



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 11:52 AM UTC

PDB ID : 4JKR / pdb_00004jkr
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

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

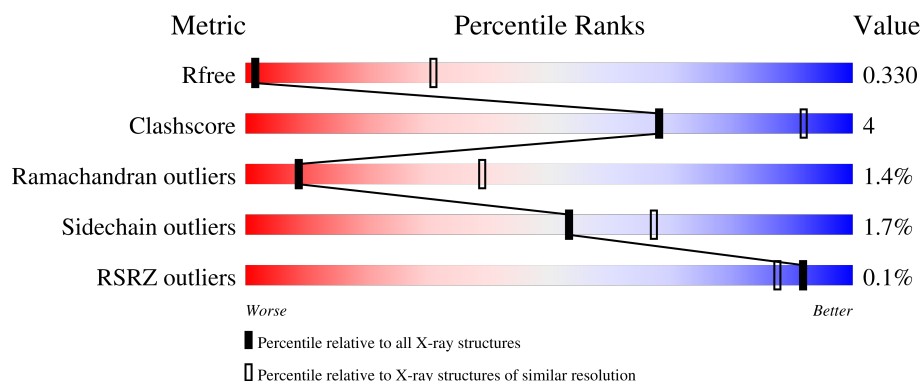
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	329	% 63% 6% 31%
1	B	329	62% 7% 31%
1	G	329	64% 5% 31%
1	H	329	66% . 31%
2	C	1342	87% 13%

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Mol	Chain	Length	Quality of chain
2	I	1342	88% 12%
3	D	1416	81% 13% 5%
3	J	1416	81% 13% 6%
4	E	90	90% 10%
4	K	90	94% 6%
5	F	628	69% 7% 23%
5	L	628	68% 8% 23%

2 Entry composition

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
1	A	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	B	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	G	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	H	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			

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

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

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

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

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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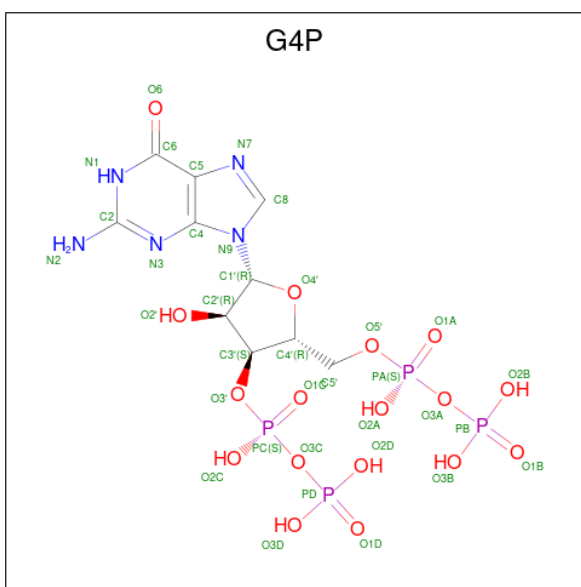
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	THR	-	expression tag	UNP P00579
F	-3	ASP	-	expression tag	UNP P00579
F	-2	GLN	-	expression tag	UNP P00579
F	-1	PHE	-	expression 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 (CCD ID: SR) (formula: Sr).

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

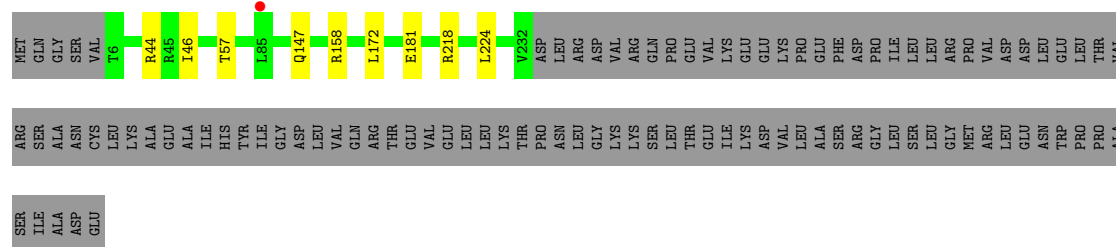
- Molecule 7 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄).



