Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2025 – 02:17 PM JST

PDB ID	:	8YH1
Title	:	Crystal structure of Thermus thermophilus UMP kinase complexed with a phosphoryl group acceptor and donor.
Authors	:	Fukui, K.; Nishiwaki, A.; Nakagawa, N.; Kuramitsu, S.; Masui, R.
Deposited on	:	2024-02-27
Resolution	:	2.60 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:

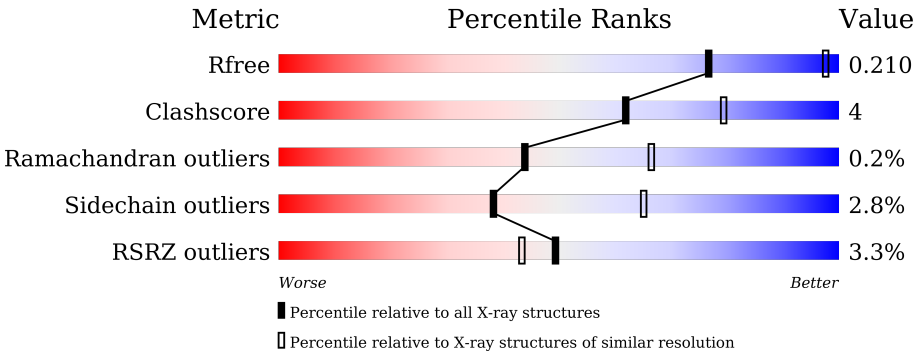
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 2.60 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	233	89% 9%
1	B	233	3% 87% 12%
1	C	233	2% 90% 9%
1	D	233	2% 91% 9%
1	E	233	3% 91% 9%
1	F	233	2% 90% 10%

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Mol	Chain	Length	Quality of chain
1	G	233	5% 90% 10%
1	H	233	5% 91% 9%
1	I	233	8% 89% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	G	304	-	-	X	-
6	MG	I	303	-	-	-	X

2 Entry composition (i)

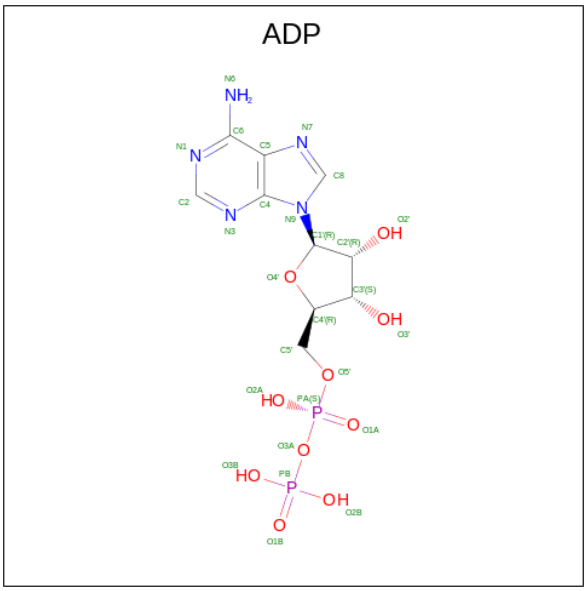
There are 8 unique types of molecules in this entry. The entry contains 16937 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridylate kinase.

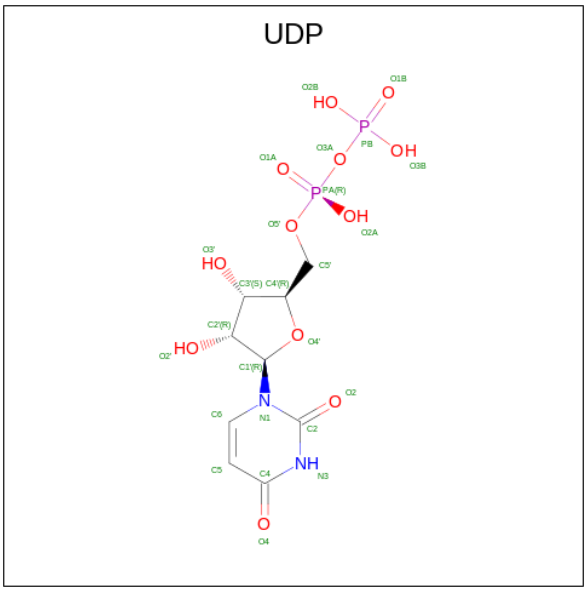
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1764	1123	305	328	8			
1	B	233	Total	C	N	O	S	0	0	0
			1766	1123	307	328	8			
1	C	233	Total	C	N	O	S	0	0	0
			1764	1123	307	326	8			
1	D	233	Total	C	N	O	S	0	0	0
			1749	1114	299	328	8			
1	E	233	Total	C	N	O	S	0	0	0
			1754	1114	304	328	8			
1	F	233	Total	C	N	O	S	0	0	0
			1754	1114	304	328	8			
1	G	233	Total	C	N	O	S	0	0	0
			1742	1109	300	325	8			
1	H	233	Total	C	N	O	S	0	0	0
			1752	1115	303	326	8			
1	I	231	Total	C	N	O	S	0	0	0
			1705	1082	295	320	8			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



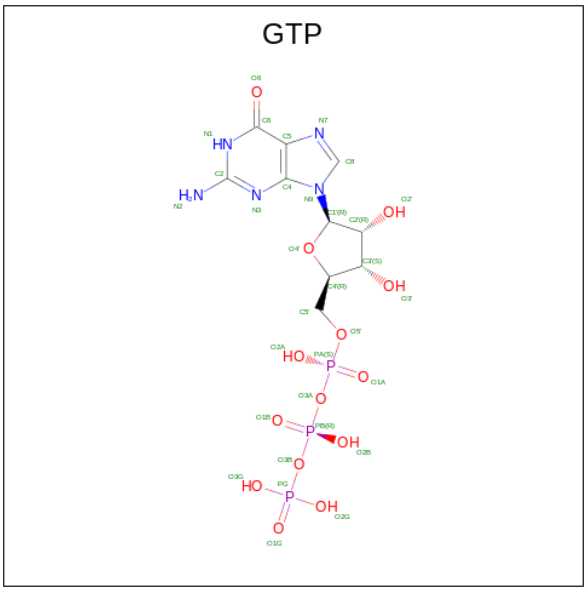
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



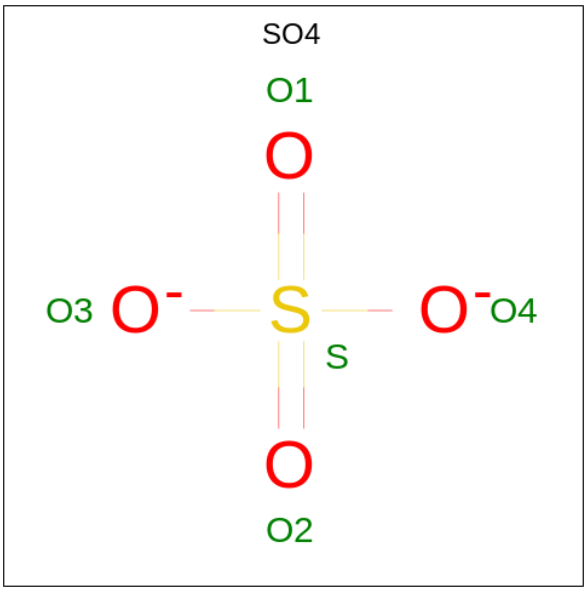
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	I	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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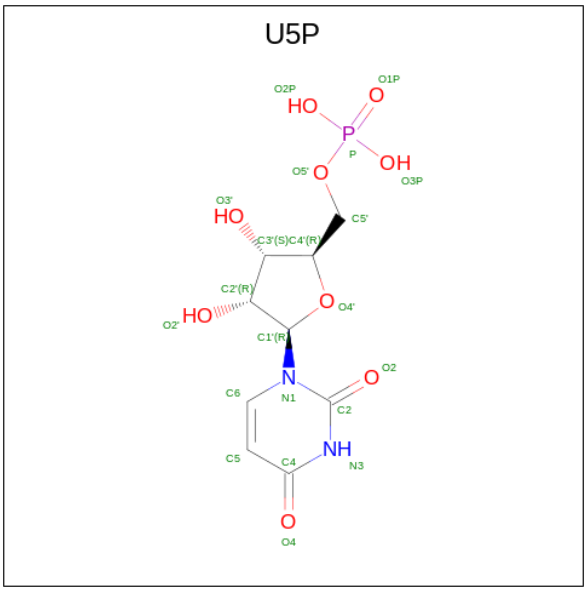
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	E	1	Total Mg 1 1	0	0
6	G	1	Total Mg 1 1	0	0
6	H	1	Total Mg 1 1	0	0
6	I	1	Total Mg 1 1	0	0

- Molecule 7 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C N O P 21 9 2 9 1	0	0
7	F	1	Total C N O P 21 9 2 9 1	0	0
7	G	1	Total C N O P 21 9 2 9 1	0	0
7	H	1	Total C N O P 21 9 2 9 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	91	Total O 91 91	0	0
8	B	78	Total O 78 78	0	0
8	C	60	Total O 60 60	0	0
8	D	53	Total O 53 53	0	0
8	E	47	Total O 47 47	0	0
8	F	35	Total O 35 35	0	0
8	G	32	Total O 32 32	0	0
8	H	37	Total O 37 37	0	0

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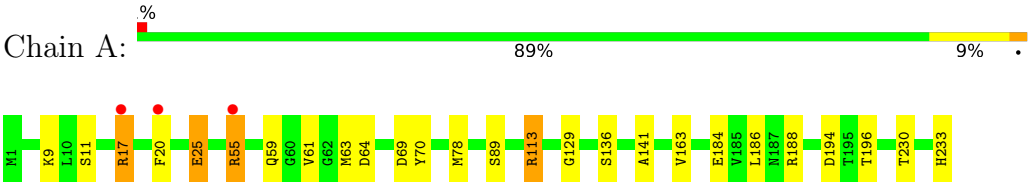
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	21	Total	O	0	0
			21	21		

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.

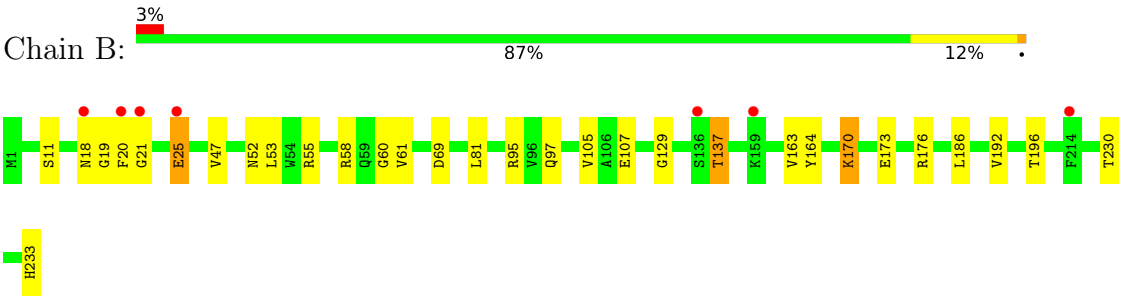
• Molecule 1: Uridylate kinase

Chain A:



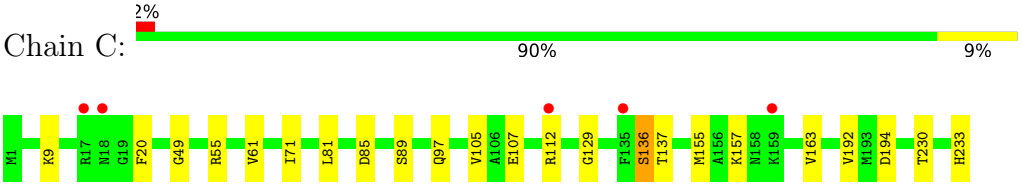
• Molecule 1: Uridylate kinase

Chain B:



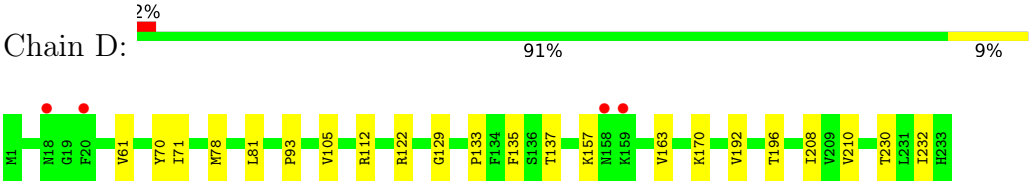
• Molecule 1: Uridylate kinase

Chain C:



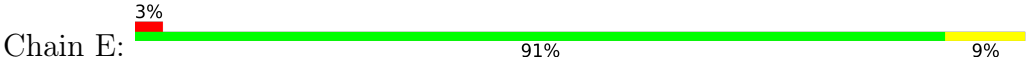
• Molecule 1: Uridylate kinase

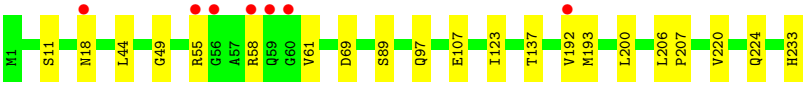
Chain D:



• Molecule 1: Uridylate kinase

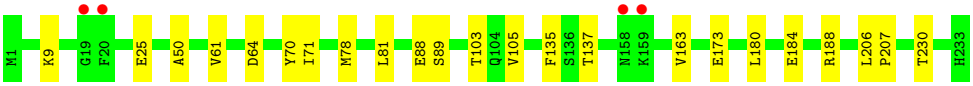
Chain E:





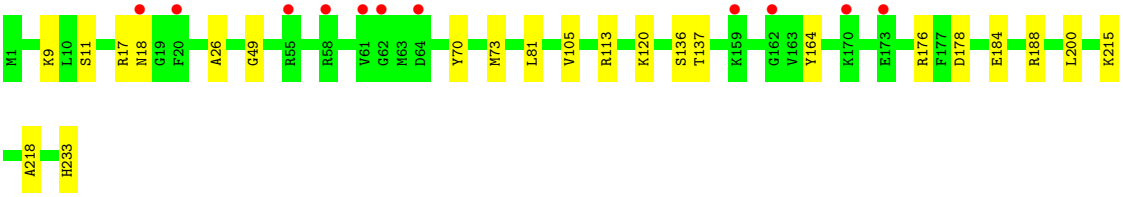
• Molecule 1: Uridylate kinase

Chain F:



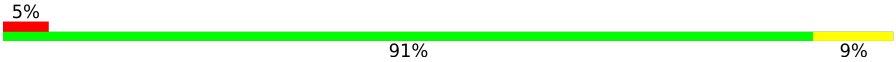
• Molecule 1: Uridylate kinase

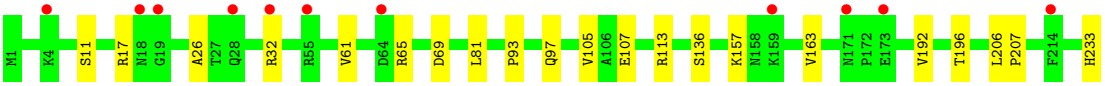
Chain G:



• Molecule 1: Uridylate kinase

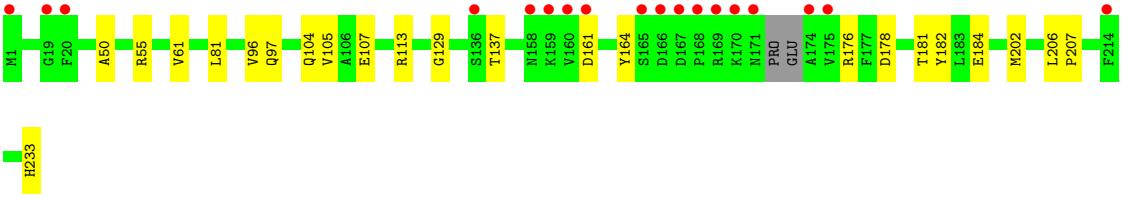
Chain H:





• Molecule 1: Uridylate kinase

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	150.22Å 232.20Å 284.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.32 – 2.60 26.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.32-2.60) 99.8 (26.32-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.15 (at 2.60Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.188 , 0.210 0.188 , 0.210	Depositor DCC
R_{free} test set	150054 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16937	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ADP, SO4, U5P, MG, UDP

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	0.26	0/1789	0.52	0/2422
1	B	0.29	0/1791	0.53	0/2425
1	C	0.25	0/1789	0.52	0/2422
1	D	0.25	0/1774	0.50	0/2406
1	E	0.26	0/1778	0.51	0/2409
1	F	0.25	0/1778	0.50	0/2409
1	G	0.26	0/1767	0.51	0/2398
1	H	0.26	0/1777	0.52	0/2409
1	I	0.24	0/1727	0.51	0/2345
All	All	0.26	0/15970	0.51	0/21645

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

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	1764	0	1817	16	0
1	B	1766	0	1817	22	0
1	C	1764	0	1817	14	0
1	D	1749	0	1779	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1754	0	1799	9	0
1	F	1754	0	1799	15	0
1	G	1742	0	1767	19	0
1	H	1752	0	1791	13	0
1	I	1705	0	1709	14	0
2	A	27	0	12	1	0
2	B	27	0	12	2	0
2	C	27	0	12	3	0
2	D	27	0	12	0	0
2	E	27	0	12	1	0
2	F	27	0	12	2	0
2	G	27	0	12	3	0
2	H	27	0	12	2	0
3	A	25	0	11	2	0
3	B	25	0	11	3	0
3	C	25	0	11	1	0
3	D	25	0	11	3	0
3	I	25	0	11	3	0
4	A	32	0	12	2	0
4	B	32	0	12	0	0
4	C	32	0	12	0	0
4	D	32	0	12	0	0
4	E	32	0	12	0	0
4	G	32	0	12	7	0
5	A	15	0	0	0	0
5	B	30	0	0	1	0
5	C	20	0	0	0	0
5	D	10	0	0	0	0
5	E	10	0	0	0	0
5	F	10	0	0	0	0
5	G	10	0	0	2	0
5	I	5	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
7	E	21	0	11	1	0
7	F	21	0	11	2	0
7	G	21	0	11	0	0
7	H	21	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	91	0	0	0	0
8	B	78	0	0	1	0
8	C	60	0	0	0	0
8	D	53	0	0	1	0
8	E	47	0	0	0	0
8	F	35	0	0	1	0
8	G	32	0	0	0	0
8	H	37	0	0	1	0
8	I	21	0	0	1	0
All	All	16937	0	16362	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (132) 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:G:120:LYS:NZ	4:G:303:GTP:PG	2.30	1.04
1:G:120:LYS:HZ2	4:G:303:GTP:PG	1.91	0.93
1:G:120:LYS:HZ1	4:G:303:GTP:PG	1.96	0.89
1:F:50:ALA:H	7:F:302:U5P:H5'1	1.43	0.80
1:D:112:ARG:NH1	8:D:401:HOH:O	2.25	0.69
1:H:17:ARG:HG2	1:H:26:ALA:HB2	1.74	0.69
1:F:9:LYS:NZ	2:F:301:ADP:O2B	2.27	0.67
1:I:129:GLY:HA3	3:I:301:UDP:C5	2.29	0.67
1:A:17:ARG:NH2	1:A:25:GLU:OE1	2.27	0.66
1:D:163:VAL:HG13	1:D:192:VAL:HG21	1.77	0.66
1:B:163:VAL:HG13	1:B:192:VAL:HG21	1.77	0.66
1:H:163:VAL:HG13	1:H:192:VAL:HG21	1.79	0.64
1:A:113:ARG:NH2	4:A:303:GTP:O1A	2.30	0.64
1:G:215:LYS:NZ	5:G:304:SO4:O4	2.31	0.64
1:B:95:ARG:NH1	5:B:306:SO4:O4	2.23	0.63
1:A:196:THR:HG23	1:B:196:THR:HG23	1.82	0.61
1:B:20:PHE:HE1	1:B:53:LEU:HD23	1.66	0.60
1:B:97:GLN:HG2	1:B:107:GLU:HG3	1.84	0.60
1:C:81:LEU:HD11	1:C:105:VAL:HG13	1.85	0.59
1:F:184:GLU:HG2	1:F:188:ARG:HH21	1.67	0.58
1:D:196:THR:HG23	1:H:196:THR:HG23	1.87	0.56
1:C:97:GLN:HG2	1:C:107:GLU:HG3	1.87	0.56
1:I:113:ARG:NH2	8:I:402:HOH:O	2.36	0.56
1:B:192:VAL:HG22	2:B:301:ADP:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:161:ASP:OD1	1:I:161:ASP:N	2.38	0.56
1:C:49:GLY:HA2	1:C:137:THR:HG21	1.88	0.55
1:D:81:LEU:HD11	1:D:105:VAL:HG13	1.89	0.55
1:F:206:LEU:HD12	1:F:207:PRO:HD2	1.89	0.54
1:C:192:VAL:HG22	2:C:301:ADP:C6	2.43	0.54
1:H:192:VAL:HG22	2:H:301:ADP:C6	2.42	0.54
1:B:20:PHE:CE1	1:B:53:LEU:HD23	2.43	0.54
1:C:9:LYS:NZ	2:C:301:ADP:O2B	2.42	0.53
1:G:215:LYS:NZ	5:G:304:SO4:S	2.82	0.53
1:I:181:THR:OG1	1:I:184:GLU:HG3	2.09	0.53
1:B:129:GLY:HA3	3:B:302:UDP:C5	2.43	0.52
1:B:129:GLY:HA3	3:B:302:UDP:C4	2.45	0.52
1:E:49:GLY:HA2	1:E:137:THR:HG21	1.91	0.52
1:I:50:ALA:HB3	3:I:301:UDP:H4'	1.92	0.52
1:G:120:LYS:NZ	4:G:303:GTP:O2G	2.29	0.52
1:D:71:ILE:HG23	1:F:78:MET:HG2	1.93	0.51
1:D:208:ILE:HB	1:D:232:ILE:HB	1.93	0.51
1:F:137:THR:OG1	7:F:302:U5P:H5'2	2.10	0.51
1:A:20:PHE:HB2	1:C:20:PHE:CE2	2.45	0.51
1:C:136:SER:HB3	1:C:194:ASP:OD2	2.11	0.50
1:F:81:LEU:HD11	1:F:105:VAL:HG13	1.93	0.50
1:H:107:GLU:OE2	1:H:113:ARG:NE	2.45	0.50
1:F:25:GLU:H	1:F:25:GLU:CD	2.16	0.49
1:I:104:GLN:OE1	1:I:104:GLN:N	2.31	0.49
2:G:301:ADP:H2'	2:G:301:ADP:N3	2.28	0.49
1:H:65:ARG:NH2	8:H:401:HOH:O	2.47	0.48
1:H:17:ARG:HH11	1:H:17:ARG:HG3	1.79	0.48
1:B:18:ASN:O	1:B:20:PHE:N	2.43	0.47
1:C:163:VAL:HG13	1:C:192:VAL:HG21	1.95	0.47
4:A:303:GTP:O1B	4:A:303:GTP:H3'	2.14	0.47
1:B:164:TYR:CE2	1:B:176:ARG:HB2	2.49	0.47
1:C:157:LYS:HA	1:C:157:LYS:HD3	1.70	0.47
1:D:78:MET:HG2	1:F:71:ILE:HG23	1.96	0.47
1:B:81:LEU:HD11	1:B:105:VAL:HG13	1.95	0.47
1:B:163:VAL:HB	1:B:230:THR:HG21	1.96	0.47
1:D:137:THR:OG1	3:D:302:UDP:O1A	2.30	0.47
1:D:70:TYR:HB3	1:F:105:VAL:HG22	1.97	0.47
1:H:69:ASP:HB3	7:H:302:U5P:O2	2.15	0.47
1:E:69:ASP:HB3	7:E:302:U5P:O2	2.15	0.46
1:G:113:ARG:HH22	4:G:303:GTP:PB	2.38	0.46
1:I:81:LEU:HD11	1:I:105:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:GLY:HA2	1:G:137:THR:HG21	1.98	0.46
1:I:129:GLY:HA3	3:I:301:UDP:C4	2.50	0.46
1:B:60:GLY:HA2	8:B:433:HOH:O	2.16	0.46
1:D:163:VAL:HB	1:D:230:THR:HG21	1.98	0.46
1:E:192:VAL:HG23	1:E:193:MET:HG2	1.98	0.45
1:A:78:MET:HG2	1:C:71:ILE:HG23	1.99	0.45
1:G:11:SER:HB2	2:G:301:ADP:O3B	2.15	0.45
1:A:69:ASP:HB3	3:A:302:UDP:O2	2.16	0.45
1:G:9:LYS:NZ	2:G:301:ADP:O2B	2.50	0.45
1:I:97:GLN:HG2	1:I:107:GLU:HG3	1.98	0.45
1:I:206:LEU:HD12	1:I:207:PRO:HD2	1.99	0.45
1:D:129:GLY:HA3	3:D:302:UDP:C4	2.52	0.45
1:G:215:LYS:HG2	1:G:218:ALA:HB2	1.98	0.45
1:E:97:GLN:HG2	1:E:107:GLU:HG3	1.99	0.44
1:B:69:ASP:HB3	3:B:302:UDP:O2	2.16	0.44
1:A:184:GLU:O	1:A:188:ARG:HG3	2.18	0.44
1:H:206:LEU:HD12	1:H:207:PRO:HD2	2.00	0.44
1:B:11:SER:HB2	2:B:301:ADP:O3B	2.17	0.44
1:E:44:LEU:HB3	1:E:123:ILE:HG12	1.99	0.44
1:G:81:LEU:HD11	1:G:105:VAL:HG13	1.99	0.44
1:B:20:PHE:CG	1:B:21:GLY:N	2.86	0.43
1:A:129:GLY:HA3	3:A:302:UDP:C5	2.53	0.43
1:B:25:GLU:H	1:B:25:GLU:CD	2.21	0.43
1:H:81:LEU:HD11	1:H:105:VAL:HG13	2.01	0.43
1:B:20:PHE:CD1	1:B:52:ASN:O	2.72	0.43
1:D:163:VAL:HG22	1:D:192:VAL:HG11	2.00	0.43
1:A:70:TYR:HB3	1:C:105:VAL:HG22	2.00	0.43
1:A:136:SER:HB3	1:A:194:ASP:OD2	2.18	0.43
1:H:97:GLN:HA	1:H:107:GLU:O	2.19	0.43
1:F:135:PHE:HE1	1:G:200:LEU:HD11	1.84	0.43
1:B:47:VAL:HG12	1:B:137:THR:HG22	2.01	0.42
1:C:163:VAL:HB	1:C:230:THR:HG21	2.01	0.42
3:D:302:UDP:O2	3:D:302:UDP:H2'	2.18	0.42
1:E:206:LEU:HD12	1:E:207:PRO:HD2	2.01	0.42
1:F:163:VAL:HB	1:F:230:THR:HG21	2.01	0.42
1:F:180:LEU:HD22	1:F:184:GLU:HB3	2.01	0.42
1:D:133:PRO:C	1:D:135:PHE:H	2.23	0.42
1:D:157:LYS:HG2	1:D:210:VAL:HG13	2.01	0.42
1:F:88:GLU:HG2	8:F:435:HOH:O	2.19	0.42
1:E:11:SER:HB2	2:E:301:ADP:O3B	2.19	0.42
2:F:301:ADP:N3	2:F:301:ADP:H2'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:TYR:CG	1:I:202:MET:HB2	2.54	0.42
1:D:170:LYS:HB3	1:D:170:LYS:HE2	1.90	0.42
1:G:184:GLU:O	1:G:188:ARG:HG3	2.20	0.41
2:C:301:ADP:N3	2:C:301:ADP:H2'	2.35	0.41
1:G:164:TYR:CZ	1:G:176:ARG:HB2	2.56	0.41
1:H:11:SER:HB2	2:H:301:ADP:O3B	2.20	0.41
1:H:157:LYS:HD2	1:H:157:LYS:HA	1.67	0.41
1:D:93:PRO:HB2	1:D:122:ARG:HG2	2.02	0.41
1:I:164:TYR:CZ	1:I:176:ARG:HB2	2.55	0.41
1:A:11:SER:HB2	2:A:301:ADP:O3B	2.20	0.41
1:A:63:MET:HA	1:C:85:ASP:OD2	2.21	0.41
1:G:113:ARG:NH2	4:G:303:GTP:O3B	2.54	0.41
1:G:120:LYS:NZ	4:G:303:GTP:O3G	2.43	0.41
1:B:58:ARG:H	1:B:58:ARG:HG3	1.69	0.41
1:C:129:GLY:HA3	3:C:302:UDP:C5	2.56	0.41
1:G:70:TYR:HA	1:G:73:MET:HE3	2.03	0.41
1:A:55:ARG:HG2	1:A:59:GLN:OE1	2.20	0.41
1:D:105:VAL:HG22	1:F:70:TYR:HB3	2.02	0.41
1:A:9:LYS:HG3	1:A:141:ALA:HB2	2.04	0.40
1:E:200:LEU:HD12	1:E:200:LEU:HA	1.89	0.40
1:G:17:ARG:HD2	1:G:26:ALA:HB2	2.03	0.40
1:I:181:THR:HA	1:I:233:HIS:O	2.22	0.40
1:E:220:VAL:O	1:E:224:GLN:HG2	2.21	0.40
1:A:186:LEU:HD13	1:B:186:LEU:HD13	2.03	0.40
1:A:163:VAL:HB	1:A:230:THR:HG21	2.04	0.40
1:I:96:VAL:O	1:I:107:GLU:HG2	2.22	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	231/233 (99%)	229 (99%)	2 (1%)	0	100	100
1	B	231/233 (99%)	224 (97%)	5 (2%)	2 (1%)	14	31
1	C	231/233 (99%)	229 (99%)	2 (1%)	0	100	100
1	D	231/233 (99%)	225 (97%)	6 (3%)	0	100	100
1	E	231/233 (99%)	225 (97%)	5 (2%)	1 (0%)	30	52
1	F	231/233 (99%)	225 (97%)	6 (3%)	0	100	100
1	G	231/233 (99%)	224 (97%)	6 (3%)	1 (0%)	30	52
1	H	231/233 (99%)	226 (98%)	5 (2%)	0	100	100
1	I	227/233 (97%)	220 (97%)	6 (3%)	1 (0%)	30	52
All	All	2075/2097 (99%)	2027 (98%)	43 (2%)	5 (0%)	44	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	137	THR
1	G	18	ASN
1	B	170	LYS
1	E	18	ASN
1	B	19	GLY

