Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 01:38 AM EDT

PDB ID	:	6PC1
Title	:	Crystal structure of Helicobacter pylori PPX/GppA (E143A) in complex with ppGpp
Authors	:	Song, H.; Wang, C.; Shaw, G.X.; Ji, X.
Deposited on	:	2019-06-15
Resolution	:	2.76 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*
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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.76 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15700 atoms, of which 4 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 Guanosine pentaphosphate phosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3803	2467	650	668	18			
1	B	483	Total	C	N	O	S	0	0	0
			3808	2470	651	669	18			
1	C	482	Total	C	N	O	S	0	0	0
			3803	2467	650	668	18			
1	D	468	Total	C	N	O	S	0	0	0
			3688	2392	633	646	17			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP B5ZA44
A	-9	ARG	-	expression tag	UNP B5ZA44
A	-8	GLY	-	expression tag	UNP B5ZA44
A	-7	SER	-	expression tag	UNP B5ZA44
A	-6	HIS	-	expression tag	UNP B5ZA44
A	-5	HIS	-	expression tag	UNP B5ZA44
A	-4	HIS	-	expression tag	UNP B5ZA44
A	-3	HIS	-	expression tag	UNP B5ZA44
A	-2	HIS	-	expression tag	UNP B5ZA44
A	-1	HIS	-	expression tag	UNP B5ZA44
A	0	GLY	-	expression tag	UNP B5ZA44
A	1	SER	-	expression tag	UNP B5ZA44
A	143	ALA	GLU	engineered mutation	UNP B5ZA44
B	-10	MET	-	initiating methionine	UNP B5ZA44
B	-9	ARG	-	expression tag	UNP B5ZA44
B	-8	GLY	-	expression tag	UNP B5ZA44
B	-7	SER	-	expression tag	UNP B5ZA44
B	-6	HIS	-	expression tag	UNP B5ZA44
B	-5	HIS	-	expression tag	UNP B5ZA44
B	-4	HIS	-	expression tag	UNP B5ZA44
B	-3	HIS	-	expression tag	UNP B5ZA44

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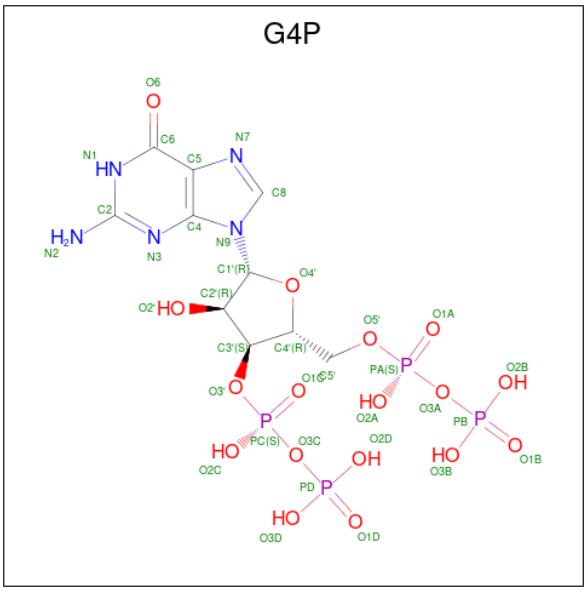
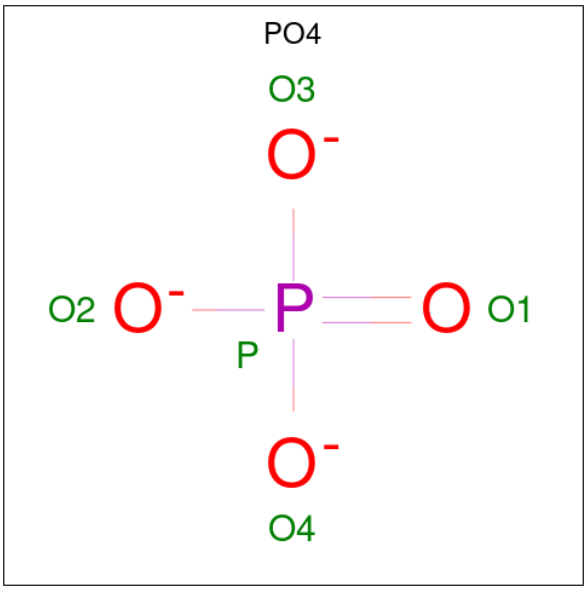
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP B5ZA44
B	-1	HIS	-	expression tag	UNP B5ZA44
B	0	GLY	-	expression tag	UNP B5ZA44
B	1	SER	-	expression tag	UNP B5ZA44
B	143	ALA	GLU	engineered mutation	UNP B5ZA44
C	-10	MET	-	initiating methionine	UNP B5ZA44
C	-9	ARG	-	expression tag	UNP B5ZA44
C	-8	GLY	-	expression tag	UNP B5ZA44
C	-7	SER	-	expression tag	UNP B5ZA44
C	-6	HIS	-	expression tag	UNP B5ZA44
C	-5	HIS	-	expression tag	UNP B5ZA44
C	-4	HIS	-	expression tag	UNP B5ZA44
C	-3	HIS	-	expression tag	UNP B5ZA44
C	-2	HIS	-	expression tag	UNP B5ZA44
C	-1	HIS	-	expression tag	UNP B5ZA44
C	0	GLY	-	expression tag	UNP B5ZA44
C	1	SER	-	expression tag	UNP B5ZA44
C	143	ALA	GLU	engineered mutation	UNP B5ZA44
D	-10	MET	-	initiating methionine	UNP B5ZA44
D	-9	ARG	-	expression tag	UNP B5ZA44
D	-8	GLY	-	expression tag	UNP B5ZA44
D	-7	SER	-	expression tag	UNP B5ZA44
D	-6	HIS	-	expression tag	UNP B5ZA44
D	-5	HIS	-	expression tag	UNP B5ZA44
D	-4	HIS	-	expression tag	UNP B5ZA44
D	-3	HIS	-	expression tag	UNP B5ZA44
D	-2	HIS	-	expression tag	UNP B5ZA44
D	-1	HIS	-	expression tag	UNP B5ZA44
D	0	GLY	-	expression tag	UNP B5ZA44
D	1	SER	-	expression tag	UNP B5ZA44
D	143	ALA	GLU	engineered mutation	UNP B5ZA44

