



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2024 – 10:55 AM EST

PDB ID : 4JKR  
Title : Crystal Structure of E. coli RNA Polymerase in complex with ppGpp  
Authors : Zuo, Y.; Wang, Y.; Steitz, T.A.  
Deposited on : 2013-03-11  
Resolution : 4.20 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

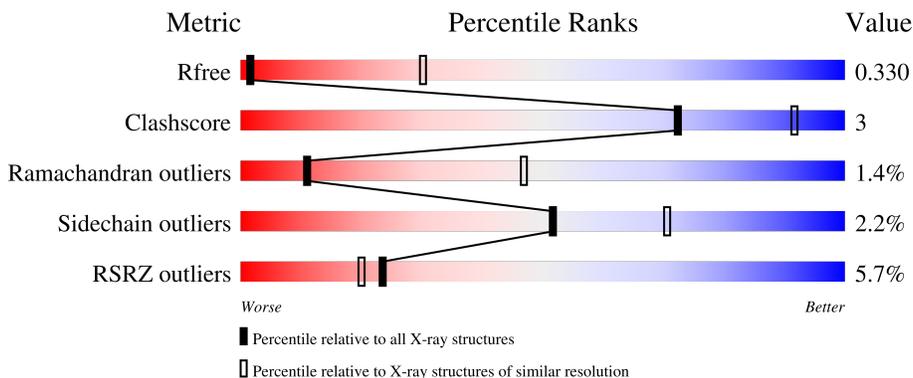
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 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))
$R_{free}$	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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  $\geq 3$ , 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	329	 2% 62% 7% 31%
1	B	329	 2% 62% 7% 31%
1	G	329	 % 63% 6% 31%
1	H	329	 5% 66% . 31%
2	C	1342	 2% 87% 12%

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Mol	Chain	Length	Quality of chain
2	I	1342	<p>3% 87% 12% 5%</p>
3	D	1416	<p>9% 81% 13% 5%</p>
3	J	1416	<p>9% 80% 14% 6%</p>
4	E	90	<p>89% 11%</p>
4	K	90	<p>16% 94% 6%</p>
5	F	628	<p>4% 68% 8% 23%</p>
5	L	628	<p>4% 67% 9% 23%</p>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 58326 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	1759	1096	311	346	6	0	0	0
1	B	227	1759	1096	311	346	6	0	0	0
1	G	227	1759	1096	311	346	6	0	0	0
1	H	227	1759	1096	311	346	6	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1340	10569	6631	1841	2054	43	0	0	0
2	I	1340	10569	6631	1841	2054	43	0	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT BETA'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1342	10431	6551	1860	1971	49	0	0	0
3	J	1338	10401	6533	1854	1965	49	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	expression tag	UNP C5A0S8
D	1409	GLU	-	expression tag	UNP C5A0S8
D	1410	VAL	-	expression tag	UNP C5A0S8
D	1411	HIS	-	expression tag	UNP C5A0S8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1412	HIS	-	expression tag	UNP C5A0S8
D	1413	HIS	-	expression tag	UNP C5A0S8
D	1414	HIS	-	expression tag	UNP C5A0S8
D	1415	HIS	-	expression tag	UNP C5A0S8
D	1416	HIS	-	expression tag	UNP C5A0S8
J	1408	LEU	-	expression tag	UNP C5A0S8
J	1409	GLU	-	expression tag	UNP C5A0S8
J	1410	VAL	-	expression tag	UNP C5A0S8
J	1411	HIS	-	expression tag	UNP C5A0S8
J	1412	HIS	-	expression tag	UNP C5A0S8
J	1413	HIS	-	expression tag	UNP C5A0S8
J	1414	HIS	-	expression tag	UNP C5A0S8
J	1415	HIS	-	expression tag	UNP C5A0S8
J	1416	HIS	-	expression tag	UNP C5A0S8

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	K	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	481	Total	C	N	O	S	0	0	0
			3910	2445	699	743	23			
5	L	481	Total	C	N	O	S	0	0	0
			3910	2445	699	743	23			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	expression tag	UNP P00579
F	-13	ARG	-	expression tag	UNP P00579
F	-12	GLY	-	expression tag	UNP P00579
F	-11	SER	-	expression tag	UNP P00579
F	-10	HIS	-	expression tag	UNP P00579
F	-9	HIS	-	expression tag	UNP P00579
F	-8	HIS	-	expression tag	UNP P00579
F	-7	HIS	-	expression tag	UNP P00579

