



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 01:57 PM UTC

PDB ID : 1V9P / pdb_00001v9p
Title : Crystal Structure Of Nad⁺-Dependent DNA Ligase
Authors : Lee, J.Y.; Chang, C.; Song, H.K.; Moon, J.; Yang, J.K.; Kim, H.K.; Kwon, S.K.; Suh, S.W.
Deposited on : 2004-01-27
Resolution : 2.90 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

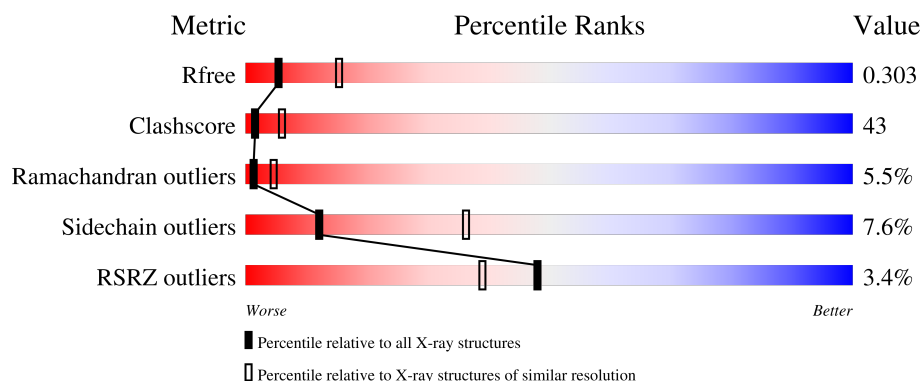
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	584	2% 39% 49% 10% .
1	B	584	5% 39% 52% 8% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9768 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.

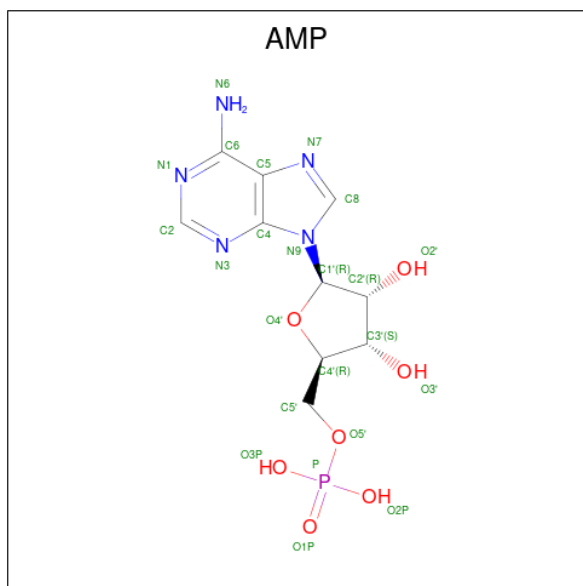
- Molecule 1 is a protein called DNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4742	3000	860	871	11			
1	B	584	Total	C	N	O	S	0	0	0
			4742	3000	860	871	11			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 22	C 10	N 5	O 6	P 1	0	0
3	B	1	Total 22	C 10	N 5	O 6	P 1	0	0

