



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:53 PM UTC

PDB ID : 6PC1 / pdb_00006pc1
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	:	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

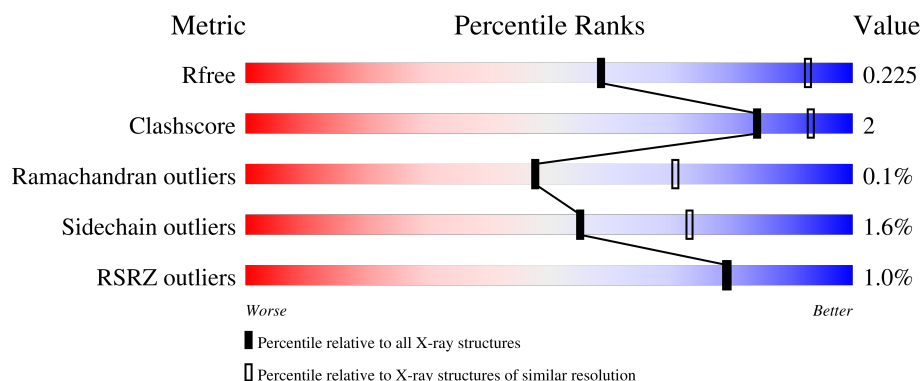
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	495	93% 2% 93% 5% 2%
1	B	495	94% 94% 5% 2%
1	C	495	92% 92% 5% 2%
1	D	495	87% 2% 87% 6% 5%

2 Entry composition

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:

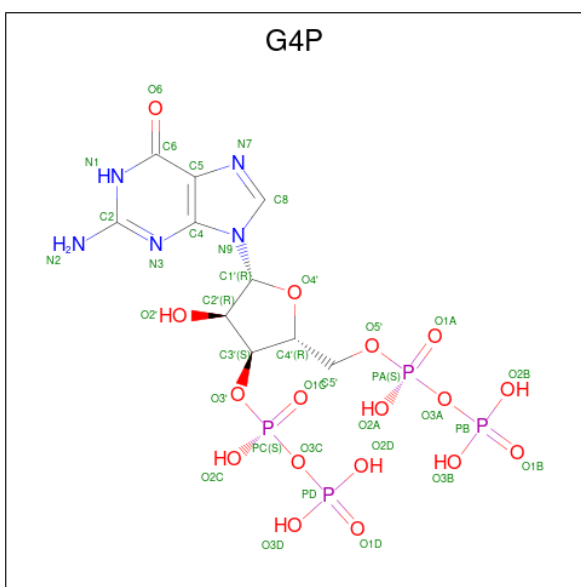
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP B5ZA44
A	-9	ARG	-	expression tag	UNP B5ZA44
A	-8	GLY	-	expression tag	UNP B5ZA44
A	-7	SER	-	expression tag	UNP B5ZA44
A	-6	HIS	-	expression tag	UNP B5ZA44
A	-5	HIS	-	expression tag	UNP B5ZA44
A	-4	HIS	-	expression tag	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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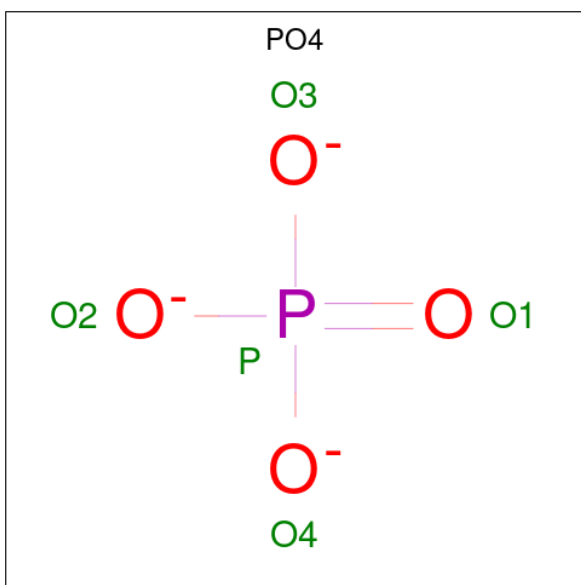
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP B5ZA44
B	-1	HIS	-	expression tag	UNP B5ZA44
B	0	GLY	-	expression tag	UNP B5ZA44
B	1	SER	-	expression tag	UNP B5ZA44
B	143	ALA	GLU	engineered mutation	UNP B5ZA44
C	-10	MET	-	initiating methionine	UNP B5ZA44
C	-9	ARG	-	expression 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 (CCD ID: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$) (labeled as "Ligand of Interest" by depositor).



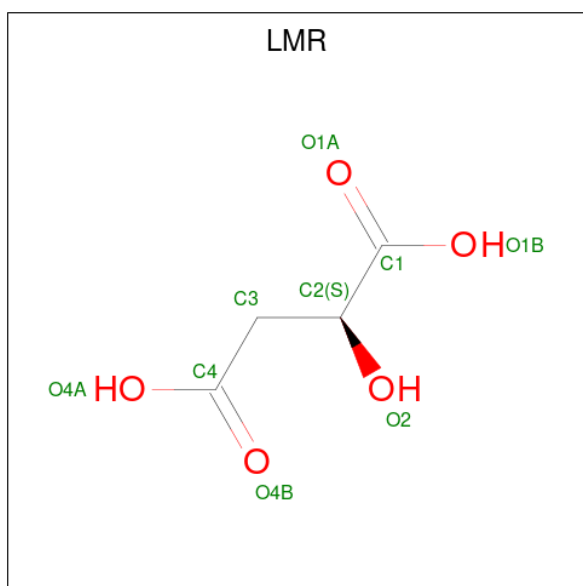
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 36	C 10	N 5	O 17	P 4	0	0
2	B	1	Total 36	C 10	N 5	O 17	P 4	0	0
2	C	1	Total 36	C 10	N 5	O 17	P 4	0	0
2	D	1	Total 36	C 10	N 5	O 17	P 4	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: 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 (CCD ID: 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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

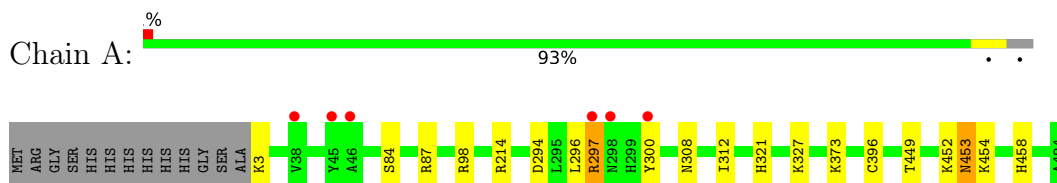
- Molecule 7 is water.

