



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2020 – 12:20 PM EDT

PDB ID : 6VWP
Title : Crystal structure of E. coli guanosine kinase in complex with ppGpp
Authors : Wang, B.; Grant, R.A.; Laub, M.T.
Deposited on : 2020-02-20
Resolution : 3.45 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 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 : 2.14.6
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) : 2.14.6

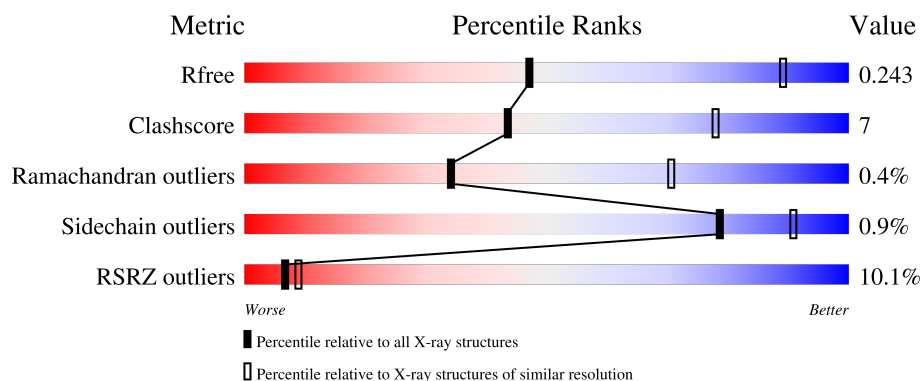
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	437	<div> <div>4%</div> <div>86%13%</div> </div>
1	B	437	<div> <div>5%</div> <div>82%15%</div> </div>
1	C	437	<div> <div>3%</div> <div>86%11%</div> </div>
1	D	437	<div> <div>7%</div> <div>83%16%</div> </div>
1	E	437	<div> <div>8%</div> <div>82%14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	437	
1	G	437	
1	H	437	

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
4	K	C	505	-	-	-	X
4	K	G	504	-	-	-	X
5	MG	D	505	-	-	-	X
5	MG	E	506	-	-	-	X
5	MG	F	505	-	-	-	X
5	MG	H	506	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 51473 atoms, of which 24272 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 Inosine-guanosine kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	435	Total	C	H	N	O	S	0	0	0
			6389	2148	2984	588	653	16			
1	B	428	Total	C	H	N	O	S	0	0	0
			6368	2123	3006	579	643	17			
1	C	429	Total	C	H	N	O	S	0	0	0
			6365	2120	3009	580	640	16			
1	D	435	Total	C	H	N	O	S	0	0	0
			6415	2148	3010	588	653	16			
1	E	422	Total	C	H	N	O	S	0	0	0
			6316	2089	3006	571	634	16			
1	F	412	Total	C	H	N	O	S	0	0	0
			6248	2039	3022	555	616	16			
1	G	421	Total	C	H	N	O	S	0	0	0
			6321	2095	3005	573	632	16			
1	H	408	Total	C	H	N	O	S	0	0	0
			6128	2023	2934	547	608	16			

There are 24 discrepancies between the modelled and reference sequences:

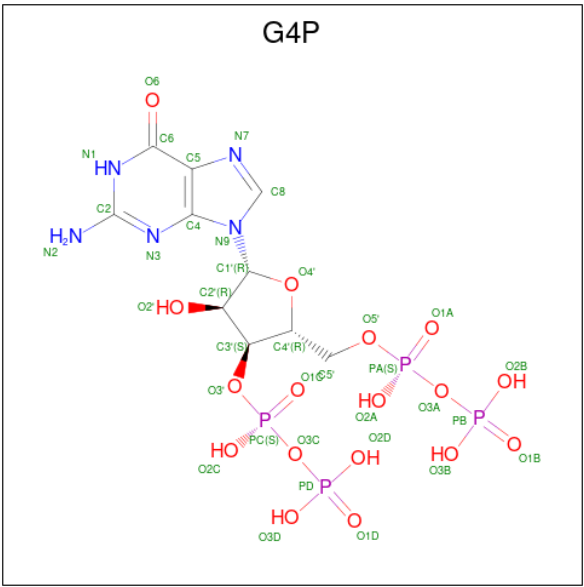
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P0AEW6
A	-1	SER	-	expression tag	UNP P0AEW6
A	0	HIS	-	expression tag	UNP P0AEW6
B	-2	GLY	-	expression tag	UNP P0AEW6
B	-1	SER	-	expression tag	UNP P0AEW6
B	0	HIS	-	expression tag	UNP P0AEW6
C	-2	GLY	-	expression tag	UNP P0AEW6
C	-1	SER	-	expression tag	UNP P0AEW6
C	0	HIS	-	expression tag	UNP P0AEW6
D	-2	GLY	-	expression tag	UNP P0AEW6
D	-1	SER	-	expression tag	UNP P0AEW6
D	0	HIS	-	expression tag	UNP P0AEW6
E	-2	GLY	-	expression tag	UNP P0AEW6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP P0AEW6
E	0	HIS	-	expression tag	UNP P0AEW6
F	-2	GLY	-	expression tag	UNP P0AEW6
F	-1	SER	-	expression tag	UNP P0AEW6
F	0	HIS	-	expression tag	UNP P0AEW6
G	-2	GLY	-	expression tag	UNP P0AEW6
G	-1	SER	-	expression tag	UNP P0AEW6
G	0	HIS	-	expression tag	UNP P0AEW6
H	-2	GLY	-	expression tag	UNP P0AEW6
H	-1	SER	-	expression tag	UNP P0AEW6
H	0	HIS	-	expression tag	UNP P0AEW6

- Molecule 2 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄) (labeled as "Ligand of Interest" by author).



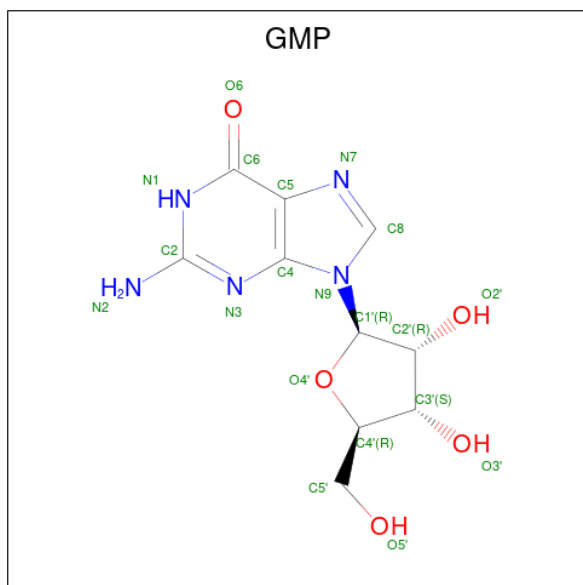
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 47	C 10	H 11	N 5	O 17	P 4	0	0
2	B	1	Total 47	C 10	H 11	N 5	O 17	P 4	0	0
2	C	1	Total 47	C 10	H 11	N 5	O 17	P 4	0	0
2	D	1	Total 47	C 10	H 11	N 5	O 17	P 4	0	0
2	E	1	Total 47	C 10	H 11	N 5	O 17	P 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	H	N	O	0	0
			47	10	11	5	17		
2	G	1	Total	C	H	N	O	0	0
			47	10	11	5	17		
2	H	1	Total	C	H	N	O	0	0
			47	10	11	5	17		

- Molecule 3 is GUANOSINE (three-letter code: GMP) (formula: $C_{10}H_{13}N_5O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	A	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	B	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	B	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	C	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	C	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	D	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	D	1	Total	C	H	N	O	0	0
			33	10	13	5	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	E	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	F	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	F	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	G	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	G	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	H	1	Total	C	H	N	O	0	0
			33	10	13	5	5		
3	H	1	Total	C	H	N	O	0	0
			33	10	13	5	5		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	E	2	Total	K	0	0
			2	2		
4	H	2	Total	K	0	0
			2	2		
4	B	2	Total	K	0	0
			2	2		
4	C	2	Total	K	0	0
			2	2		
4	A	1	Total	K	0	0
			1	1		
4	F	1	Total	K	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mg	0	0
			1	1		

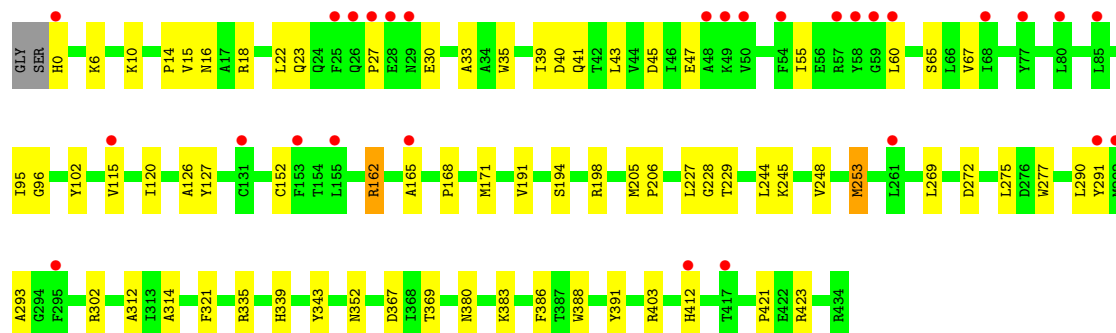
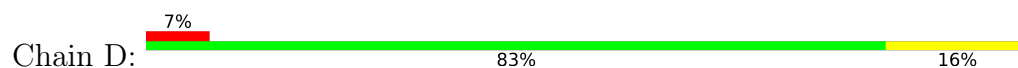
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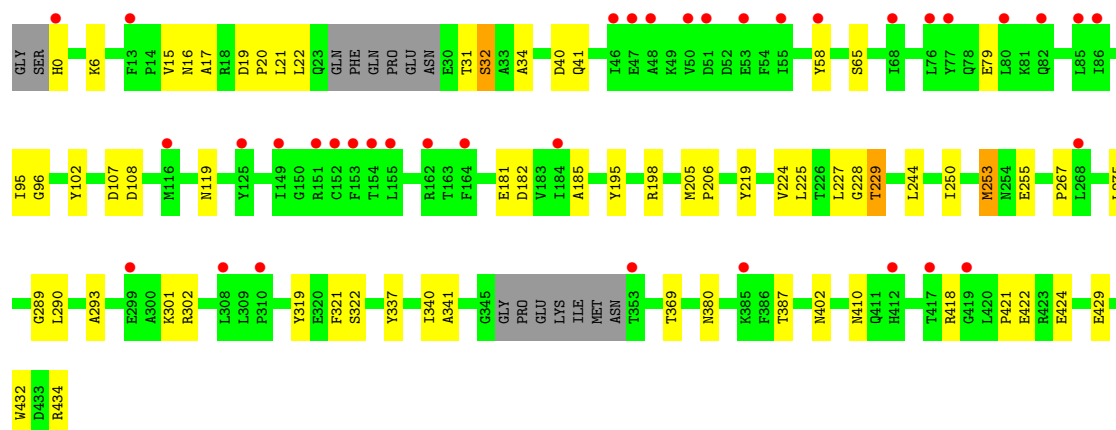
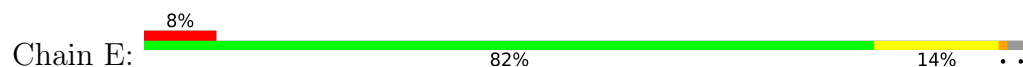
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 1	Mg 1	0	0
5	E	1	Total 1	Mg 1	0	0
5	H	1	Total 1	Mg 1	0	0
5	C	1	Total 1	Mg 1	0	0
5	A	1	Total 1	Mg 1	0	0
5	F	1	Total 1	Mg 1	0	0



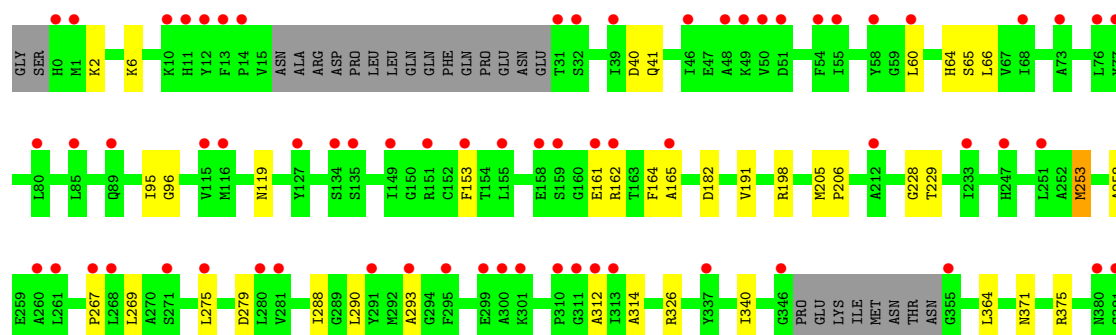
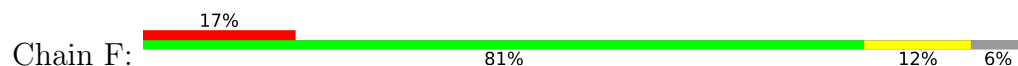
- Molecule 1: Inosine-guanosine kinase

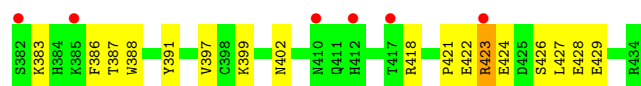


- Molecule 1: Inosine-guanosine kinase

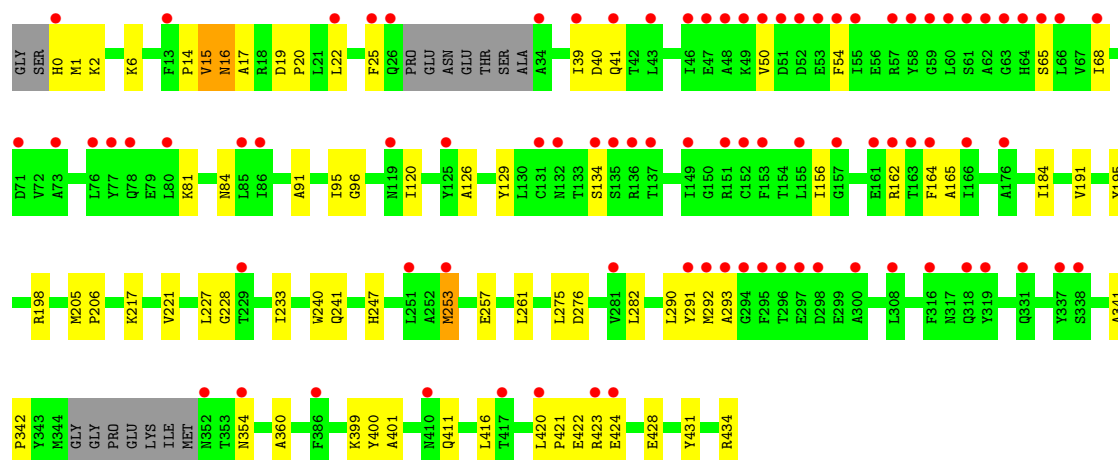
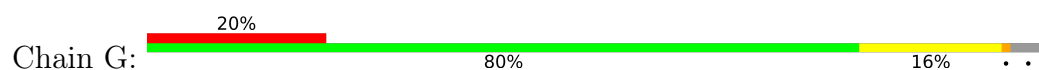


- Molecule 1: Inosine-guanosine kinase

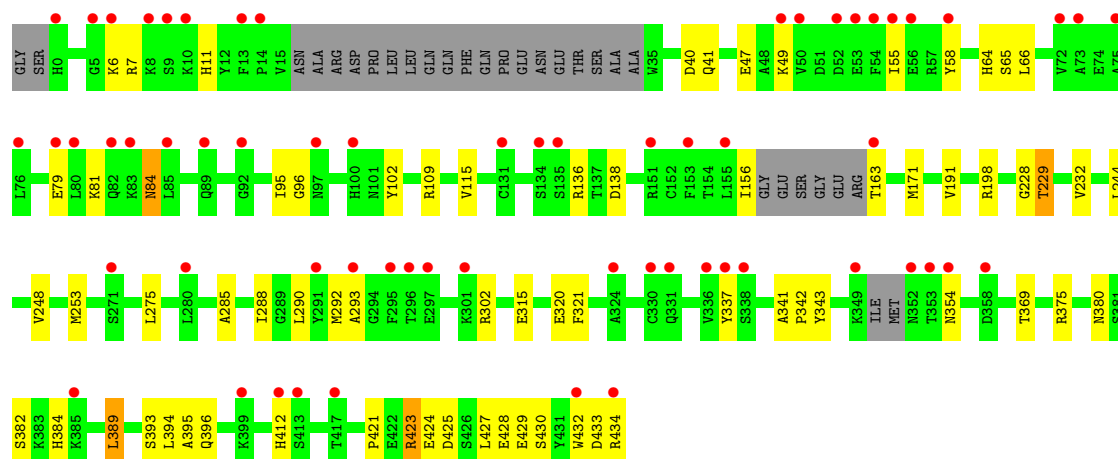
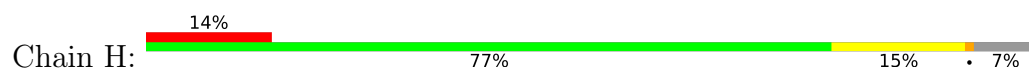




• Molecule 1: Inosine-guanosine kinase



• Molecule 1: Inosine-guanosine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.95Å 245.95Å 221.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.16 – 3.45 49.16 – 3.42	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.16-3.45) 94.0 (49.16-3.42)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.200 , 0.242 0.200 , 0.243	Depositor DCC
R_{free} test set	1991 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	133.5	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 108.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51473	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G4P, K, GMP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/3485	0.53	0/4734
1	B	0.35	0/3441	0.52	0/4670
1	C	0.36	1/3434 (0.0%)	0.52	0/4662
1	D	0.32	0/3485	0.51	0/4734
1	E	0.31	0/3385	0.50	0/4593
1	F	0.28	0/3300	0.49	0/4476
1	G	0.29	0/3392	0.50	0/4602
1	H	0.32	0/3268	0.52	0/4436
All	All	0.33	1/27190 (0.0%)	0.51	0/36907

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	419	GLY	C-N	-5.51	1.21	1.34

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	3405	2984	3303	48	0
1	B	3362	3006	3273	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3356	3009	3262	33	0
1	D	3405	3010	3303	49	0
1	E	3310	3006	3224	52	0
1	F	3226	3022	3143	45	0
1	G	3316	3005	3229	54	0
1	H	3194	2934	3103	66	0
2	A	36	11	11	0	0
2	B	36	11	11	0	0
2	C	36	11	11	0	0
2	D	36	11	11	3	0
2	E	36	11	11	1	0
2	F	36	11	11	1	0
2	G	36	11	11	0	0
2	H	36	11	11	0	0
3	A	40	26	26	0	0
3	B	40	26	26	0	0
3	C	40	26	26	0	0
3	D	40	26	26	0	0
3	E	40	26	26	2	0
3	F	40	26	26	1	0
3	G	40	26	26	1	0
3	H	40	26	26	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
All	All	27201	24272	26136	356	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 7.