- Molecule 2 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$) (labeled as "Ligand of Interest" by depositor).



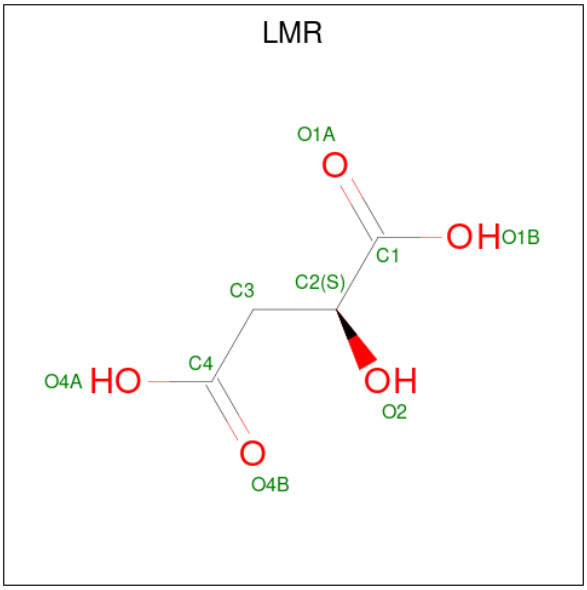
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
2	B	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
2	C	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
2	D	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