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

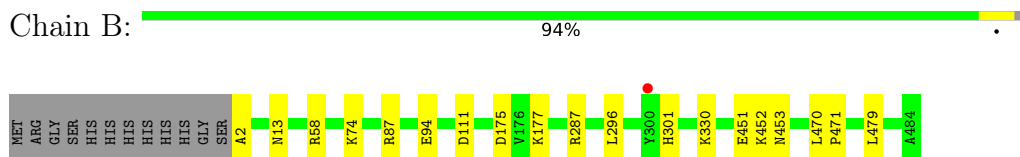
3 Residue-property plots [i](#)

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.

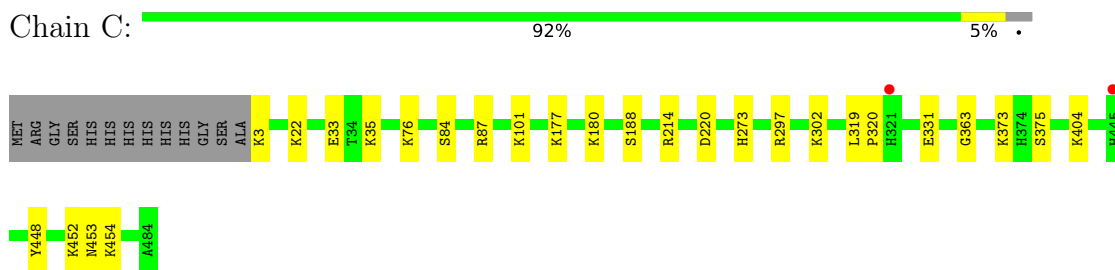
- Molecule 1: Guanosine pentaphosphate phosphohydrolase



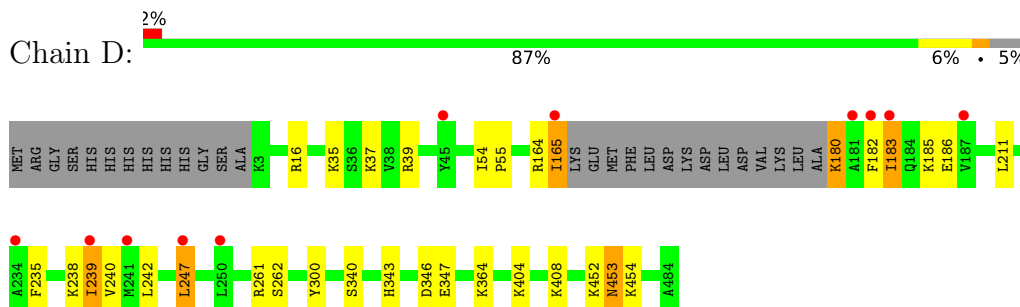
- Molecule 1: Guanosine pentaphosphate phosphohydrolase



- Molecule 1: Guanosine pentaphosphate phosphohydrolase



- Molecule 1: Guanosine pentaphosphate phosphohydrolase



4 Data and refinement statistics

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 40.00 – 2.76	Depositor EDS
% Data completeness (in resolution range)	96.3 (40.00-2.76) 96.2 (40.00-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.77Å)	Xtriage
Refinement program	PHENIX (dev_3352: ???)	Depositor
R, R_{free}	0.178 , 0.222 0.181 , 0.225	Depositor DCC
R_{free} test set	1001 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
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.*

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: PO4, LMR, G4P, MG, EDO

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	0.27	0/3873	0.37	0/5205
1	B	0.12	0/3878	0.27	0/5212
1	C	0.17	0/3873	0.34	0/5205
1	D	0.22	0/3756	0.42	0/5048
All	All	0.20	0/15380	0.35	0/20670

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3803	0	4020	11	0
1	B	3808	0	4025	13	0
1	C	3803	0	4020	18	0
1	D	3688	0	3897	30	0
2	A	36	0	11	0	0
2	B	36	0	11	0	0
2	C	36	0	11	2	0
2	D	36	0	11	1	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	10	0	0	1	0
3	D	5	0	0	0	0
4	A	18	4	8	0	0
4	B	9	0	4	0	0
4	C	9	0	4	0	0
4	D	9	0	4	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
7	A	85	0	0	7	0
7	B	115	0	0	4	0
7	C	103	0	0	8	0
7	D	66	0	0	6	0
All	All	15696	4	16038	72	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 2.

