



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:36 AM UTC

PDB ID : 1WAF / pdb_00001waf
Title : DNA POLYMERASE FROM BACTERIOPHAGE RB69
Authors : Wang, J.; Satter, A.K.M.A.; Wang, C.C.; Karam, J.D.; Konigsberg, W.H.;
Steitz, T.A.
Deposited on : 1997-04-13
Resolution : 3.20 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

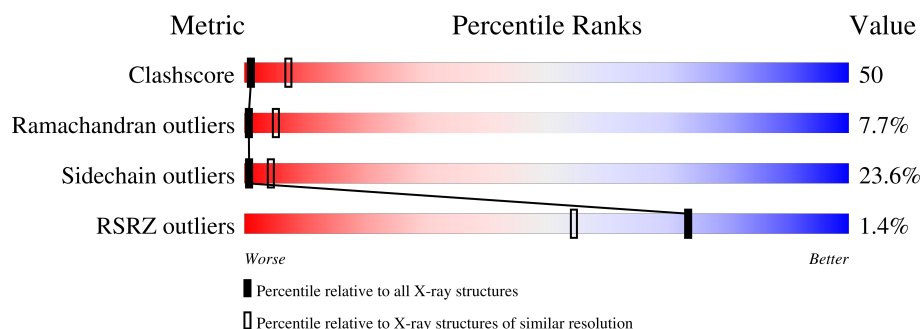
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	903	2% 24% 50% 21% 5%
1	B	903	% 25% 49% 21% 5%

2 Entry composition [i](#)

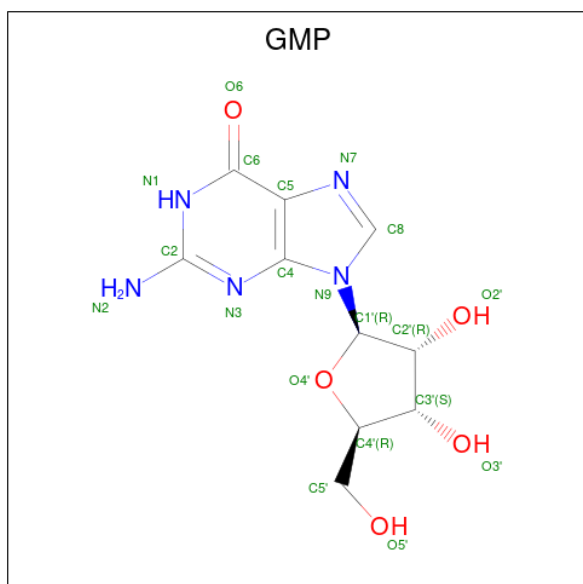
There are 2 unique types of molecules in this entry. The entry contains 14800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	0	0
			7380	4739	1226	1382	33			
1	B	903	Total	C	N	O	S	0	0	0
			7380	4739	1226	1382	33			

- Molecule 2 is GUANOSINE (CCD ID: GMP) (formula: $C_{10}H_{13}N_5O_5$).