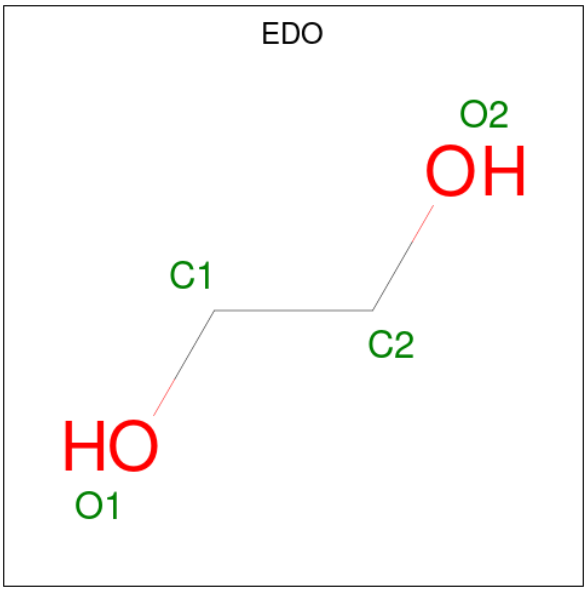
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 4 5	0	0
4	A	1	Total C H O 13 4 4 5	0	0
4	B	1	Total C O 9 4 5	0	0
4	C	1	Total C O 9 4 5	0	0
4	D	1	Total C O 9 4 5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	C	2	Total Mg 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	85	Total O 85 85	0	0
7	B	115	Total O 115 115	0	0
7	C	103	Total O 103 103	0	0
7	D	66	Total O 66 66	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	194.51Å 194.51Å 136.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.76	Depositor
% Data completeness (in resolution range)	96.3 (40.00-2.76)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.77Å)	Xtriage
Refinement program	PHENIX (dev_3352: ???)	Depositor
R, R_{free}	0.178 , 0.222	Depositor
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.452	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
Total number of atoms	15700	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	PO4	B	503	6	4,4,4	0.92	0	6,6,6	0.40	0
5	EDO	B	505	-	3,3,3	0.49	0	2,2,2	0.25	0
4	LMR	A	604	-	8,8,8	1.06	0	10,10,10	1.29	2 (20%)
2	G4P	A	601	-	30,38,38	1.29	3 (10%)	42,61,61	1.92	8 (19%)
4	LMR	A	603	-	8,8,8	1.73	2 (25%)	10,10,10	1.51	1 (10%)
2	G4P	D	601	-	30,38,38	1.30	3 (10%)	42,61,61	1.96	8 (19%)
4	LMR	C	504	-	8,8,8	2.44	4 (50%)	10,10,10	1.60	1 (10%)
5	EDO	A	605	-	3,3,3	0.64	0	2,2,2	0.39	0
3	PO4	D	602	-	4,4,4	0.91	0	6,6,6	0.43	0
3	PO4	A	602	-	4,4,4	0.95	0	6,6,6	0.35	0
2	G4P	B	502	-	30,38,38	1.30	3 (10%)	42,61,61	1.90	8 (19%)
4	LMR	B	504	-	8,8,8	0.69	0	10,10,10	1.50	1 (10%)
4	LMR	D	603	-	8,8,8	2.46	4 (50%)	10,10,10	1.54	1 (10%)
2	G4P	C	502	6	30,38,38	1.34	3 (10%)	42,61,61	1.93	8 (19%)
3	PO4	C	503	6	4,4,4	0.90	0	6,6,6	0.50	0
3	PO4	C	506	-	4,4,4	0.88	0	6,6,6	0.44	0