All (72) 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:A:294:ASP:O	1:A:297:ARG:HD3	1.61	1.00
1:D:165:ILE:CG2	1:D:262:SER:HB2	2.02	0.89
1:D:453:ASN:O	1:D:453:ASN:ND2	2.07	0.88
1:D:211:LEU:CD1	1:D:235:PHE:HE2	1.98	0.77
1:D:211:LEU:HD11	1:D:235:PHE:HE2	1.51	0.75
1:D:180:LYS:HG2	1:D:180:LYS:O	1.88	0.74
1:C:3:LYS:HB3	1:C:76:LYS:HE2	1.70	0.74
1:D:233:LEU:C	1:D:233:LEU:HD12	2.13	0.73
1:D:211:LEU:HD11	1:D:235:PHE:CE2	2.23	0.73
1:D:233:LEU:HD12	1:D:233:LEU:O	1.91	0.71
1:D:165:ILE:HG22	1:D:262:SER:HB2	1.74	0.67
1:C:35:LYS:NZ	2:C:502:G4P:O1C	2.34	0.60
1:D:165:ILE:O	1:D:165:ILE:HG23	2.01	0.59
1:D:239:ILE:O	1:D:261:ARG:HG2	2.04	0.58
1:D:364:LYS:NZ	7:D:708:HOH:O	2.37	0.57
1:B:2:ALA:N	7:B:605:HOH:O	2.38	0.56
1:D:16:ARG:NH2	2:D:601:G4P:O2D	2.37	0.56
1:D:239:ILE:HA	1:D:242:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LYS:NZ	7:C:607:HOH:O	2.39	0.55
1:D:300:TYR:CD1	1:D:300:TYR:N	2.72	0.54
1:C:404:LYS:NZ	7:C:603:HOH:O	2.34	0.54
1:C:3:LYS:N	7:C:611:HOH:O	2.41	0.53
1:A:373:LYS:NZ	7:A:715:HOH:O	2.42	0.53
1:D:242:LEU:HD13	1:D:247:LEU:HD21	1.91	0.52
1:D:229:ALA:O	1:D:233:LEU:HB2	2.10	0.51
1:D:39:ARG:NE	7:D:712:HOH:O	2.40	0.51
7:A:706:HOH:O	1:B:74:LYS:HE3	2.11	0.50
1:D:238:LYS:O	1:D:240:VAL:N	2.45	0.50
1:C:452:LYS:HD3	1:C:452:LYS:O	2.12	0.50
1:A:453:ASN:HD22	1:A:453:ASN:N	2.09	0.50
1:D:37:LYS:NZ	7:D:710:HOH:O	2.40	0.50
1:A:214:ARG:NH1	7:A:712:HOH:O	2.41	0.50
1:C:220:ASP:OD1	7:C:601:HOH:O	2.20	0.48
1:C:373:LYS:NZ	7:C:616:HOH:O	2.46	0.48
1:C:188:SER:HA	1:C:273:HIS:CE1	2.49	0.48
1:D:35:LYS:NZ	7:D:710:HOH:O	2.47	0.47
1:B:87:ARG:HD3	1:B:111:ASP:HA	1.96	0.47
1:C:331:GLU:OE1	1:C:448:TYR:OH	2.28	0.47
1:C:84:SER:HA	1:C:87:ARG:HG2	1.96	0.47
1:D:239:ILE:O	1:D:239:ILE:HG22	2.15	0.47
1:C:214:ARG:NE	7:C:617:HOH:O	2.47	0.47
1:A:300:TYR:CD1	1:A:300:TYR:N	2.81	0.46
1:D:39:ARG:HB2	7:D:712:HOH:O	2.15	0.46
1:B:94:GLU:N	1:B:94:GLU:OE1	2.48	0.46
1:A:98:ARG:NH2	7:A:711:HOH:O	2.41	0.46
1:A:308:ASN:O	1:A:312:ILE:HG13	2.16	0.45
1:A:449:THR:HG23	1:A:458:HIS:CE1	2.51	0.45
1:D:180:LYS:O	1:D:183:ILE:HG22	2.17	0.45
1:D:340:SER:HA	1:D:343:HIS:CE1	2.52	0.44
1:B:296:LEU:O	1:B:301:HIS:HD2	2.00	0.44
1:D:231:LYS:HD3	1:D:232:ASN:ND2	2.32	0.44
2:C:502:G4P:O2B	1:D:404:LYS:NZ	2.43	0.44
1:C:180:LYS:NZ	3:C:506:PO4:O3	2.51	0.44
1:C:177:LYS:NZ	7:C:622:HOH:O	2.51	0.43
7:A:706:HOH:O	1:B:74:LYS:CE	2.65	0.43
1:B:13:ASN:HB3	7:B:677:HOH:O	2.18	0.43
1:B:287:ARG:HB2	7:B:654:HOH:O	2.19	0.43
1:A:84:SER:HA	1:A:87:ARG:HG2	2.01	0.42
1:C:3:LYS:NZ	1:C:22:LYS:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:GLY:H	1:C:375:SER:HG	1.68	0.42
1:B:451:GLU:O	1:B:452:LYS:C	2.62	0.41
1:D:54:ILE:HB	1:D:55:PRO:HD3	2.02	0.41
1:D:37:LYS:HE3	7:D:712:HOH:O	2.19	0.41
1:B:452:LYS:O	1:B:453:ASN:ND2	2.54	0.41
1:B:470:LEU:N	1:B:471:PRO:CD	2.84	0.41
1:D:346:ASP:OD1	1:D:347:GLU:N	2.53	0.41
1:B:58:ARG:HD3	7:B:698:HOH:O	2.20	0.41
1:A:3:LYS:HB3	7:A:774:HOH:O	2.21	0.41
1:C:319:LEU:O	1:C:320:PRO:C	2.64	0.41
1:A:321:HIS:ND1	7:A:706:HOH:O	2.36	0.40
1:B:175:ASP:OD2	1:B:177:LYS:NZ	2.49	0.40
1:C:101:LYS:NZ	7:C:626:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/495 (97%)	464 (97%)	16 (3%)	0	100	100
1	B	481/495 (97%)	471 (98%)	10 (2%)	0	100	100
1	C	480/495 (97%)	465 (97%)	15 (3%)	0	100	100
1	D	464/495 (94%)	447 (96%)	16 (3%)	1 (0%)	43	64
All	All	1905/1980 (96%)	1847 (97%)	57 (3%)	1 (0%)	48	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	239	ILE

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	419/429 (98%)	412 (98%)	7 (2%)	53	71
1	B	419/429 (98%)	417 (100%)	2 (0%)	81	89
1	C	419/429 (98%)	415 (99%)	4 (1%)	68	81
1	D	406/429 (95%)	392 (97%)	14 (3%)	32	57
All	All	1663/1716 (97%)	1636 (98%)	27 (2%)	55	73

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	LEU
1	A	297	ARG
1	A	327	LYS
1	A	396	CYS
1	A	452	LYS
1	A	453	ASN
1	A	454	LYS
1	B	330	LYS
1	B	479	LEU
1	C	33	GLU
1	C	297	ARG
1	C	453	ASN
1	C	454	LYS
1	D	164	ARG
1	D	165	ILE
1	D	180	LYS
1	D	182	PHE
1	D	183	ILE
1	D	185	LYS
1	D	186	GLU
1	D	231	LYS
1	D	233	LEU
1	D	247	LEU
1	D	408	LYS

