



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:16 AM UTC

PDB ID : 1ZYQ / pdb_00001zyq
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

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

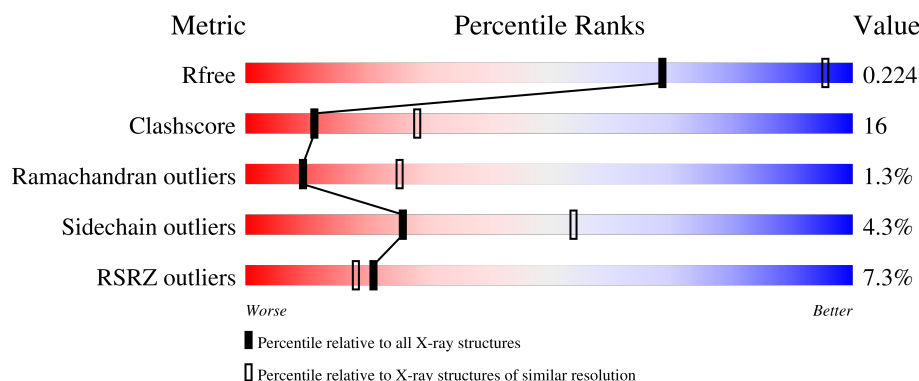
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	18% 14% 41% 5% 41%
2	T	26	12% 31% 19% • • 42%
3	A	698	7% 66% 28% • •
4	B	108	6% 56% 40% • •

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

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
1	P	13	Total	C	N	O	P	0	0	0
			266	125	52	76	13			

- 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
2	T	15	Total	C	N	O	P	0	0	0
			308	144	57	92	15			

- Molecule 3 is a protein called DNA polymerase.

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

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

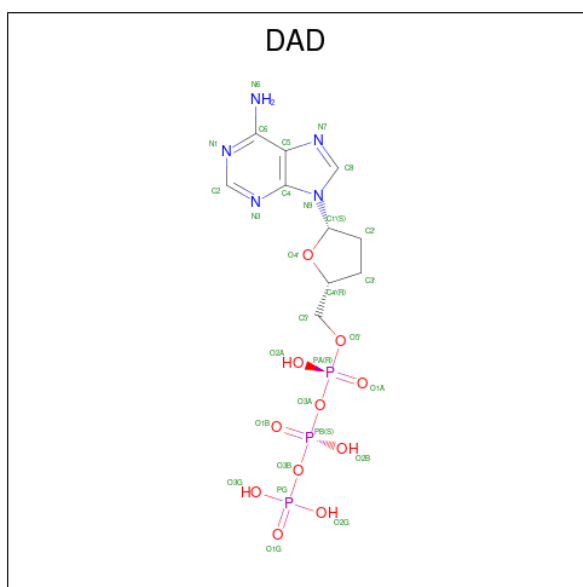
- Molecule 4 is a protein called Thioredoxin 1.

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is 2',3'-DIDEOXYADENOSINE-5'-TRIPHOSPHATE (CCD ID: DAD) (formula: C₁₀H₁₆N₅O₁₁P₃).



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

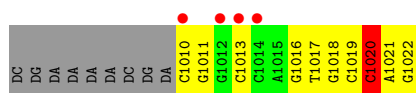
- Molecule 7 is water.

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

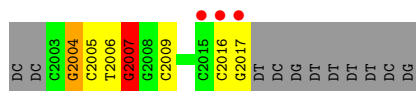
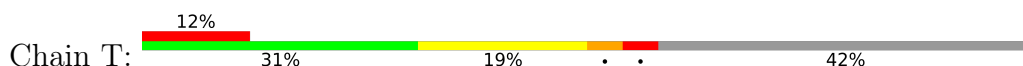
3 Residue-property plots

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.