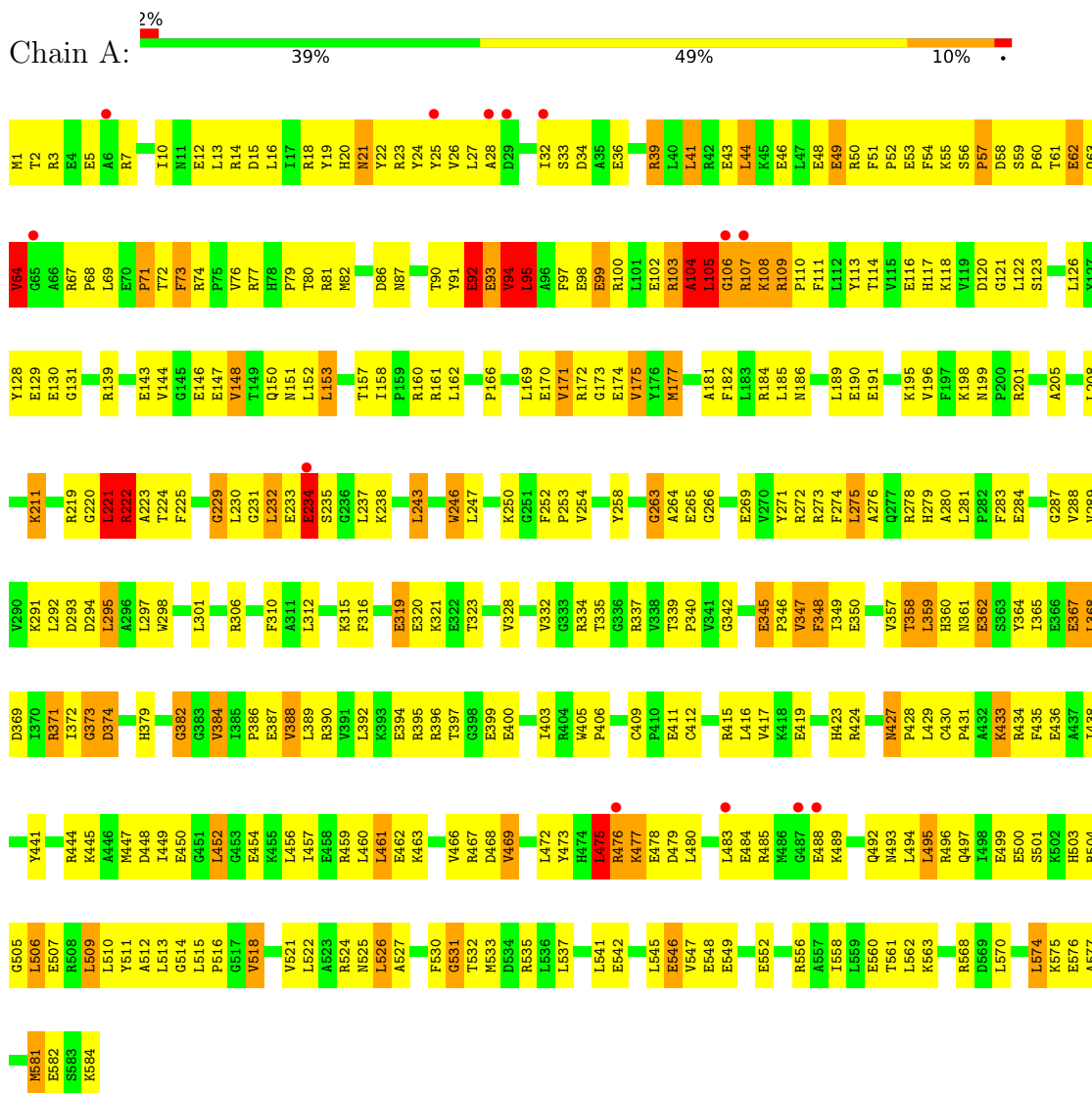
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total 120	O 120	0	0
4	B	118	Total 118	O 118	0	0