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Mol	Chain	Res	Type
1	D	452	LYS
1	D	453	ASN
1	D	454	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	453	ASN
1	A	458	HIS
1	B	130	ASN
1	B	301	HIS
1	B	453	ASN
1	C	273	HIS
1	C	444	HIS
1	D	232	ASN
1	D	321	HIS
1	D	400	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	G4P	C	502	6	36,38,38	1.10	2 (5%)	56,61,61	1.54	9 (16%)
4	LMR	D	603	-	8,8,8	2.53	4 (50%)	10,10,10	1.58	2 (20%)
3	PO4	B	503	6	4,4,4	0.96	0	6,6,6	0.43	0
2	G4P	A	601	-	36,38,38	1.10	2 (5%)	56,61,61	1.55	11 (19%)
4	LMR	C	504	-	8,8,8	2.51	4 (50%)	10,10,10	1.64	1 (10%)
3	PO4	A	602	-	4,4,4	1.00	0	6,6,6	0.38	0
2	G4P	D	601	-	36,38,38	1.07	1 (2%)	56,61,61	1.55	9 (16%)
3	PO4	C	503	6	4,4,4	0.94	0	6,6,6	0.54	0
4	LMR	A	604	-	8,8,8	1.11	0	10,10,10	1.33	2 (20%)
5	EDO	A	605	-	3,3,3	0.60	0	2,2,2	0.43	0
2	G4P	B	502	-	36,38,38	1.11	2 (5%)	56,61,61	1.56	10 (17%)
3	PO4	C	506	-	4,4,4	0.93	0	6,6,6	0.47	0
5	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.30	0
4	LMR	B	504	-	8,8,8	0.69	0	10,10,10	1.53	1 (10%)
4	LMR	A	603	-	8,8,8	1.77	2 (25%)	10,10,10	1.53	1 (10%)
3	PO4	D	602	-	4,4,4	0.95	0	6,6,6	0.46	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
2	G4P	C	502	6	-	7/27/43/43	0/3/3/3
4	LMR	D	603	-	-	2/8/8/8	-
2	G4P	A	601	-	-	3/27/43/43	0/3/3/3
4	LMR	C	504	-	-	2/8/8/8	-
2	G4P	D	601	-	-	8/27/43/43	0/3/3/3
4	LMR	A	604	-	-	4/8/8/8	-
5	EDO	A	605	-	-	1/1/1/1	-
5	EDO	B	505	-	-	1/1/1/1	-
2	G4P	B	502	-	-	5/27/43/43	0/3/3/3
4	LMR	B	504	-	-	4/8/8/8	-
4	LMR	A	603	-	-	4/8/8/8	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	LMR	O1A-C1	4.28	1.34	1.22
4	C	504	LMR	O1A-C1	4.28	1.34	1.22
4	D	603	LMR	O4B-C4	3.88	1.34	1.22
4	C	504	LMR	O4B-C4	3.78	1.34	1.22
4	A	603	LMR	O4B-C4	3.74	1.34	1.22
4	D	603	LMR	O1B-C1	-2.98	1.21	1.30
4	C	504	LMR	O1B-C1	-2.93	1.21	1.30
4	A	603	LMR	O4A-C4	-2.91	1.21	1.30
4	C	504	LMR	O4A-C4	-2.91	1.21	1.30
4	D	603	LMR	O4A-C4	-2.87	1.21	1.30
2	A	601	G4P	PA-O3A	2.39	1.62	1.59
2	D	601	G4P	PA-O3A	2.36	1.62	1.59
2	B	502	G4P	PC-O3C	2.33	1.62	1.59
2	B	502	G4P	PA-O3A	2.32	1.62	1.59
2	C	502	G4P	PA-O3A	2.25	1.61	1.59
2	A	601	G4P	PC-O3C	2.22	1.61	1.59
2	C	502	G4P	PC-O3C	2.09	1.61	1.59

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	G4P	C5-C4-N3	-5.39	119.81	128.39
2	C	502	G4P	C5-C4-N3	-5.37	119.84	128.39
2	D	601	G4P	C5-C4-N3	-5.19	120.13	128.39
2	B	502	G4P	C2-N3-C4	5.18	121.22	112.30
2	A	601	G4P	C5-C4-N3	-5.17	120.16	128.39
2	D	601	G4P	C2-N3-C4	5.10	121.09	112.30
2	A	601	G4P	C2-N3-C4	5.07	121.04	112.30
2	C	502	G4P	C2-N3-C4	5.05	121.01	112.30
2	B	502	G4P	N9-C4-N3	3.96	133.87	125.95
2	C	502	G4P	N9-C4-N3	3.94	133.84	125.95
2	D	601	G4P	N9-C4-N3	3.83	133.60	125.95
2	A	601	G4P	N9-C4-N3	3.80	133.54	125.95
4	C	504	LMR	O1B-C1-C2	3.62	120.39	112.74
4	D	603	LMR	O1B-C1-C2	3.50	120.14	112.74
4	B	504	LMR	O1B-C1-C2	3.42	119.97	112.74
4	A	603	LMR	O1B-C1-C2	3.25	119.62	112.74
2	C	502	G4P	C8-N7-C5	2.91	109.45	104.26
4	A	604	LMR	O1B-C1-C2	2.87	118.81	112.74
2	B	502	G4P	C8-N7-C5	2.86	109.35	104.26
2	A	601	G4P	C8-N7-C5	2.82	109.29	104.26
2	D	601	G4P	C8-N7-C5	2.79	109.23	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	G4P	C2-N1-C6	-2.59	120.41	125.11
2	A	601	G4P	C2-N1-C6	-2.57	120.45	125.11
2	B	502	G4P	C2-N1-C6	-2.56	120.47	125.11
2	D	601	G4P	C2-N1-C6	-2.47	120.63	125.11
2	A	601	G4P	C6-C5-N7	2.39	134.64	130.29
2	A	601	G4P	PA-O5'-C5'	-2.33	108.00	121.35
2	D	601	G4P	C6-C5-N7	2.32	134.52	130.29
2	B	502	G4P	PA-O5'-C5'	-2.30	108.14	121.35
2	B	502	G4P	C6-C5-N7	2.30	134.47	130.29
2	B	502	G4P	C4-C5-N7	-2.24	107.12	110.67
2	C	502	G4P	C4-C5-N7	-2.23	107.13	110.67
2	A	601	G4P	C4-C5-N7	-2.20	107.18	110.67
2	D	601	G4P	C4-C5-N7	-2.17	107.23	110.67
2	C	502	G4P	C6-C5-N7	2.16	134.22	130.29
2	A	601	G4P	O6-C6-C5	-2.14	120.88	126.53
4	A	604	LMR	O1A-C1-C2	-2.13	118.34	122.60
2	D	601	G4P	O6-C6-C5	-2.12	120.94	126.53
2	C	502	G4P	O6-C6-C5	-2.10	121.00	126.53
2	B	502	G4P	O6-C6-C5	-2.09	121.01	126.53
2	C	502	G4P	PA-O5'-C5'	-2.09	109.39	121.35
2	A	601	G4P	N9-C8-N7	-2.04	109.62	113.40
2	D	601	G4P	PA-O5'-C5'	-2.02	109.75	121.35
4	D	603	LMR	O4A-C4-C3	2.02	120.29	114.00
2	A	601	G4P	C5-C6-N1	2.02	118.40	113.25
2	B	502	G4P	C5-C6-N1	2.00	118.35	113.25

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-O3A
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	B	504	LMR	O1A-C1-C2-O2