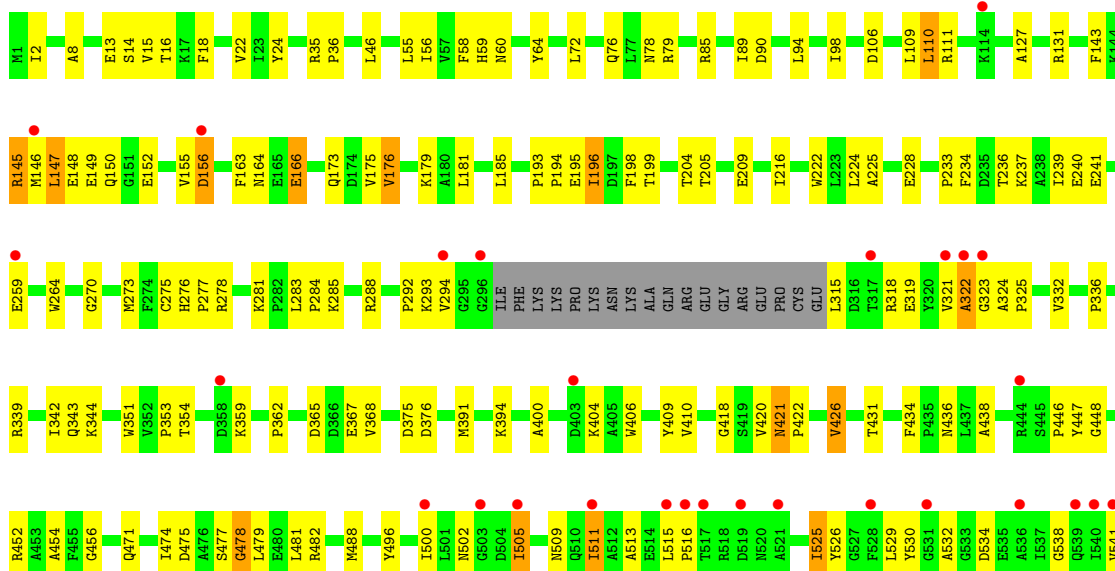
- Molecule 1: 5'-D(*CP*GP*AP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*AP*(DDG))-3'

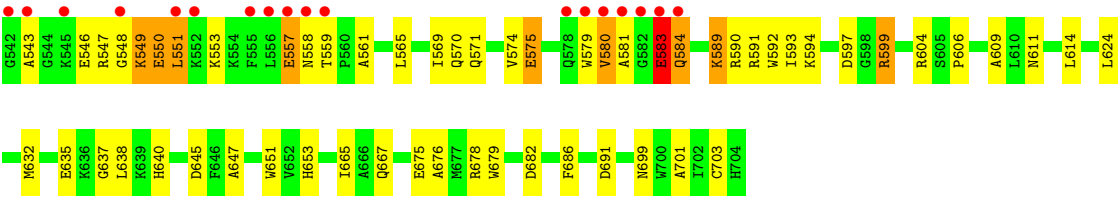


- Molecule 2: 5'-D(*CP*CP*CP*(8OG)P*CP*TP*GP*GP*CP*AP*CP*TP*GP*GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3'

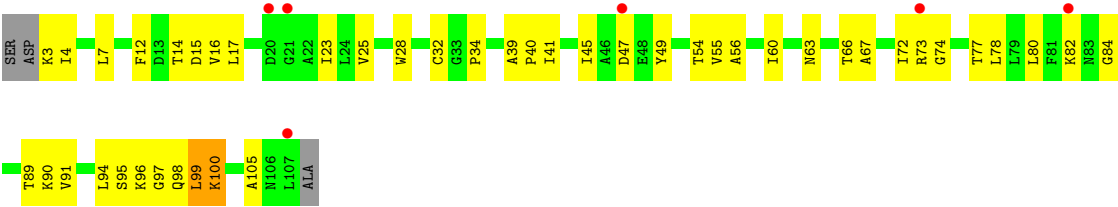


- Molecule 3: DNA polymerase





● Molecule 4: Thioredoxin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.15Å 213.01Å 52.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 2.70 47.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.5 (47.60-2.70) 94.5 (47.60-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.272 0.225 , 0.224	Depositor DCC
R_{free} test set	1958 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7041	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage'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.*

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: DDG, DAD, 8OG, MG

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	0.34	0/274	0.78	1/420 (0.2%)
2	T	0.35	0/317	0.80	1/484 (0.2%)
3	A	0.45	0/5545	0.93	18/7503 (0.2%)
4	B	0.42	0/817	0.96	4/1108 (0.4%)
All	All	0.44	0/6953	0.92	24/9515 (0.3%)