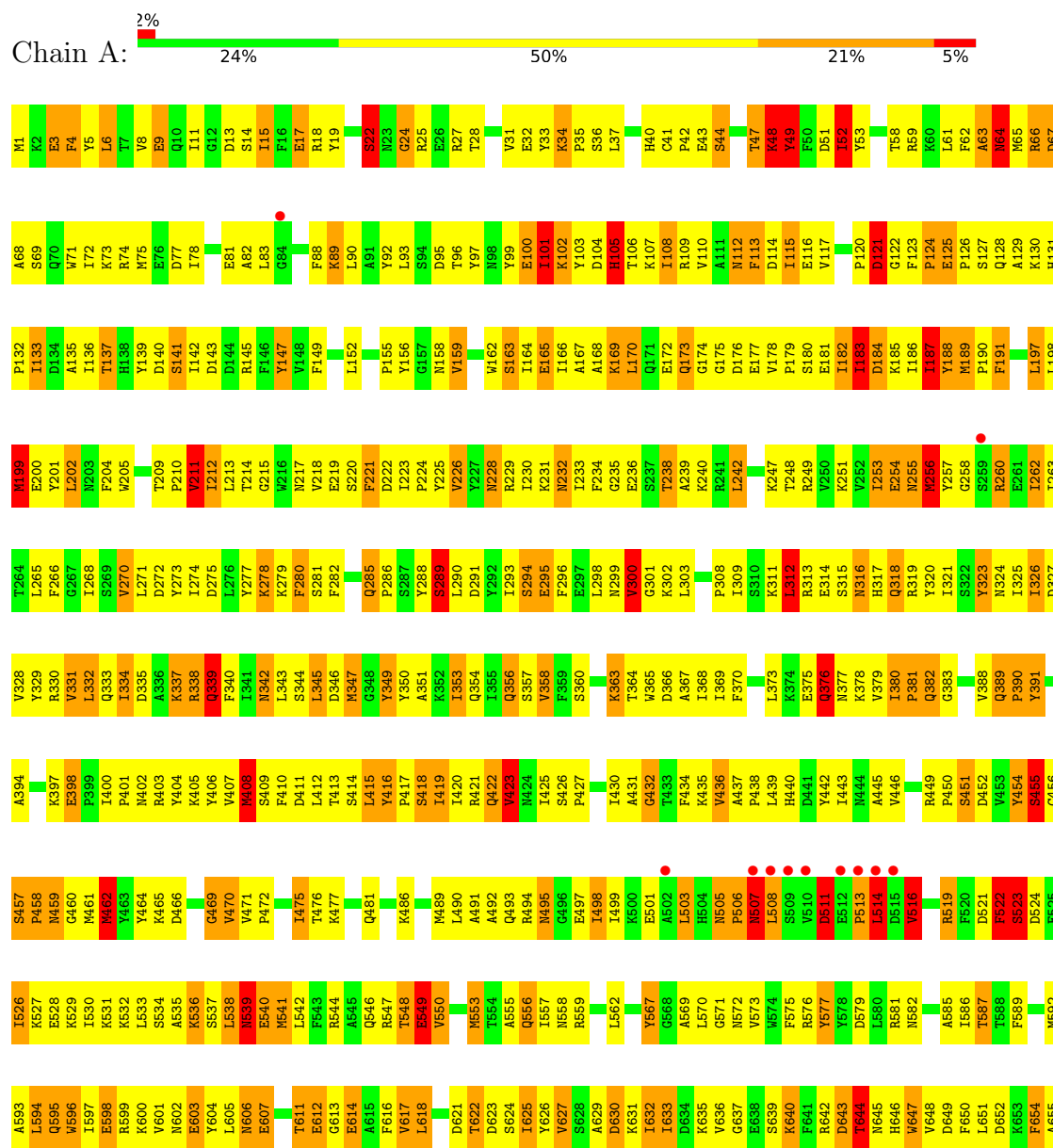


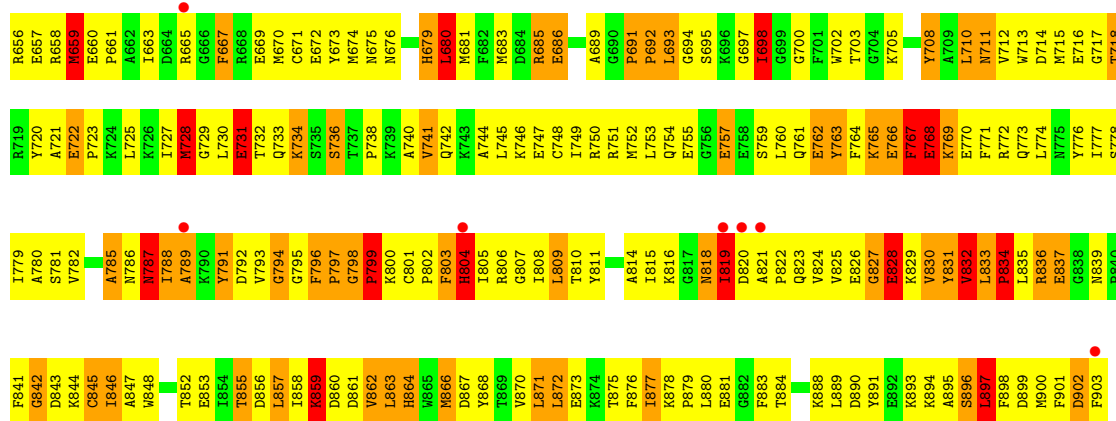
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	10	5	5		
2	B	1	Total	C	N	O	0	0
			20	10	5	5		