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
4	LMR	A	604	-	-	4/8/8/8	-
2	G4P	A	601	-	-	3/23/43/43	0/3/3/3
4	LMR	A	603	-	-	4/8/8/8	-
2	G4P	D	601	-	-	8/23/43/43	0/3/3/3
4	LMR	C	504	-	-	2/8/8/8	-
2	G4P	B	502	-	-	5/23/43/43	0/3/3/3
4	LMR	B	504	-	-	4/8/8/8	-
4	LMR	D	603	-	-	2/8/8/8	-
5	EDO	B	505	-	-	1/1/1/1	-
2	G4P	C	502	6	-	7/23/43/43	0/3/3/3
5	EDO	A	605	-	-	1/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	LMR	O1A-C1	4.15	1.34	1.22
4	C	504	LMR	O1A-C1	4.14	1.34	1.22
4	D	603	LMR	O4B-C4	3.81	1.34	1.22
4	C	504	LMR	O4B-C4	3.71	1.34	1.22
4	A	603	LMR	O4B-C4	3.68	1.34	1.22
2	C	502	G4P	O4'-C1'	3.38	1.45	1.41
2	A	601	G4P	O4'-C1'	3.16	1.45	1.41
2	B	502	G4P	O4'-C1'	3.05	1.45	1.41
2	D	601	G4P	O4'-C1'	3.04	1.45	1.41
4	D	603	LMR	O1B-C1	-2.87	1.21	1.30
4	A	603	LMR	O4A-C4	-2.84	1.21	1.30
4	C	504	LMR	O4A-C4	-2.83	1.21	1.30
4	C	504	LMR	O1B-C1	-2.82	1.21	1.30
4	D	603	LMR	O4A-C4	-2.80	1.21	1.30
2	C	502	G4P	C5-C6	-2.74	1.41	1.47
2	D	601	G4P	C5-C6	-2.70	1.41	1.47
2	A	601	G4P	C5-C6	-2.68	1.42	1.47
2	C	502	G4P	C8-N7	-2.68	1.30	1.35
2	B	502	G4P	C5-C6	-2.67	1.42	1.47
2	B	502	G4P	C8-N7	-2.58	1.30	1.35
2	D	601	G4P	C8-N7	-2.58	1.30	1.35
2	A	601	G4P	C8-N7	-2.46	1.30	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	G4P	PC-O3C-PD	-7.35	107.62	132.83
2	C	502	G4P	PC-O3C-PD	-6.92	109.08	132.83
2	B	502	G4P	PC-O3C-PD	-6.76	109.64	132.83
2	C	502	G4P	PA-O3A-PB	-6.62	110.11	132.83
2	A	601	G4P	PC-O3C-PD	-6.60	110.18	132.83
2	D	601	G4P	PA-O3A-PB	-6.53	110.42	132.83
2	A	601	G4P	PA-O3A-PB	-6.41	110.82	132.83
2	B	502	G4P	PA-O3A-PB	-6.27	111.31	132.83
4	C	504	LMR	O1B-C1-C2	3.49	120.39	112.72
2	C	502	G4P	C8-N7-C5	3.39	109.45	102.99
4	D	603	LMR	O1B-C1-C2	3.38	120.14	112.72
2	B	502	G4P	C8-N7-C5	3.34	109.35	102.99
2	A	601	G4P	C8-N7-C5	3.31	109.29	102.99
4	B	504	LMR	O1B-C1-C2	3.30	119.97	112.72
2	D	601	G4P	C8-N7-C5	3.28	109.23	102.99
2	B	502	G4P	O3C-PC-O3'	3.22	108.98	102.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	G4P	O3C-PC-O3'	3.22	108.98	102.48
4	A	603	LMR	O1B-C1-C2	3.14	119.62	112.72
2	C	502	G4P	O3C-PC-O3'	3.05	108.64	102.48
4	A	604	LMR	O1B-C1-C2	2.77	118.81	112.72
2	A	601	G4P	PC-O3'-C3'	-2.71	109.54	119.41
2	D	601	G4P	O3C-PC-O3'	2.61	107.75	102.48
2	D	601	G4P	PC-O3'-C3'	-2.58	110.01	119.41
2	C	502	G4P	C2-N1-C6	-2.55	120.41	125.10
2	A	601	G4P	C2-N1-C6	-2.53	120.45	125.10
2	A	601	G4P	C5-C6-N1	2.52	118.40	113.95
2	B	502	G4P	C2-N1-C6	-2.51	120.47	125.10
2	B	502	G4P	C5-C6-N1	2.49	118.35	113.95
2	D	601	G4P	C5-C6-N1	2.44	118.26	113.95
2	D	601	G4P	C2-N1-C6	-2.43	120.63	125.10
2	C	502	G4P	C5-C6-N1	2.42	118.22	113.95
2	A	601	G4P	PA-O5'-C5'	-2.33	108.00	121.68
2	C	502	G4P	PC-O3'-C3'	-2.33	110.94	119.41
2	B	502	G4P	PA-O5'-C5'	-2.31	108.14	121.68
2	B	502	G4P	PC-O3'-C3'	-2.21	111.36	119.41
4	A	604	LMR	O1A-C1-C2	-2.15	118.34	122.54
2	C	502	G4P	PA-O5'-C5'	-2.10	109.39	121.68
2	D	601	G4P	PA-O5'-C5'	-2.03	109.75	121.68

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	502	G4P	PA-O3A-PB-O2B
2	B	502	G4P	C5'-O5'-PA-O1A
2	C	502	G4P	PB-O3A-PA-O5'
2	C	502	G4P	C5'-O5'-PA-O3A
2	C	502	G4P	C5'-O5'-PA-O1A
2	C	502	G4P	C5'-O5'-PA-O2A
2	D	601	G4P	C5'-O5'-PA-O1A
2	D	601	G4P	C5'-O5'-PA-O2A
4	A	603	LMR	O1A-C1-C2-O2
4	A	603	LMR	O1B-C1-C2-O2
4	A	604	LMR	O2-C2-C3-C4
4	B	504	LMR	O1A-C1-C2-O2
4	B	504	LMR	O1B-C1-C2-O2
4	C	504	LMR	O1A-C1-C2-O2
4	C	504	LMR	O1B-C1-C2-O2