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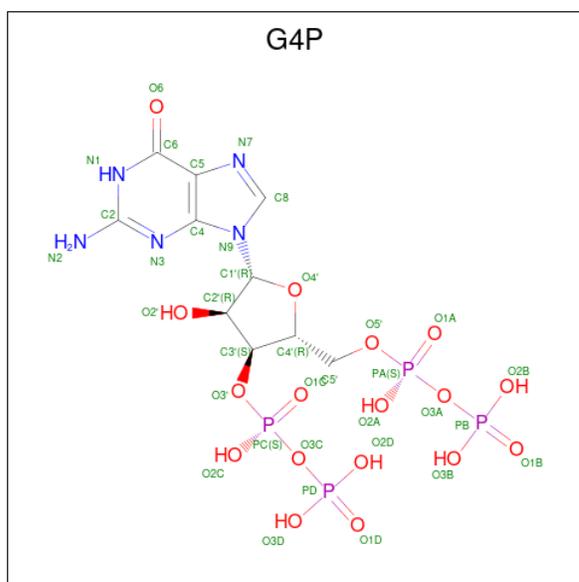
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	THR	-	expression tag	UNP P00579
F	-3	ASP	-	expression tag	UNP P00579
F	-2	GLN	-	expression tag	UNP P00579
F	-1	PHE	-	expression tag	UNP P00579
F	0	THR	-	expression tag	UNP P00579
L	-14	MET	-	expression tag	UNP P00579
L	-13	ARG	-	expression tag	UNP P00579
L	-12	GLY	-	expression tag	UNP P00579
L	-11	SER	-	expression tag	UNP P00579
L	-10	HIS	-	expression tag	UNP P00579
L	-9	HIS	-	expression tag	UNP P00579
L	-8	HIS	-	expression tag	UNP P00579
L	-7	HIS	-	expression tag	UNP P00579
L	-6	HIS	-	expression tag	UNP P00579
L	-5	HIS	-	expression tag	UNP P00579
L	-4	THR	-	expression tag	UNP P00579
L	-3	ASP	-	expression tag	UNP P00579
L	-2	GLN	-	expression tag	UNP P00579
L	-1	PHE	-	expression tag	UNP P00579
L	0	THR	-	expression tag	UNP P00579

- Molecule 6 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Sr 1 1	0	0
6	C	2	Total Sr 2 2	0	0
6	D	1	Total Sr 1 1	0	0
6	E	1	Total Sr 1 1	0	0
6	F	1	Total Sr 1 1	0	0
6	I	1	Total Sr 1 1	0	0
6	J	1	Total Sr 1 1	0	0

- Molecule 7 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>5</sub>O<sub>17</sub>P<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	D	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
7	K	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

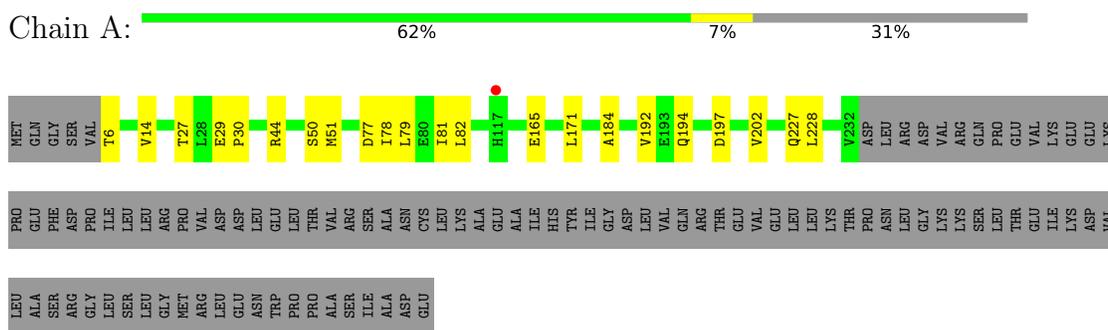
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	J	2	Total	Zn	0	0
			2	2		

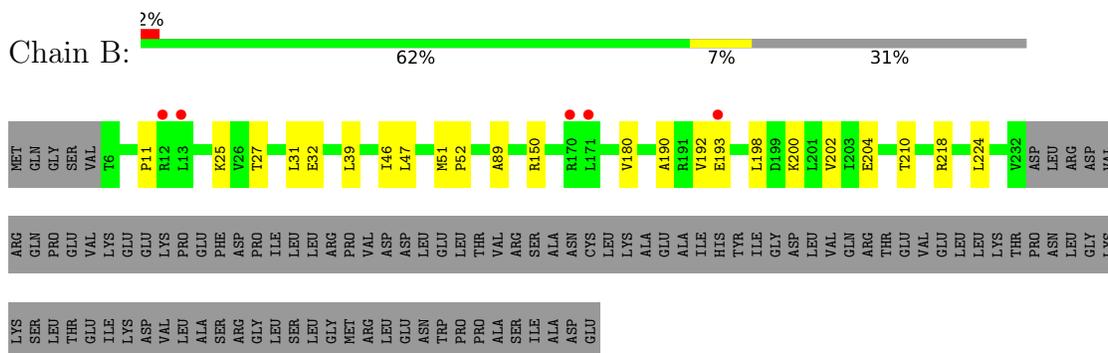
### 3 Residue-property plots [i](#)

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.

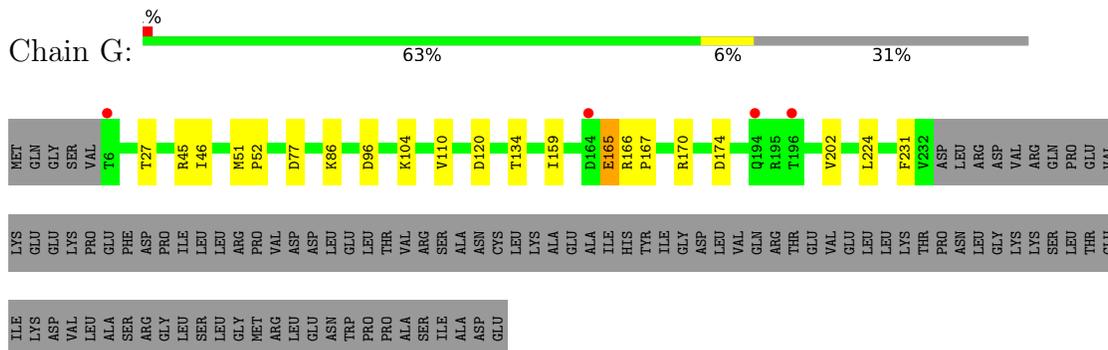
- Molecule 1: DNA-directed RNA polymerase subunit alpha



