W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 05:27 AM EDT

PDB ID	:	7MPQ
Title	:	Bartonella henselae NrnC cleaving pGG in the presence of Mn2+
Authors	:	Lormand, J.D.; Sondermann, H.
Deposited on	:	2021-05-04
Resolution	:	2.35 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

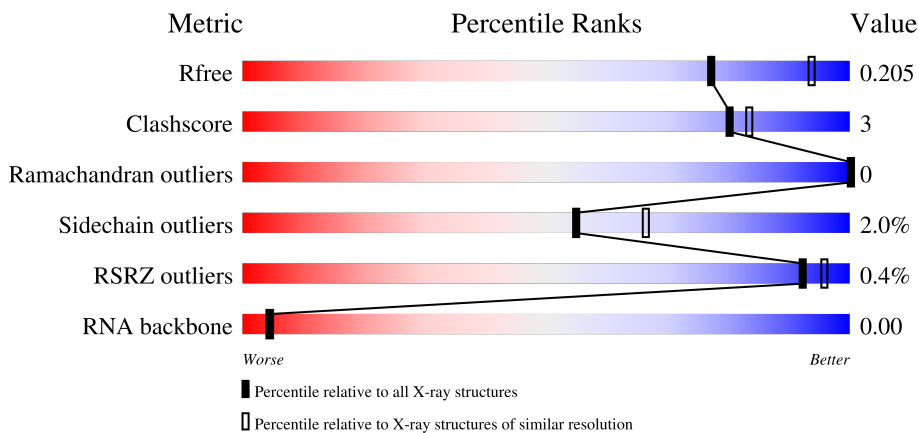|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.35 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.
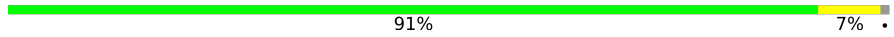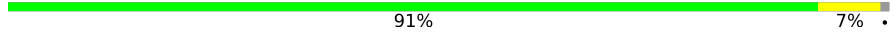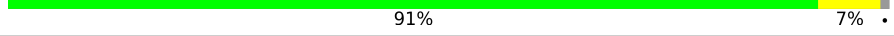
Metric	Percentile Ranks	Value
Rfree		0.205
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		2.0%
RSRZ outliers		0.4%
RNA backbone		0.00

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)
RNA backbone	3102	1006 (2.74-1.98)

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 <=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	207	95% •
1	C	207	91% 7% •
1	E	207	92% 7% •
1	G	207	93% 6% •

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	207	91% 7% ·
1	K	207	89% 10% ·
1	M	207	91% 7% ·
1	O	207	% 91% 7% ·
2	R	2	100% 50% 50%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 14235 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 NanoRNase C.

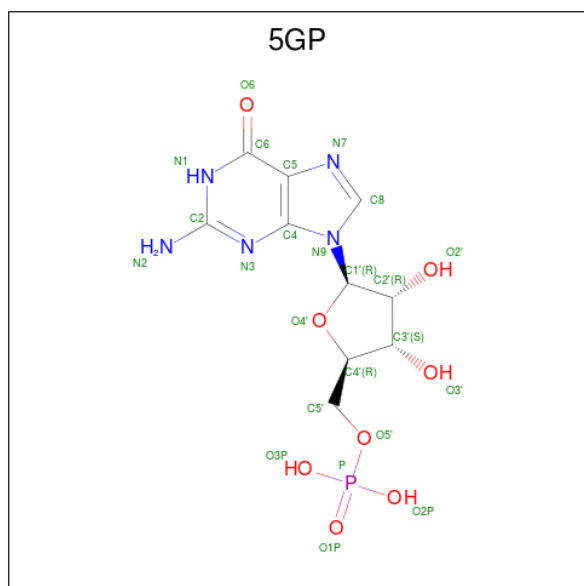| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total 1667	C 1049	N 295	O 316	S 7	0	6	0
1	C	205	Total 1660	C 1045	N 294	O 314	S 7	0	5	0
1	E	205	Total 1653	C 1040	N 296	O 311	S 6	0	3	0
1	G	205	Total 1655	C 1041	N 293	O 315	S 6	0	4	0
1	I	205	Total 1650	C 1038	N 294	O 312	S 6	0	3	0
1	K	205	Total 1652	C 1039	N 297	O 310	S 6	0	3	0
1	M	204	Total 1646	C 1036	N 295	O 309	S 6	0	3	0
1	O	204	Total 1631	C 1026	N 291	O 308	S 6	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP X5MEI1
C	0	SER	-	expression tag	UNP X5MEI1
E	0	SER	-	expression tag	UNP X5MEI1
G	0	SER	-	expression tag	UNP X5MEI1
I	0	SER	-	expression tag	UNP X5MEI1
K	0	SER	-	expression tag	UNP X5MEI1
M	0	SER	-	expression tag	UNP X5MEI1
O	0	SER	-	expression tag	UNP X5MEI1

- Molecule 2 is a RNA chain called 5'-phosphorylated GG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			

- Molecule 3 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	E	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	E	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	I	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	I	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	I	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	K	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	K	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	K	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	M	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	M	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	O	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		
4	C	2	Total	Mn	0	0
			2	2		
4	E	2	Total	Mn	0	0
			2	2		
4	G	2	Total	Mn	0	0
			2	2		
4	I	2	Total	Mn	0	0
			2	2		
4	K	2	Total	Mn	0	0
			2	2		
4	M	2	Total	Mn	0	0
			2	2		
4	O	2	Total	Mn	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	100	Total	O	0	0
			100	100		
5	C	97	Total	O	0	0
			97	97		
5	E	87	Total	O	0	0
			87	87		
5	G	86	Total	O	0	0
			86	86		
5	I	85	Total	O	0	0
			85	85		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	64	Total 64	O 64	0	0
5	M	63	Total 63	O 63	0	0
5	O	38	Total 38	O 38	0	0
5	R	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

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: NanoRNase C

Chain A:

- Molecule 1: NanoRNase C

Chain C:
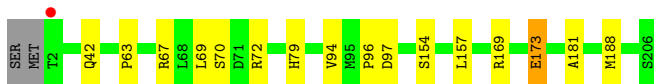
- Molecule 1: NanoRNase C

Chain E:

- Molecule 1: NanoRNase C

Chain G:

- Molecule 1: NanoRNase C
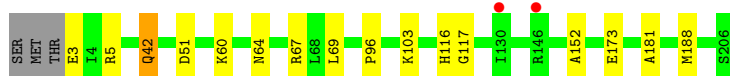
Chain I:

- Molecule 1: NanoRNase C

Chain K:

SER MET T2 E3 D10 L11 E27 T28 L29 V40 V41 Q42 T49 P63 L69 P96 K103 D114 R115 H116 G117 E120 R169 E173 A181 M188 S206

• Molecule 1: NanoRNase C

Chain M:

91%   7%   •

SER MET THR E3 L69 P96 D97 K103 N127 K132 S136 E150 L162 E173 A181 M188 D193 S198 S206

• Molecule 1: NanoRNase C

Chain O:

.%

91%   7%   •

SER MET THR E3 I4 R5 Q42 D51 K60 N64 R67 L68 L69 P96 K103 H116 G117 I130 R146 A152 E173 A181 M188 S206
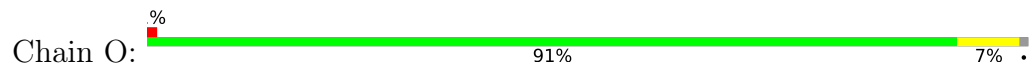
• Molecule 2: 5'-phosphorylated GG

Chain R:

100%

50%   50%

G603 G604

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.68Å 127.80Å 128.81Å 90.00° 94.87° 90.00°	Depositor
Resolution (Å)	128.34 – 2.35 128.34 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.8 (128.34-2.35) 97.8 (128.34-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.162 , 0.206 0.165 , 0.205	Depositor DCC
R_{free} test set	4388 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å^2)	48.7	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14235	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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.

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: 5GP, MN

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	0.42	0/1713	0.57	0/2314
1	C	0.39	0/1703	0.57	0/2300
1	E	0.41	0/1690	0.55	0/2282
1	G	0.38	0/1695	0.56	0/2290
1	I	0.38	0/1687	0.54	0/2279
1	K	0.37	0/1689	0.54	0/2281
1	M	0.37	0/1683	0.55	0/2272
1	O	0.33	0/1662	0.51	0/2245
2	R	1.72	1/52 (1.9%)	1.09	0/78
All	All	0.40	1/13574 (0.0%)	0.55	0/18341

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	603	G	OP3-P	-10.28	1.48	1.61

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	1667	0	1672	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1660	0	1664	11	0
1	E	1653	0	1658	8	0
1	G	1655	0	1653	7	0
1	I	1650	0	1651	10	0
1	K	1652	0	1658	12	0
1	M	1646	0	1651	8	0
1	O	1631	0	1628	11	0
2	R	47	0	23	1	0
3	A	48	0	23	1	0
3	C	24	0	12	1	0
3	E	48	0	24	1	0
3	I	72	0	36	5	0
3	K	72	0	36	8	0
3	M	48	0	24	1	0
3	O	24	0	12	2	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
4	G	2	0	0	0	0
4	I	2	0	0	0	0
4	K	2	0	0	0	0
4	M	2	0	0	0	0
4	O	2	0	0	0	0
5	A	100	0	0	5	0
5	C	97	0	0	4	0
5	E	87	0	0	3	0
5	G	86	0	0	2	0
5	I	85	0	0	3	0
5	K	64	0	0	4	0
5	M	63	0	0	2	0
5	O	38	0	0	1	0
5	R	2	0	0	0	0
All	All	14235	0	13425	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 74 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:A:302:5GP:N2	5:A:402:HOH:O	2.00	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:THR:O	5:I:401:HOH:O	1.92	0.88
1:A:4:ILE:O	5:A:401:HOH:O	1.92	0.86
1:I:2:THR:OG1	1:I:3:GLU:N	2.13	0.80
3:I:303:5GP:O3P	1:O:103:LYS:NZ	2.18	0.76

There are no symmetry-related clashes.

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	210/207 (101%)	209 (100%)	1 (0%)	0	100	100
1	C	208/207 (100%)	207 (100%)	1 (0%)	0	100	100
1	E	206/207 (100%)	204 (99%)	2 (1%)	0	100	100
1	G	207/207 (100%)	207 (100%)	0	0	100	100
1	I	206/207 (100%)	206 (100%)	0	0	100	100
1	K	206/207 (100%)	205 (100%)	1 (0%)	0	100	100
1	M	205/207 (99%)	205 (100%)	0	0	100	100
1	O	203/207 (98%)	199 (98%)	4 (2%)	0	100	100
All	All	1651/1656 (100%)	1642 (100%)	9 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	184/180 (102%)	180 (98%)	4 (2%)	52	63
1	C	183/180 (102%)	179 (98%)	4 (2%)	52	63
1	E	181/180 (101%)	177 (98%)	4 (2%)	52	63
1	G	182/180 (101%)	179 (98%)	3 (2%)	62	75
1	I	181/180 (101%)	177 (98%)	4 (2%)	52	63
1	K	181/180 (101%)	177 (98%)	4 (2%)	52	63
1	M	180/180 (100%)	175 (97%)	5 (3%)	43	53
1	O	178/180 (99%)	176 (99%)	2 (1%)	73	84
All	All	1450/1440 (101%)	1420 (98%)	30 (2%)	55	65

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	173	GLU
1	M	206	SER
1	I	97	ASP
1	O	173	GLU
1	M	103	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	135	GLN
1	G	32	GLN
1	O	8	GLN
1	O	54	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	1/2 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6　Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 16 are monoatomic - leaving 14 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	5GP	E	302	4	22,26,26	1.17	2 (9%)	26,40,40	1.40	6 (23%)
3	5GP	C	301	4	22,26,26	1.07	2 (9%)	26,40,40	1.41	5 (19%)
3	5GP	O	301	4	22,26,26	1.08	1 (4%)	26,40,40	1.26	3 (11%)
3	5GP	I	301	4	22,26,26	1.11	2 (9%)	26,40,40	1.23	4 (15%)
3	5GP	M	301	4	22,26,26	1.13	2 (9%)	26,40,40	1.23	3 (11%)
3	5GP	K	302	4	22,26,26	1.07	2 (9%)	26,40,40	1.23	4 (15%)
3	5GP	I	302	-	22,26,26	1.19	2 (9%)	26,40,40	1.24	3 (11%)
3	5GP	M	302	4	22,26,26	1.04	1 (4%)	26,40,40	1.22	2 (7%)
3	5GP	I	303	4	22,26,26	1.17	1 (4%)	26,40,40	1.39	4 (15%)
3	5GP	A	302	4	22,26,26	1.12	1 (4%)	26,40,40	1.42	5 (19%)
3	5GP	K	301	4	22,26,26	1.19	1 (4%)	26,40,40	1.31	3 (11%)
3	5GP	A	301	4	22,26,26	1.09	2 (9%)	26,40,40	1.29	3 (11%)
3	5GP	K	303	4	22,26,26	1.12	1 (4%)	26,40,40	1.26	3 (11%)
3	5GP	E	301	4	22,26,26	1.09	1 (4%)	26,40,40	1.26	4 (15%)