3 Residue-property plots

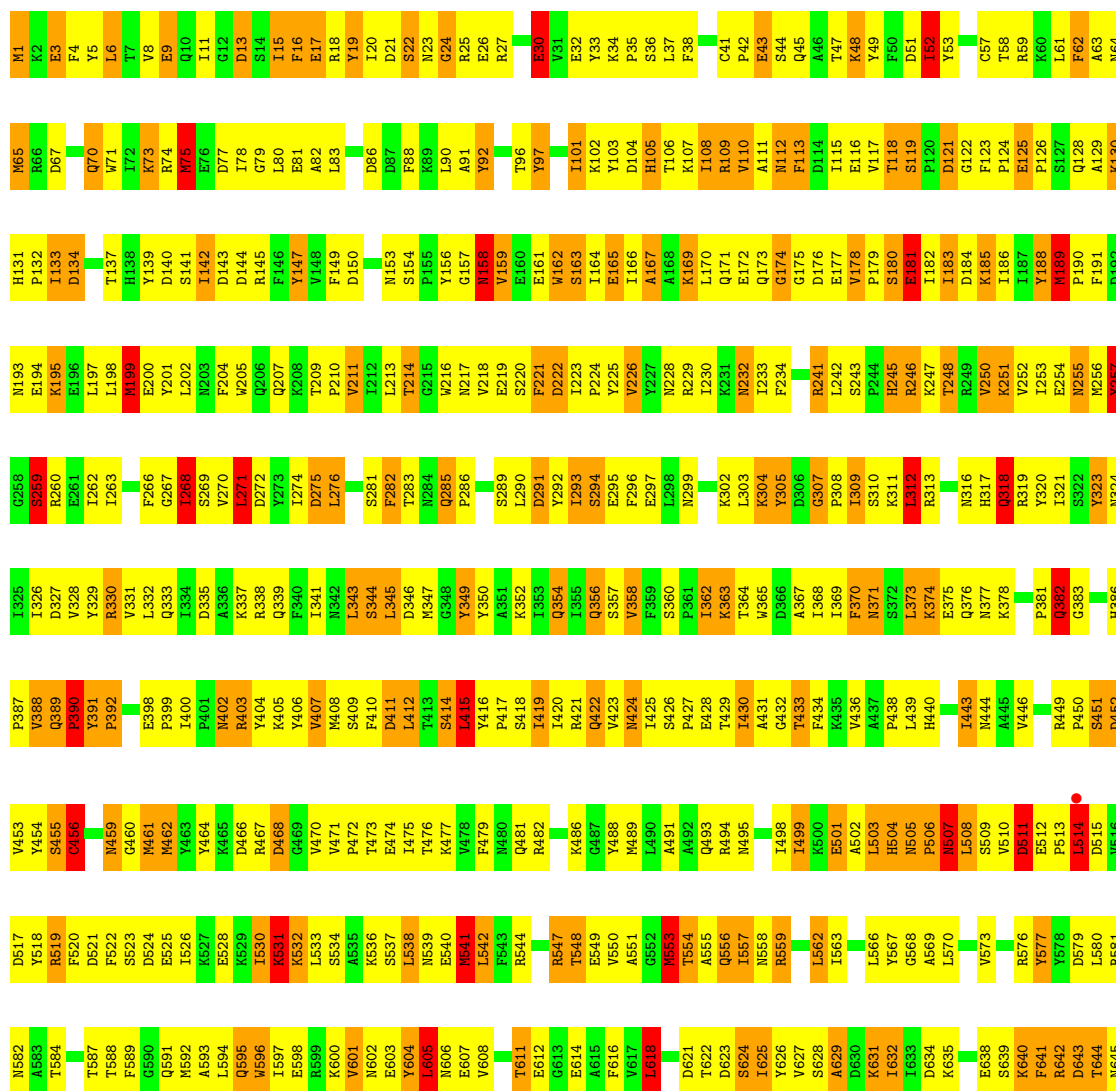
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 POLYMERASE





