



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:34 PM UTC

PDB ID : 1X9N / pdb_00001x9n
Title : Crystal Structure of Human DNA Ligase I bound to 5'-adenylated, nicked DNA
Authors : Pascal, J.M.; O'Brien, P.J.; Tomkinson, A.E.; Ellenberger, T.
Deposited on : 2004-08-23
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

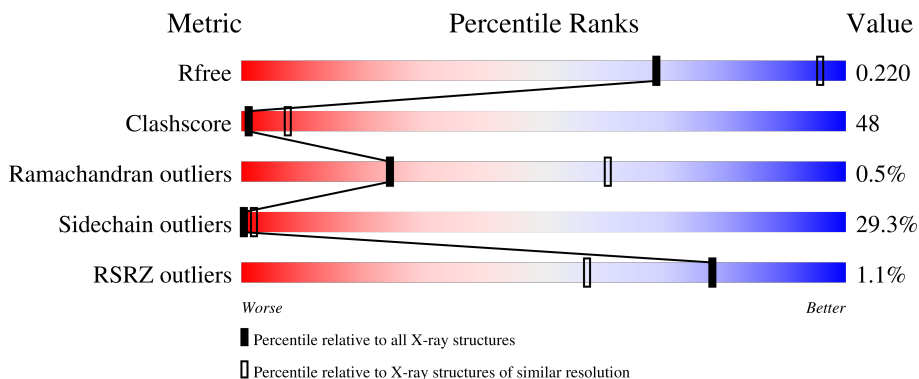
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	B	13	8% 62% 23% 15%
2	C	15	7% 7% 47% 7% 40%
3	D	28	4% 11% 57% • 29%
4	A	688	% 30% 45% 16% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5730 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 dideoxy terminated DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	11	Total	C	N	O	P	0	0	0
			222	107	40	65	10			

- Molecule 2 is a DNA chain called 5'-phosphorylated DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			187	88	35	55	9			

- Molecule 3 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	20	Total	C	N	O	P	0	0	0
			404	192	78	115	19			

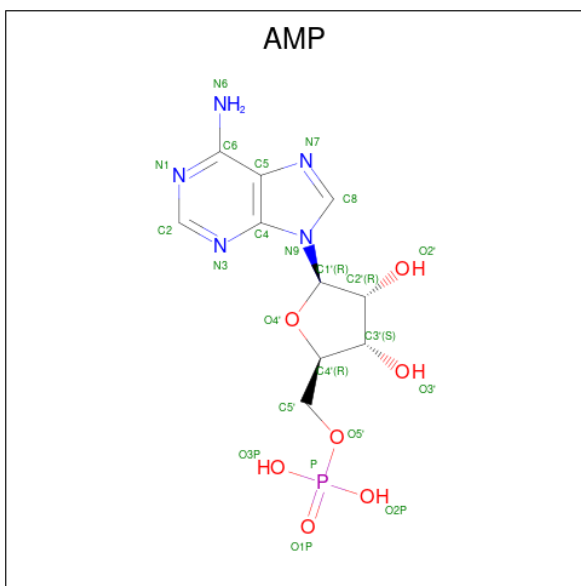
- Molecule 4 is a protein called DNA ligase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	A	632	Total	C	N	O	S	Se	0	0	0
			4894	3109	849	920	10	6			

There are 7 discrepancies between the modelled and reference sequences:

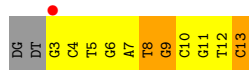
Chain	Residue	Modelled	Actual	Comment	Reference
A	232	MET	-	initiating methionine	UNP P18858
A	308	MSE	MET	modified residue	UNP P18858
A	393	MSE	MET	modified residue	UNP P18858
A	480	MSE	MET	modified residue	UNP P18858
A	501	MSE	MET	modified residue	UNP P18858
A	543	MSE	MET	modified residue	UNP P18858
A	723	MSE	MET	modified residue	UNP P18858

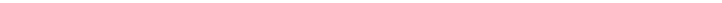
- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

