



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 03:59 am BST

PDB ID : 5VSW
Title : X-ray crystal structure of Escherichia coli RNA polymerase and DksA/ppGpp complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2017-05-12
Resolution : 4.29 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 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

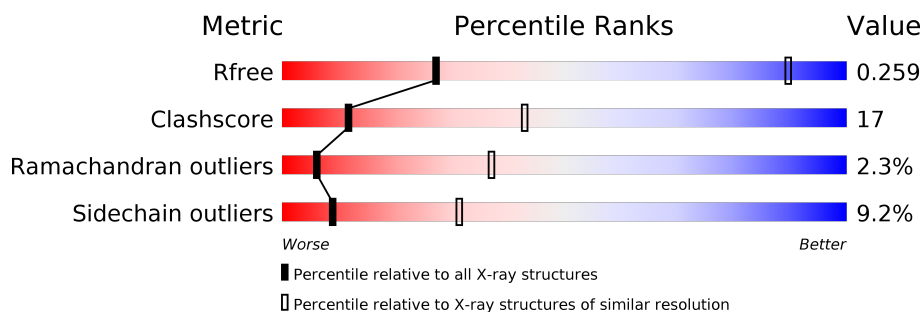
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.29 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)

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 ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	329	50% (Green), 36% (Yellow), 9% (Orange), 5% (Red), 0% (Grey)
1	B	329	43% (Green), 38% (Yellow), 7% (Orange), 10% (Red), 2% (Grey)
1	G	329	42% (Green), 24% (Yellow), 0% (Orange), 31% (Red), 3% (Grey)
1	H	329	40% (Green), 24% (Yellow), 0% (Orange), 34% (Red), 2% (Grey)
2	C	1342	60% (Green), 36% (Yellow), 0% (Orange), 0% (Red), 4% (Grey)
2	I	1342	61% (Green), 35% (Yellow), 0% (Orange), 0% (Red), 4% (Grey)
3	D	1407	49% (Green), 30% (Yellow), 0% (Orange), 0% (Red), 21% (Grey)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	1407	 48% 31% • 18%
4	E	91	 60% 33% • •
4	K	91	 52% 27% 7% • 13%
5	F	613	 49% 25% • 24%
5	L	613	 47% 27% • 23%
6	M	151	 44% 46% • 7%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 57643 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	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	297	Total	C	N	O	S	0	0	0
			2297	1439	403	447	8			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	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
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1173	Total	C	N	O	S	0	0	0
			9095	5718	1628	1703	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is a protein called RNA polymerase-binding transcription factor DksA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	140	Total	C	N	O	S	0	0	0
			1140	703	206	224	7			

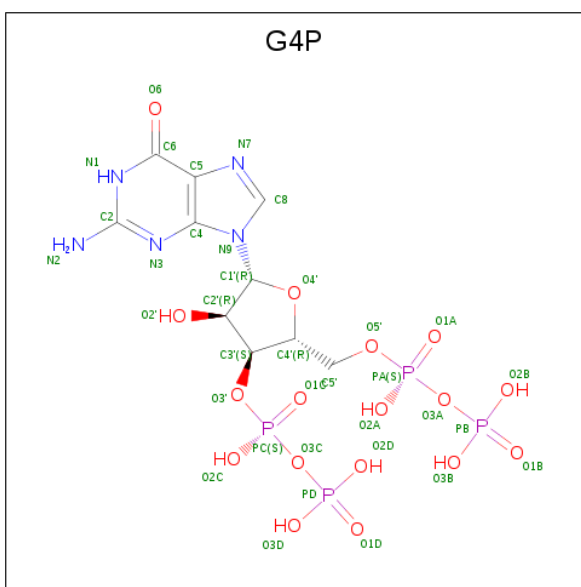
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