All (356) 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:C:424:GLU:OE2	1:D:423:ARG:HG3	1.60	1.01
1:A:421:PRO:HB3	1:B:422:GLU:HB3	1.47	0.96
1:A:109:ARG:NH2	1:A:138:ASP:OD2	2.12	0.82
1:B:228:GLY:O	1:B:229:THR:OG1	1.97	0.82
1:E:341:ALA:O	1:E:402:ASN:ND2	2.14	0.80
1:E:424:GLU:OE1	1:F:423:ARG:HB3	1.80	0.80
1:A:424:GLU:HG2	1:B:6:LYS:HZ1	1.44	0.80
1:H:423:ARG:NH1	1:H:423:ARG:HB2	1.99	0.77
1:F:427:LEU:HD12	1:H:382:SER:HB3	1.66	0.77
1:E:65:SER:O	1:E:198:ARG:NH1	2.18	0.76
1:B:47:GLU:OE1	1:B:412:HIS:NE2	2.18	0.76
1:A:343:TYR:OH	1:B:428:GLU:HG2	1.86	0.76
1:E:19:ASP:OD1	1:E:20:PRO:HD2	1.86	0.75
1:H:228:GLY:O	1:H:229:THR:OG1	2.05	0.75
1:H:102:TYR:OH	1:H:369:THR:HG21	1.86	0.75
1:F:6:LYS:NZ	1:F:421:PRO:O	2.21	0.74
1:H:47:GLU:OE1	1:H:412:HIS:NE2	2.21	0.74
1:A:352:ASN:O	1:A:409:LEU:HD23	1.87	0.74
1:F:40:ASP:OD1	1:F:41:GLN:N	2.20	0.74
1:A:21:LEU:H	1:A:21:LEU:HD12	1.52	0.74
1:A:40:ASP:OD1	1:A:41:GLN:N	2.21	0.73
1:F:228:GLY:O	1:F:229:THR:OG1	2.04	0.73
1:A:421:PRO:CB	1:B:422:GLU:HB3	2.19	0.73
1:G:227:LEU:HD12	1:G:253:MET:HG3	1.71	0.73
1:B:40:ASP:OD1	1:B:41:GLN:N	2.22	0.72
1:H:424:GLU:HG3	1:H:428:GLU:HB2	1.69	0.72
1:E:198:ARG:NH2	3:E:502:GMP:O6	2.22	0.72
1:B:17:ALA:HA	1:B:22:LEU:HD23	1.73	0.71
1:D:228:GLY:O	1:D:229:THR:OG1	2.07	0.71
1:G:275:LEU:HD11	1:G:293:ALA:HB1	1.73	0.71
1:A:224:VAL:HG22	1:A:250:ILE:HB	1.72	0.70
1:A:220:ASN:OD1	1:A:328:LYS:NZ	2.22	0.70
1:A:228:GLY:O	1:A:229:THR:OG1	2.07	0.69
1:E:302:ARG:HD2	1:E:321:PHE:O	1.93	0.68
1:G:6:LYS:NZ	1:G:421:PRO:O	2.24	0.68
1:G:241:GLN:NE2	1:G:261:LEU:O	2.26	0.68
1:D:269:LEU:HD21	1:D:312:ALA:HB1	1.76	0.68
1:F:65:SER:O	1:F:198:ARG:NH1	2.25	0.68
1:E:40:ASP:OD1	1:E:41:GLN:N	2.27	0.68
1:C:40:ASP:OD1	1:C:41:GLN:N	2.27	0.68
1:D:33:ALA:HB1	1:D:35:TRP:HZ3	1.59	0.67
1:H:55:ILE:HD12	1:H:163:THR:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:TYR:OH	1:C:369:THR:HG21	1.94	0.67
1:A:50:VAL:O	1:A:157:GLY:HA2	1.94	0.67
1:H:292:MET:HB3	1:H:394:LEU:HD11	1.77	0.67
1:A:6:LYS:NZ	1:A:421:PRO:O	2.28	0.66
1:G:40:ASP:OD1	1:G:41:GLN:N	2.29	0.66
1:H:40:ASP:OD1	1:H:41:GLN:N	2.28	0.66
1:C:47:GLU:OE1	1:C:412:HIS:NE2	2.28	0.66
1:D:47:GLU:OE1	1:D:412:HIS:NE2	2.29	0.66
1:H:424:GLU:HG3	1:H:428:GLU:CB	2.25	0.66
1:D:40:ASP:OD1	1:D:41:GLN:N	2.28	0.65
1:E:40:ASP:OD2	1:E:96:GLY:N	2.29	0.65
1:H:389:LEU:O	1:H:389:LEU:HD12	1.98	0.64
1:H:424:GLU:HB2	1:H:428:GLU:HG3	1.78	0.64
1:G:162:ARG:HB2	1:G:354:ASN:ND2	2.12	0.64
1:G:423:ARG:NH2	1:H:432:TRP:HB2	2.12	0.64
1:H:423:ARG:HH11	1:H:423:ARG:HB2	1.63	0.64
1:G:399:LYS:NZ	1:H:434:ARG:O	2.26	0.64
1:G:428:GLU:HG2	1:H:343:TYR:OH	1.99	0.63
1:E:17:ALA:O	1:E:22:LEU:HD11	1.98	0.63
1:C:95:ILE:HD12	1:C:191:VAL:HG12	1.80	0.63
1:B:314:ALA:HB2	1:D:380:ASN:HB3	1.80	0.63
1:E:432:TRP:HA	1:F:399:LYS:HE2	1.79	0.63
1:G:40:ASP:OD2	1:G:96:GLY:N	2.31	0.63
1:C:14:PRO:HB3	1:C:22:LEU:HD22	1.81	0.62
1:D:14:PRO:CB	1:D:22:LEU:HD11	2.29	0.62
1:A:422:GLU:HG2	1:B:421:PRO:HB3	1.81	0.61
1:G:227:LEU:HD13	1:G:233:ILE:HD11	1.82	0.61
1:F:95:ILE:HD12	1:F:191:VAL:HG12	1.81	0.61
1:G:227:LEU:HD13	1:G:233:ILE:CD1	2.30	0.61
1:H:58:TYR:OH	1:H:79:GLU:OE1	2.15	0.61
1:C:65:SER:O	1:C:198:ARG:NH1	2.31	0.61
1:E:102:TYR:OH	1:E:369:THR:HG21	2.01	0.60
1:D:102:TYR:OH	1:D:369:THR:HG21	2.01	0.60
1:C:290:LEU:O	1:C:290:LEU:HD12	2.02	0.59
1:H:244:LEU:HD23	1:H:248:VAL:HG21	1.83	0.59
1:A:272:ASP:OD2	1:A:337:TYR:OH	2.13	0.59
1:E:432:TRP:O	1:F:399:LYS:NZ	2.32	0.58
1:G:17:ALA:O	1:G:22:LEU:HD11	2.03	0.58
1:D:290:LEU:O	1:D:290:LEU:HD12	2.02	0.58
1:H:275:LEU:HD11	1:H:293:ALA:HB1	1.85	0.58
1:A:417:THR:O	1:B:418:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:LEU:HD11	1:D:293:ALA:HB1	1.85	0.58
1:H:424:GLU:HB2	1:H:428:GLU:HB2	1.84	0.58
1:B:6:LYS:NZ	1:B:421:PRO:O	2.37	0.57
1:C:275:LEU:HD11	1:C:293:ALA:HB1	1.85	0.57
1:D:60:LEU:HD11	1:D:165:ALA:HB2	1.86	0.57
1:E:225:LEU:HD23	1:E:244:LEU:HD21	1.85	0.57
1:E:410:ASN:OD1	1:H:380:ASN:ND2	2.37	0.57
1:D:314:ALA:HB2	1:E:380:ASN:HB3	1.85	0.57
1:H:433:ASP:OD1	1:H:434:ARG:N	2.37	0.57
1:B:423:ARG:HG3	1:B:423:ARG:HH11	1.70	0.57
1:E:119:ASN:ND2	1:F:119:ASN:OD1	2.38	0.57
1:G:65:SER:OG	3:G:502:GMP:N7	2.31	0.57
1:B:17:ALA:HA	1:B:22:LEU:CD2	2.34	0.56
1:G:411:GLN:OE1	1:G:416:LEU:HD23	2.05	0.56
1:D:65:SER:O	1:D:198:ARG:NH1	2.31	0.56
1:A:65:SER:O	1:A:198:ARG:NH1	2.38	0.55
1:G:434:ARG:O	1:G:434:ARG:HG2	2.05	0.55
1:E:424:GLU:OE1	1:F:423:ARG:NE	2.39	0.55
1:G:233:ILE:HG23	1:G:240:TRP:CD1	2.42	0.55
1:G:290:LEU:HD12	1:G:290:LEU:O	2.06	0.55
1:H:40:ASP:OD2	1:H:96:GLY:N	2.37	0.55
1:B:157:GLY:O	1:B:158:GLU:HB2	2.06	0.55
1:A:424:GLU:HG2	1:B:6:LYS:NZ	2.20	0.54
1:D:95:ILE:HD12	1:D:191:VAL:HG12	1.89	0.54
1:A:422:GLU:HG2	1:B:421:PRO:CB	2.37	0.54
1:E:424:GLU:HB3	1:F:6:LYS:HZ1	1.70	0.54
1:E:0:HIS:HA	1:E:16:ASN:HA	1.89	0.54
1:G:156:ILE:HG12	1:G:162:ARG:HG2	1.90	0.54
1:H:81:LYS:O	1:H:84:ASN:ND2	2.41	0.54
1:C:205:MET:HB3	1:C:206:PRO:HD3	1.90	0.54
1:E:58:TYR:OH	1:E:79:GLU:OE1	2.21	0.54
1:H:424:GLU:HB2	1:H:428:GLU:CB	2.38	0.54
1:E:19:ASP:OD1	1:E:21:LEU:HD12	2.07	0.53
1:F:269:LEU:HD21	1:F:312:ALA:HB1	1.90	0.53
1:C:14:PRO:CB	1:C:22:LEU:HD22	2.38	0.53
1:G:424:GLU:HG3	1:H:6:LYS:HZ1	1.73	0.53
1:D:162:ARG:NH2	1:D:352:ASN:HA	2.23	0.53
1:H:228:GLY:O	1:H:229:THR:CB	2.57	0.53
1:C:19:ASP:HB3	1:C:22:LEU:HB3	1.91	0.53
1:D:269:LEU:HD21	1:D:312:ALA:CB	2.39	0.53
1:A:40:ASP:OD2	1:A:96:GLY:N	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:GLU:HG3	1:F:423:ARG:NH2	2.23	0.53
1:C:429:GLU:HG3	1:D:423:ARG:HD3	1.90	0.52
1:C:24:GLN:HG2	1:F:267:PRO:HD2	1.90	0.52
1:D:0:HIS:HA	1:D:16:ASN:HA	1.92	0.52
1:A:347:PRO:HB3	1:A:410:ASN:OD1	2.10	0.52
1:D:27:PRO:O	1:D:30:GLU:HG2	2.10	0.52
1:F:6:LYS:CE	1:F:421:PRO:O	2.57	0.52
1:B:228:GLY:O	1:B:229:THR:CB	2.57	0.52
1:B:360:ALA:HB1	1:B:401:ALA:HB1	1.91	0.52
1:D:10:LYS:HE2	2:D:501:G4P:O2D	2.10	0.51
1:A:95:ILE:HD12	1:A:191:VAL:HG12	1.91	0.51
1:C:425:ASP:OD1	1:C:427:LEU:HB3	2.10	0.51
1:E:224:VAL:HG22	1:E:250:ILE:HB	1.92	0.51
1:H:65:SER:O	1:H:198:ARG:NH1	2.44	0.51
1:C:244:LEU:HD23	1:C:248:VAL:HG21	1.93	0.51
1:F:364:LEU:HD13	1:F:397:VAL:HG11	1.93	0.51
1:B:49:LYS:HG2	1:B:156:ILE:HB	1.93	0.51
1:H:430:SER:O	1:H:434:ARG:HG3	2.11	0.51
1:D:244:LEU:HD23	1:D:248:VAL:HG21	1.92	0.51
1:E:301:LYS:HD2	1:E:319:TYR:CE2	2.46	0.51
1:H:424:GLU:CG	1:H:428:GLU:HB2	2.37	0.51
1:A:107:ASP:OD1	1:B:417:THR:OG1	2.27	0.51
1:C:20:PRO:HB2	1:F:288:ILE:HD13	1.93	0.51
1:D:40:ASP:OD2	1:D:96:GLY:N	2.42	0.51
1:E:228:GLY:O	1:E:229:THR:HG23	2.10	0.51
1:B:224:VAL:HG22	1:B:250:ILE:HB	1.93	0.50
1:E:275:LEU:HD11	1:E:293:ALA:HB1	1.93	0.50
1:F:40:ASP:OD2	1:F:96:GLY:N	2.43	0.50
1:A:47:GLU:OE1	1:A:412:HIS:NE2	2.44	0.50
1:H:6:LYS:CE	1:H:421:PRO:O	2.59	0.50
1:G:95:ILE:HD12	1:G:191:VAL:HG12	1.93	0.50
1:F:198:ARG:NH2	3:F:502:GMP:O6	2.45	0.50
1:G:360:ALA:HB1	1:G:401:ALA:HB1	1.94	0.50
1:E:228:GLY:O	1:E:229:THR:OG1	2.27	0.49
1:E:421:PRO:HB3	1:F:422:GLU:HG3	1.93	0.49
1:G:400:TYR:HE1	1:G:420:LEU:HD12	1.78	0.49
1:A:276:ASP:OD1	1:A:335:ARG:NH2	2.38	0.49
1:G:19:ASP:OD1	1:G:20:PRO:HD2	2.13	0.49
1:E:6:LYS:NZ	1:E:421:PRO:O	2.43	0.49
1:H:229:THR:OG1	1:H:232:VAL:HG23	2.13	0.49
1:E:6:LYS:HD2	1:E:421:PRO:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:LEU:HD11	1:F:293:ALA:HB1	1.93	0.49
1:D:383:LYS:CE	2:D:501:G4P:O2B	2.61	0.49
1:F:269:LEU:HD21	1:F:312:ALA:CB	2.43	0.49
1:H:109:ARG:NH2	1:H:138:ASP:OD2	2.43	0.49
1:H:302:ARG:NH1	1:H:321:PHE:O	2.46	0.49
1:H:321:PHE:HA	1:H:393:SER:OG	2.13	0.49
1:G:14:PRO:HB3	1:G:22:LEU:HD23	1.94	0.48
1:H:424:GLU:HB2	1:H:428:GLU:CG	2.41	0.48
1:G:65:SER:O	1:G:198:ARG:NH1	2.45	0.48
1:H:7:ARG:HD2	1:H:396:GLN:OE1	2.14	0.48
1:G:65:SER:HA	1:G:164:PHE:HB2	1.95	0.48
1:A:76:LEU:O	1:A:76:LEU:HD23	2.12	0.48
1:B:275:LEU:HD11	1:B:293:ALA:HB1	1.95	0.48
1:A:340:ILE:HG21	1:A:402:ASN:HB2	1.95	0.48
1:H:430:SER:O	1:H:433:ASP:OD1	2.32	0.48
1:A:364:LEU:HD13	1:A:397:VAL:HG11	1.95	0.48
1:B:26:GLN:HG2	1:B:27:PRO:HD2	1.96	0.48
1:G:423:ARG:HH21	1:H:429:GLU:HA	1.79	0.48
1:F:371:ASN:O	1:F:375:ARG:HB2	2.14	0.48
1:C:420:LEU:HD12	1:C:421:PRO:HD2	1.95	0.47
1:D:115:VAL:HG21	1:D:171:MET:HA	1.97	0.47
1:E:418:ARG:HD2	1:F:2:LYS:HE2	1.97	0.47
1:F:65:SER:HA	1:F:164:PHE:HB2	1.96	0.47
1:H:290:LEU:O	1:H:290:LEU:HD12	2.15	0.47
1:B:22:LEU:O	1:B:26:GLN:N	2.48	0.47
1:B:31:THR:O	1:B:32:SER:HB2	2.14	0.47
1:C:290:LEU:C	1:C:290:LEU:HD12	2.34	0.47
1:E:31:THR:O	1:E:32:SER:HB3	2.14	0.47
1:A:228:GLY:O	1:A:229:THR:CB	2.62	0.47
1:H:95:ILE:HD12	1:H:191:VAL:HG12	1.97	0.47
1:B:420:LEU:HB3	1:B:421:PRO:HD2	1.97	0.47
1:B:6:LYS:CE	1:B:421:PRO:O	2.63	0.47
1:D:14:PRO:HB2	1:D:22:LEU:HD11	1.96	0.47
1:D:18:ARG:HA	1:D:23:GLN:NE2	2.30	0.47
1:F:427:LEU:HD12	1:H:382:SER:CB	2.41	0.47
1:F:60:LEU:HD11	1:F:165:ALA:HB2	1.97	0.47
1:D:194:SER:OG	1:D:228:GLY:N	2.48	0.46
1:F:205:MET:HB3	1:F:206:PRO:HD3	1.97	0.46
1:A:182:ASP:OD1	1:A:182:ASP:N	2.46	0.46
1:D:302:ARG:NH1	1:D:321:PHE:O	2.48	0.46
1:H:320:GLU:HG2	1:H:395:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:GLU:HB2	1:E:267:PRO:HG3	1.98	0.46
1:G:424:GLU:HG3	1:H:6:LYS:NZ	2.31	0.46
1:G:422:GLU:HB3	1:H:421:PRO:CB	2.46	0.46
1:C:40:ASP:OD2	1:C:96:GLY:N	2.43	0.46
1:F:340:ILE:HG21	1:F:402:ASN:HB2	1.98	0.46
1:E:185:ALA:HB2	1:E:219:TYR:CE2	2.51	0.46
1:F:182:ASP:N	1:F:182:ASP:OD1	2.48	0.46
1:A:17:ALA:HA	1:A:22:LEU:HD23	1.98	0.46
1:D:43:LEU:HD21	1:D:152:CYS:HB2	1.98	0.46
1:F:290:LEU:HD12	1:F:290:LEU:O	2.16	0.46
1:G:162:ARG:HB2	1:G:354:ASN:HD21	1.79	0.46
1:B:22:LEU:HD21	1:B:377:ASN:ND2	2.31	0.45
1:B:382:SER:HB3	1:H:315:GLU:OE1	2.16	0.45
1:B:40:ASP:OD2	1:B:96:GLY:N	2.46	0.45
1:C:428:GLU:HG2	1:D:343:TYR:OH	2.16	0.45
1:F:424:GLU:HB2	1:F:428:GLU:HB3	1.97	0.45
1:H:393:SER:HB3	1:H:396:GLN:HG3	1.98	0.45
1:B:423:ARG:HG3	1:B:423:ARG:NH1	2.30	0.45
1:E:228:GLY:O	1:E:229:THR:CB	2.64	0.45
1:H:424:GLU:CB	1:H:428:GLU:HB2	2.46	0.45
1:B:290:LEU:HD12	1:B:290:LEU:O	2.15	0.45
1:E:225:LEU:HD23	1:E:244:LEU:CD2	2.47	0.45
1:G:195:TYR:CZ	1:G:228:GLY:HA3	2.52	0.45
1:G:290:LEU:C	1:G:290:LEU:HD12	2.37	0.45
1:D:383:LYS:HE3	2:D:501:G4P:O2B	2.17	0.45
1:E:181:GLU:OE2	1:E:219:TYR:OH	2.32	0.45
1:G:81:LYS:O	1:G:84:ASN:ND2	2.49	0.45
1:H:11:HIS:CE1	1:H:382:SER:HB2	2.52	0.45
1:A:6:LYS:CE	1:A:421:PRO:O	2.65	0.45
1:B:115:VAL:HG21	1:B:171:MET:HA	1.98	0.45
1:C:95:ILE:CD1	1:C:191:VAL:HG12	2.45	0.45
1:B:269:LEU:HD21	1:B:312:ALA:CB	2.47	0.45
1:E:182:ASP:OD1	1:E:182:ASP:N	2.50	0.45
1:A:423:ARG:HB2	1:B:424:GLU:OE1	2.17	0.44
1:B:65:SER:O	1:B:198:ARG:NH1	2.45	0.44
1:C:182:ASP:N	1:C:182:ASP:OD1	2.49	0.44
1:C:228:GLY:O	1:C:229:THR:OG1	2.22	0.44
1:D:33:ALA:HB1	1:D:35:TRP:CZ3	2.45	0.44
1:G:422:GLU:HB3	1:H:421:PRO:HB3	1.98	0.44
1:F:64:HIS:HB3	1:F:66:LEU:HG	1.99	0.44
1:G:341:ALA:HB1	1:G:342:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:LYS:NZ	1:H:421:PRO:O	2.51	0.44
1:B:40:ASP:HB2	1:B:95:ILE:HB	1.99	0.44
1:C:6:LYS:HD2	1:C:421:PRO:O	2.18	0.44
1:A:0:HIS:O	1:A:0:HIS:CG	2.71	0.44
2:E:501:G4P:O3B	2:E:501:G4P:O1A	2.36	0.44
1:H:341:ALA:HB1	1:H:342:PRO:HD2	1.99	0.44
1:B:0:HIS:CG	1:B:0:HIS:O	2.69	0.44
1:D:205:MET:HB3	1:D:206:PRO:HD3	2.00	0.44
1:G:0:HIS:HA	1:G:16:ASN:HA	2.00	0.44
1:C:176:ALA:HB2	1:C:208:ALA:HA	1.99	0.43
1:E:302:ARG:HG2	1:E:322:SER:HA	2.00	0.43
1:A:20:PRO:HB3	1:C:288:ILE:HD13	2.00	0.43
1:D:227:LEU:HD12	1:D:253:MET:HG3	1.99	0.43
1:E:422:GLU:HB3	1:F:421:PRO:CB	2.48	0.43
1:B:319:TYR:HB2	1:B:336:VAL:HG12	2.01	0.43
1:G:282:LEU:HD13	1:G:292:MET:CG	2.48	0.43
1:H:425:ASP:OD1	1:H:427:LEU:HB3	2.17	0.43
1:G:227:LEU:HB2	1:G:257:GLU:OE1	2.18	0.43
1:A:40:ASP:HB2	1:A:95:ILE:HB	2.00	0.43
1:F:386:PHE:O	1:F:388:TRP:CD1	2.72	0.43
1:H:64:HIS:HB3	1:H:66:LEU:HG	1.99	0.43
1:E:40:ASP:HB2	1:E:95:ILE:HB	2.00	0.43
1:C:0:HIS:ND1	1:C:16:ASN:HB3	2.33	0.43
1:E:289:GLY:HA3	1:E:340:ILE:O	2.19	0.43
1:H:389:LEU:C	1:H:389:LEU:HD12	2.38	0.43
1:H:40:ASP:HB2	1:H:95:ILE:HB	2.01	0.43
1:A:227:LEU:HD12	1:A:253:MET:HG3	2.01	0.43
1:B:303:LYS:HB2	1:B:303:LYS:HE3	1.89	0.43
1:C:253:MET:SD	1:C:258:ALA:HB2	2.59	0.43
1:E:290:LEU:O	1:E:290:LEU:HD12	2.19	0.43
1:F:161:GLU:HG3	1:F:162:ARG:N	2.33	0.43
1:G:217:LYS:NZ	1:G:247:HIS:HA	2.32	0.43
1:B:102:TYR:OH	1:B:369:THR:HG21	2.18	0.43
1:H:136:ARG:HG3	1:H:136:ARG:O	2.19	0.43
1:C:142:LEU:HD12	1:D:127:TYR:OH	2.18	0.43
1:E:195:TYR:CD2	3:E:502:GMP:C6	3.07	0.42
1:B:413:SER:OG	1:B:414:PRO:HD2	2.19	0.42
1:B:94:THR:HG23	1:B:358:ASP:OD2	2.18	0.42
1:D:291:TYR:CE1	1:D:339:HIS:CD2	3.07	0.42
1:G:91:ALA:HB1	1:G:129:TYR:CE1	2.54	0.42
1:H:375:ARG:HB2	1:H:384:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:HD12	1:A:290:LEU:C	2.40	0.42
1:D:386:PHE:O	1:D:388:TRP:CD1	2.71	0.42
1:G:0:HIS:O	1:G:0:HIS:CG	2.72	0.42
1:D:272:ASP:OD1	1:D:335:ARG:NH1	2.47	0.42
1:F:253:MET:SD	1:F:258:ALA:HA	2.60	0.42
1:G:205:MET:HB3	1:G:206:PRO:HD3	2.01	0.42
1:A:269:LEU:HD21	1:A:312:ALA:HB1	2.02	0.42
1:F:426:SER:O	1:F:429:GLU:HB3	2.19	0.42
1:H:49:LYS:HG2	1:H:156:ILE:HB	2.01	0.42
1:B:244:LEU:HD23	1:B:248:VAL:HG21	2.02	0.42
1:A:21:LEU:H	1:A:21:LEU:CD1	2.28	0.42
1:B:229:THR:OG1	1:B:232:VAL:HG23	2.20	0.42
1:G:15:VAL:HG12	1:G:16:ASN:N	2.35	0.42
1:A:424:GLU:OE1	1:B:423:ARG:NH1	2.53	0.42
1:D:290:LEU:C	1:D:290:LEU:HD12	2.41	0.42
1:D:67:VAL:HG13	1:D:168:PRO:CG	2.50	0.42
1:F:279:ASP:OD2	1:F:326:ARG:HB3	2.20	0.42
1:A:290:LEU:O	1:A:290:LEU:HD12	2.19	0.41
1:B:227:LEU:HD12	1:B:253:MET:HG2	2.02	0.41
1:G:68:ILE:HD13	1:G:165:ALA:HB1	2.02	0.41
1:G:431:TYR:CE2	1:H:343:TYR:HD2	2.38	0.41
1:H:423:ARG:CZ	1:H:423:ARG:HB2	2.49	0.41
1:D:245:LYS:HG2	1:D:277:TRP:CD1	2.55	0.41
1:D:67:VAL:HG13	1:D:168:PRO:HG3	2.02	0.41
1:H:115:VAL:HG21	1:H:171:MET:HA	2.02	0.41
1:A:136:ARG:HD3	1:B:417:THR:HG21	2.02	0.41
1:B:62:ALA:HB1	1:B:161:GLU:OE1	2.21	0.41
1:A:422:GLU:CG	1:B:421:PRO:HB3	2.49	0.41
1:B:425:ASP:OD1	1:B:428:GLU:HG3	2.20	0.41
1:C:43:LEU:HD23	1:C:150:GLY:C	2.41	0.41
1:E:434:ARG:OXT	1:F:399:LYS:NZ	2.47	0.41
1:F:153:PHE:HB2	1:F:165:ALA:HB3	2.01	0.41
1:G:50:VAL:HB	1:G:54:PHE:HB3	2.02	0.41
1:G:40:ASP:HB2	1:G:95:ILE:HB	2.03	0.41
1:G:39:ILE:O	1:G:95:ILE:HG21	2.21	0.41
1:A:244:LEU:HD23	1:A:248:VAL:HG21	2.02	0.41
2:F:501:G4P:O3B	2:F:501:G4P:O1A	2.38	0.41
1:G:423:ARG:HG2	1:H:424:GLU:OE1	2.20	0.41
1:B:1:MET:CE	1:B:370:ALA:HA	2.51	0.41
1:F:383:LYS:HE3	1:F:391:TYR:CZ	2.56	0.41
1:G:341:ALA:HB1	1:G:342:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ILE:O	1:D:95:ILE:HG21	2.20	0.41
1:G:120:ILE:HG23	1:G:126:ALA:HB3	2.03	0.41
1:B:156:ILE:HG22	1:B:158:GLU:H	1.86	0.41
1:C:380:ASN:HB3	1:F:314:ALA:HB2	2.02	0.41
1:G:1:MET:HG2	1:G:2:LYS:N	2.36	0.41
1:G:184:ILE:O	1:G:221:VAL:HG21	2.21	0.41
1:E:34:ALA:O	1:E:108:ASP:OD2	2.39	0.41
1:H:337:TYR:CD1	1:H:337:TYR:N	2.88	0.41
1:A:164:PHE:HE2	1:A:354:ASN:HD22	1.68	0.41
1:A:418:ARG:NH1	1:B:422:GLU:OE1	2.54	0.41
1:B:325:MET:HG3	1:B:388:TRP:CE3	2.55	0.40
1:B:425:ASP:N	1:B:425:ASP:OD1	2.55	0.40
1:D:6:LYS:HD2	1:D:421:PRO:O	2.20	0.40
1:E:107:ASP:OD2	1:F:418:ARG:NH1	2.54	0.40
1:E:302:ARG:CD	1:E:321:PHE:O	2.66	0.40
1:E:337:TYR:N	1:E:337:TYR:CD1	2.88	0.40
1:A:76:LEU:C	1:A:76:LEU:HD23	2.40	0.40
1:D:60:LEU:CD1	1:D:165:ALA:HB2	2.49	0.40
1:E:227:LEU:HD12	1:E:253:MET:HG3	2.02	0.40
1:H:285:ALA:HB1	1:H:288:ILE:HB	2.03	0.40
1:D:367:ASP:OD1	1:D:391:TYR:N	2.54	0.40
1:D:55:ILE:HG22	1:D:60:LEU:O	2.22	0.40
1:C:367:ASP:OD1	1:C:391:TYR:N	2.53	0.40
1:D:120:ILE:HG23	1:D:126:ALA:HB3	2.03	0.40
1:E:195:TYR:CZ	1:E:228:GLY:HA3	2.57	0.40
1:E:205:MET:HB3	1:E:206:PRO:HD3	2.02	0.40
1:H:424:GLU:HG3	1:H:428:GLU:HB3	2.01	0.40