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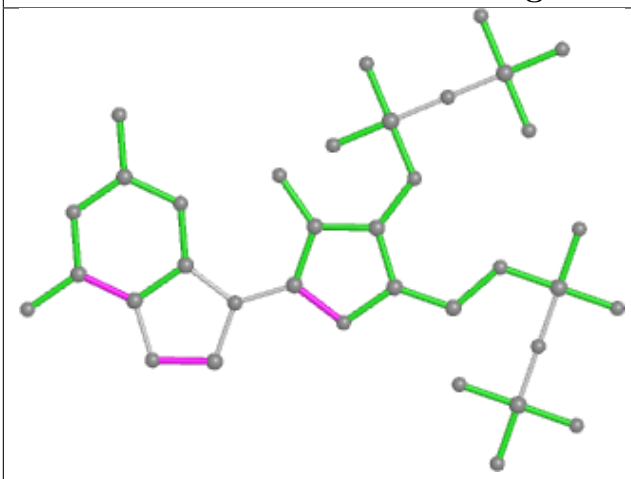
Mol	Chain	Res	Type	Atoms
2	D	601	G4P	C3'-C4'-C5'-O5'
2	A	601	G4P	O4'-C4'-C5'-O5'
2	A	601	G4P	C3'-C4'-C5'-O5'
2	C	502	G4P	O4'-C4'-C5'-O5'
2	C	502	G4P	C3'-C4'-C5'-O5'
2	D	601	G4P	O4'-C4'-C5'-O5'
5	A	605	EDO	O1-C1-C2-O2
4	D	603	LMR	O1A-C1-C2-O2
4	D	603	LMR	O1B-C1-C2-O2
2	B	502	G4P	O4'-C4'-C5'-O5'
4	A	603	LMR	O1A-C1-C2-C3
4	A	603	LMR	O1B-C1-C2-C3
4	B	504	LMR	O1A-C1-C2-C3
4	B	504	LMR	O1B-C1-C2-C3
2	A	601	G4P	PD-O3C-PC-O3'
2	B	502	G4P	PD-O3C-PC-O3'
2	C	502	G4P	PD-O3C-PC-O3'
2	D	601	G4P	PD-O3C-PC-O3'
2	B	502	G4P	C3'-C4'-C5'-O5'
4	A	604	LMR	C1-C2-C3-C4
2	D	601	G4P	C5'-O5'-PA-O3A
5	B	505	EDO	O1-C1-C2-O2
4	A	604	LMR	O1B-C1-C2-O2
2	D	601	G4P	PB-O3A-PA-O1A
2	D	601	G4P	PB-O3A-PA-O2A
4	A	604	LMR	O1A-C1-C2-O2

There are no ring outliers.

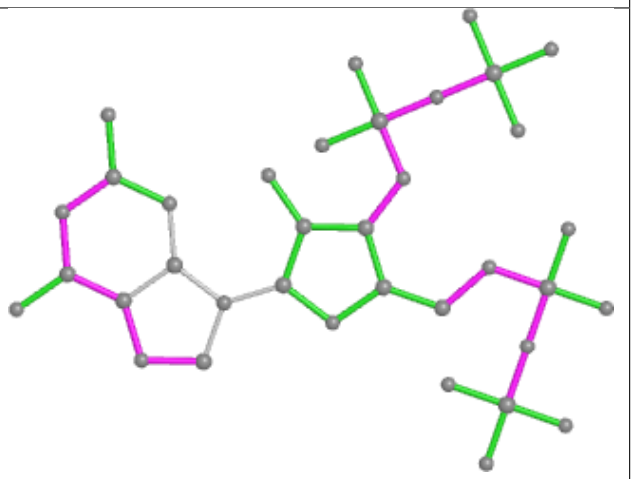
No monomer is involved in short contacts.

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 then 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.