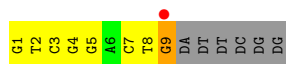


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 1: dideoxy terminated DNA

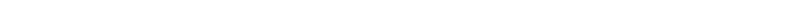


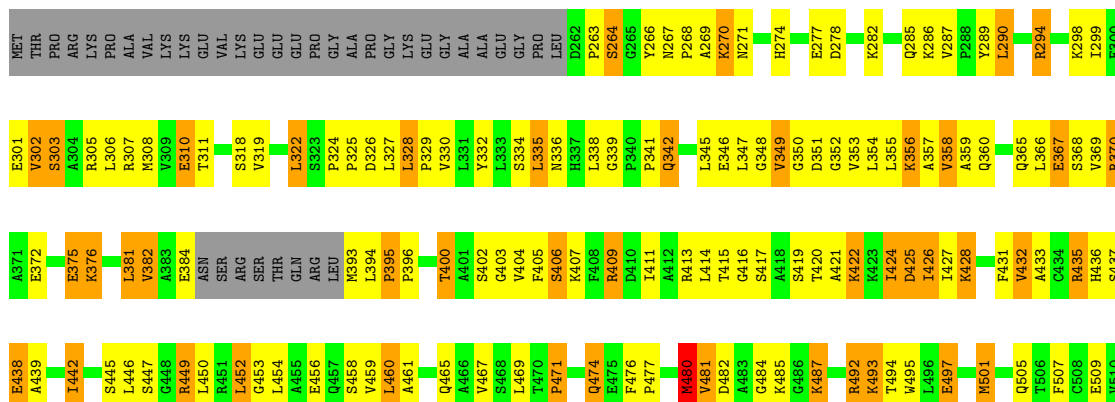
- Chain C:  7% 7% 47% 7% 40%



- Chain D: 4% 11% 57% . 29%



- Chain A:  %



GLY	E843	L780	F710	V646	L579	P511
GLU	A781	A781	L711	D647	E580	D512
ASP	S782	S782	E712	A648	G581	L513
SER	K345	S783	E713	S649	V584	D514
GLY	A847	D784	S714	E650	K585	R515
SER	D848	E785	V715	I651	I586	I516
ASP	L349	D786	K716	Q652	I517	I517
PRO	S850	S787		V653	V519	P518
GLU	L851	E788	C719	Q654	R589	
ASP	S852	E789	E720	V655	N590	E522
THR	P853	L790	G721	C656	Q591	H523
TYR	I854	Q791	L722	L657		
	Y855	A792	M723	Y658	K597	
	P856	I793	V724		Y598	E526
	A857	K794	K725	D661	P599	R527
		K795	T726	L662	D600	L528
		L796	L727	I663	I601	P529
				Y664	I602	E530
				T732	S603	H531
	D863	T798	Y733	L665	R604	C532
	S864	G799	E734	M666	I605	K533
	K866	P800	E735	G667	P606	L534
	G867	I868	A736	S668	K607	S535
	I868	S869	K737	S669	I608	P536
	S870	L870	R738	V671	K609	
	R871	H808	S739	A672	L610	L540
	F872	H809	H740	E673	P611	K541
	P873	Q810	N741	S674	P542	P542
	R874	S811	W742	L675	M543	M543
	F875	L812	L743	S676	T614	L544
	I876	K813	K744	R677	S615	A545
	R877	A814	L745	R678	F616	H546
	V878	L815	K746	R679	I617	P547
		W816	K747	Q680	L618	T548
	K882	L817	D748	L681	D619	R549
	Q883	P818	Y749	L682	T620	G550
	P884	S819	L750	R683	E621	I551
	E885	P820	D751	E684	A622	
	Q886	R821	G752	R685	V623	V554
	A887	P822	W753	F686	A624	L555
	T888	W823	G754	V687	W625	K556
	T889	W824	D755	E688	D626	
	S890	R825	T756	T689		E559
	A891	D826	L757		K629	A562
	Q892	D827	D758	F693	K630	F563
	V893	G828	L759	V694	Q631	T564
	A894	A829	W760	F695	T632	C565
	C895	W830	V761	A696	Q633	E566
	L896	I831	I762	T697	P634	Y567
	Y897	P832		S698	F635	K568
	R898	D833	Y765	L699	Q636	Y569
	K899	H834		D700	V637	D570
	Q900	W835	R768	T701	L638	G571
	S901	L836	G769	K702	T639	Q572
	GLN	D837	K770	D703	T640	
	TLE	P838	R771	I704	R641	
	GLN	S839		E705	K642	Q576
	ASN	A840		Q706	R643	I576
	GLN	W841	R774	I707	K644	H577
	GLN	W842	L779		E645	A578