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
3	5GP	E	302	4	-	0/6/26/26	0/3/3/3
3	5GP	C	301	4	-	5/6/26/26	0/3/3/3
3	5GP	O	301	4	-	6/6/26/26	0/3/3/3
3	5GP	I	301	4	-	3/6/26/26	0/3/3/3
3	5GP	M	301	4	-	5/6/26/26	0/3/3/3
3	5GP	K	302	4	-	0/6/26/26	0/3/3/3
3	5GP	I	302	-	-	1/6/26/26	0/3/3/3
3	5GP	M	302	4	-	1/6/26/26	0/3/3/3
3	5GP	I	303	4	-	3/6/26/26	0/3/3/3
3	5GP	A	302	4	-	5/6/26/26	0/3/3/3
3	5GP	K	301	4	-	5/6/26/26	0/3/3/3
3	5GP	A	301	4	-	3/6/26/26	0/3/3/3
3	5GP	K	303	4	-	5/6/26/26	0/3/3/3
3	5GP	E	301	4	-	0/6/26/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	303	5GP	C5-C6	-4.04	1.39	1.47
3	K	301	5GP	C5-C6	-3.98	1.39	1.47
3	E	302	5GP	C5-C6	-3.86	1.39	1.47
3	I	302	5GP	C5-C6	-3.84	1.39	1.47
3	E	301	5GP	C5-C6	-3.77	1.39	1.47

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	5GP	C5-C6-N1	3.38	119.92	113.95
3	E	302	5GP	C5-C6-N1	3.36	119.88	113.95
3	I	303	5GP	C5-C6-N1	3.29	119.75	113.95
3	K	301	5GP	C5-C6-N1	3.21	119.62	113.95
3	A	301	5GP	C5-C6-N1	2.99	119.23	113.95

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	5GP	C5'-O5'-P-O1P
3	A	301	5GP	C5'-O5'-P-O3P
3	A	302	5GP	C5'-O5'-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	302	5GP	C5'-O5'-P-O2P
3	A	302	5GP	C5'-O5'-P-O3P

There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	5GP	1	0
3	C	301	5GP	1	0
3	O	301	5GP	2	0
3	I	301	5GP	1	0
3	M	301	5GP	1	0
3	I	302	5GP	1	0
3	M	302	5GP	1	0
3	I	303	5GP	3	0
3	A	302	5GP	1	0
3	K	301	5GP	6	0
3	K	303	5GP	2	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 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 5GP E 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP O 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP I 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP M 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP K 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP I 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP M 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP I 303

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP A 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP K 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP A 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP K 303

Bond lengths

Bond angles

Torsions

Rings

Ligand 5GP E 301

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	206/207 (99%)	0.13	1 (0%)	91	95	29, 39, 64, 87	0
1	C	205/207 (99%)	0.13	1 (0%)	91	95	29, 40, 61, 84	0
1	E	205/207 (99%)	0.04	0	100	100	31, 42, 65, 77	0
1	G	205/207 (99%)	0.10	0	100	100	30, 43, 66, 86	0
1	I	205/207 (99%)	0.05	1 (0%)	91	95	34, 44, 68, 86	0
1	K	205/207 (99%)	0.19	0	100	100	31, 50, 71, 85	0
1	M	204/207 (98%)	0.20	0	100	100	34, 47, 71, 85	0
1	O	204/207 (98%)	0.25	2 (0%)	82	88	37, 55, 80, 96	0
2	R	2/2 (100%)	2.49	2 (100%)	0	0	86, 86, 86, 91	0
All	All	1641/1658 (98%)	0.14	7 (0%)	92	96	29, 45, 70, 96	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	130	ILE	3.1
1	A	1	MET	2.8
1	I	2	THR	2.7
2	R	603	G	2.6
2	R	604	G	2.4