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.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	259	GLU	N-CA-C	-7.52	103.72	113.12
3	A	127	ALA	N-CA-C	7.15	119.75	111.02
3	A	550	GLU	N-CA-C	-6.88	103.83	111.82
3	A	589	LYS	N-CA-C	-6.50	104.39	112.90
4	B	91	VAL	N-CA-C	6.49	117.19	108.11
3	A	166	GLU	N-CA-C	-6.08	104.73	111.36
3	A	703	CYS	N-CA-C	5.96	119.52	112.72
3	A	324	ALA	CA-C-N	5.95	125.86	119.85
3	A	324	ALA	C-N-CA	5.95	125.86	119.85
3	A	479	LEU	N-CA-C	5.87	120.99	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	199	THR	N-CA-C	-5.75	106.03	113.16
4	B	66	THR	N-CA-C	5.73	117.33	111.14
3	A	354	THR	N-CA-C	-5.60	107.45	114.56
3	A	400	ALA	N-CA-C	5.57	122.66	110.80
2	T	2007	DG	N9-C1'-C2'	-5.50	105.24	113.50
1	P	1020	DC	N1-C1'-C2'	-5.47	105.30	113.50
3	A	575	GLU	N-CA-C	-5.38	106.77	113.55
3	A	421	ASN	CA-C-N	5.23	126.38	119.84
3	A	421	ASN	C-N-CA	5.23	126.38	119.84
4	B	63	ASN	CA-C-N	5.05	125.13	119.87
4	B	63	ASN	C-N-CA	5.05	125.13	119.87
3	A	196	ILE	CB-CA-C	-5.05	104.30	111.21
3	A	225	ALA	N-CA-C	-5.04	105.97	111.82
3	A	477	SER	N-CA-C	5.00	117.56	110.10

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	171	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7041	0	6432	215	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 16.

All (215) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:97:GLY:C	7:B:5020:HOH:O	2.42	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
3:A:488:MET:HE2	3:A:496:TYR:HB2	1.83	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
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
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:273:MET:HE1	3:A:284:PRO:HG3	1.88	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:534:ASP:CG	3:A:549:LYS:HG2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:143:PHE:O	3:A:147:LEU:HB2	2.07	0.54
3:A:593:ILE:HG22	3:A:594:LYS:N	2.21	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:13:GLU:H	3:A:13:GLU:CD	2.16	0.53
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
3:A:195:GLU:H	3:A:195:GLU:CD	2.17	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:18:PHE:H	3:A:76:GLN:NE2	2.08	0.51
3:A:682:ASP:C	3:A:682:ASP:OD2	2.54	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
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
3:A:264:TRP:CD1	3:A:344:LYS:HZ3	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:145:ARG:O	3:A:149:GLU:HG3	2.12	0.48
3:A:375:ASP:O	3:A:376:ASP:C	2.57	0.48
3:A:583:GLU:OE1	3:A:583:GLU:C	2.56	0.48
3:A:583:GLU:CD	3:A:584:GLN:N	2.72	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: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
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:146:MET:HE2	3:A:149:GLU:OE1	2.16	0.45
3:A:436:ASN:OD1	3:A:438:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:436:ASN:C	3:A:438:ALA:H	2.25	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:575:GLU:CD	3:A:589:LYS:HE2	2.43	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
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:22:VAL:HB	3:A:175:VAL:HG21	1.99	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:391:MET:HE2	3:A:446:PRO:HB3	2.00	0.42
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
3:A:195:GLU:CD	3:A:195:GLU:N	2.78	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:635:GLU:C	3:A:637:GLY:H	2.27	0.41
3:A:632:MET:HE1	3:A:675:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:148:GLU:C	3:A:150:GLN:H	2.27	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:488:MET:HE3	3:A:561:ALA:HB3	2.04	0.40
3:A:155:VAL:O	3:A:156:ASP:C	2.64	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	672/698 (96%)	618 (92%)	44 (6%)	10 (2%)	8	22
4	B	103/108 (95%)	94 (91%)	9 (9%)	0	100	100
All	All	775/806 (96%)	712 (92%)	53 (7%)	10 (1%)	9	25

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 ⓘ

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%)	538 (96%)	23 (4%)	27	56
4	B	85/87 (98%)	80 (94%)	5 (6%)	18	42
All	All	646/665 (97%)	618 (96%)	28 (4%)	26	54

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	147	LEU
3	A	176	VAL
3	A	181	LEU
3	A	285	LYS
3	A	332	VAL
3	A	368	VAL
3	A	426	VAL
3	A	475	ASP
3	A	505	ILE
3	A	511	ILE

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Mol	Chain	Res	Type
3	A	525	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	667	GLN
3	A	686	PHE
4	B	14	THR
4	B	73	ARG
4	B	89	THR
4	B	99	LEU
4	B	100	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	227	GLN
3	A	276	HIS
3	A	347	GLN
3	A	417	HIS
3	A	450	GLN
3	A	509	ASN
3	A	510	GLN
3	A	520	ASN
3	A	570	GLN
3	A	667	GLN
4	B	106	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	20,23,24	0.42	0	27,33,36	0.49	0
2	8OG	T	2004	2	22,25,26	0.92	1 (4%)	26,37,40	1.52	4 (15%)