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	433/437 (99%)	411 (95%)	20 (5%)	2 (0%)	29	66
1	B	424/437 (97%)	406 (96%)	17 (4%)	1 (0%)	47	80
1	C	425/437 (97%)	408 (96%)	15 (4%)	2 (0%)	29	66
1	D	433/437 (99%)	410 (95%)	22 (5%)	1 (0%)	47	80
1	E	416/437 (95%)	399 (96%)	14 (3%)	3 (1%)	22	60
1	F	406/437 (93%)	390 (96%)	15 (4%)	1 (0%)	47	80
1	G	415/437 (95%)	400 (96%)	14 (3%)	1 (0%)	47	80
1	H	400/437 (92%)	385 (96%)	14 (4%)	1 (0%)	41	75
All	All	3352/3496 (96%)	3209 (96%)	131 (4%)	12 (0%)	34	70

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	229	THR
1	H	229	THR
1	A	229	THR
1	B	229	THR
1	E	15	VAL
1	F	387	THR
1	C	351	MET
1	G	15	VAL
1	E	32	SER
1	A	385	LYS
1	C	15	VAL
1	D	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	364/369 (99%)	363 (100%)	1 (0%)	92	98
1	B	361/369 (98%)	358 (99%)	3 (1%)	81	92
1	C	358/369 (97%)	356 (99%)	2 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	364/369 (99%)	360 (99%)	4 (1%)	73	88
1	E	355/369 (96%)	353 (99%)	2 (1%)	86	95
1	F	345/369 (94%)	343 (99%)	2 (1%)	86	95
1	G	356/369 (96%)	350 (98%)	6 (2%)	60	82
1	H	342/369 (93%)	337 (98%)	5 (2%)	65	84
All	All	2845/2952 (96%)	2820 (99%)	25 (1%)	78	91

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	386	PHE
1	B	25	PHE
1	B	284	THR
1	B	291	TYR
1	C	253	MET
1	C	386	PHE
1	D	45	ASP
1	D	162	ARG
1	D	253	MET
1	D	403	ARG
1	E	253	MET
1	E	387	THR
1	F	253	MET
1	F	423	ARG
1	G	16	ASN
1	G	25	PHE
1	G	134	SER
1	G	253	MET
1	G	276	ASP
1	G	291	TYR
1	H	84	ASN
1	H	253	MET
1	H	354	ASN
1	H	389	LEU
1	H	423	ARG

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

Mol	Chain	Res	Type
1	A	64	HIS
1	C	384	HIS
1	E	327	HIS
1	G	354	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 19 are monoatomic - leaving 24 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	GMP	C	502	-	18,22,22	1.13	1 (5%)	20,33,33	2.60	4 (20%)
3	GMP	H	502	-	18,22,22	1.16	1 (5%)	20,33,33	2.63	4 (20%)
3	GMP	G	502	-	18,22,22	1.16	1 (5%)	20,33,33	2.61	4 (20%)
3	GMP	C	503	-	18,22,22	1.16	1 (5%)	20,33,33	2.56	4 (20%)
3	GMP	H	503	-	18,22,22	1.20	1 (5%)	20,33,33	2.60	4 (20%)
2	G4P	F	501	-	30,38,38	1.12	2 (6%)	43,61,61	1.78	9 (20%)
2	G4P	D	501	-	30,38,38	1.12	2 (6%)	43,61,61	1.90	10 (23%)
2	G4P	G	501	-	30,38,38	1.12	2 (6%)	43,61,61	2.10	11 (25%)
3	GMP	B	502	-	18,22,22	1.13	1 (5%)	20,33,33	2.60	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GMP	B	503	-	18,22,22	1.20	1 (5%)	20,33,33	2.59	4 (20%)
2	G4P	A	501	-	30,38,38	1.10	2 (6%)	43,61,61	2.12	12 (27%)
3	GMP	D	502	-	18,22,22	1.16	1 (5%)	20,33,33	2.59	4 (20%)
3	GMP	E	502	-	18,22,22	1.15	1 (5%)	20,33,33	2.60	4 (20%)
2	G4P	H	501	-	30,38,38	1.06	2 (6%)	43,61,61	1.82	10 (23%)
3	GMP	F	502	-	18,22,22	1.16	1 (5%)	20,33,33	2.62	4 (20%)
2	G4P	B	501	-	30,38,38	1.16	3 (10%)	43,61,61	2.10	12 (27%)
3	GMP	D	503	-	18,22,22	1.18	1 (5%)	20,33,33	2.58	4 (20%)
2	G4P	E	501	-	30,38,38	1.14	2 (6%)	43,61,61	1.95	9 (20%)
2	G4P	C	501	-	30,38,38	1.09	3 (10%)	43,61,61	1.92	11 (25%)
3	GMP	A	502	-	18,22,22	1.13	1 (5%)	20,33,33	2.61	4 (20%)
3	GMP	E	503	-	18,22,22	1.18	1 (5%)	20,33,33	2.61	4 (20%)
3	GMP	A	503	-	18,22,22	1.14	1 (5%)	20,33,33	2.59	4 (20%)
3	GMP	G	503	-	18,22,22	1.18	1 (5%)	20,33,33	2.59	4 (20%)
3	GMP	F	503	-	18,22,22	1.19	1 (5%)	20,33,33	2.60	4 (20%)

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	GMP	C	502	-	-	0/2/22/22	0/3/3/3
3	GMP	H	502	-	-	0/2/22/22	0/3/3/3
3	GMP	G	502	-	-	0/2/22/22	0/3/3/3
3	GMP	C	503	-	-	2/2/22/22	0/3/3/3
3	GMP	H	503	-	-	0/2/22/22	0/3/3/3
2	G4P	F	501	-	-	4/23/43/43	0/3/3/3
2	G4P	D	501	-	-	1/23/43/43	0/3/3/3
2	G4P	G	501	-	-	4/23/43/43	0/3/3/3
3	GMP	B	502	-	-	0/2/22/22	0/3/3/3
3	GMP	B	503	-	-	2/2/22/22	0/3/3/3
2	G4P	A	501	-	-	3/23/43/43	0/3/3/3
3	GMP	D	502	-	-	0/2/22/22	0/3/3/3
3	GMP	E	502	-	-	0/2/22/22	0/3/3/3
2	G4P	H	501	-	-	4/23/43/43	0/3/3/3
3	GMP	F	502	-	-	0/2/22/22	0/3/3/3
2	G4P	B	501	-	-	0/23/43/43	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GMP	D	503	-	-	2/2/22/22	0/3/3/3
2	G4P	E	501	-	-	3/23/43/43	0/3/3/3
2	G4P	C	501	-	-	5/23/43/43	0/3/3/3
3	GMP	A	502	-	-	0/2/22/22	0/3/3/3
3	GMP	E	503	-	-	0/2/22/22	0/3/3/3
3	GMP	A	503	-	-	2/2/22/22	0/3/3/3
3	GMP	G	503	-	-	2/2/22/22	0/3/3/3
3	GMP	F	503	-	-	2/2/22/22	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	G4P	C6-C5	4.71	1.49	1.41
2	B	501	G4P	C6-C5	4.56	1.49	1.41
2	F	501	G4P	C6-C5	4.54	1.49	1.41
2	G	501	G4P	C6-C5	4.42	1.49	1.41
2	D	501	G4P	C6-C5	4.38	1.48	1.41
2	H	501	G4P	C6-C5	4.17	1.48	1.41
3	B	503	GMP	C6-N1	4.09	1.40	1.33
3	G	503	GMP	C6-N1	4.09	1.40	1.33
3	H	503	GMP	C6-N1	4.07	1.40	1.33
3	D	502	GMP	C6-N1	4.07	1.40	1.33
2	A	501	G4P	C6-C5	4.07	1.48	1.41
3	H	502	GMP	C6-N1	4.06	1.40	1.33
3	F	502	GMP	C6-N1	4.06	1.40	1.33
2	C	501	G4P	C6-C5	4.05	1.48	1.41
3	E	503	GMP	C6-N1	4.05	1.40	1.33
3	G	502	GMP	C6-N1	4.05	1.40	1.33
3	F	503	GMP	C6-N1	4.05	1.40	1.33
3	E	502	GMP	C6-N1	3.98	1.40	1.33
3	D	503	GMP	C6-N1	3.98	1.40	1.33
3	A	503	GMP	C6-N1	3.96	1.39	1.33
3	B	502	GMP	C6-N1	3.94	1.39	1.33
3	C	503	GMP	C6-N1	3.94	1.39	1.33
3	A	502	GMP	C6-N1	3.92	1.39	1.33
3	C	502	GMP	C6-N1	3.88	1.39	1.33
2	C	501	G4P	O4'-C1'	2.44	1.44	1.41
2	D	501	G4P	C5-C4	2.30	1.47	1.40
2	H	501	G4P	C5-C4	2.27	1.46	1.40
2	G	501	G4P	C5-C4	2.24	1.46	1.40
2	F	501	G4P	C5-C4	2.23	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	G4P	C5-C4	2.13	1.46	1.40
2	B	501	G4P	C5-C4	2.13	1.46	1.40
2	B	501	G4P	O4'-C1'	2.10	1.44	1.41
2	C	501	G4P	C5-C4	2.06	1.46	1.40
2	A	501	G4P	C5-C4	2.05	1.46	1.40

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	502	GMP	C5-C6-N1	-8.85	111.33	123.43
3	F	503	GMP	C5-C6-N1	-8.84	111.34	123.43
3	A	503	GMP	C5-C6-N1	-8.82	111.37	123.43
3	H	502	GMP	C5-C6-N1	-8.82	111.37	123.43
3	G	503	GMP	C5-C6-N1	-8.81	111.38	123.43
3	G	502	GMP	C5-C6-N1	-8.81	111.38	123.43
3	E	502	GMP	C5-C6-N1	-8.80	111.39	123.43
3	E	503	GMP	C5-C6-N1	-8.80	111.39	123.43
3	B	503	GMP	C5-C6-N1	-8.78	111.42	123.43
3	H	503	GMP	C5-C6-N1	-8.75	111.46	123.43
3	A	502	GMP	C5-C6-N1	-8.75	111.46	123.43
3	D	503	GMP	C5-C6-N1	-8.73	111.48	123.43
3	C	502	GMP	C5-C6-N1	-8.73	111.49	123.43
3	D	502	GMP	C5-C6-N1	-8.73	111.50	123.43
3	B	502	GMP	C5-C6-N1	-8.71	111.52	123.43
3	C	503	GMP	C5-C6-N1	-8.71	111.52	123.43
3	F	502	GMP	C6-N1-C2	5.90	125.31	115.93
3	F	503	GMP	C6-N1-C2	5.90	125.30	115.93
3	H	503	GMP	C6-N1-C2	5.90	125.30	115.93
3	E	503	GMP	C6-N1-C2	5.89	125.29	115.93
3	H	502	GMP	C6-N1-C2	5.89	125.29	115.93
3	A	502	GMP	C6-N1-C2	5.87	125.26	115.93
3	C	502	GMP	C6-N1-C2	5.87	125.26	115.93
3	G	503	GMP	C6-N1-C2	5.87	125.25	115.93
3	A	503	GMP	C6-N1-C2	5.85	125.22	115.93
3	G	502	GMP	C6-N1-C2	5.83	125.19	115.93
3	D	503	GMP	C6-N1-C2	5.83	125.19	115.93
3	E	502	GMP	C6-N1-C2	5.82	125.18	115.93
3	B	502	GMP	C6-N1-C2	5.81	125.17	115.93
2	B	501	G4P	PC-O3C-PD	-5.81	112.88	132.83
3	B	503	GMP	C6-N1-C2	5.81	125.16	115.93
3	D	502	GMP	C6-N1-C2	5.79	125.14	115.93
3	C	503	GMP	C6-N1-C2	5.74	125.05	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	G4P	PC-O3C-PD	-5.44	114.17	132.83
2	E	501	G4P	C2-N3-C4	5.39	121.51	115.36
2	G	501	G4P	O3C-PC-O3'	-5.11	92.19	102.48
2	F	501	G4P	C2-N3-C4	4.99	121.05	115.36
2	D	501	G4P	C2-N3-C4	4.83	120.88	115.36
2	A	501	G4P	C2-N3-C4	4.83	120.87	115.36
2	G	501	G4P	C6-C5-C4	-4.74	116.27	120.80
2	B	501	G4P	C2-N3-C4	4.72	120.75	115.36
2	G	501	G4P	C2-N3-C4	4.68	120.70	115.36
2	H	501	G4P	C2-N3-C4	4.50	120.49	115.36
2	C	501	G4P	C2-N3-C4	4.42	120.40	115.36
2	H	501	G4P	C5-C6-N1	-4.39	117.43	123.43
2	A	501	G4P	C5-C6-N1	-4.31	117.54	123.43
2	C	501	G4P	C5-C6-N1	-4.30	117.55	123.43
2	D	501	G4P	PC-O3C-PD	-4.30	118.08	132.83
2	E	501	G4P	C4-C5-N7	-4.20	105.02	109.40
2	B	501	G4P	C5-C6-N1	-4.18	117.72	123.43
2	D	501	G4P	C5-C6-N1	-4.12	117.79	123.43
2	C	501	G4P	C6-N1-C2	4.09	122.42	115.93
2	A	501	G4P	C6-N1-C2	4.05	122.36	115.93
2	G	501	G4P	C6-N1-C2	4.02	122.32	115.93
2	E	501	G4P	C6-C5-C4	-4.02	116.96	120.80
2	B	501	G4P	C6-C5-C4	-3.99	116.99	120.80
2	F	501	G4P	C5-C6-N1	-3.96	118.02	123.43
2	B	501	G4P	C6-N1-C2	3.87	122.07	115.93
2	H	501	G4P	C6-N1-C2	3.85	122.05	115.93
2	G	501	G4P	C5-C6-N1	-3.82	118.20	123.43
2	A	501	G4P	C6-C5-C4	-3.79	117.18	120.80
2	C	501	G4P	C4-C5-N7	-3.78	105.46	109.40
2	D	501	G4P	C6-N1-C2	3.78	121.93	115.93
2	B	501	G4P	C4-C5-N7	-3.64	105.60	109.40
2	F	501	G4P	C6-C5-C4	-3.63	117.33	120.80
2	C	501	G4P	C6-C5-C4	-3.61	117.35	120.80
2	E	501	G4P	C5-C6-N1	-3.59	118.52	123.43
2	E	501	G4P	C6-N1-C2	3.58	121.61	115.93
2	H	501	G4P	C4-C5-N7	-3.57	105.68	109.40
2	G	501	G4P	C4-C5-N7	-3.52	105.73	109.40
2	F	501	G4P	C4-C5-N7	-3.51	105.74	109.40
2	F	501	G4P	C6-N1-C2	3.47	121.44	115.93
2	E	501	G4P	PC-O3C-PD	-3.43	121.07	132.83
2	D	501	G4P	C4-C5-N7	-3.40	105.85	109.40
2	H	501	G4P	C6-C5-C4	-3.40	117.55	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	G4P	C4-C5-N7	-3.33	105.92	109.40
2	G	501	G4P	N3-C2-N1	-3.33	122.78	127.22
2	B	501	G4P	O3C-PC-O3'	-3.26	95.92	102.48
2	G	501	G4P	C1'-N9-C4	-3.23	120.96	126.64
2	A	501	G4P	N3-C2-N1	-3.21	122.94	127.22
2	B	501	G4P	PA-O3A-PB	-3.19	121.89	132.83
2	D	501	G4P	C6-C5-C4	-3.18	117.76	120.80
2	H	501	G4P	PC-O3C-PD	-3.11	122.17	132.83
2	C	501	G4P	PC-O3C-PD	-3.11	122.17	132.83
2	E	501	G4P	PA-O3A-PB	-3.10	122.20	132.83
2	E	501	G4P	N3-C2-N1	-3.08	123.11	127.22
2	C	501	G4P	N3-C2-N1	-2.98	123.25	127.22
2	B	501	G4P	N3-C2-N1	-2.98	123.25	127.22
2	G	501	G4P	PC-O3'-C3'	2.97	130.23	119.41
2	F	501	G4P	PC-O3C-PD	-2.95	122.71	132.83
2	D	501	G4P	N3-C2-N1	-2.90	123.36	127.22
3	E	503	GMP	C2-N3-C4	-2.86	112.09	115.36
3	H	503	GMP	N3-C2-N1	-2.86	123.41	127.22
3	B	502	GMP	N3-C2-N1	-2.83	123.45	127.22
3	F	503	GMP	C2-N3-C4	-2.83	112.13	115.36
3	C	502	GMP	N3-C2-N1	-2.81	123.47	127.22
3	E	502	GMP	C2-N3-C4	-2.80	112.16	115.36
3	F	502	GMP	N3-C2-N1	-2.80	123.49	127.22
3	D	503	GMP	N3-C2-N1	-2.80	123.49	127.22
3	A	502	GMP	N3-C2-N1	-2.79	123.50	127.22
3	H	502	GMP	N3-C2-N1	-2.79	123.50	127.22
3	D	502	GMP	N3-C2-N1	-2.79	123.50	127.22
3	G	502	GMP	C2-N3-C4	-2.79	112.17	115.36
3	E	503	GMP	N3-C2-N1	-2.77	123.53	127.22
3	H	502	GMP	C2-N3-C4	-2.77	112.20	115.36
3	G	503	GMP	C2-N3-C4	-2.76	112.20	115.36
2	F	501	G4P	N3-C2-N1	-2.76	123.54	127.22
3	A	503	GMP	C2-N3-C4	-2.75	112.21	115.36
3	F	502	GMP	C2-N3-C4	-2.74	112.22	115.36
3	G	503	GMP	N3-C2-N1	-2.74	123.57	127.22
3	A	502	GMP	C2-N3-C4	-2.74	112.23	115.36
3	F	503	GMP	N3-C2-N1	-2.74	123.57	127.22
3	C	502	GMP	C2-N3-C4	-2.73	112.23	115.36
3	B	503	GMP	N3-C2-N1	-2.73	123.59	127.22
2	H	501	G4P	N3-C2-N1	-2.73	123.59	127.22
3	G	502	GMP	N3-C2-N1	-2.70	123.61	127.22
3	C	503	GMP	C2-N3-C4	-2.70	112.28	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	503	GMP	C2-N3-C4	-2.70	112.28	115.36
3	B	502	GMP	C2-N3-C4	-2.70	112.28	115.36
3	D	502	GMP	C2-N3-C4	-2.69	112.28	115.36
2	D	501	G4P	PA-O3A-PB	-2.69	123.60	132.83
3	B	503	GMP	C2-N3-C4	-2.69	112.29	115.36
3	E	502	GMP	N3-C2-N1	-2.68	123.64	127.22
2	C	501	G4P	C1'-N9-C4	-2.68	121.94	126.64
3	A	503	GMP	N3-C2-N1	-2.66	123.67	127.22
2	A	501	G4P	PA-O3A-PB	-2.64	123.76	132.83
3	D	503	GMP	C2-N3-C4	-2.64	112.35	115.36
3	C	503	GMP	N3-C2-N1	-2.60	123.76	127.22
2	A	501	G4P	O3C-PC-O3'	-2.48	97.49	102.48
2	G	501	G4P	O3'-C3'-C2'	-2.44	102.83	111.68
2	G	501	G4P	PA-O3A-PB	-2.42	124.52	132.83
2	A	501	G4P	O3D-PD-O2D	2.33	116.55	107.64
2	B	501	G4P	C1'-N9-C4	-2.32	122.56	126.64
2	C	501	G4P	C5'-C4'-C3'	-2.32	106.70	114.40
2	D	501	G4P	O3D-PD-O2D	2.32	116.49	107.64
2	E	501	G4P	C3'-C2'-C1'	2.31	105.00	99.89
2	D	501	G4P	C3'-C2'-C1'	2.29	104.97	99.89
2	C	501	G4P	O3B-PB-O2B	2.28	116.36	107.64
2	F	501	G4P	PA-O3A-PB	-2.26	125.06	132.83
2	F	501	G4P	C3'-C2'-C1'	2.26	104.90	99.89
2	A	501	G4P	O2'-C2'-C3'	-2.22	104.85	111.17
2	B	501	G4P	C3'-C2'-C1'	2.20	104.76	99.89
2	H	501	G4P	PC-O3'-C3'	2.19	127.38	119.41
2	H	501	G4P	PA-O3A-PB	-2.19	125.32	132.83
2	C	501	G4P	PA-O3A-PB	-2.17	125.38	132.83
2	A	501	G4P	O3'-C3'-C2'	-2.16	103.85	111.68
2	H	501	G4P	C1'-N9-C4	-2.09	122.97	126.64
2	B	501	G4P	O3D-PD-O2D	2.06	115.51	107.64

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	501	G4P	PA-O3A-PB-O2B
2	F	501	G4P	PA-O3A-PB-O3B
2	G	501	G4P	PA-O3A-PB-O2B
2	G	501	G4P	PA-O3A-PB-O3B
3	B	503	GMP	O4'-C4'-C5'-O5'
3	B	503	GMP	C3'-C4'-C5'-O5'