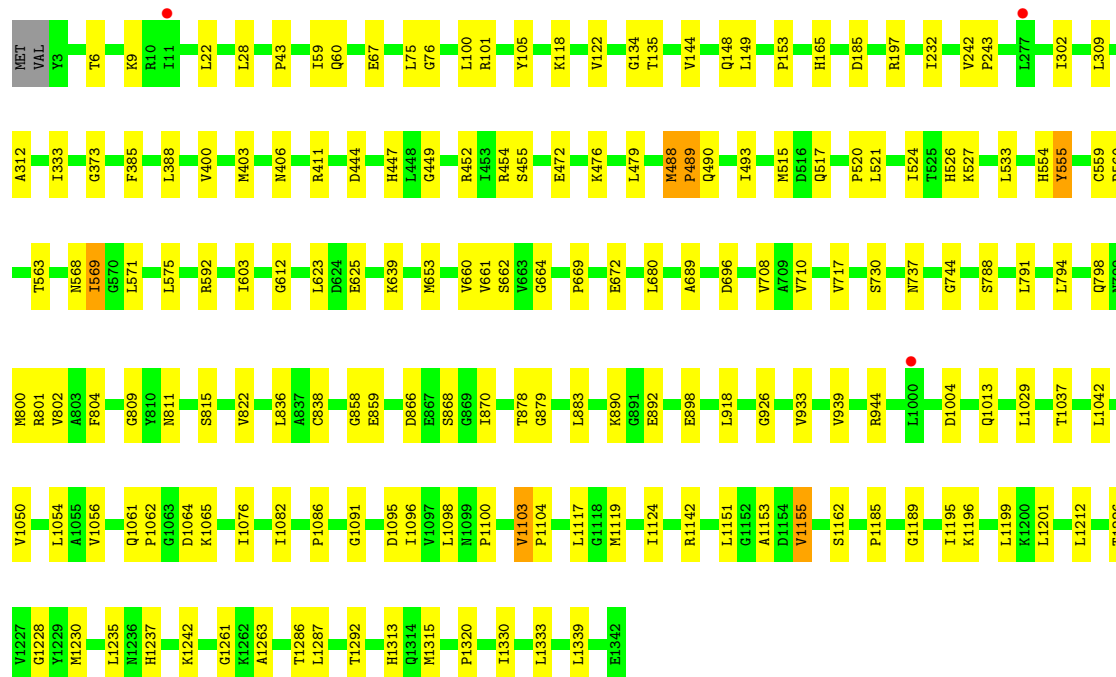
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	D	1	Total 36	C 10	N 5	O 17	P 4	0	0
7	K	1	Total 36	C 10	N 5	O 17	P 4	0	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

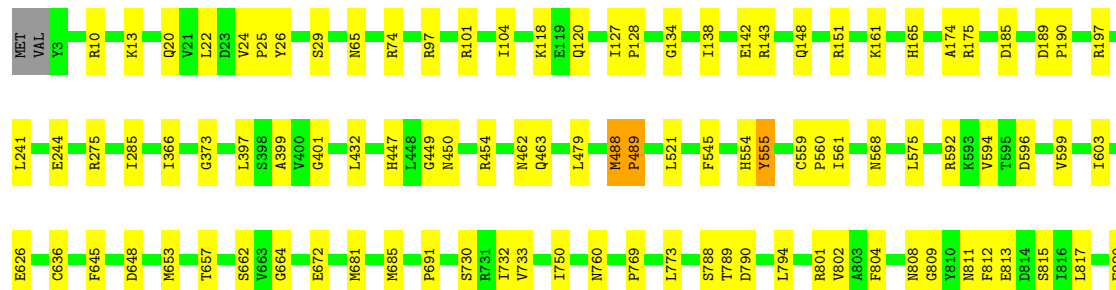
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	2	Total Zn 2 2	0	0
8	J	2	Total Zn 2 2	0	0