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 monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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(Å^2)	Q<0.9
4	MN	O	303	1/1	0.77	0.08	111,111,111,111	0
3	5GP	O	301	24/24	0.85	0.27	48,96,115,122	0
4	MN	K	305	1/1	0.86	0.06	86,86,86,86	0
3	5GP	M	302	24/24	0.86	0.26	61,107,115,120	0
3	5GP	A	302	24/24	0.88	0.25	37,86,94,96	24
3	5GP	I	303	24/24	0.88	0.24	52,84,103,105	24
4	MN	M	304	1/1	0.89	0.11	82,82,82,82	0
3	5GP	E	302	24/24	0.89	0.23	44,73,88,93	24
4	MN	I	305	1/1	0.90	0.06	90,90,90,90	0
3	5GP	K	303	24/24	0.90	0.27	50,86,92,95	24
3	5GP	I	302	24/24	0.90	0.27	43,80,93,101	24
3	5GP	K	301	24/24	0.90	0.21	42,84,97,100	24
3	5GP	I	301	24/24	0.91	0.19	54,82,88,91	0
3	5GP	C	301	24/24	0.93	0.18	42,77,87,89	0
4	MN	C	303	1/1	0.93	0.11	78,78,78,78	0
3	5GP	K	302	24/24	0.93	0.24	60,87,94,98	0
4	MN	A	304	1/1	0.94	0.13	78,78,78,78	0
3	5GP	E	301	24/24	0.94	0.23	63,78,83,84	0
3	5GP	A	301	24/24	0.94	0.19	43,75,83,88	0
4	MN	C	302	1/1	0.95	0.07	84,84,84,84	0
3	5GP	M	301	24/24	0.95	0.20	49,74,92,102	0
4	MN	G	302	1/1	0.95	0.05	81,81,81,81	0
4	MN	O	302	1/1	0.95	0.10	116,116,116,116	0
