



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:36 PM UTC

PDB ID : 5IIM / pdb_00005iim
Title : Crystal structure of the pre-catalytic ternary extension complex of DNA polymerase lambda with an 8-oxo-dG:dA base-pair
Authors : Burak, M.J.; Guja, K.E.; Garcia-Diaz, M.
Deposited on : 2016-03-01
Resolution : 1.94 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

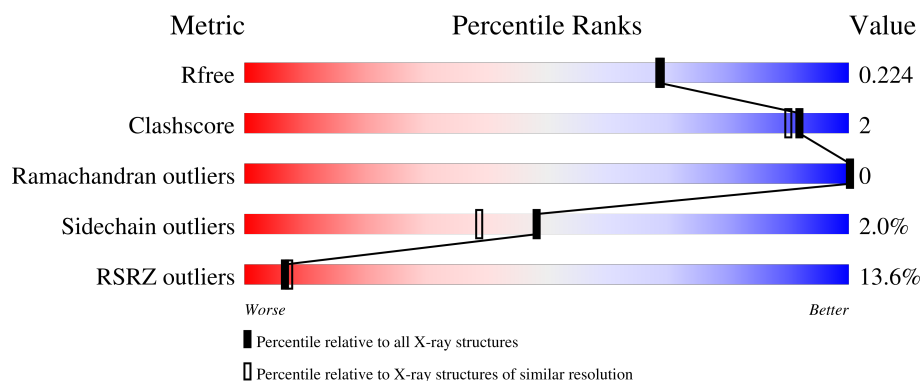
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	334	14% 93% ...
2	D	4	100%
3	P	6	100%
4	T	11	91% 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3301 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 DNA polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	2	0
			2493	1567	451	463	12			

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			

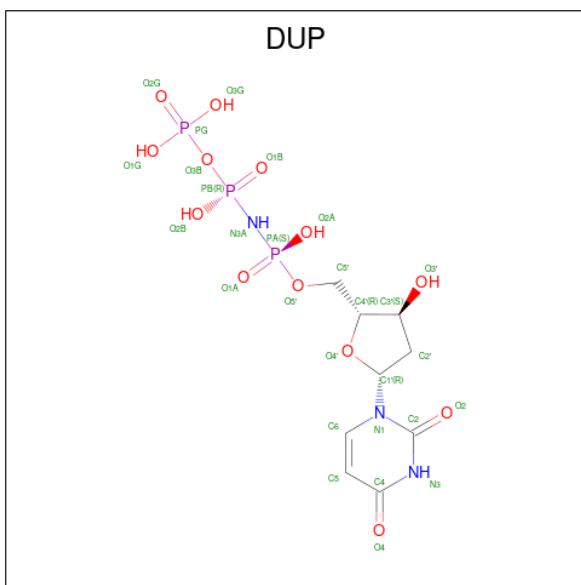
- Molecule 3 is a DNA chain called DNA (5'-D(*CP*AP*GP*TP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	6	Total	C	N	O	P	0	0	0
			121	59	25	32	5			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*GP*CP*AP*(8OG)P*TP*AP*CP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	11	Total	C	N	O	P	0	0	0
			225	107	43	65	10			

- Molecule 5 is 2'-DEOXYURIDINE 5'-ALPHA,BETA-IMIDO-TRIPHOSPHATE (CCD ID: DUP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

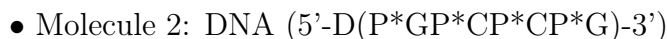
- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Na	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	245	Total	O	0	0
			245	245		
7	D	11	Total	O	0	0
			11	11		
7	P	32	Total	O	0	0
			32	32		
7	T	61	Total	O	0	0
			61	61		

- Molecule 1: DNA polymerase lambda



- Molecule 3: DNA (5'-D(*CP*AP*GP*TP*AP*A)-3')



- Molecule 4: DNA (5'-D(*CP*GP*GP*CP*AP*(8OG)P*TP*AP*CP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.27Å 63.70Å 140.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.95 – 1.94 43.95 – 1.94	Depositor EDS
% Data completeness (in resolution range)	94.4 (43.95-1.94) 94.6 (43.95-1.94)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.183 , 0.216 0.193 , 0.224	Depositor DCC
R_{free} test set	3602 reflections (9.42%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.1	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	0.93	EDS
Total number of atoms	3301	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DUP, 8OG

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	0.28	0/2550	0.44	0/3452
2	D	0.27	0/92	0.48	0/138
3	P	0.38	0/136	0.59	0/208
4	T	0.44	0/225	0.71	0/343
All	All	0.30	0/3003	0.48	0/4141

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2493	0	2429	9	0
2	D	83	0	45	0	0
3	P	121	0	69	0	0
4	T	225	0	125	0	0
5	A	28	0	12	0	0
6	A	2	0	0	0	0
7	A	245	0	0	4	1
7	D	11	0	0	0	0
7	P	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T	61	0	0	0	1
All	All	3301	0	2680	9	1

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 2.