Molecule 1: DNA POLYMERASE



H646	H647	V648	D649	F650	L651	D652	K653	F654	A655	R656	E657	R658	E659	E660	P661	A662	I663	D664	R665	G666	F667	R668	E669	M670	M674	M675	M676	K677	Q678	H679	L680	M681	F682	M683	D684	R685	E686	A687	I688	A689	G690	P691	P692	L693	G694	S695	L698	G699	G700	F701	W702	T703	K706	R707	Y708	A709
L710	N711	W712	W713	E716	R719	Y720	A721	E722	P723	K724	L725	K726	I727	M728	G729	I663	D664	R665	G666	F667	R668	E669	M670	M674	M675	M676	K677	Q678	H679	L680	M681	F682	M683	D684	R685	E686	A687	I688	A689	G690	P691	P692	L693	G694	S695	L698	G699	G700	F701	W702	T703	K706	R707	Y708	A709	
S778	I779	A780	S781	A785	N786	N787	I788	A789	K790	Y791	D792	V793	G794	F796	P797	G798	P799	P802	F803	H804	I805	R806	G807	I808	L809	T810	Y811	H812	R813	A814	I815	K816	G817	H818	I819	D820	A821	P822	H823	V824	G827	E828	K829	Y830	Y831	H832	L833	P834	L835	R836	H837	G838	I839	P840	F841	
G842	D843	K844	C845	I846	A847	S850	E853	I854	T855	H856	L857	I858	K859	D860	D861	V862	L863	H864	W865	W866	D867	Y868	T869	W870	L871	L872	E873	F876	I877	K878	P879	L880	E881	G882	F883	T884	H885	A886	L889	D890	K894	A895	S896	L897	F898	D899	W900	F901	D902	F903						

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.32Å 196.86Å 118.31Å 90.00° 92.57° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 82.2 (40.00-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 3.18Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.198 , 0.274 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14800	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: GMP

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	1.04	12/7561 (0.2%)	1.45	126/10217 (1.2%)
1	B	1.02	9/7561 (0.1%)	1.44	125/10217 (1.2%)
All	All	1.03	21/15122 (0.1%)	1.45	251/20434 (1.2%)

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	A	0	4
1	B	0	6
All	All	0	10

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	MET	SD-CE	8.22	2.00	1.79
1	B	268	ILE	CA-CB	7.42	1.64	1.54
1	B	1	MET	SD-CE	7.39	1.98	1.79
1	A	199	MET	SD-CE	7.17	1.97	1.79
1	B	553	MET	SD-CE	6.93	1.96	1.79

The worst 5 of 251 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	VAL	N-CA-C	-16.47	97.40	111.56
1	B	788	ILE	N-CA-C	-16.01	94.29	110.62
1	A	461	MET	N-CA-C	14.43	131.73	113.55
1	B	101	ILE	N-CA-C	13.72	123.60	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	211	VAL	N-CA-C	-13.11	101.26	111.62

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	TYR	Sidechain
1	A	349	TYR	Sidechain
1	A	350	TYR	Sidechain
1	A	567	TYR	Sidechain
1	B	188	TYR	Sidechain

5.2 Too-close contacts

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	7380	0	7265	754	0
1	B	7380	0	7265	724	0
2	A	20	0	13	2	0
2	B	20	0	13	2	0
All	All	14800	0	14556	1478	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 50.