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	161.89Å 161.89Å 88.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	50.0 (20.00-3.00) 98.6 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.1.80	Depositor
R, R_{free}	0.235 , 0.268 0.215 , 0.220	Depositor DCC
R_{free} test set	1287 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5730	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: DOC, AMP

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	B	0.44	0/228	1.50	6/351 (1.7%)
2	C	0.64	0/209	1.44	1/321 (0.3%)
3	D	0.54	0/453	1.29	2/696 (0.3%)
4	A	0.75	4/4987 (0.1%)	1.06	9/6753 (0.1%)
All	All	0.72	4/5877 (0.1%)	1.12	18/8121 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	480	MSE	SE-CE	6.81	2.15	1.95
4	A	471	PRO	CA-CB	-5.56	1.49	1.54
4	A	480	MSE	CA-C	-5.49	1.47	1.53
4	A	501	MSE	SE-CE	5.37	2.11	1.95

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	DT	O4'-C1'-N1	8.54	121.21	108.40
3	D	18	DC	P-O5'-C5'	-7.66	108.52	120.00
1	B	8	DT	C5'-C4'-O4'	7.10	120.05	109.40
1	B	8	DT	O5'-C5'-C4'	7.06	121.39	110.80
1	B	8	DT	O3'-P-O5'	-6.75	93.87	104.00

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	B	222	0	126	18	0
2	C	187	0	102	15	0
3	D	404	0	224	30	0
4	A	4894	0	4925	479	0
5	C	23	0	12	3	0
All	All	5730	0	5389	531	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 48.

The worst 5 of 531 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)
4:A:480:MSE:SE	4:A:480:MSE:CE	2.15	1.44
4:A:548:THR:CG2	4:A:745:LEU:HD13	1.72	1.19
2:C:7:DC:H2''	2:C:8:DT:H5''	1.24	1.15
4:A:400:THR:HG22	4:A:403:GLY:H	1.08	1.14
4:A:551:ILE:CD1	4:A:707:ILE:HG22	1.79	1.13

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
4	A	628/688 (91%)	559 (89%)	66 (10%)	3 (0%)	24 60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	748	ASP
4	A	753	VAL
4	A	644	LYS

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
4	A	525/576 (91%)	371 (71%)	154 (29%)	0 2

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	745	LEU
4	A	866	LYS
4	A	756	THR
4	A	815	LEU
4	A	885	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	810	GLN
4	A	886	GLN
4	A	594	ASN
4	A	652	GLN
4	A	706	GLN

5.3.3 RNA [i](#)

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	$\# Z > 2$
1	DOC	B	13	3,1	16,19,20	0.71	0	20,26,29	1.65	3 (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	DOC	B	13	3,1	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	DOC	C2'-C1'-N1	-3.88	105.04	112.40
1	B	13	DOC	C4'-O4'-C1'	-3.39	106.61	109.81
1	B	13	DOC	C3'-C2'-C1'	-3.13	99.26	102.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	13	DOC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
5	AMP	C	100	2	25,25,25	1.13	3 (12%)	37,38,38	1.87	9 (24%)

