



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:09 am BST

PDB ID : 4FF3  
Title : N4 mini-vRNAP transcription initiation complex, 3 min after soaking GTP, ATP and Mn  
Authors : Murakami, K.S.; Basu, R.S.  
Deposited on : 2012-05-30  
Resolution : 2.00 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

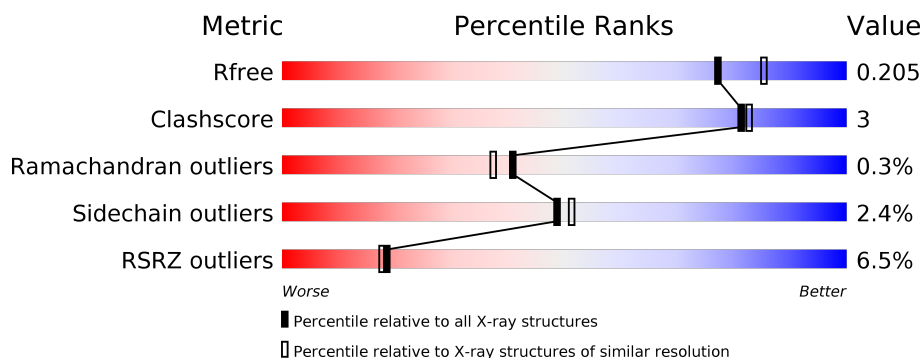
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1118	<div> <div>6%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	B	1118	<div> <div>7%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
2	C	36	<div> <div>42%</div> <div>14%</div> <div>44%</div> </div>
2	D	36	<div> <div>44%</div> <div>8%</div> <div>44%</div> <div>.</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19046 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 Virion RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1095	Total	C	N	O	S	0	0	0
			8454	5306	1435	1672	41			
1	B	1095	Total	C	N	O	S	0	0	0
			8454	5306	1435	1672	41			

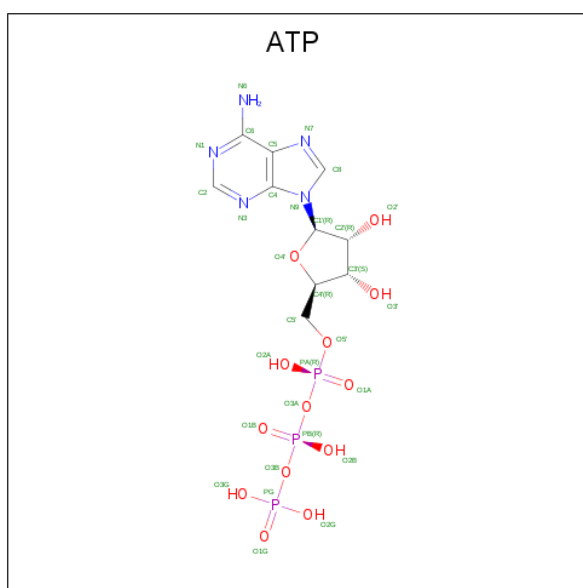
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q859P9
A	-10	GLY	-	EXPRESSION TAG	UNP Q859P9
A	-9	GLY	-	EXPRESSION TAG	UNP Q859P9
A	-8	SER	-	EXPRESSION TAG	UNP Q859P9
A	-7	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-6	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-5	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-4	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-3	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-2	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-1	ARG	-	EXPRESSION TAG	UNP Q859P9
A	0	SER	-	EXPRESSION TAG	UNP Q859P9
B	-11	MET	-	EXPRESSION TAG	UNP Q859P9
B	-10	GLY	-	EXPRESSION TAG	UNP Q859P9
B	-9	GLY	-	EXPRESSION TAG	UNP Q859P9
B	-8	SER	-	EXPRESSION TAG	UNP Q859P9
B	-7	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-6	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-5	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-4	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-3	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-2	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-1	ARG	-	EXPRESSION TAG	UNP Q859P9
B	0	SER	-	EXPRESSION TAG	UNP Q859P9

- Molecule 2 is a DNA chain called Bacteriophage N4 P2 promoter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			413	196	80	117	20			
2	D	20	Total	C	N	O	P	0	0	0
			413	196	80	117	20			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

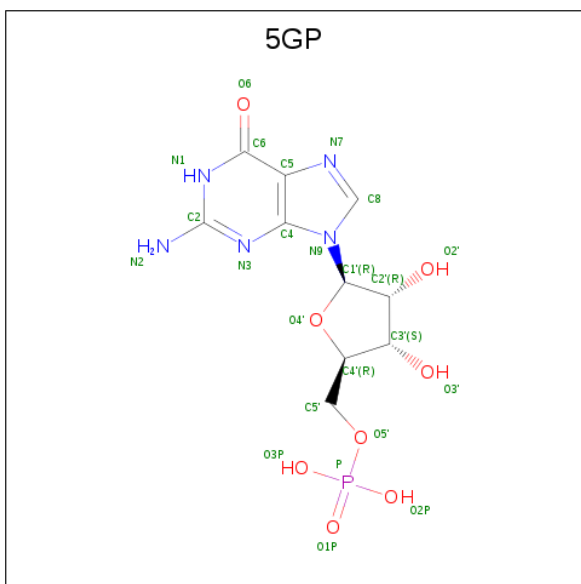
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula:  $C_{10}H_{14}N_5O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