All (9) 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:382:ASP:OD2	7:A:701:HOH:O	2.06	0.73
1:A:459:ASP:OD2	7:A:702:HOH:O	2.12	0.68
1:A:436:ASP:OD1	1:A:437:GLY:N	2.33	0.61
1:A:346[B]:THR:HG23	7:A:868:HOH:O	2.11	0.50
1:A:350:GLN:NE2	7:A:704:HOH:O	2.32	0.48
1:A:311:GLU:HA	1:A:314:ILE:HG22	1.97	0.46
1:A:422:LYS:NZ	1:A:574:ASP:OD2	2.51	0.43
1:A:429:ASP:HB3	1:A:506:PHE:CZ	2.55	0.42
1:A:427:ASP:OD1	1:A:427:ASP:C	2.64	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:741:HOH:O	7:T:121:HOH:O[4_555]	2.02	0.18

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	326/334 (98%)	321 (98%)	5 (2%)	0	100 100

There are no Ramachandran outliers to report.

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
1	A	255/280 (91%)	250 (98%)	5 (2%)	48 39

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	SER
1	A	422	LYS
1	A	506	PHE
1	A	515	SER
1	A	549	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
4	8OG	T	6	4,3	22,25,26	4.19	16 (72%)	26,37,40	1.83	8 (30%)

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	8OG	T	6	4,3	-	0/7/21/22	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	6	8OG	C3'-C4'	-7.49	1.33	1.53
4	T	6	8OG	O4'-C4'	7.39	1.61	1.45
4	T	6	8OG	C8-N7	6.73	1.50	1.38
4	T	6	8OG	C2-N3	5.81	1.47	1.33
4	T	6	8OG	C8-N9	5.67	1.50	1.40
4	T	6	8OG	O4'-C1'	-4.94	1.31	1.42
4	T	6	8OG	C4-N3	4.91	1.45	1.34
4	T	6	8OG	C2-N1	4.35	1.48	1.37
4	T	6	8OG	C2-N2	4.25	1.44	1.34
4	T	6	8OG	C5-N7	4.00	1.44	1.37
4	T	6	8OG	C5-C4	3.87	1.42	1.37
4	T	6	8OG	C6-N1	3.05	1.44	1.38
4	T	6	8OG	C5-C6	3.02	1.50	1.41
4	T	6	8OG	O3'-C3'	2.85	1.49	1.43
4	T	6	8OG	O8-C8	-2.53	1.18	1.23
4	T	6	8OG	C4-N9	2.17	1.43	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	6	8OG	C2-N3-C4	3.67	118.62	112.30
4	T	6	8OG	C4'-O4'-C1'	-3.59	100.98	109.51
4	T	6	8OG	O6-C6-C5	-3.22	119.50	127.26
4	T	6	8OG	C2-N1-C6	-2.94	119.77	125.11
4	T	6	8OG	N9-C4-N3	2.56	129.33	126.13
4	T	6	8OG	C4-C5-N7	2.46	110.57	106.06
4	T	6	8OG	C5-C6-N1	2.32	118.50	112.13
4	T	6	8OG	C5-N7-C8	-2.20	106.44	109.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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	$\# Z > 2$
5	DUP	A	601	6	28,29,29	2.96	14 (50%)	39,45,45	1.57	7 (17%)

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
5	DUP	A	601	6	-	3/19/34/34	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	DUP	O4'-C1'	8.43	1.61	1.42
5	A	601	DUP	O4'-C4'	-6.13	1.31	1.45
5	A	601	DUP	C2'-C1'	-5.67	1.37	1.52
5	A	601	DUP	PB-N3A	3.85	1.73	1.63
5	A	601	DUP	PA-N3A	3.77	1.73	1.63
5	A	601	DUP	PB-O1B	3.32	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	DUP	PB-O3B	2.76	1.62	1.59
5	A	601	DUP	PA-O1A	2.75	1.50	1.46
5	A	601	DUP	O3'-C3'	-2.62	1.37	1.43
5	A	601	DUP	O4-C4	-2.61	1.19	1.24
5	A	601	DUP	C5-C4	-2.53	1.38	1.43
5	A	601	DUP	PA-O2A	-2.35	1.50	1.56
5	A	601	DUP	C4-N3	-2.07	1.35	1.38
5	A	601	DUP	PA-O5'	2.01	1.64	1.57