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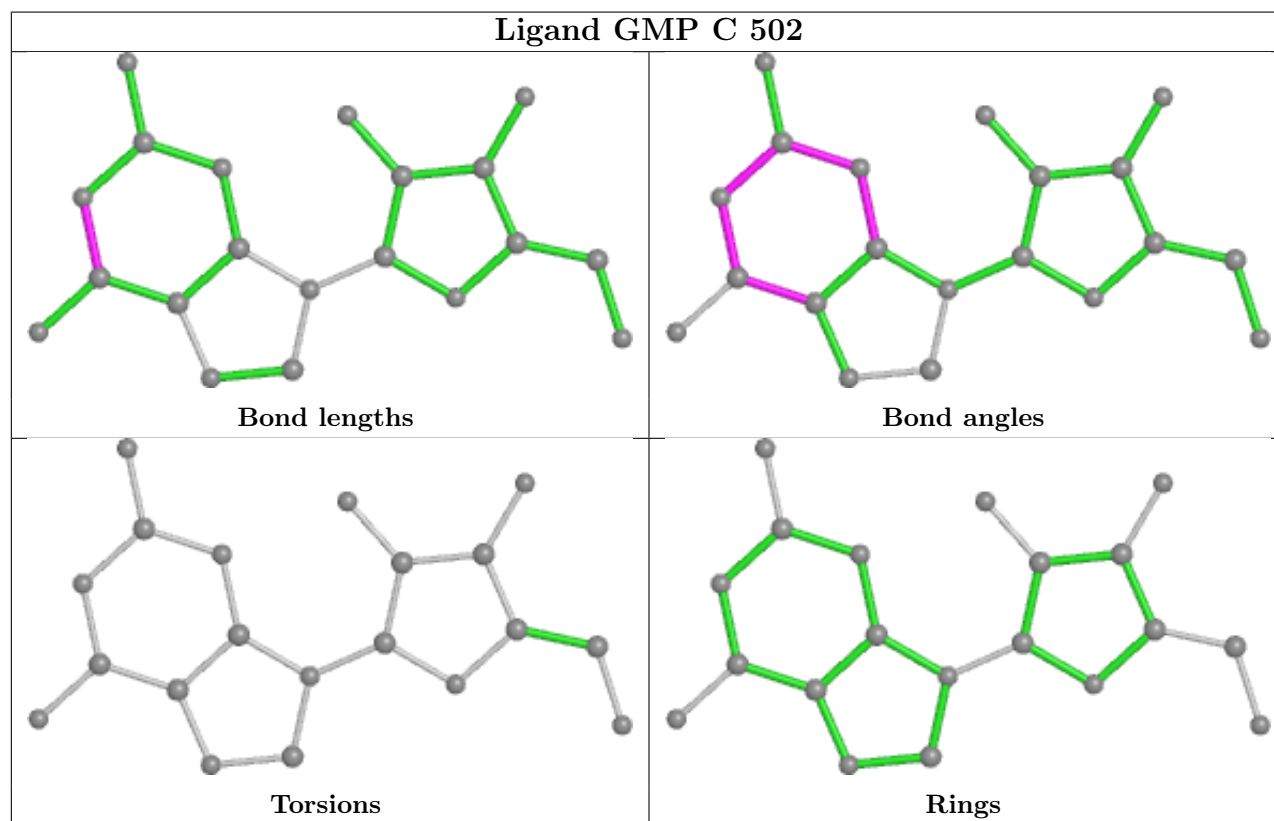
Mol	Chain	Res	Type	Atoms
2	A	501	G4P	PA-O3A-PB-O3B
2	H	501	G4P	PA-O3A-PB-O2B
2	H	501	G4P	PA-O3A-PB-O3B
2	H	501	G4P	C4'-C3'-O3'-PC
3	A	503	GMP	O4'-C4'-C5'-O5'
3	A	503	GMP	C3'-C4'-C5'-O5'
3	D	503	GMP	O4'-C4'-C5'-O5'
3	D	503	GMP	C3'-C4'-C5'-O5'
2	E	501	G4P	PA-O3A-PB-O2B
2	E	501	G4P	PA-O3A-PB-O3B
2	C	501	G4P	PA-O3A-PB-O2B
2	C	501	G4P	PA-O3A-PB-O3B
3	G	503	GMP	O4'-C4'-C5'-O5'
3	G	503	GMP	C3'-C4'-C5'-O5'
3	F	503	GMP	O4'-C4'-C5'-O5'
3	F	503	GMP	C3'-C4'-C5'-O5'
2	D	501	G4P	C3'-O3'-PC-O3C
3	C	503	GMP	O4'-C4'-C5'-O5'
2	A	501	G4P	PA-O3A-PB-O2B
2	H	501	G4P	PB-O3A-PA-O1A
3	C	503	GMP	C3'-C4'-C5'-O5'
2	C	501	G4P	C3'-O3'-PC-O3C
2	F	501	G4P	PA-O3A-PB-O1B
2	A	501	G4P	PA-O3A-PB-O1B
2	F	501	G4P	PB-O3A-PA-O1A
2	G	501	G4P	PB-O3A-PA-O1A
2	E	501	G4P	PB-O3A-PA-O1A
2	C	501	G4P	PD-O3C-PC-O2C
2	G	501	G4P	PA-O3A-PB-O1B
2	C	501	G4P	PA-O3A-PB-O1B

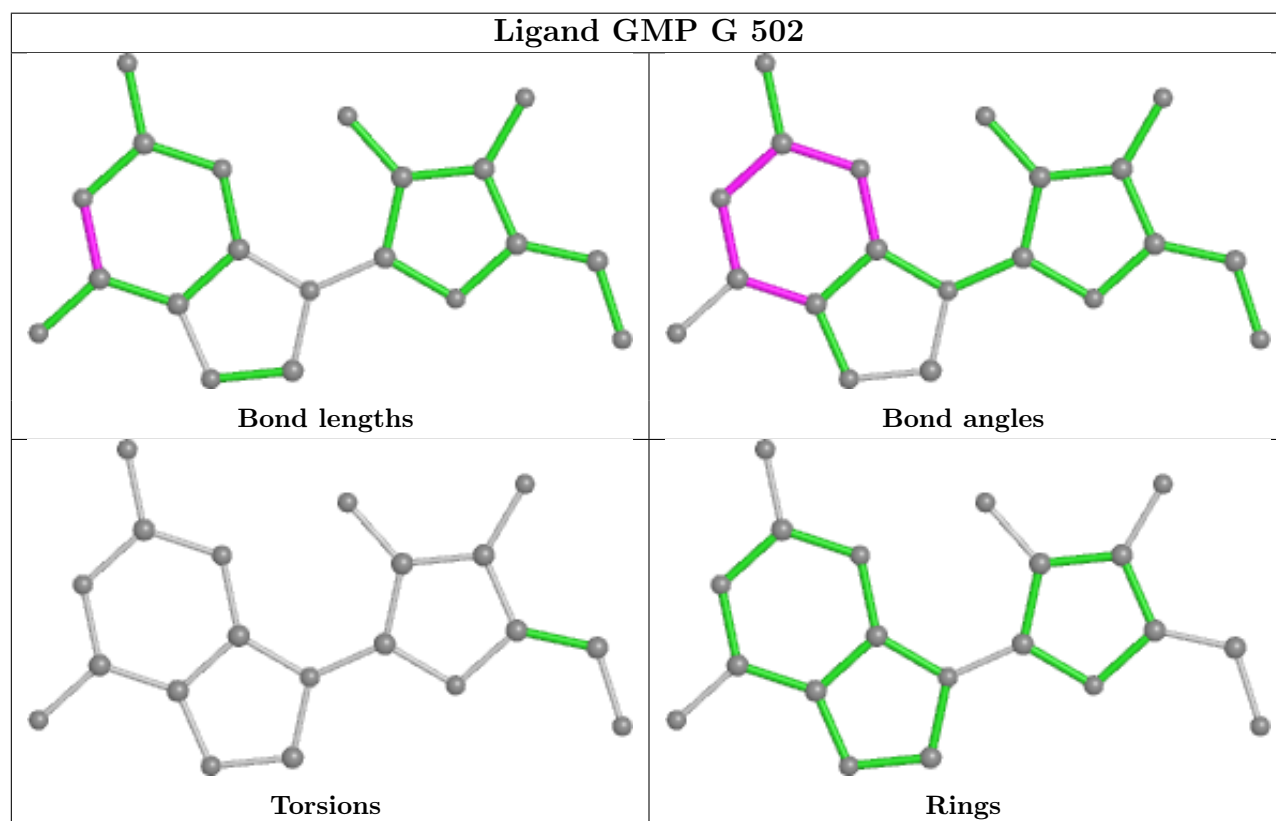
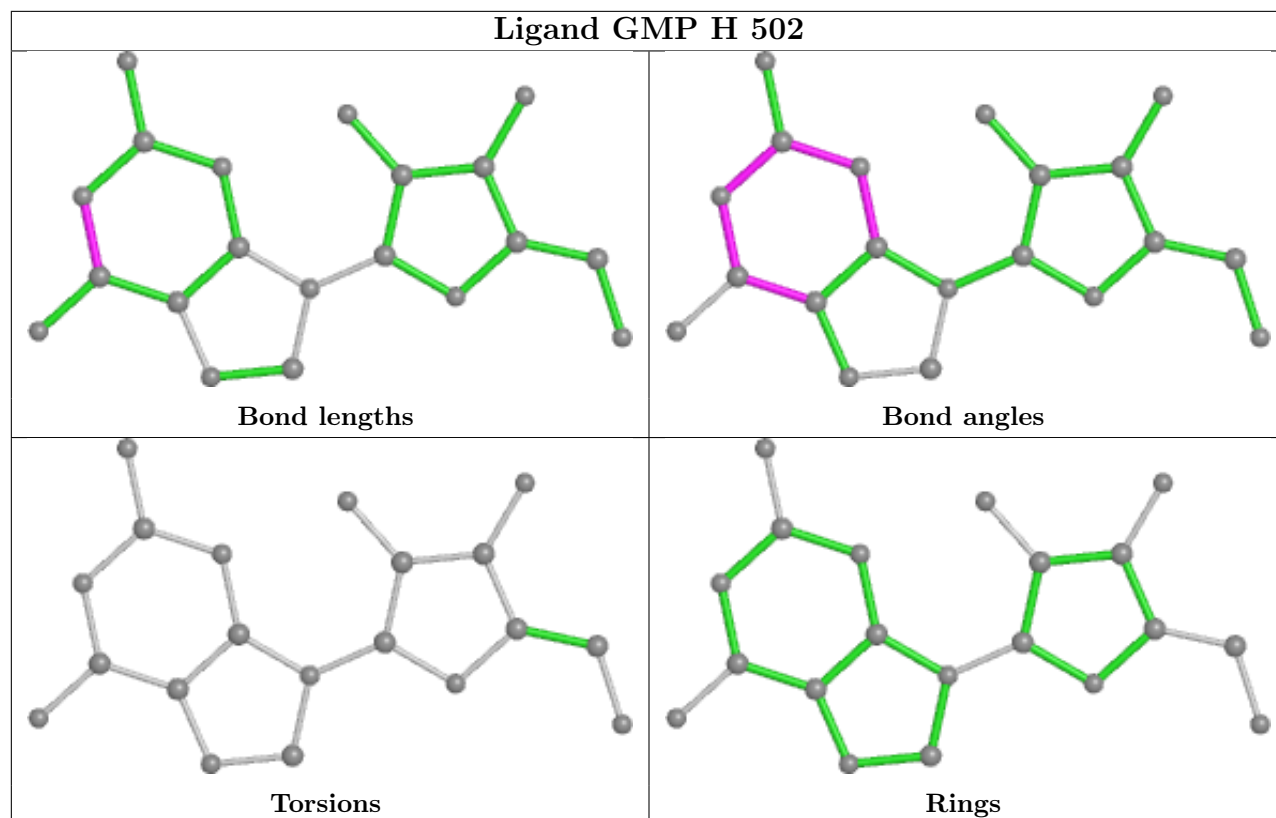
There are no ring outliers.

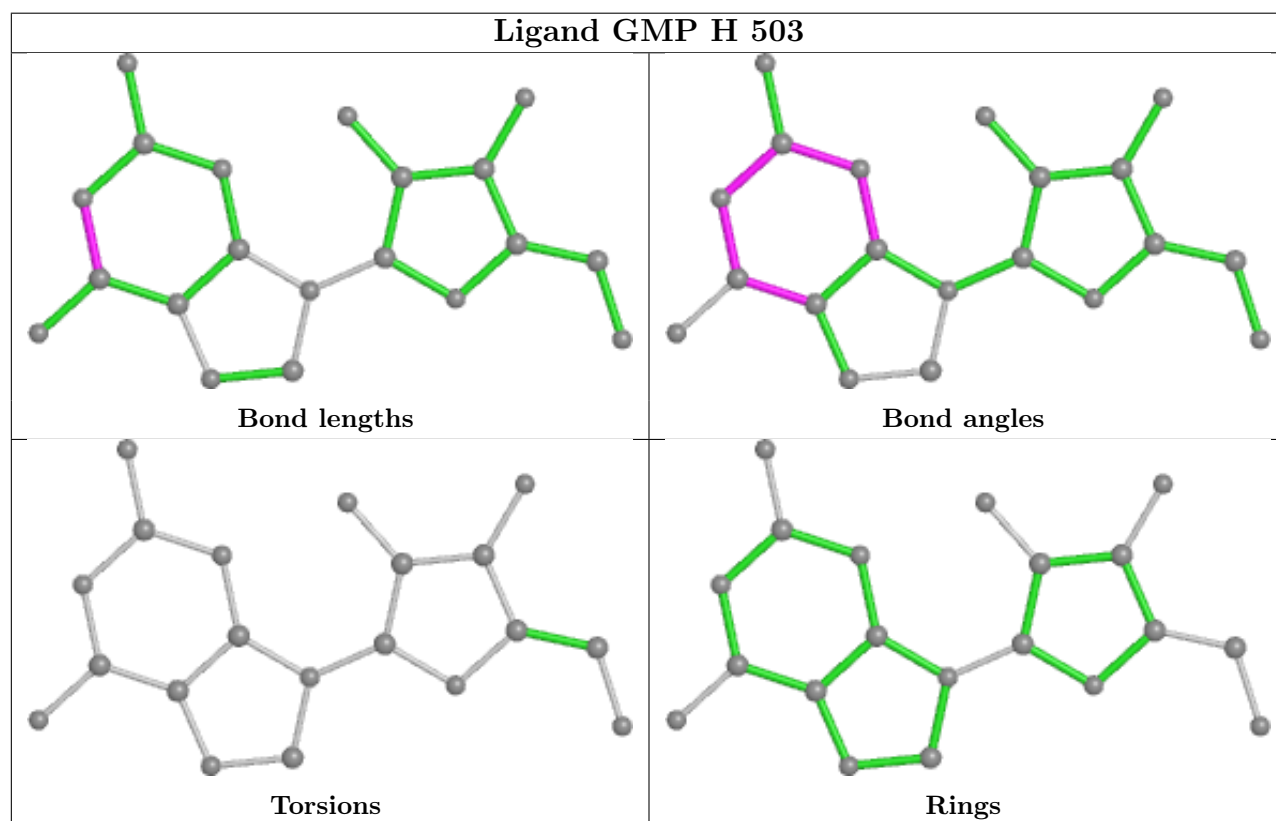
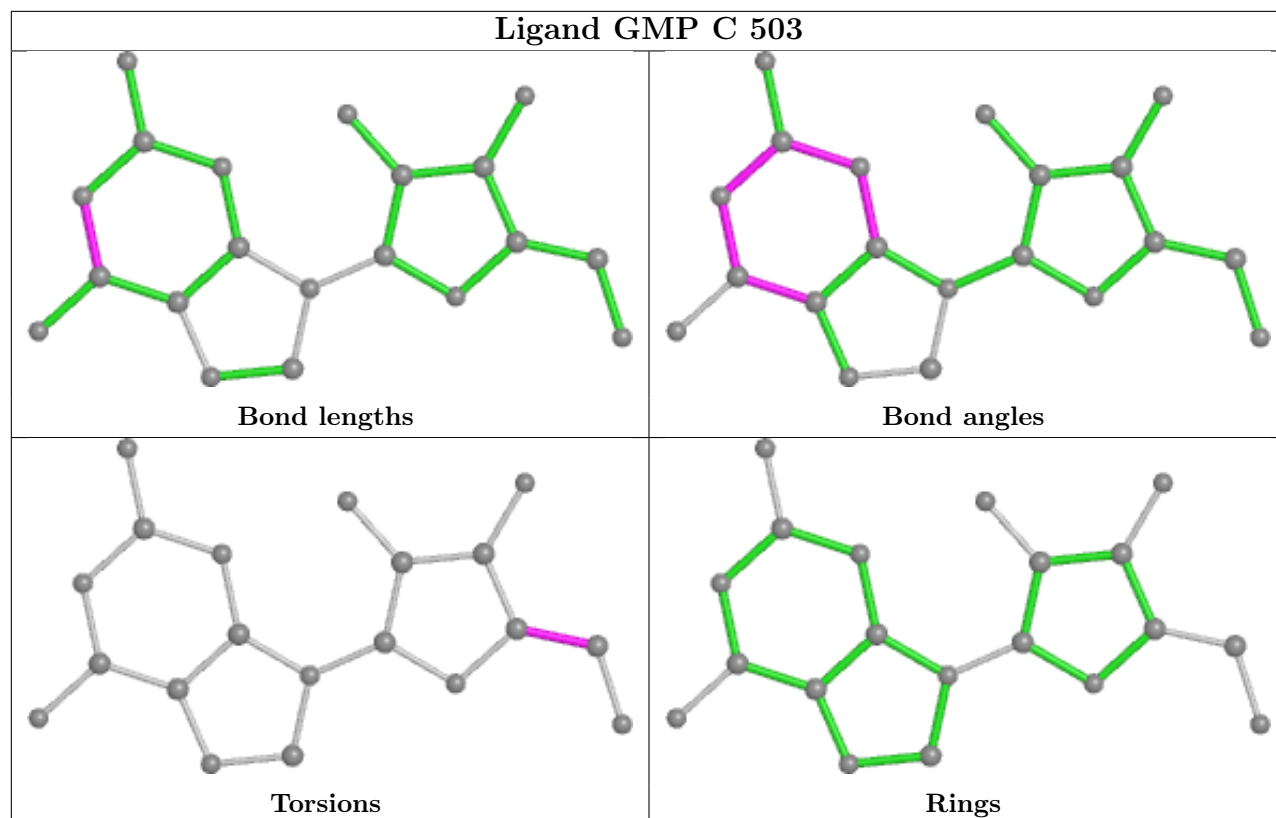
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	502	GMP	1	0
2	F	501	G4P	1	0
2	D	501	G4P	3	0
3	E	502	GMP	2	0
3	F	502	GMP	1	0
2	E	501	G4P	1	0

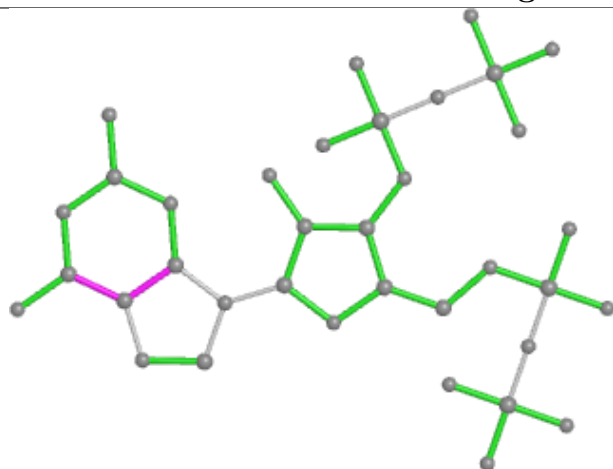
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