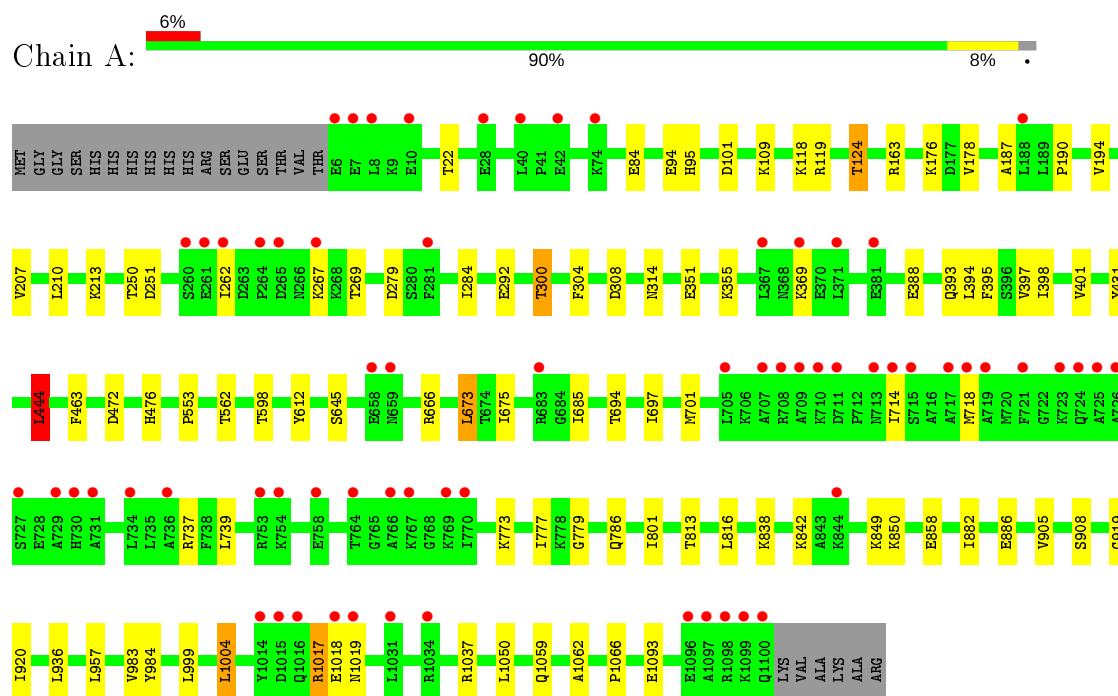
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	546	Total 546	O 546	0	0
7	C	42	Total 42	O 42	0	0
7	B	624	Total 624	O 624	0	0
7	D	33	Total 33	O 33	0	0

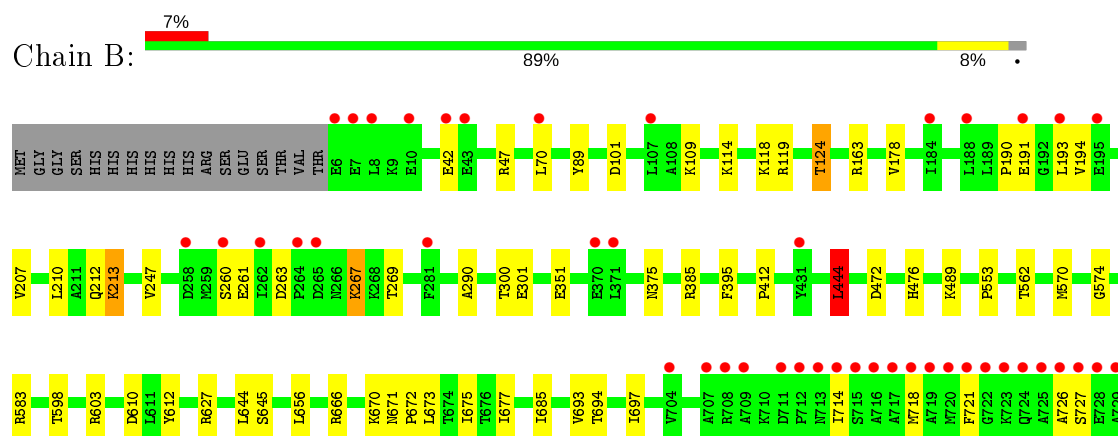
### 3 Residue-property plots [i](#)

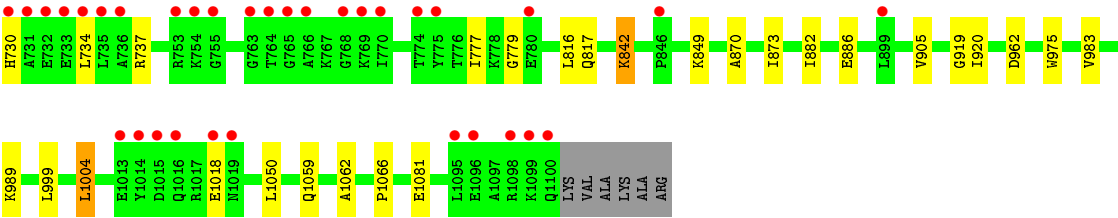
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