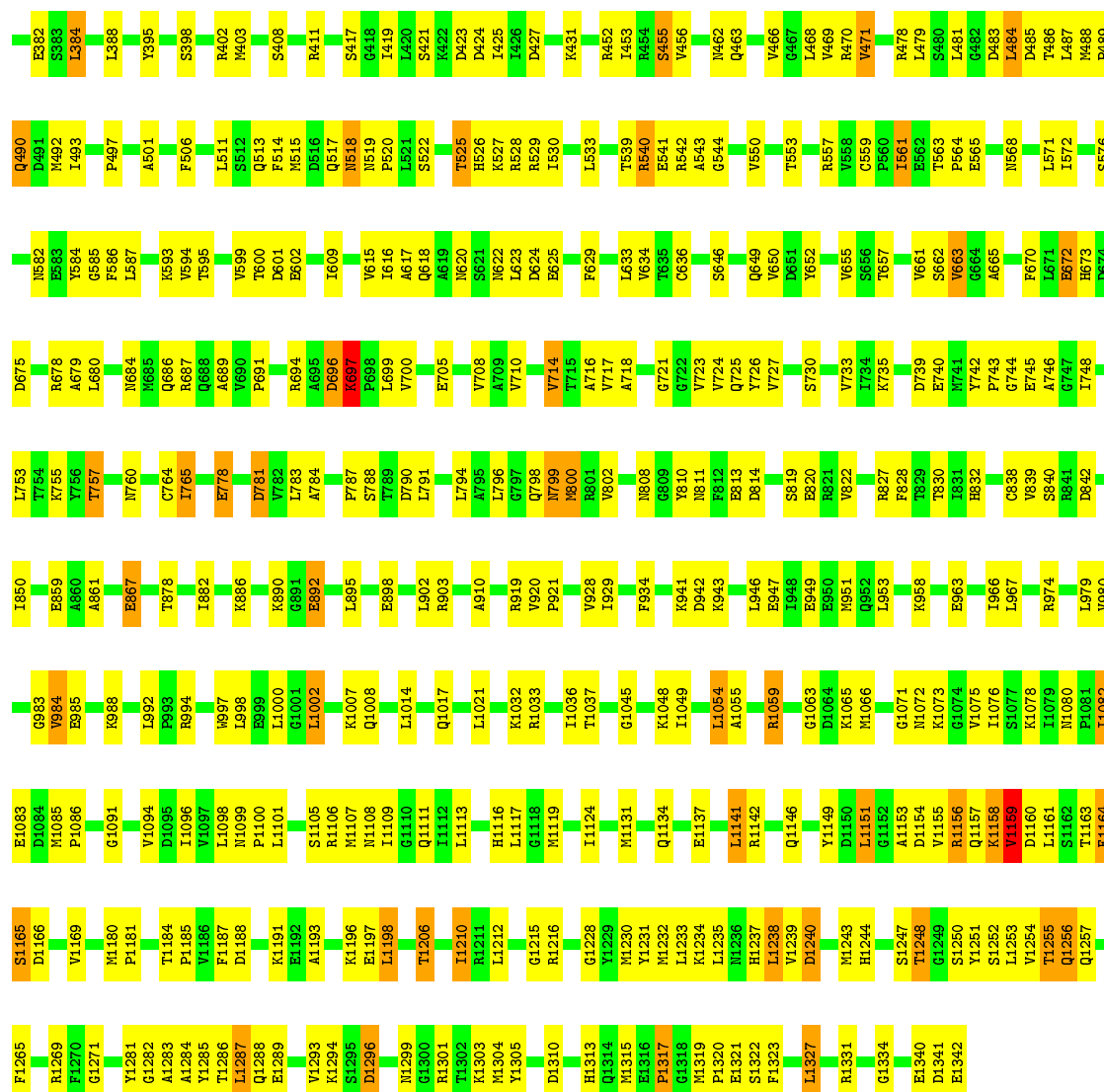
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		
8	M	1	Total	Zn	0	0
			1	1		

- Molecule 9 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄).

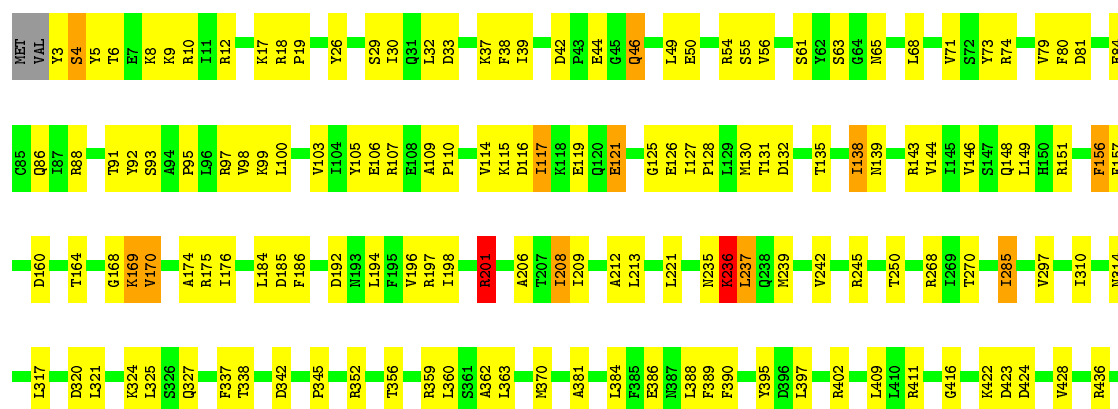


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total 36	C 10	N 5	O 17	P 4	0	0
9	J	1	Total 36	C 10	N 5	O 17	P 4	0	0
9	M	1	Total 36	C 10	N 5	O 17	P 4	0	0



• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I: 61% 35%



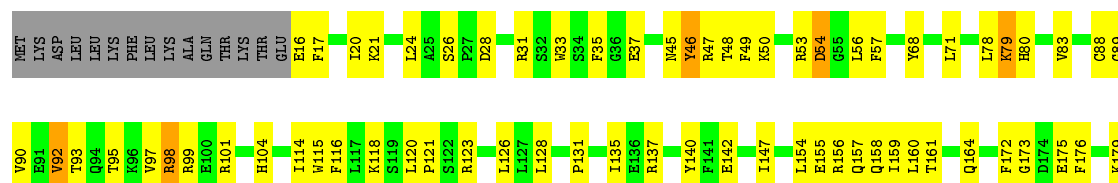


Response	Percentage
Yes, U.S. should take action to reduce greenhouse gas emissions	49%
No, U.S. should focus on other issues	30%
Don't know	1%
Other	17%