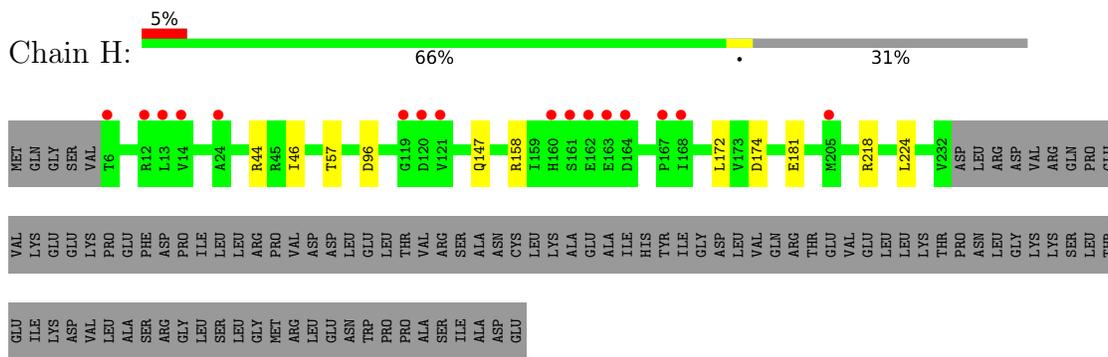
- Molecule 1: DNA-directed RNA polymerase subunit alpha



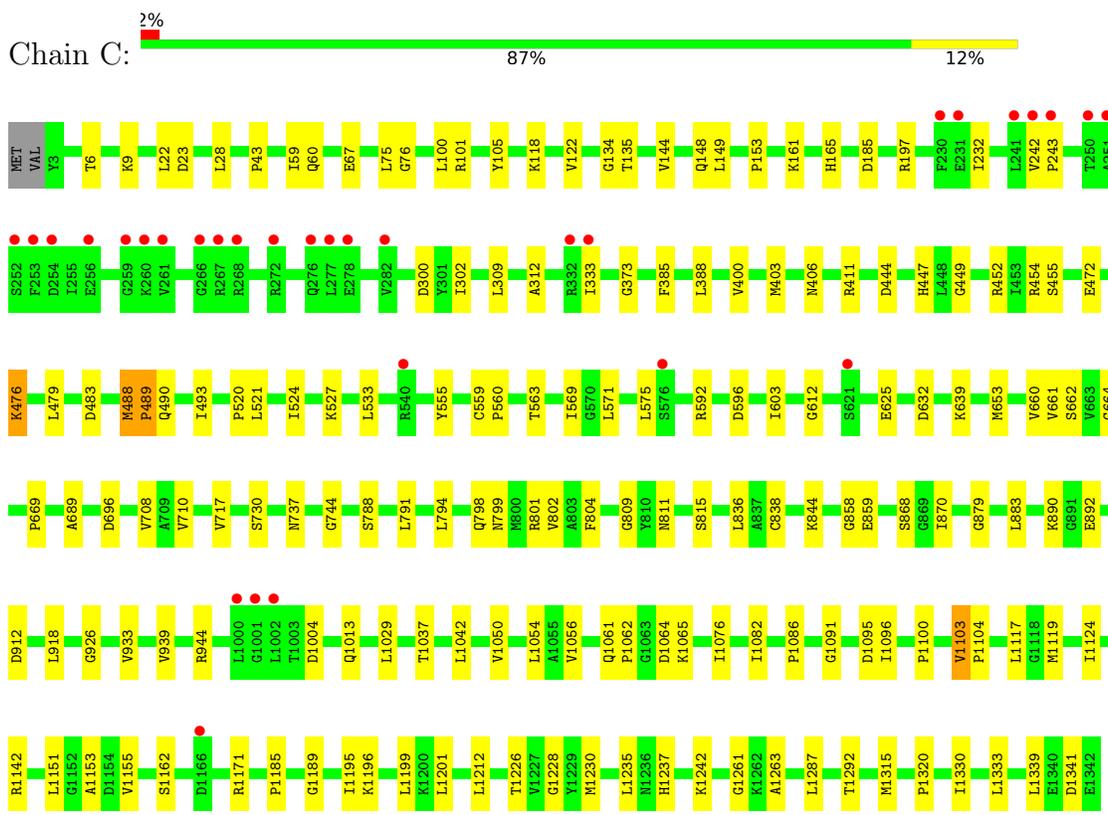
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