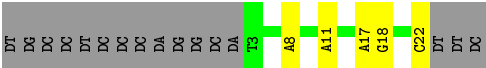


#### • Molecule 1: Virion RNA polymerase

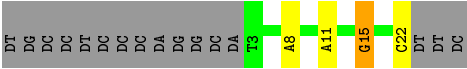




● Molecule 2: Bacteriophage N4 P2 promoter



● Molecule 2: Bacteriophage N4 P2 promoter





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.02Å 111.65Å 276.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.38 – 2.00 42.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.9 (42.38-2.00) 84.7 (42.38-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.182 , 0.211 0.174 , 0.205	Depositor DCC
$R_{free}$ test set	2000 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19046	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, 5GP, ATP, MN

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	0.25	0/8583	0.44	1/11609 (0.0%)
1	B	0.25	0/8583	0.44	1/11609 (0.0%)
2	C	0.49	0/464	1.10	0/714
2	D	0.52	0/464	1.12	2/714 (0.3%)
All	All	0.27	0/18094	0.50	4/24646 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	LEU	CA-CB-CG	7.77	133.16	115.30
2	D	15	DG	O4'-C1'-N9	7.09	112.96	108.00
1	B	444	LEU	CA-CB-CG	6.73	130.79	115.30
2	D	15	DG	C3'-C2'-C1'	-5.99	95.31	102.50

There are no chirality outliers.

There are no planarity outliers.

### 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	8454	0	8479	44	0
1	B	8454	0	8479	50	0
2	C	413	0	225	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	413	0	225	4	0
3	A	31	0	12	0	0
4	A	2	0	0	0	0
5	A	5	0	0	1	0
5	B	5	0	0	1	0
6	C	24	0	12	0	0
7	A	546	0	0	0	0
7	B	624	0	0	4	0
7	C	42	0	0	0	0
7	D	33	0	0	1	0
All	All	19046	0	17432	92	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 3.