4	MN	I	304	1/1	0.95	0.05	96,96,96,96	0
4	MN	E	303	1/1	0.96	0.07	75,75,75,75	0
4	MN	G	301	1/1	0.97	0.08	88,88,88,88	0
4	MN	A	303	1/1	0.97	0.05	80,80,80,80	0
4	MN	K	304	1/1	0.99	0.13	110,110,110,110	0
4	MN	E	304	1/1	0.99	0.06	88,88,88,88	0
4	MN	M	303	1/1	0.99	0.05	83,83,83,83	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.
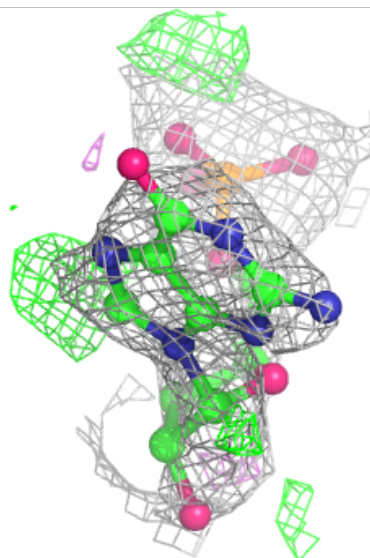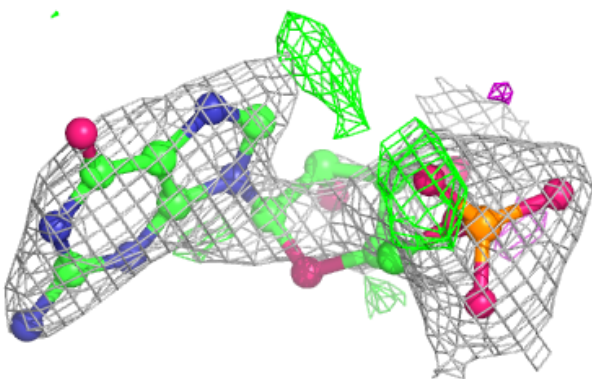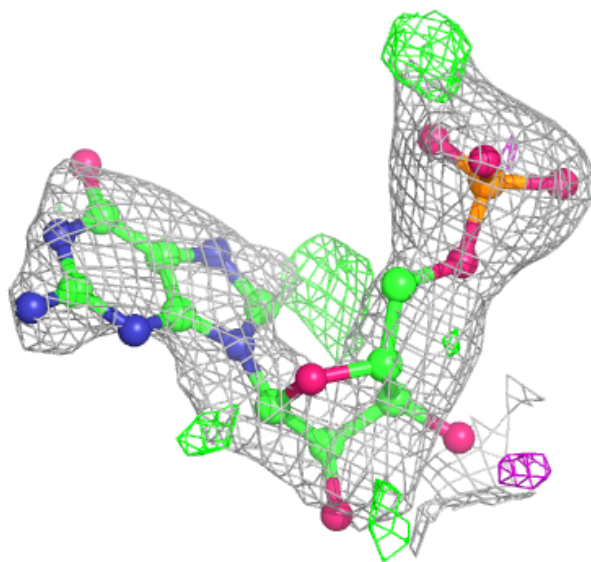
Electron density around 5GP O 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
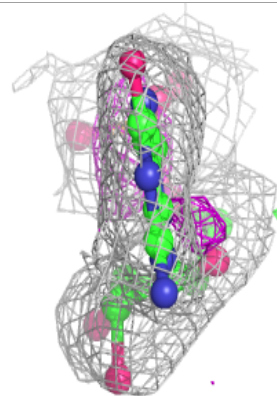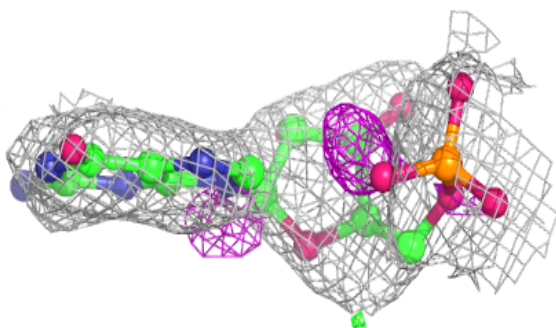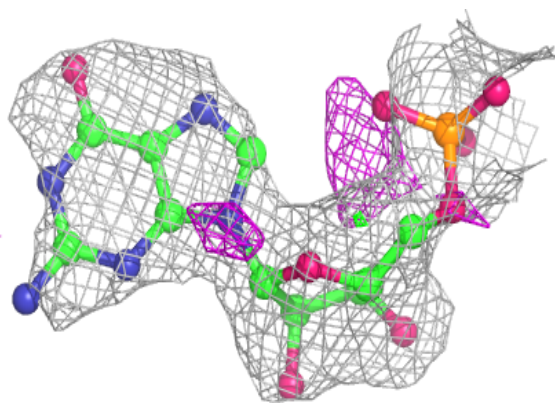
Electron density around 5GP M 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
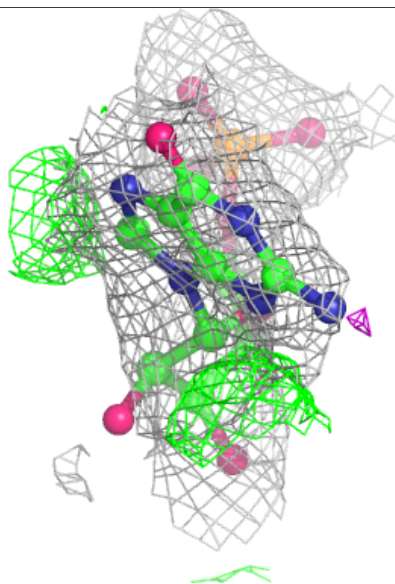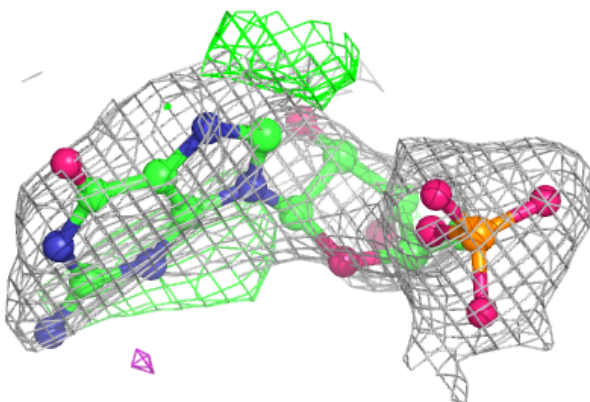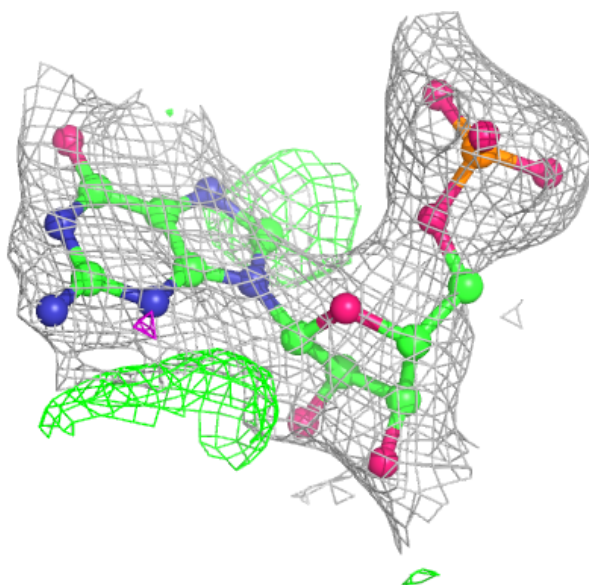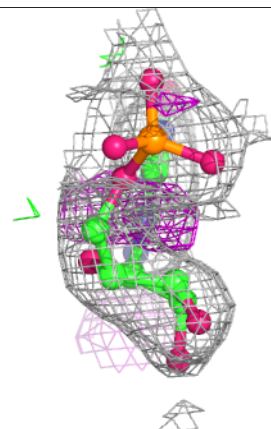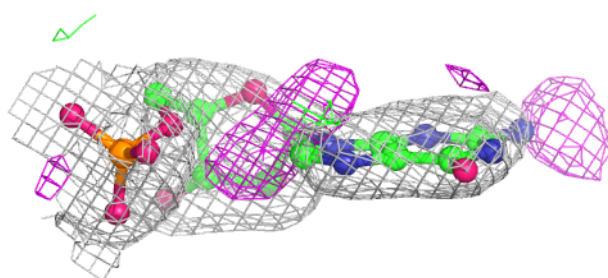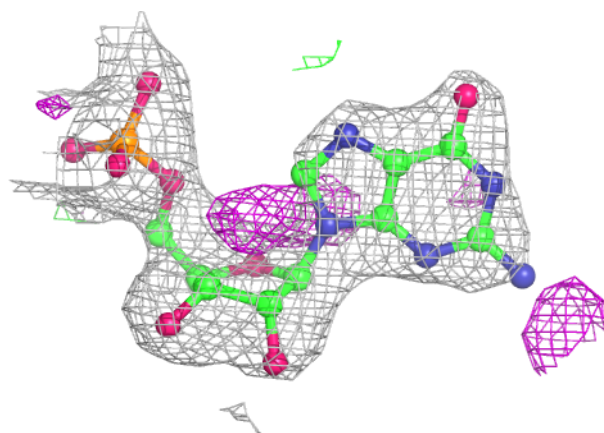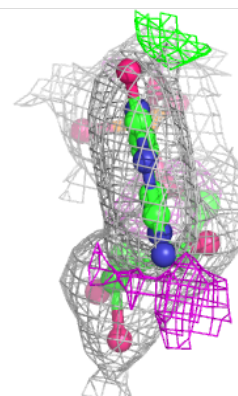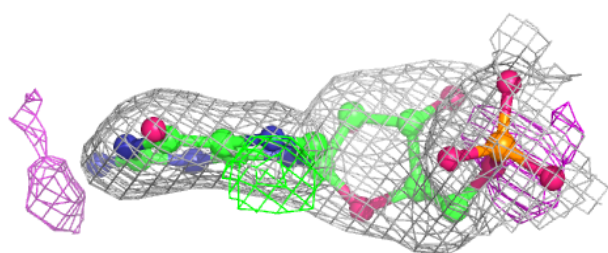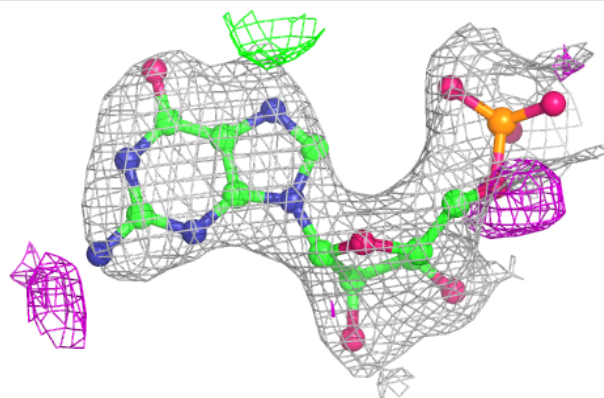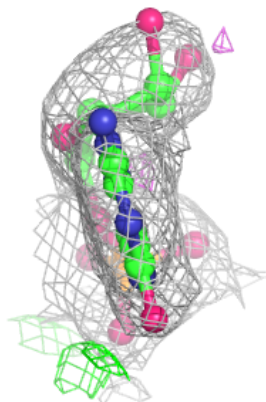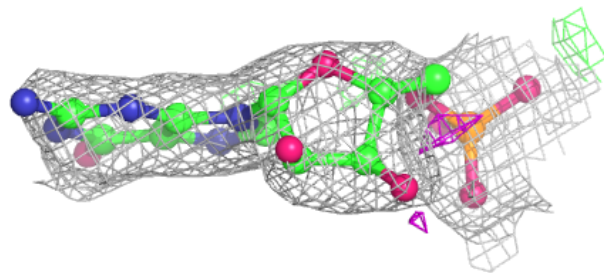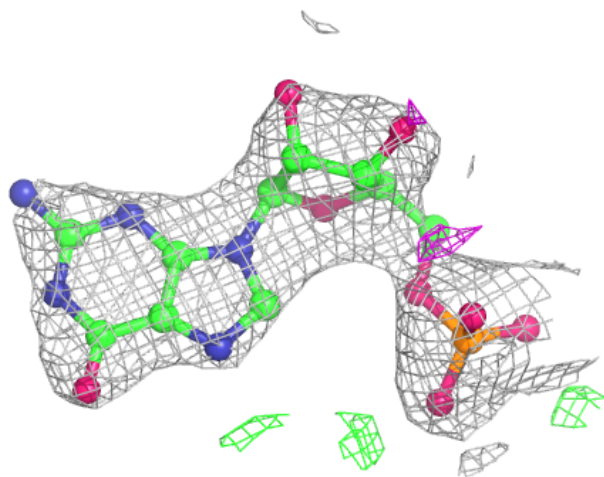and green (positive)