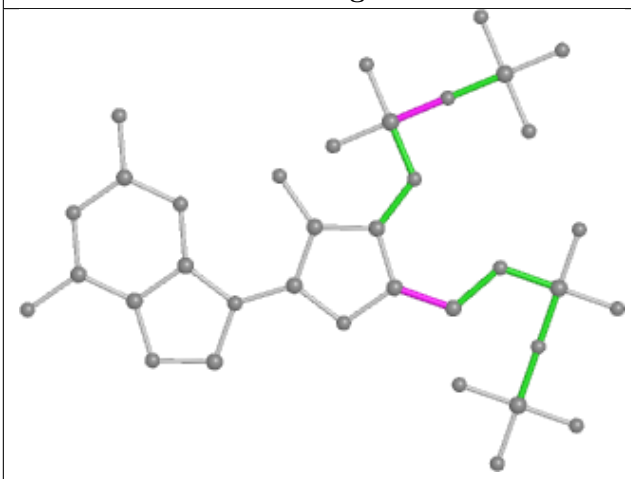
Ligand G4P A 601



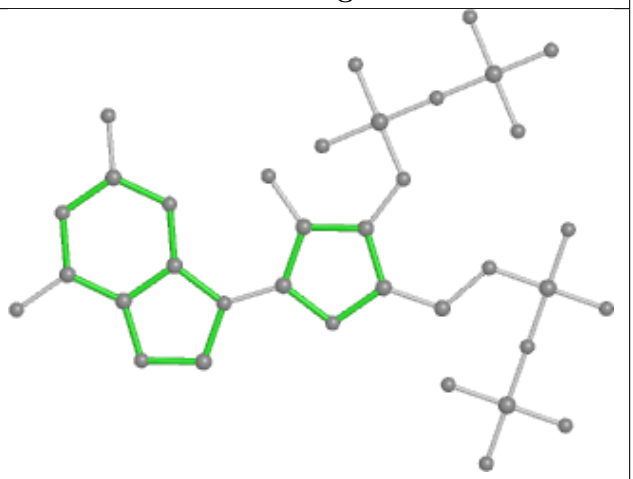
Bond lengths



Bond angles

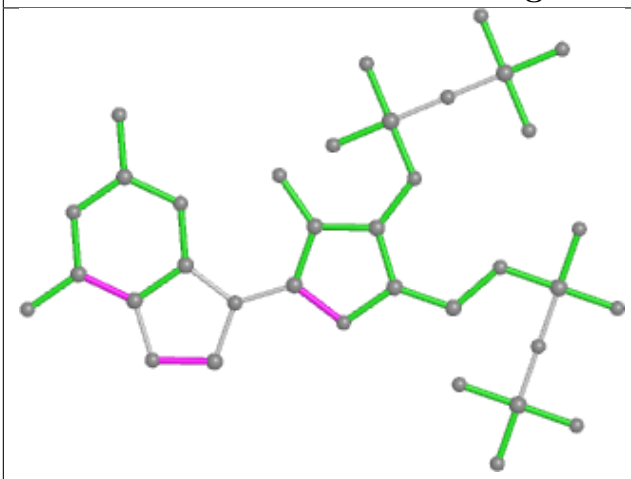


Torsions

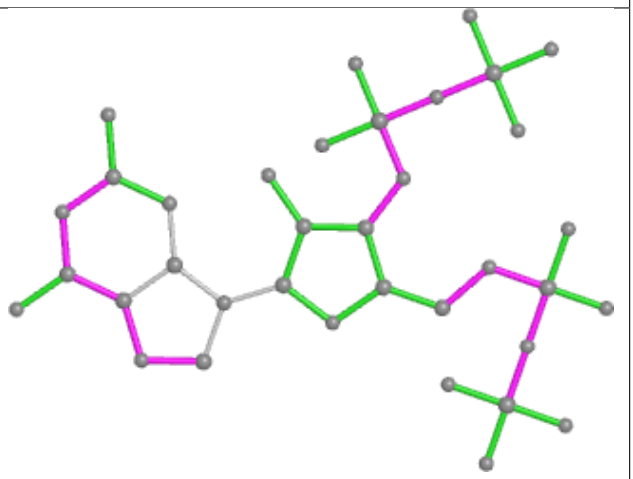


Rings