All (92) 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)
2:D:22:DC:O3'	7:D:109:HOH:O	2.10	0.69
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.75	0.67
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.77	0.66
1:B:583:ARG:NH2	1:B:1081:GLU:OE2	2.29	0.66
1:B:476:HIS:ND1	5:B:1201:PO4:O2	2.24	0.65
1:B:694:THR:HG22	1:B:777:ILE:HD12	1.79	0.65
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.80	0.63
1:A:101:ASP:OD1	1:B:109:LYS:NZ	2.28	0.62
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.82	0.62
1:A:999:LEU:HB2	1:A:1004:LEU:HD22	1.82	0.60
1:B:570:MET:HE2	1:B:975:TRP:HB3	1.84	0.59
1:B:207:VAL:HG11	1:B:905:VAL:HG21	1.84	0.59
1:A:444:LEU:HG	1:A:553:PRO:HB2	1.87	0.56
1:A:694:THR:HG22	1:A:777:ILE:HD12	1.88	0.56
1:B:817:GLN:HB2	1:B:920:ILE:HD11	1.87	0.56
1:A:675:ILE:HD11	1:A:685:ILE:HG12	1.87	0.55
1:A:476:HIS:ND1	5:A:1204:PO4:O2	2.24	0.55
1:A:94:GLU:HG2	1:B:247:VAL:HG12	1.88	0.55
1:A:119:ARG:O	1:A:124:THR:HG23	2.07	0.55
1:B:671:ASN:HB3	1:B:672:PRO:HD3	1.89	0.54
1:B:119:ARG:O	1:B:124:THR:HG23	2.08	0.53
1:B:726:ALA:HB3	1:B:730:HIS:NE2	2.25	0.52
1:A:190:PRO:HG2	1:A:262:ILE:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:THR:O	1:A:920:ILE:HD11	2.09	0.52
1:B:213:LYS:HE2	1:B:301:GLU:OE2	2.09	0.52
1:A:886:GLU:O	2:C:8:DA:H4'	2.10	0.51
1:B:610:ASP:OD2	1:B:666:ARG:NH1	2.43	0.51
1:A:645:SER:OG	1:A:737:ARG:HD2	2.11	0.50
1:B:191:GLU:HG2	1:B:375:ASN:O	2.12	0.50
1:B:114:LYS:NZ	2:D:15:DG:N7	2.59	0.49
1:B:677:ILE:O	1:B:920:ILE:HG21	2.13	0.49
1:B:816:LEU:HD13	1:B:983:VAL:HG21	1.93	0.48
1:A:393:GLN:HG3	1:A:431:TYR:CD2	2.48	0.48
1:B:269:THR:O	2:D:11:DA:H5'	2.14	0.48
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.43	0.48
1:A:562:THR:HG22	1:A:612:TYR:CE1	2.50	0.47
1:A:109:LYS:NZ	1:B:101:ASP:OD1	2.33	0.47
1:A:187:ALA:HB1	1:A:786:GLN:HE22	1.79	0.47
1:B:886:GLU:O	2:D:8:DA:H4'	2.15	0.47
1:B:999:LEU:HB2	1:B:1004:LEU:HD22	1.96	0.47
1:B:612:TYR:CE2	1:B:673:LEU:HD23	2.50	0.46
1:B:351:GLU:HG3	1:B:395:PHE:CE2	2.50	0.46
1:A:351:GLU:HG3	1:A:395:PHE:CE2	2.50	0.46
1:B:574:GLY:O	7:B:1626:HOH:O	2.21	0.46
1:B:47:ARG:NH2	7:B:1374:HOH:O	2.40	0.46
1:B:693:VAL:O	1:B:697:ILE:HG23	2.16	0.46
1:B:645:SER:OG	1:B:737:ARG:HD2	2.16	0.45
1:B:714:ILE:HD11	1:B:718:MET:HB3	1.99	0.45
1:A:849:LYS:NZ	2:C:17:DA:OP2	2.44	0.45
1:A:882:ILE:HD13	1:A:919:GLY:HA2	1.99	0.45
1:A:369:LYS:O	1:A:773:LYS:NZ	2.50	0.45
1:B:849:LYS:HE3	7:B:1777:HOH:O	2.17	0.45
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.52	0.45
1:B:444:LEU:HG	1:B:553:PRO:HB2	1.98	0.44
1:A:394:LEU:O	1:A:398:ILE:HG12	2.17	0.44
1:A:118:LYS:HE3	1:A:118:LYS:HB2	1.79	0.44
1:B:882:ILE:HD13	1:B:919:GLY:HA2	2.00	0.44
1:A:673:LEU:HD12	1:A:801:ILE:HG12	2.00	0.44
1:A:463:PHE:HA	1:A:957:LEU:HD13	2.00	0.44
1:A:984:TYR:CE1	1:A:1037:ARG:HB2	2.53	0.44
1:B:721:PHE:HB3	1:B:734:LEU:HD12	2.00	0.44
1:B:267:LYS:HG2	1:B:267:LYS:H	1.64	0.43
1:B:603:ARG:NH1	7:B:1413:HOH:O	2.22	0.43
1:A:95:HIS:NE2	1:A:251:ASP:OD2	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:SER:HB2	1:B:730:HIS:CE1	2.53	0.43
1:B:873:ILE:HD13	1:B:983:VAL:HG22	2.00	0.43
1:A:292:GLU:OE2	1:A:300:THR:HG23	2.19	0.43
1:A:714:ILE:HD11	1:A:718:MET:HB3	2.00	0.43
1:B:118:LYS:HE3	1:B:118:LYS:HB2	1.77	0.42
1:A:355:LYS:HD2	1:A:388:GLU:HG3	2.00	0.42
1:A:267:LYS:HD3	2:C:22:DC:C5	2.54	0.42
1:B:675:ILE:HD11	1:B:685:ILE:HG12	2.01	0.42
1:A:304:PHE:HB3	1:A:308:ASP:O	2.20	0.42
1:A:697:ILE:O	1:A:701:MET:HG2	2.20	0.42
1:B:842:LYS:HD2	1:B:842:LYS:HA	1.63	0.42
1:A:397:VAL:O	1:A:401:VAL:HG23	2.19	0.42
1:B:612:TYR:CZ	1:B:670:LYS:HG3	2.55	0.42
1:B:190:PRO:HD2	1:B:193:LEU:HD22	2.02	0.42
1:B:627:ARG:HH21	1:B:644:LEU:HD12	1.85	0.42
1:A:850:LYS:NZ	2:C:18:DG:OP1	2.37	0.41
1:A:842:LYS:HD3	1:A:842:LYS:HA	1.76	0.41
1:B:1004:LEU:HD13	1:B:1004:LEU:HA	1.94	0.41
1:B:598:THR:HG22	1:B:1066:PRO:HD3	2.03	0.41
1:A:598:THR:HG22	1:A:1066:PRO:HD3	2.02	0.41
1:B:260:SER:HA	1:B:263:ASP:O	2.20	0.41
1:A:1017:ARG:O	1:A:1019:ASN:N	2.53	0.41
1:B:42:GLU:HG2	1:B:42:GLU:H	1.75	0.41
1:B:562:THR:HG22	1:B:612:TYR:CE1	2.56	0.41
1:A:838:LYS:HE2	1:A:858:GLU:HG2	2.02	0.40
1:B:870:ALA:HB2	1:B:989:LYS:HD3	2.03	0.40
1:A:187:ALA:HB1	1:A:786:GLN:NE2	2.36	0.40
1:A:269:THR:O	2:C:11:DA:H5'	2.22	0.40