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

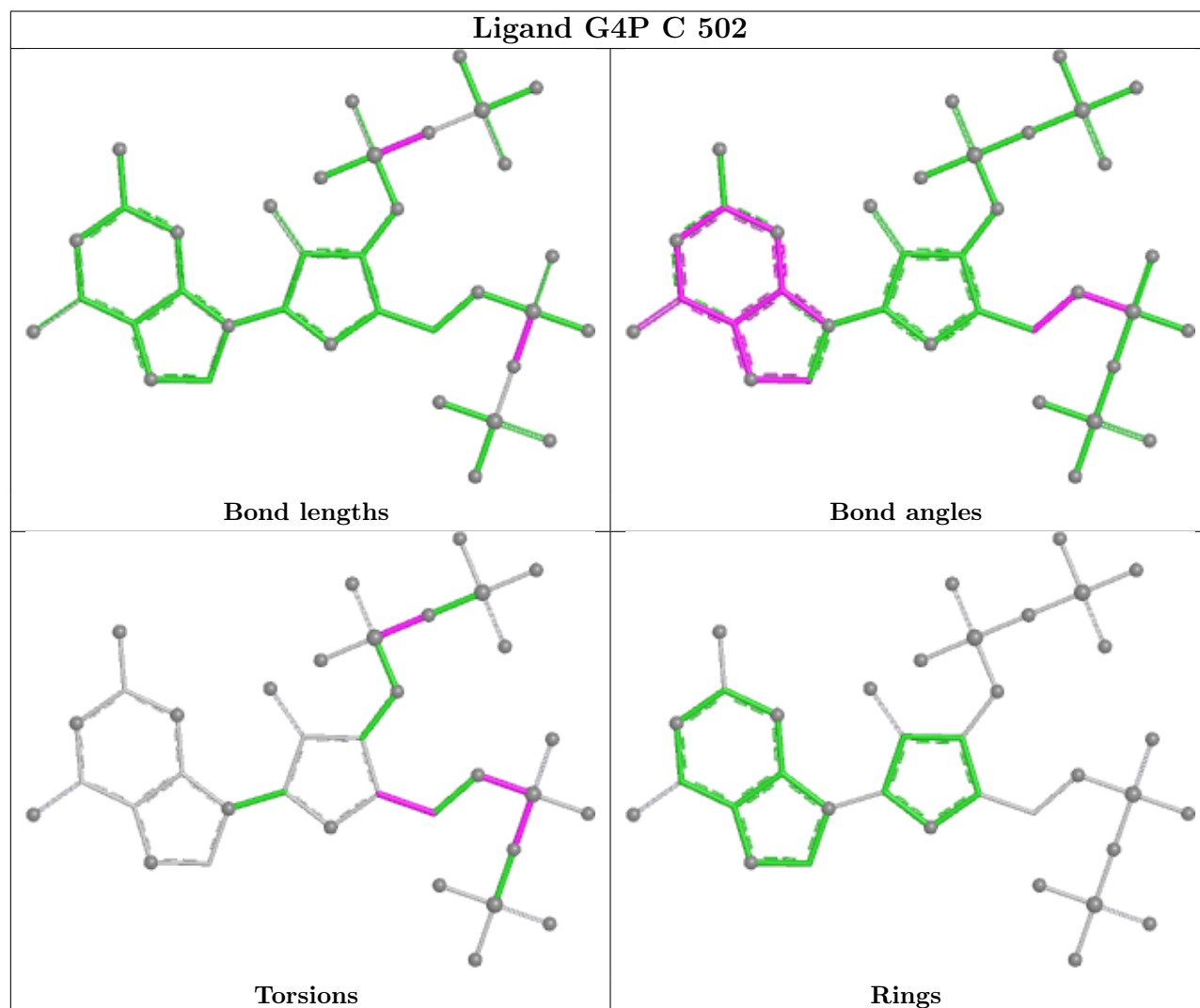
There are no ring outliers.

3 monomers are involved in 4 short contacts:

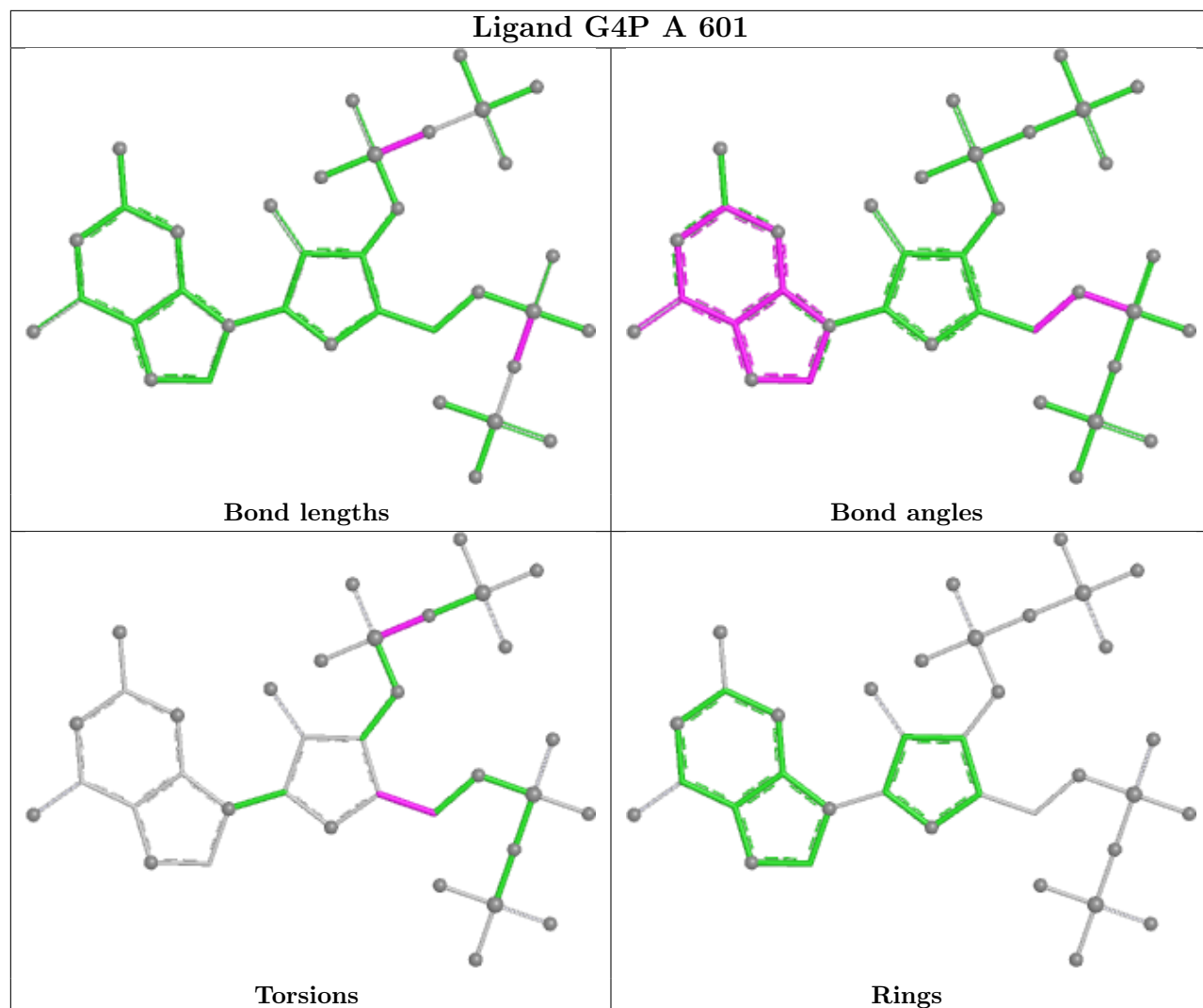
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	G4P	2	0
2	D	601	G4P	1	0
3	C	506	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