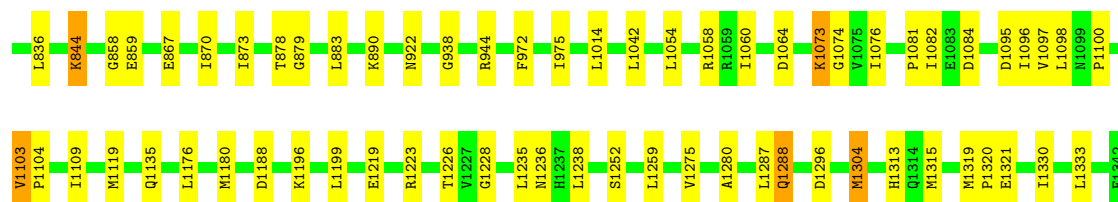


- Chain C: 87% 13%



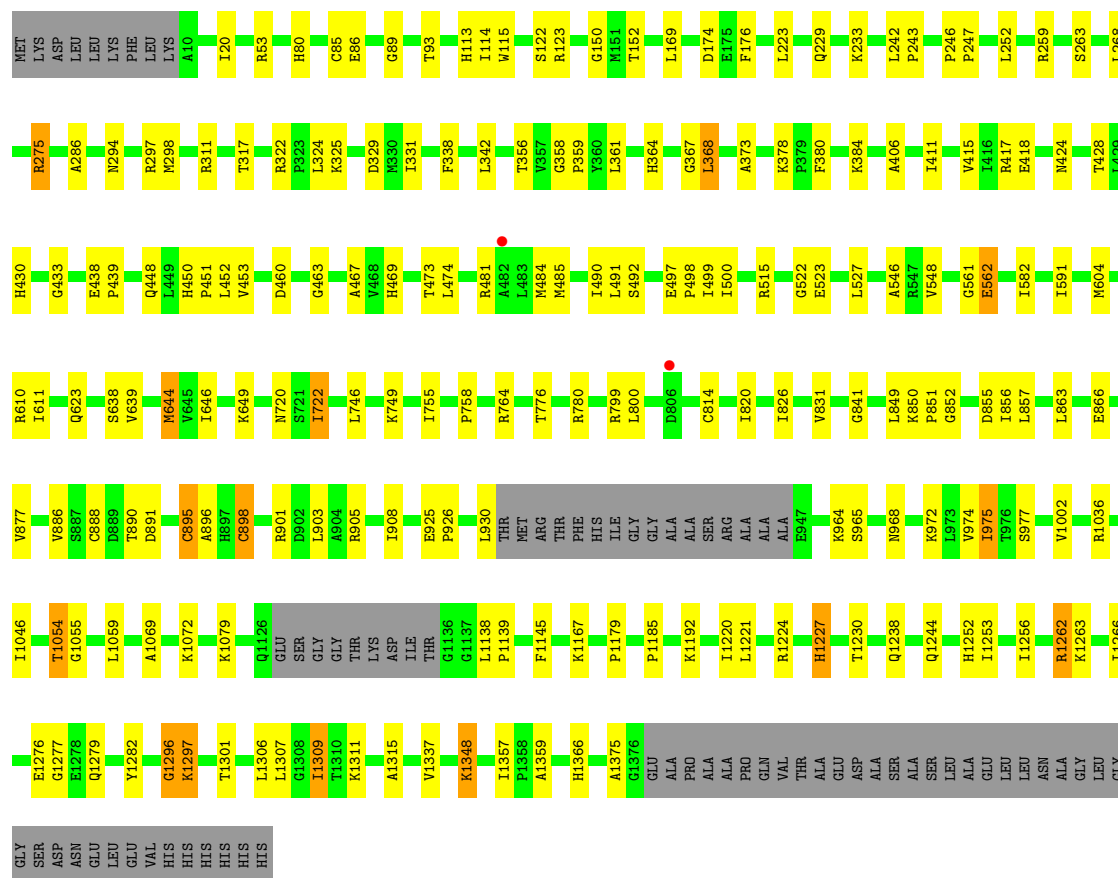
- Chain I: 88% 12%





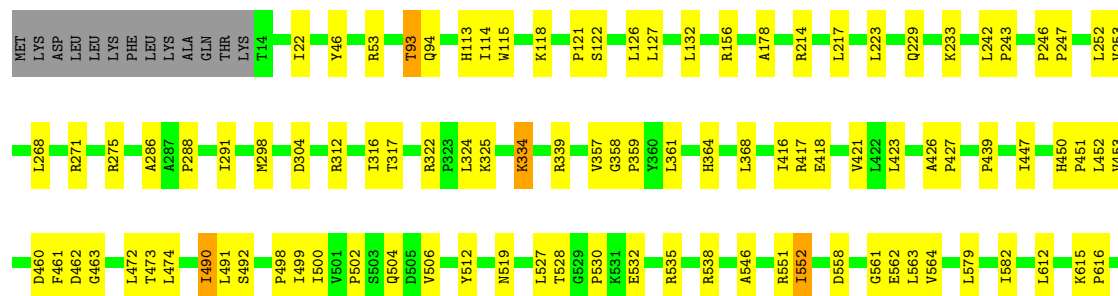
• Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT BETA'

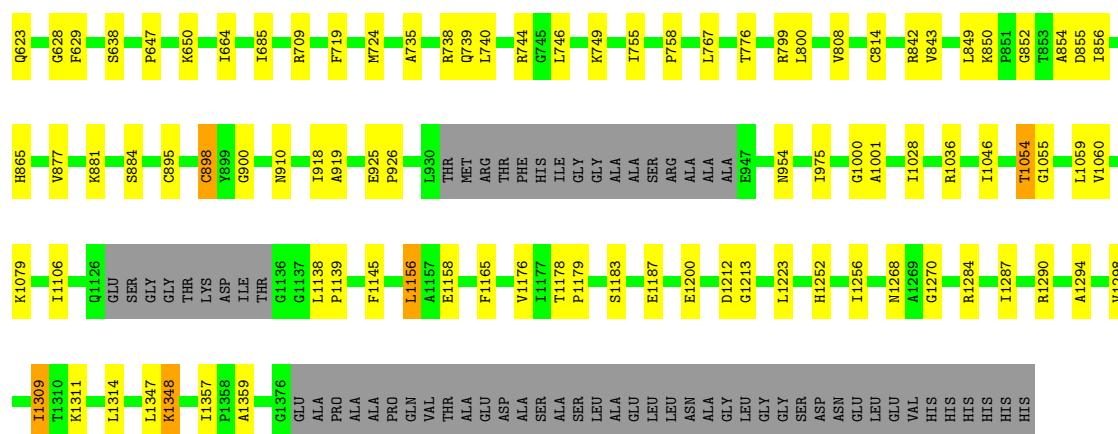
Chain D: 81% 13% • 5%



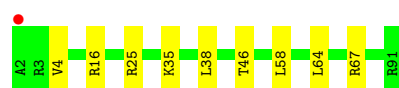
• Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT BETA'

