	2004	2	-	1/3/21/22	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	2004	8OG	C6-N1	4.00	1.40	1.33
1	P	1022	DDG	C6-N1	3.63	1.39	1.33
2	T	2004	8OG	C8-N7	-2.22	1.31	1.34
1	P	1022	DDG	C8-N7	-2.18	1.30	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	1022	DDG	C5-C6-N1	-8.68	111.56	123.43
2	T	2004	8OG	C5-C6-N1	-8.66	111.59	123.43
1	P	1022	DDG	C6-N1-C2	5.87	125.25	115.93
2	T	2004	8OG	C6-N1-C2	5.78	125.11	115.93
2	T	2004	8OG	C2'-C1'-N9	-5.74	109.75	116.01
1	P	1022	DDG	C2-N3-C4	-3.08	111.84	115.36
2	T	2004	8OG	C2-N3-C4	-2.95	111.99	115.36
2	T	2004	8OG	N3-C2-N1	-2.53	123.85	127.22
1	P	1022	DDG	N3-C2-N1	-2.52	123.86	127.22
2	T	2004	8OG	C6-C5-C4	-2.15	118.75	120.80
1	P	1022	DDG	C6-C5-C4	-2.02	118.87	120.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	2004	8OG	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	1022	DDG	3	0
2	T	2004	8OG	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z  > 2$
6	DAD	A	1024	5	25,31,31	0.73	0	26,48,48	1.04	2 (7%)

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
6	DAD	A	1024	5	2/2/5/5	5/18/31/31	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1024	DAD	O2G-PG-O1G	2.36	119.92	110.68
6	A	1024	DAD	PA-O3A-PB	-2.33	124.82	132.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1024	DAD	C4'
6	A	1024	DAD	C1'

All (5) torsion outliers are listed below:

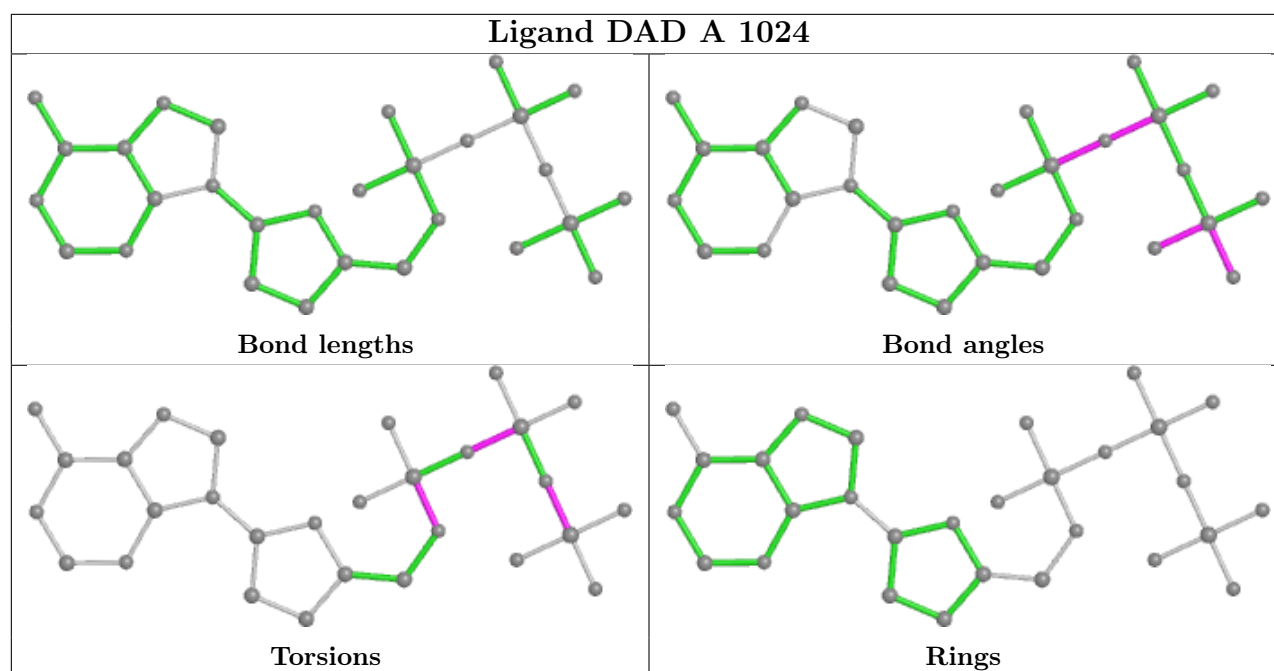
Mol	Chain	Res	Type	Atoms
6	A	1024	DAD	C5'-O5'-PA-O2A
6	A	1024	DAD	C5'-O5'-PA-O3A
6	A	1024	DAD	PA-O3A-PB-O2B
6	A	1024	DAD	PB-O3B-PG-O2G
6	A	1024	DAD	PB-O3B-PG-O3G

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1024	DAD	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	293:LYS	C	294:VAL	N	3.69
1	A	541:VAL	C	542:GLY	N	3.02