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	1093/1118 (98%)	1068 (98%)	21 (2%)	4 (0%)	34	30
1	B	1093/1118 (98%)	1071 (98%)	20 (2%)	2 (0%)	47	44
All	All	2186/2236 (98%)	2139 (98%)	41 (2%)	6 (0%)	41	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1018	GLU
1	A	1062	ALA
1	B	1062	ALA
1	A	779	GLY
1	A	1017	ARG
1	B	779	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	
1	A	916/935 (98%)	893 (98%)	23 (2%)	47	49
1	B	916/935 (98%)	895 (98%)	21 (2%)	50	53
All	All	1832/1870 (98%)	1788 (98%)	44 (2%)	49	51

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	84	GLU
1	A	124	THR
1	A	163	ARG
1	A	176	LYS
1	A	210	LEU
1	A	213	LYS
1	A	250	THR
1	A	279	ASP
1	A	284	ILE

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Mol	Chain	Res	Type
1	A	300	THR
1	A	314	ASN
1	A	444	LEU
1	A	472	ASP
1	A	666	ARG
1	A	673	LEU
1	A	739	LEU
1	A	908	SER
1	A	936	LEU
1	A	1004	LEU
1	A	1050	LEU
1	A	1059	GLN
1	A	1093	GLU
1	B	70	LEU
1	B	124	THR
1	B	163	ARG
1	B	210	LEU
1	B	212	GLN
1	B	213	LYS
1	B	261	GLU
1	B	267	LYS
1	B	300	THR
1	B	385	ARG
1	B	412	PRO
1	B	444	LEU
1	B	472	ASP
1	B	489	LYS
1	B	656	LEU
1	B	842	LYS
1	B	962	ASP
1	B	1004	LEU
1	B	1018	GLU
1	B	1050	LEU
1	B	1059	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	PO4	B	1201	-	4,4,4	0.88	0	6,6,6	0.43	0
5	PO4	A	1204	-	4,4,4	0.92	0	6,6,6	0.37	0
6	5GP	C	101	4	22,26,26	0.60	0	27,40,40	1.76	5 (18%)
3	ATP	A	1201	4	26,33,33	0.99	2 (7%)	31,52,52	1.20	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
6	5GP	C	101	4	-	5/6/26/26	0/3/3/3
3	ATP	A	1201	4	-	7/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	ATP	C5-C4	2.38	1.47	1.40
3	A	1201	ATP	C2-N3	2.21	1.35	1.32

All (8) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	101	5GP	N3-C2-N1	-4.69	120.96	127.22
6	C	101	5GP	C2-N3-C4	4.60	120.61	115.36
3	A	1201	ATP	N3-C2-N1	-3.42	123.34	128.68
6	C	101	5GP	C6-N1-C2	3.08	120.83	115.93
6	C	101	5GP	C5-C6-N1	-2.91	119.46	123.43
3	A	1201	ATP	C4-C5-N7	-2.67	106.61	109.40
3	A	1201	ATP	PB-O3B-PG	-2.53	124.14	132.83
6	C	101	5GP	O3P-P-O5'	-2.39	100.38	106.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	ATP	C5'-O5'-PA-O2A
6	C	101	5GP	C5'-O5'-P-O1P
6	C	101	5GP	C5'-O5'-P-O2P
6	C	101	5GP	C5'-O5'-P-O3P
6	C	101	5GP	C3'-C4'-C5'-O5'
6	C	101	5GP	O4'-C4'-C5'-O5'
3	A	1201	ATP	C5'-O5'-PA-O3A
3	A	1201	ATP	C5'-O5'-PA-O1A
3	A	1201	ATP	PB-O3B-PG-O1G
3	A	1201	ATP	PB-O3B-PG-O3G
3	A	1201	ATP	PA-O3A-PB-O1B
3	A	1201	ATP	PA-O3A-PB-O2B