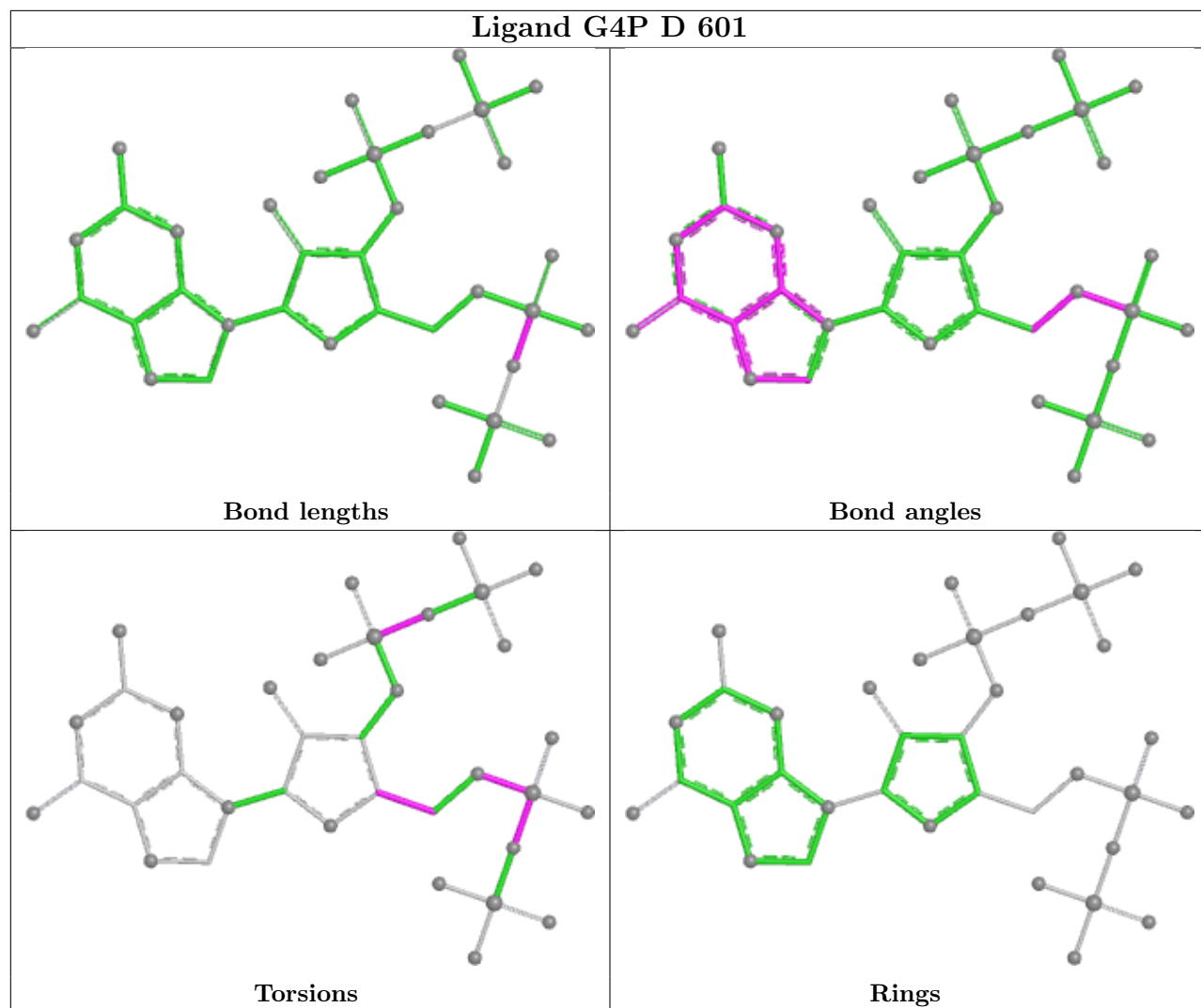
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