5.3.2 Protein sidechains (i)

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	181/183 (99%)	173 (96%)	8 (4%)	24	48
1	B	181/183 (99%)	174 (96%)	7 (4%)	27	53
1	C	180/183 (98%)	173 (96%)	7 (4%)	27	53
1	D	177/183 (97%)	176 (99%)	1 (1%)	84	94
1	E	179/183 (98%)	174 (97%)	5 (3%)	38	65
1	F	179/183 (98%)	174 (97%)	5 (3%)	38	65
1	G	175/183 (96%)	172 (98%)	3 (2%)	56	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	178/183 (97%)	173 (97%)	5 (3%)	38 65
1	I	168/183 (92%)	165 (98%)	3 (2%)	54 77
All	All	1598/1647 (97%)	1554 (97%)	44 (3%)	38 65

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	25	GLU
1	A	55	ARG
1	A	61	VAL
1	A	64	ASP
1	A	89	SER
1	A	113	ARG
1	A	233	HIS
1	B	25	GLU
1	B	55	ARG
1	B	61	VAL
1	B	137	THR
1	B	170	LYS
1	B	173	GLU
1	B	233	HIS
1	C	55	ARG
1	C	61	VAL
1	C	89	SER
1	C	112	ARG
1	C	136	SER
1	C	155	MET
1	C	233	HIS
1	D	61	VAL
1	E	55	ARG
1	E	58	ARG
1	E	61	VAL
1	E	89	SER
1	E	233	HIS
1	F	61	VAL
1	F	64	ASP
1	F	89	SER
1	F	103	THR
1	F	173	GLU
1	G	136	SER

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Mol	Chain	Res	Type
1	G	178	ASP
1	G	233	HIS
1	H	32	ARG
1	H	61	VAL
1	H	93	PRO
1	H	136	SER
1	H	233	HIS
1	I	55	ARG
1	I	61	VAL
1	I	178	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	224	GLN
1	B	18	ASN
1	B	28	GLN
1	D	18	ASN
1	D	28	GLN
1	I	18	ASN

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 51 ligands modelled in this entry, 6 are monoatomic - leaving 45 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	$\#\|Z\| > 2$
4	GTP	B	303	-	26,34,34	1.12	2 (7%)	32,54,54	1.61	6 (18%)
3	UDP	I	301	-	24,26,26	0.48	0	37,40,40	0.51	0
5	SO4	F	304	-	4,4,4	0.13	0	6,6,6	0.06	0
2	ADP	B	301	-	24,29,29	0.93	1 (4%)	29,45,45	1.46	4 (13%)
3	UDP	D	302	-	24,26,26	0.43	0	37,40,40	0.69	1 (2%)
5	SO4	G	304	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	C	306	-	4,4,4	0.15	0	6,6,6	0.05	0
2	ADP	F	301	-	24,29,29	0.95	1 (4%)	29,45,45	1.39	4 (13%)
5	SO4	B	304	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	309	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	E	304	-	4,4,4	0.14	0	6,6,6	0.05	0
2	ADP	G	301	6	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)
4	GTP	E	303	-	26,34,34	1.12	2 (7%)	32,54,54	1.50	7 (21%)
7	U5P	H	302	6	22,22,22	0.42	0	33,33,33	0.38	0
5	SO4	B	306	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	B	308	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	C	307	-	4,4,4	0.14	0	6,6,6	0.09	0
3	UDP	B	302	-	24,26,26	0.50	0	37,40,40	0.48	0
5	SO4	B	307	-	4,4,4	0.13	0	6,6,6	0.07	0
4	GTP	C	303	-	26,34,34	1.10	2 (7%)	32,54,54	1.38	5 (15%)
5	SO4	A	305	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	E	305	-	4,4,4	0.12	0	6,6,6	0.11	0
7	U5P	F	302	-	22,22,22	0.45	0	33,33,33	0.97	1 (3%)
4	GTP	D	303	-	26,34,34	1.10	2 (7%)	32,54,54	1.42	5 (15%)
5	SO4	B	305	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	D	304	-	4,4,4	0.13	0	6,6,6	0.06	0
7	U5P	G	302	6	22,22,22	0.42	0	33,33,33	0.41	0
2	ADP	D	301	-	24,29,29	0.98	1 (4%)	29,45,45	1.35	4 (13%)
2	ADP	C	301	6	24,29,29	0.94	1 (4%)	29,45,45	1.47	4 (13%)
5	SO4	C	305	-	4,4,4	0.14	0	6,6,6	0.04	0
3	UDP	C	302	6	24,26,26	0.48	0	37,40,40	0.57	0
2	ADP	H	301	6	24,29,29	0.96	1 (4%)	29,45,45	1.43	4 (13%)
5	SO4	D	305	-	4,4,4	0.13	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	I	302	-	4,4,4	0.14	0	6,6,6	0.05	0
2	ADP	A	301	6	24,29,29	0.93	1 (4%)	29,45,45	1.43	4 (13%)
4	GTP	G	303	-	26,34,34	0.99	2 (7%)	32,54,54	1.02	2 (6%)
4	GTP	A	303	-	26,34,34	1.10	2 (7%)	32,54,54	1.42	6 (18%)
5	SO4	A	304	-	4,4,4	0.13	0	6,6,6	0.11	0
5	SO4	A	306	-	4,4,4	0.14	0	6,6,6	0.04	0
2	ADP	E	301	6	24,29,29	0.94	1 (4%)	29,45,45	1.39	4 (13%)
3	UDP	A	302	-	24,26,26	0.52	0	37,40,40	0.47	0
5	SO4	G	305	-	4,4,4	0.13	0	6,6,6	0.06	0
5	SO4	F	303	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	304	-	4,4,4	0.13	0	6,6,6	0.05	0
7	U5P	E	302	6	22,22,22	0.42	0	33,33,33	0.37	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	GTP	B	303	-	-	5/18/38/38	0/3/3/3
3	UDP	I	301	-	-	6/16/32/32	0/2/2/2
2	ADP	B	301	-	-	4/12/32/32	0/3/3/3
3	UDP	D	302	-	-	6/16/32/32	0/2/2/2
2	ADP	F	301	-	-	3/12/32/32	0/3/3/3
2	ADP	G	301	6	-	5/12/32/32	0/3/3/3
4	GTP	E	303	-	-	9/18/38/38	0/3/3/3
7	U5P	H	302	6	-	5/10/26/26	0/2/2/2
3	UDP	B	302	-	-	9/16/32/32	0/2/2/2
4	GTP	C	303	-	-	6/18/38/38	0/3/3/3
7	U5P	F	302	-	-	4/10/26/26	0/2/2/2
4	GTP	D	303	-	-	6/18/38/38	0/3/3/3
7	U5P	G	302	6	-	1/10/26/26	0/2/2/2
2	ADP	D	301	-	-	4/12/32/32	0/3/3/3
2	ADP	C	301	6	-	4/12/32/32	0/3/3/3
3	UDP	C	302	6	-	3/16/32/32	0/2/2/2
2	ADP	H	301	6	-	6/12/32/32	0/3/3/3
2	ADP	A	301	6	-	3/12/32/32	0/3/3/3
4	GTP	G	303	-	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	303	-	-	2/18/38/38	0/3/3/3
2	ADP	E	301	6	-	3/12/32/32	0/3/3/3
3	UDP	A	302	-	-	7/16/32/32	0/2/2/2
7	U5P	E	302	6	-	5/10/26/26	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	GTP	C5-C6	-4.03	1.39	1.47
4	E	303	GTP	C5-C6	-3.99	1.39	1.47
4	C	303	GTP	C5-C6	-3.96	1.39	1.47
4	D	303	GTP	C5-C6	-3.90	1.39	1.47
4	A	303	GTP	C5-C6	-3.90	1.39	1.47
4	G	303	GTP	C5-C6	-2.64	1.42	1.47
2	H	301	ADP	C5-C4	2.62	1.47	1.40
2	C	301	ADP	C5-C4	2.61	1.47	1.40
2	G	301	ADP	C5-C4	2.60	1.47	1.40
2	F	301	ADP	C5-C4	2.59	1.47	1.40
2	E	301	ADP	C5-C4	2.59	1.47	1.40
2	A	301	ADP	C5-C4	2.57	1.47	1.40
2	D	301	ADP	C5-C4	2.55	1.47	1.40
2	B	301	ADP	C5-C4	2.54	1.47	1.40
4	A	303	GTP	C2-N3	2.24	1.38	1.33
4	C	303	GTP	C2-N3	2.23	1.38	1.33
4	B	303	GTP	C2-N3	2.21	1.38	1.33
4	D	303	GTP	C2-N3	2.19	1.38	1.33
4	E	303	GTP	C2-N3	2.18	1.38	1.33
4	G	303	GTP	C8-N7	-2.11	1.31	1.35

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	303	GTP	PB-O3B-PG	-4.36	117.87	132.83
2	B	301	ADP	PA-O3A-PB	-4.00	119.09	132.83
2	C	301	ADP	PA-O3A-PB	-3.98	119.18	132.83
2	G	301	ADP	PA-O3A-PB	-3.92	119.37	132.83
2	A	301	ADP	PA-O3A-PB	-3.64	120.34	132.83
7	F	302	U5P	O3P-P-O5'	-3.60	97.16	106.73
2	H	301	ADP	PA-O3A-PB	-3.59	120.50	132.83
2	F	301	ADP	PA-O3A-PB	-3.40	121.17	132.83
2	G	301	ADP	C3'-C2'-C1'	3.32	105.98	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	ADP	PA-O3A-PB	-3.30	121.50	132.83
4	D	303	GTP	PB-O3B-PG	-3.27	121.59	132.83
2	E	301	ADP	N3-C2-N1	-3.27	123.56	128.68
4	E	303	GTP	PB-O3B-PG	-3.23	121.73	132.83
2	G	301	ADP	N3-C2-N1	-3.21	123.66	128.68
2	B	301	ADP	N3-C2-N1	-3.21	123.66	128.68
4	A	303	GTP	C5-C6-N1	3.21	119.61	113.95
2	A	301	ADP	N3-C2-N1	-3.19	123.70	128.68
2	H	301	ADP	N3-C2-N1	-3.19	123.70	128.68
2	H	301	ADP	C3'-C2'-C1'	3.18	105.77	100.98
2	D	301	ADP	N3-C2-N1	-3.17	123.72	128.68
4	B	303	GTP	C5-C6-N1	3.17	119.55	113.95
4	E	303	GTP	C5-C6-N1	3.17	119.55	113.95
2	C	301	ADP	N3-C2-N1	-3.16	123.75	128.68
4	C	303	GTP	C5-C6-N1	3.15	119.51	113.95
2	C	301	ADP	C3'-C2'-C1'	3.13	105.69	100.98
4	D	303	GTP	C5-C6-N1	3.13	119.47	113.95
2	D	301	ADP	C3'-C2'-C1'	3.09	105.64	100.98
2	F	301	ADP	C3'-C2'-C1'	3.09	105.63	100.98
2	F	301	ADP	N3-C2-N1	-3.08	123.86	128.68
2	B	301	ADP	C3'-C2'-C1'	3.05	105.57	100.98
4	E	303	GTP	C8-N7-C5	3.02	108.74	102.99
4	C	303	GTP	PB-O3B-PG	-3.00	122.53	132.83
4	B	303	GTP	C8-N7-C5	3.00	108.70	102.99
2	A	301	ADP	C3'-C2'-C1'	2.98	105.47	100.98
4	D	303	GTP	C8-N7-C5	2.96	108.64	102.99
4	C	303	GTP	C8-N7-C5	2.95	108.61	102.99
4	A	303	GTP	C8-N7-C5	2.94	108.59	102.99
2	E	301	ADP	C3'-C2'-C1'	2.90	105.35	100.98
2	D	301	ADP	PA-O3A-PB	-2.88	122.93	132.83
4	A	303	GTP	PB-O3B-PG	-2.87	122.98	132.83
4	B	303	GTP	C2-N1-C6	-2.84	119.87	125.10
4	A	303	GTP	C2-N1-C6	-2.83	119.88	125.10
4	C	303	GTP	C2-N1-C6	-2.83	119.89	125.10
4	E	303	GTP	C2-N1-C6	-2.82	119.90	125.10
4	B	303	GTP	PA-O3A-PB	-2.80	123.22	132.83
4	E	303	GTP	PA-O3A-PB	-2.79	123.26	132.83
4	D	303	GTP	C2-N1-C6	-2.79	119.96	125.10
4	G	303	GTP	O2G-PG-O3B	-2.60	95.92	104.64
4	A	303	GTP	PA-O3A-PB	-2.57	124.01	132.83
2	H	301	ADP	C4-C5-N7	-2.53	106.77	109.40
2	D	301	ADP	C4-C5-N7	-2.52	106.77	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	ADP	C4-C5-N7	-2.42	106.88	109.40
2	G	301	ADP	C4-C5-N7	-2.40	106.90	109.40
2	E	301	ADP	C4-C5-N7	-2.39	106.91	109.40
2	C	301	ADP	C4-C5-N7	-2.36	106.94	109.40
4	G	303	GTP	O3G-PG-O2G	2.36	116.64	107.64
2	B	301	ADP	C4-C5-N7	-2.32	106.98	109.40
3	D	302	UDP	O3B-PB-O3A	2.24	112.14	104.64
4	B	303	GTP	O6-C6-C5	-2.18	120.11	124.37
4	E	303	GTP	O6-C6-C5	-2.16	120.16	124.37
4	A	303	GTP	O6-C6-C5	-2.16	120.16	124.37
4	C	303	GTP	O6-C6-C5	-2.14	120.19	124.37
4	E	303	GTP	C3'-C2'-C1'	2.12	104.17	100.98
4	D	303	GTP	O6-C6-C5	-2.11	120.25	124.37
2	A	301	ADP	C4-C5-N7	-2.10	107.21	109.40

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	ADP	C5'-O5'-PA-O1A
2	C	301	ADP	C5'-O5'-PA-O3A
2	D	301	ADP	C5'-O5'-PA-O3A
2	D	301	ADP	C3'-C4'-C5'-O5'
2	E	301	ADP	PA-O3A-PB-O2B
2	E	301	ADP	PA-O3A-PB-O3B
2	F	301	ADP	C5'-O5'-PA-O2A
2	F	301	ADP	C5'-O5'-PA-O3A
2	G	301	ADP	C5'-O5'-PA-O1A
2	G	301	ADP	C5'-O5'-PA-O3A
2	G	301	ADP	C3'-C4'-C5'-O5'
2	H	301	ADP	C5'-O5'-PA-O1A
3	A	302	UDP	C5'-O5'-PA-O1A
3	A	302	UDP	C5'-O5'-PA-O2A
3	B	302	UDP	C5'-O5'-PA-O1A
3	B	302	UDP	C5'-O5'-PA-O2A
3	D	302	UDP	C4'-C5'-O5'-PA
3	I	301	UDP	O4'-C4'-C5'-O5'
3	I	301	UDP	C5'-O5'-PA-O1A
3	I	301	UDP	C5'-O5'-PA-O2A
4	B	303	GTP	PB-O3A-PA-O5'
4	B	303	GTP	C5'-O5'-PA-O1A
4	C	303	GTP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
4	C	303	GTP	C5'-O5'-PA-O1A
4	C	303	GTP	C5'-O5'-PA-O2A
4	D	303	GTP	PB-O3A-PA-O5'
4	D	303	GTP	C5'-O5'-PA-O1A
4	D	303	GTP	C5'-O5'-PA-O2A
4	E	303	GTP	PB-O3A-PA-O5'
4	E	303	GTP	C5'-O5'-PA-O1A
4	E	303	GTP	C5'-O5'-PA-O2A
4	G	303	GTP	PB-O3B-PG-O2G
7	E	302	U5P	C5'-O5'-P-O1P
7	E	302	U5P	C5'-O5'-P-O2P
7	E	302	U5P	C5'-O5'-P-O3P
7	F	302	U5P	C5'-O5'-P-O2P
7	F	302	U5P	C5'-O5'-P-O3P
7	H	302	U5P	C5'-O5'-P-O1P
7	H	302	U5P	C5'-O5'-P-O2P
7	H	302	U5P	C5'-O5'-P-O3P
3	B	302	UDP	O4'-C4'-C5'-O5'
3	D	302	UDP	C3'-C4'-C5'-O5'
3	I	301	UDP	C3'-C4'-C5'-O5'
4	G	303	GTP	C3'-C4'-C5'-O5'
2	D	301	ADP	O4'-C4'-C5'-O5'
4	G	303	GTP	O4'-C4'-C5'-O5'
2	G	301	ADP	O4'-C4'-C5'-O5'
3	B	302	UDP	C3'-C4'-C5'-O5'
4	D	303	GTP	O4'-C4'-C5'-O5'
4	E	303	GTP	O4'-C4'-C5'-O5'
3	A	302	UDP	PA-O3A-PB-O1B
7	F	302	U5P	C5'-O5'-P-O1P
3	D	302	UDP	O4'-C4'-C5'-O5'
4	E	303	GTP	C3'-C4'-C5'-O5'
3	D	302	UDP	PB-O3A-PA-O5'
4	G	303	GTP	PB-O3A-PA-O5'
4	E	303	GTP	PB-O3B-PG-O1G
2	B	301	ADP	C4'-C5'-O5'-PA
3	B	302	UDP	C4'-C5'-O5'-PA
3	A	302	UDP	PA-O3A-PB-O2B
4	G	303	GTP	PB-O3B-PG-O3G
2	H	301	ADP	C5'-O5'-PA-O3A
4	C	303	GTP	C5'-O5'-PA-O3A
4	D	303	GTP	C3'-C4'-C5'-O5'
2	A	301	ADP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	H	301	ADP	PB-O3A-PA-O2A
4	B	303	GTP	PA-O3A-PB-O2B
2	E	301	ADP	C4'-C5'-O5'-PA
3	A	302	UDP	C4'-C5'-O5'-PA
2	C	301	ADP	C5'-O5'-PA-O2A
2	D	301	ADP	C5'-O5'-PA-O1A
2	F	301	ADP	C5'-O5'-PA-O1A
2	G	301	ADP	C5'-O5'-PA-O2A
4	B	303	GTP	C5'-O5'-PA-O2A
4	G	303	GTP	C5'-O5'-PA-O2A
4	A	303	GTP	O4'-C4'-C5'-O5'
2	A	301	ADP	C4'-C5'-O5'-PA
2	B	301	ADP	C3'-C4'-C5'-O5'
3	B	302	UDP	PA-O3A-PB-O1B
7	E	302	U5P	C4'-C5'-O5'-P
2	H	301	ADP	C3'-C4'-C5'-O5'
4	C	303	GTP	O4'-C4'-C5'-O5'
2	B	301	ADP	PB-O3A-PA-O2A
2	H	301	ADP	PB-O3A-PA-O1A
3	C	302	UDP	C4'-C5'-O5'-PA
7	H	302	U5P	C4'-C5'-O5'-P
7	G	302	U5P	C4'-C5'-O5'-P
3	C	302	UDP	C3'-C4'-C5'-O5'
3	D	302	UDP	C2'-C1'-N1-C6
3	C	302	UDP	O4'-C4'-C5'-O5'
4	A	303	GTP	C3'-C4'-C5'-O5'
3	D	302	UDP	C2'-C1'-N1-C2
3	A	302	UDP	O4'-C4'-C5'-O5'
3	I	301	UDP	PA-O3A-PB-O1B
4	G	303	GTP	PB-O3B-PG-O1G
2	C	301	ADP	C3'-C4'-C5'-O5'
7	H	302	U5P	O4'-C4'-C5'-O5'
3	B	302	UDP	PA-O3A-PB-O2B
3	B	302	UDP	PA-O3A-PB-O3B
4	E	303	GTP	PB-O3B-PG-O2G
4	E	303	GTP	PB-O3B-PG-O3G
3	A	302	UDP	C5'-O5'-PA-O3A
3	B	302	UDP	C5'-O5'-PA-O3A
3	I	301	UDP	C5'-O5'-PA-O3A
4	D	303	GTP	C5'-O5'-PA-O3A
4	E	303	GTP	C5'-O5'-PA-O3A
4	G	303	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
7	E	302	U5P	O4'-C4'-C5'-O5'
2	B	301	ADP	PB-O3A-PA-O1A
4	B	303	GTP	PA-O3A-PB-O1B
4	C	303	GTP	PA-O3A-PB-O2B
2	A	301	ADP	C5'-O5'-PA-O1A
7	F	302	U5P	O4'-C4'-C5'-O5'
2	H	301	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