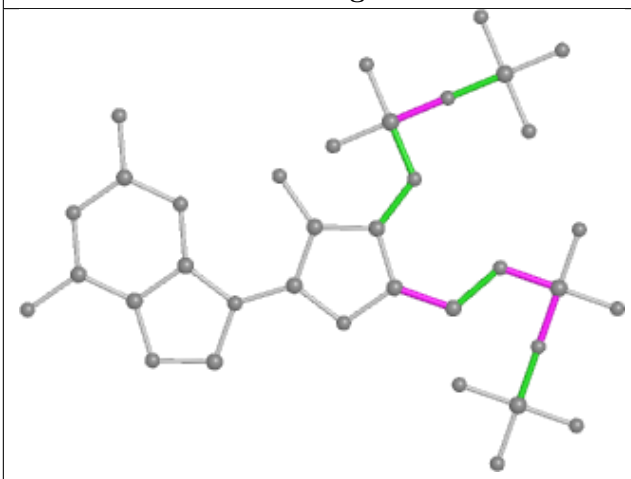
Ligand G4P D 601



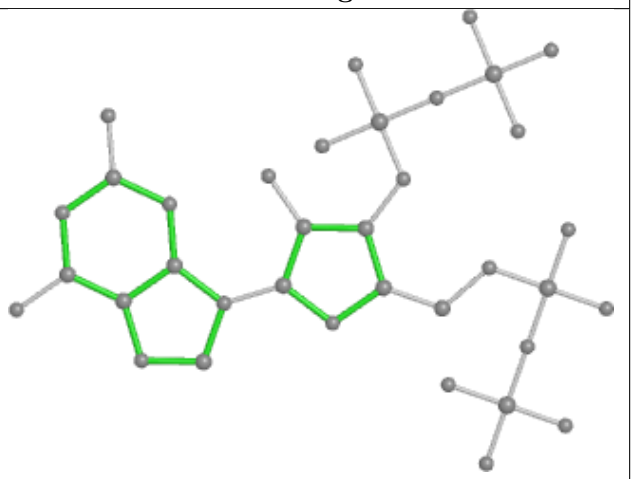
Bond lengths



Bond angles

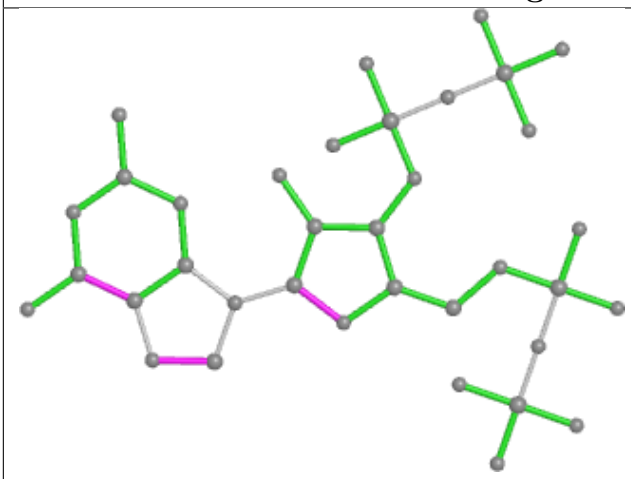


Torsions

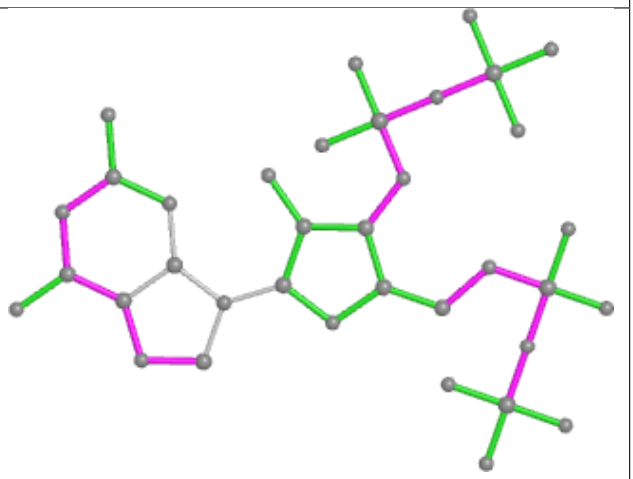


Rings

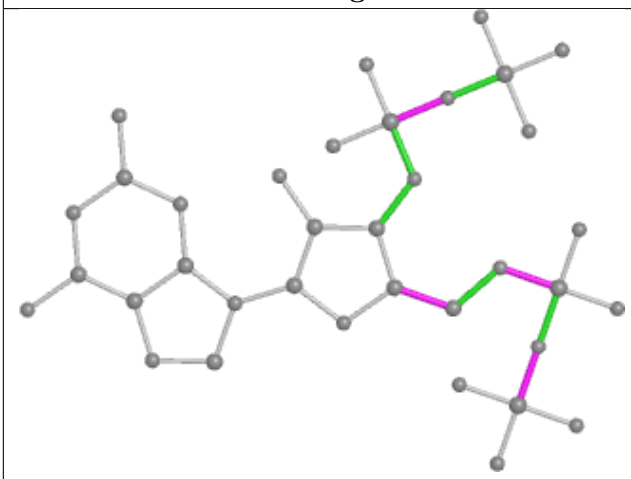