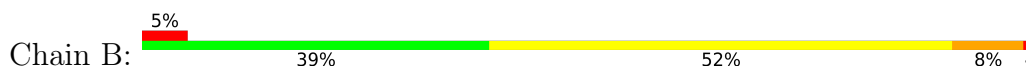
3 Residue-property plots

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: DNA ligase



• Molecule 1: DNA ligase



M2001	A2066	G2131	L2221	D2286	I2365	P2496	L2495	V2571
T2002	R2067	V2132	R2222	L2292	L2368	N2427	R2496	R2572
R2003	P2068		A2223	L2293	L2369	P2428	Q2497	R2573
E2004		T2138	T2224	D2293	D2369	L2428	L2498	L2574
A2005	P2071	R2139	F2225	G2294	I2370	C2430	E2499	K2575
E2006	T2072	G2140	Y2226	L2295	R2371	A2432	E2500	
R2007	D2141	D2140	A2227	A2296	G2372	K2433	S2501	M2581
R2008	F2073	D2142	L2228	L2297	G2373	K2434	K2502	E2582
R2009	P2074	E2143	G2229	K2298	D2374	R2435	H2503	S2583
L2010	R2075	O2143	L2230	E2300	V2376	E2436	R2504	K2584
N2011	V2076	G2145	L2231	E2300	V2376		G2505	
E2012	R2077	G2145	L2232	L2301	L2377	A2437	L2506	
L2013	H2078	E2146	E2233	G2302	V2378	I2438	E2507	
R2014	T2080	E2147	E2234	Y2303	H2379	R2439	R2508	
D2015		V2148	E2235	T2304	K2380	H2440	L2509	
L2016	D2086	Q2150	G2236	P2304	A2381	Y2441	L2510	
L2017	N2087	Q2150	L2237	P2308	G2382	A2442	V2511	
R2018	A2088	N2151	K2238	R2309	G2383	S2443	A2512	
Y2019	F2089	L2153	S2239		V2384	R2444	L2513	
H2020	T2090		Q2240	K2315	L2385	K2445	G2514	
N2021	Y2091	T2157	Y2241	F2316	P2386	A2446	L2515	
Y2022	E2092		E2242	P2317	E2387	M2447		
R2023	E2093	R2160	L2243	E2320	V2388		V2518	
Y2024	V2094	R2161	L2244		L2389	G2451	G2519	
Y2025	L2095	L2162	W2246		R2390	L2452	E2520	
V2026	A2096		L2247		V2391		V2521	
L2027	F2097	P2166			L2392	K2455	L2522	
A2028	E2098				K2393	L2456	A2523	
D2029	E2099	L2169	K2250	D2327	E2394	I2457		
P2030	R2100	E2170	G2251	V2329	R2395		L2526	
E2031	L2101	V2171	F2252	F2330	R2396		A2527	
L2032	L2102	R2172	P2253	R2331	T2397	L2461		
S2033	R2103	G2173	V2254	V2332	G2398	E2462	F2530	
	A2104	E2174	E2255	G2333	E2399	K2463	G2531	
E2036	L2105	V2175	H2256	R2334	E2400	L2464	T2532	
Y2037	G2106		G2257	T2335	R2401	V2465	M2533	
D2038	R2107		Y2258	G2336	P2402	V2466		
R2039	K2108		E2259	R2337	F2403	R2467	A2539	
L2041	R2109		K2260	T2338	R2404	D2468	S2540	
R2042	F2111		A2261	T2339	W2405	V2469	L2541	
E2043	L2112		L2262	P2340	P2406	A2470	E2542	
K2044	Y2113		G2263	V2341	E2407		E2543	
E2046	T2114		E2264	G2342	T2408	Y2473	E2546	
L2047	V2115		G2266		C2409	H2474	V2547	
E2048	E2116		V2267	E2345	F2410	L2475	E2548	
R2049	H2117		E2268	P2346	E2411	R2476	E2549	
R2050	K2118		E2269	F2348	G2412	K2477		
	V2119			E2350	G2413	E2478		
	D2120		R2273	G2351	H2414		E2552	
F2054	G2121				R2415	E2484	L2553	
K2055	L2122		Q2277	V2357	L2416	R2485	T2554	
S2056	S2123		R2278	V2357	K2417	P2486	A2555	
D2058	V2124		H2279	T2358	E2418	E2487	R2556	
	N2125		A2280	L2359	E2419	K2488		
E2062	L2126		L2281	R2360	G2420	K2489	K2563	
Q2063	Y2127		P2282	V2361	V2422	A2491	D2564	
V2064	Y2128		F2283	E2362	R2423	Q2492	P2565	
	E2129		E2284	S2363	R2424	N2493	A2566	
G2065	E2130		A2285	Y2364	C2425	L2494	L2570	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.21Å 117.33Å 97.48Å 90.00° 115.09° 90.00°	Depositor
Resolution (Å)	19.93 – 2.90 19.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.4 (19.93-2.90) 95.5 (19.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.293 0.244 , 0.303	Depositor DCC
R_{free} test set	3869 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9768	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: AMP, ZN

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	0.60	6/4832 (0.1%)	1.11	41/6514 (0.6%)
1	B	0.53	5/4832 (0.1%)	1.04	29/6514 (0.4%)
All	All	0.57	11/9664 (0.1%)	1.08	70/13028 (0.5%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	LEU	N-CA	-10.07	1.33	1.46
1	B	2120	ASP	C-N	-8.30	1.21	1.33
1	B	2360	HIS	C-N	-8.10	1.22	1.33
1	B	2359	LEU	C-N	-7.51	1.23	1.33
1	B	2361	ASN	CA-C	-7.17	1.43	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	LEU	N-CA-C	-11.51	97.37	112.68
1	A	359	LEU	CB-CA-C	10.93	132.16	110.42
1	A	359	LEU	N-CA-C	-10.67	88.08	110.80
1	B	2360	HIS	N-CA-C	9.88	131.85	110.80
1	A	94	VAL	CB-CA-C	-8.97	96.57	111.29

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	4742	0	4797	416	0
1	B	4742	0	4794	399	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	12	2	0
3	B	22	0	12	1	0
4	A	120	0	0	15	0
4	B	118	0	0	6	0
All	All	9768	0	9615	815	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 43.