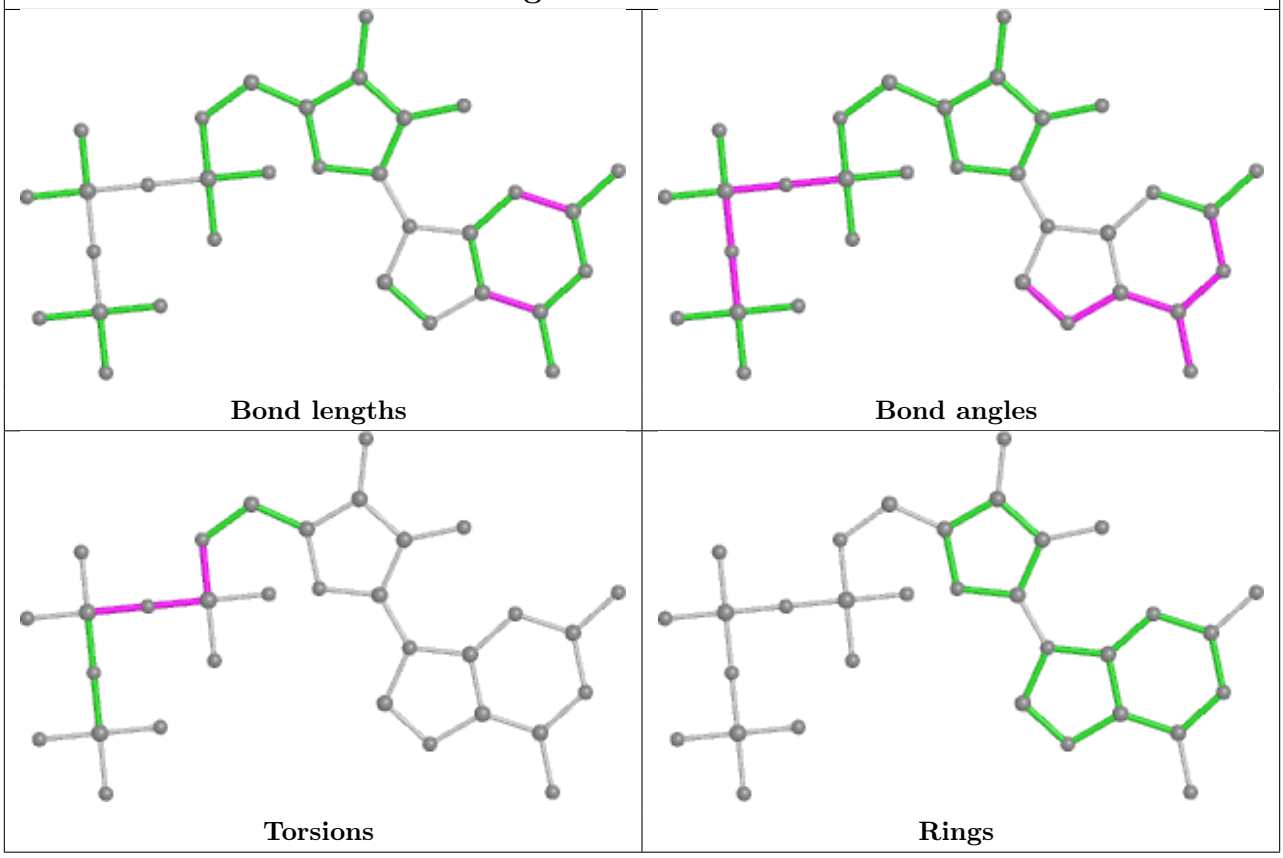
19 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	301	UDP	3	0
2	B	301	ADP	2	0
3	D	302	UDP	3	0
5	G	304	SO4	2	0
2	F	301	ADP	2	0
2	G	301	ADP	3	0
7	H	302	U5P	1	0
5	B	306	SO4	1	0
3	B	302	UDP	3	0
7	F	302	U5P	2	0
2	C	301	ADP	3	0
3	C	302	UDP	1	0
2	H	301	ADP	2	0
2	A	301	ADP	1	0
4	G	303	GTP	7	0
4	A	303	GTP	2	0
2	E	301	ADP	1	0
3	A	302	UDP	2	0
7	E	302	U5P	1	0

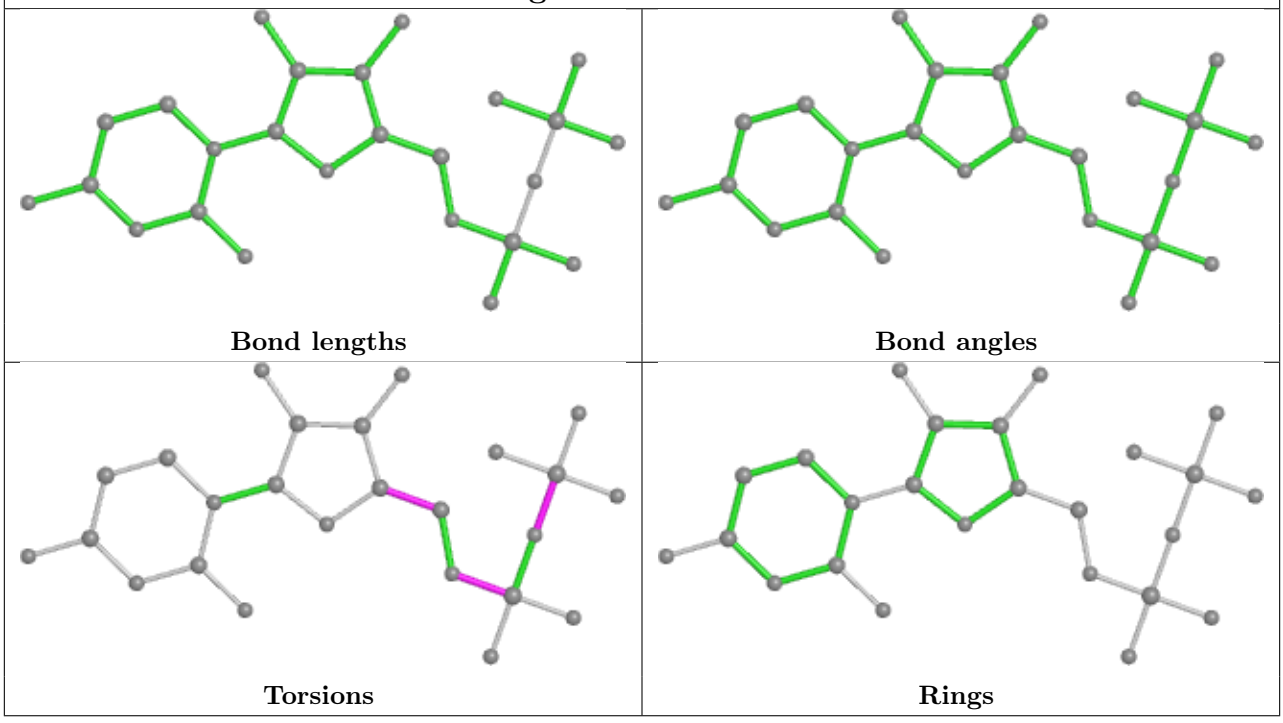
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

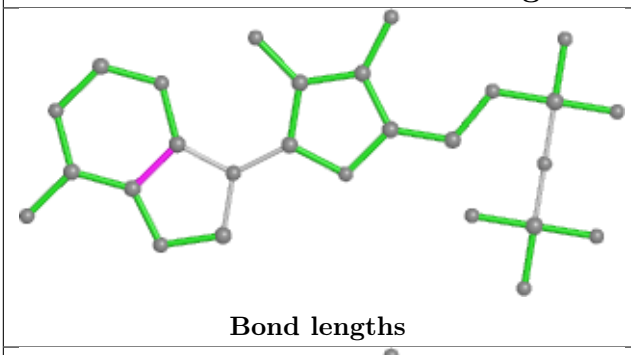
Ligand GTP B 303



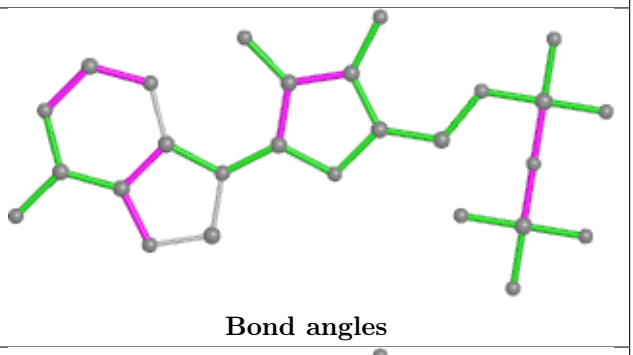
Ligand UDP I 301



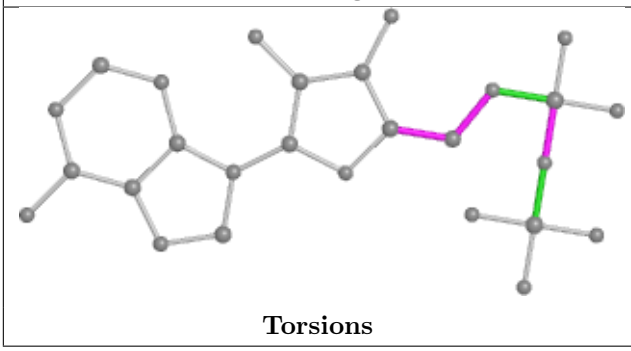
Ligand ADP B 301



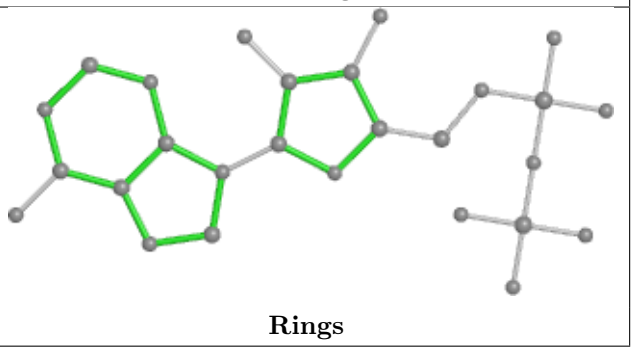
Bond lengths



Bond angles

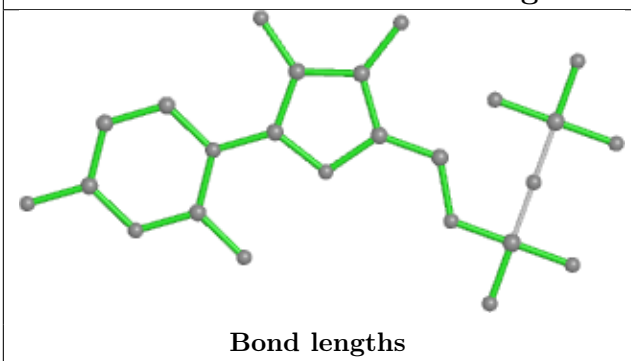


Torsions

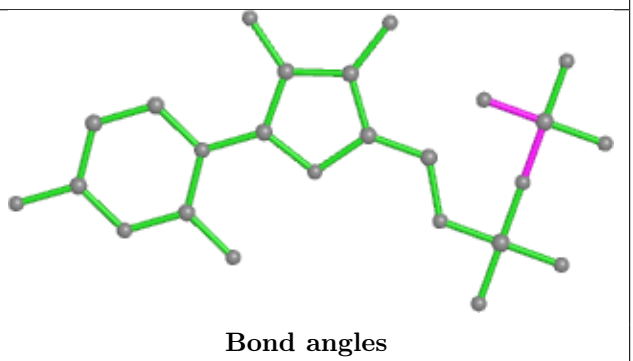


Rings

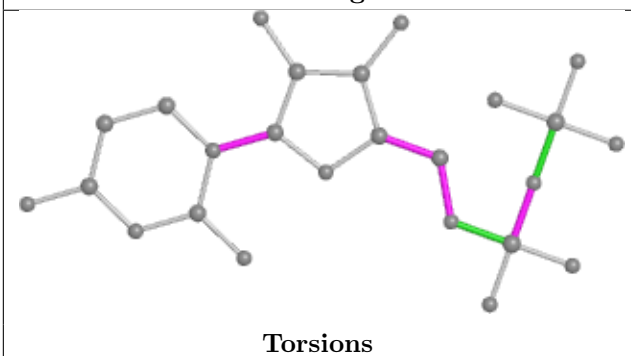
Ligand UDP D 302



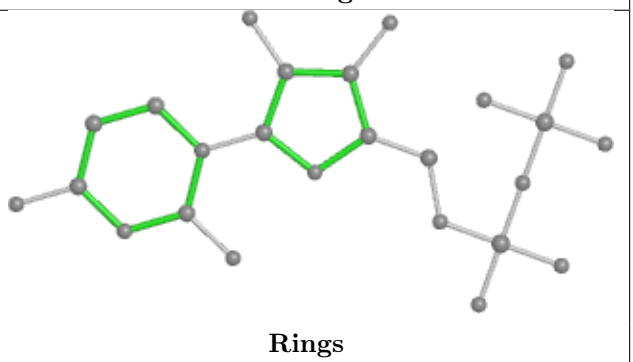
Bond lengths



Bond angles

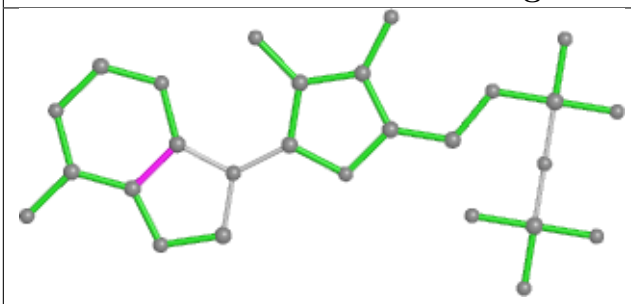


Torsions



Rings

Ligand ADP F 301



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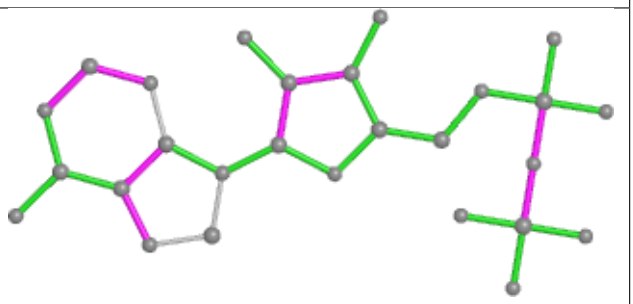

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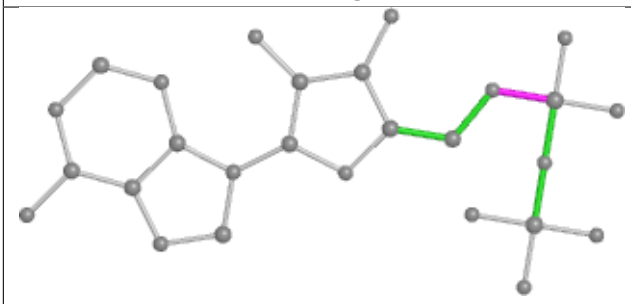
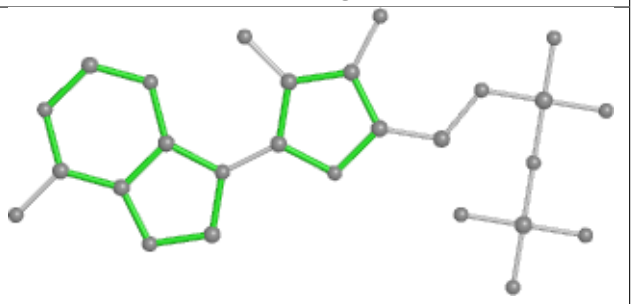
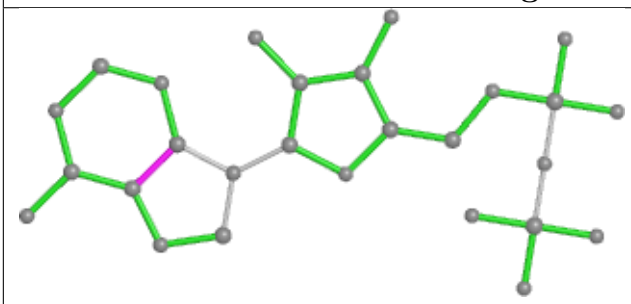


Torsions



Rings

Ligand ADP G 301



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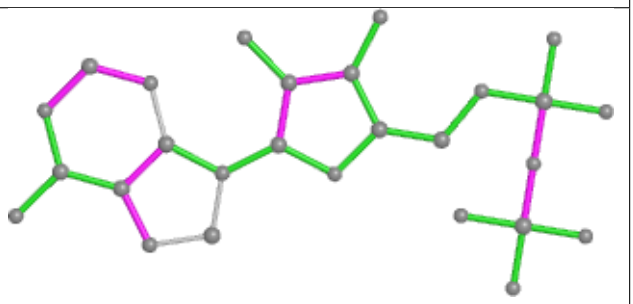

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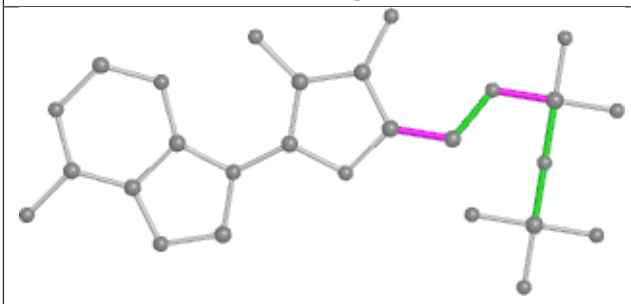

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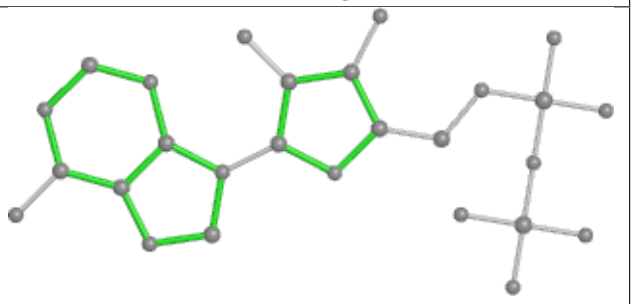
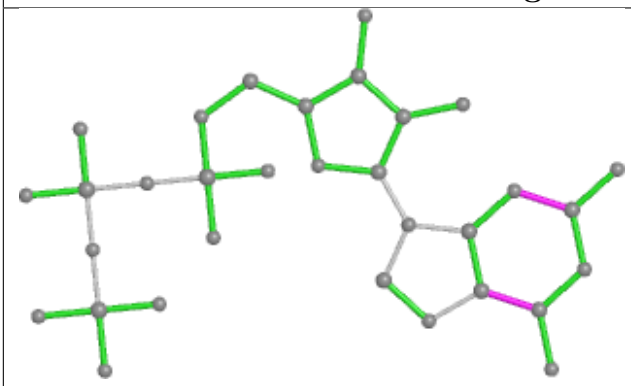


Rings

Ligand GTP E 303



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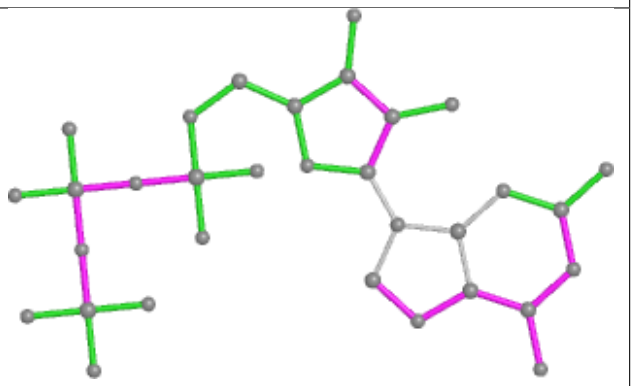

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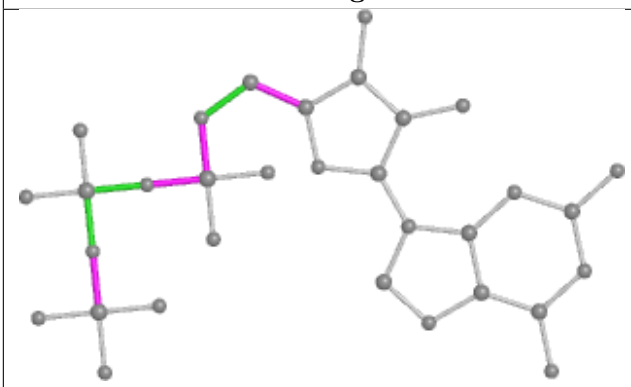

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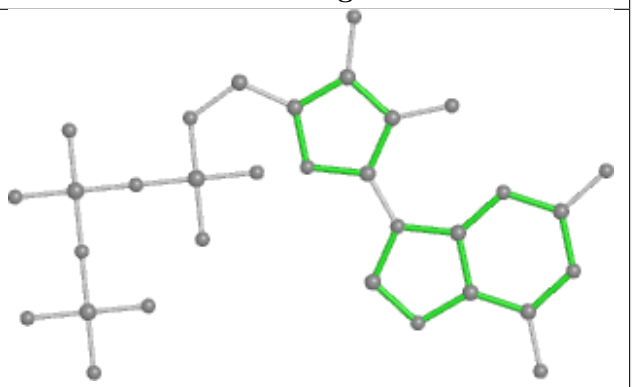
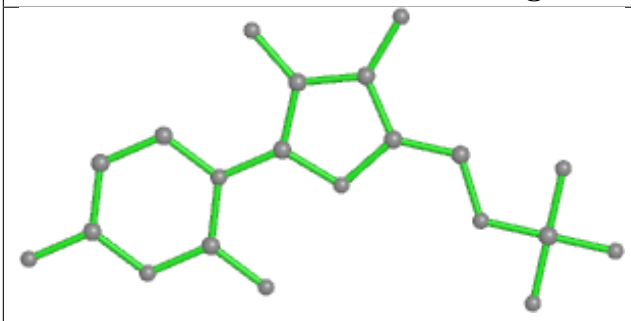


Rings

Ligand U5P H 302



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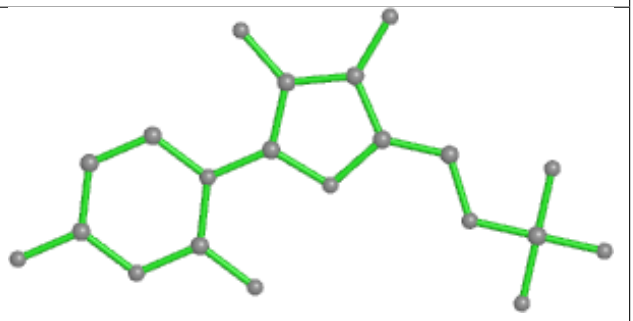
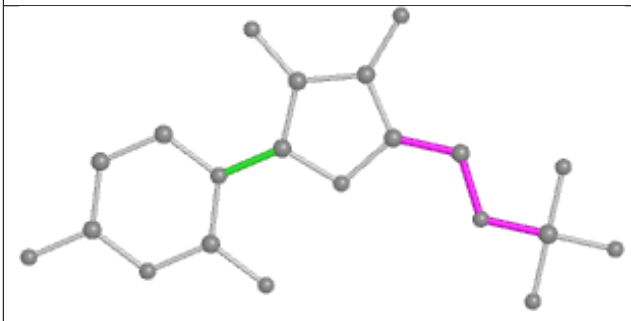


Bond angles



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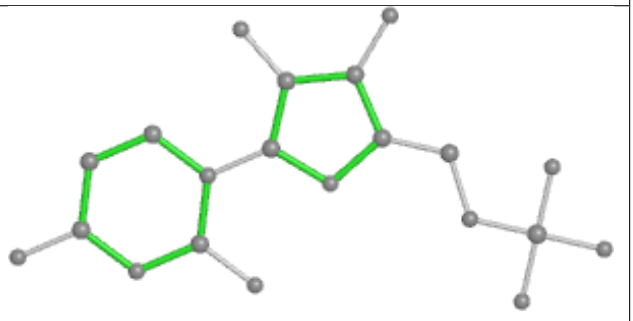
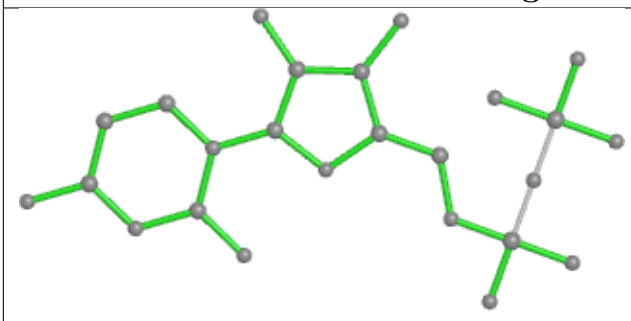


Rings

Ligand UDP B 302



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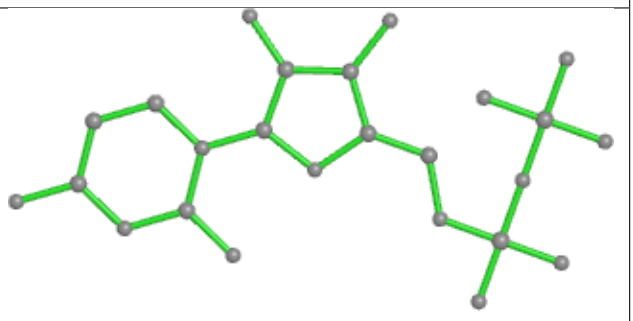