The worst 5 of 1478 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:253:ILE:CG2	1:B:260:ARG:HB2	1.63	1.26
1:B:246:ARG:HG2	1:B:246:ARG:HH11	1.06	1.13
1:B:253:ILE:HG22	1:B:260:ARG:HB2	1.20	1.12
1:B:253:ILE:HG12	1:B:254:GLU:H	1.18	1.09
1:A:796:PHE:HB3	1:A:797:PRO:HD2	1.33	1.08

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	901/903 (100%)	657 (73%)	170 (19%)	74 (8%)	0	4
1	B	901/903 (100%)	659 (73%)	177 (20%)	65 (7%)	1	6
All	All	1802/1806 (100%)	1316 (73%)	347 (19%)	139 (8%)	1	5

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	255	ASN
1	A	312	LEU
1	A	316	ASN
1	A	405	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	
1	A	802/802 (100%)	617 (77%)	185 (23%)	1	5
1	B	802/802 (100%)	608 (76%)	194 (24%)	1	4
All	All	1604/1604 (100%)	1225 (76%)	379 (24%)	1	4

5 of 379 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	248	THR

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Mol	Chain	Res	Type
1	B	511	ASP
1	B	268	ILE
1	B	390	PRO
1	B	556	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	217	ASN
1	B	389	GLN
1	B	245	HIS
1	B	339	GLN
1	B	422	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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
2	GMP	B	999	-	22,22,22	1.73	4 (18%)	33,33,33	1.42	3 (9%)
2	GMP	A	999	-	22,22,22	1.53	2 (9%)	33,33,33	1.15	3 (9%)

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
2	GMP	B	999	-	-	1/6/22/22	0/3/3/3
2	GMP	A	999	-	-	0/6/22/22	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	GMP	O3'-C3'	4.33	1.53	1.43
2	A	999	GMP	C6-N1	3.94	1.46	1.38
2	B	999	GMP	C6-N1	3.03	1.44	1.38
2	B	999	GMP	C4-N3	2.91	1.40	1.34
2	B	999	GMP	C2-N1	2.22	1.43	1.37

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	999	GMP	C2'-C3'-C4'	-4.20	94.49	102.61
2	A	999	GMP	C5'-C4'-C3'	-3.18	107.58	115.10
2	B	999	GMP	N1-C2-N3	-2.47	118.81	123.32
2	A	999	GMP	O4'-C4'-C5'	2.44	114.37	109.22
2	B	999	GMP	O4'-C1'-C2'	-2.24	101.82	106.62

There are no chirality outliers.

All (1) torsion outliers are listed below:

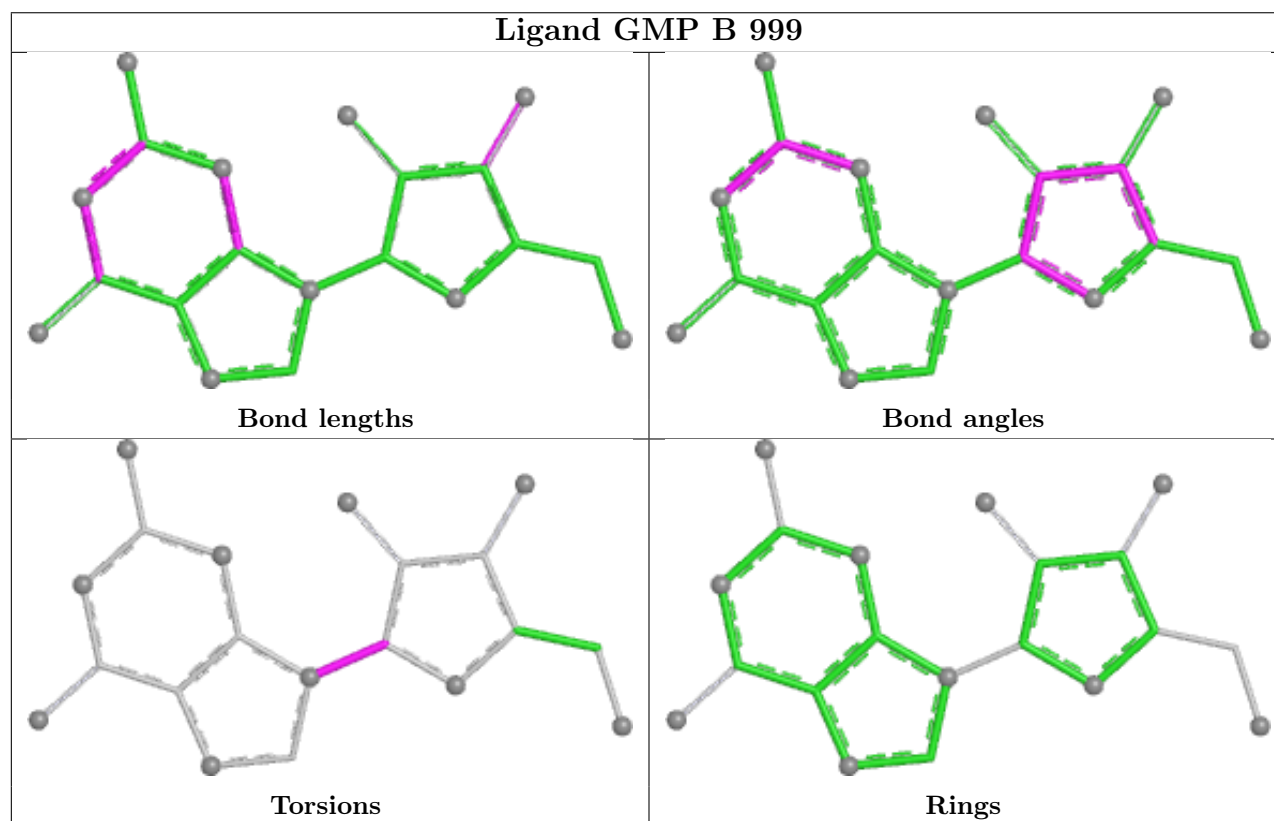
Mol	Chain	Res	Type	Atoms
2	B	999	GMP	O4'-C1'-N9-C4

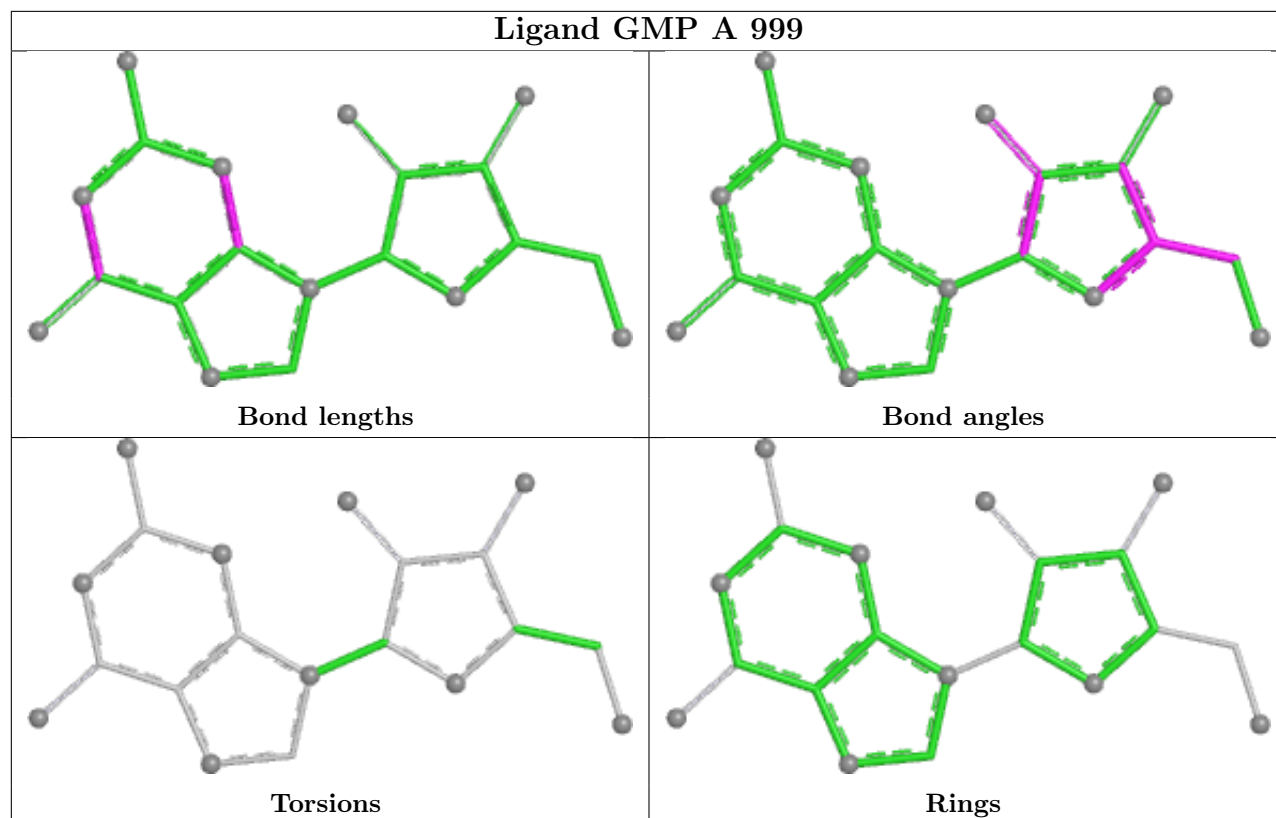
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	999	GMP	2	0
2	A	999	GMP	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	903/903 (100%)	-0.03	18 (1%) 65 45	40, 68, 100, 100	0
1	B	903/903 (100%)	-0.06	7 (0%) 82 67	39, 68, 100, 100	0
All	All	1806/1806 (100%)	-0.04	25 (1%) 73 54	39, 68, 100, 100	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	665	ARG	4.7
1	A	903	PHE	3.8
1	A	514	LEU	3.8
1	A	508	LEU	3.7
1	A	821	ALA	3.5