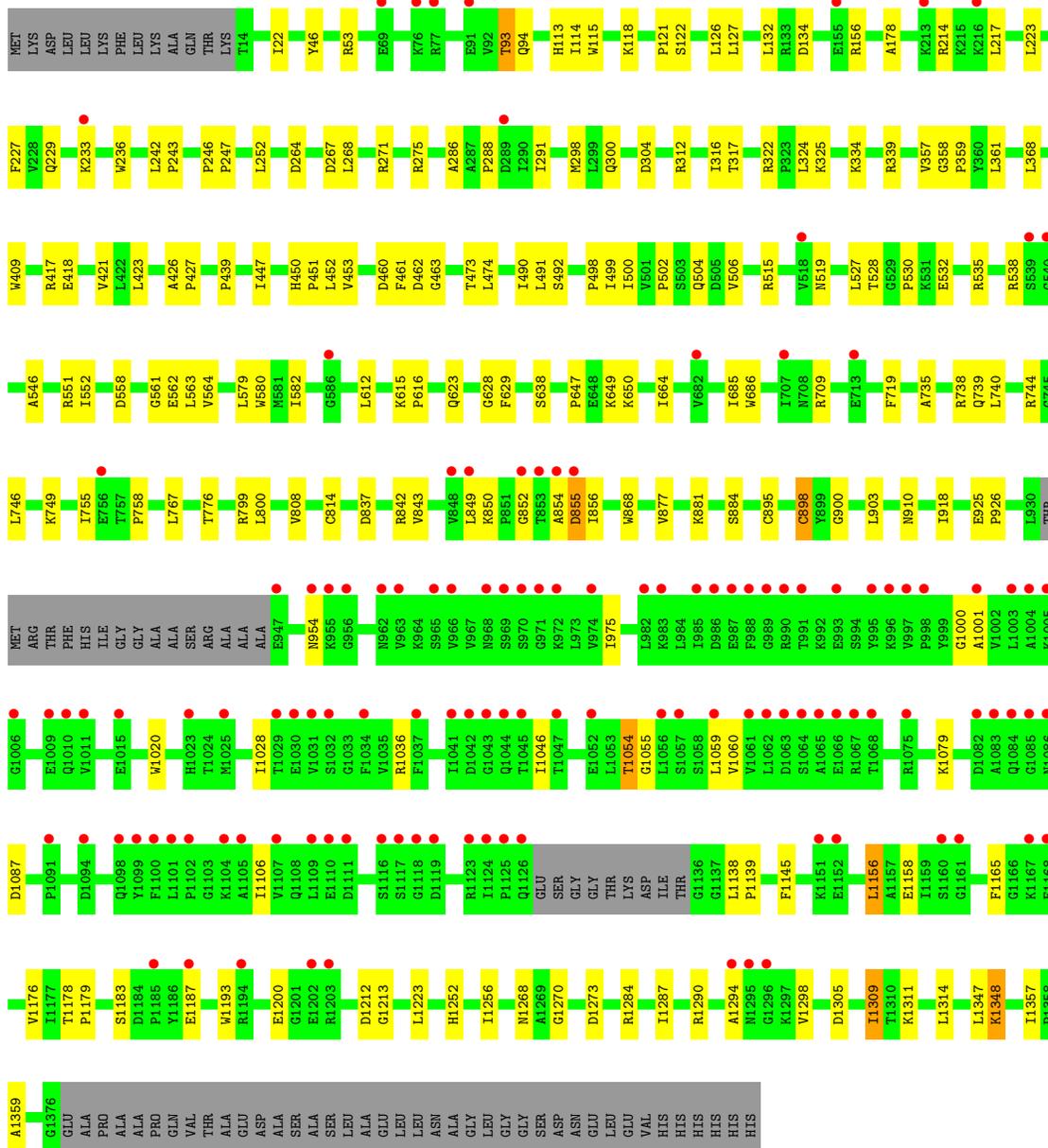




HIS  
HIS  
HIS

• Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT BETA'

Chain J: 9% 80% 14% 6%



• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 89% 11%



• Molecule 4: DNA-directed RNA polymerase subunit omega



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.57Å 206.16Å 311.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 4.20 39.94 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.97-4.20) 99.7 (39.94-4.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 4.13Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.247 , 0.318 0.260 , 0.330	Depositor DCC
$R_{free}$ test set	4396 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	167.3	Xtrriage
Anisotropy	0.268	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 202.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	58326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	280.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: G4P, ZN, SR

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	0.45	0/1781	0.49	1/2414 (0.0%)
1	B	0.43	0/1781	0.51	1/2414 (0.0%)
1	G	0.41	0/1781	0.47	0/2414
1	H	0.40	0/1781	0.47	0/2414
2	C	0.50	0/10738	0.54	1/14489 (0.0%)
2	I	0.42	2/10738 (0.0%)	0.49	0/14489
3	D	0.50	5/10588 (0.0%)	0.53	2/14295 (0.0%)
3	J	0.45	7/10558 (0.1%)	0.51	1/14255 (0.0%)
4	E	0.53	0/710	0.56	0/956
4	K	0.39	0/710	0.51	0/956
5	F	0.45	3/3964 (0.1%)	0.52	0/5330
5	L	0.43	4/3964 (0.1%)	0.49	0/5330
All	All	0.46	21/59094 (0.0%)	0.51	6/79756 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	479	GLU	CD-OE1	-6.85	1.18	1.25
2	I	807	TRP	CD2-CE2	5.79	1.48	1.41
3	D	580	TRP	CD2-CE2	5.54	1.48	1.41
3	D	33	TRP	CD2-CE2	5.48	1.48	1.41
3	J	868	TRP	CD2-CE2	5.42	1.47	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	C	1341	ASP	CB-CG-OD1	6.31	123.98	118.30
3	D	479	GLU	OE1-CD-OE2	-6.14	115.94	123.30
3	D	855	ASP	CB-CG-OD2	5.23	123.00	118.30
3	J	855	ASP	CB-CG-OD2	5.21	122.99	118.30

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	1759	0	1785	10	0
1	B	1759	0	1785	14	0
1	G	1759	0	1785	11	0
1	H	1759	0	1785	5	0
2	C	10569	0	10582	75	0
2	I	10569	0	10582	77	0
3	D	10431	0	10649	104	0
3	J	10401	0	10616	103	0
4	E	708	0	719	5	0
4	K	708	0	719	3	0
5	F	3910	0	3970	23	0
5	L	3910	0	3970	22	0
6	A	1	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	D	36	0	11	1	0
7	K	36	0	11	0	0
8	D	2	0	0	1	0
8	J	2	0	0	0	0
All	All	58326	0	58969	404	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.