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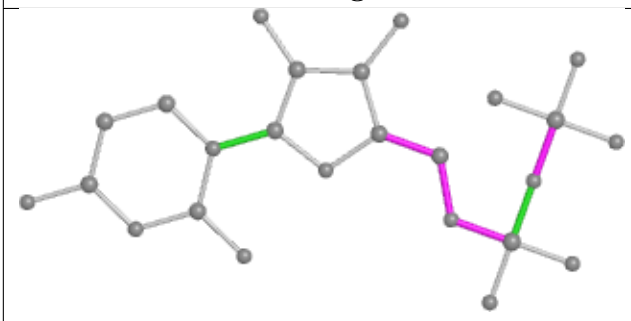

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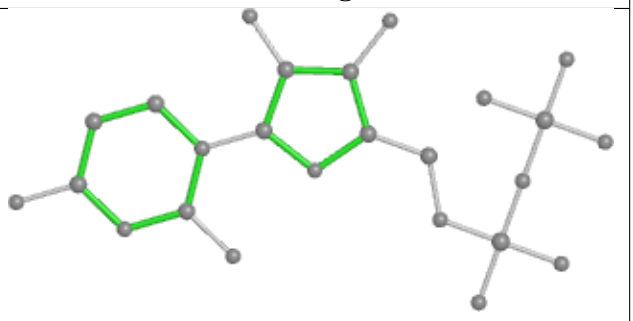
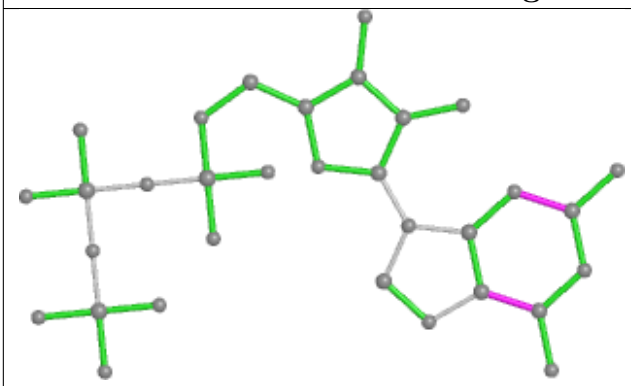


Rings

Ligand GTP C 303



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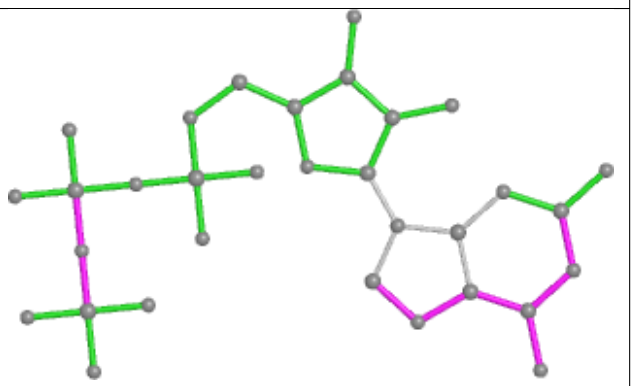

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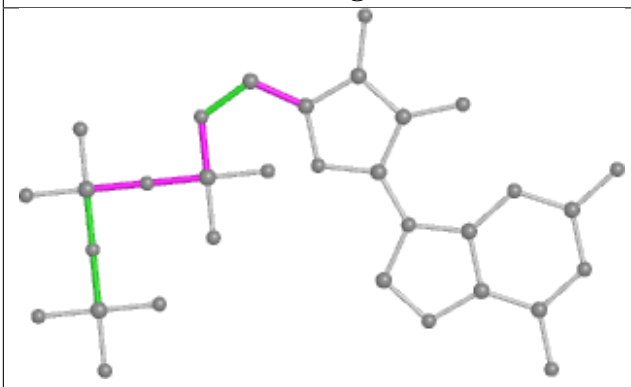

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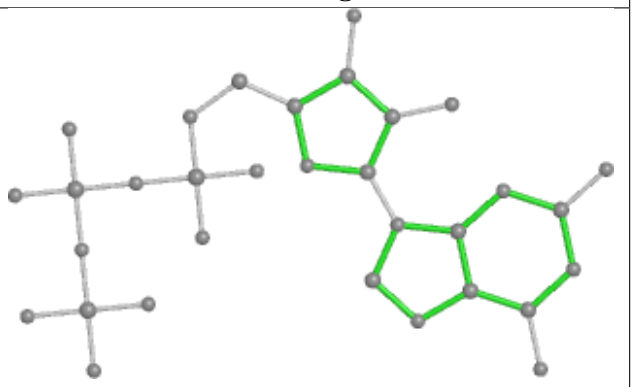
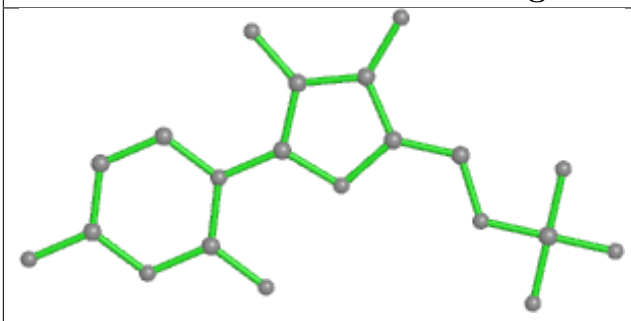


Rings

Ligand U5P F 302



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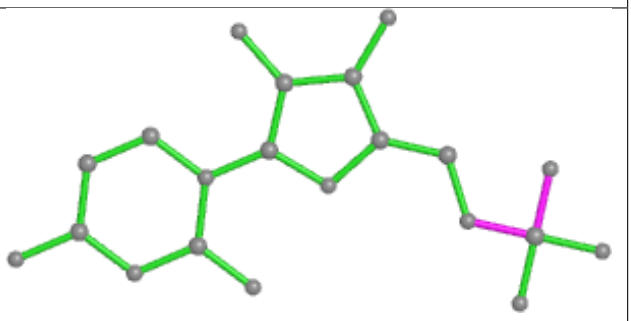

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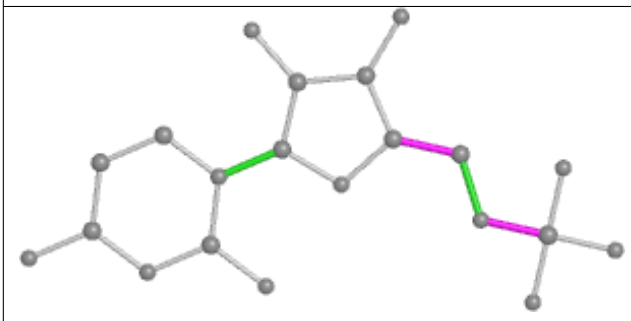

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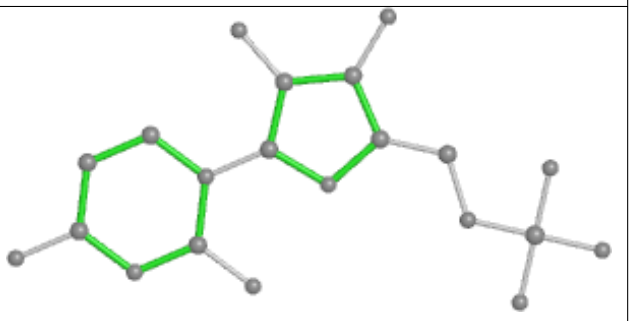
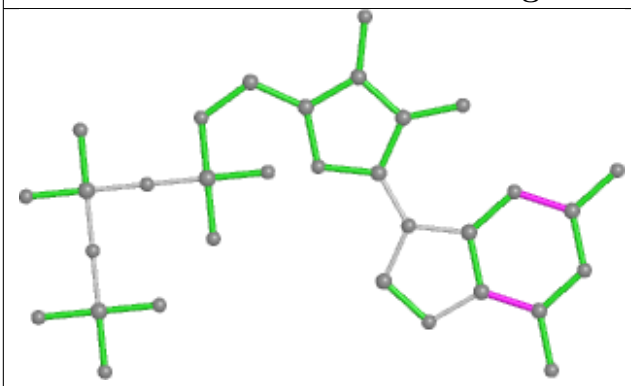


Rings

Ligand GTP D 303



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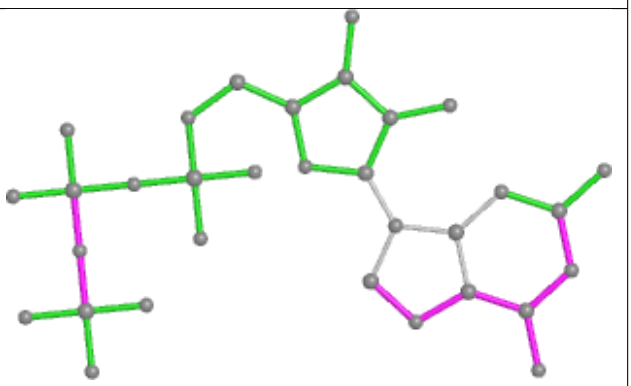

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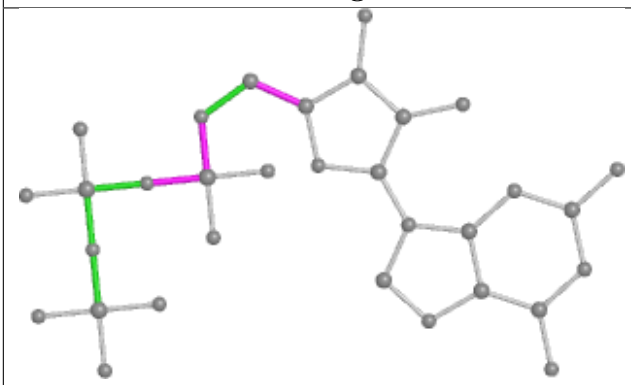

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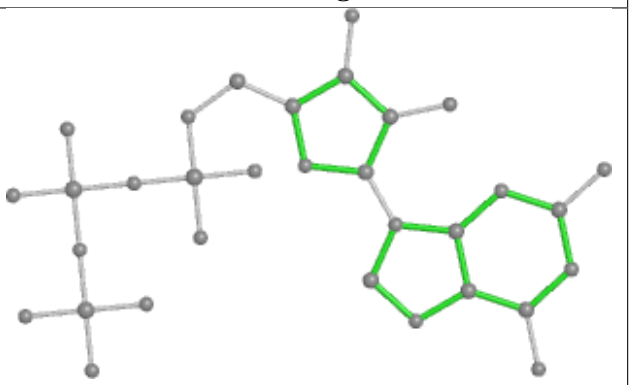
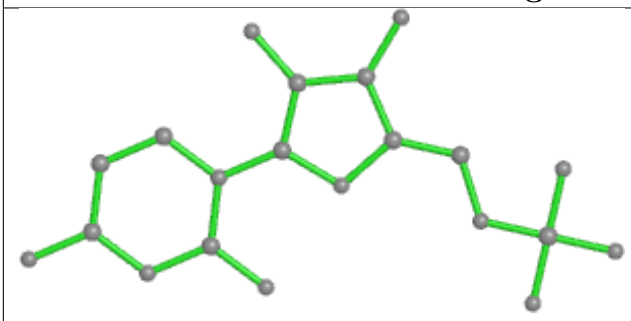


Rings

Ligand U5P G 302



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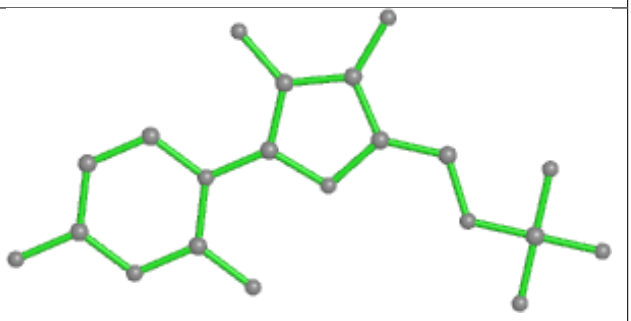

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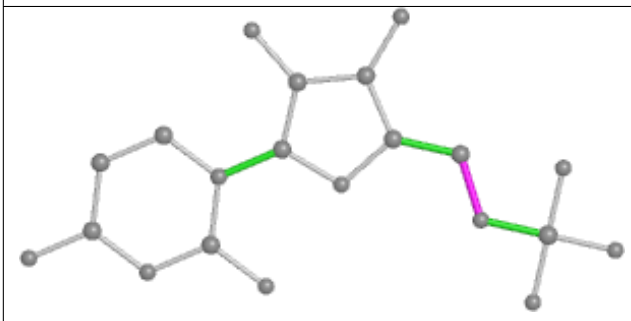

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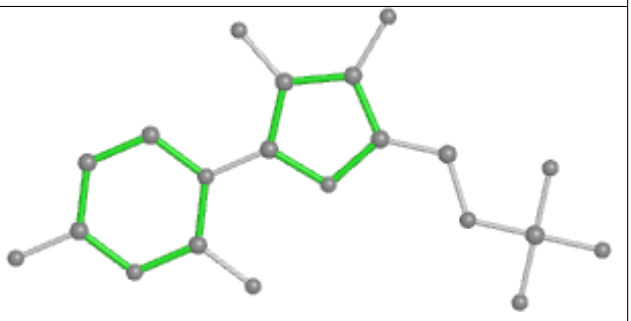
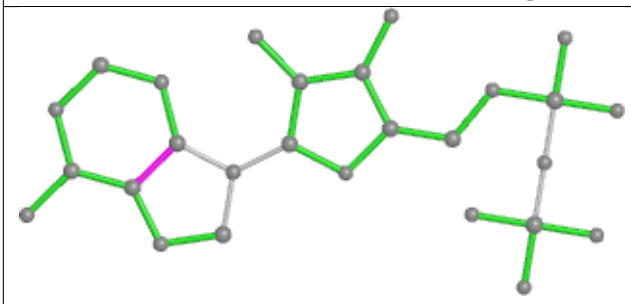


Rings

Ligand ADP D 301



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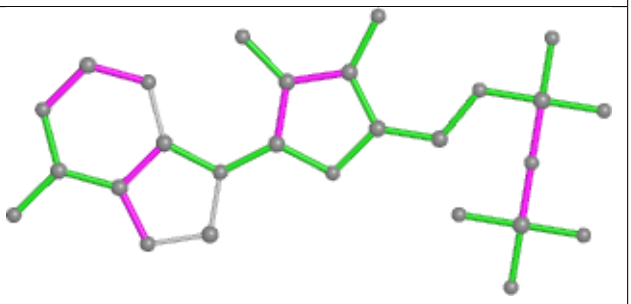

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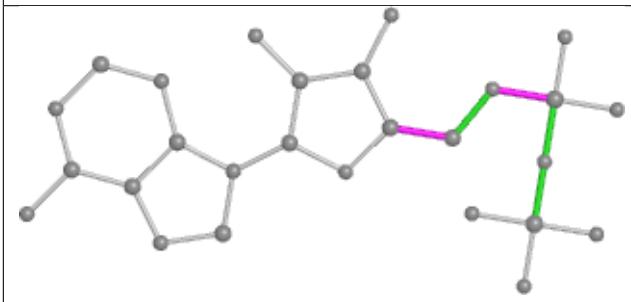
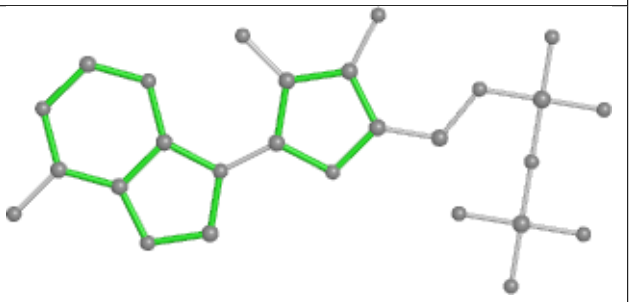
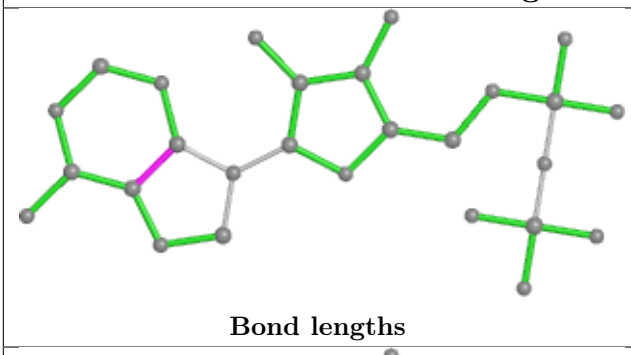


Torsions



Rings

Ligand ADP C 301



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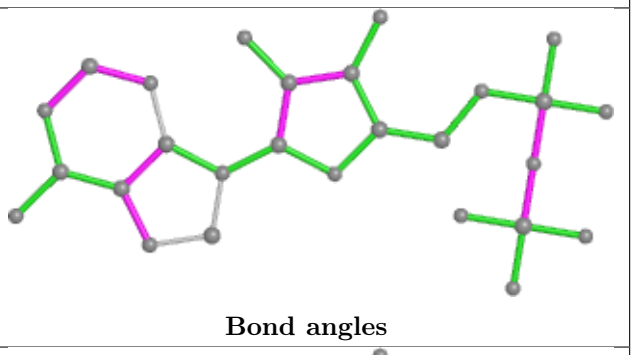
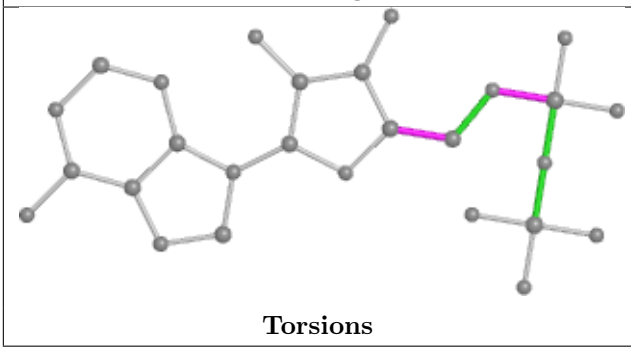


Bond angles



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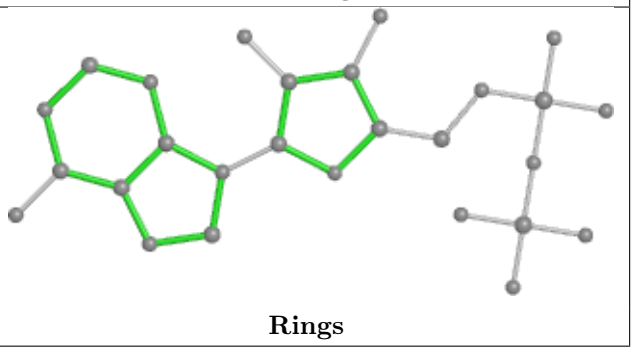
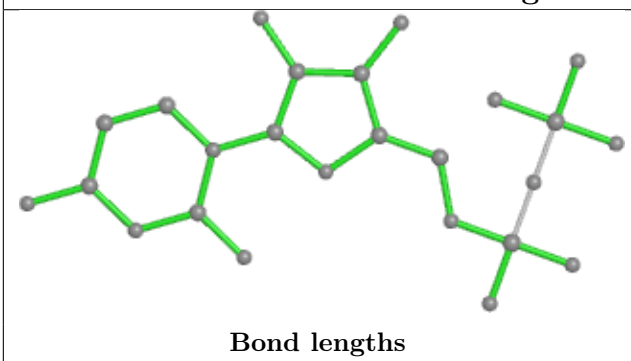


Rings

Ligand UDP C 302



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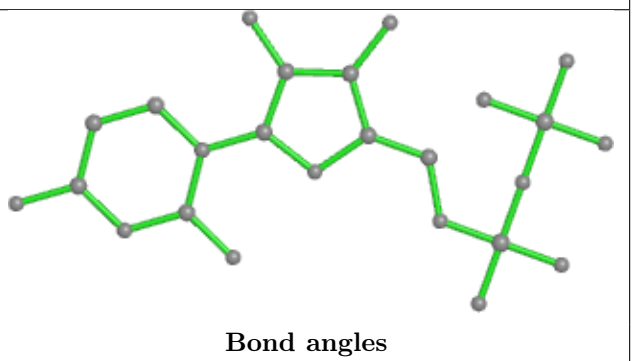

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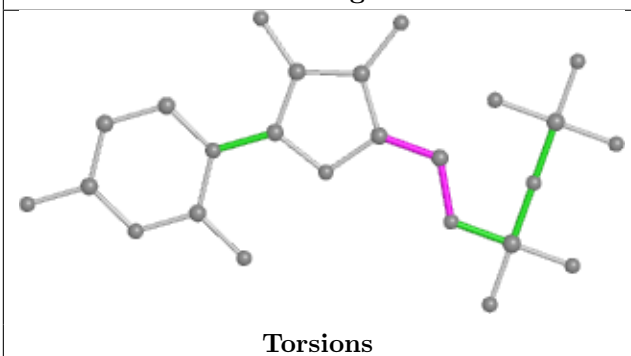

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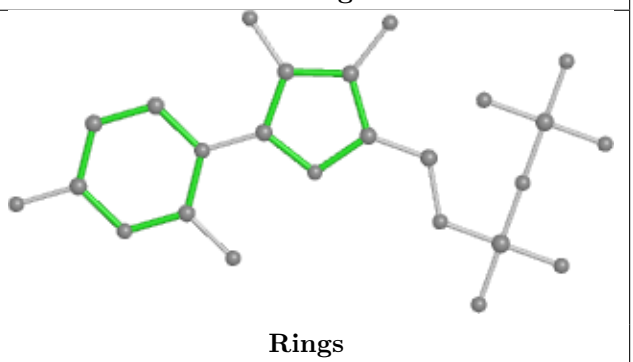
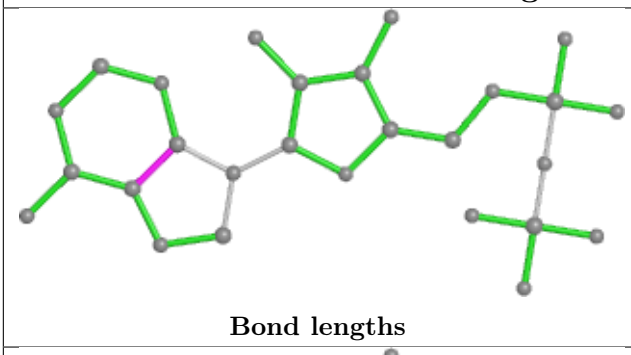


Rings

Ligand ADP H 301



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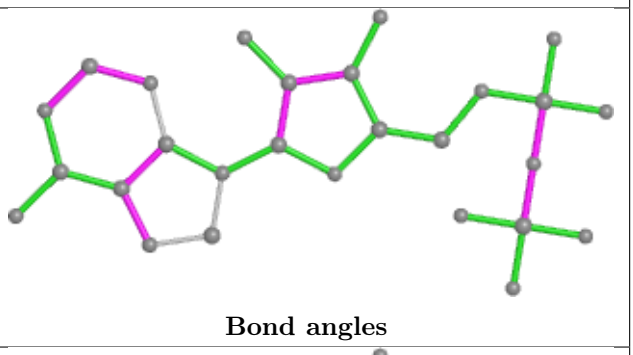
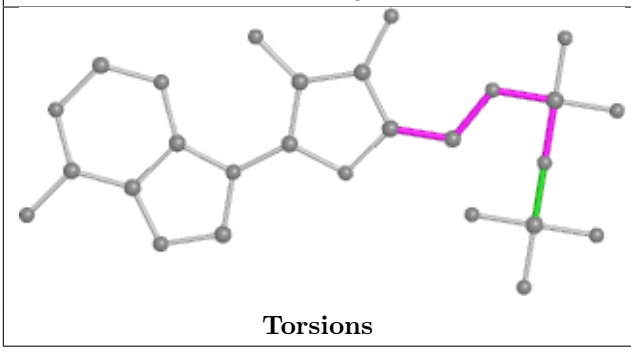
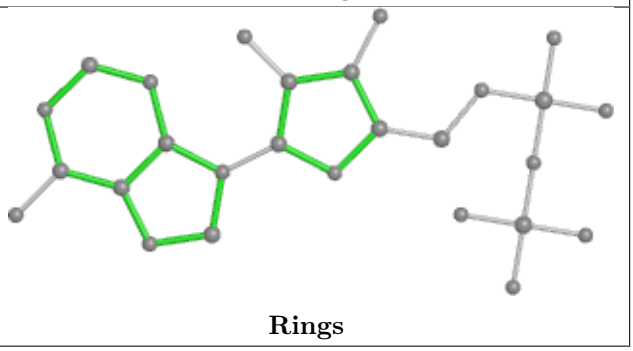