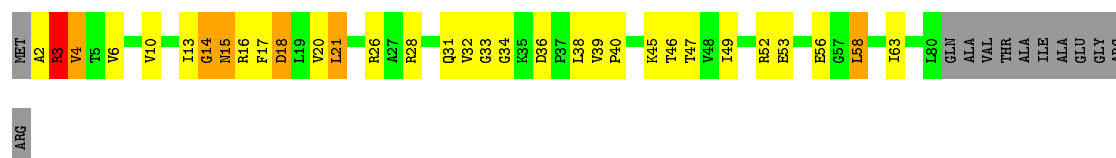


Frequency	Percentage
Daily	48%
Often	31%
Sometimes	1%
Never	18%

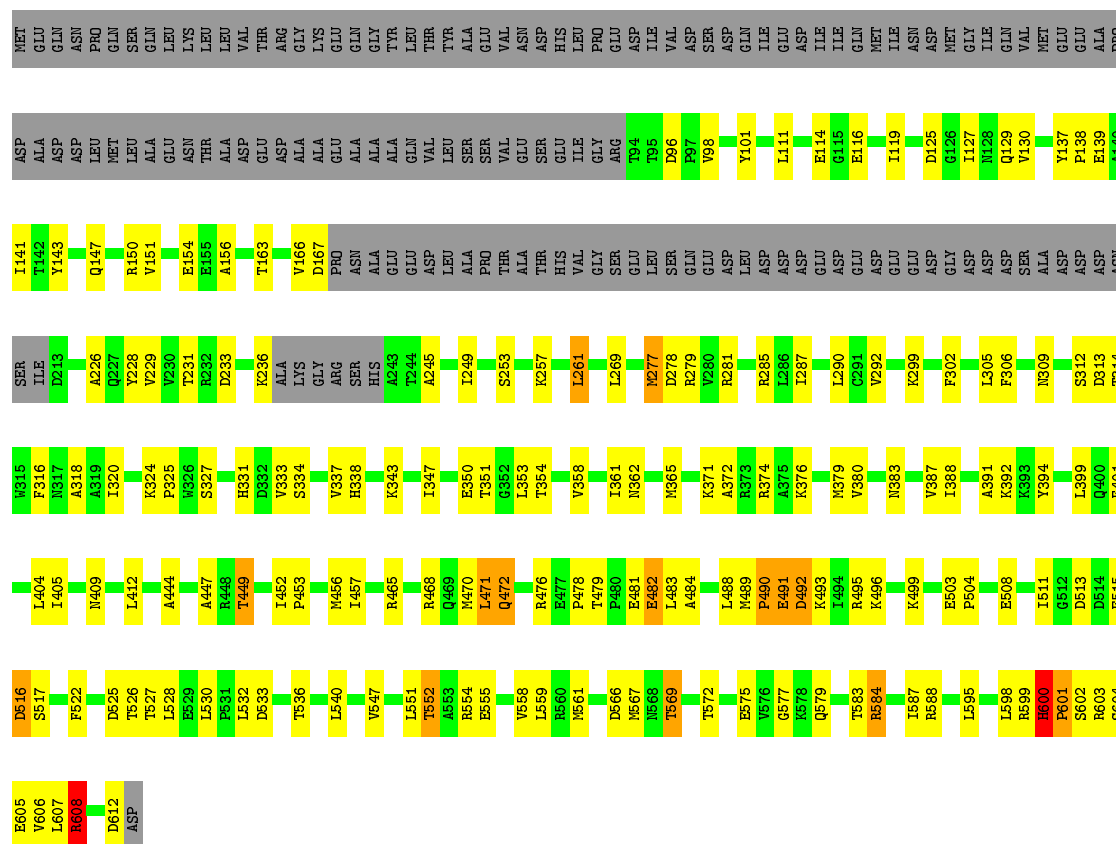




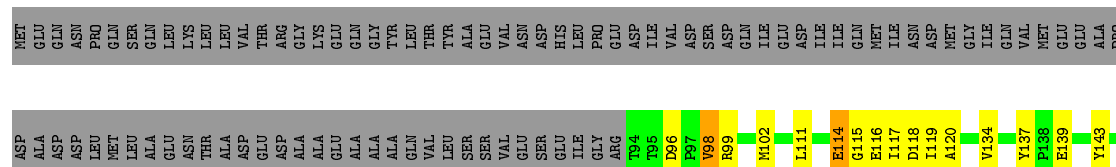
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.27Å 205.26Å 311.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.82 – 4.29 49.55 – 4.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (46.82-4.29) 81.4 (49.55-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.221 , 0.259 0.221 , 0.259	Depositor DCC
R_{free} test set	1967 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	187.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 225.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	57643	wwPDB-VP
Average B, all atoms (Å ²)	279.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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: G4P, ZN, MG