The worst 5 of 815 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:B:2360:HIS:O	1:B:2361:ASN:HB3	1.37	1.11
1:A:10:ILE:HG23	1:A:14:ARG:NH1	1.68	1.09
1:A:166:PRO:CG	1:A:234:GLU:HB3	1.88	1.03
1:A:537:LEU:HD22	1:A:568:ARG:HE	1.24	1.02
1:B:2360:HIS:O	1:B:2361:ASN:CB	2.00	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	582/584 (100%)	478 (82%)	71 (12%)	33 (6%)	1 4
1	B	582/584 (100%)	463 (80%)	88 (15%)	31 (5%)	1 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1164/1168 (100%)	941 (81%)	159 (14%)	64 (6%)	1 4

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	64	VAL
1	A	94	VAL
1	A	104	ALA
1	A	109	ARG

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	499/499 (100%)	460 (92%)	39 (8%)	11 35
1	B	499/499 (100%)	462 (93%)	37 (7%)	13 38
All	All	998/998 (100%)	922 (92%)	76 (8%)	12 36

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2240	GLN
1	B	2506	LEU
1	B	2255	GLU
1	B	2409	CYS
1	B	2526	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2150	GLN
1	B	2210	GLN
1	B	2497	GLN

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Mol	Chain	Res	Type
1	B	2277	GLN
1	B	2202	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AMP	B	2700	-	21,24,25	1.58	3 (14%)	30,35,38	2.34	8 (26%)
3	AMP	A	700	-	21,24,25	1.51	4 (19%)	30,35,38	2.32	9 (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
3	AMP	B	2700	-	-	0/7/25/26	0/3/3/3
3	AMP	A	700	-	-	1/7/25/26	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	AMP	C5-N7	-4.60	1.30	1.39
3	B	2700	AMP	C5-N7	-4.54	1.30	1.39
3	B	2700	AMP	C1'-N9	2.78	1.54	1.46
3	A	700	AMP	C1'-N9	2.44	1.53	1.46
3	B	2700	AMP	C5-C4	2.35	1.43	1.39

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2700	AMP	N3-C2-N1	-6.60	118.58	128.58
3	A	700	AMP	N3-C2-N1	-6.34	118.99	128.58
3	B	2700	AMP	C5-C4-N3	-5.56	119.06	126.72
3	A	700	AMP	C5-C4-N3	-5.49	119.16	126.72
3	B	2700	AMP	C2-N3-C4	4.56	122.97	111.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