The worst 5 of 404 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)
3:J:895:CYS:HB2	3:J:898:CYS:SG	1.76	1.24
3:D:888:CYS:SG	3:D:895:CYS:SG	2.60	0.99
3:J:895:CYS:CB	3:J:898:CYS:SG	2.53	0.97
3:J:895:CYS:N	3:J:898:CYS:SG	2.42	0.93
3:D:898:CYS:O	3:D:898:CYS:SG	2.29	0.90

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	225/329 (68%)	216 (96%)	6 (3%)	3 (1%)	12	48
1	B	225/329 (68%)	213 (95%)	12 (5%)	0	100	100
1	G	225/329 (68%)	214 (95%)	10 (4%)	1 (0%)	34	72
1	H	225/329 (68%)	217 (96%)	7 (3%)	1 (0%)	34	72
2	C	1338/1342 (100%)	1208 (90%)	107 (8%)	23 (2%)	9	44
2	I	1338/1342 (100%)	1186 (89%)	131 (10%)	21 (2%)	9	45
3	D	1336/1416 (94%)	1206 (90%)	110 (8%)	20 (2%)	10	46
3	J	1332/1416 (94%)	1207 (91%)	111 (8%)	14 (1%)	14	52
4	E	88/90 (98%)	82 (93%)	5 (6%)	1 (1%)	14	52
4	K	88/90 (98%)	83 (94%)	5 (6%)	0	100	100
5	F	477/628 (76%)	432 (91%)	36 (8%)	9 (2%)	8	41
5	L	477/628 (76%)	442 (93%)	27 (6%)	8 (2%)	9	44
All	All	7374/8268 (89%)	6706 (91%)	567 (8%)	101 (1%)	11	47

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	488	MET

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Mol	Chain	Res	Type
2	C	489	PRO
2	C	555	TYR
2	C	569	ILE
5	F	243	ALA

### 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	195/286 (68%)	192 (98%)	3 (2%)	65	80
1	B	195/286 (68%)	195 (100%)	0	100	100
1	G	195/286 (68%)	191 (98%)	4 (2%)	53	71
1	H	195/286 (68%)	193 (99%)	2 (1%)	76	86
2	C	1155/1157 (100%)	1133 (98%)	22 (2%)	57	74
2	I	1155/1157 (100%)	1122 (97%)	33 (3%)	42	64
3	D	1123/1177 (95%)	1098 (98%)	25 (2%)	52	70
3	J	1120/1177 (95%)	1090 (97%)	30 (3%)	44	66
4	E	74/74 (100%)	72 (97%)	2 (3%)	44	66
4	K	74/74 (100%)	73 (99%)	1 (1%)	67	80
5	F	427/554 (77%)	419 (98%)	8 (2%)	57	74
5	L	427/554 (77%)	415 (97%)	12 (3%)	43	65
All	All	6335/7068 (90%)	6193 (98%)	142 (2%)	52	70

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	551	ARG
3	J	881	LYS
5	L	96	ASP
3	D	1305	ASP
3	D	1266	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	799	ASN
3	J	1227	HIS
2	I	1312	ASN
3	J	488	ASN
5	L	129	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 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	$\# Z  > 2$
7	G4P	D	2001	-	30,38,38	1.32	3 (10%)	42,61,61	1.47	4 (9%)
7	G4P	K	101	-	30,38,38	1.11	2 (6%)	42,61,61	1.30	4 (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
7	G4P	D	2001	-	-	1/23/43/43	0/3/3/3
7	G4P	K	101	-	-	1/23/43/43	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	2001	G4P	C6-N1	-3.24	1.33	1.37
7	K	101	G4P	O4'-C1'	3.17	1.45	1.41
7	D	2001	G4P	O4'-C1'	3.04	1.45	1.41
7	K	101	G4P	C6-N1	-2.72	1.33	1.37
7	D	2001	G4P	PB-O2B	-2.13	1.46	1.54

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	2001	G4P	PA-O3A-PB	-4.53	117.28	132.83
7	K	101	G4P	PC-O3C-PD	-3.76	119.91	132.83
7	D	2001	G4P	PC-O3C-PD	-3.68	120.21	132.83
7	K	101	G4P	PA-O3A-PB	-3.65	120.30	132.83
7	D	2001	G4P	C5-C6-N1	2.88	119.03	113.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	2001	G4P	PB-O3A-PA-O1A
7	K	101	G4P	PB-O3A-PA-O1A