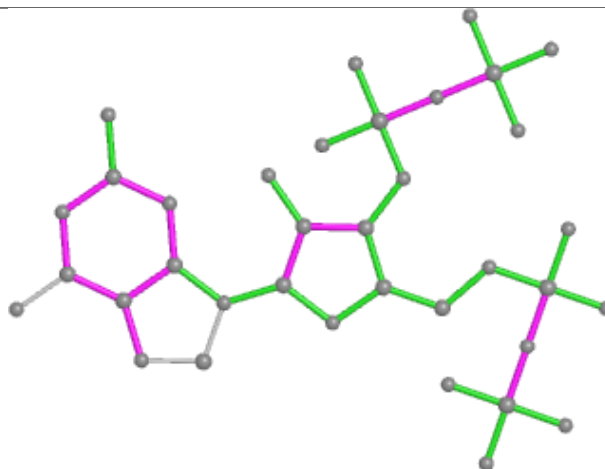




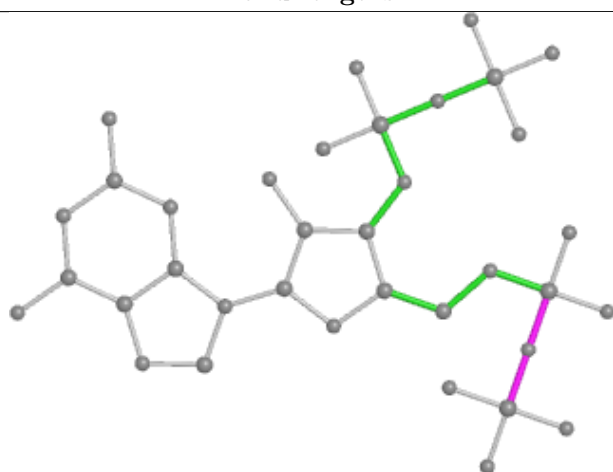
Ligand G4P F 501



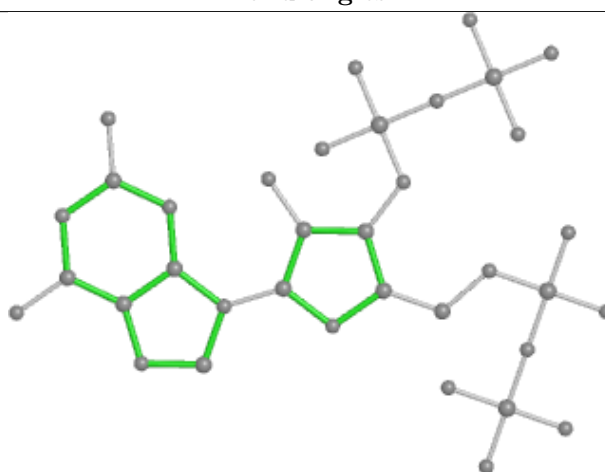
Bond lengths



Bond angles

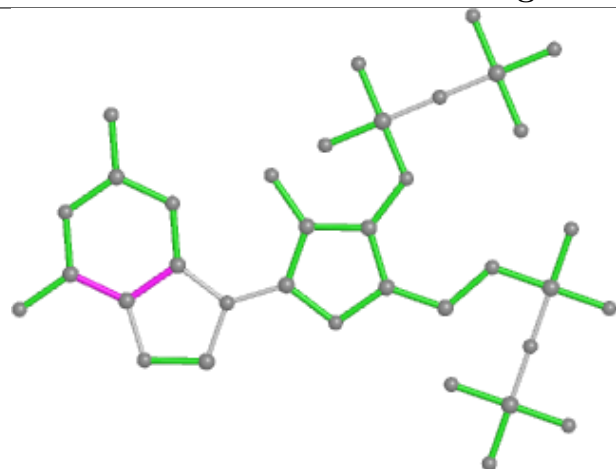


Torsions

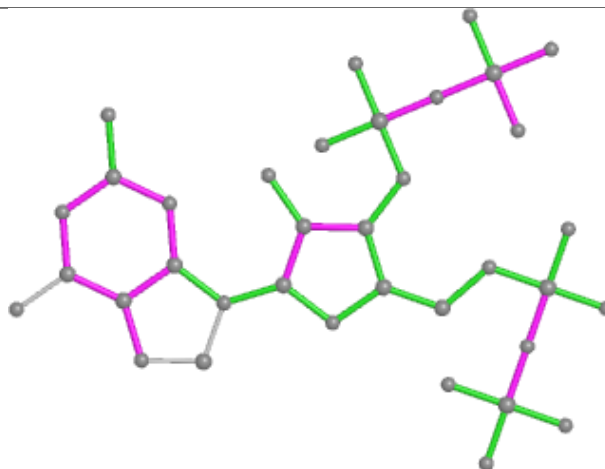


Rings

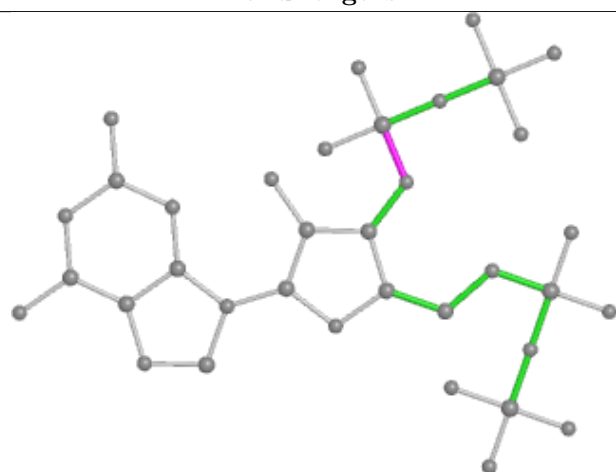
Ligand G4P D 501



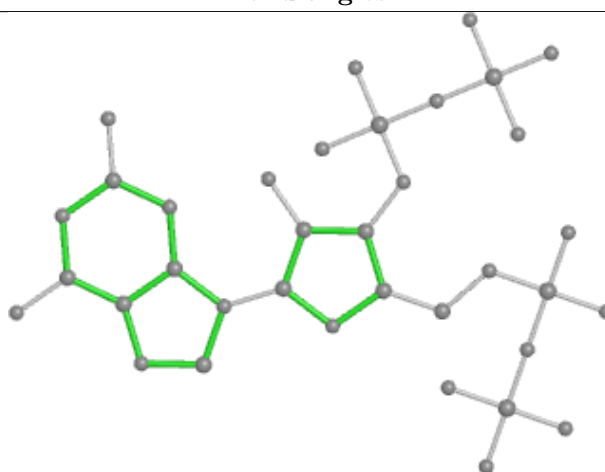
Bond lengths



Bond angles

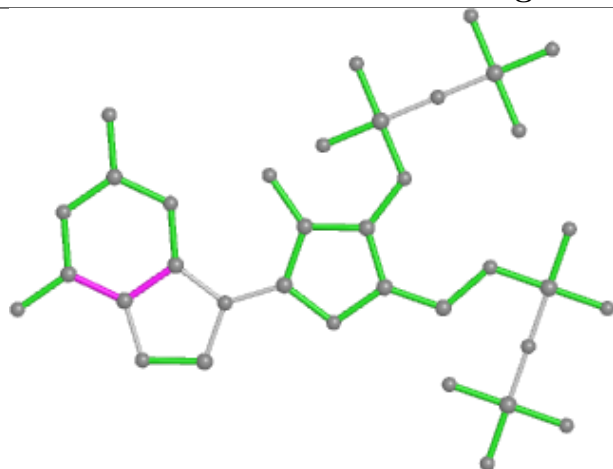


Torsions

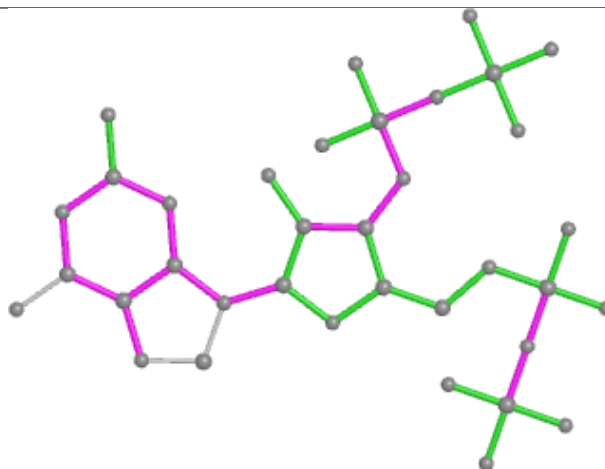


Rings

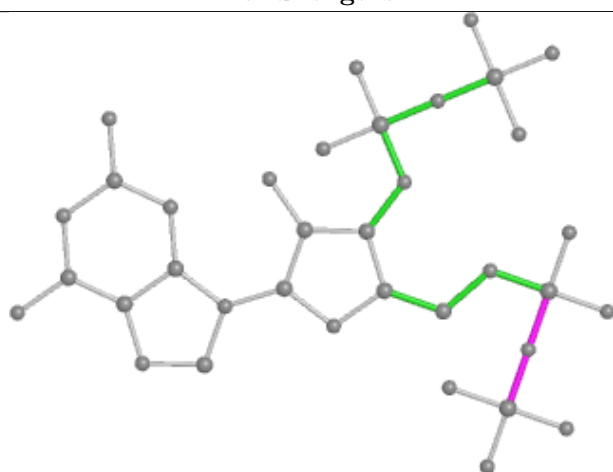
Ligand G4P G 501



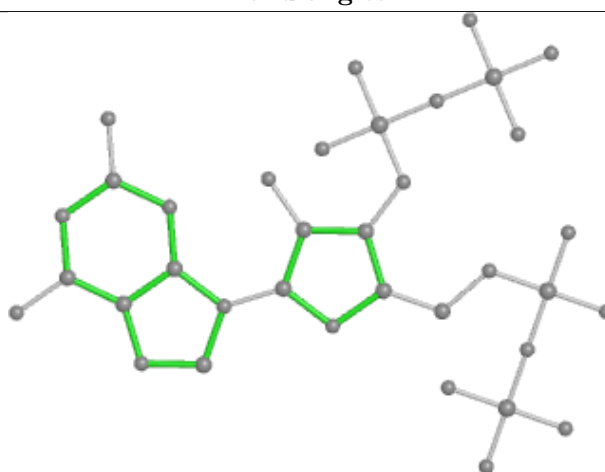
Bond lengths



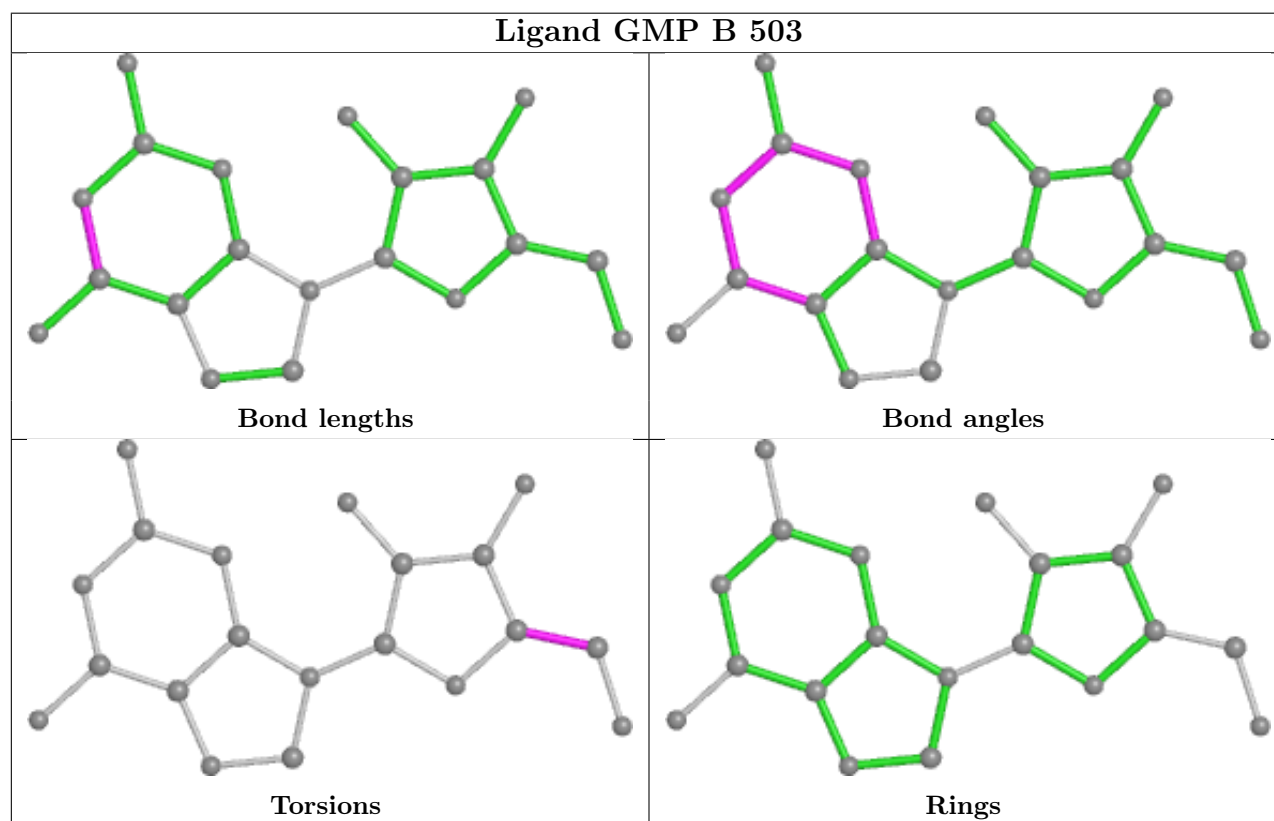
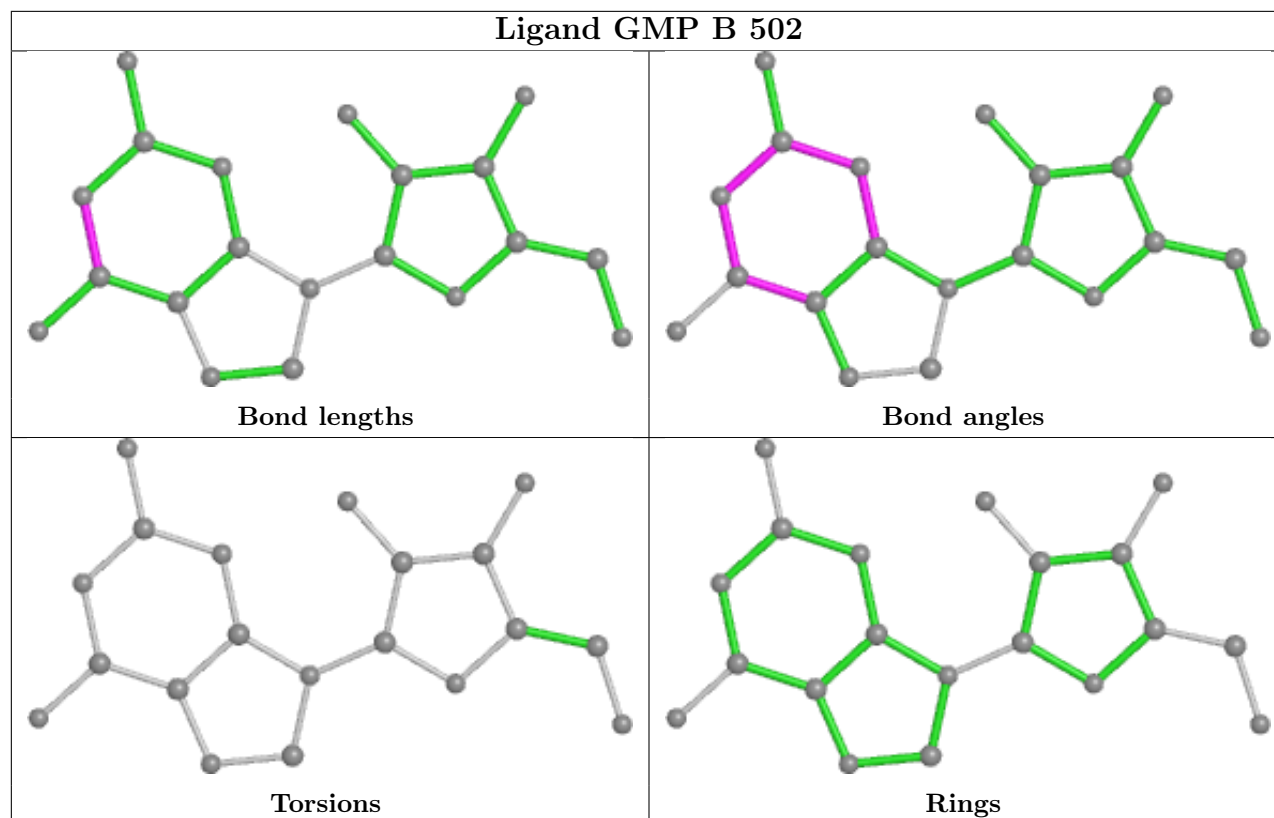
Bond angles



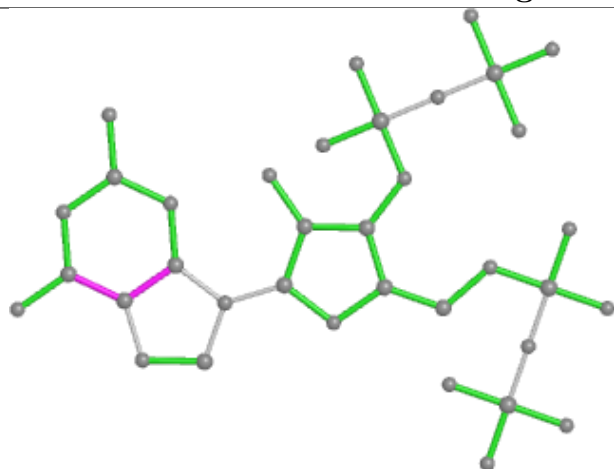
Torsions



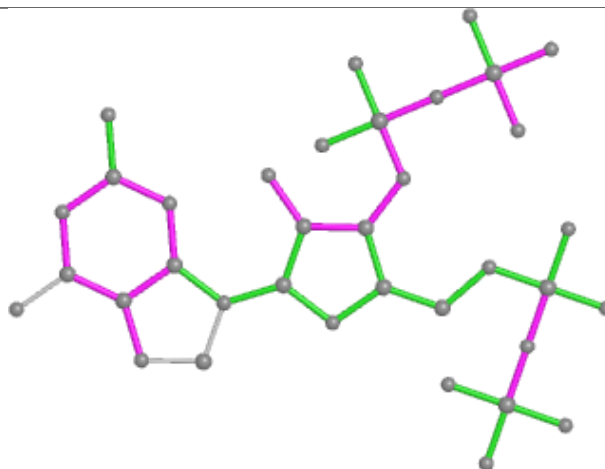
Rings



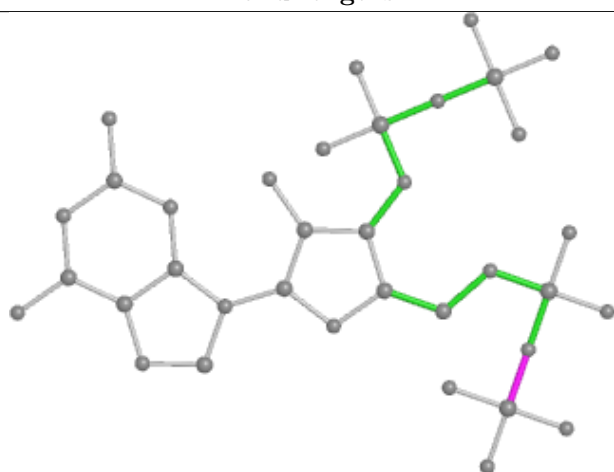
Ligand G4P A 501



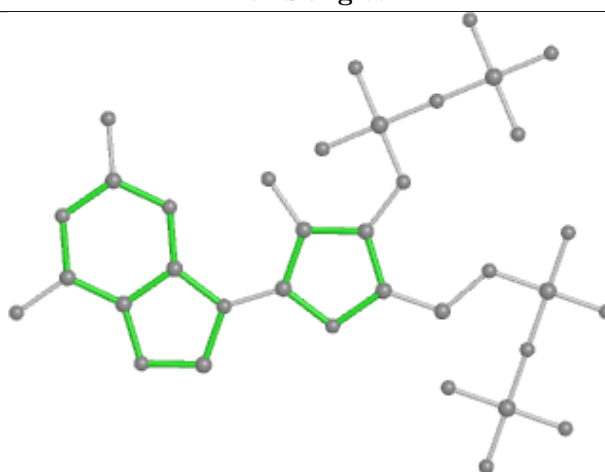
Bond lengths



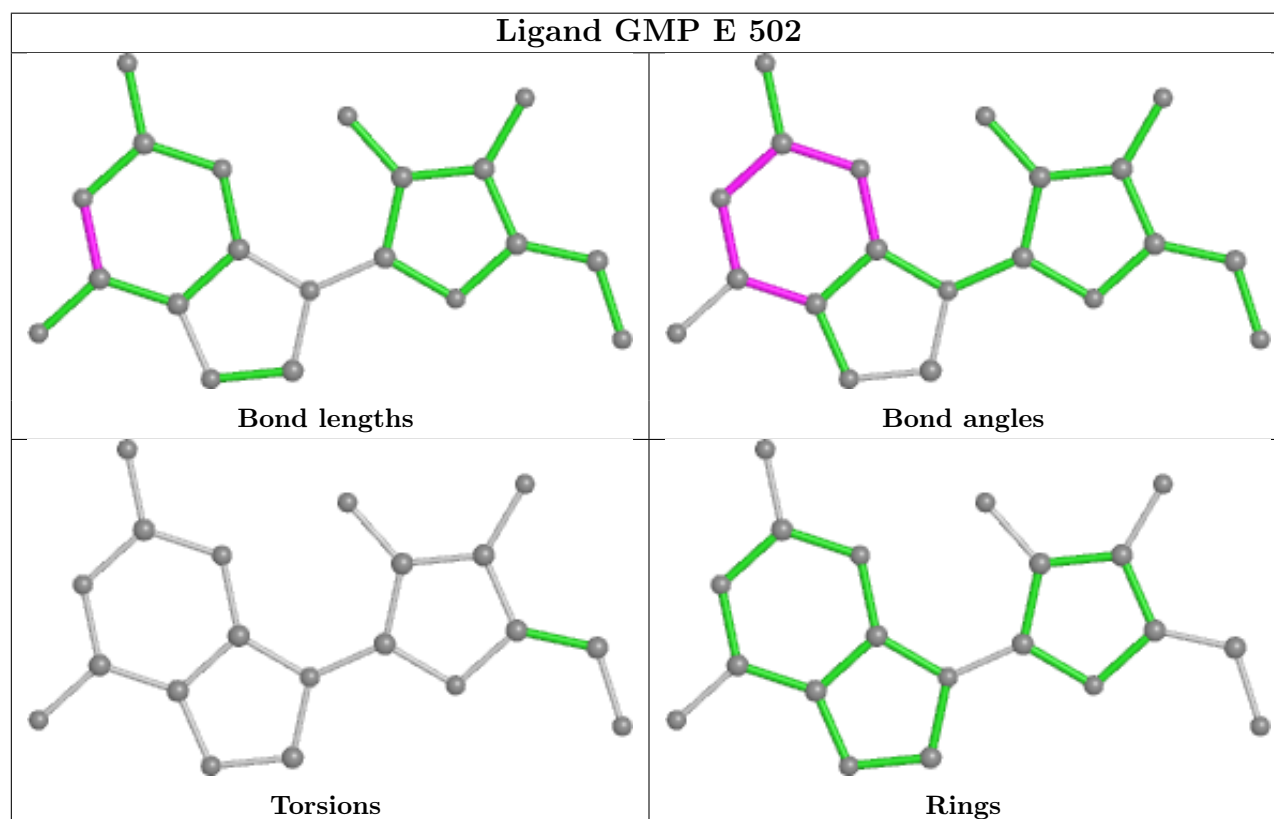
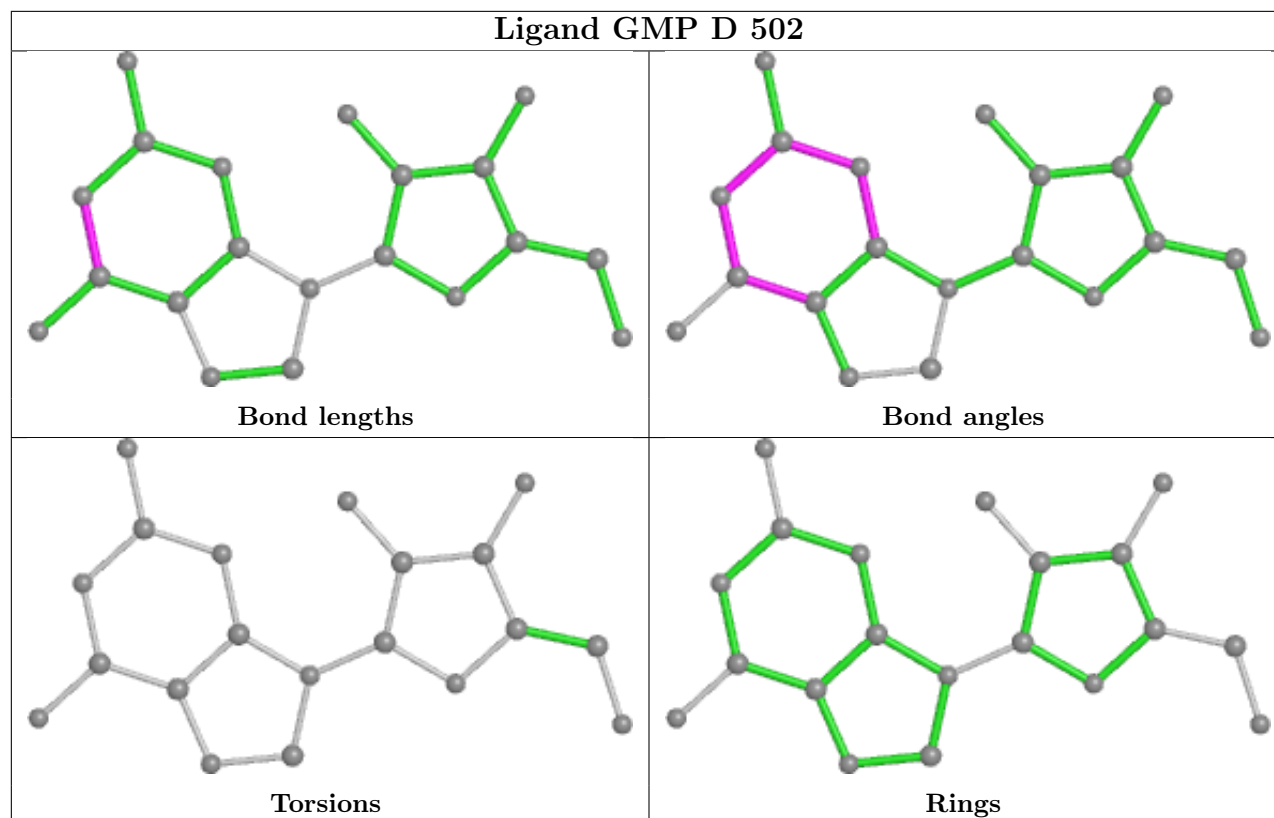
Bond angles