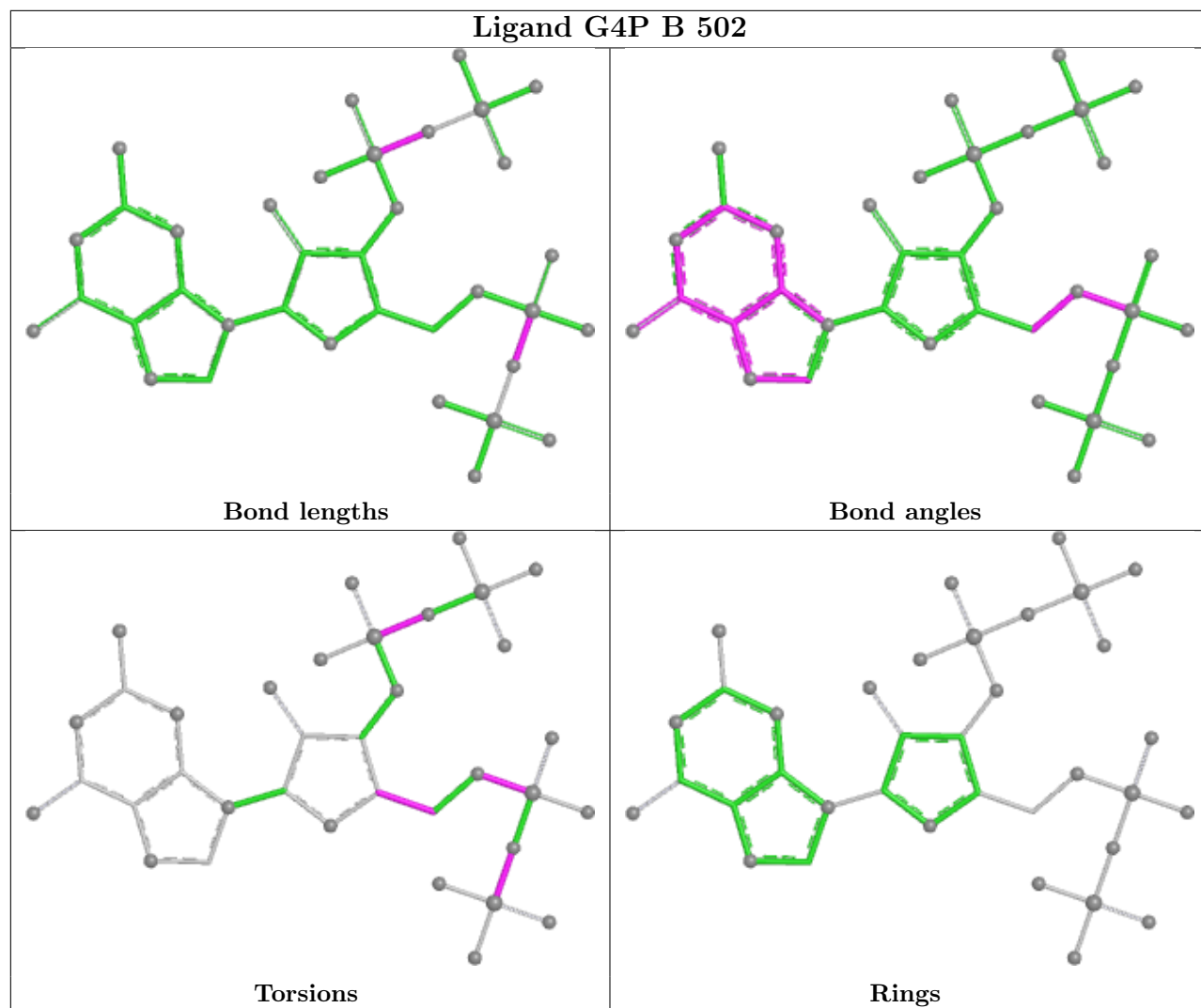


Ligand G4P A 601



Ligand G4P D 601





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	482/495 (97%)	-0.32	6 (1%) 76 76	28, 46, 80, 119	0
1	B	483/495 (97%)	-0.49	1 (0%) 91 92	27, 41, 69, 96	0
1	C	482/495 (97%)	-0.37	2 (0%) 88 89	30, 45, 76, 110	0
1	D	468/495 (94%)	-0.09	11 (2%) 59 57	31, 54, 106, 135	0
All	All	1915/1980 (96%)	-0.32	20 (1%) 79 79	27, 46, 86, 135	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	165	ILE	4.9
1	D	183	ILE	4.4
1	A	45	TYR	3.7
1	A	46	ALA	3.2
1	D	187	VAL	3.0
1	A	300	TYR	2.9
1	A	298	ASN	2.6
1	C	321	HIS	2.5
1	C	445	HIS	2.4
1	B	300	TYR	2.3
1	D	250	LEU	2.3
1	D	239	ILE	2.2
1	D	45	TYR	2.2
1	D	241	MET	2.2
1	D	181	ALA	2.2
1	D	182	PHE	2.1
1	A	297	ARG	2.1
1	D	234	ALA	2.1
1	D	247	LEU	2.0
1	A	38	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

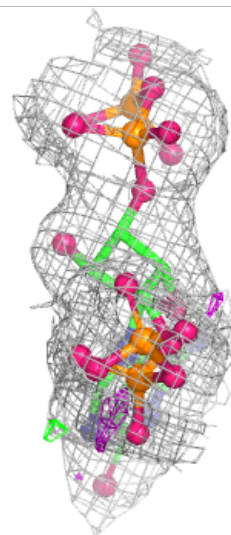
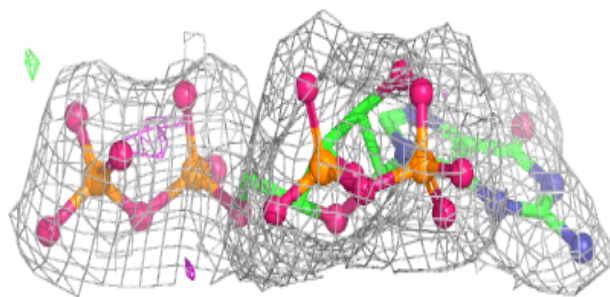
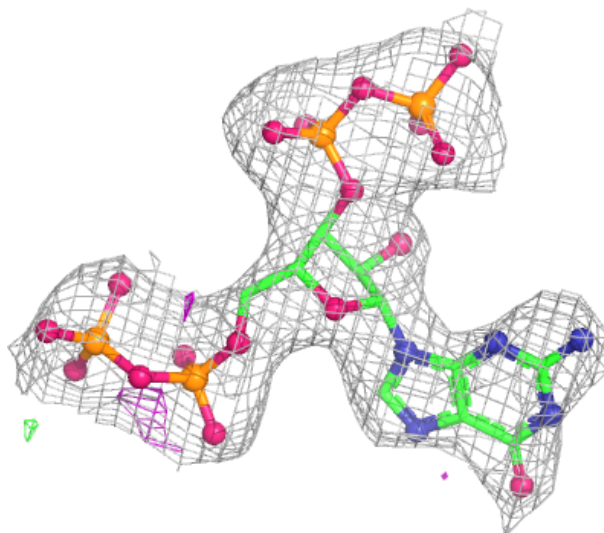
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	EDO	B	505	4/4	0.61	0.22	52,60,61,67	0
6	MG	C	505	1/1	0.71	0.13	83,83,83,83	0
4	LMR	A	604	9/9	0.73	0.13	76,99,122,127	0
5	EDO	A	605	4/4	0.76	0.19	51,54,64,71	0
3	PO4	C	506	5/5	0.87	0.13	80,93,117,130	0
4	LMR	A	603	9/9	0.88	0.13	44,48,57,63	0
4	LMR	D	603	9/9	0.89	0.11	65,67,86,87	0
3	PO4	D	602	5/5	0.89	0.12	98,98,113,130	0
2	G4P	D	601	36/36	0.90	0.09	53,75,100,103	0
4	LMR	C	504	9/9	0.91	0.13	36,45,69,70	0
4	LMR	B	504	9/9	0.92	0.12	37,46,54,59	0
3	PO4	A	602	5/5	0.92	0.12	65,67,82,87	0
2	G4P	B	502	36/36	0.93	0.08	36,51,88,104	0
2	G4P	A	601	36/36	0.94	0.08	43,65,98,114	0
2	G4P	C	502	36/36	0.95	0.07	38,57,98,110	0
3	PO4	B	503	5/5	0.95	0.09	47,54,60,60	0
3	PO4	C	503	5/5	0.98	0.06	42,46,47,55	0
6	MG	C	501	1/1	0.99	0.06	50,50,50,50	0
6	MG	B	501	1/1	0.99	0.12	72,72,72,72	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.