Bond angles

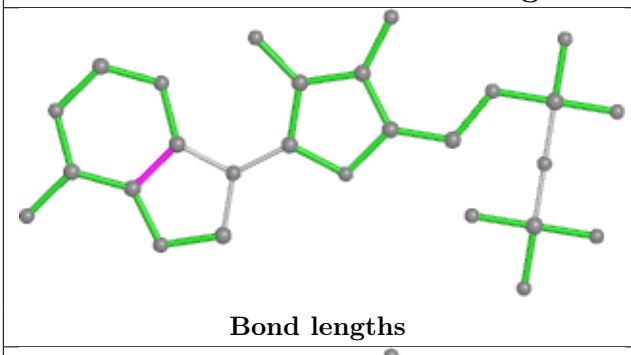


Torsions

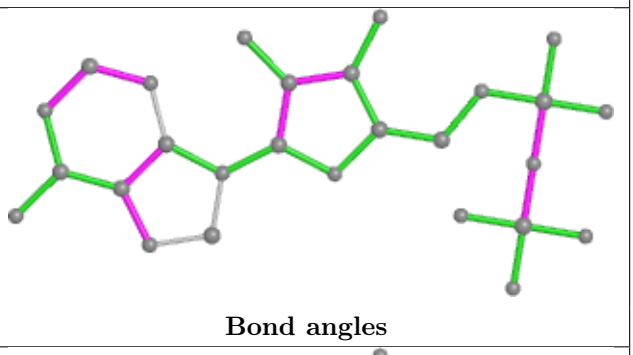


Rings

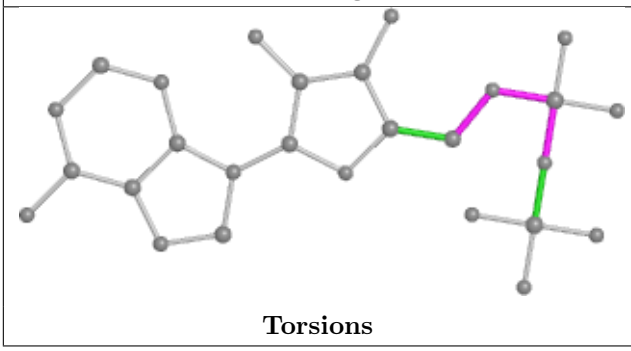
Ligand ADP A 301



Bond lengths



Bond angles



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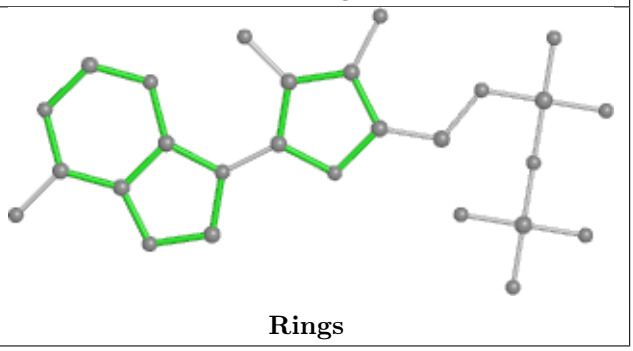
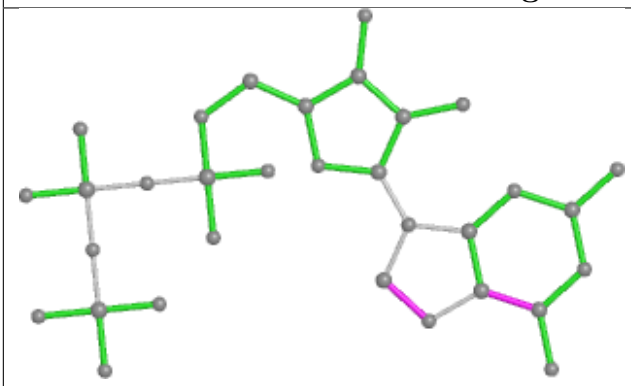


Rings

Ligand GTP G 303



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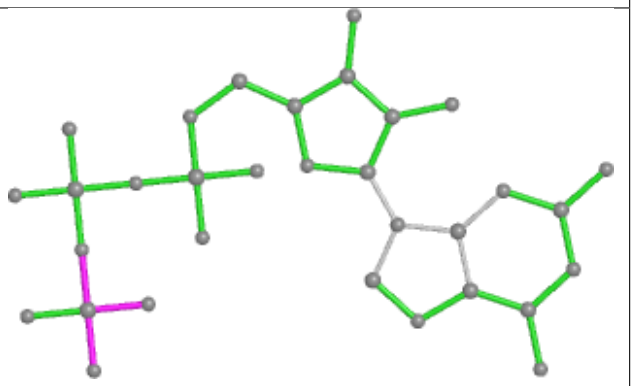
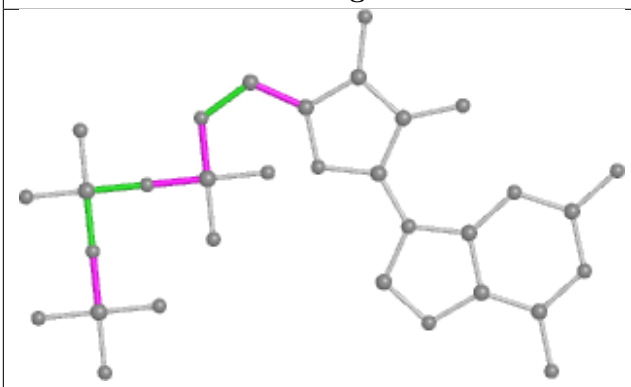
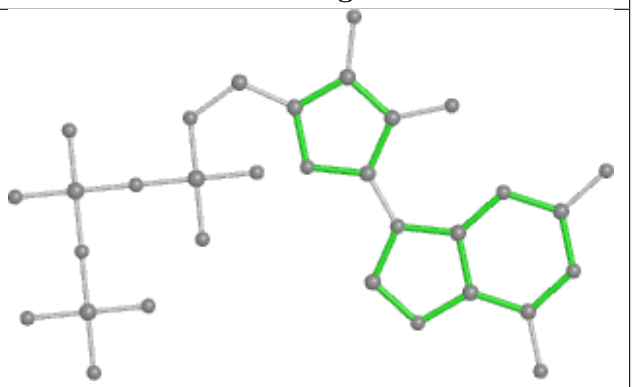


Bond angles

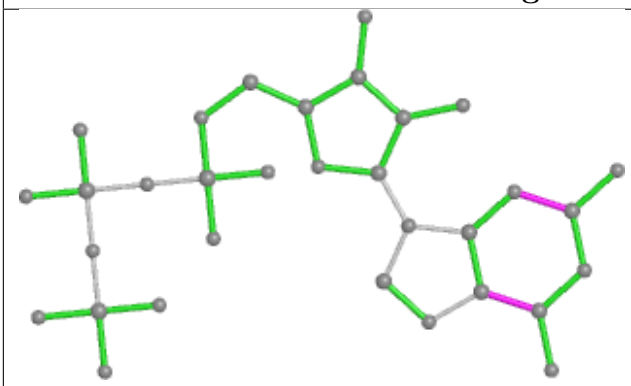


Torsions

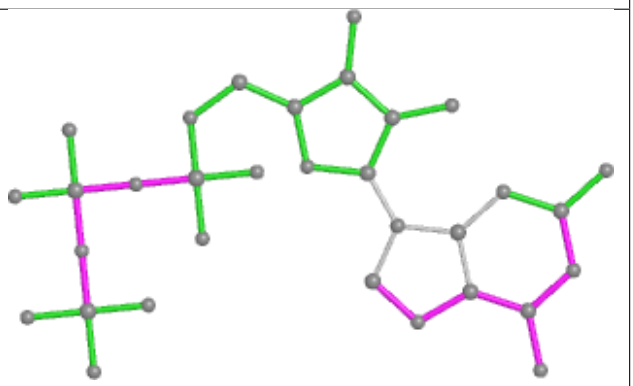


Rings

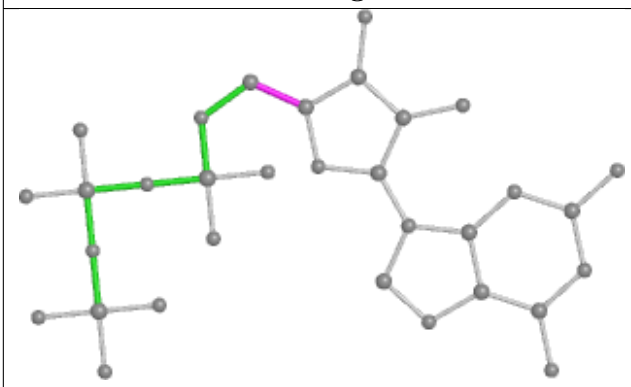
Ligand GTP A 303



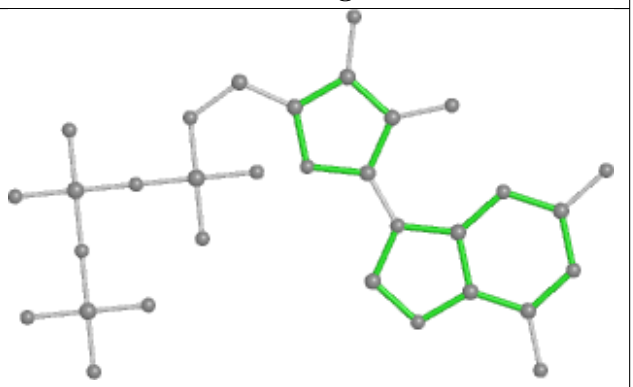
Bond lengths



Bond angles

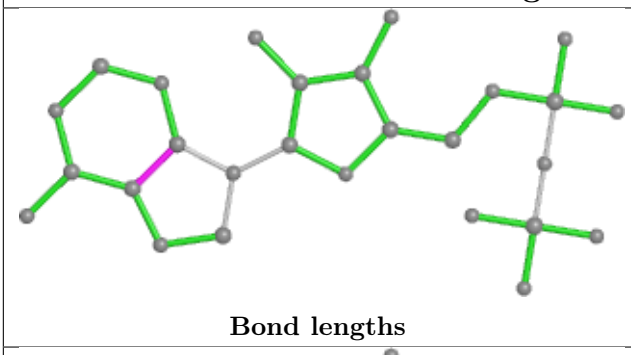


Torsions

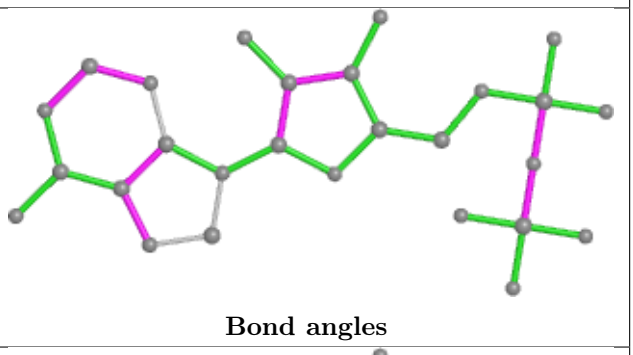


Rings

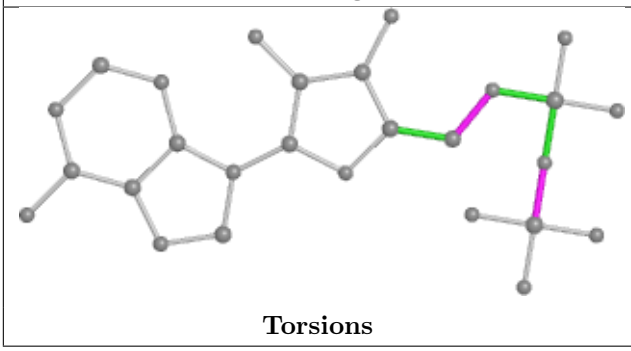
Ligand ADP E 301



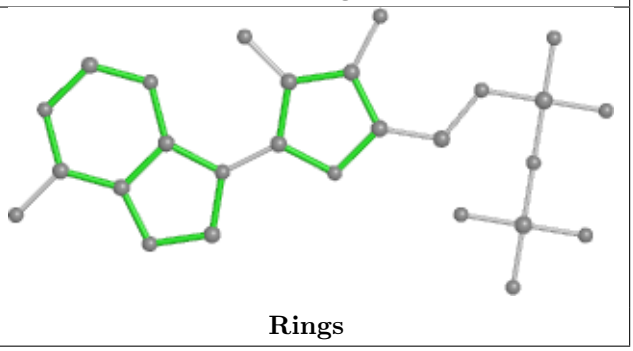
Bond lengths



Bond angles

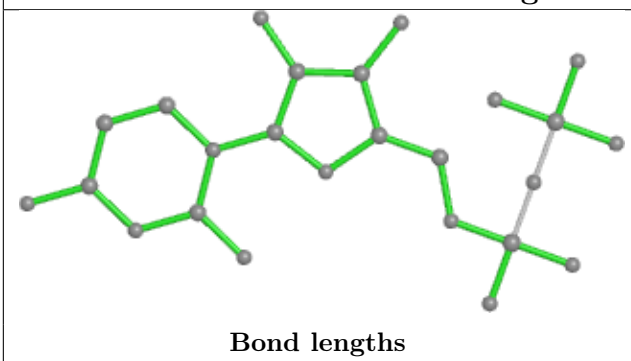


Torsions

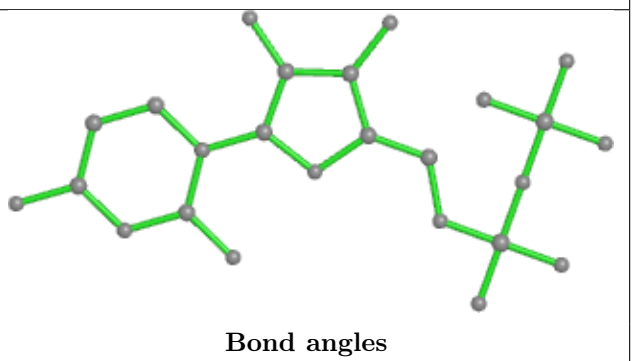


Rings

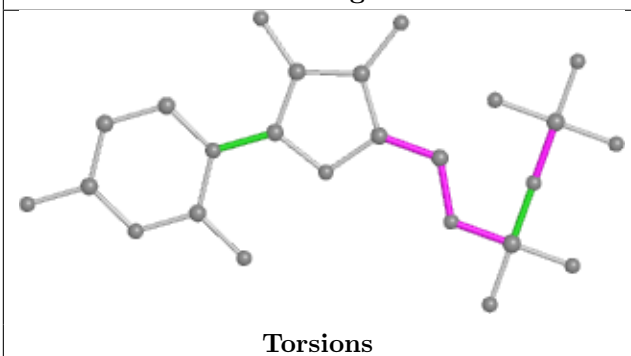
Ligand UDP A 302



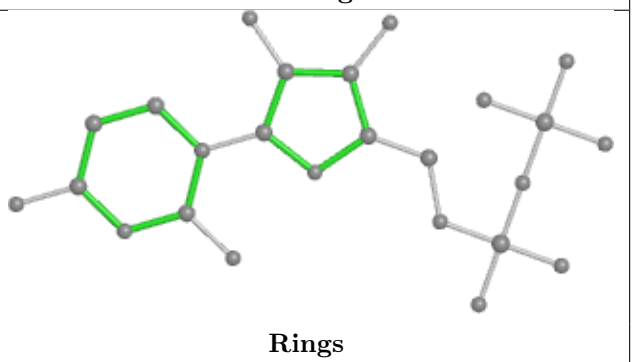
Bond lengths



Bond angles

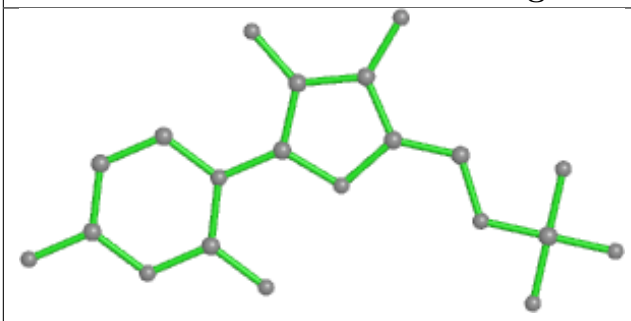


Torsions

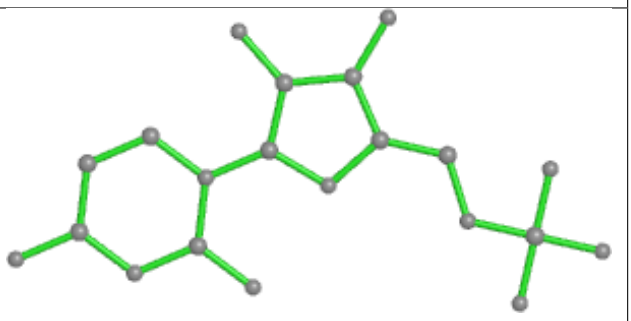


Rings

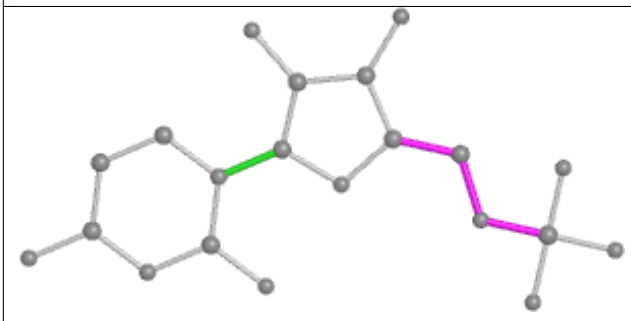
Ligand U5P E 302



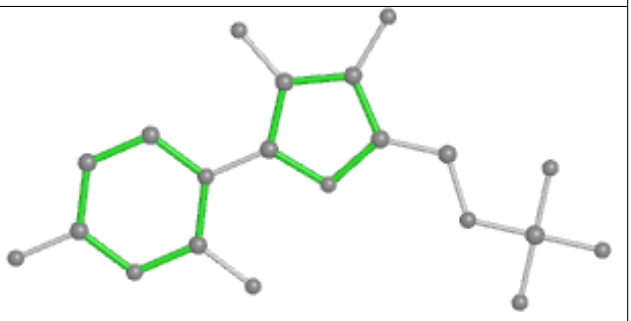
Bond lengths



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

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, 95^{th} 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	233/233 (100%)	-0.65	3 (1%)	74	70	21, 32, 53, 66	0
1	B	233/233 (100%)	-0.36	7 (3%)	52	46	20, 36, 61, 77	0
1	C	233/233 (100%)	-0.42	5 (2%)	63	58	20, 36, 59, 79	0
1	D	233/233 (100%)	-0.44	4 (1%)	69	64	29, 41, 59, 68	0
1	E	233/233 (100%)	-0.17	7 (3%)	52	46	30, 42, 63, 86	0
1	F	233/233 (100%)	-0.18	4 (1%)	69	64	31, 46, 64, 80	0
1	G	233/233 (100%)	0.02	11 (4%)	37	32	31, 47, 70, 85	0
1	H	233/233 (100%)	0.17	11 (4%)	37	32	34, 50, 74, 90	0
1	I	231/233 (99%)	0.32	18 (7%)	20	17	34, 57, 94, 120	0
All	All	2095/2097 (99%)	-0.19	70 (3%)	49	43	20, 43, 69, 120	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	PHE	5.7
1	I	158	ASN	5.5
1	I	20	PHE	5.0
1	B	21	GLY	4.8
1	I	159	LYS	4.6
1	F	159	LYS	4.5
1	I	175	VAL	4.5
1	G	58	ARG	4.4
1	I	174	ALA	4.3
1	E	55	ARG	4.1
1	I	160	VAL	4.0
1	E	58	ARG	3.9
1	C	112	ARG	3.9
1	E	59	GLN	3.6
1	B	214	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	214	PHE	3.5
1	G	173	GLU	3.5
1	G	55	ARG	3.5
1	F	19	GLY	3.3
1	I	166	ASP	3.2
1	E	56	GLY	3.2
1	G	18	ASN	3.1
1	H	159	LYS	3.1
1	I	161	ASP	3.0
1	I	214	PHE	3.0
1	G	61	VAL	3.0
1	I	170	LYS	2.9
1	A	20	PHE	2.9
1	E	60	GLY	2.9
1	I	168	PRO	2.9
1	D	18	ASN	2.8
1	I	165	SER	2.8
1	B	159	LYS	2.8
1	G	170	LYS	2.8
1	H	55	ARG	2.8
1	I	169	ARG	2.7
1	D	158	ASN	2.7
1	I	167	ASP	2.6
1	I	136	SER	2.6
1	A	55	ARG	2.6
1	H	19	GLY	2.6
1	H	64	ASP	2.5
1	A	17	ARG	2.5
1	F	158	ASN	2.5
1	I	19	GLY	2.5
1	G	159	LYS	2.5
1	F	20	PHE	2.4
1	B	25	GLU	2.3
1	B	136	SER	2.3
1	H	18	ASN	2.3
1	C	18	ASN	2.3
1	H	32	ARG	2.3
1	H	171	ASN	2.3
1	D	159	LYS	2.2
1	C	135	PHE	2.2
1	E	18	ASN	2.2
1	I	171	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	20	PHE	2.2
1	H	173	GLU	2.2
1	G	62	GLY	2.2
1	H	28	GLN	2.2
1	E	192	VAL	2.1
1	G	162	GLY	2.1
1	C	159	LYS	2.1
1	B	18	ASN	2.1
1	C	17	ARG	2.1
1	G	64	ASP	2.1
1	H	4	LYS	2.0
1	I	1	MET	2.0
1	D	20	PHE	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 monosaccharides 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, 95^{th} 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	GTP	C	303	32/32	0.67	0.26	43,67,97,100	32
5	SO4	G	305	5/5	0.69	0.27	89,101,123,130	0
4	GTP	E	303	32/32	0.70	0.24	47,68,90,101	32
4	GTP	D	303	32/32	0.72	0.22	39,69,98,101	32
4	GTP	G	303	32/32	0.73	0.27	42,63,89,96	32
4	GTP	A	303	32/32	0.73	0.22	35,69,92,102	32
6	MG	I	303	1/1	0.75	0.66	82,82,82,82	0
4	GTP	B	303	32/32	0.76	0.23	34,61,90,95	32
5	SO4	E	305	5/5	0.76	0.18	69,85,116,129	0
5	SO4	B	306	5/5	0.77	0.19	74,83,117,138	0

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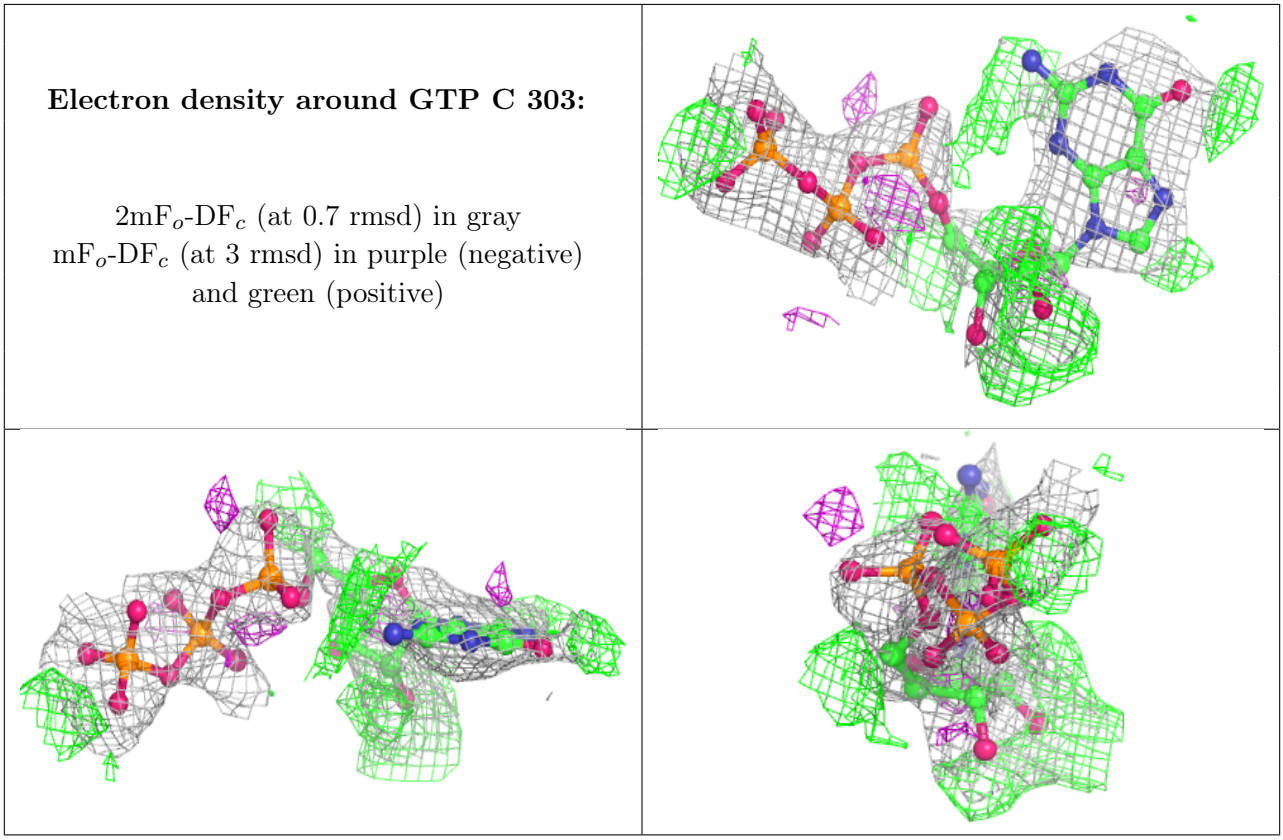
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	U5P	F	302	21/21	0.77	0.26	44,77,93,103	0
5	SO4	A	304	5/5	0.78	0.20	67,82,109,131	0
5	SO4	B	309	5/5	0.78	0.23	82,93,123,123	0
5	SO4	A	306	5/5	0.79	0.24	99,103,113,125	0
5	SO4	A	305	5/5	0.80	0.24	70,73,115,117	0
3	UDP	D	302	25/25	0.81	0.29	42,60,85,92	25
5	SO4	I	302	5/5	0.81	0.21	88,98,125,150	0
5	SO4	C	306	5/5	0.82	0.29	75,78,101,130	0
5	SO4	B	307	5/5	0.82	0.22	75,88,113,136	0
5	SO4	F	303	5/5	0.83	0.20	75,95,98,114	0
5	SO4	F	304	5/5	0.83	0.23	71,91,115,150	0
5	SO4	C	305	5/5	0.83	0.22	100,107,110,110	0
5	SO4	D	304	5/5	0.84	0.20	75,77,95,97	0
5	SO4	C	304	5/5	0.84	0.18	77,81,126,126	0
6	MG	A	307	1/1	0.84	0.22	70,70,70,70	0
2	ADP	G	301	27/27	0.84	0.14	46,68,89,104	0
3	UDP	I	301	25/25	0.84	0.20	45,63,80,96	25
5	SO4	B	304	5/5	0.85	0.23	64,73,87,96	0
6	MG	H	303	1/1	0.85	0.22	69,69,69,69	0
5	SO4	D	305	5/5	0.87	0.17	87,100,125,127	0
2	ADP	D	301	27/27	0.87	0.13	35,59,112,150	0
6	MG	G	306	1/1	0.88	0.23	53,53,53,53	0
5	SO4	B	308	5/5	0.88	0.15	72,90,119,126	0
2	ADP	C	301	27/27	0.88	0.13	40,59,104,113	0
5	SO4	G	304	5/5	0.88	0.18	57,98,114,127	0
3	UDP	B	302	25/25	0.89	0.18	32,50,65,85	25
6	MG	C	308	1/1	0.89	0.14	79,79,79,79	0
2	ADP	H	301	27/27	0.89	0.12	38,60,99,105	0
2	ADP	F	301	27/27	0.90	0.12	33,66,118,139	0
5	SO4	C	307	5/5	0.90	0.22	74,75,106,115	0
5	SO4	E	304	5/5	0.90	0.14	69,76,96,106	0
2	ADP	B	301	27/27	0.91	0.11	31,57,99,108	0
6	MG	E	306	1/1	0.91	0.21	54,54,54,54	0
3	UDP	C	302	25/25	0.91	0.14	28,44,70,85	25
2	ADP	E	301	27/27	0.93	0.09	29,45,65,68	0
2	ADP	A	301	27/27	0.93	0.10	27,46,78,84	0
5	SO4	B	305	5/5	0.93	0.24	73,81,98,100	0
7	U5P	E	302	21/21	0.94	0.10	38,43,61,68	0
3	UDP	A	302	25/25	0.94	0.10	31,46,61,84	0
7	U5P	H	302	21/21	0.94	0.10	39,49,63,72	0
7	U5P	G	302	21/21	0.96	0.09	37,53,63,65	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.