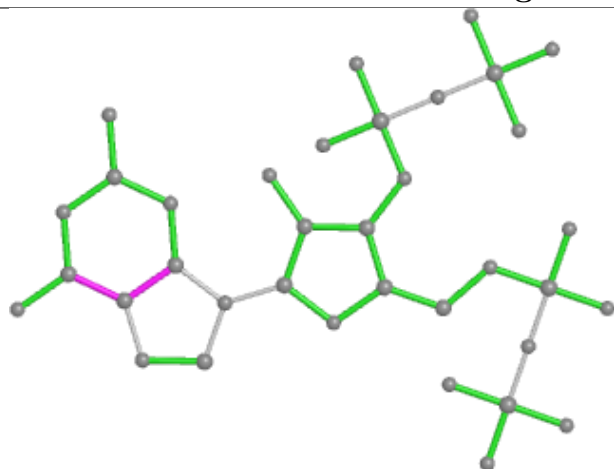
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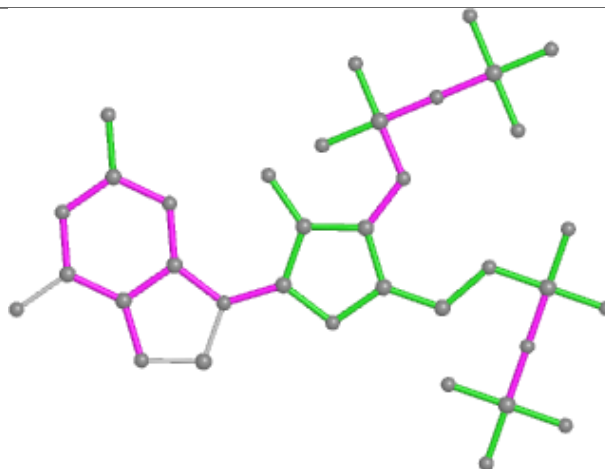
Rings



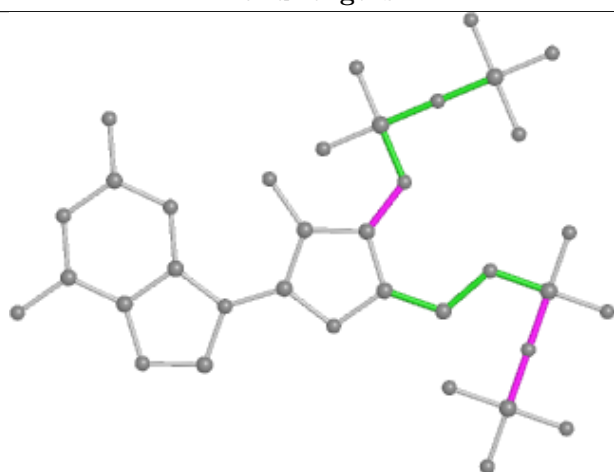
Ligand G4P H 501



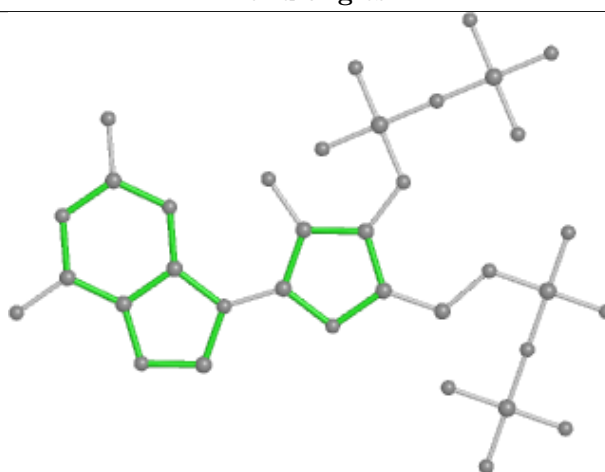
Bond lengths



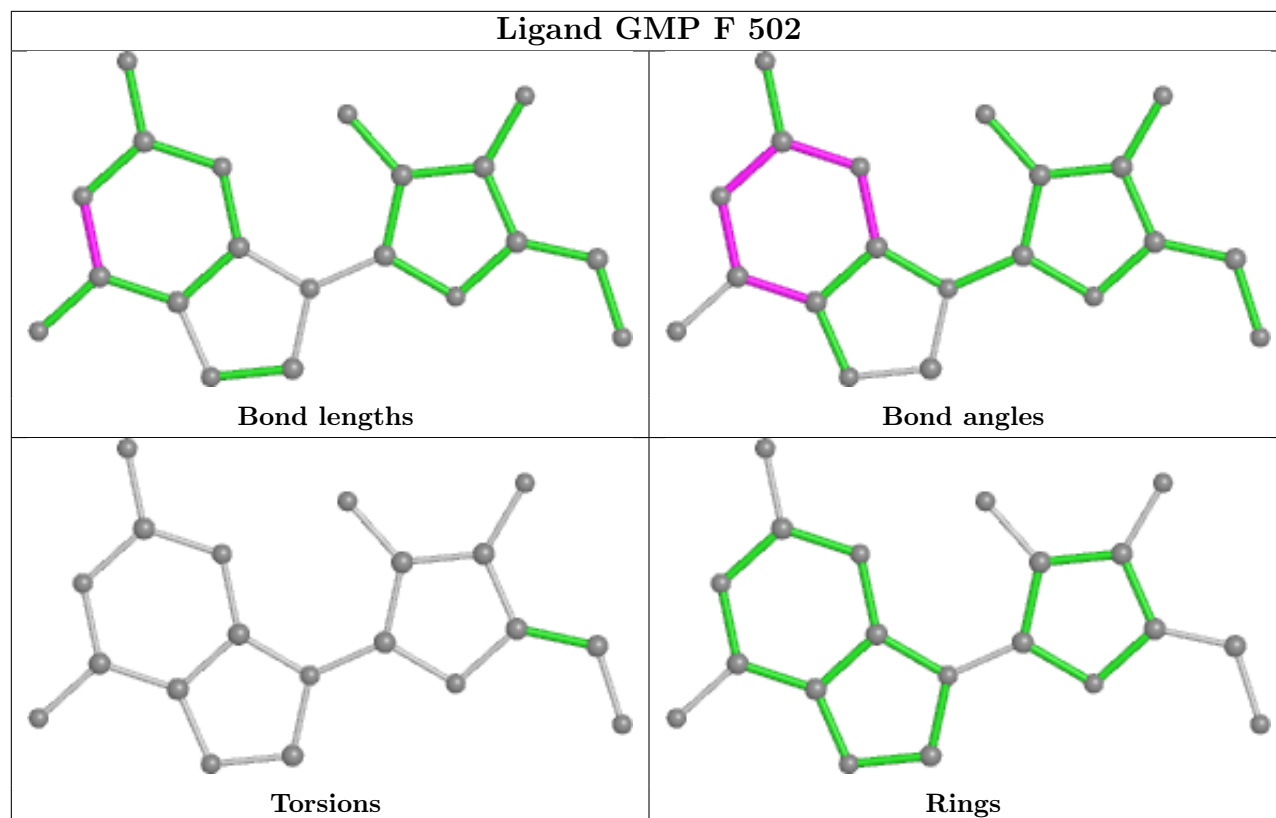
Bond angles



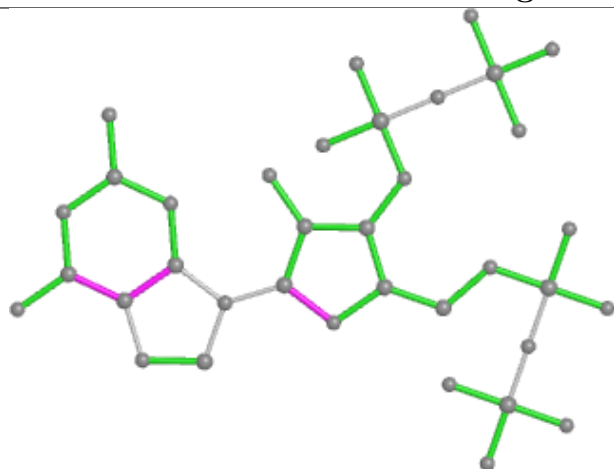
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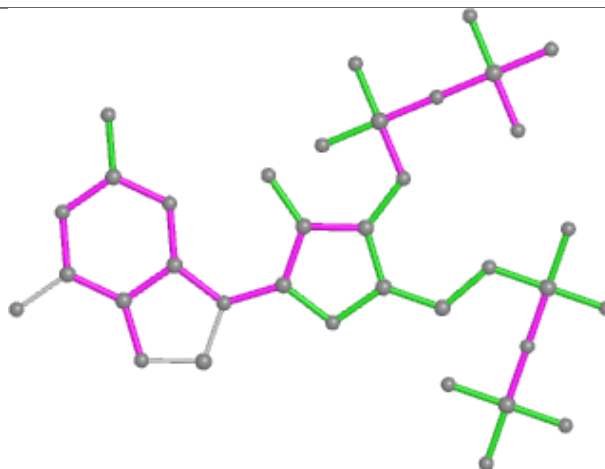
Rings