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	AMP	C	100	2	-	1/10/26/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	100	AMP	C5-N7	-2.77	1.34	1.39
5	C	100	AMP	C2-N3	2.45	1.38	1.33
5	C	100	AMP	C2-N1	2.42	1.38	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	100	AMP	N3-C2-N1	-5.10	120.87	128.58
5	C	100	AMP	C5-C4-N3	-4.99	119.85	126.72
5	C	100	AMP	C5-N7-C8	3.47	108.90	103.45
5	C	100	AMP	N9-C8-N7	-3.46	109.03	113.94
5	C	100	AMP	C2-N3-C4	3.32	119.95	111.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

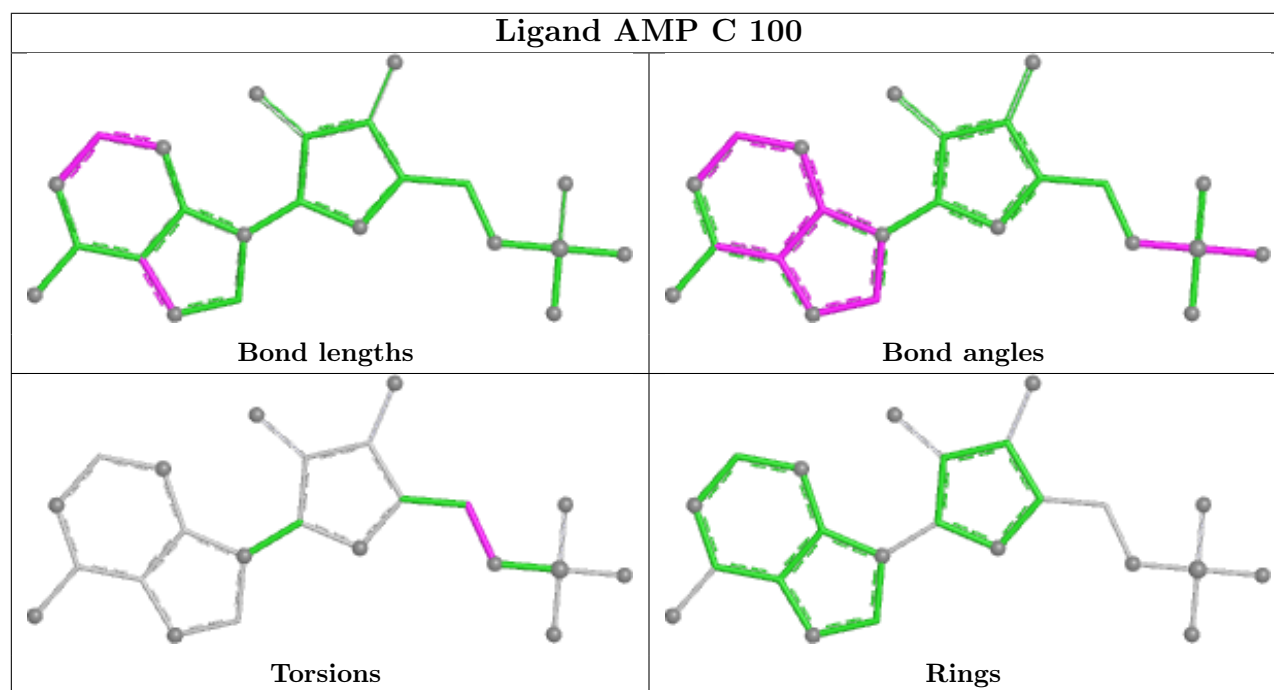
Mol	Chain	Res	Type	Atoms
5	C	100	AMP	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	100	AMP	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	B	10/13 (76%)	0.40	1 (10%) 12 7	44, 50, 65, 66	0
2	C	9/15 (60%)	0.52	1 (11%) 10 6	40, 46, 55, 61	0
3	D	20/28 (71%)	0.51	1 (5%) 34 18	38, 46, 58, 70	0
4	A	626/688 (90%)	-0.05	4 (0%) 85 69	26, 41, 50, 61	0
All	All	665/744 (89%)	-0.02	7 (1%) 78 57	26, 41, 52, 70	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	26	DC	3.6
4	A	581	GLY	2.7
4	A	644	LYS	2.6
1	B	3	DG	2.6
2	C	9	DG	2.6