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	0.29	0/2524	0.62	1/3421 (0.0%)
1	B	0.31	0/2326	0.77	2/3153 (0.1%)
1	G	0.27	0/1777	0.56	0/2408
1	H	0.27	0/1681	0.61	1/2278 (0.0%)
2	C	0.29	0/10739	0.56	1/14489 (0.0%)
2	I	0.28	0/10735	0.54	1/14484 (0.0%)
3	D	0.29	0/9235	0.57	0/12472
3	J	0.28	0/9140	0.57	1/12341 (0.0%)
4	E	0.28	0/693	0.49	0/935
4	K	0.26	0/629	0.58	1/847 (0.1%)
5	F	0.26	0/3864	0.53	1/5194 (0.0%)
5	L	0.27	0/3872	0.51	0/5205
6	M	0.36	0/1155	0.65	1/1549 (0.1%)
All	All	0.29	0/58370	0.57	10/78776 (0.0%)

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	B	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	3	ARG	N-CA-C	-6.51	93.41	111.00
1	A	318	LEU	CA-CB-CG	6.18	129.50	115.30
3	J	1221	LEU	CA-CB-CG	5.99	129.08	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	236	LYS	N-CA-C	5.86	126.82	111.00
1	B	318	LEU	CA-CB-CG	5.77	128.56	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	323	PRO	Peptide

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	2490	0	2542	123	0
1	B	2297	0	2350	144	1
1	G	1755	0	1773	60	0
1	H	1662	0	1687	57	0
2	C	10570	0	10582	390	0
2	I	10566	0	10576	362	0
3	D	9095	0	9222	376	0
3	J	9001	0	9167	366	1
4	E	691	0	695	25	0
4	K	627	0	634	28	0
5	F	3813	0	3880	125	0
5	L	3821	0	3884	119	0
6	M	1140	0	1119	63	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
8	M	1	0	0	0	0
9	E	36	0	11	3	0
9	J	36	0	11	4	0
9	M	36	0	11	7	0
All	All	57643	0	58144	2018	1

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 17.

The worst 5 of 2018 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:29:GLU:HB3	1:B:30:PRO:CD	1.26	1.46
1:B:29:GLU:CB	1:B:30:PRO:HD2	1.35	1.45
1:B:279:GLY:HA3	1:B:321:TRP:CZ2	1.55	1.41
5:F:600:HIS:O	5:F:604:SER:HB3	1.33	1.29
1:B:253:LEU:O	1:B:321:TRP:HZ2	0.98	1.26

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ASP:OD2	3:J:675:ALA:N[2_555]	2.03	0.17

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	317/329 (96%)	249 (78%)	53 (17%)	15 (5%)	2	24
1	B	291/329 (88%)	225 (77%)	45 (16%)	21 (7%)	1	16
1	G	225/329 (68%)	200 (89%)	21 (9%)	4 (2%)	8	42
1	H	212/329 (64%)	197 (93%)	11 (5%)	4 (2%)	8	41
2	C	1338/1342 (100%)	1201 (90%)	114 (8%)	23 (2%)	9	43
2	I	1338/1342 (100%)	1196 (89%)	119 (9%)	23 (2%)	9	43
3	D	1169/1407 (83%)	1042 (89%)	99 (8%)	28 (2%)	6	36
3	J	1151/1407 (82%)	1024 (89%)	100 (9%)	27 (2%)	6	37
4	E	87/91 (96%)	81 (93%)	4 (5%)	2 (2%)	6	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	77/91 (85%)	68 (88%)	5 (6%)	4 (5%)	2	22
5	F	462/613 (75%)	425 (92%)	28 (6%)	9 (2%)	8	41
5	L	463/613 (76%)	424 (92%)	32 (7%)	7 (2%)	10	46
6	M	138/151 (91%)	128 (93%)	7 (5%)	3 (2%)	6	38
All	All	7268/8373 (87%)	6460 (89%)	638 (9%)	170 (2%)	6	37

5 of 170 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	167	PRO
1	A	242	VAL

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	278/286 (97%)	230 (83%)	48 (17%)	2	13
1	B	256/286 (90%)	224 (88%)	32 (12%)	4	22
1	G	193/286 (68%)	169 (88%)	24 (12%)	4	22
1	H	183/286 (64%)	171 (93%)	12 (7%)	16	43
2	C	1155/1157 (100%)	1053 (91%)	102 (9%)	10	34
2	I	1154/1157 (100%)	1059 (92%)	95 (8%)	11	37
3	D	962/1168 (82%)	879 (91%)	83 (9%)	10	35
3	J	960/1168 (82%)	875 (91%)	85 (9%)	9	33
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	25
4	K	67/75 (89%)	60 (90%)	7 (10%)	7	27
5	F	417/540 (77%)	387 (93%)	30 (7%)	14	41
5	L	418/540 (77%)	380 (91%)	38 (9%)	9	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	M	121/131 (92%)	111 (92%)	10 (8%)	11	37
All	All	6236/7155 (87%)	5662 (91%)	574 (9%)	9	31

5 of 574 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1289	ASN
1	G	187	VAL
5	L	261	LEU
4	E	18	ASP
5	F	526	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	406	GLN
2	I	357	ASN
5	L	362	ASN
5	F	446	GLN
5	F	600	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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
9	G4P	E	101	-	30,38,38	1.82	7 (23%)	43,61,61	1.62	8 (18%)
9	G4P	M	202	-	30,38,38	1.95	9 (30%)	43,61,61	1.62	7 (16%)
9	G4P	J	2004	-	30,38,38	1.96	9 (30%)	43,61,61	1.53	8 (18%)