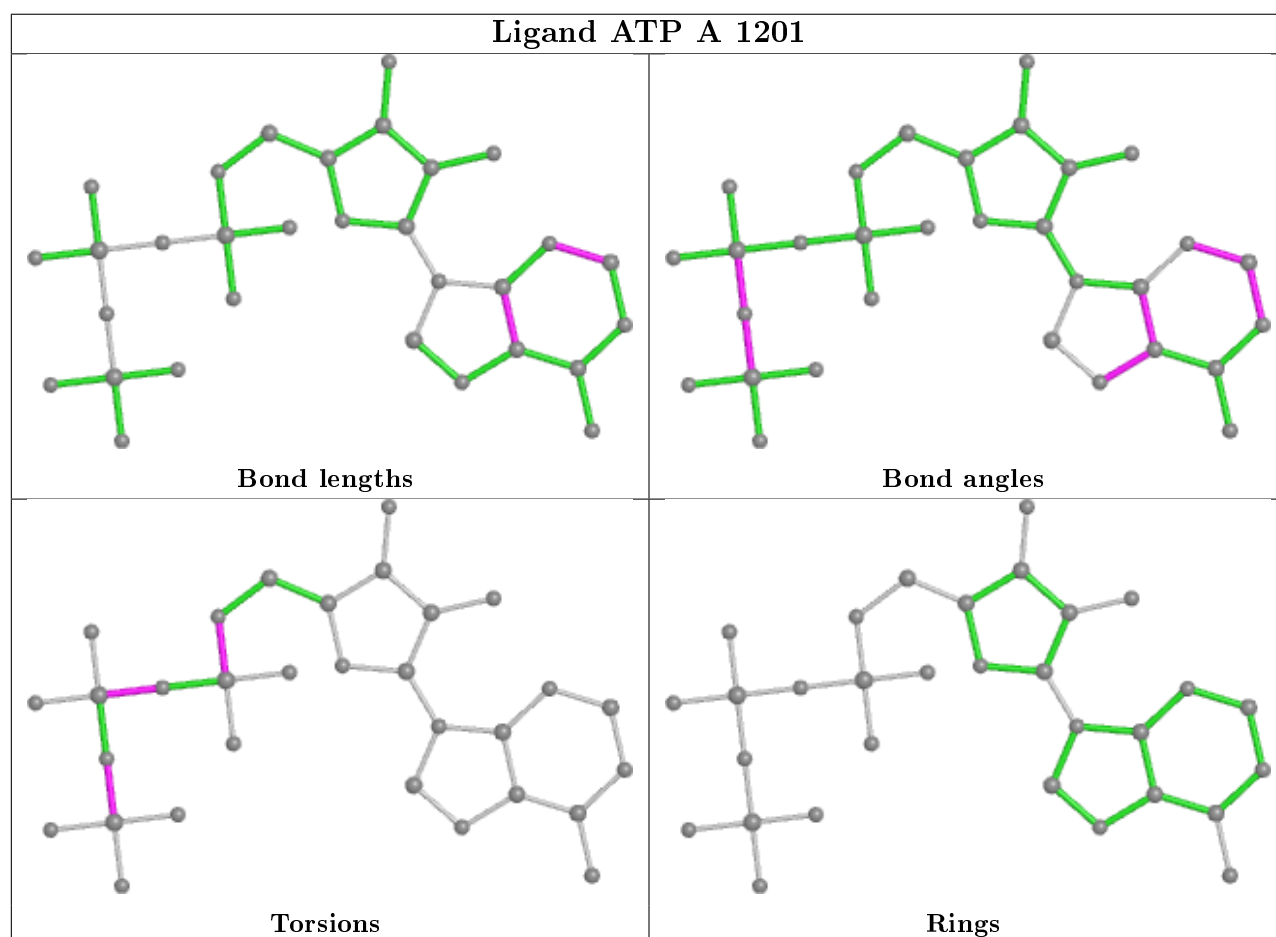
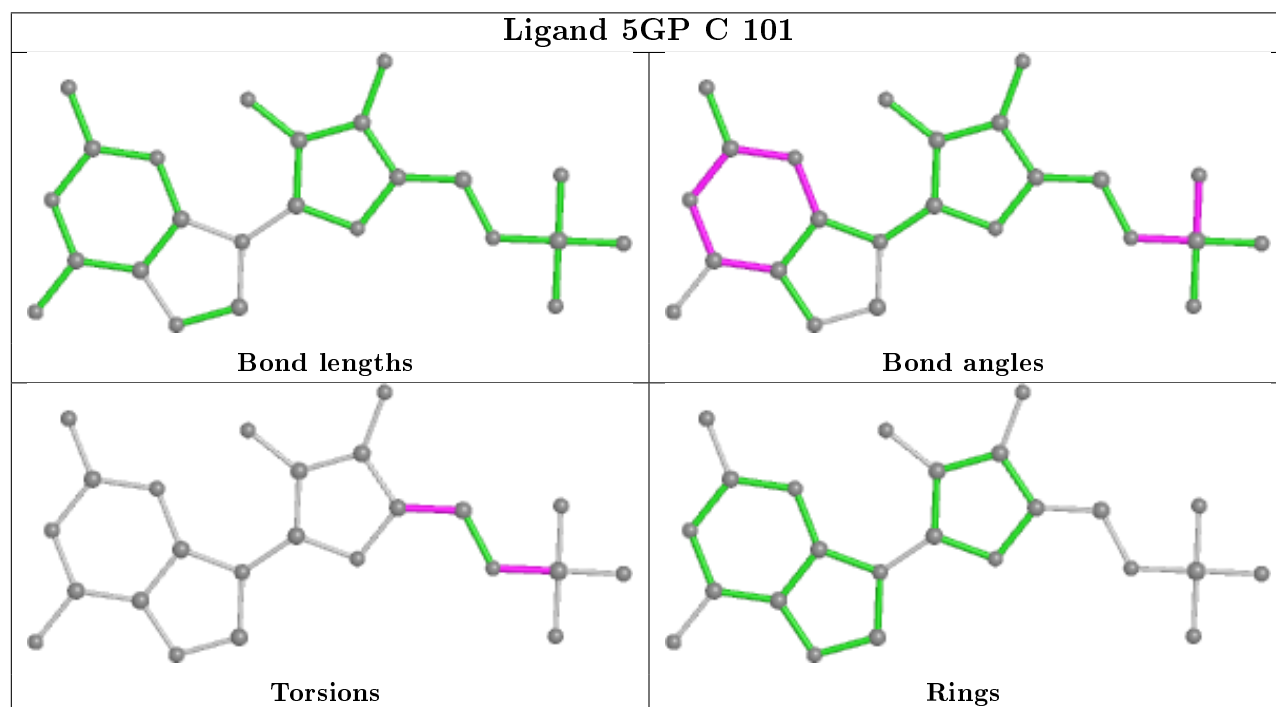
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1201	PO4	1	0
5	A	1204	PO4	1	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1095/1118 (97%)	0.29	67 (6%)	21	20	12, 29, 69, 107	0
1	B	1095/1118 (97%)	0.40	78 (7%)	16	15	13, 28, 69, 144	0
2	C	20/36 (55%)	-0.33	0	100	100	29, 36, 57, 60	0
2	D	20/36 (55%)	-0.16	0	100	100	22, 37, 53, 79	0
All	All	2230/2308 (96%)	0.33	145 (6%)	18	18	12, 29, 69, 144	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	ALA	12.5
1	B	727	SER	9.7
1	B	729	ALA	9.3
1	B	725	ALA	7.1
1	A	725	ALA	6.8
1	B	1099	LYS	6.6
1	B	730	HIS	6.5
1	A	8	LEU	6.4
1	B	713	ASN	6.4
1	A	729	ALA	6.2
1	B	718	MET	5.9
1	B	722	GLY	5.7
1	B	714	ILE	5.7
1	B	8	LEU	5.6
1	B	723	LYS	5.5
1	A	1014	TYR	5.1
1	A	723	LYS	4.9
1	A	262	ILE	4.9
1	A	734	LEU	4.9
1	B	704	VAL	4.8
1	A	726	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	28	GLU	4.7
1	B	1014	TYR	4.6
1	B	7	GLU	4.6
1	A	658	GLU	4.6
1	A	7	GLU	4.5
1	B	724	GLN	4.5
1	A	714	ILE	4.2
1	B	262	ILE	4.1
1	B	264	PRO	4.1
1	A	264	PRO	4.1
1	B	195	GLU	4.0
1	B	711	ASP	4.0
1	A	711	ASP	4.0
1	B	1015	ASP	4.0
1	A	727	SER	4.0
1	B	770	ILE	3.9
1	B	42	GLU	3.9
1	A	721	PHE	3.9
1	B	1100	GLN	3.9
1	B	769	LYS	3.8
1	A	707	ALA	3.8
1	A	709	ALA	3.8
1	B	708	ARG	3.8
1	B	260	SER	3.7
1	B	728	GLU	3.6
1	A	770	ILE	3.6
1	B	707	ALA	3.5
1	A	730	HIS	3.4
1	A	260	SER	3.4
1	B	1095	LEU	3.4
1	B	719	ALA	3.4
1	B	717	ALA	3.3
1	B	1098	ARG	3.3
1	A	719	ALA	3.3
1	A	1015	ASP	3.3
1	A	705	LEU	3.3