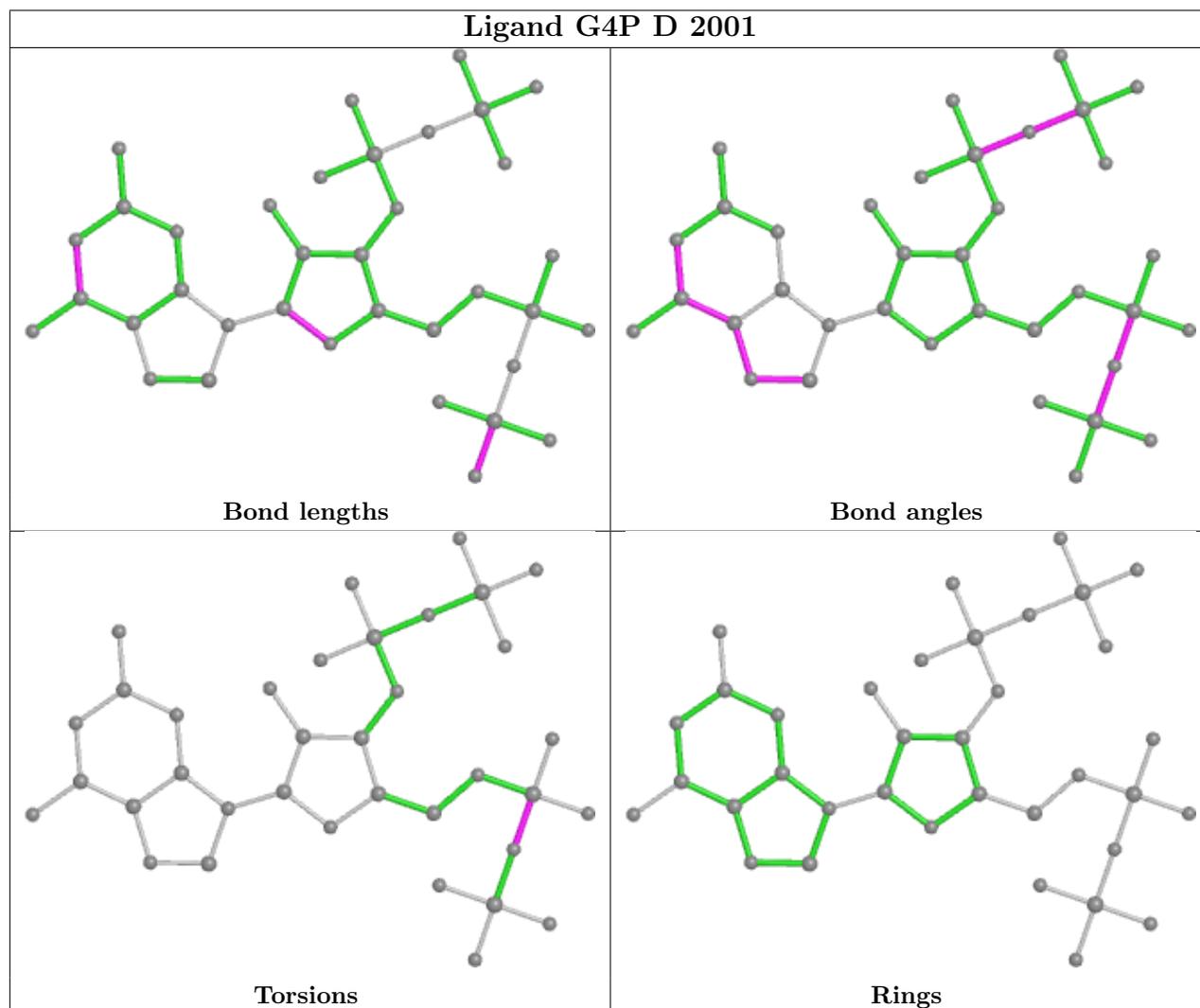
There are no ring outliers.