Chain J: 81% 13% • 6%





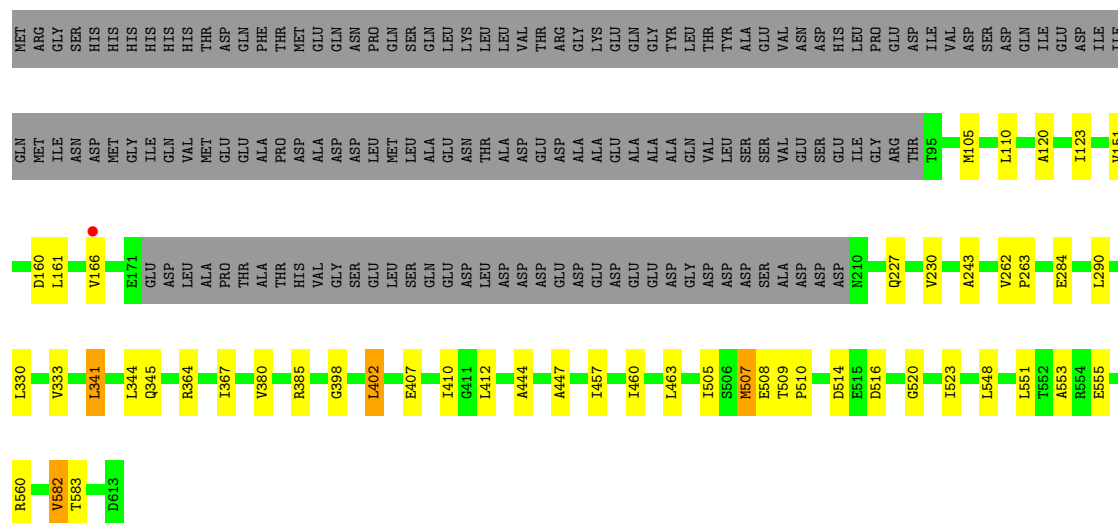
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 5: RNA polymerase sigma factor RpoD



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.57Å 206.16Å 311.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 4.20 39.97 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.97-4.20) 99.6 (39.97-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.247 , 0.318 0.260 , 0.330	Depositor DCC
R_{free} test set	4401 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	167.3	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 253.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	58326	wwPDB-VP
Average B, all atoms (Å ²)	280.0	wwPDB-VP

Xtriage'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.*

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: SR, G4P, 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	0.67	0/1781	0.73	0/2414
1	B	0.65	0/1781	0.73	0/2414
1	G	0.61	0/1781	0.71	0/2414
1	H	0.60	0/1781	0.69	0/2414
2	C	0.64	5/10738 (0.0%)	0.77	1/14489 (0.0%)
2	I	0.55	0/10738	0.74	0/14489
3	D	0.64	6/10588 (0.1%)	0.78	0/14295
3	J	0.59	2/10558 (0.0%)	0.76	1/14255 (0.0%)
4	E	0.63	0/710	0.86	0/956
4	K	0.47	0/710	0.78	0/956
5	F	0.55	0/3964	0.80	2/5330 (0.0%)
5	L	0.53	0/3964	0.78	0/5330
All	All	0.60	13/59094 (0.0%)	0.76	4/79756 (0.0%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	364	HIS	CE1-NE2	8.87	1.41	1.32
2	C	1313	HIS	CG-CD2	7.31	1.43	1.35
2	C	1313	HIS	ND1-CE1	6.99	1.39	1.32
3	D	364	HIS	CG-CD2	6.80	1.43	1.35
3	D	469	HIS	CG-CD2	6.07	1.42	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	866	ASP	N-CA-C	6.01	113.70	108.78
3	J	253	VAL	N-CA-C	5.94	113.74	108.63
5	F	262	VAL	CA-C-N	5.19	126.33	119.84
5	F	262	VAL	C-N-CA	5.19	126.33	119.84

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	81	0
2	I	10569	0	10582	82	0
3	D	10431	0	10649	108	0
3	J	10401	0	10616	107	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	23	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	421	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 4.