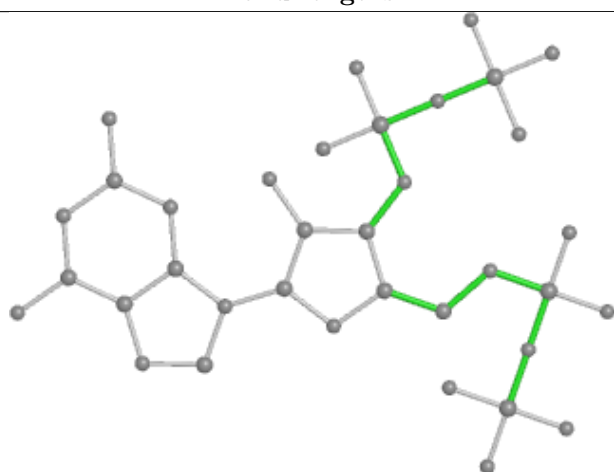
Ligand G4P B 501



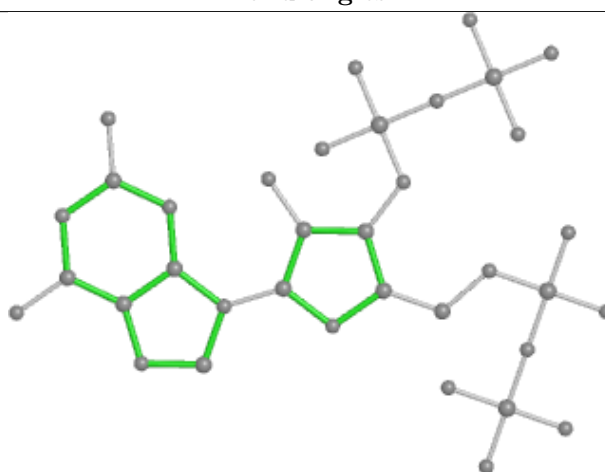
Bond lengths



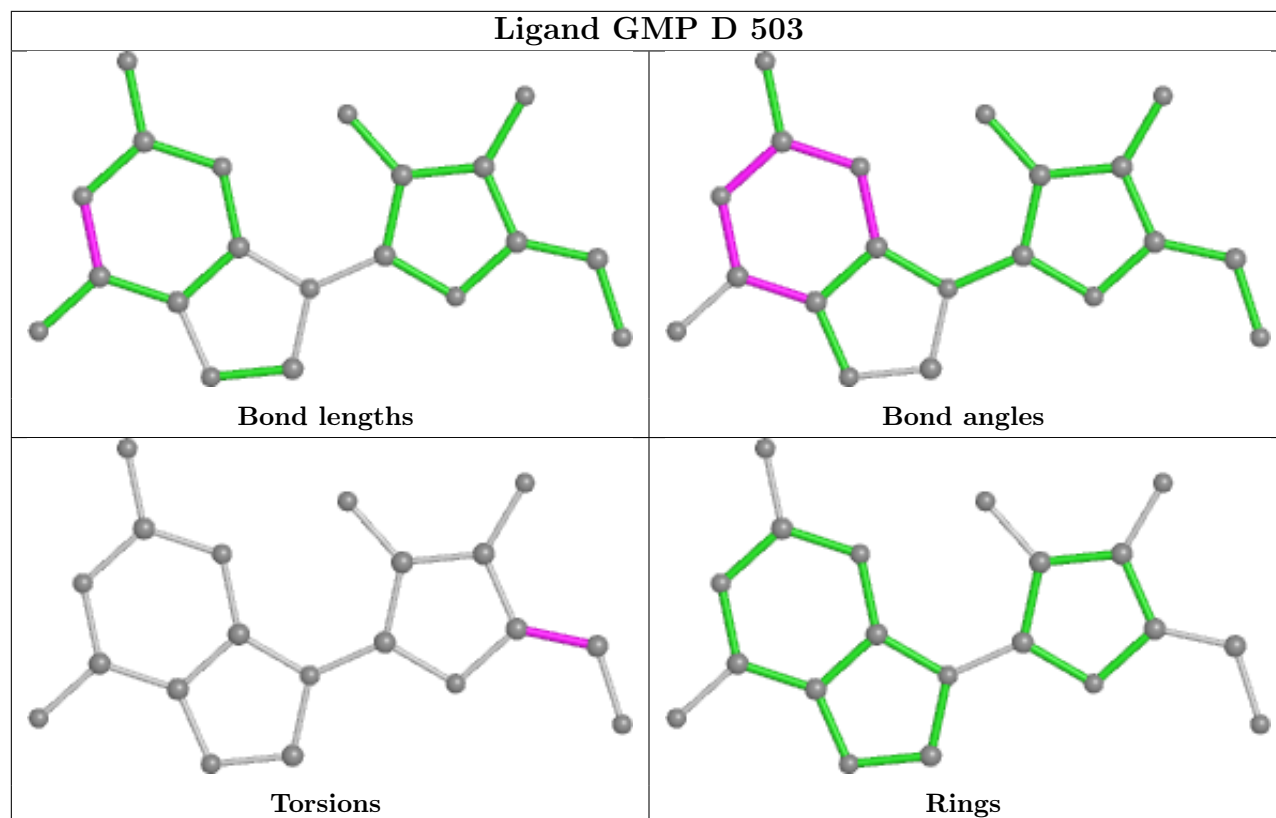
Bond angles



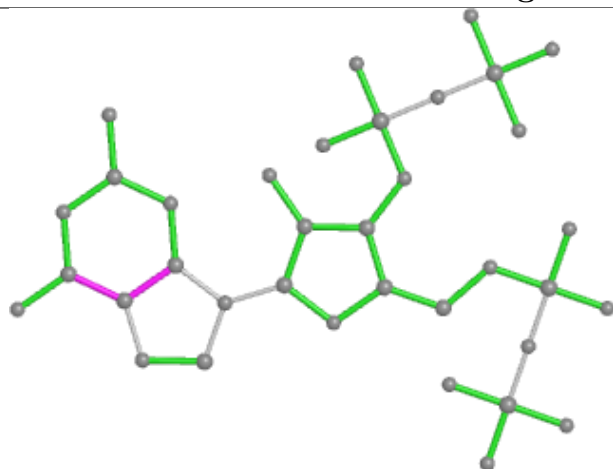
Torsions



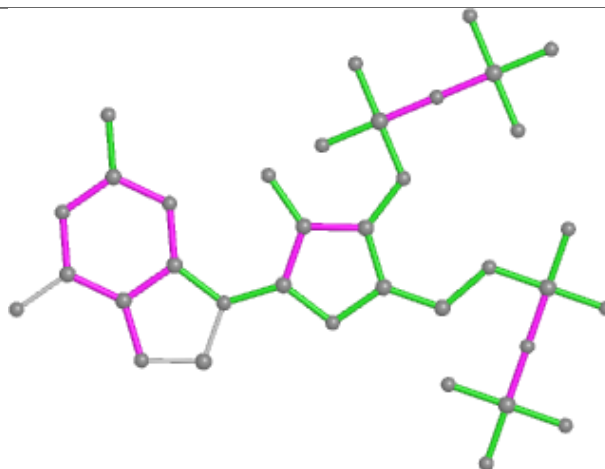
Rings



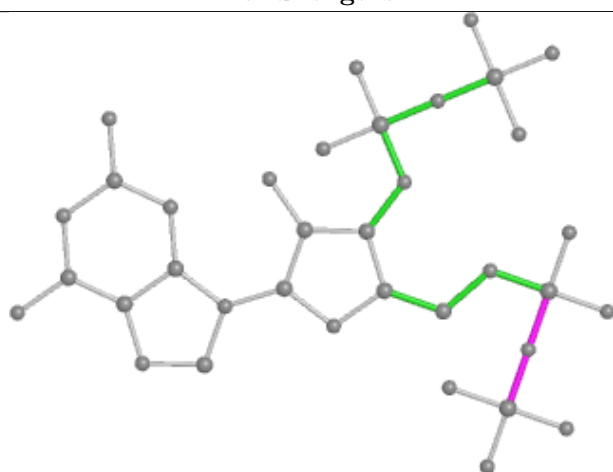
Ligand G4P E 501



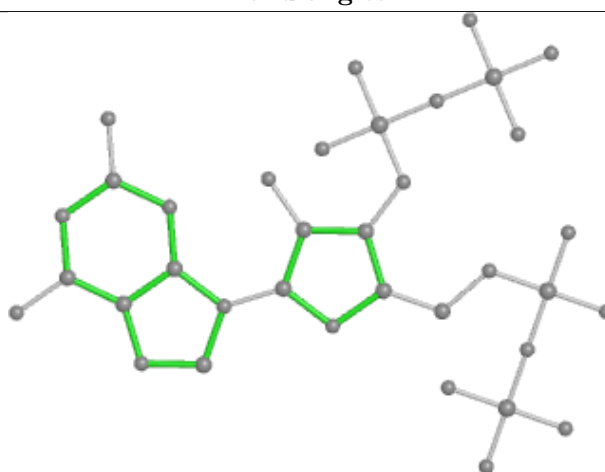
Bond lengths



Bond angles

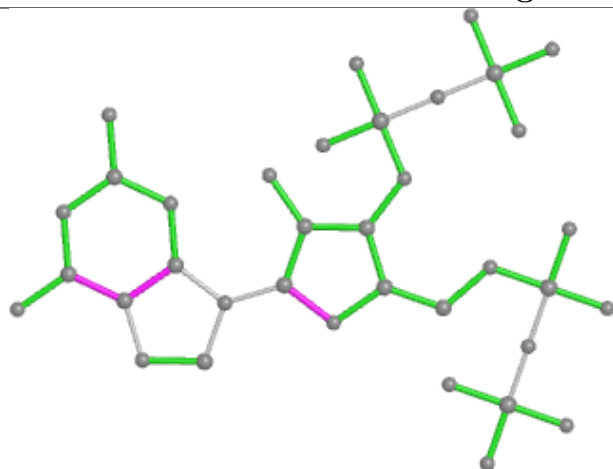


Torsions

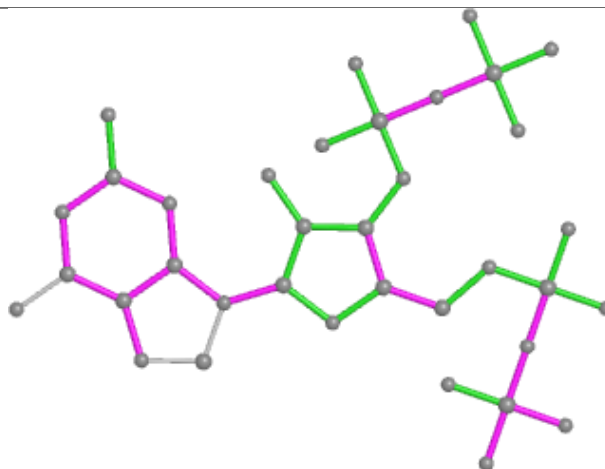


Rings

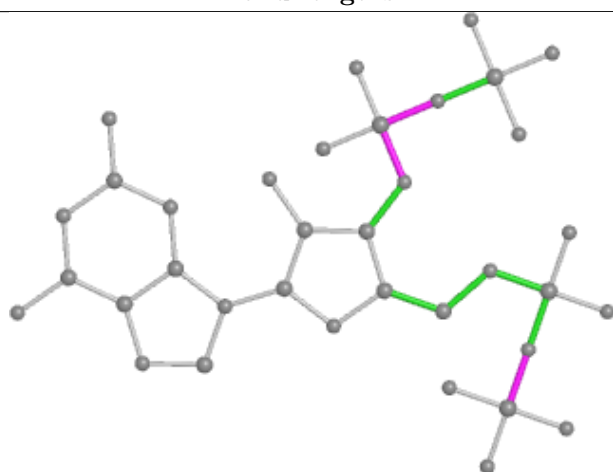
Ligand G4P C 501



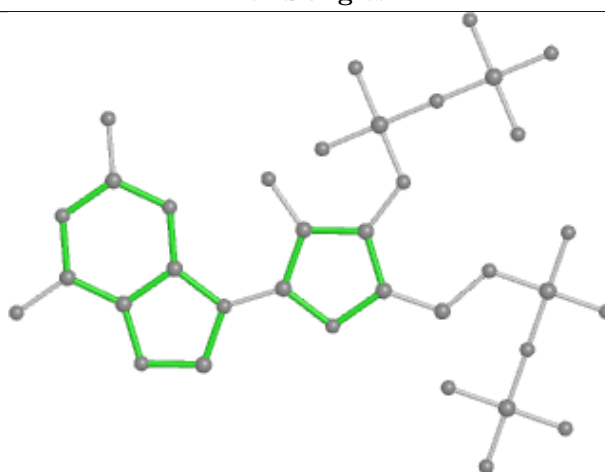
Bond lengths



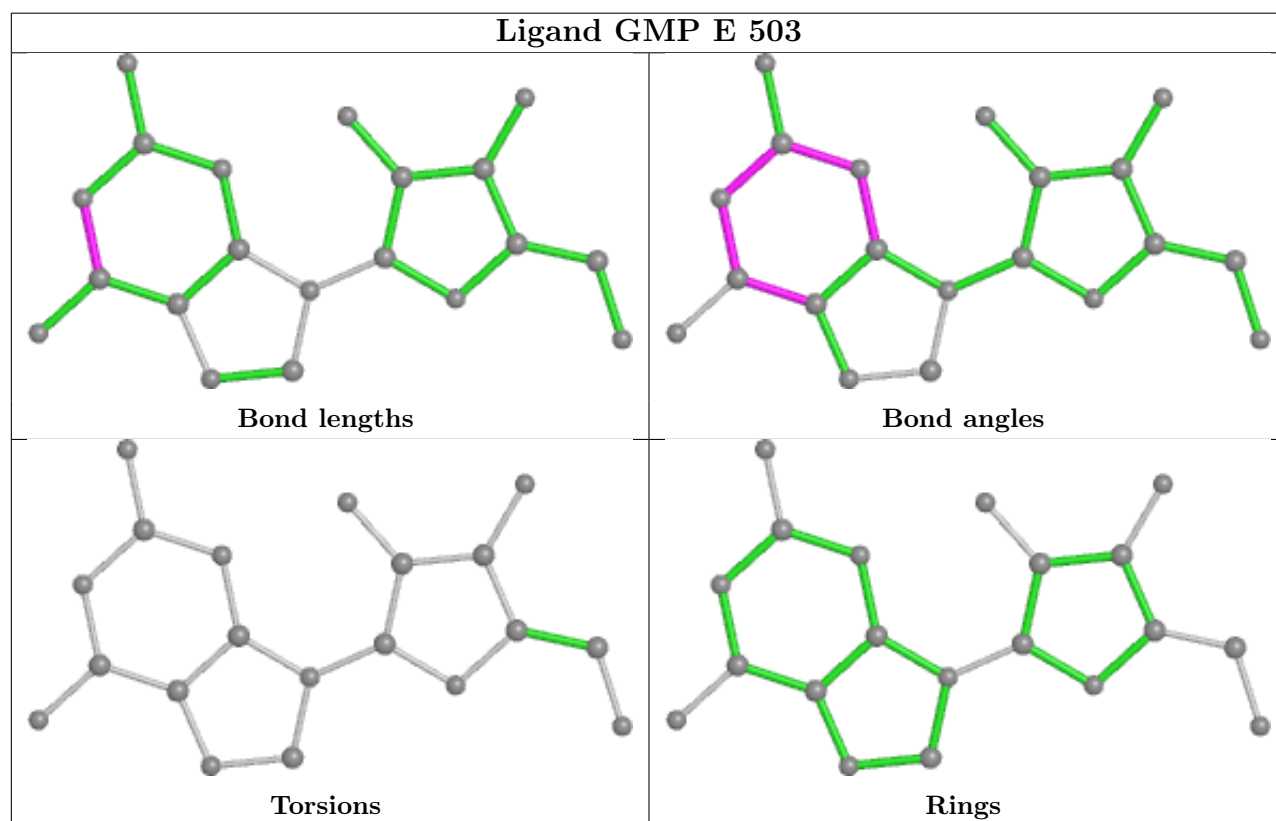
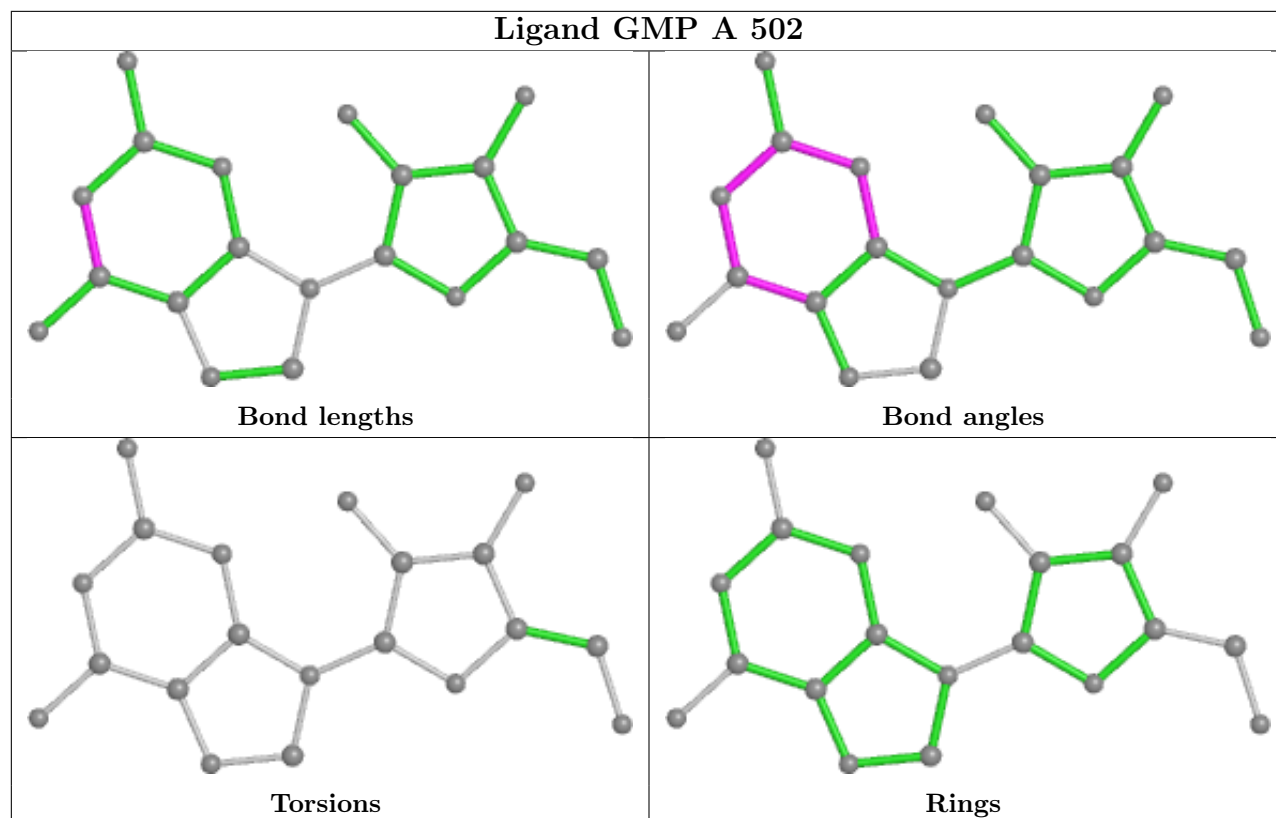
Bond angles

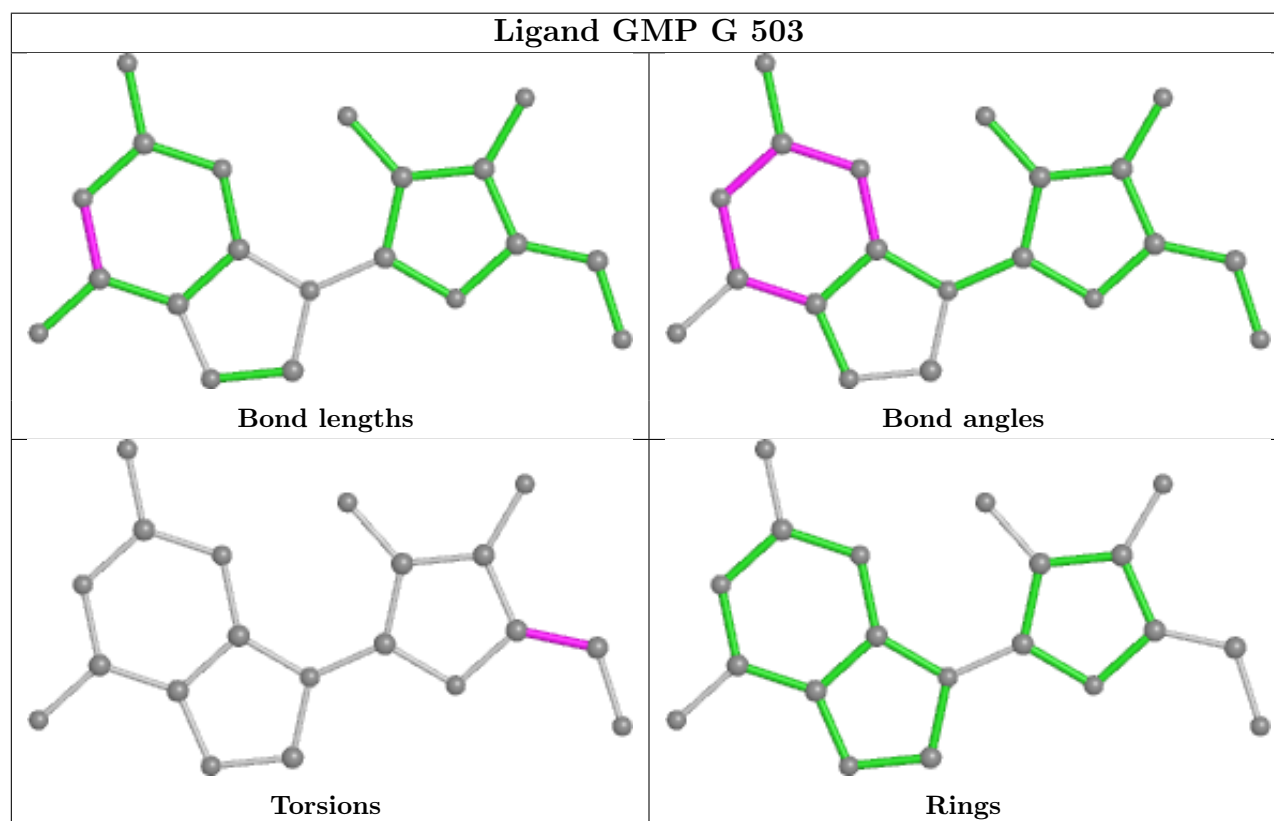
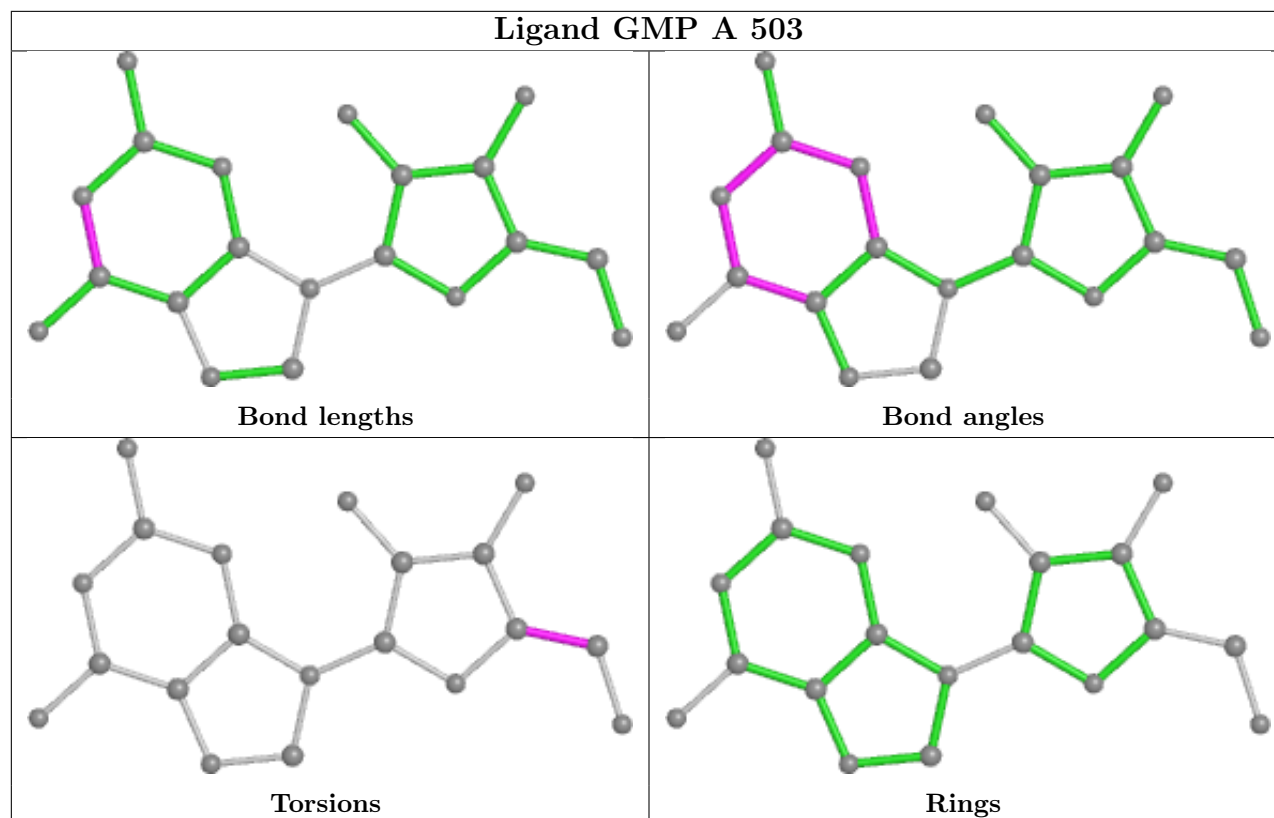


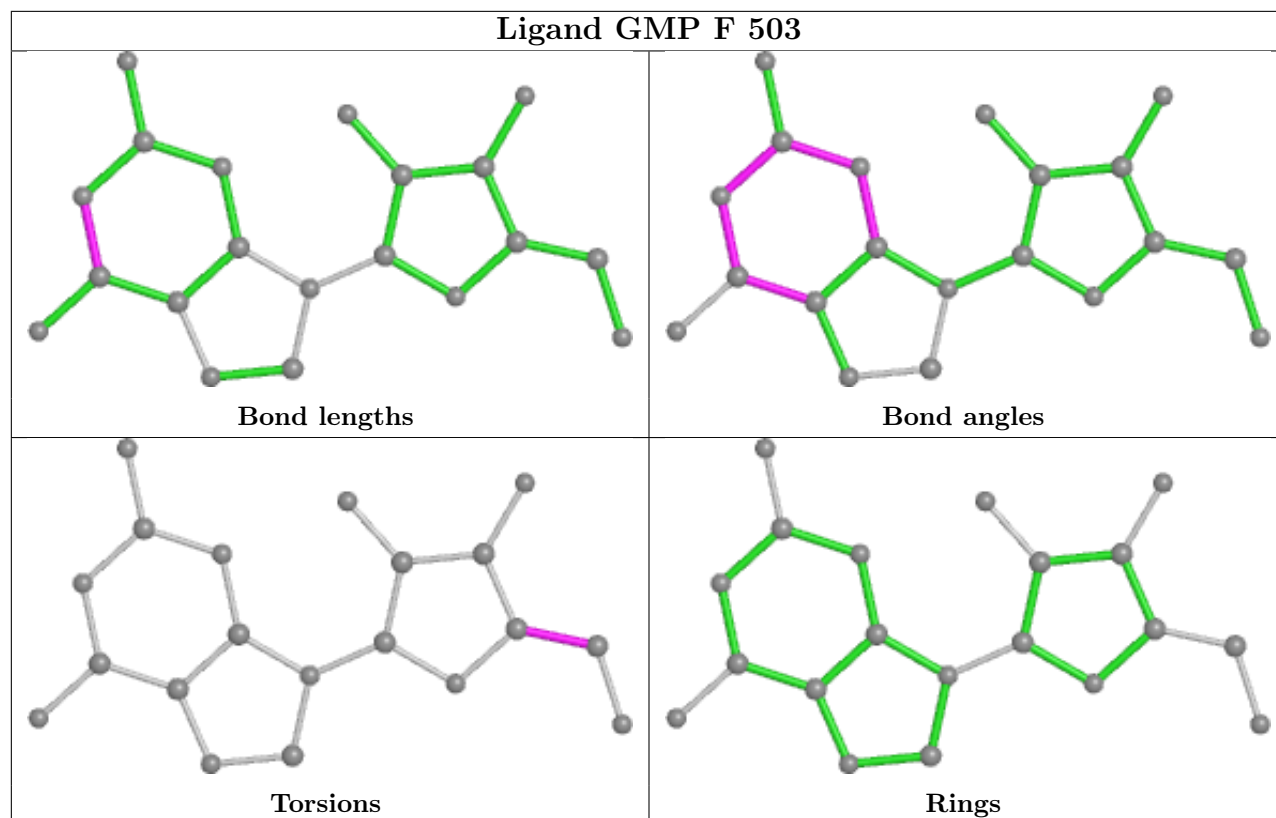
Torsions



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	435/437 (99%)	0.46	17 (3%) 39 38	96, 118, 169, 209	0
1	B	428/437 (97%)	0.62	24 (5%) 24 24	95, 121, 170, 219	0
1	C	429/437 (98%)	0.44	14 (3%) 46 44	95, 120, 169, 202	0
1	D	435/437 (99%)	0.63	29 (6%) 17 19	95, 137, 196, 218	0
1	E	422/437 (96%)	0.64	37 (8%) 10 12	105, 144, 190, 220	0
1	F	412/437 (94%)	0.95	73 (17%) 1 2	116, 169, 207, 223	0
1	G	421/437 (96%)	1.11	86 (20%) 1 1	131, 182, 212, 228	0
1	H	408/437 (93%)	0.89	62 (15%) 2 3	106, 141, 201, 227	0
All	All	3390/3496 (96%)	0.71	342 (10%) 7 9	95, 141, 201, 228	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	50	VAL	8.8
1	G	60	LEU	7.1
1	B	355	GLY	6.7
1	F	50	VAL	6.5
1	C	25	PHE	6.1
1	F	153	PHE	6.1
1	H	352	ASN	6.0
1	G	296	THR	5.9
1	F	68	ILE	5.9
1	F	346	GLY	5.8
1	E	86	ILE	5.7
1	G	68	ILE	5.6
1	G	25	PHE	5.5
1	F	60	LEU	5.3
1	G	58	TYR	5.2
1	F	31	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	G	354	ASN	5.0
1	E	80	LEU	5.0
1	F	355	GLY	4.9
1	E	162	ARG	4.9
1	G	149	ILE	4.9
1	G	155	LEU	4.8
1	F	382	SER	4.6
1	G	46	ILE	4.5
1	G	54	PHE	4.5
1	G	61	SER	4.5
1	E	153	PHE	4.4
1	F	54	PHE	4.4
1	G	48	ALA	4.4
1	G	49	LYS	4.4
1	G	85	LEU	4.3
1	H	80	LEU	4.2
1	E	308	LEU	4.2
1	D	60	LEU	4.1
1	H	54	PHE	4.1
1	G	76	LEU	4.1
1	A	29	ASN	4.1
1	D	48	ALA	4.0
1	G	151	ARG	4.0
1	G	352	ASN	4.0
1	G	0	HIS	4.0
1	H	417	THR	4.0
1	G	22	LEU	4.0
1	G	300	ALA	3.9
1	G	337	TYR	3.9
1	E	155	LEU	3.9
1	D	50	VAL	3.9
1	H	349	LYS	3.9
1	B	347	PRO	3.9
1	G	86	ILE	3.9
1	H	55	ILE	3.9
1	F	89	GLN	3.8
1	G	297	GLU	3.8
1	D	58	TYR	3.8
1	G	62	ALA	3.8
1	H	72	VAL	3.8
1	F	0	HIS	3.8
1	C	21	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	0	HIS	3.7
1	E	353	THR	3.7
1	G	338	SER	3.7
1	F	310	PRO	3.7
1	G	135	SER	3.7
1	A	54	PHE	3.7
1	G	295	PHE	3.7
1	F	271	SER	3.7
1	G	80	LEU	3.7
1	F	80	LEU	3.7
1	G	308	LEU	3.7
1	D	153	PHE	3.6
1	F	13	PHE	3.6
1	C	22	LEU	3.6
1	G	77	TYR	3.6
1	H	336	VAL	3.6
1	H	79	GLU	3.6
1	G	162	ARG	3.5
1	F	116	MET	3.5
1	F	381	SER	3.5
1	H	432	TRP	3.5
1	E	50	VAL	3.5
1	F	46	ILE	3.4
1	G	131	CYS	3.4
1	H	131	CYS	3.4
1	F	58	TYR	3.4
1	G	41	GLN	3.4
1	G	318	GLN	3.4
1	G	166	ILE	3.4
1	G	153	PHE	3.4
1	G	134	SER	3.4
1	F	312	ALA	3.4
1	F	127	TYR	3.4
1	G	161	GLU	3.3
1	F	158	GLU	3.3
1	B	49	LYS	3.3
1	E	77	TYR	3.3
1	G	59	GLY	3.3
1	E	85	LEU	3.3
1	C	0	HIS	3.2
1	D	57	ARG	3.2
1	G	163	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	316	PHE	3.2
1	G	34	ALA	3.2
1	A	25	PHE	3.2
1	D	25	PHE	3.2
1	F	85	LEU	3.2
1	H	135	SER	3.2
1	C	164	PHE	3.2
1	G	291	TYR	3.2
1	H	0	HIS	3.1
1	B	85	LEU	3.1
1	F	76	LEU	3.1
1	G	39	ILE	3.1
1	H	155	LEU	3.1
1	E	76	LEU	3.1
1	H	53	GLU	3.0
1	H	76	LEU	3.0
1	C	60	LEU	3.0
1	D	131	CYS	3.0
1	F	233	ILE	3.0
1	F	155	LEU	3.0
1	G	164	PHE	2.9
1	G	319	TYR	2.9
1	H	134	SER	2.9
1	H	83	LYS	2.9
1	G	292	MET	2.9
1	D	49	LYS	2.9
1	D	26	GLN	2.9
1	G	66	LEU	2.9
1	F	301	LYS	2.9
1	D	80	LEU	2.9
1	E	47	GLU	2.9
1	G	137	THR	2.9
1	B	29	ASN	2.9
1	D	68	ILE	2.8
1	F	14	PRO	2.8
1	G	73	ALA	2.8
1	H	9	SER	2.8
1	B	80	LEU	2.8
1	D	291	TYR	2.8
1	H	271	SER	2.8
1	E	68	ILE	2.8
1	B	50	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	152	CYS	2.8
1	F	275	LEU	2.8
1	G	298	ASP	2.8
1	B	48	ALA	2.8
1	H	324	ALA	2.8
1	F	151	ARG	2.8
1	F	385	LYS	2.8
1	F	49	LYS	2.7
1	D	155	LEU	2.7
1	H	50	VAL	2.7
1	B	358	ASP	2.7
1	G	423	ARG	2.7
1	A	131	CYS	2.7
1	A	58	TYR	2.7
1	G	65	SER	2.7
1	D	165	ALA	2.7
1	F	380	ASN	2.7
1	F	417	THR	2.7
1	D	54	PHE	2.7
1	F	162	ARG	2.7
1	F	412	HIS	2.7
1	F	77	TYR	2.7
1	G	125	TYR	2.7
1	H	73	ALA	2.7
1	B	83	LYS	2.7
1	E	419	GLY	2.7
1	A	310	PRO	2.7
1	D	28	GLU	2.7
1	F	313	ILE	2.7
1	H	52	ASP	2.6
1	E	116	MET	2.6
1	H	291	TYR	2.6
1	H	354	ASN	2.6
1	A	316	PHE	2.6
1	A	135	SER	2.6
1	B	82	GLN	2.6
1	F	149	ILE	2.6
1	D	27	PRO	2.6
1	G	331	GLN	2.6
1	E	46	ILE	2.6
1	E	53	GLU	2.6
1	H	296	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	25	PHE	2.6
1	C	115	VAL	2.6
1	G	386	PHE	2.6
1	B	60	LEU	2.6
1	G	417	THR	2.6
1	F	12	TYR	2.5
1	H	353	THR	2.5
1	G	293	ALA	2.5
1	H	56	GLU	2.5
1	B	55	ILE	2.5
1	F	51	ASP	2.5
1	G	253	MET	2.5
1	H	413	SER	2.5
1	C	165	ALA	2.5
1	D	29	ASN	2.5
1	H	58	TYR	2.5
1	A	417	THR	2.5
1	D	261	LEU	2.5
1	E	125	TYR	2.5
1	D	417	THR	2.5
1	G	13	PHE	2.5
1	C	135	SER	2.5
1	G	55	ILE	2.5
1	H	8	LYS	2.5
1	G	64	HIS	2.5
1	G	57	ARG	2.5
1	B	58	TYR	2.5
1	D	77	TYR	2.5
1	F	10	LYS	2.5
1	E	13	PHE	2.5
1	B	357	GLY	2.4
1	C	153	PHE	2.4
1	F	165	ALA	2.4
1	G	53	GLU	2.4
1	F	32	SER	2.4
1	H	399	LYS	2.4
1	G	26	GLN	2.4
1	E	154	THR	2.4
1	F	212	ALA	2.4
1	G	424	GLU	2.4
1	A	424	GLU	2.4
1	B	356	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	291	TYR	2.4
1	E	412	HIS	2.4
1	F	293	ALA	2.4
1	H	297	GLU	2.4
1	G	52	ASP	2.4
1	H	412	HIS	2.4
1	F	1	MET	2.3
1	H	385	LYS	2.3
1	G	294	GLY	2.3
1	H	331	GLN	2.3
1	E	48	ALA	2.3
1	C	24	GLN	2.3
1	F	261	LEU	2.3
1	D	59	GLY	2.3
1	F	311	GLY	2.3
1	E	417	THR	2.3
1	F	337	TYR	2.3
1	G	152	CYS	2.3
1	H	293	ALA	2.3
1	H	100	HIS	2.3
1	E	55	ILE	2.3
1	D	295	PHE	2.3
1	D	115	VAL	2.3
1	H	295	PHE	2.3
1	H	358	ASP	2.3
1	H	92	GLY	2.3
1	E	385	LYS	2.3
1	F	159	SER	2.3
1	H	85	LEU	2.3
1	F	115	VAL	2.3
1	F	410	ASN	2.3
1	H	301	LYS	2.3
1	H	280	LEU	2.3
1	G	119	ASN	2.3
1	C	55	ILE	2.3
1	H	5	GLY	2.3
1	A	80	LEU	2.3
1	F	280	LEU	2.3
1	B	155	LEU	2.2
1	H	153	PHE	2.2
1	H	337	TYR	2.2
1	E	151	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	39	ILE	2.2
1	G	47	GLU	2.2
1	G	78	GLN	2.2
1	F	268	LEU	2.2
1	F	134	SER	2.2
1	H	97	ASN	2.2
1	A	230	LYS	2.2
1	E	82	GLN	2.2
1	H	330	CYS	2.2
1	D	85	LEU	2.2
1	D	412	HIS	2.2
1	E	58	TYR	2.2
1	B	135	SER	2.2
1	F	300	ALA	2.2
1	G	43	LEU	2.2
1	H	338	SER	2.2
1	A	308	LEU	2.2
1	F	48	ALA	2.2
1	H	82	GLN	2.2
1	E	0	HIS	2.2
1	G	229	THR	2.2
1	H	434	ARG	2.2
1	A	423	ARG	2.1
1	G	51	ASP	2.1
1	G	157	GLY	2.1
1	F	260	ALA	2.1
1	E	184	ILE	2.1
1	A	76	LEU	2.1
1	G	176	ALA	2.1
1	E	149	ILE	2.1
1	G	136	ARG	2.1
1	H	6	LYS	2.1
1	H	13	PHE	2.1
1	E	299	GLU	2.1
1	F	295	PHE	2.1
1	H	151	ARG	2.1
1	F	55	ILE	2.1
1	E	268	LEU	2.1
1	F	423	ARG	2.1
1	F	11	HIS	2.1
1	B	6	LYS	2.1
1	H	10	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	0	HIS	2.1
1	G	420	LEU	2.1
1	C	131	CYS	2.1
1	F	247	HIS	2.1
1	A	309	LEU	2.1
1	G	132	ASN	2.1
1	F	267	PRO	2.1
1	H	49	LYS	2.1
1	F	251	LEU	2.1
1	B	54	PHE	2.1
1	F	161	GLU	2.1
1	H	14	PRO	2.1
1	H	75	ALA	2.1
1	H	89	GLN	2.0
1	F	299	GLU	2.0
1	A	55	ILE	2.0
1	F	281	VAL	2.0
1	G	251	LEU	2.0
1	H	163	THR	2.0
1	E	164	PHE	2.0
1	G	71	ASP	2.0
1	B	131	CYS	2.0
1	E	51	ASP	2.0
1	G	281	VAL	2.0
1	G	63	GLY	2.0
1	E	310	PRO	2.0
1	B	12	TYR	2.0
1	C	385	LYS	2.0
1	F	135	SER	2.0
1	F	73	ALA	2.0
1	D	292	MET	2.0
1	G	410	ASN	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 ⓘ

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.