## 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	P	12/22 (54%)	0.80	3 (25%) 0 0	25, 55, 120, 122	0
2	T	14/26 (53%)	0.81	3 (21%) 0 0	25, 36, 106, 110	0
3	A	680/698 (97%)	0.06	30 (4%) 34 33	9, 29, 68, 77	0
4	B	105/108 (97%)	0.27	9 (8%) 10 8	22, 36, 54, 60	0
All	All	811/854 (94%)	0.11	45 (5%) 25 24	9, 30, 68, 122	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	294	VAL	4.7
2	T	2017	DG	4.6
3	A	551	LEU	4.3
3	A	542	GLY	4.1
4	B	107	LEU	4.1
3	A	559	THR	4.0
3	A	548	GLY	3.9
3	A	505	ILE	3.8
3	A	558	ASN	3.3
3	A	320	TYR	3.2
3	A	541	VAL	3.0
3	A	358	ASP	3.0
3	A	582	GLY	2.8
4	B	103	LEU	2.8
3	A	317	THR	2.8
3	A	578	GLN	2.7
3	A	543	ALA	2.7
1	P	1011	DG	2.7
1	P	1010	DC	2.6
4	B	20	ASP	2.6
3	A	293	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	516	PRO	2.6
3	A	539	GLN	2.6
4	B	87	ALA	2.6
3	A	321	VAL	2.6
3	A	580	VAL	2.5
4	B	73	ARG	2.5
1	P	1012	DG	2.5
3	A	555	PHE	2.5
3	A	511	ILE	2.4
3	A	540	ILE	2.4
2	T	2015	DC	2.4
3	A	295	GLY	2.4
3	A	503	GLY	2.3
2	T	2016	DC	2.3
4	B	82	LYS	2.3
4	B	22	ALA	2.3
3	A	323	GLY	2.3
3	A	259	GLU	2.2
3	A	114	LYS	2.2
4	B	52	LYS	2.2
3	A	271	THR	2.2
3	A	553	LYS	2.1
4	B	21	GLY	2.1
3	A	512	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	8OG	T	2004	23/24	0.92	0.18	11,19,58,60	0
1	DDG	P	1022	21/22	0.96	0.20	24,27,30,30	0

## 6.3 Carbohydrates [i](#)

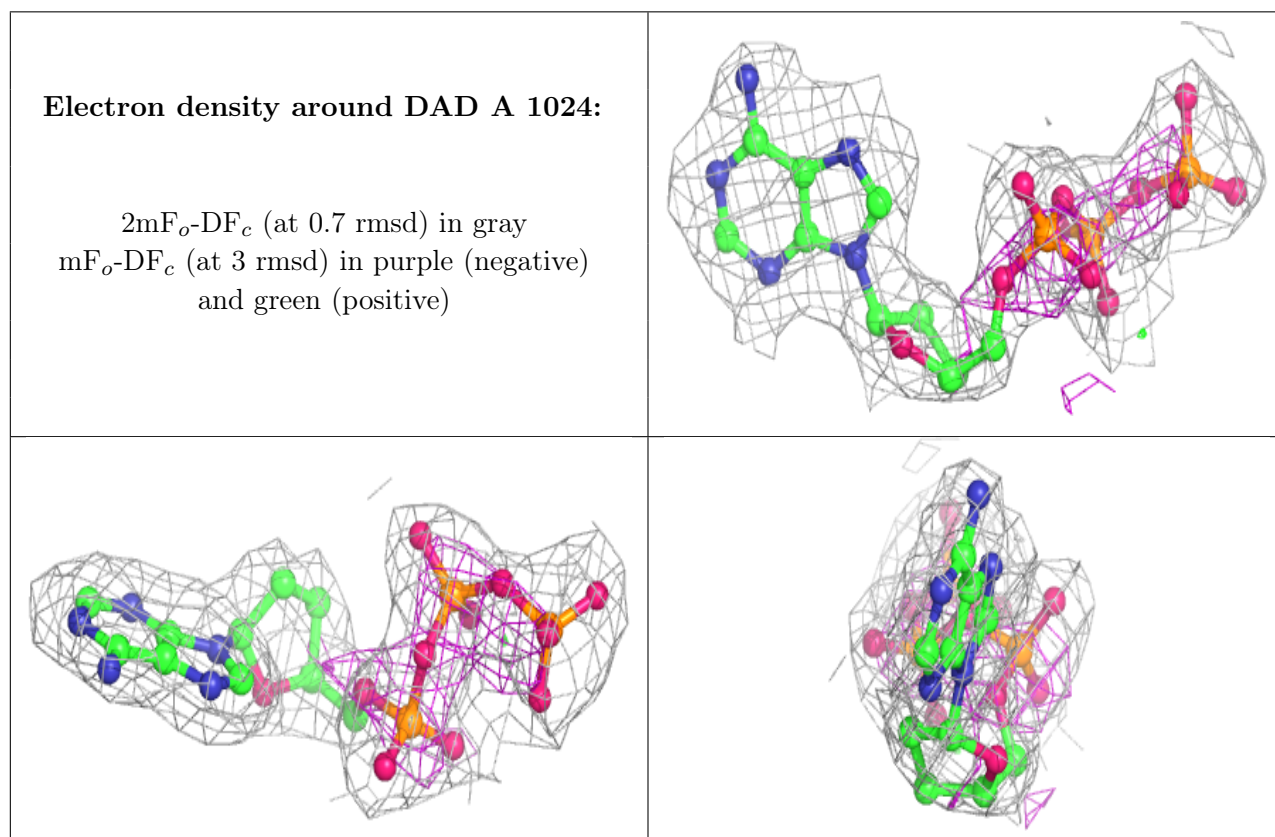
There are no monosaccharides in this entry.

## 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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	A	4003	1/1	0.61	0.29	29,29,29,29	0
5	MG	A	4001	1/1	0.83	0.12	30,30,30,30	0
5	MG	A	4002	1/1	0.90	0.39	48,48,48,48	0
6	DAD	A	1024	29/29	0.93	0.14	28,30,33,34	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.