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](#)

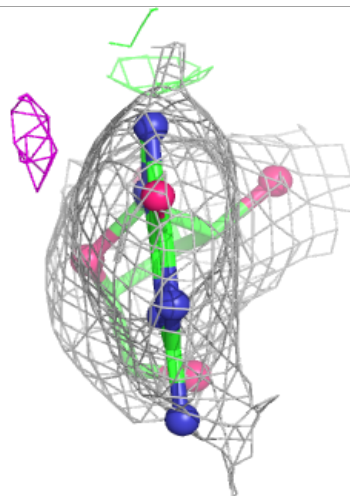
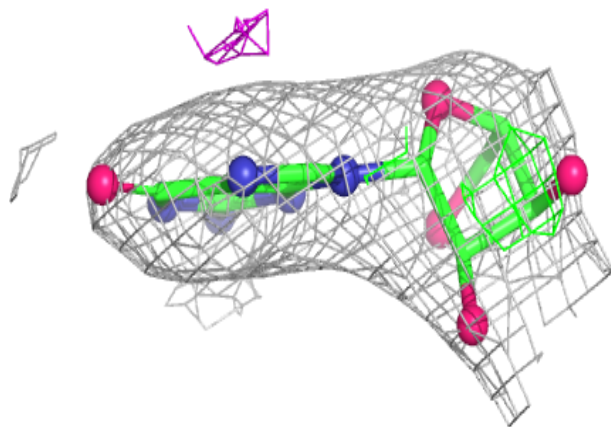
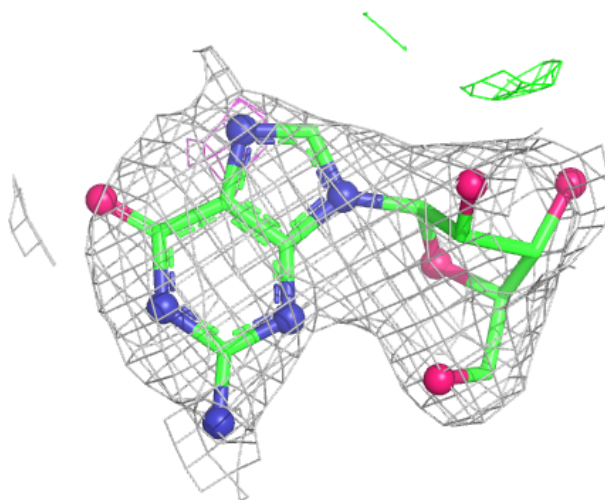
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