Ligand G4P B 502



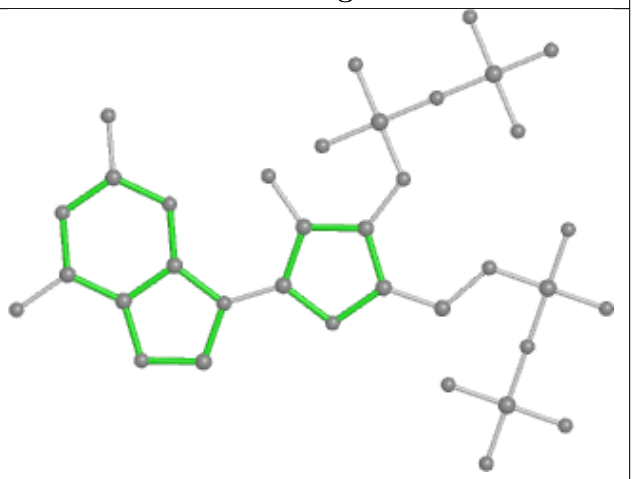
Bond lengths



Bond angles

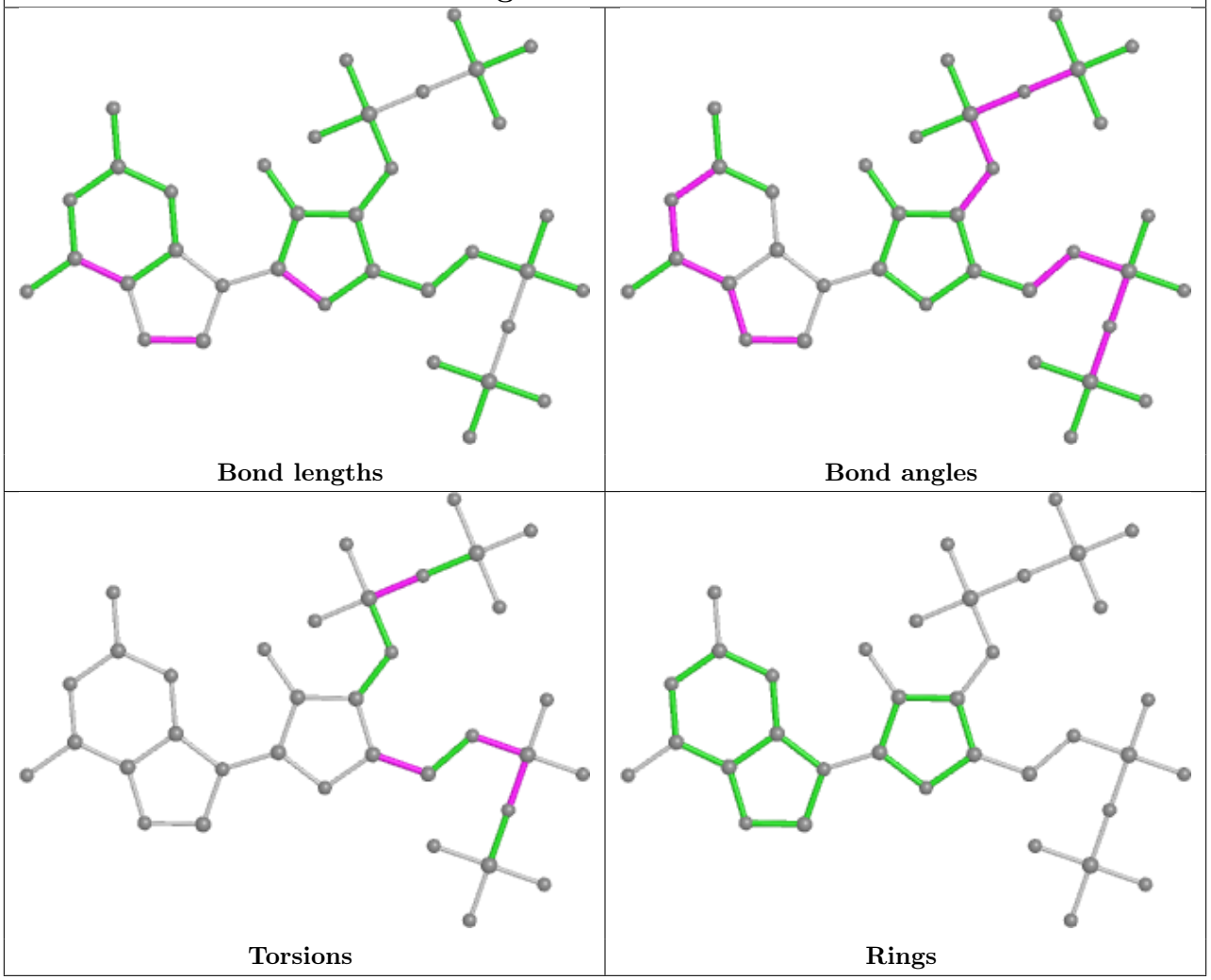


Torsions



Rings

Ligand G4P C 502



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.