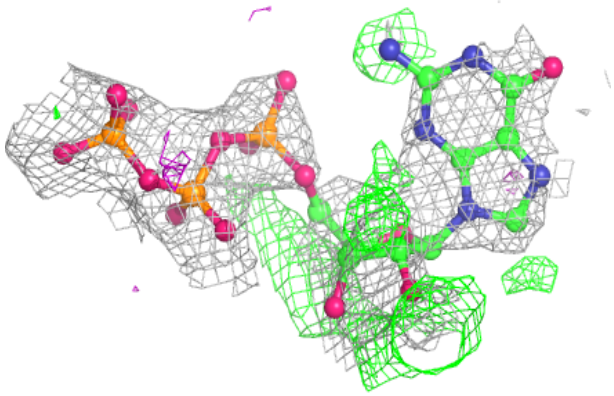
Electron density around GTP C 303:

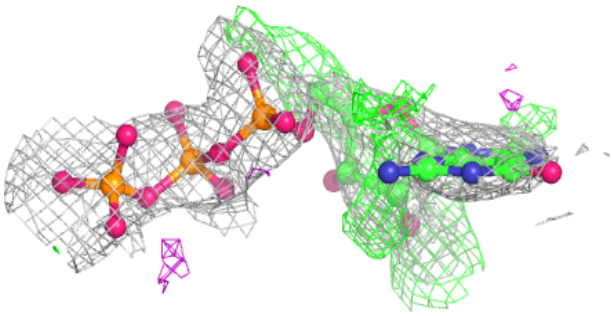
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

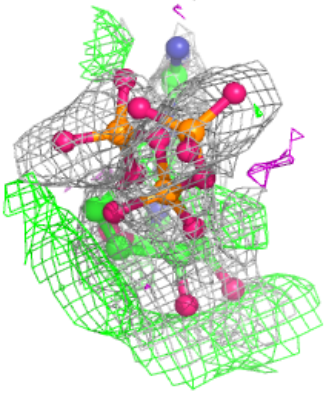


Electron density around GTP E 303:

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

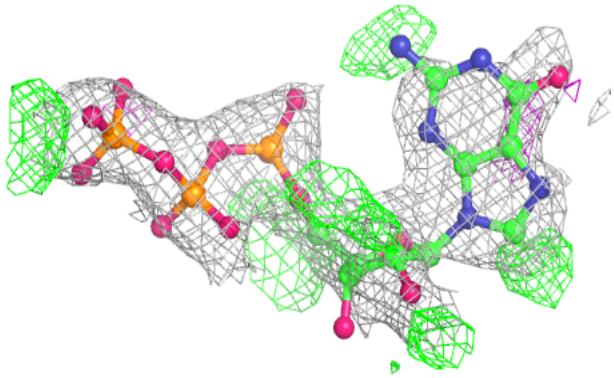


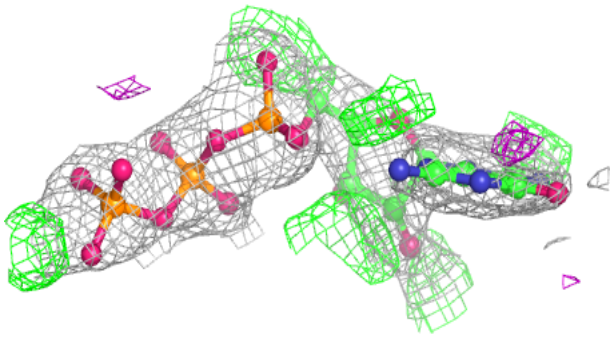


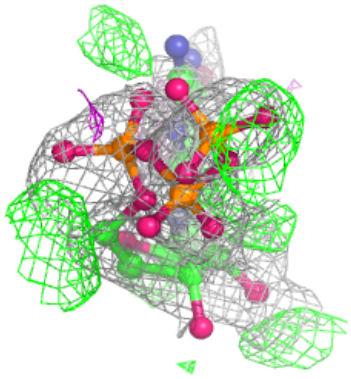


Electron density around GTP D 303:

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

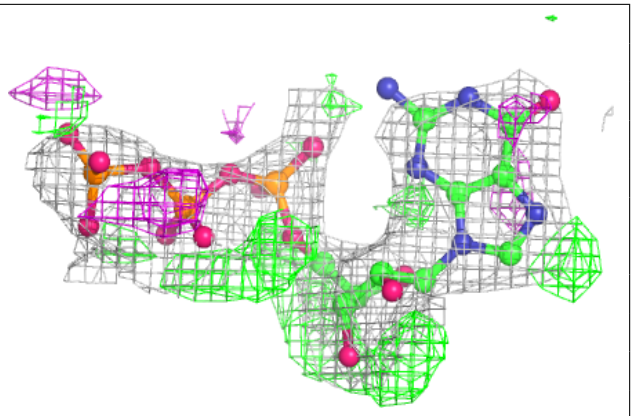


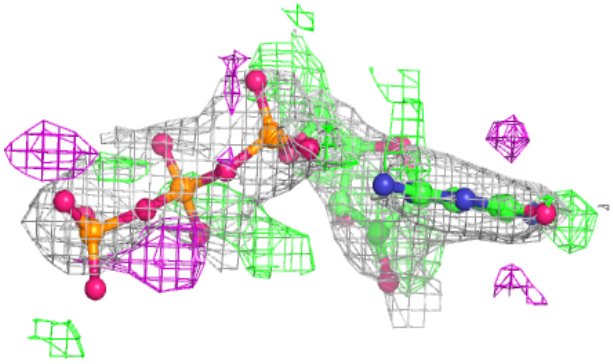


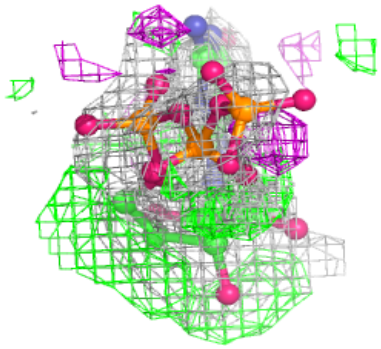


Electron density around GTP G 303:

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

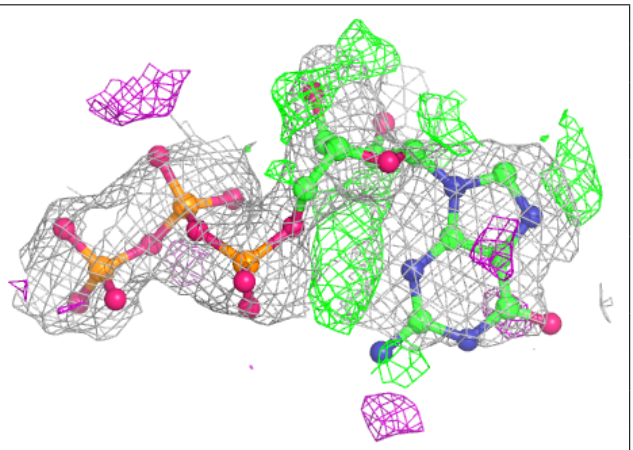


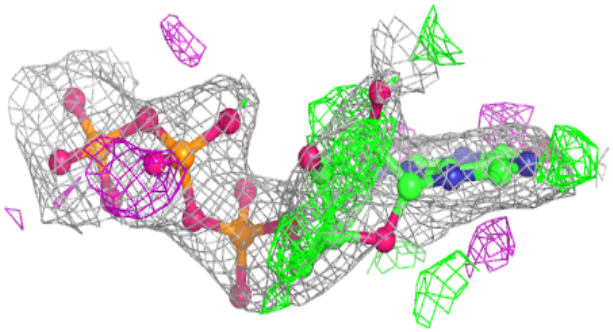


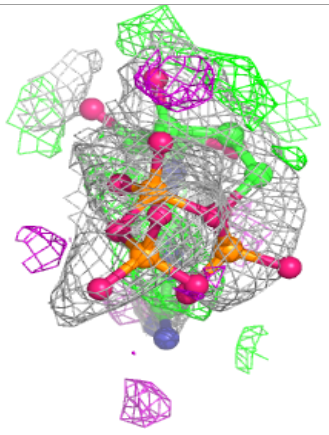


Electron density around GTP A 303:

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

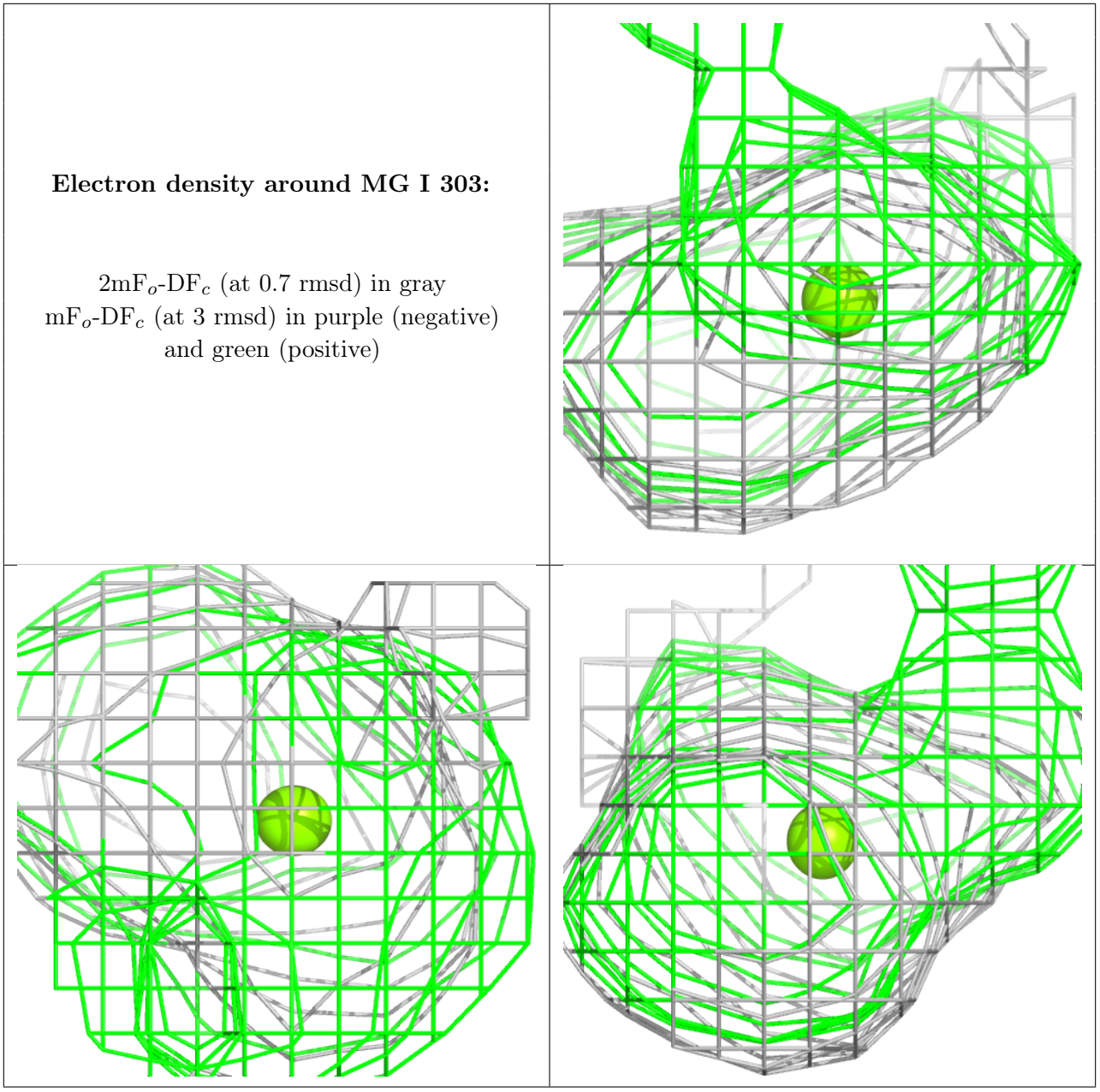






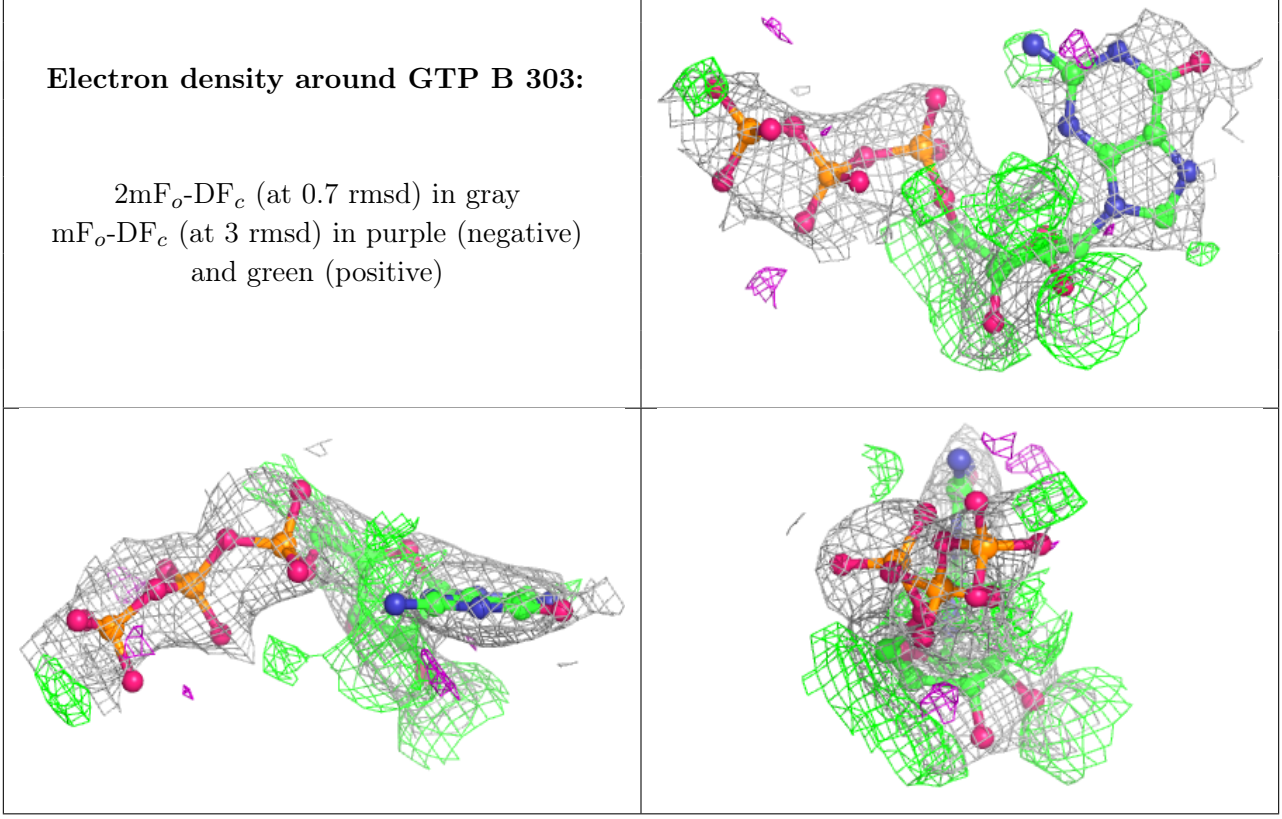
Electron density around MG I 303:

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



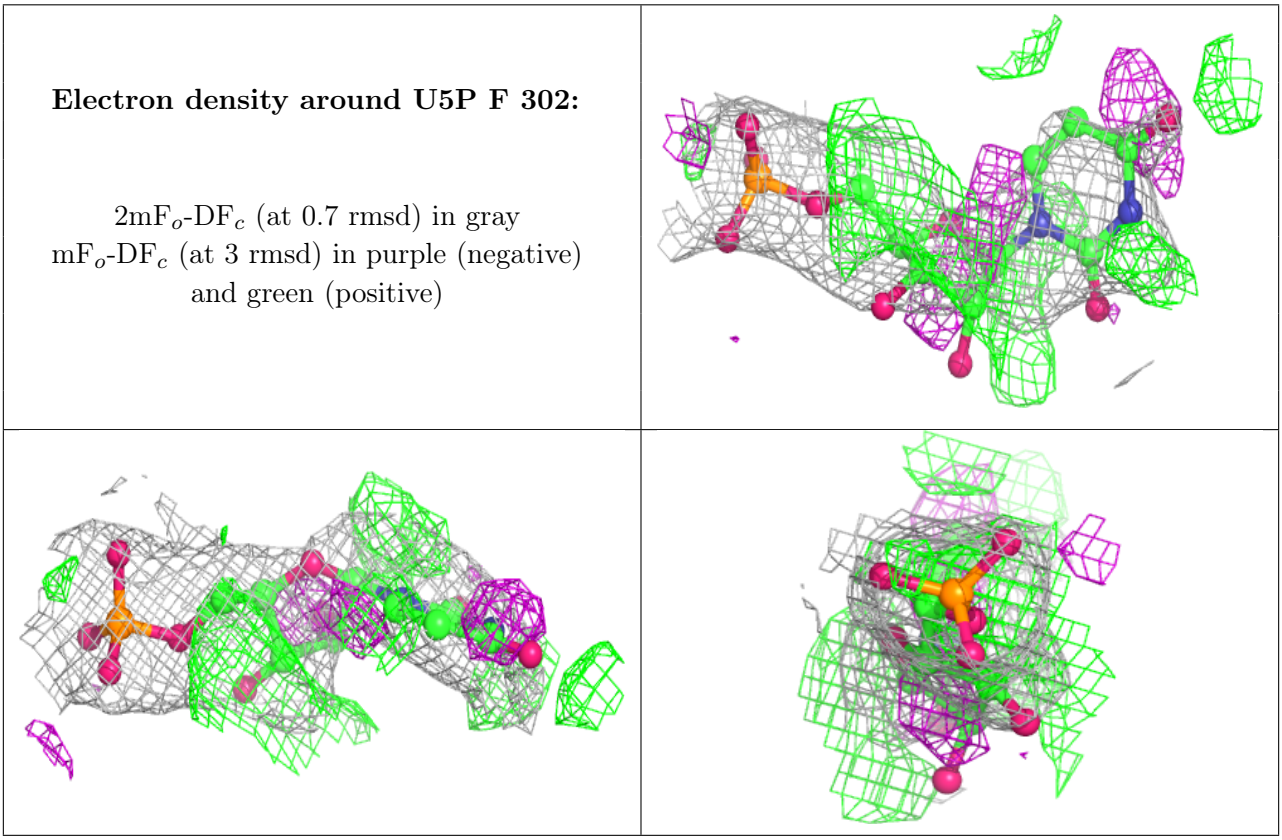
Electron density around GTP B 303:

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



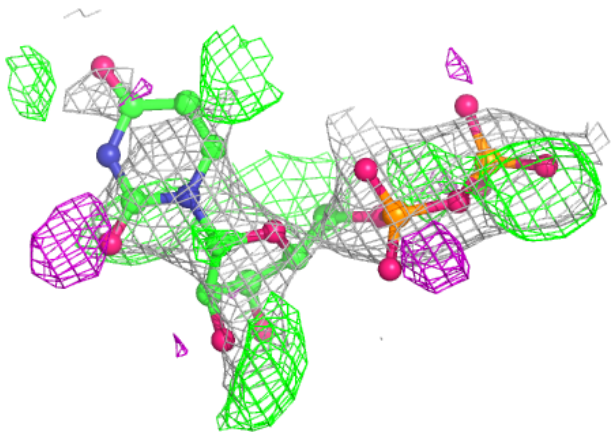
Electron density around U5P F 302:

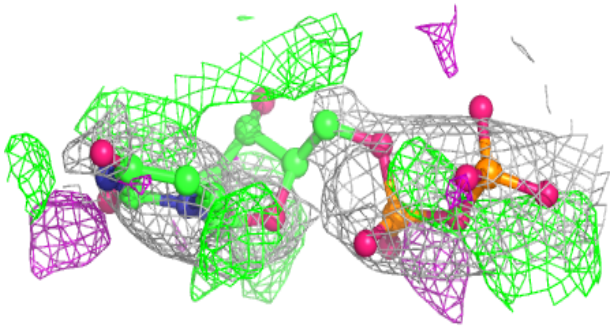
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

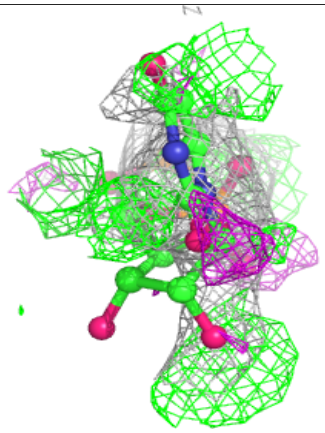


Electron density around UDP D 302:

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

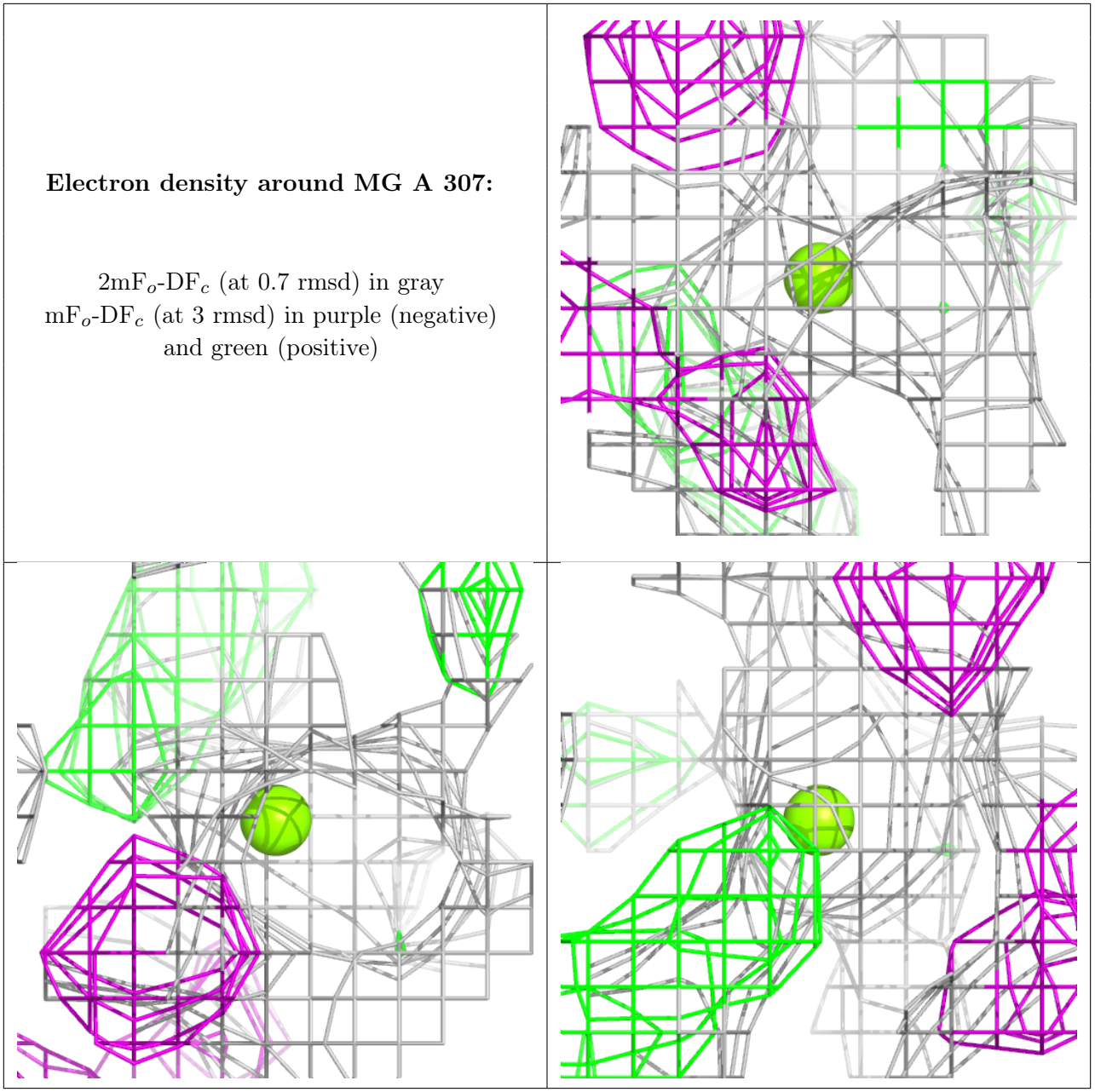






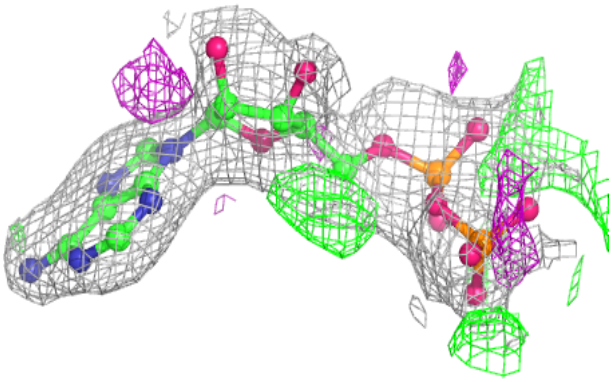
Electron density around MG A 307:

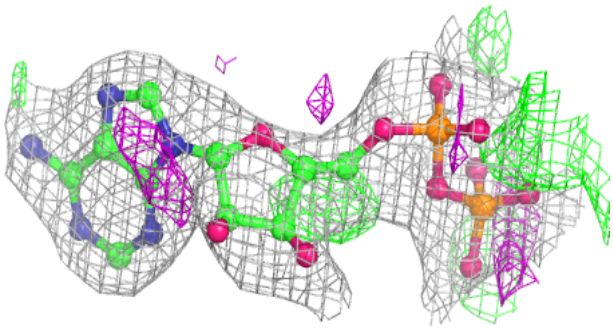
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

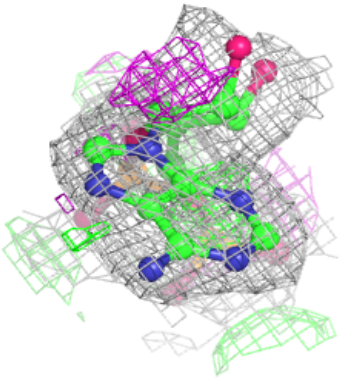


Electron density around ADP G 301:

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

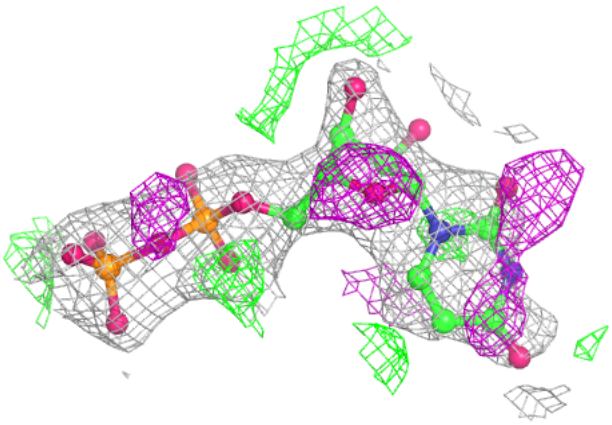


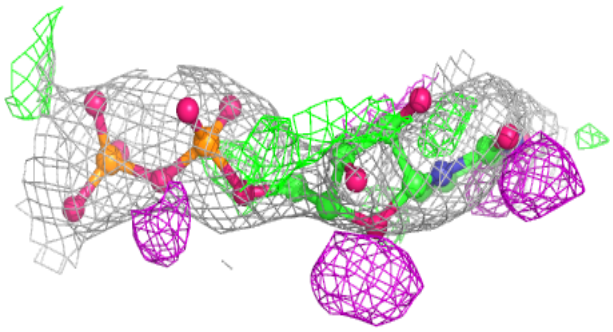


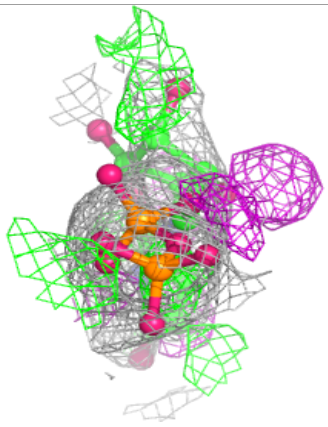


Electron density around UDP I 301:

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

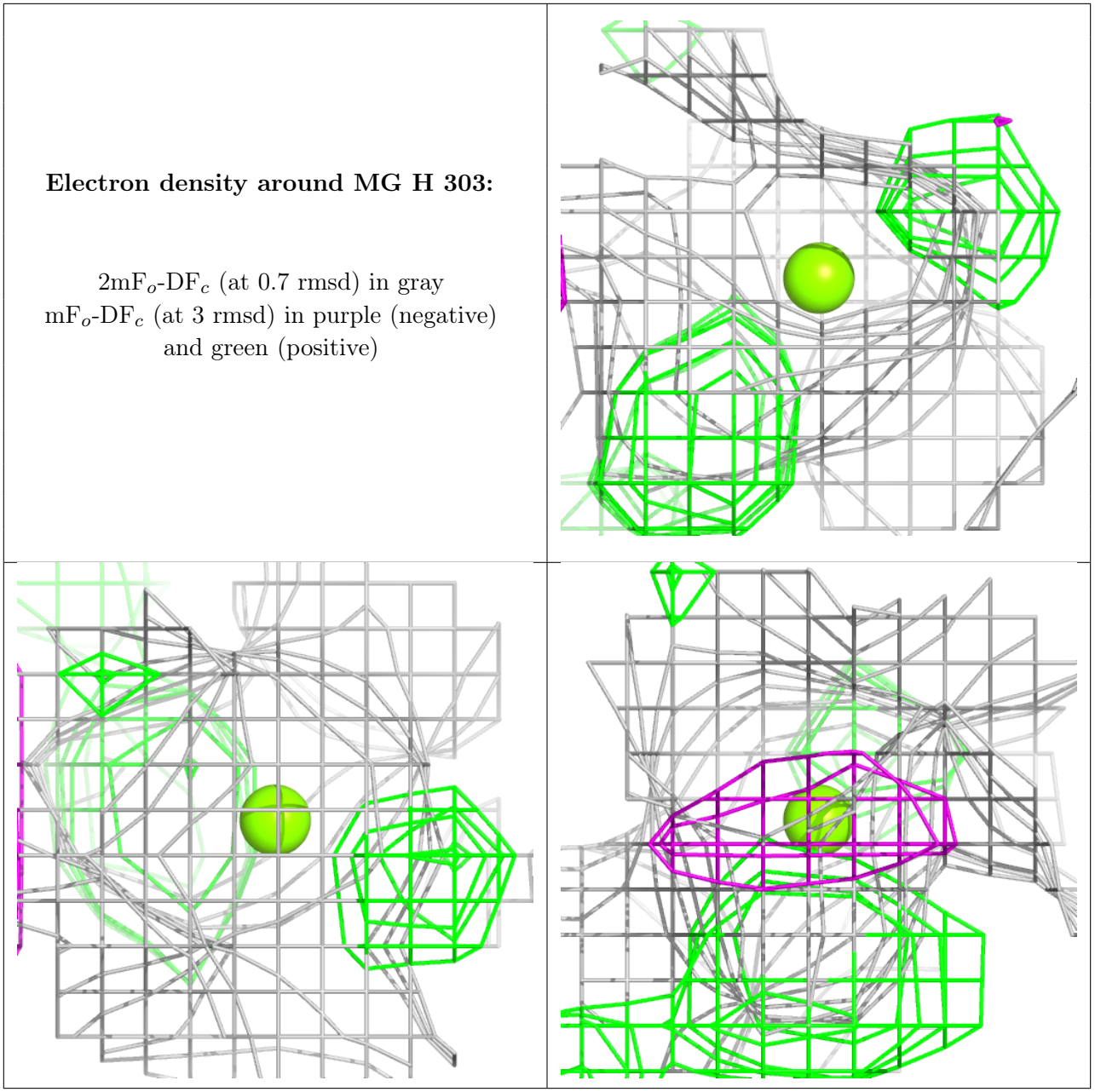






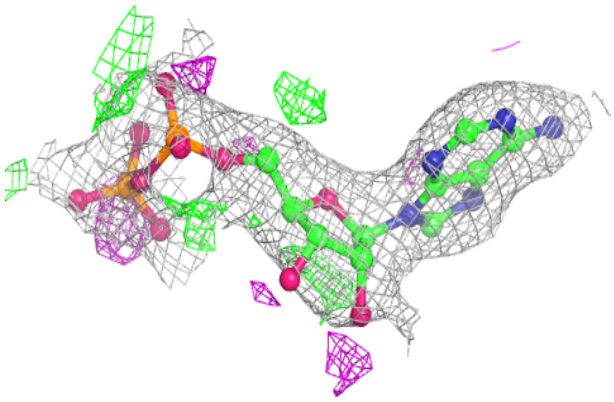
Electron density around MG H 303:

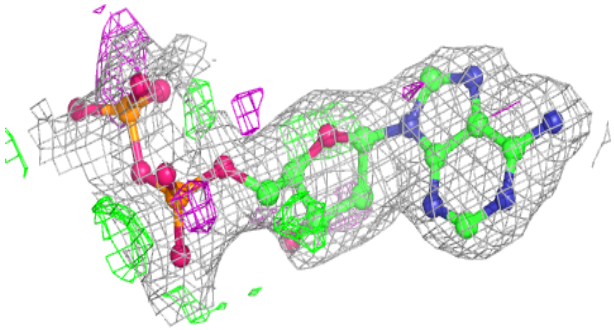
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

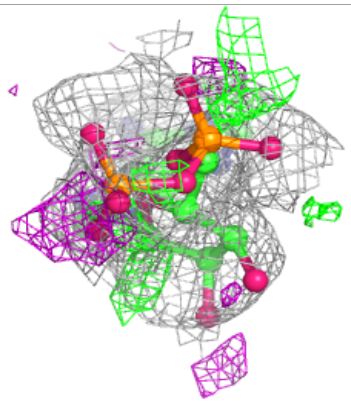


Electron density around ADP D 301:

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

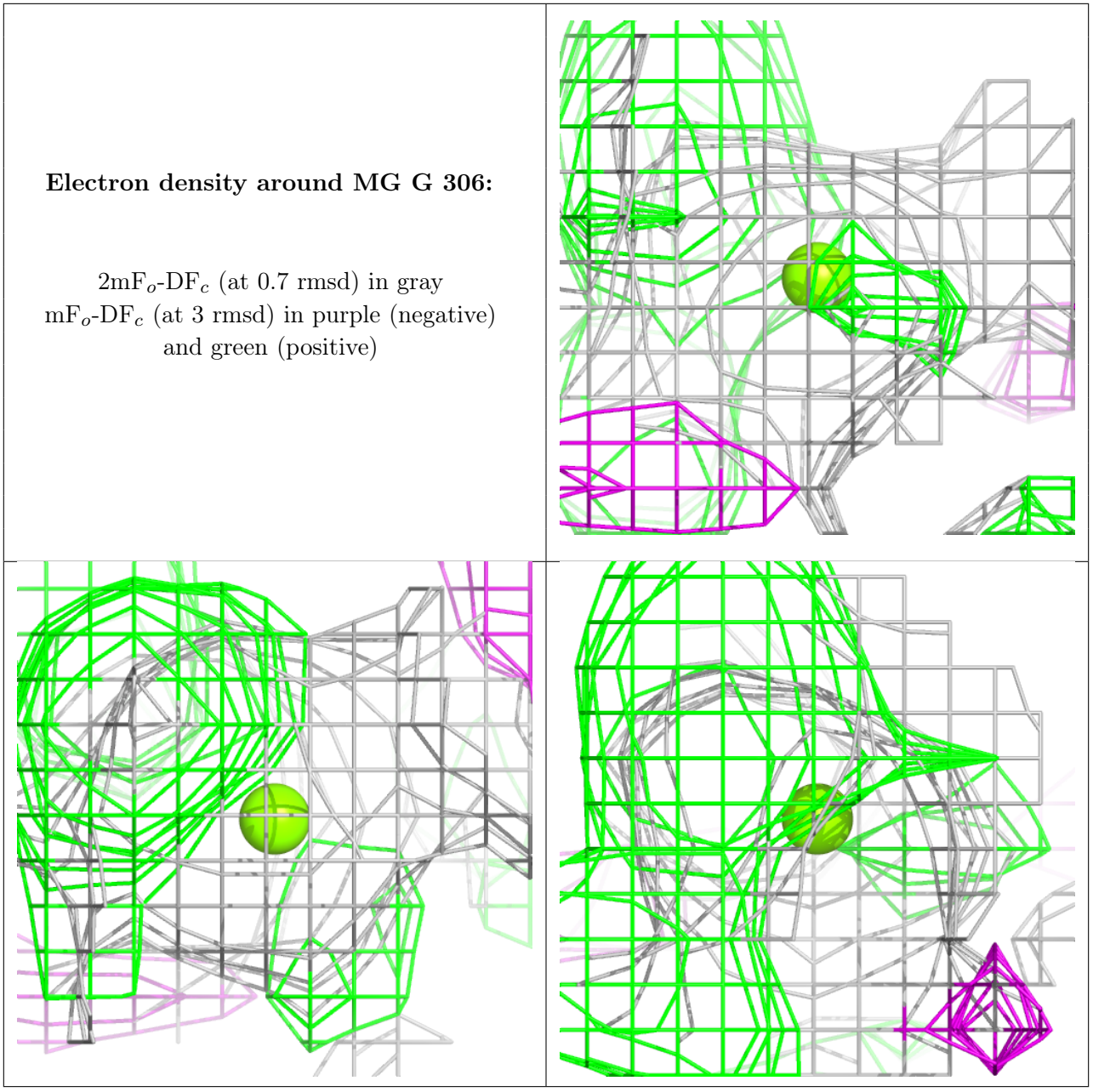






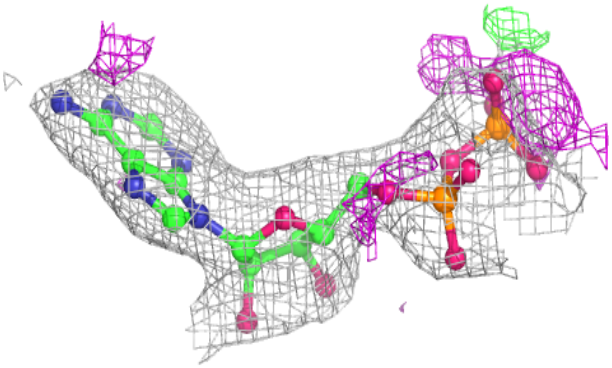
Electron density around MG G 306:

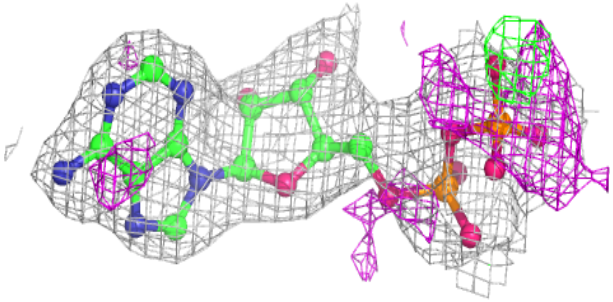
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

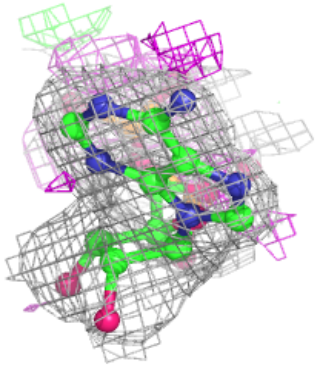


Electron density around ADP C 301:

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

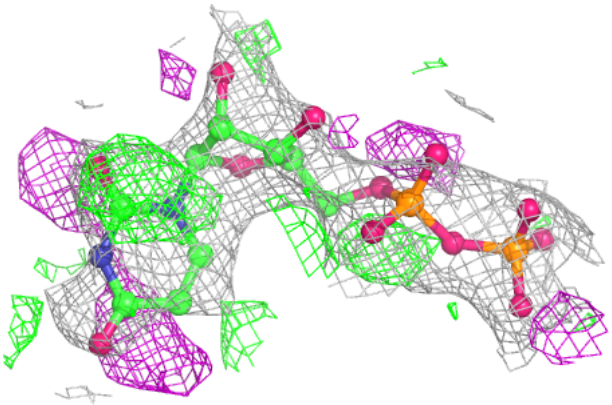


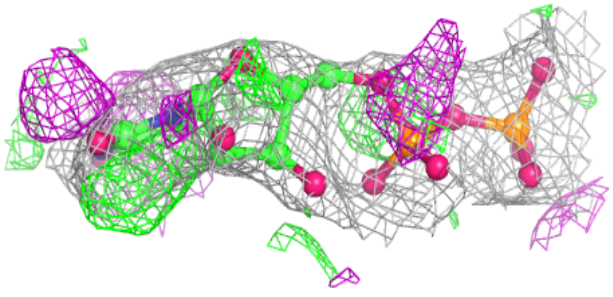


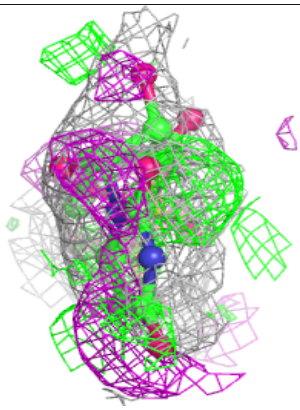


Electron density around UDP B 302:

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

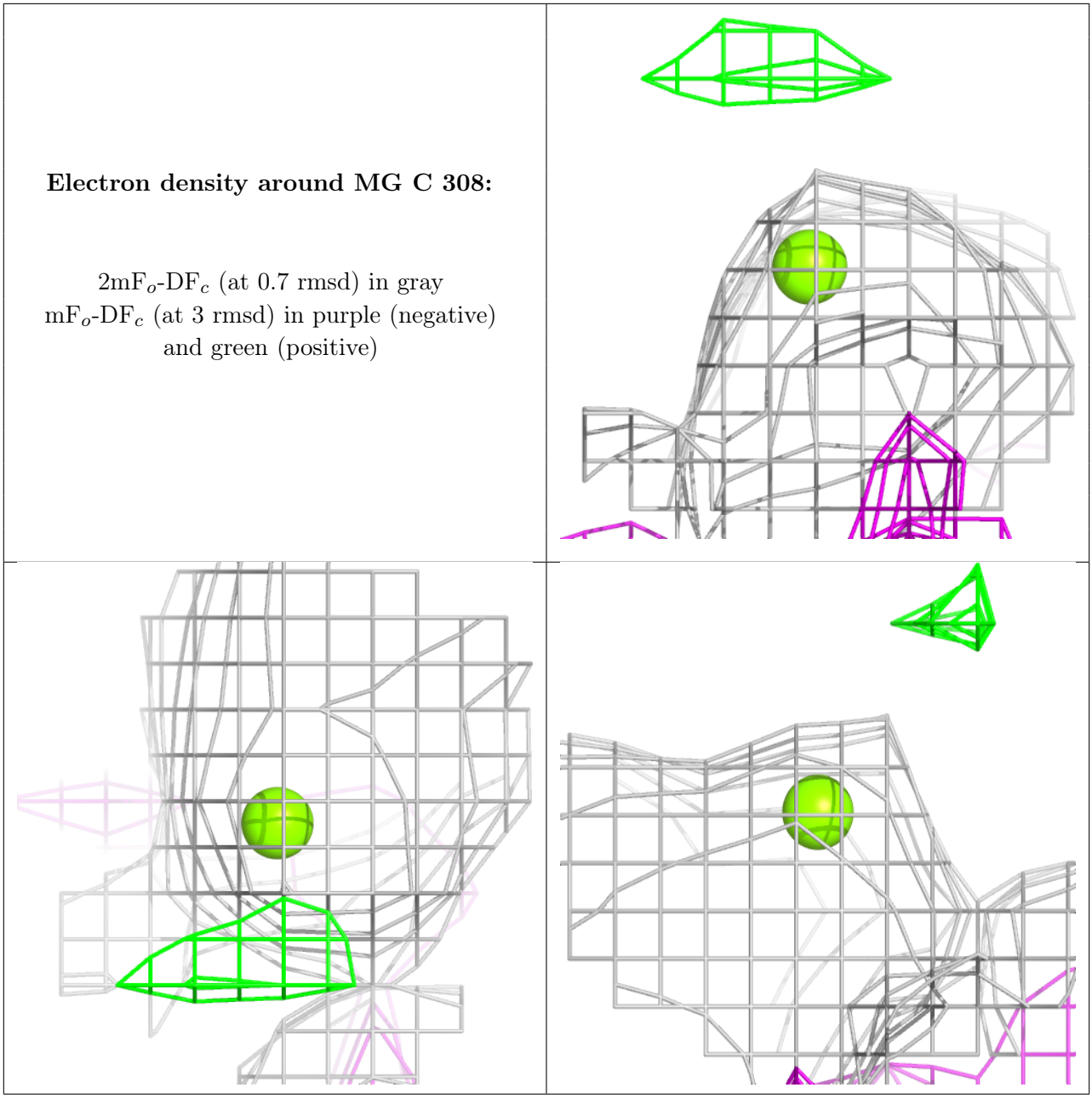






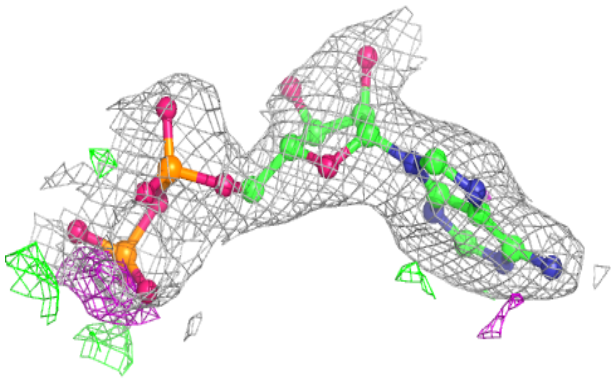
Electron density around MG C 308:

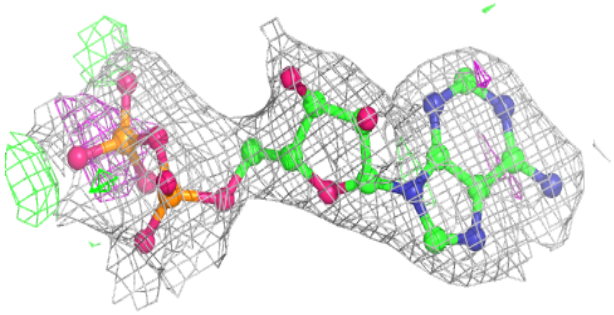
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

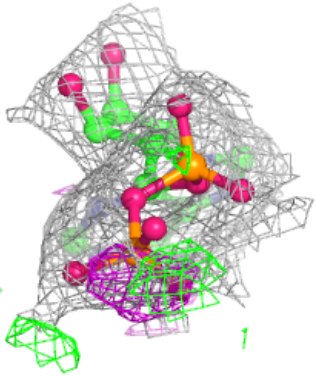


Electron density around ADP H 301:

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

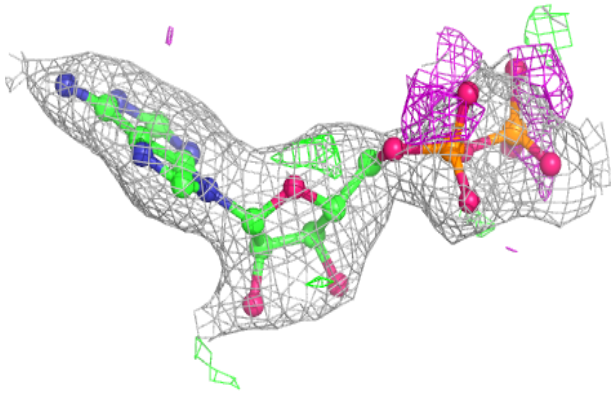


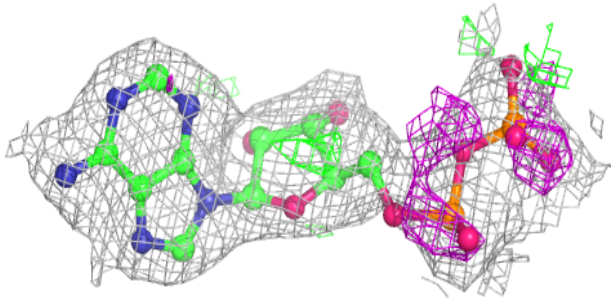


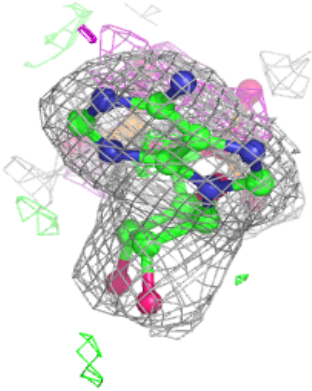


Electron density around ADP F 301:

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

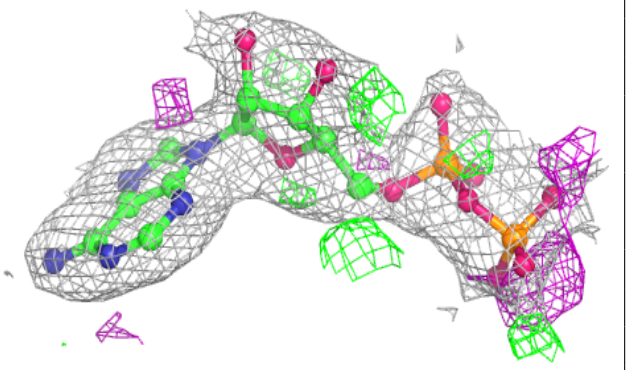


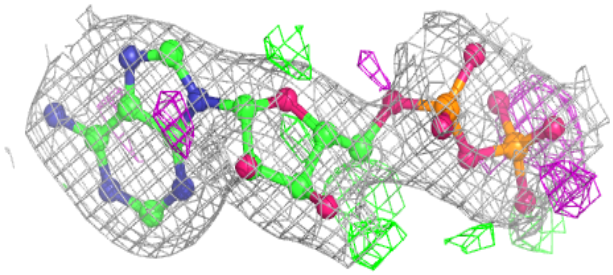


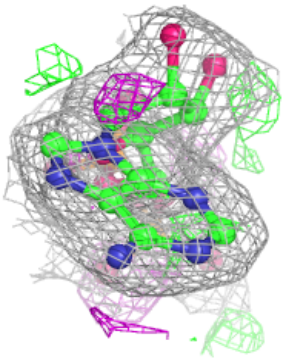


Electron density around ADP B 301:

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

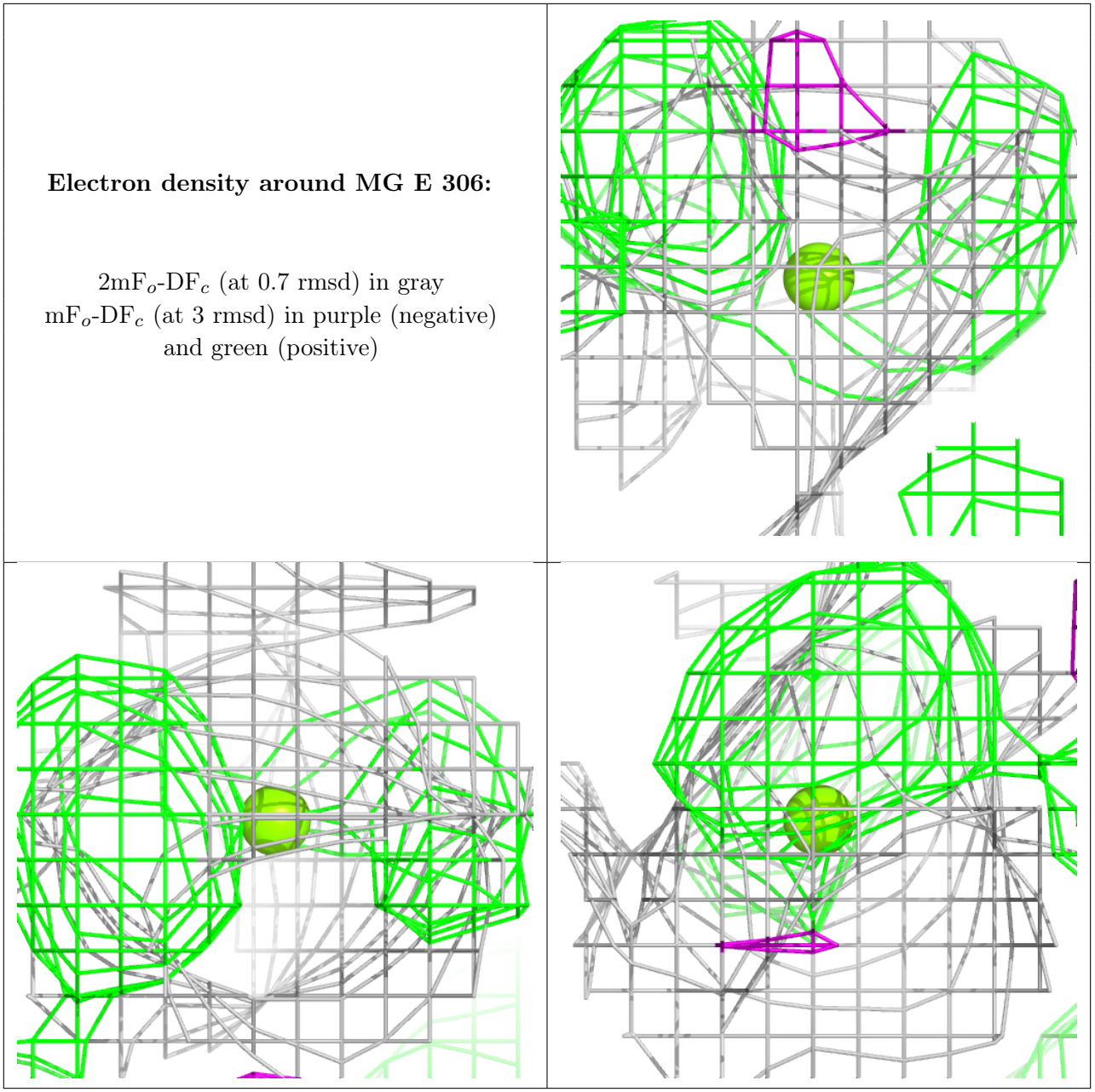






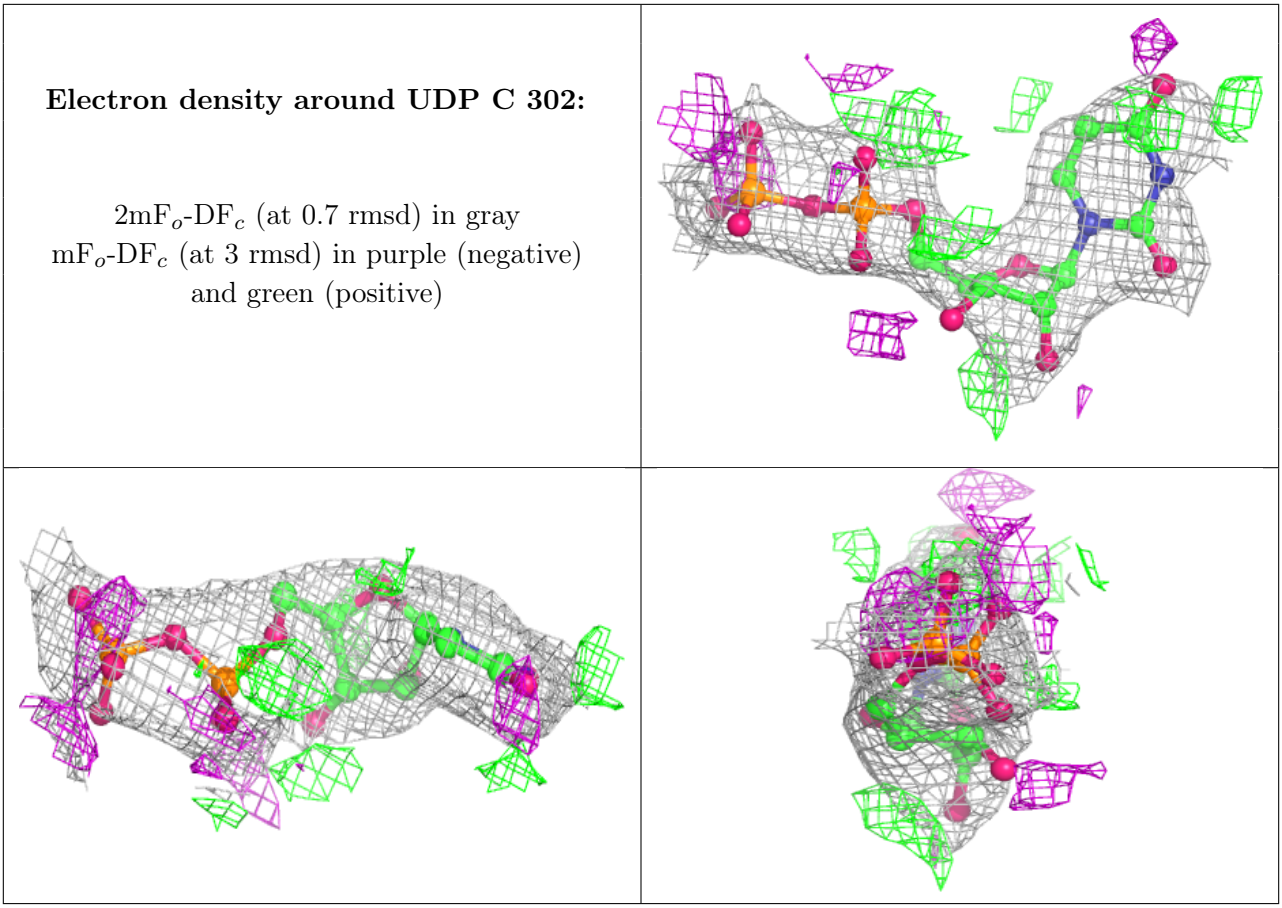
Electron density around MG E 306:

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



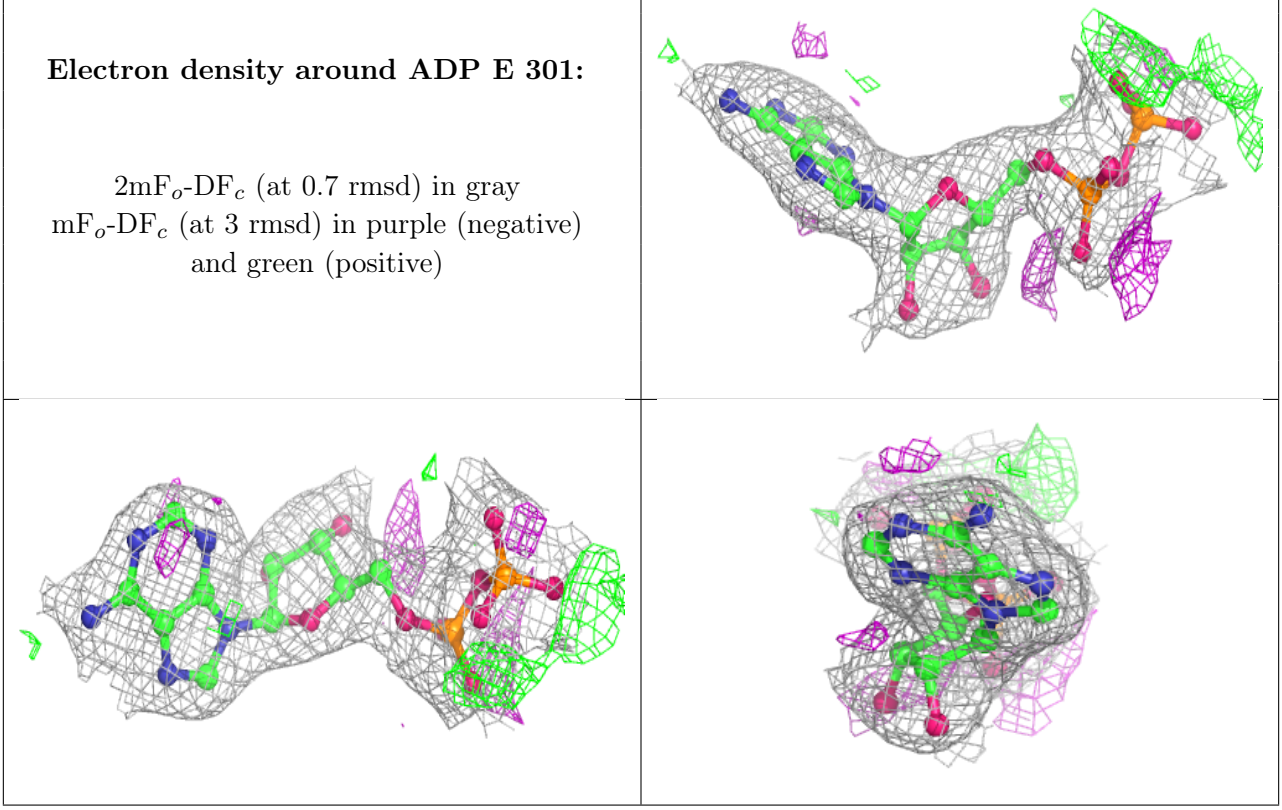
Electron density around UDP C 302:

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



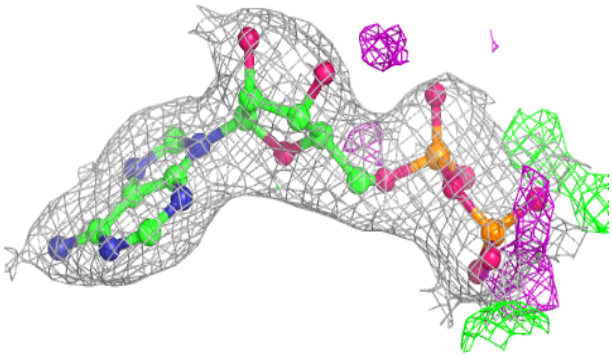
Electron density around ADP E 301:

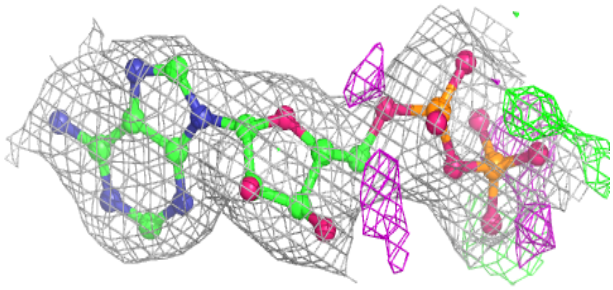
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

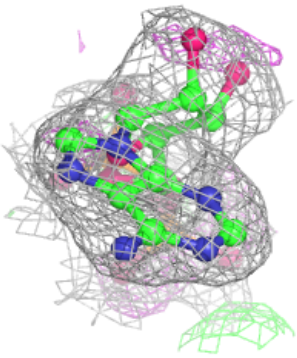


Electron density around ADP A 301:

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

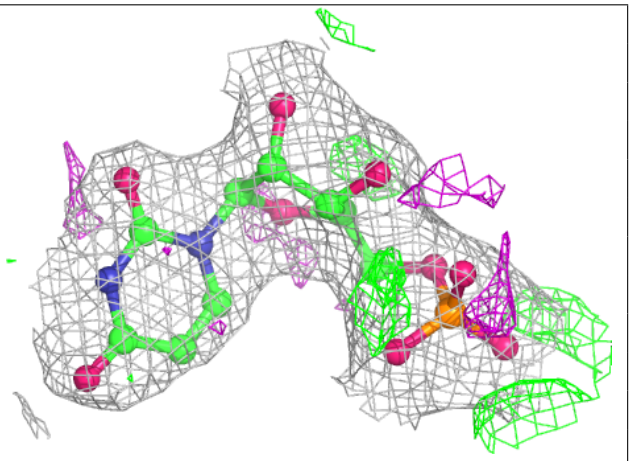


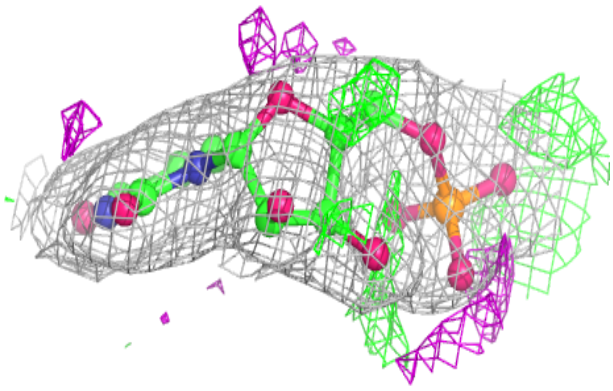


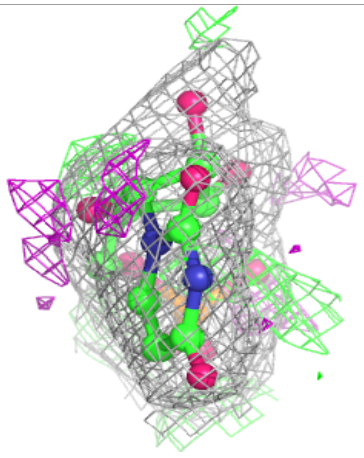


Electron density around U5P E 302:

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

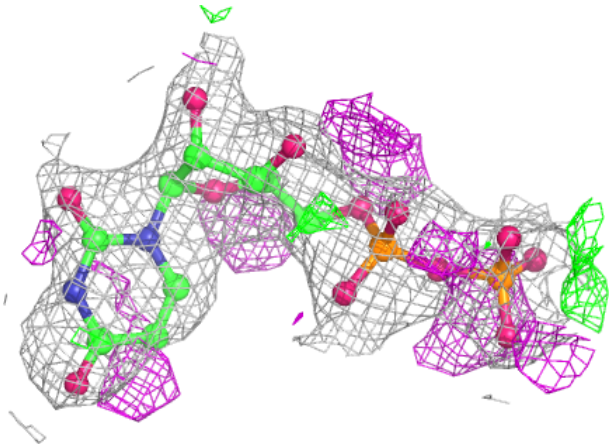


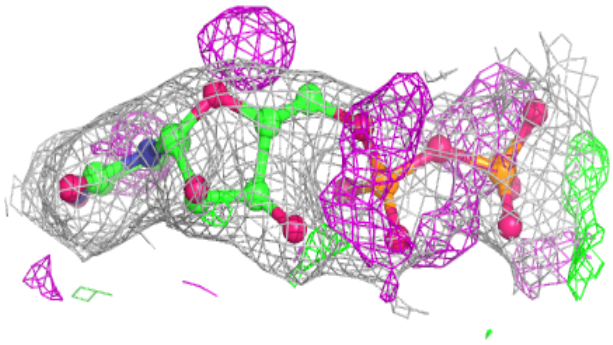


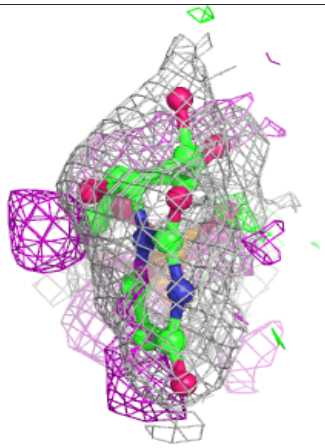


Electron density around UDP A 302:

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

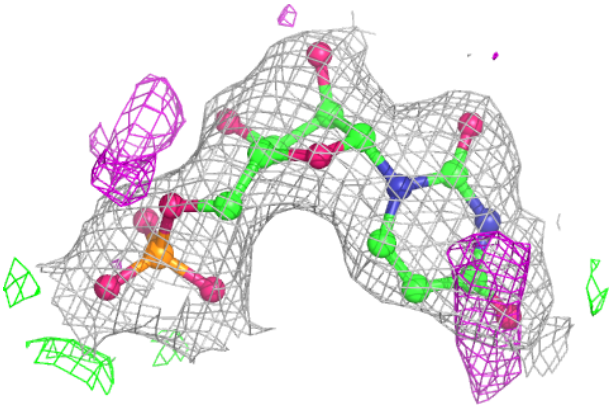


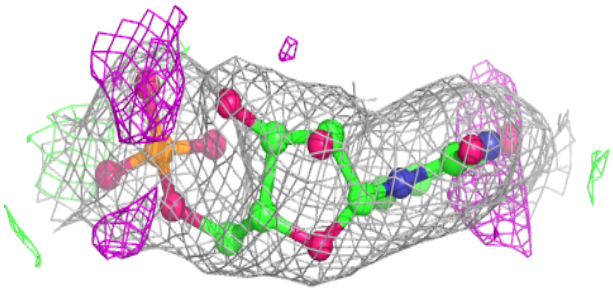


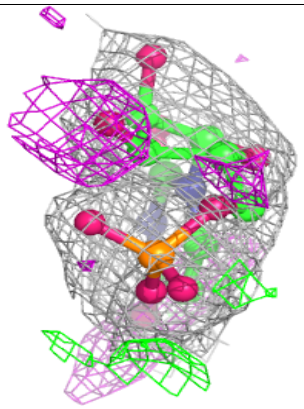


Electron density around U5P H 302:

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

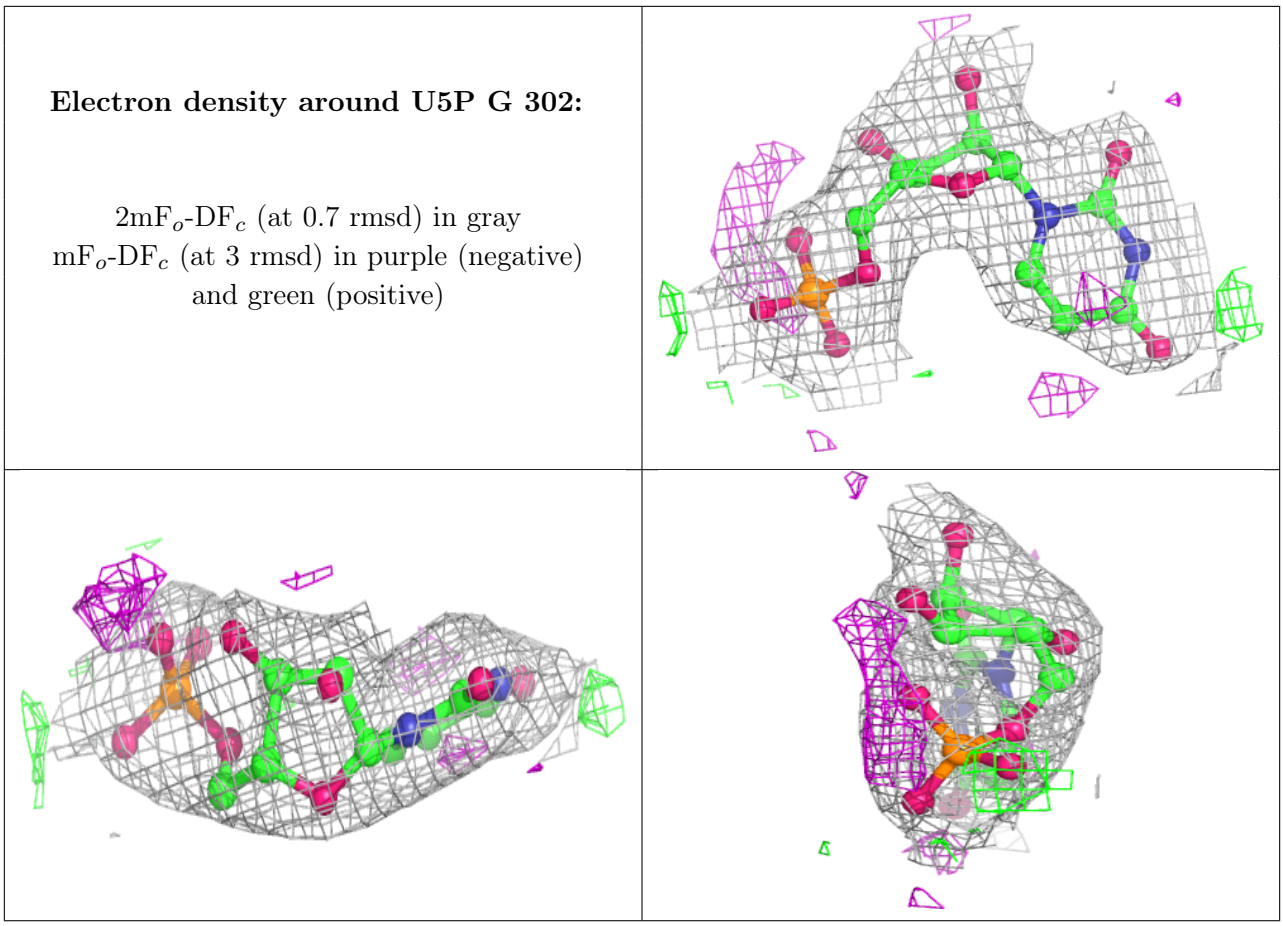






Electron density around U5P G 302:

$2mF_o$-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.