The worst 5 of 421 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%)	9	41
1	B	225/329 (68%)	213 (95%)	12 (5%)	0	100	100
1	G	225/329 (68%)	214 (95%)	10 (4%)	1 (0%)	30	66
1	H	225/329 (68%)	217 (96%)	7 (3%)	1 (0%)	30	66
2	C	1338/1342 (100%)	1208 (90%)	107 (8%)	23 (2%)	7	35
2	I	1338/1342 (100%)	1186 (89%)	131 (10%)	21 (2%)	7	37
3	D	1336/1416 (94%)	1206 (90%)	110 (8%)	20 (2%)	8	38
3	J	1332/1416 (94%)	1207 (91%)	111 (8%)	14 (1%)	11	45
4	E	88/90 (98%)	82 (93%)	5 (6%)	1 (1%)	11	45
4	K	88/90 (98%)	83 (94%)	5 (6%)	0	100	100
5	F	477/628 (76%)	432 (91%)	36 (8%)	9 (2%)	6	32
5	L	477/628 (76%)	442 (93%)	27 (6%)	8 (2%)	7	35
All	All	7374/8268 (89%)	6706 (91%)	567 (8%)	101 (1%)	9	39

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 ⓘ

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%)	194 (100%)	1 (0%)	81	81
1	B	195/286 (68%)	194 (100%)	1 (0%)	81	81
1	G	195/286 (68%)	195 (100%)	0	100	100
1	H	195/286 (68%)	195 (100%)	0	100	100
2	C	1155/1157 (100%)	1138 (98%)	17 (2%)	57	70
2	I	1155/1157 (100%)	1135 (98%)	20 (2%)	53	67
3	D	1123/1177 (95%)	1093 (97%)	30 (3%)	39	60
3	J	1120/1177 (95%)	1097 (98%)	23 (2%)	47	65
4	E	74/74 (100%)	73 (99%)	1 (1%)	59	70
4	K	74/74 (100%)	73 (99%)	1 (1%)	59	70
5	F	427/554 (77%)	421 (99%)	6 (1%)	59	70
5	L	427/554 (77%)	418 (98%)	9 (2%)	47	65
All	All	6335/7068 (90%)	6226 (98%)	109 (2%)	53	67

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	161	LYS
2	I	1082	ILE
4	K	46	THR
2	I	366	ILE
2	I	844	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	46	GLN
3	J	158	GLN
2	I	447	HIS
2	I	1099	ASN
3	J	335	GLN

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 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	-	36,38,38	1.99	6 (16%)	56,61,61	1.82	9 (16%)
7	G4P	K	101	-	36,38,38	1.35	3 (8%)	56,61,61	1.69	6 (10%)

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	-	-	2/27/43/43	0/3/3/3
7	G4P	K	101	-	-	1/27/43/43	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	2001	G4P	PC-O3C	7.11	1.67	1.59
7	D	2001	G4P	PA-O3A	5.42	1.65	1.59
7	K	101	G4P	PC-O3C	3.98	1.63	1.59
7	D	2001	G4P	C5-C4	3.34	1.47	1.38
7	D	2001	G4P	C6-N1	-3.10	1.33	1.38

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	2001	G4P	C5-C4-N3	-6.27	118.41	128.39
7	K	101	G4P	C5-C4-N3	-6.25	118.44	128.39
7	K	101	G4P	C2-N3-C4	5.16	121.18	112.30
7	D	2001	G4P	C2-N3-C4	5.03	120.96	112.30
7	D	2001	G4P	N9-C4-N3	4.90	135.74	125.95

There are no chirality outliers.

All (3) 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
7	D	2001	G4P	PB-O3A-PA-O2A