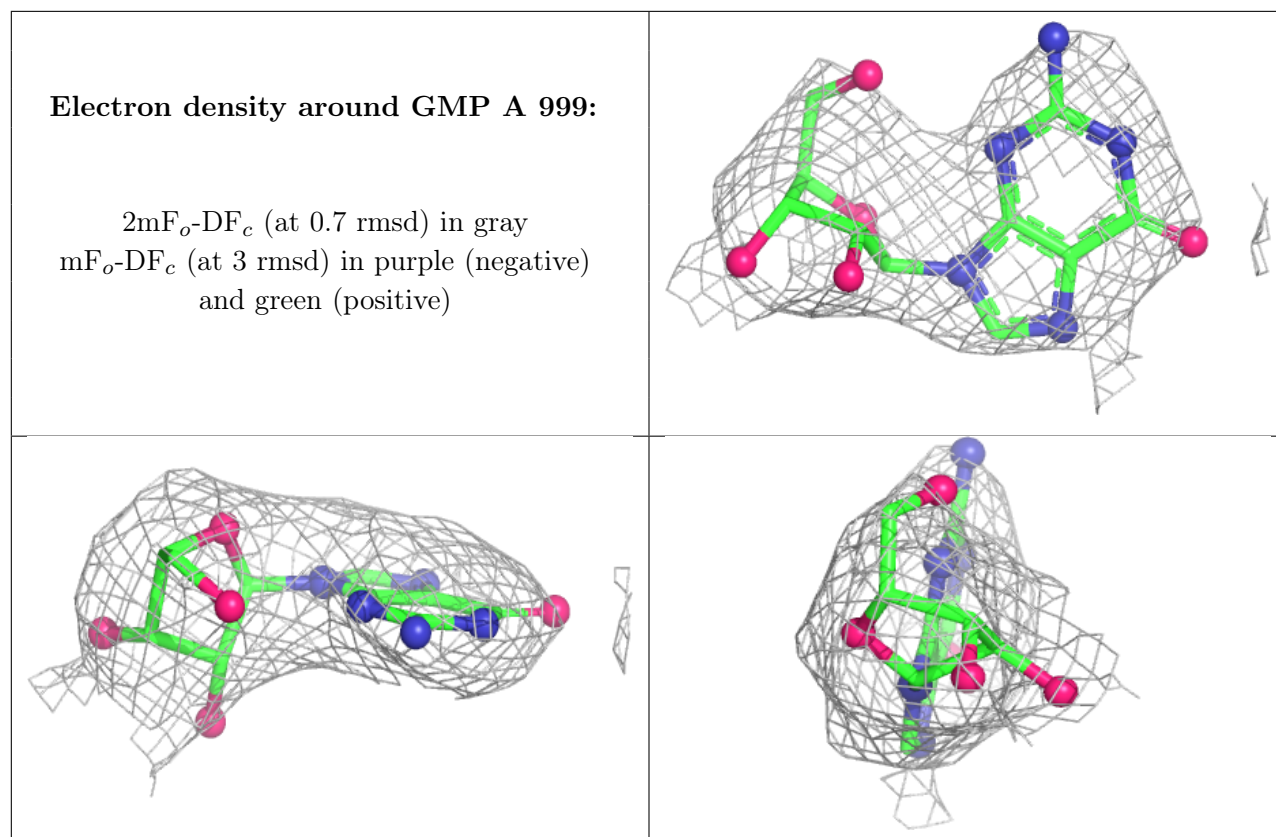
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GMP	B	999	20/20	0.93	0.11	82,82,84,84	0
2	GMP	A	999	20/20	0.95	0.11	81,82,84,84	0

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 GMP B 999:

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.