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
9	G4P	E	101	-	-	1/23/43/43	0/3/3/3
9	G4P	M	202	-	-	8/23/43/43	0/3/3/3
9	G4P	J	2004	-	-	7/23/43/43	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	2004	G4P	C2'-C1'	-5.51	1.45	1.53
9	M	202	G4P	C2'-C1'	-4.92	1.46	1.53
9	E	101	G4P	C2'-C1'	-4.82	1.46	1.53
9	M	202	G4P	C2-N2	4.50	1.42	1.33
9	J	2004	G4P	C2-N2	4.39	1.42	1.33

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	101	G4P	O3C-PC-O3'	5.63	113.83	102.48
9	M	202	G4P	O3C-PC-O3'	5.19	112.95	102.48
9	M	202	G4P	N3-C2-N1	-4.22	121.59	127.22
9	J	2004	G4P	O3C-PC-O3'	4.09	110.74	102.48
9	J	2004	G4P	PC-O3C-PD	-3.80	119.78	132.83

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	202	G4P	PA-O3A-PB-O2B
9	J	2004	G4P	C3'-O3'-PC-O1C
9	J	2004	G4P	C3'-O3'-PC-O3C
9	M	202	G4P	C4'-C5'-O5'-PA
9	M	202	G4P	PB-O3A-PA-O5'

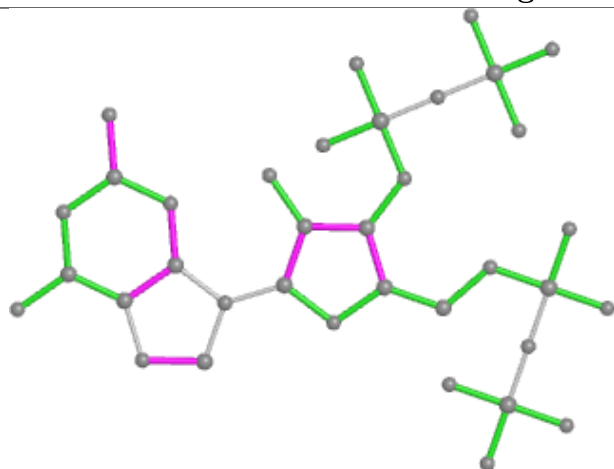
There are no ring outliers.

3 monomers are involved in 14 short contacts:

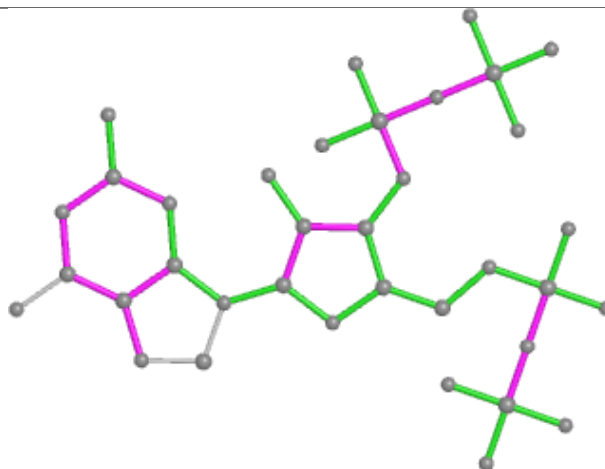
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	101	G4P	3	0
9	M	202	G4P	7	0
9	J	2004	G4P	4	0

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.