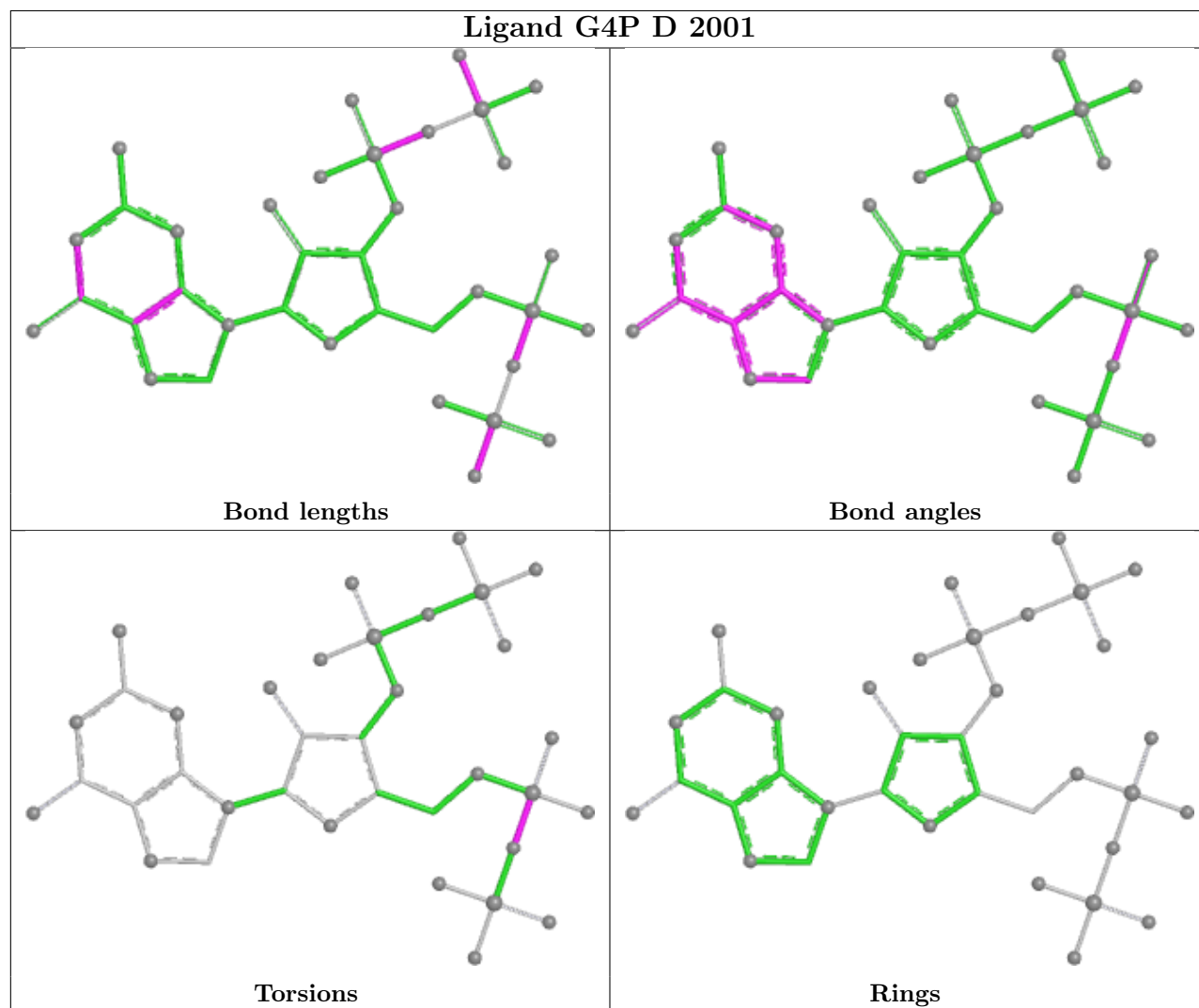
There are no ring outliers.

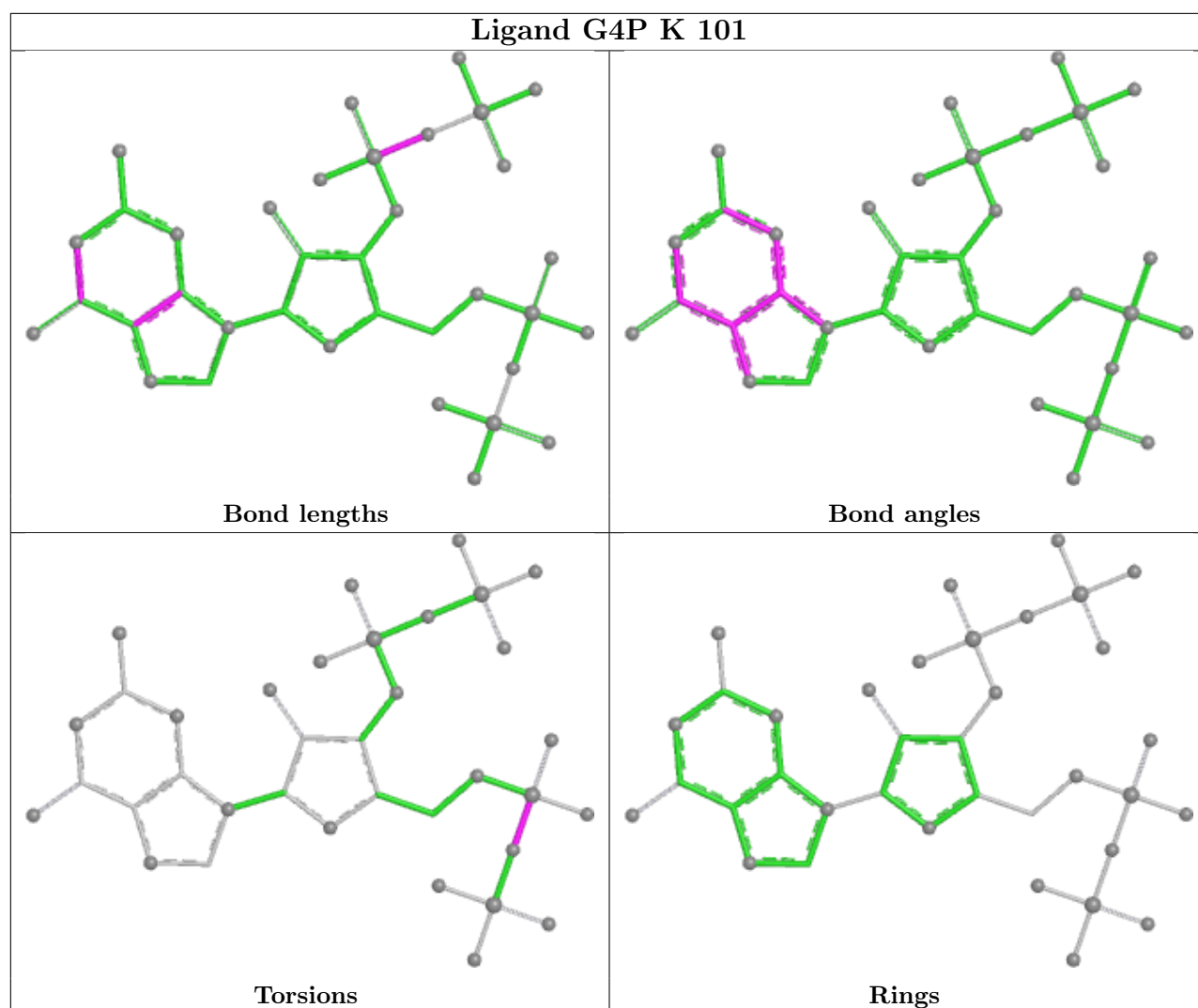
1 monomer is involved in 1 short contact:

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 ⓘ

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, 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	227/329 (68%)	-0.33	3 (1%) 75 59	148, 217, 322, 411	0
1	B	227/329 (68%)	-0.32	0 100 100	155, 276, 386, 464	0
1	G	227/329 (68%)	-0.44	0 100 100	195, 272, 381, 487	0
1	H	227/329 (68%)	-0.49	1 (0%) 88 77	209, 313, 434, 551	0
2	C	1340/1342 (99%)	-0.34	3 (0%) 91 83	116, 219, 400, 608	0
2	I	1340/1342 (99%)	-0.42	0 100 100	158, 257, 405, 600	0
3	D	1342/1416 (94%)	-0.33	2 (0%) 92 87	114, 234, 543, 696	0
3	J	1338/1416 (94%)	-0.36	0 100 100	158, 266, 556, 725	0
4	E	90/90 (100%)	-0.30	1 (1%) 78 62	147, 230, 311, 405	0
4	K	90/90 (100%)	-0.39	0 100 100	217, 322, 517, 666	0
5	F	481/628 (76%)	-0.45	1 (0%) 91 83	153, 297, 481, 614	0
5	L	481/628 (76%)	-0.54	0 100 100	182, 318, 469, 601	0
All	All	7410/8268 (89%)	-0.38	11 (0%) 92 87	114, 258, 482, 725	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	166	VAL	3.6
2	C	277	LEU	3.3
3	D	482	ALA	2.7
4	E	2	ALA	2.7
1	A	205	MET	2.7