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	-	0/7/18/19	0/3/3/3
2	8OG	T	2004	2	-	0/7/21/22	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	2004	8OG	C8-N7	-3.63	1.31	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	2004	8OG	N7-C8-N9	5.10	112.28	106.61
2	T	2004	8OG	C5-N7-C8	-3.29	104.94	109.47
2	T	2004	8OG	O8-C8-N9	-3.10	121.78	126.00
2	T	2004	8OG	C4-C5-N7	2.65	110.92	106.06

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
1	P	1022	DDG	3	0
2	T	2004	8OG	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	30,31,31	0.60	0	42,48,48	0.71	1 (2%)

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	5/22/31/31	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1024	DAD	O2G-PG-O1G	2.33	119.92	110.83

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:

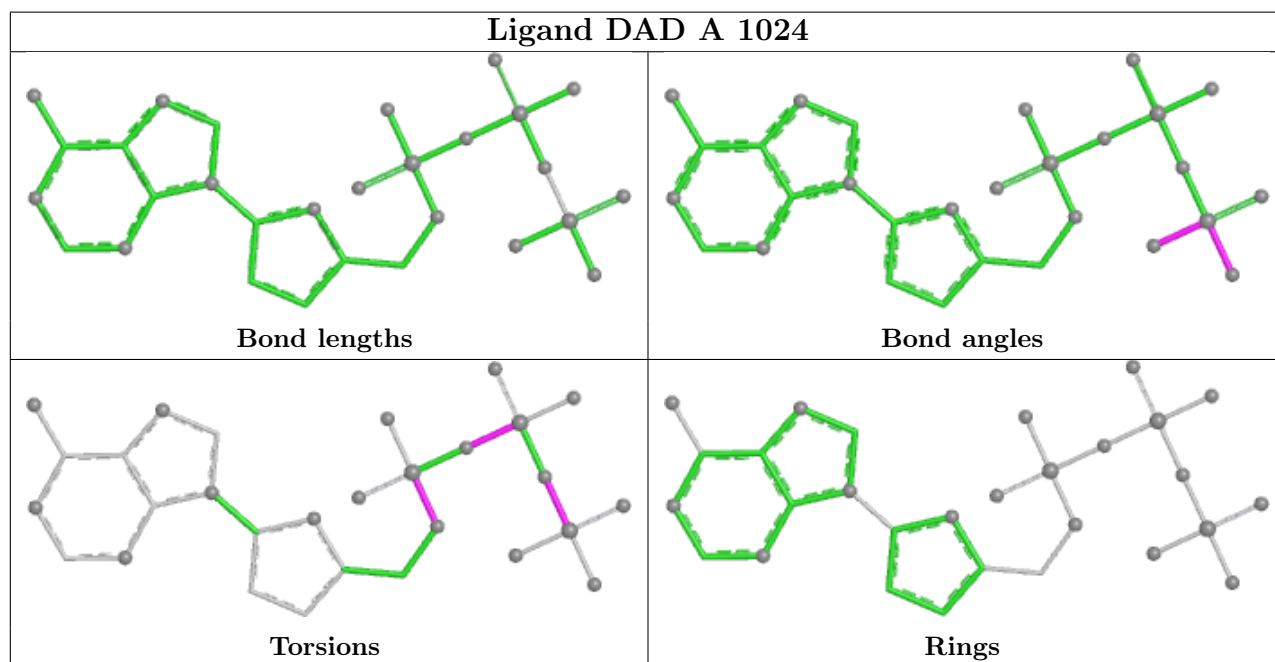
Mol	Chain	Res	Type	Atoms
6	A	1024	DAD	C5'-O5'-PA-O2A
6	A	1024	DAD	C5'-O5'-PA-O3A
6	A	1024	DAD	PA-O3A-PB-O2B
6	A	1024	DAD	PB-O3B-PG-O2G
6	A	1024	DAD	PB-O3B-PG-O3G