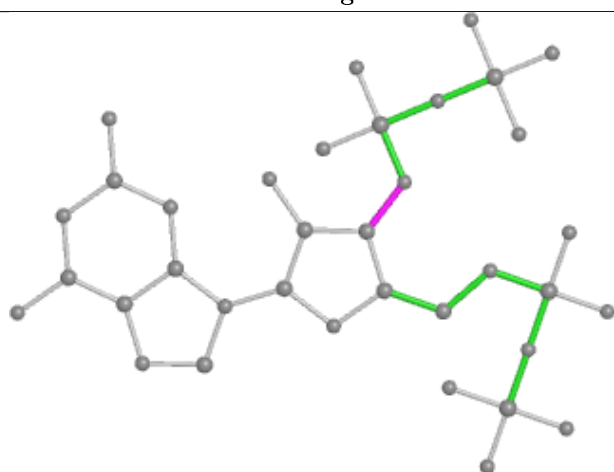
Ligand G4P E 101



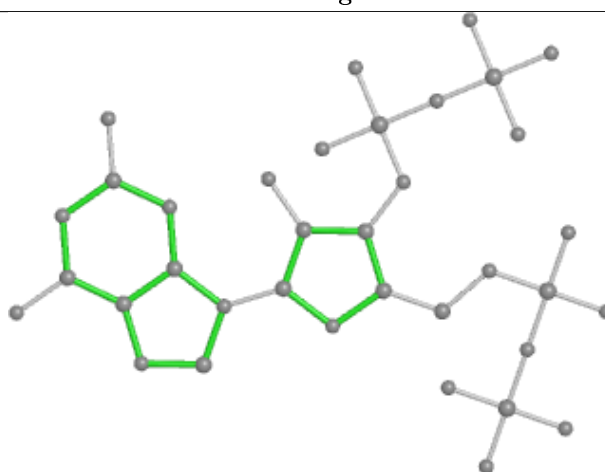
Bond lengths



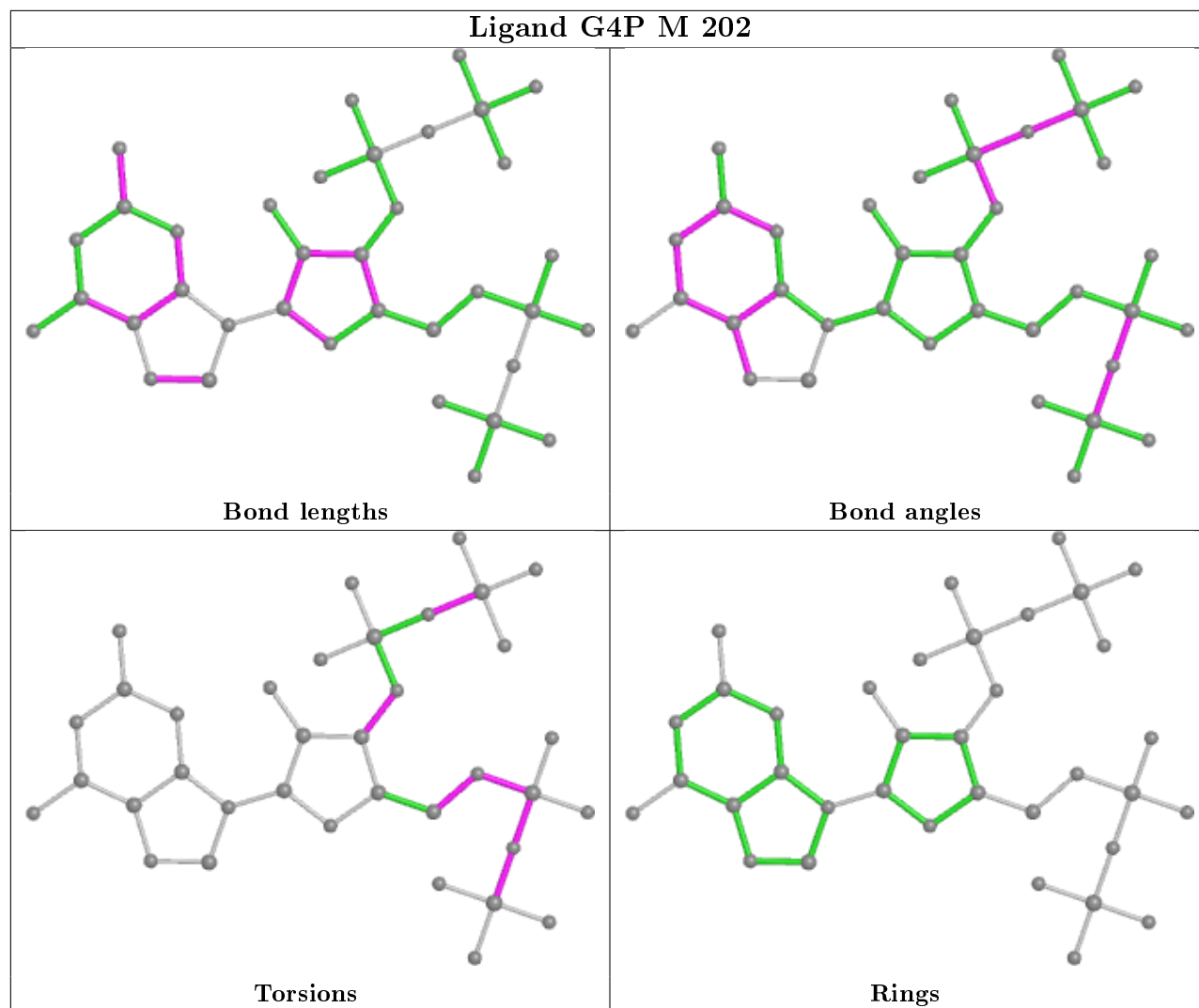
Bond angles

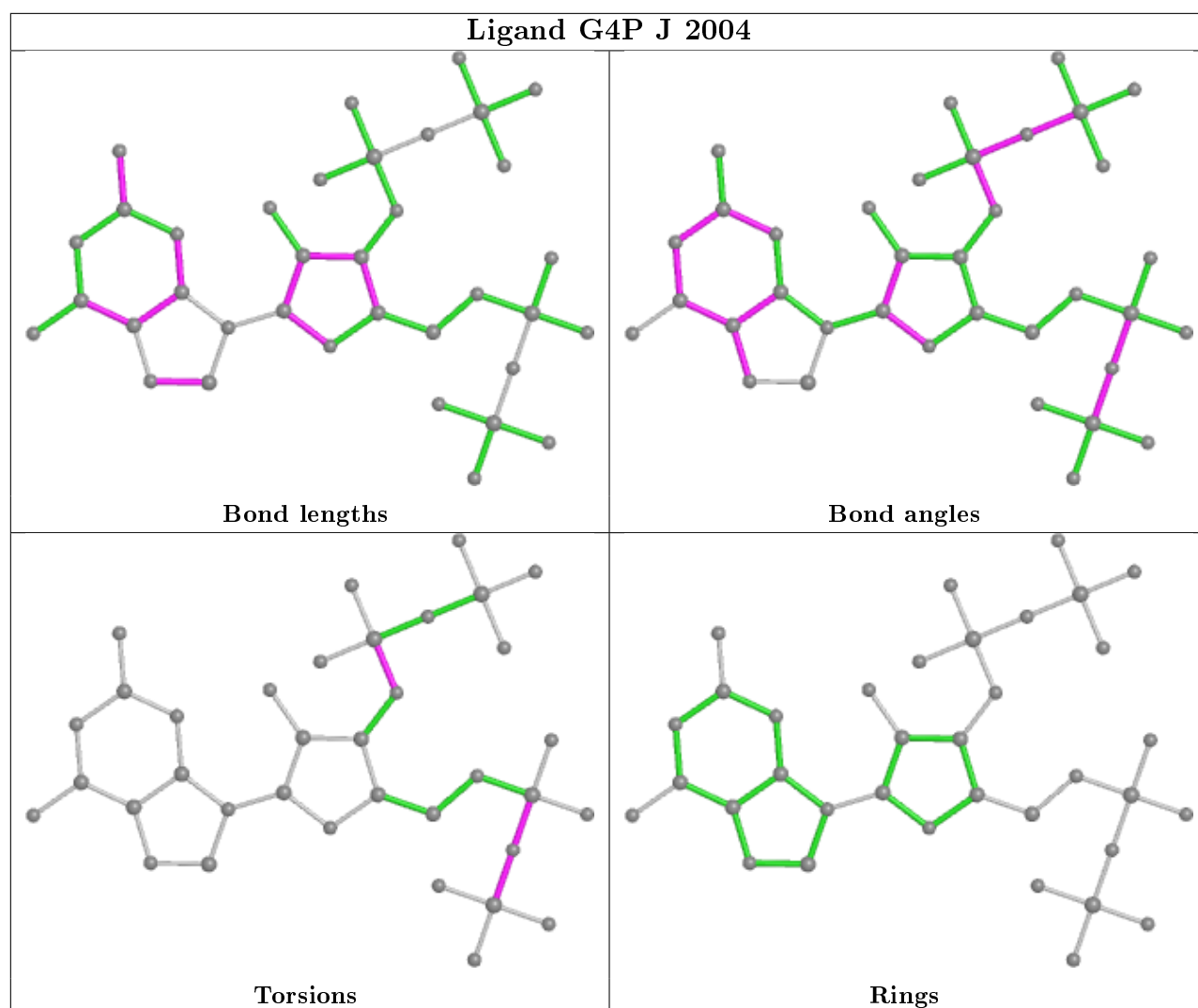


Torsions



Rings