1	B	736	ALA	3.3
1	A	10	GLU	3.2
1	B	731	ALA	3.2
1	A	718	MET	3.2
1	B	1096	GLU	3.2
1	A	1098	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	371	LEU	3.2
1	B	1018	GLU	3.2
1	A	369	LYS	3.2
1	B	43	GLU	3.1
1	A	754	LYS	3.1
1	A	724	GLN	3.0
1	B	734	LEU	3.0
1	B	721	PHE	3.0
1	A	1018	GLU	3.0
1	A	713	ASN	3.0
1	B	715	SER	2.9
1	A	766	ALA	2.9
1	B	780	GLU	2.9
1	B	1019	ASN	2.9
1	A	1099	LYS	2.9
1	A	367	LEU	2.9
1	A	659	ASN	2.9
1	A	731	ALA	2.9
1	B	371	LEU	2.9
1	B	899	LEU	2.9
1	B	10	GLU	2.9
1	A	281	PHE	2.9
1	B	766	ALA	2.9
1	B	764	THR	2.8
1	B	265	ASP	2.8
1	A	42	GLU	2.8
1	B	732	GLU	2.8
1	A	267	LYS	2.7
1	A	1019	ASN	2.7
1	A	1096	GLU	2.7
1	A	1016	GLN	2.7
1	B	735	LEU	2.6
1	A	188	LEU	2.6
1	B	191	GLU	2.6
1	A	708	ARG	2.6
1	A	753	ARG	2.6
1	A	6	GLU	2.6
1	A	261	GLU	2.6
1	A	1031	LEU	2.5
1	A	265	ASP	2.5
1	A	683	ARG	2.5
1	A	74	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	370	GLU	2.5
1	B	1016	GLN	2.5
1	B	281	PHE	2.5
1	B	184	ILE	2.4
1	B	846	PRO	2.4
1	A	1097	ALA	2.4
1	B	107	LEU	2.4
1	B	754	LYS	2.4
1	B	716	ALA	2.4
1	A	736	ALA	2.4
1	B	763	GLY	2.3
1	B	188	LEU	2.3
1	B	709	ALA	2.3
1	B	753	ARG	2.3
1	B	768	GLY	2.2
1	A	1034	ARG	2.2
1	B	765	GLY	2.2
1	A	1100	GLN	2.2
1	B	70	LEU	2.2
1	A	715	SER	2.2
1	B	258	ASP	2.2
1	A	40	LEU	2.2
1	A	769	LYS	2.2
1	A	381	GLU	2.2
1	B	6	GLU	2.2
1	B	1013	GLU	2.1
1	A	767	LYS	2.1
1	A	717	ALA	2.1
1	B	733	GLU	2.1
1	B	720	MET	2.1
1	A	758	GLU	2.1
1	A	844	LYS	2.1
1	B	431	TYR	2.1
1	B	193	LEU	2.1
1	B	712	PRO	2.1
1	A	710	LYS	2.1
1	A	764	THR	2.0
1	B	775	TYR	2.0
1	B	755	GLY	2.0
1	B	774	THR	2.0