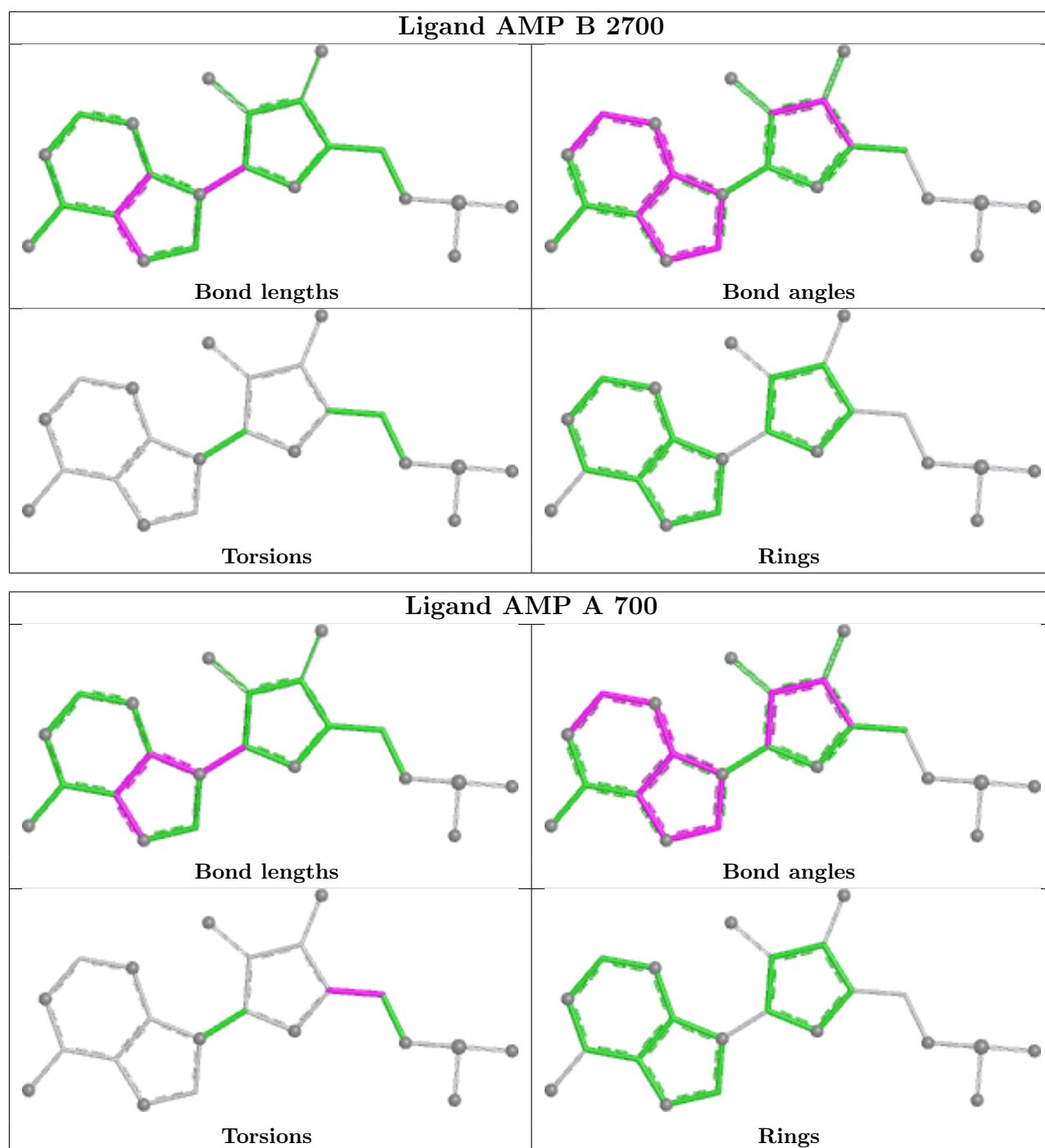
Mol	Chain	Res	Type	Atoms
3	A	700	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2700	AMP	1	0
3	A	700	AMP	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](#)

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	A	584/584 (100%)	0.08	13 (2%) 62 53	12, 46, 92, 142	0
1	B	584/584 (100%)	0.17	27 (4%) 37 29	12, 50, 98, 151	0
All	All	1168/1168 (100%)	0.13	40 (3%) 48 39	12, 48, 95, 151	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2383	GLY	5.0
1	B	2064	VAL	4.4
1	B	2121	GLY	4.2
1	B	2122	LEU	4.1
1	A	106	GLY	3.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

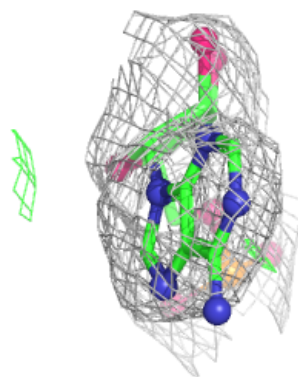
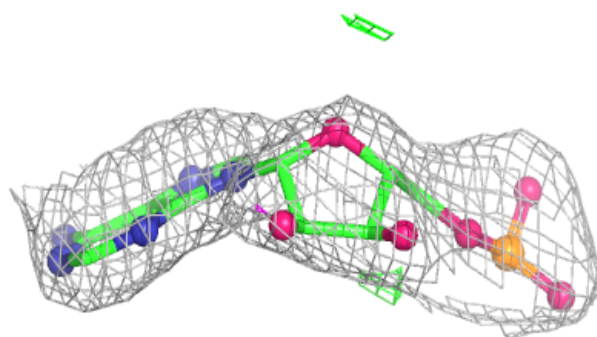
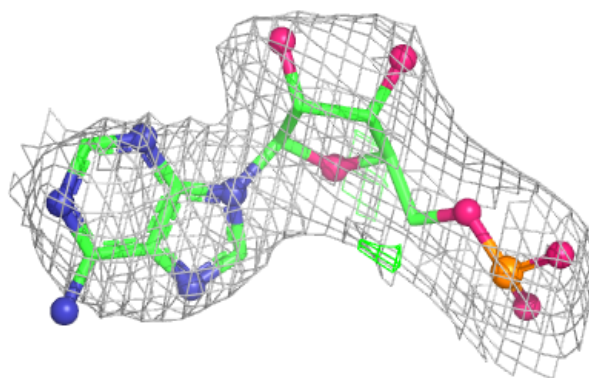
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