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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

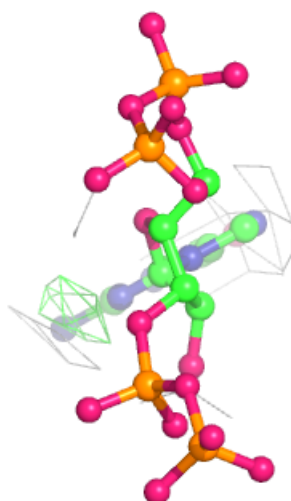
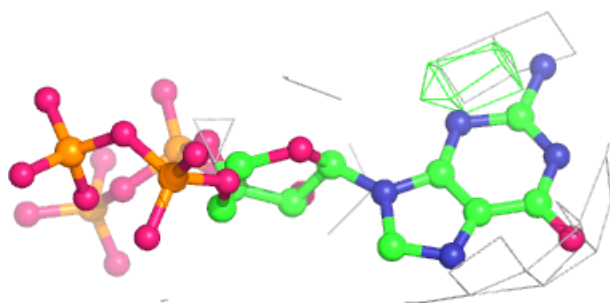
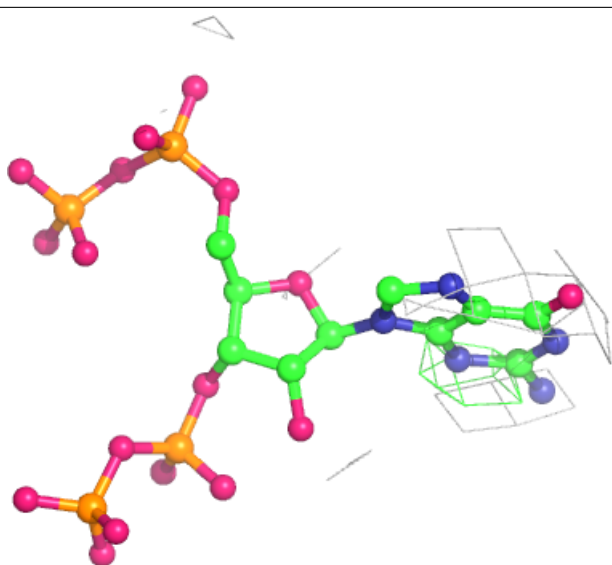
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