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	DUP	C4-N3-C2	-4.57	120.94	126.61
5	A	601	DUP	N3-C2-N1	3.53	119.49	114.89
5	A	601	DUP	C5-C4-N3	3.38	119.54	114.80
5	A	601	DUP	O4-C4-C5	-2.96	120.06	125.16
5	A	601	DUP	O1A-PA-N3A	2.45	115.37	111.77
5	A	601	DUP	O5'-PA-O1A	-2.36	107.25	114.27
5	A	601	DUP	O2-C2-N1	-2.08	120.09	122.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

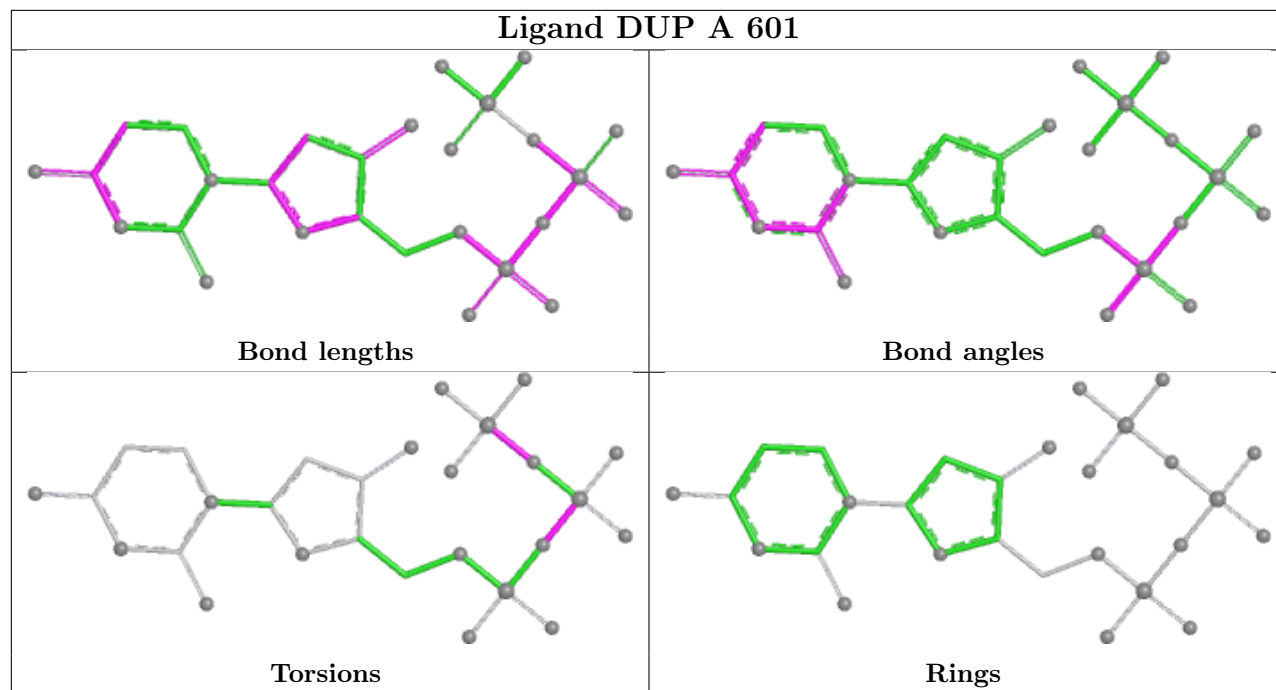
Mol	Chain	Res	Type	Atoms
5	A	601	DUP	PA-N3A-PB-O1B
5	A	601	DUP	PB-O3B-PG-O1G
5	A	601	DUP	PB-O3B-PG-O2G

There are no ring outliers.

No monomer is involved in short contacts.

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	326/334 (97%)	0.84	47 (14%) 6 7	11, 30, 58, 79	2 (0%)
2	D	4/4 (100%)	0.17	0 100 100	29, 35, 35, 36	0
3	P	6/6 (100%)	-0.86	0 100 100	15, 17, 19, 21	0
4	T	10/11 (90%)	-0.47	0 100 100	17, 20, 27, 32	0
All	All	346/355 (97%)	0.77	47 (13%) 7 7	11, 29, 58, 79	2 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	440	HIS	5.7
1	A	250	THR	5.5
1	A	289	PHE	4.8
1	A	314	ILE	4.5
1	A	575	TRP	4.3
1	A	294	THR	3.8
1	A	545	VAL	3.7
1	A	439	SER	3.6
1	A	325	LEU	3.6
1	A	326	ASP	3.5
1	A	442	GLY	3.3
1	A	303	PRO	3.3
1	A	321	HIS	3.3
1	A	446	ARG	3.3
1	A	438	ARG	3.2
1	A	255	HIS	3.2
1	A	290	HIS	3.1
1	A	252	HIS	3.1
1	A	256	ILE	3.0
1	A	292	PRO	3.0
1	A	319	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	320	GLY	3.0
1	A	406	PHE	2.9
1	A	441	ARG	2.8
1	A	317	LEU	2.7
1	A	316	ILE	2.7
1	A	295	SER	2.6
1	A	445	SER	2.6
1	A	547	PRO	2.6
1	A	449	ASP	2.6
1	A	318	GLU	2.6
1	A	546	GLY	2.6
1	A	437	GLY	2.5
1	A	543	CYS	2.5
1	A	288	SER	2.5
1	A	540	THR	2.4
1	A	287	LYS	2.3
1	A	330	GLU	2.3
1	A	291	LYS	2.3
1	A	293	VAL	2.2
1	A	327	HIS	2.2
1	A	299	ALA	2.2
1	A	296	TYR	2.2
1	A	313	ILE	2.1
1	A	436	ASP	2.1
1	A	409	GLY	2.0
1	A	284	ASN	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(Å ²)	Q<0.9
4	8OG	T	6	23/24	0.97	0.06	14,17,20,21	0