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
1	DOC	B	13	18/19	0.97	0.06	35,37,42,42	0

6.3 Carbohydrates [i](#)

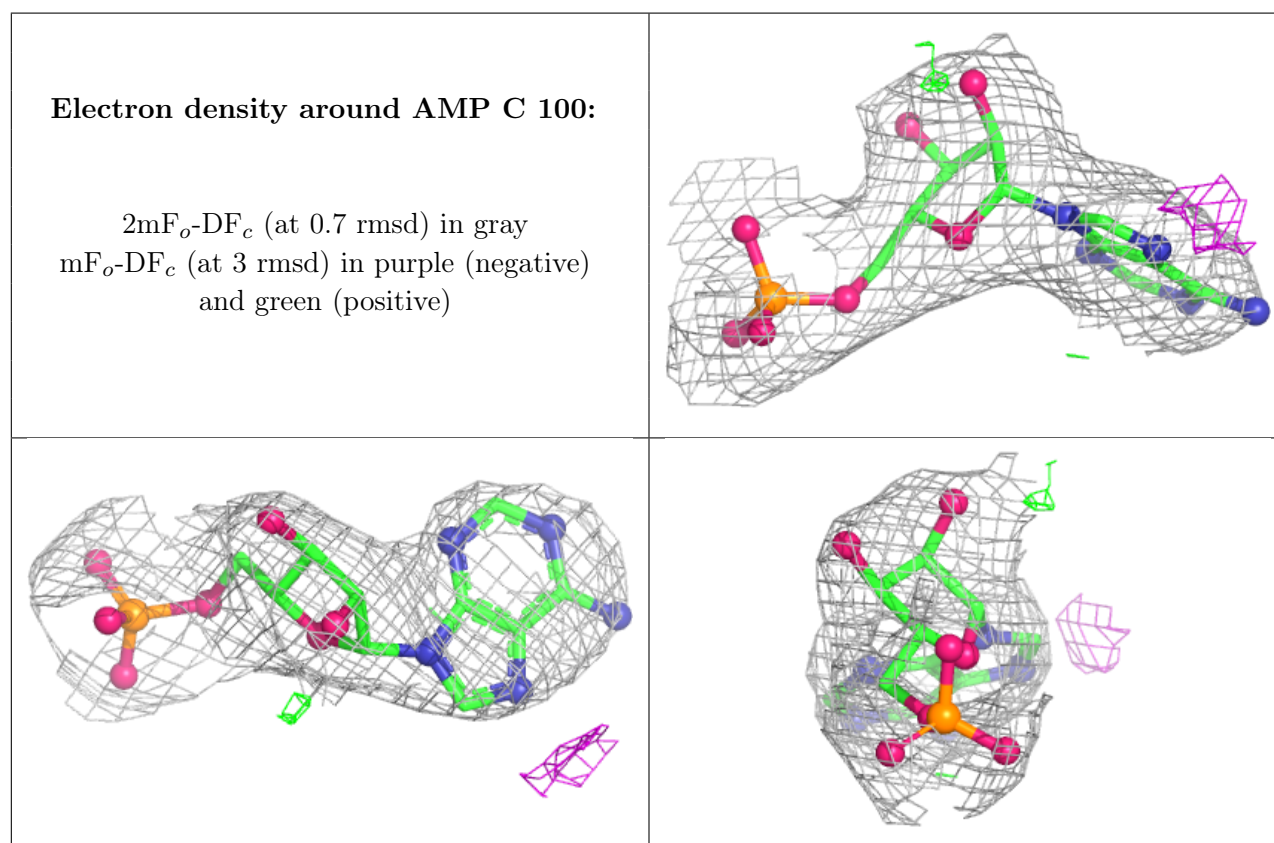
There are no oligosaccharides in this entry.

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	AMP	C	100	23/23	0.95	0.08	36,38,45,48	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.