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

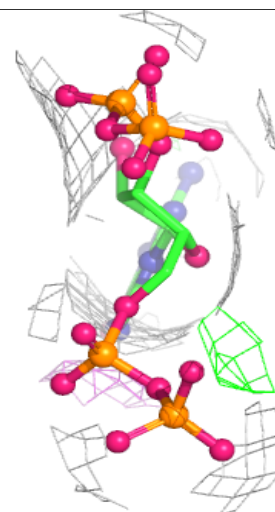
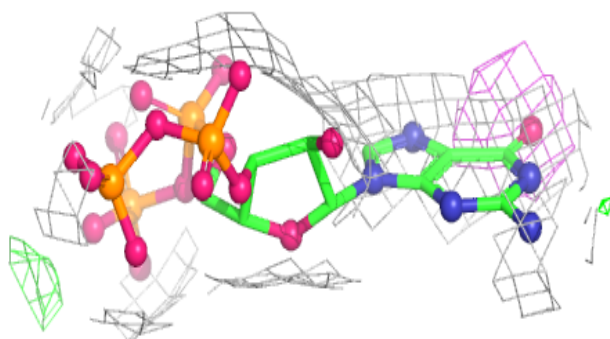
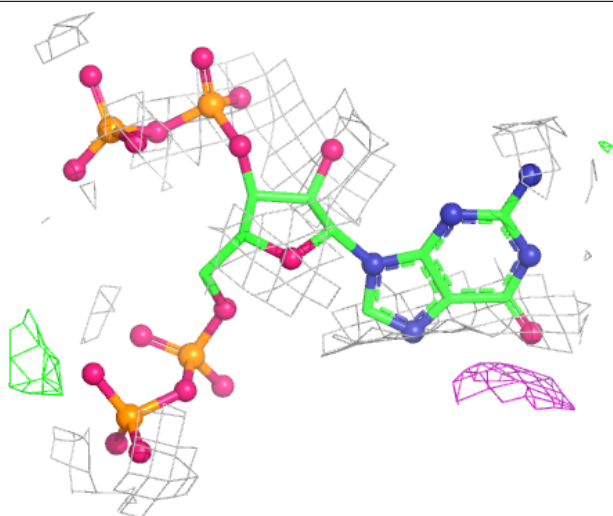
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	SR	C	1401	1/1	0.56	0.12	303,303,303,303	0
6	SR	I	1401	1/1	0.67	0.06	346,346,346,346	0
7	G4P	K	101	36/36	0.67	0.09	158,256,299,307	0
8	ZN	J	1502	1/1	0.85	0.09	256,256,256,256	0
7	G4P	D	2001	36/36	0.88	0.09	125,188,244,266	0
6	SR	J	1503	1/1	0.90	0.06	322,322,322,322	0
8	ZN	D	2003	1/1	0.90	0.09	245,245,245,245	0
6	SR	A	401	1/1	0.90	0.10	261,261,261,261	0
6	SR	E	101	1/1	0.93	0.09	328,328,328,328	0
6	SR	C	1402	1/1	0.95	0.15	212,212,212,212	0
6	SR	F	701	1/1	0.95	0.07	239,239,239,239	0
6	SR	D	2004	1/1	0.96	0.03	288,288,288,288	0
8	ZN	D	2002	1/1	0.96	0.06	261,261,261,261	0
8	ZN	J	1501	1/1	0.99	0.03	249,249,249,249	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.

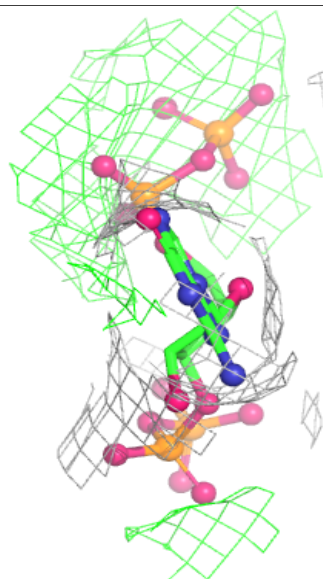
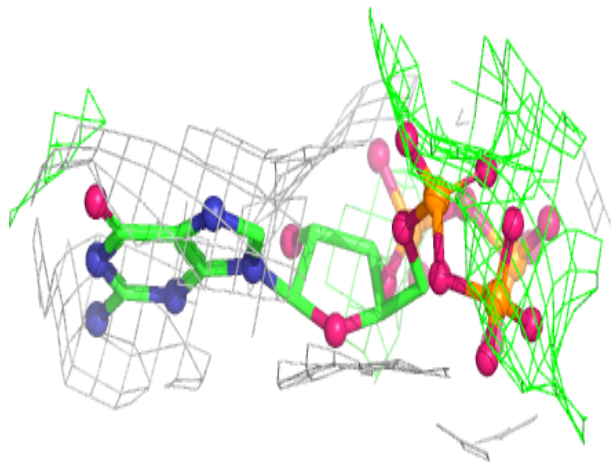
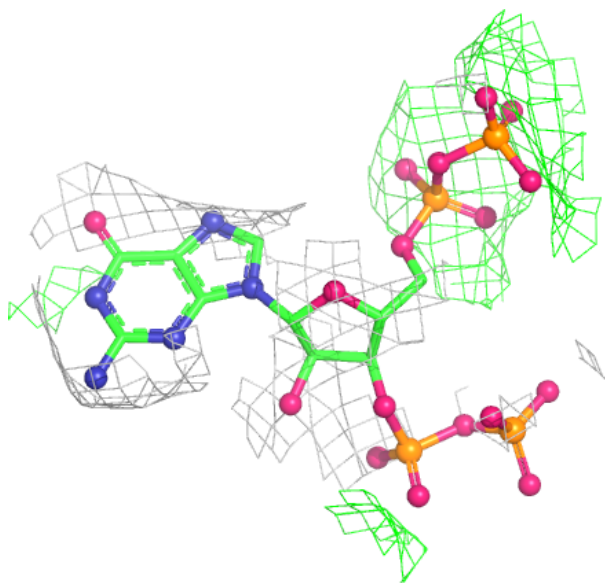
Electron density around G4P K 101:

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



Electron density around G4P D 2001:

$2mF_o - DF_c$ (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.