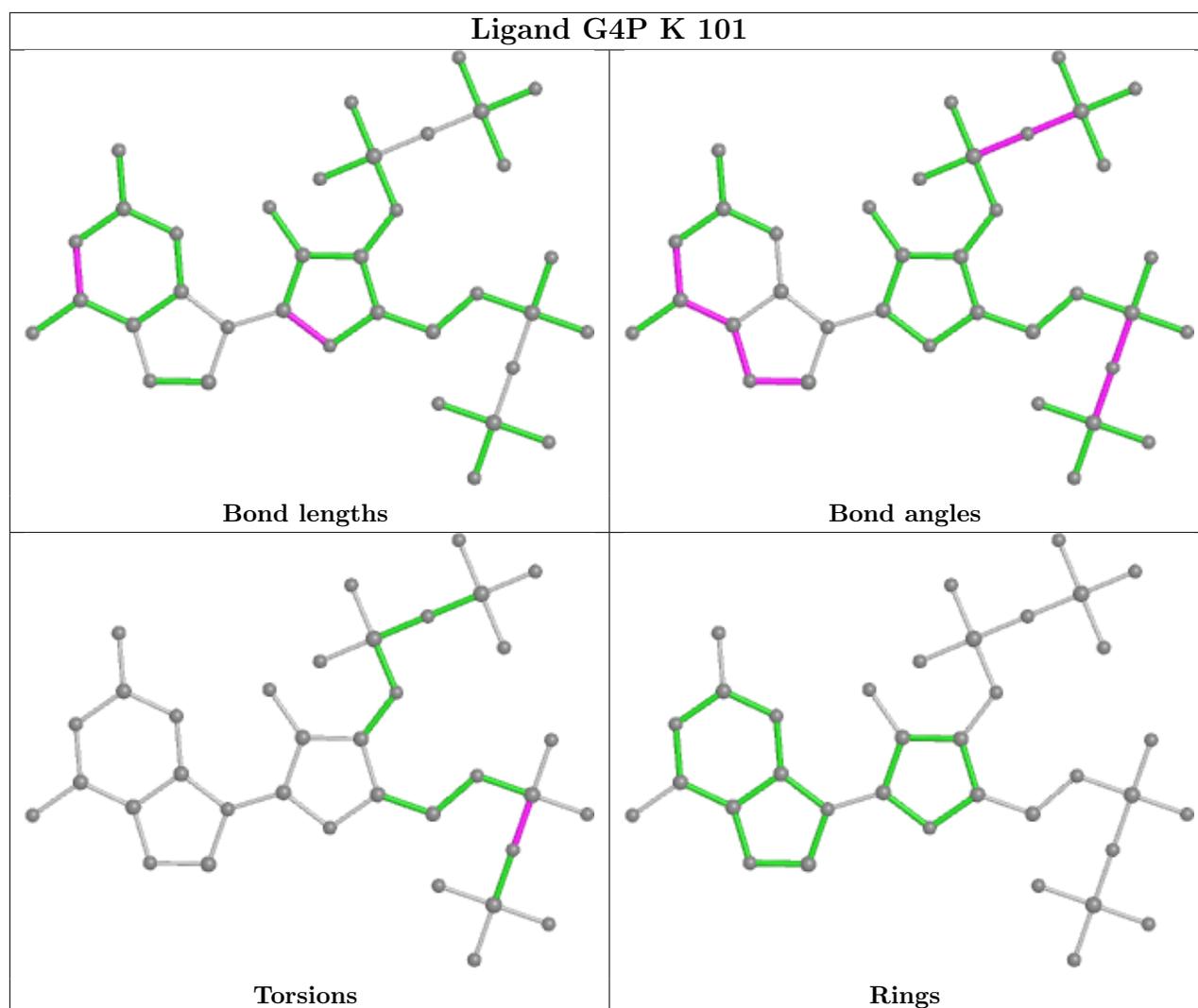
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	2001	G4P	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 [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, 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	227/329 (68%)	-0.14	1 (0%) 92 87	148, 217, 322, 411	0
1	B	227/329 (68%)	-0.00	5 (2%) 62 52	155, 276, 386, 464	0
1	G	227/329 (68%)	-0.09	4 (1%) 68 59	195, 272, 381, 487	0
1	H	227/329 (68%)	0.30	16 (7%) 16 13	209, 313, 434, 551	0
2	C	1340/1342 (99%)	-0.13	31 (2%) 60 51	116, 219, 400, 608	0
2	I	1340/1342 (99%)	-0.03	43 (3%) 47 37	158, 257, 405, 600	0
3	D	1342/1416 (94%)	0.29	128 (9%) 8 8	114, 234, 543, 696	0
3	J	1338/1416 (94%)	0.38	127 (9%) 8 8	158, 266, 556, 725	0
4	E	90/90 (100%)	-0.12	0 100 100	147, 230, 311, 405	0
4	K	90/90 (100%)	0.73	14 (15%) 2 2	217, 322, 517, 666	0
5	F	481/628 (76%)	0.03	25 (5%) 27 23	153, 297, 481, 614	0
5	L	481/628 (76%)	0.12	27 (5%) 24 21	182, 318, 469, 601	0
All	All	7410/8268 (89%)	0.11	421 (5%) 23 20	114, 258, 482, 725	0

The worst 5 of 421 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1073	ASP	22.8
3	J	1118	GLY	18.5
3	J	1125	PRO	17.7
3	D	983	LYS	16.8
3	J	1057	SER	12.1

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

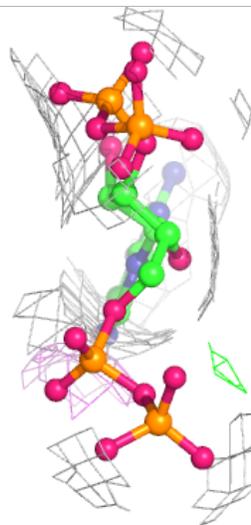
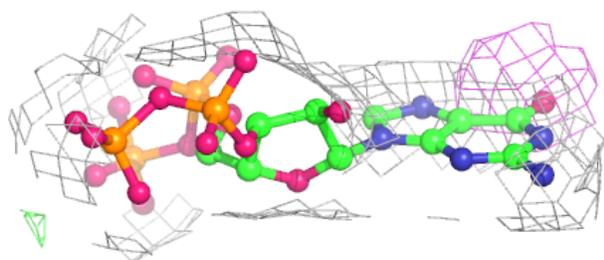
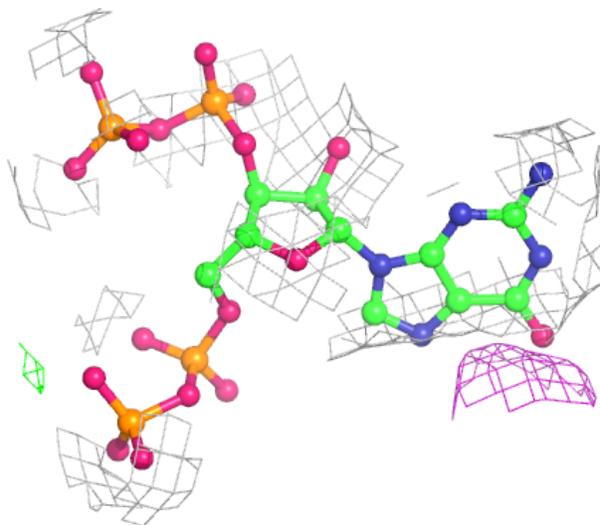
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