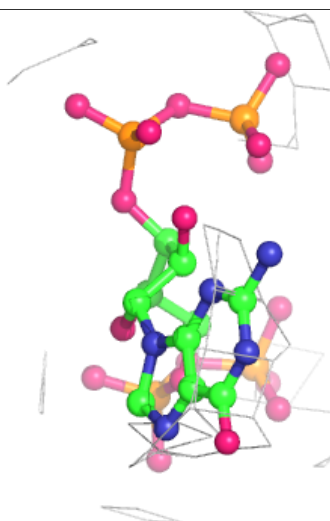
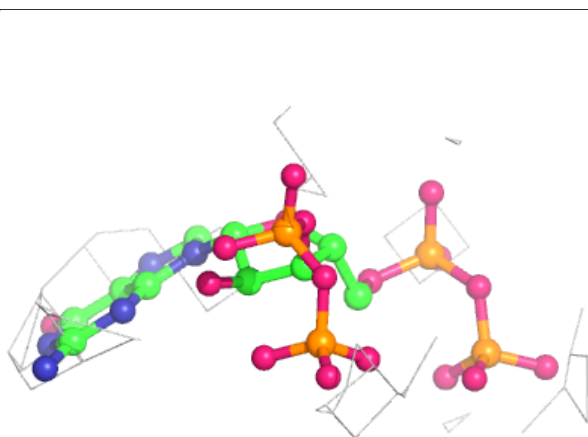
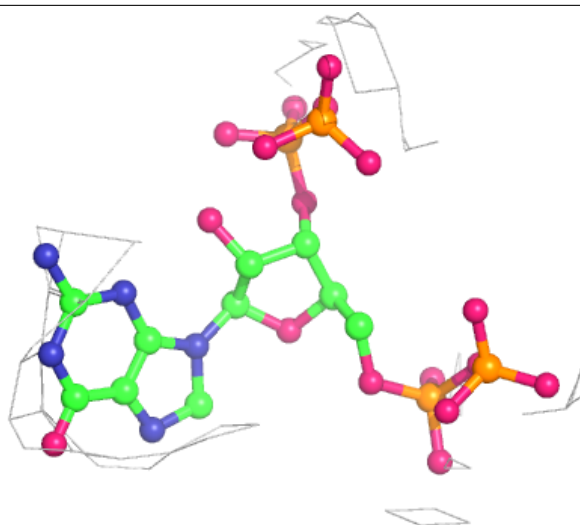
Electron density around G4P E 101:

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



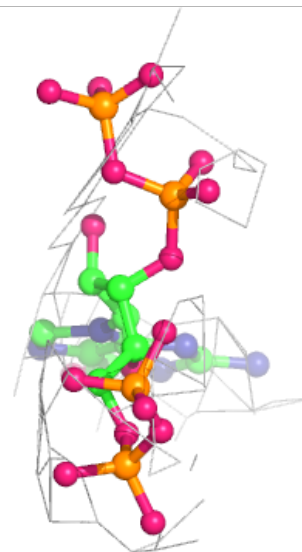
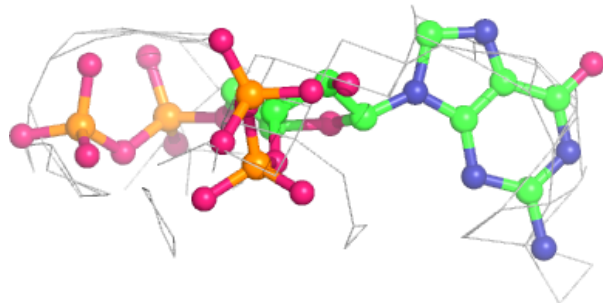
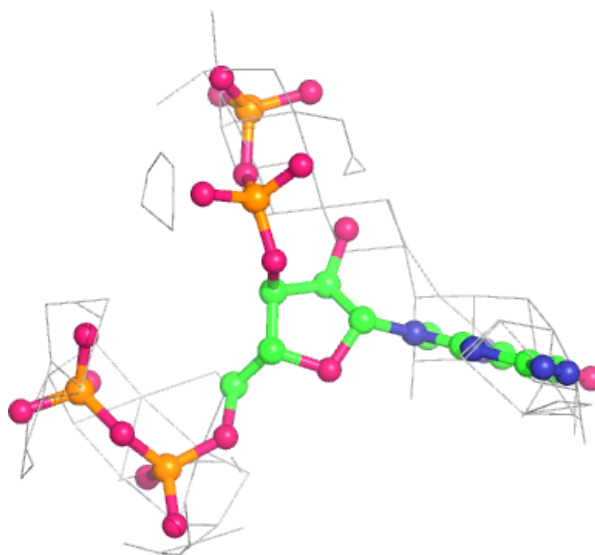
Electron density around G4P M 202:

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



Electron density around G4P J 2004:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.