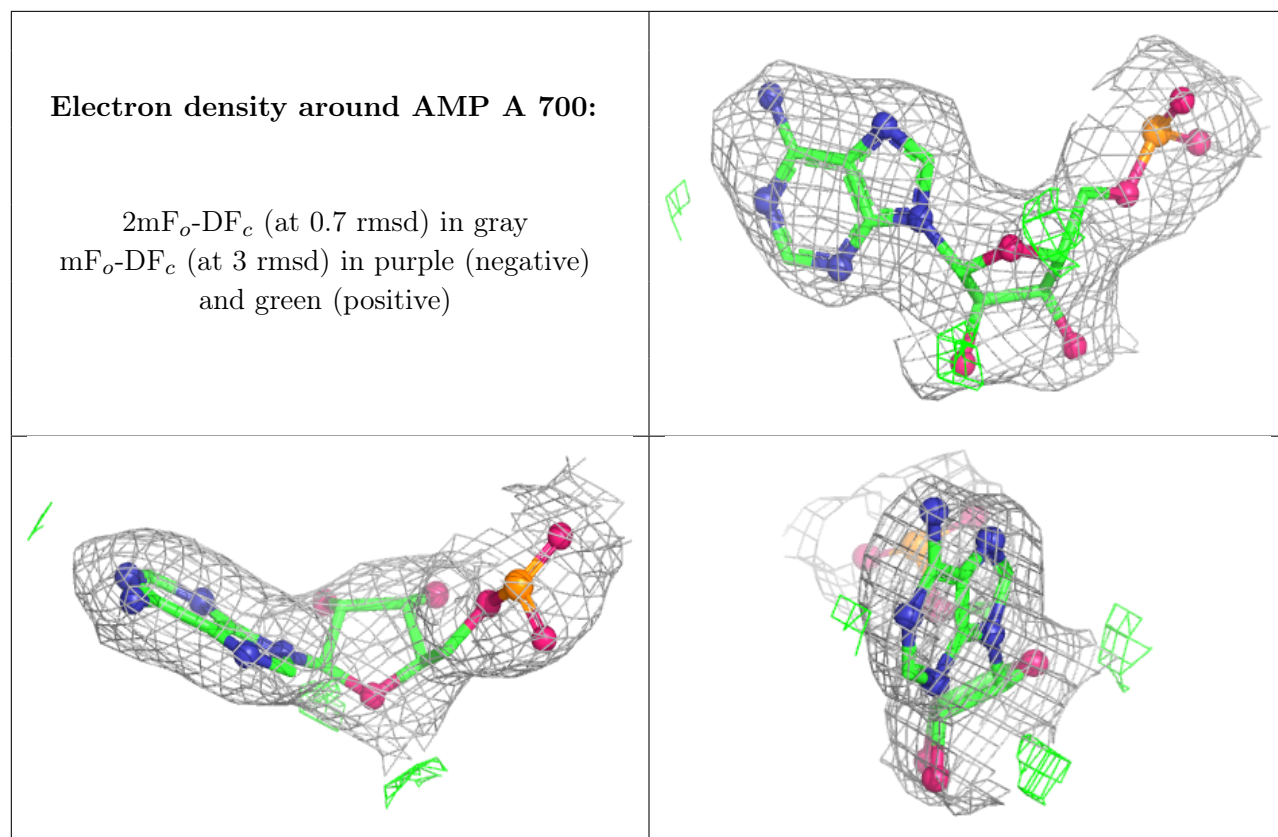
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AMP	B	2700	22/23	0.90	0.13	81,90,93,93	0
3	AMP	A	700	22/23	0.92	0.10	49,53,56,57	0
2	ZN	B	2701	1/1	0.98	0.04	29,29,29,29	0
2	ZN	A	701	1/1	0.99	0.04	19,19,19,19	0

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 AMP B 2700:

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.