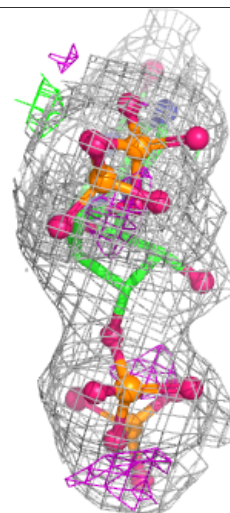
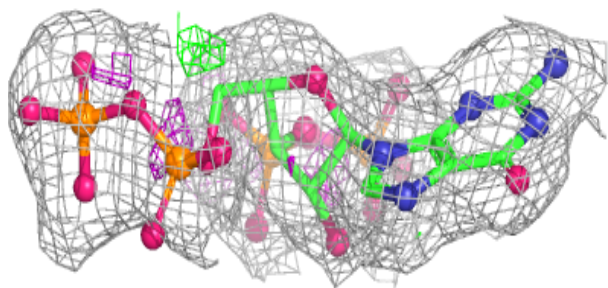
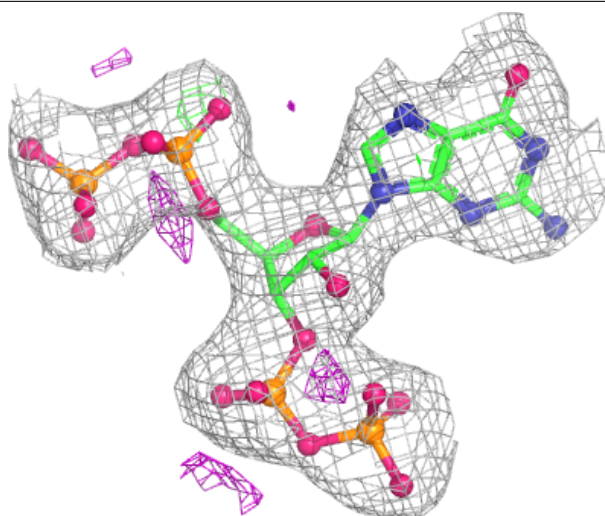
Electron density around G4P D 601:

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



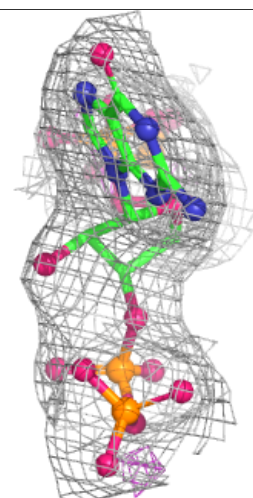
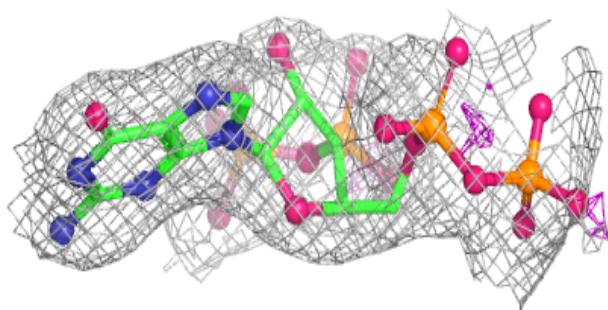
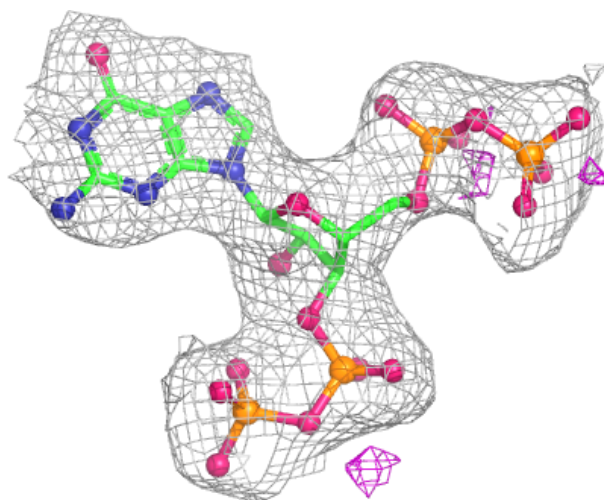
Electron density around G4P B 502:

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



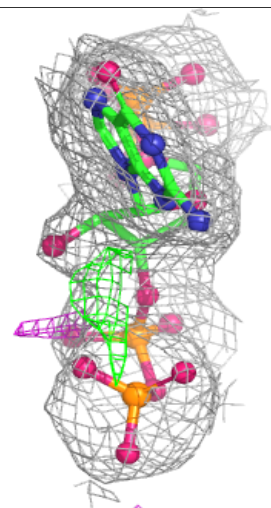
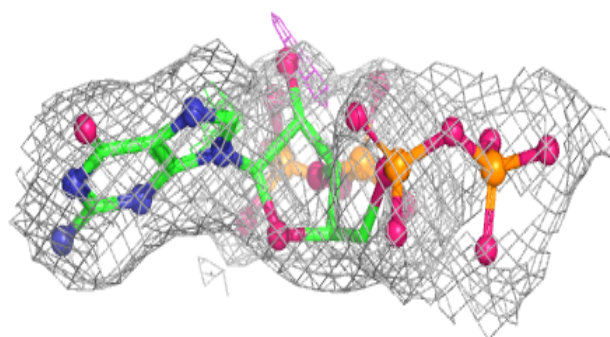
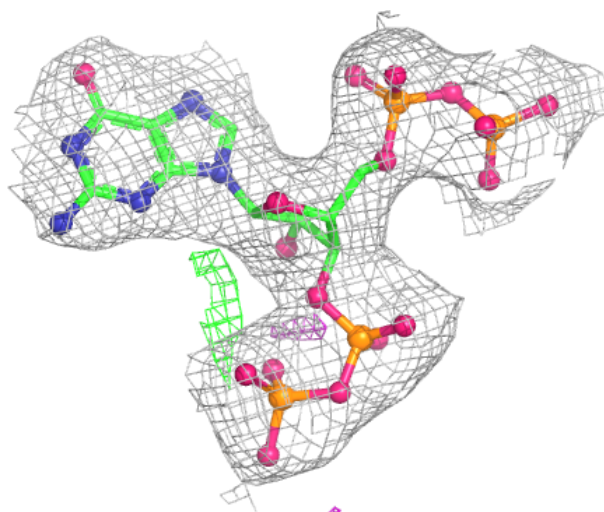
Electron density around G4P A 601:

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



Electron density around G4P C 502:

$2mF_o-DF_c$ (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.