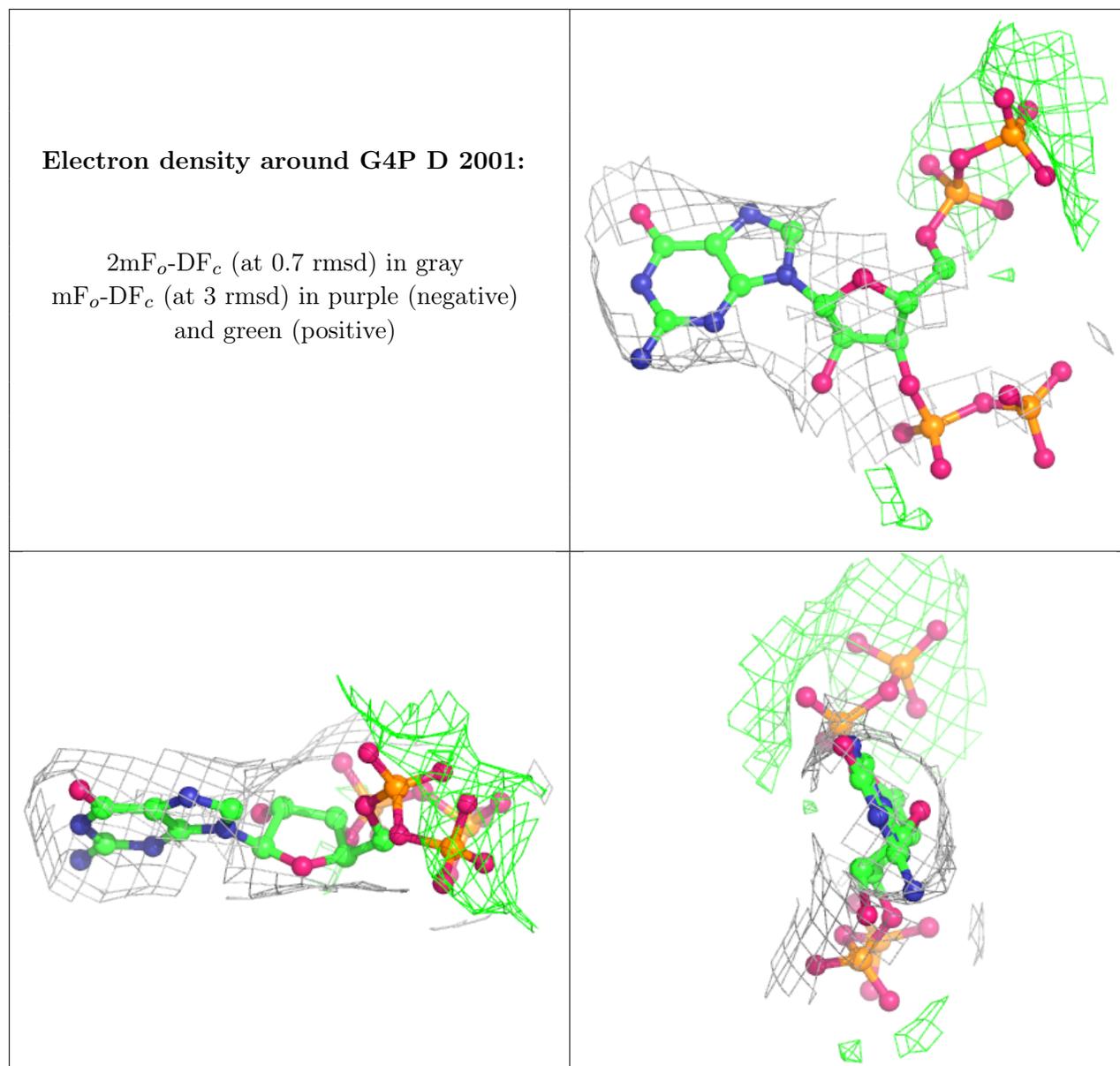
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SR	E	101	1/1	0.69	0.28	328,328,328,328	0
6	SR	I	1401	1/1	0.76	0.39	346,346,346,346	0
7	G4P	K	101	36/36	0.76	0.26	158,256,299,307	0
8	ZN	J	1502	1/1	0.84	0.12	256,256,256,256	0
6	SR	C	1401	1/1	0.85	0.46	303,303,303,303	0
8	ZN	D	2003	1/1	0.88	0.12	245,245,245,245	0
7	G4P	D	2001	36/36	0.90	0.32	125,188,244,266	0
6	SR	A	401	1/1	0.90	0.15	261,261,261,261	0
8	ZN	D	2002	1/1	0.94	0.04	261,261,261,261	0
6	SR	F	701	1/1	0.94	0.44	239,239,239,239	0
6	SR	D	2004	1/1	0.94	0.17	288,288,288,288	0
6	SR	J	1503	1/1	0.95	0.29	322,322,322,322	0
8	ZN	J	1501	1/1	0.96	0.03	249,249,249,249	0
6	SR	C	1402	1/1	0.96	0.62	212,212,212,212	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 G4P K 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.