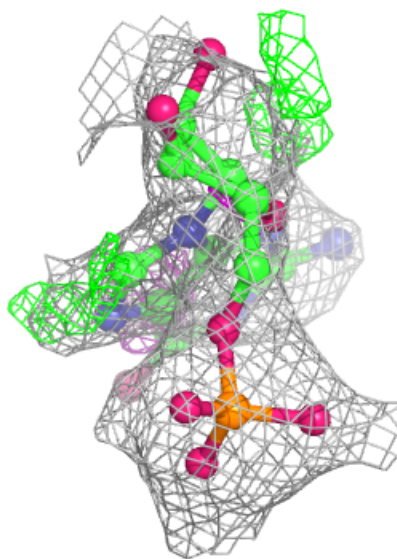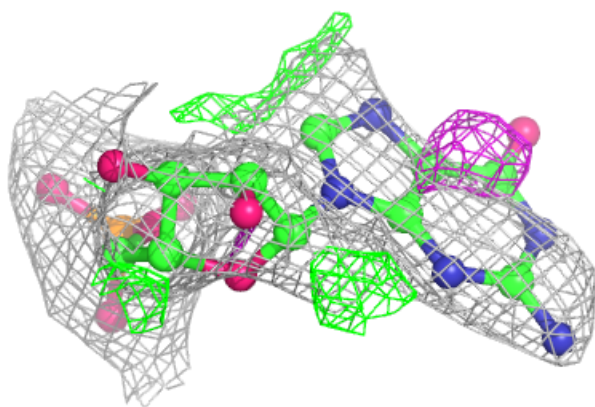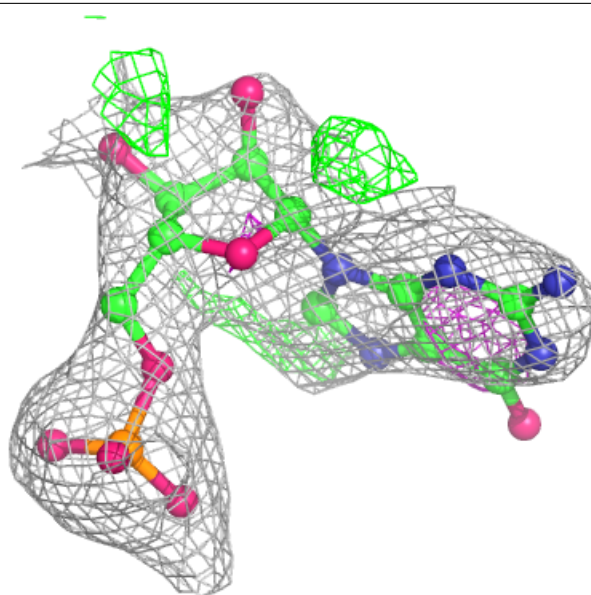
Electron density around 5GP A 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
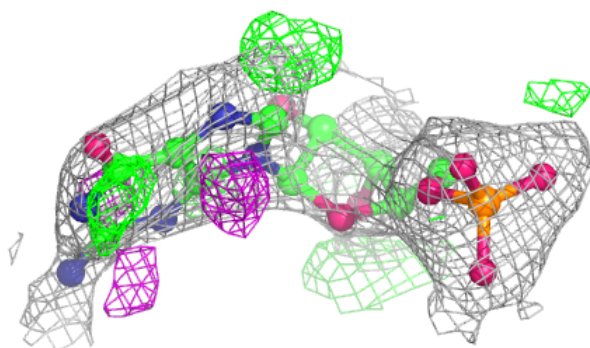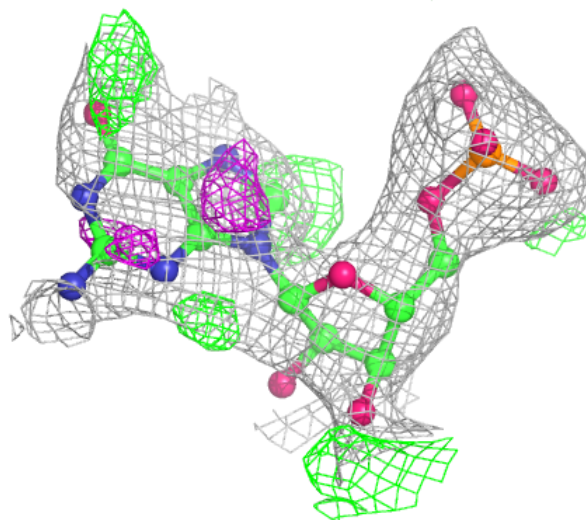
Electron density around 5GP I 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
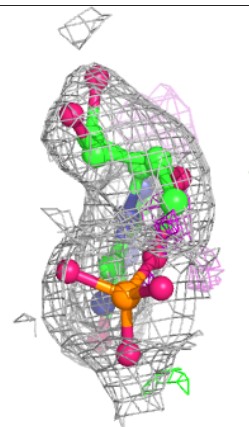and green (positive)
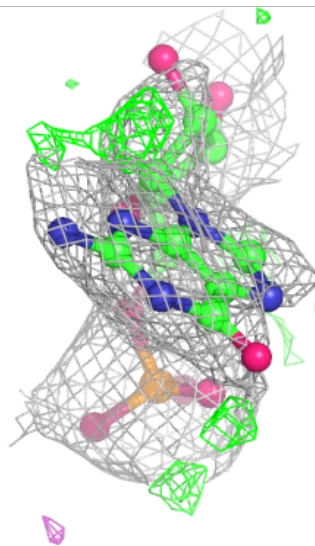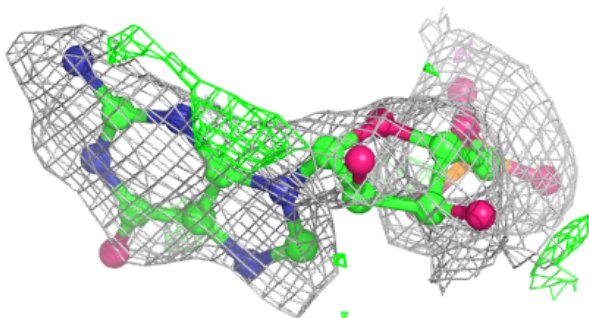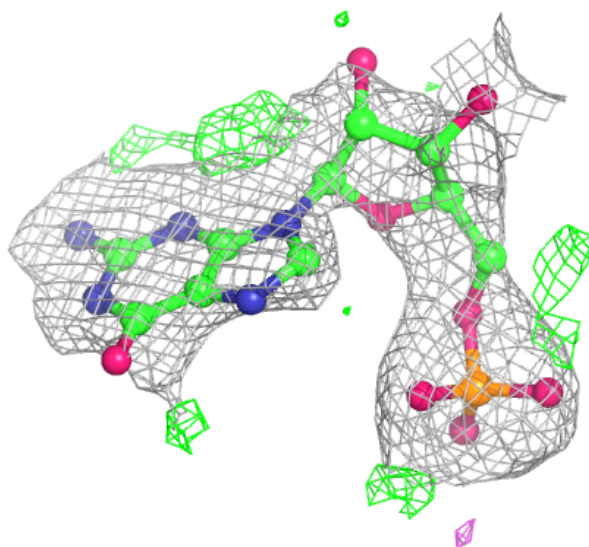
Electron density around 5GP E 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
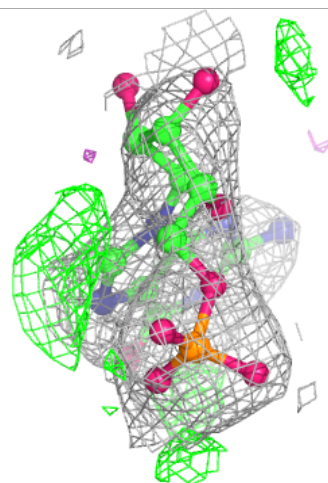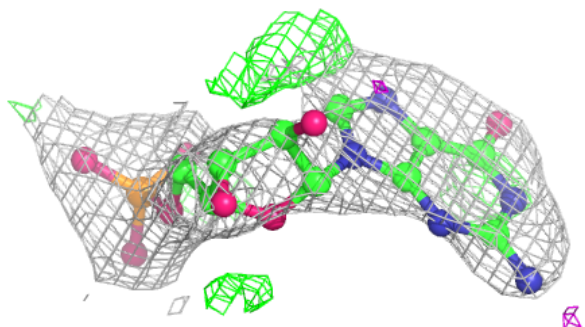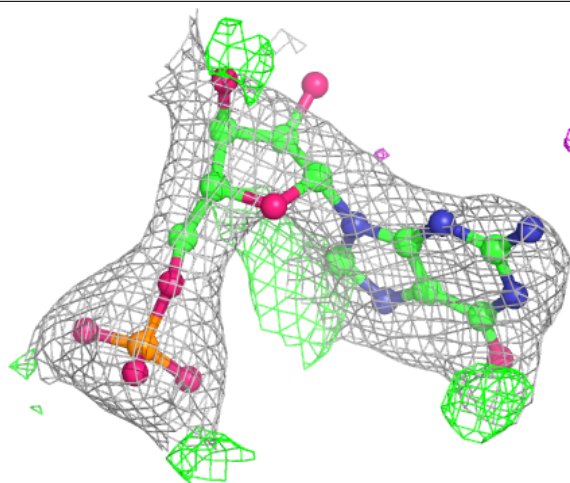
Electron density around 5GP K 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
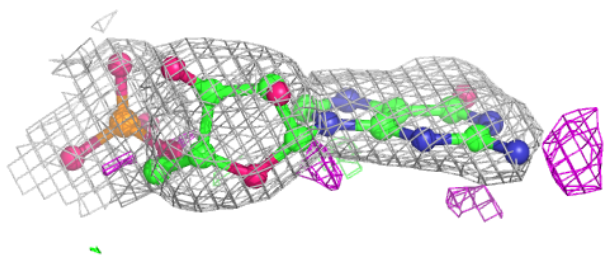and green (positive)
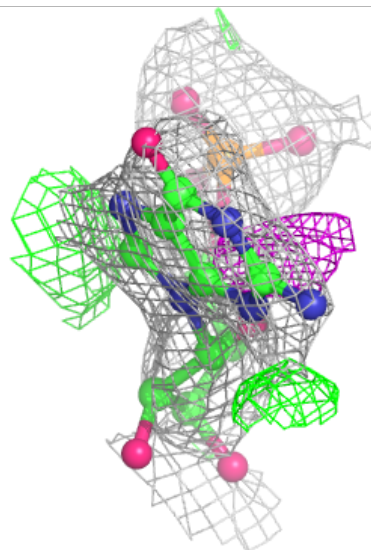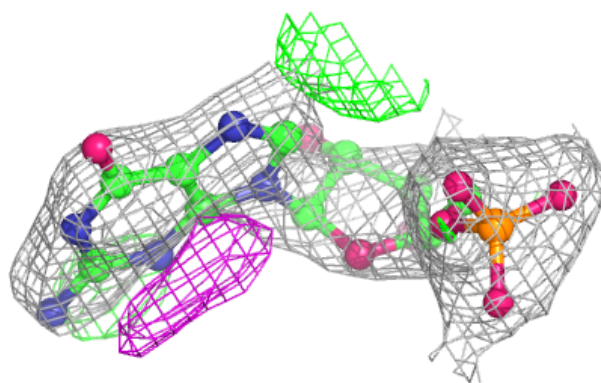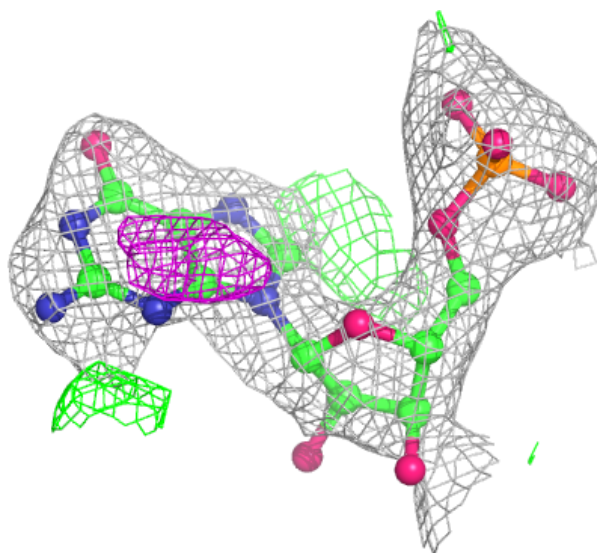
Electron density around 5GP I 302:

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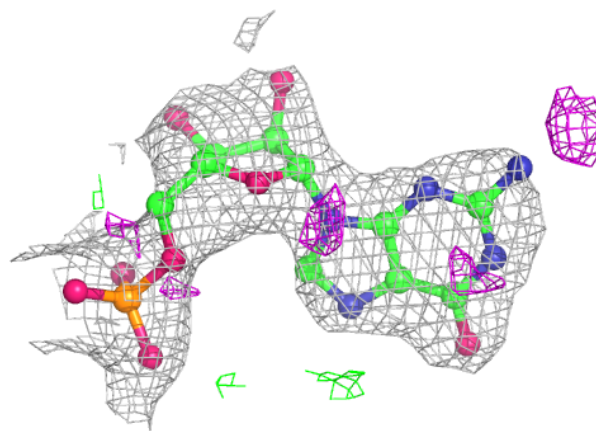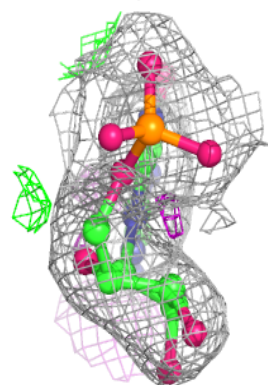and green (positive)

Electron density around 5GP K 301:

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 5GP I 301:

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

Electron density around 5GP C 301:

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

Electron density around 5GP K 302:

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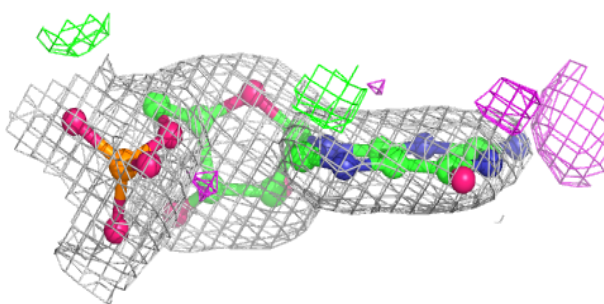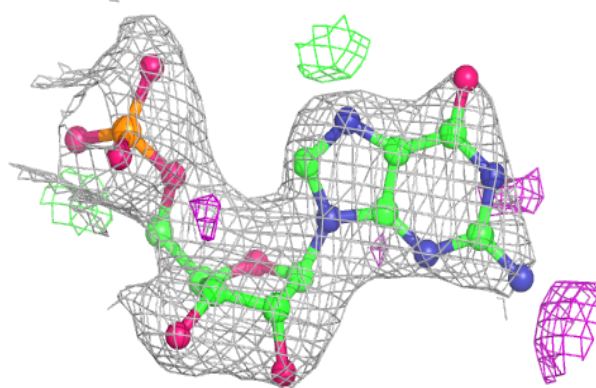mF_o-DF_c (at 3 rmsd) in purple (negative)
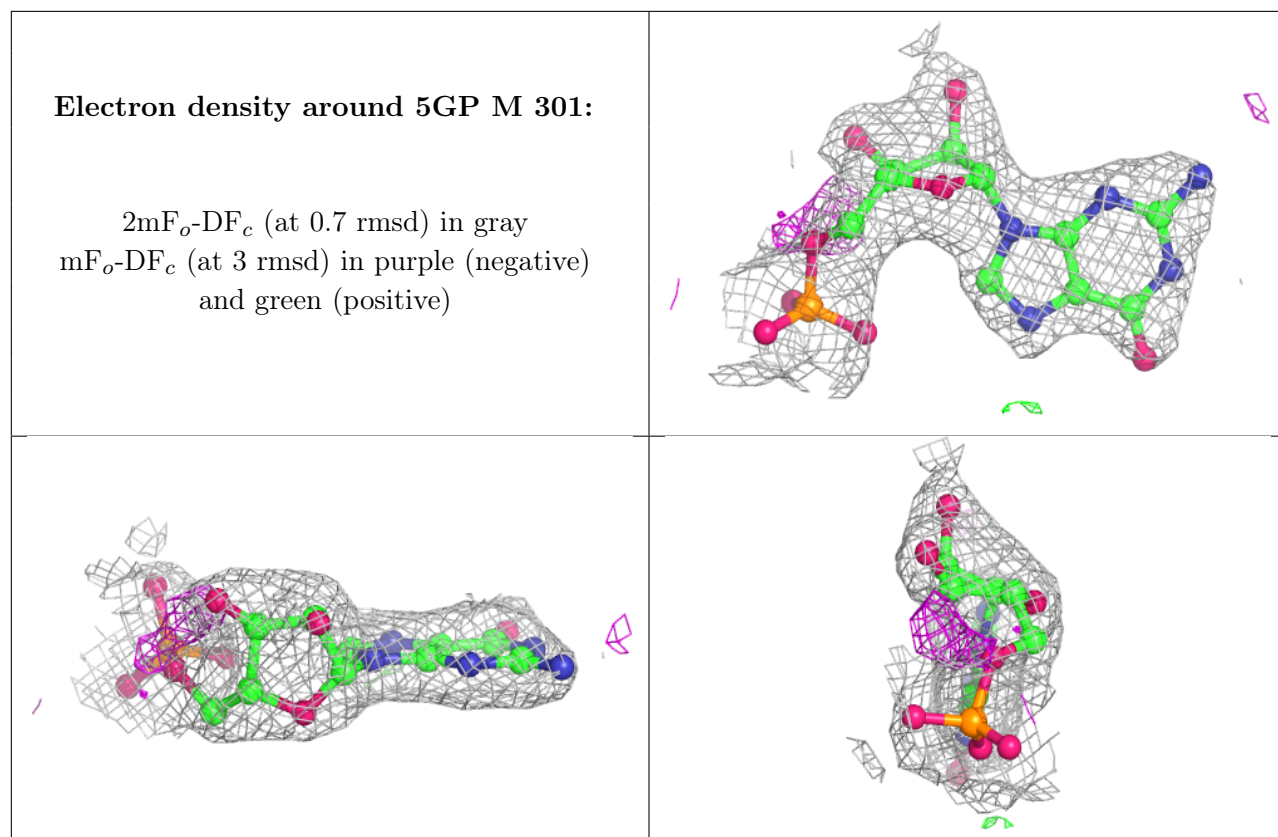and green (positive)

Electron density around 5GP E 301:

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

Electron density around 5GP A 301:

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

Electron density around 5GP M 301:

$2mF_o$-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 ⓘ

There are no such residues in this entry.