6.3 Carbohydrates [i](#)

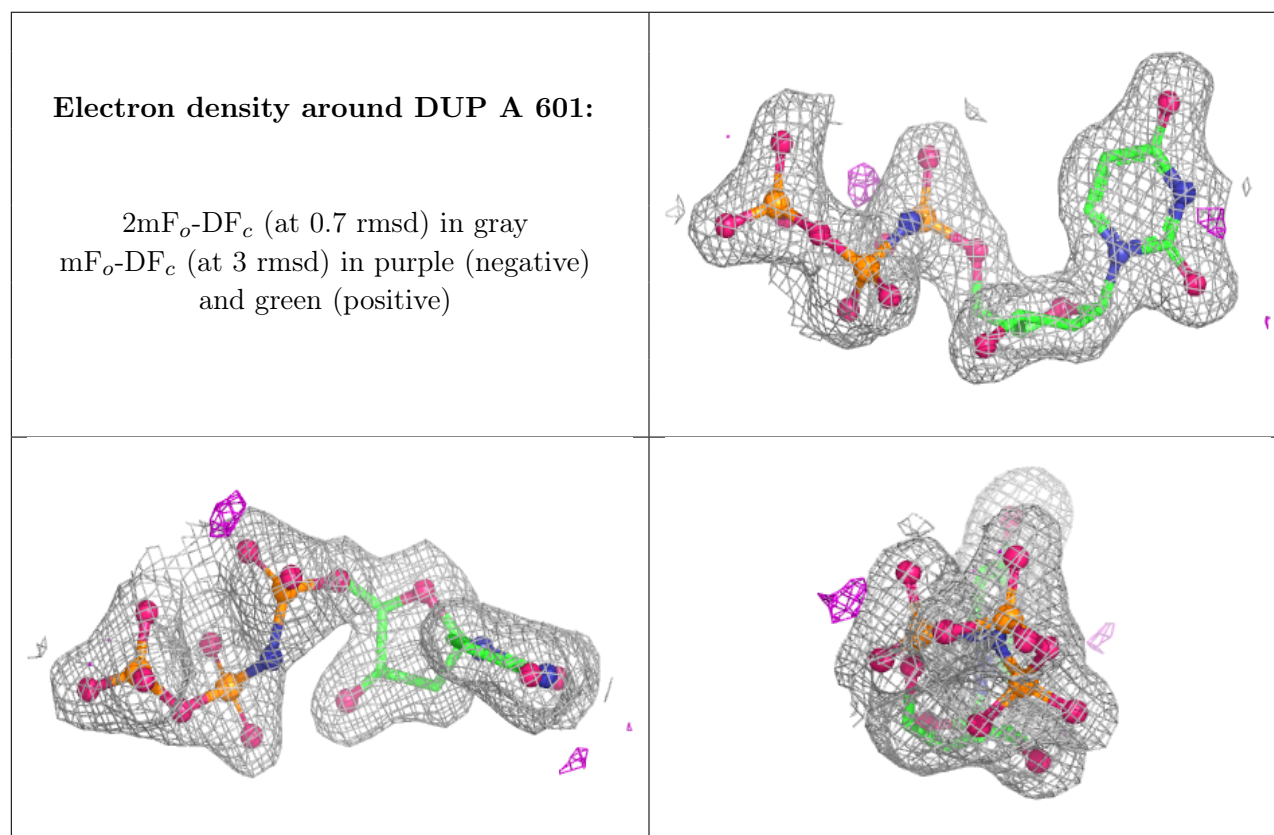
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
5	DUP	A	601	28/28	0.98	0.06	13,17,21,22	0
6	NA	A	602	1/1	0.98	0.05	17,17,17,17	0
6	NA	A	603	1/1	0.99	0.03	16,16,16,16	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.