## 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 carbohydrates 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, 95<sup>th</sup> 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.

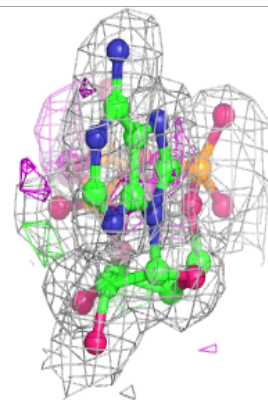
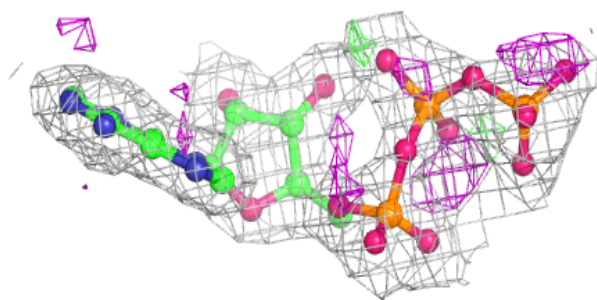
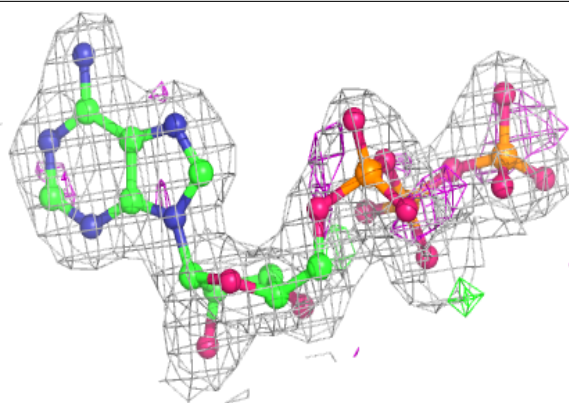
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MN	A	1202	1/1	0.89	0.08	56,56,56,56	0
3	ATP	A	1201	31/31	0.92	0.13	16,26,42,124	0
6	5GP	C	101	24/24	0.92	0.14	31,41,78,81	0
5	PO4	B	1201	5/5	0.96	0.11	39,43,54,54	0
4	MN	A	1203	1/1	0.97	0.06	35,35,35,35	0
5	PO4	A	1204	5/5	0.98	0.10	28,34,37,44	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.

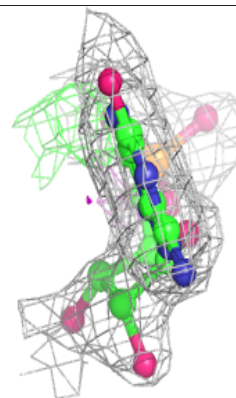
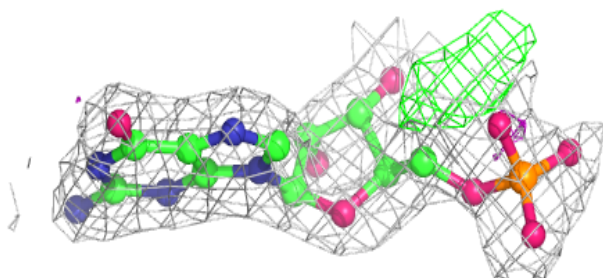
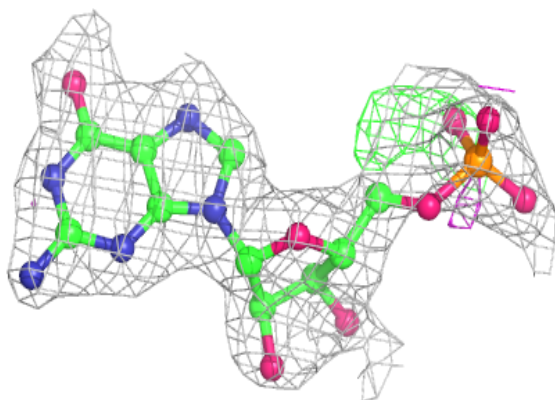


**Electron density around ATP A 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 5GP C 101:**

$2mF_o-DF_c$  (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.