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, 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	P	12/22 (54%)	0.96	4 (33%) 1 1	25, 55, 120, 122	0
2	T	14/26 (53%)	0.55	3 (21%) 2 2	25, 36, 106, 110	0
3	A	680/698 (97%)	0.20	46 (6%) 23 20	9, 29, 68, 77	0
4	B	105/108 (97%)	0.39	6 (5%) 29 26	22, 36, 54, 60	0
All	All	811/854 (94%)	0.24	59 (7%) 21 18	9, 30, 68, 122	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	551	LEU	4.6
3	A	296	GLY	4.1
3	A	358	ASP	4.0
2	T	2017	DG	3.8
3	A	555	PHE	3.6
3	A	156	ASP	3.5
3	A	516	PRO	3.4
3	A	583	GLU	3.4
3	A	505	ILE	3.3
3	A	559	THR	3.2
3	A	323	GLY	3.1
3	A	536	ALA	3.1
4	B	20	ASP	3.0
2	T	2016	DC	3.0
3	A	580	VAL	2.9
3	A	579	TRP	2.9
3	A	540	ILE	2.9
3	A	556	LEU	2.8
3	A	321	VAL	2.8
3	A	542	GLY	2.7
3	A	541	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	503	GLY	2.7
3	A	259	GLU	2.7
1	P	1014	DC	2.6
2	T	2015	DC	2.6
3	A	584	GLN	2.6
3	A	114	LYS	2.5
3	A	548	GLY	2.5
3	A	578	GLN	2.5
3	A	511	ILE	2.5
3	A	528	PHE	2.4
3	A	582	GLY	2.4
3	A	545	LYS	2.4
3	A	539	GLN	2.4
3	A	317	THR	2.4
4	B	21	GLY	2.4
3	A	146	MET	2.4
4	B	82	LYS	2.4
3	A	581	ALA	2.4
3	A	552	LYS	2.3
3	A	521	ALA	2.3
3	A	500	ILE	2.3
3	A	322	ALA	2.2
1	P	1010	DC	2.2
1	P	1012	DG	2.2
4	B	47	ASP	2.2
3	A	557	GLU	2.2
1	P	1013	DC	2.2
3	A	294	VAL	2.2
3	A	515	LEU	2.2
3	A	543	ALA	2.1
3	A	531	GLY	2.1
3	A	403	ASP	2.1
4	B	107	LEU	2.1
3	A	517	THR	2.1
3	A	558	ASN	2.1
3	A	444	ARG	2.0
4	B	73	ARG	2.0
3	A	519	ASP	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, 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
2	8OG	T	2004	23/24	0.89	0.15	11,19,58,60	0
1	DDG	P	1022	21/22	0.96	0.09	24,27,30,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

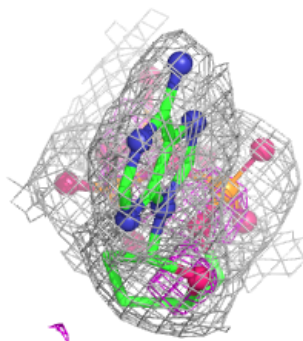
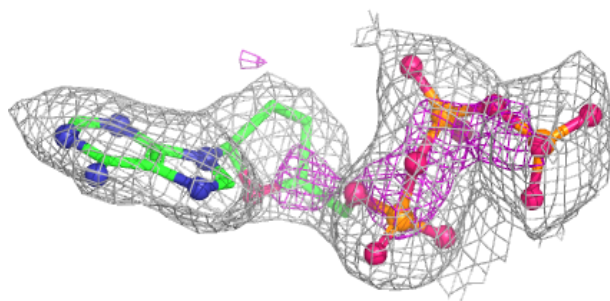
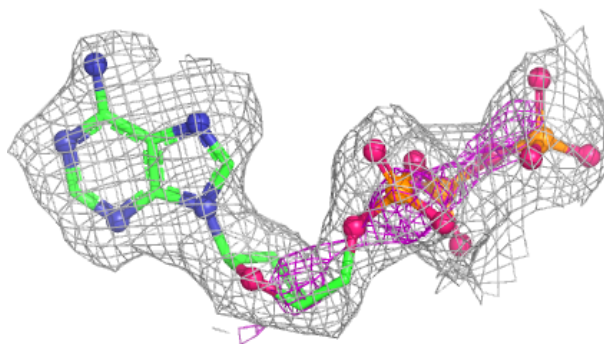
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	MG	A	4003	1/1	0.79	0.20	29,29,29,29	0
5	MG	A	4001	1/1	0.90	0.06	30,30,30,30	0
5	MG	A	4002	1/1	0.94	0.16	48,48,48,48	0
6	DAD	A	1024	29/29	0.94	0.10	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.

Electron density around DAD A 1024:

$2mF_o-DF_c$ (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.