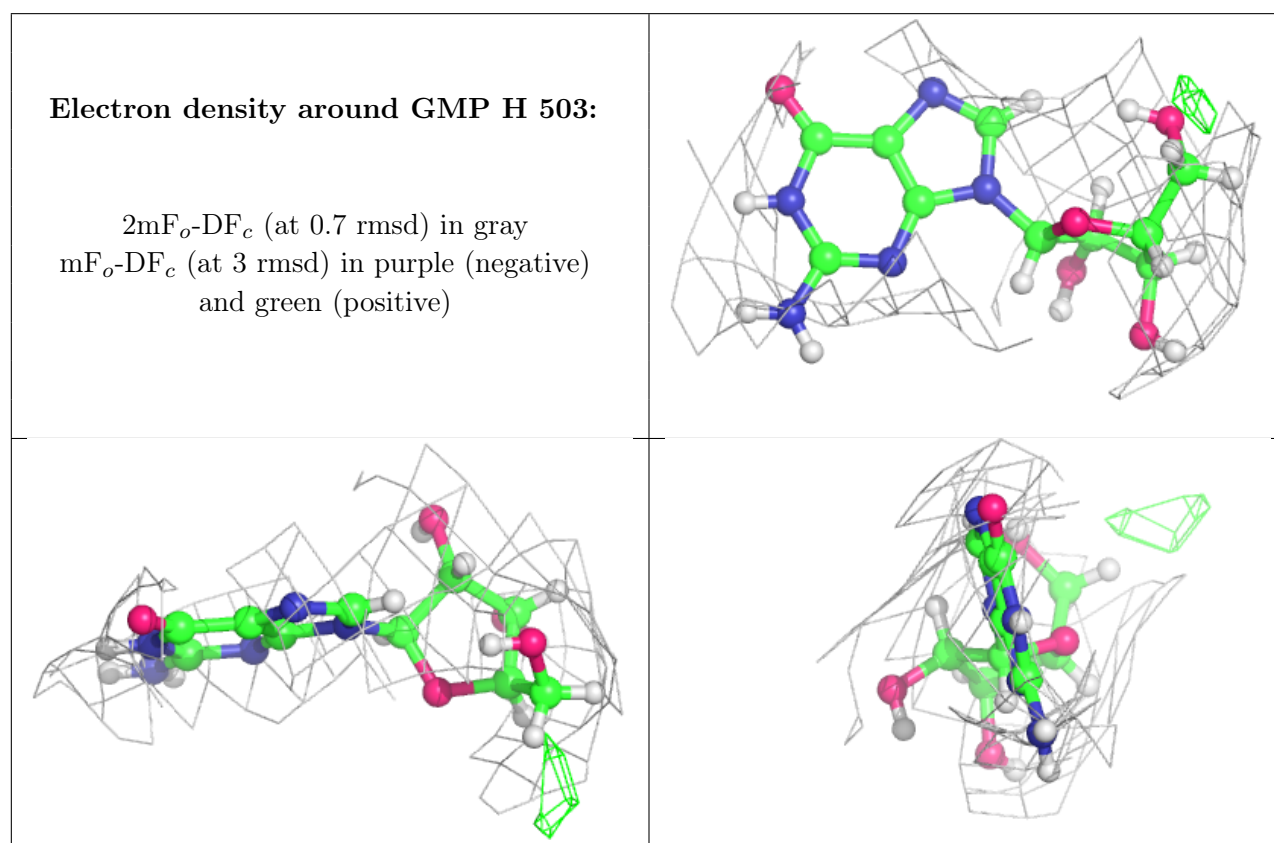
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	F	504	1/1	0.50	0.29	392,392,392,392	0
5	MG	E	506	1/1	0.56	2.37	146,146,146,146	0
4	K	C	505	1/1	0.65	0.43	198,198,198,198	0
5	MG	H	506	1/1	0.73	1.50	133,133,133,133	0
4	K	G	504	1/1	0.74	0.73	210,210,210,210	0
5	MG	D	505	1/1	0.77	0.78	143,143,143,143	0
3	GMP	H	503	20/20	0.77	0.24	119,168,224,228	0
3	GMP	C	503	20/20	0.79	0.34	105,147,201,221	0
3	GMP	F	503	20/20	0.79	0.26	174,215,279,282	0
5	MG	F	505	1/1	0.80	0.84	148,148,148,148	0
3	GMP	G	503	20/20	0.82	0.21	184,212,266,273	0
4	K	B	505	1/1	0.82	0.66	294,294,294,294	0
5	MG	G	505	1/1	0.83	0.78	177,177,177,177	0
5	MG	C	506	1/1	0.84	0.78	131,131,131,131	0
4	K	D	504	1/1	0.84	0.16	202,202,202,202	0
4	K	E	505	1/1	0.85	0.43	128,128,128,128	0
3	GMP	G	502	20/20	0.85	0.25	175,201,249,250	0
3	GMP	B	503	20/20	0.85	0.27	135,167,227,238	0
3	GMP	D	503	20/20	0.86	0.28	148,189,241,253	0
3	GMP	A	503	20/20	0.86	0.21	115,149,214,223	0
2	G4P	F	501	36/36	0.86	0.23	135,183,249,272	0
3	GMP	E	503	20/20	0.87	0.18	116,182,240,247	0
2	G4P	H	501	36/36	0.87	0.22	136,171,232,249	0
2	G4P	G	501	36/36	0.88	0.13	137,178,227,239	0
4	K	H	505	1/1	0.89	0.34	183,183,183,183	0
3	GMP	F	502	20/20	0.89	0.20	163,182,220,240	0
5	MG	A	505	1/1	0.89	0.78	139,139,139,139	0
2	G4P	A	501	36/36	0.90	0.19	94,133,192,226	0
2	G4P	E	501	36/36	0.90	0.19	117,151,220,257	0
3	GMP	E	502	20/20	0.91	0.28	137,161,197,213	0
4	K	H	504	1/1	0.92	0.65	160,160,160,160	0
2	G4P	D	501	36/36	0.93	0.18	94,123,187,212	0
2	G4P	C	501	36/36	0.93	0.17	94,121,198,233	0
3	GMP	D	502	20/20	0.94	0.24	125,152,194,229	0
2	G4P	B	501	36/36	0.94	0.15	97,135,196,219	0
4	K	E	504	1/1	0.94	0.30	135,135,135,135	0
3	GMP	A	502	20/20	0.94	0.27	95,116,164,203	0

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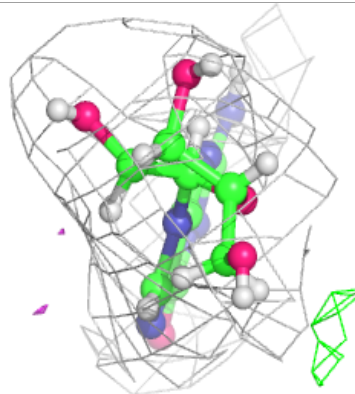
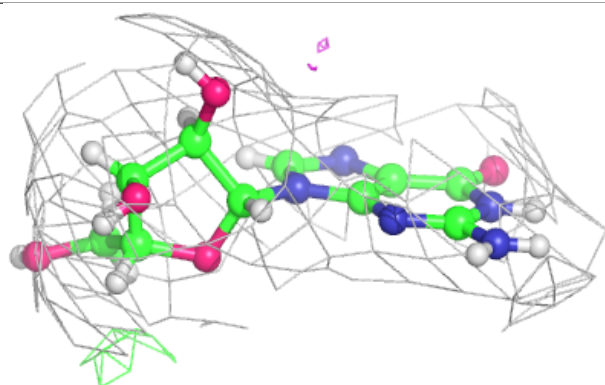
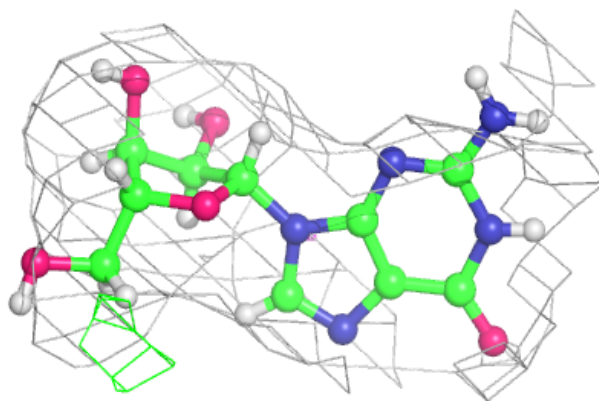
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GMP	B	502	20/20	0.94	0.27	94,108,131,187	0
3	GMP	C	502	20/20	0.95	0.29	94,124,169,215	0
3	GMP	H	502	20/20	0.96	0.35	108,137,192,196	0
4	K	B	504	1/1	0.97	0.41	113,113,113,113	0
4	K	C	504	1/1	0.97	0.32	94,94,94,94	0
4	K	A	504	1/1	0.97	0.52	145,145,145,145	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.

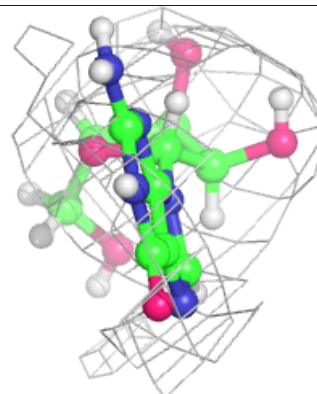
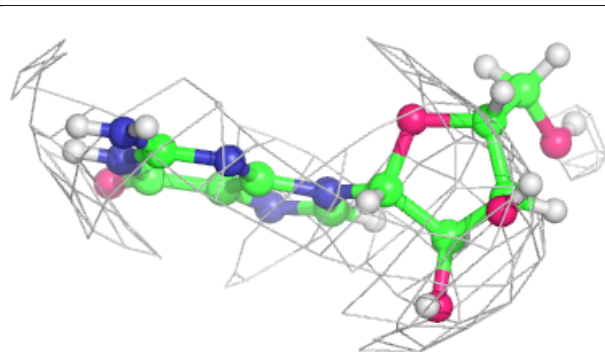
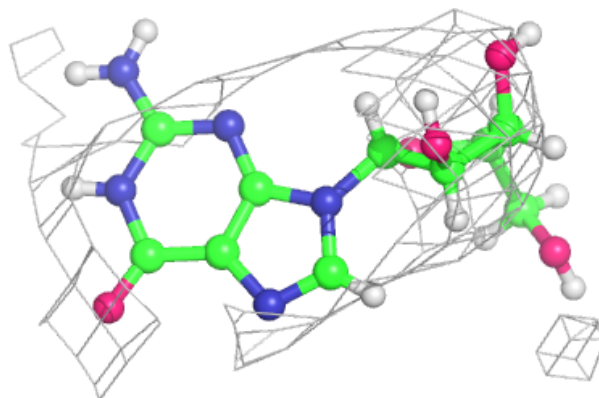


Electron density around GMP C 503:

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

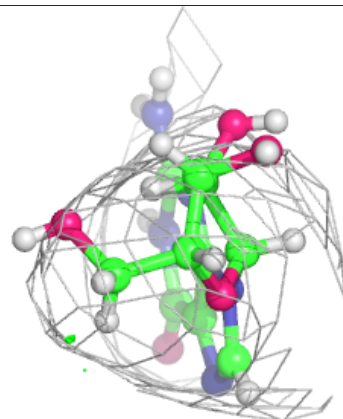
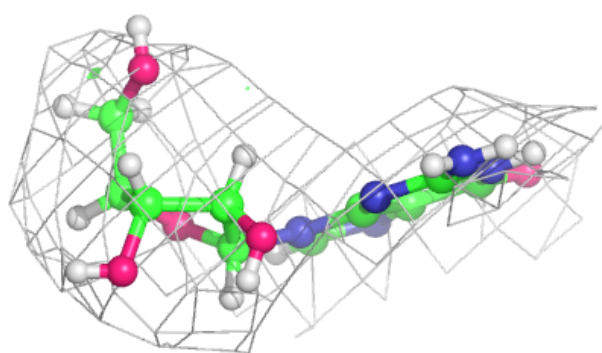
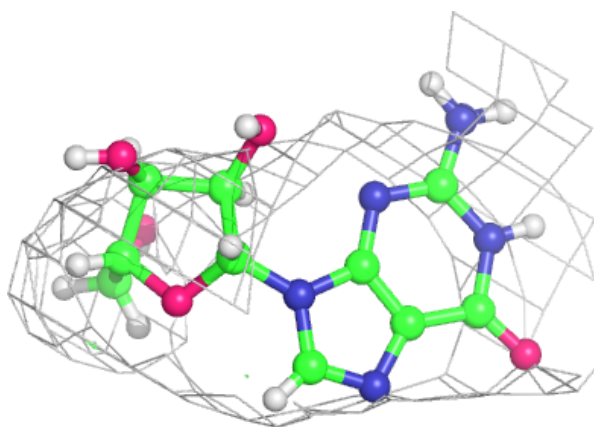
**Electron density around GMP F 503:**

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

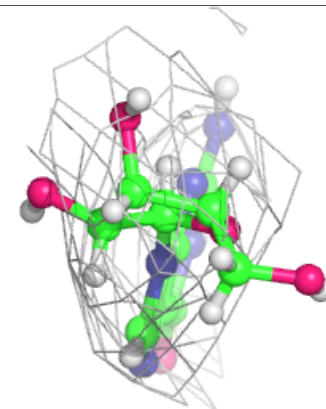
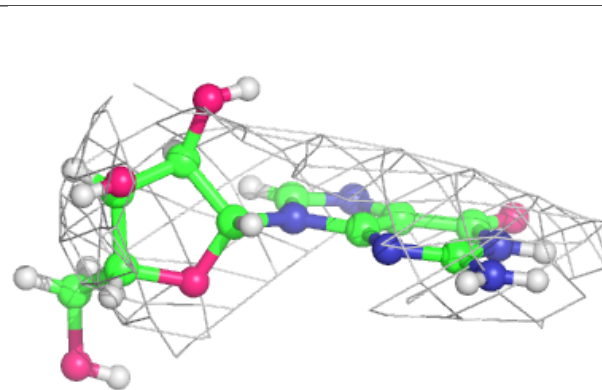
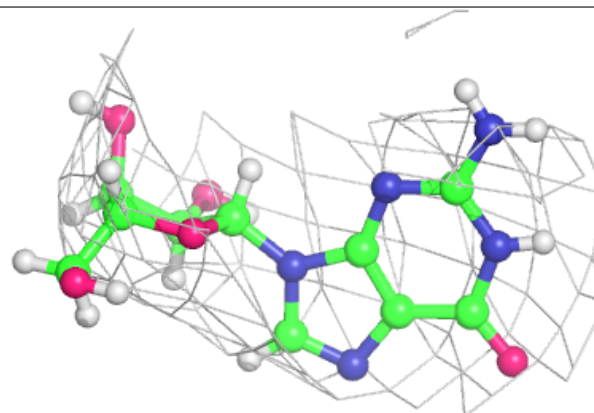


Electron density around GMP G 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

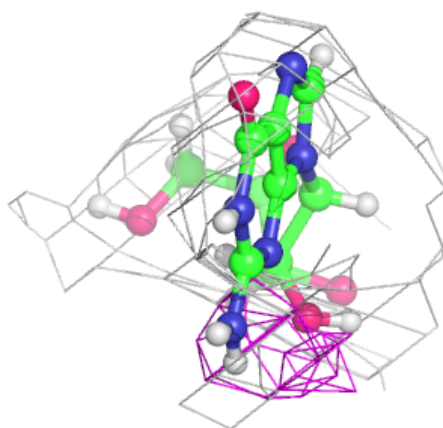
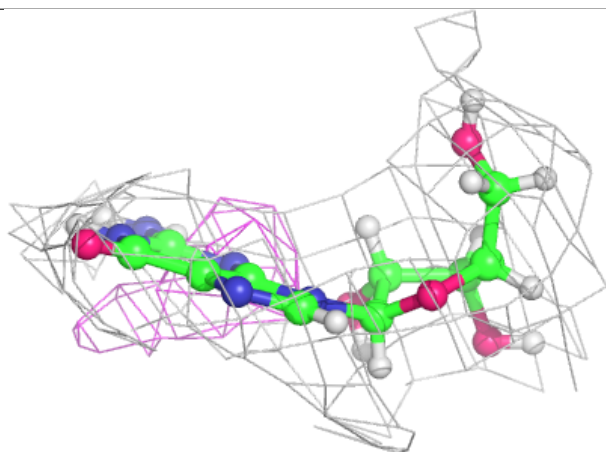
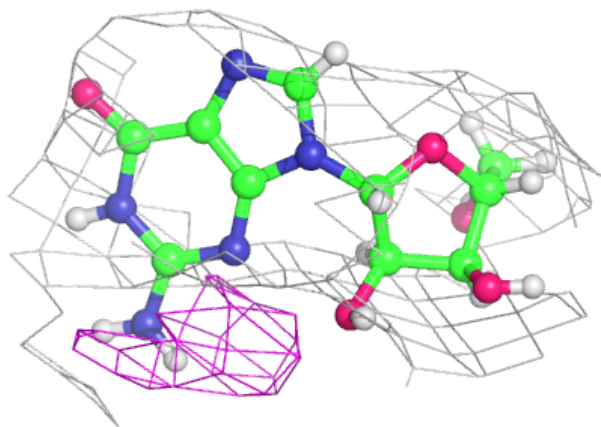
**Electron density around GMP G 502:**

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



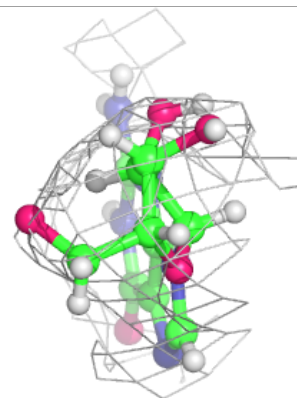
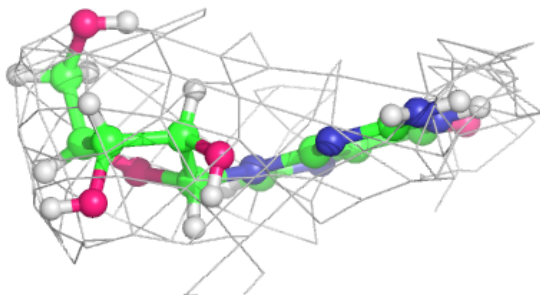
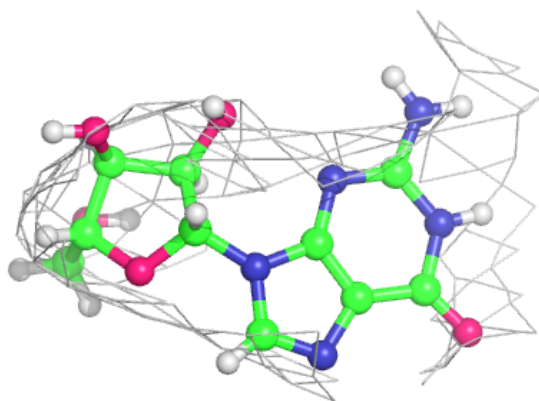
Electron density around GMP B 503:

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

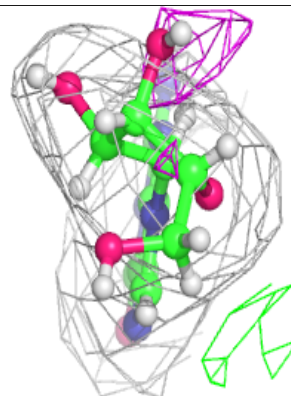
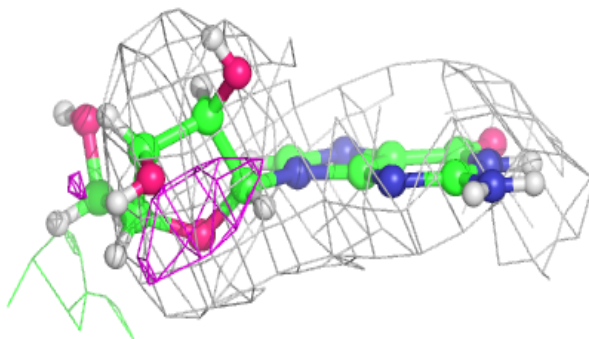
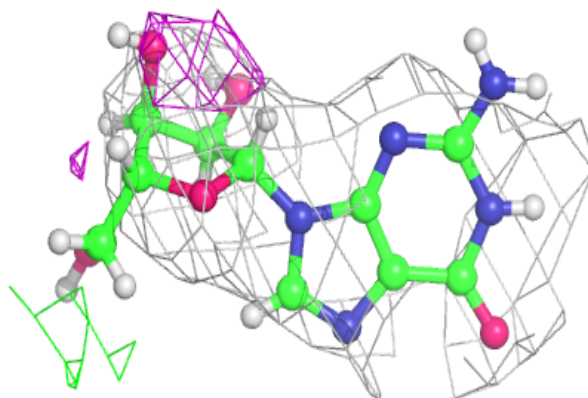


Electron density around GMP D 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

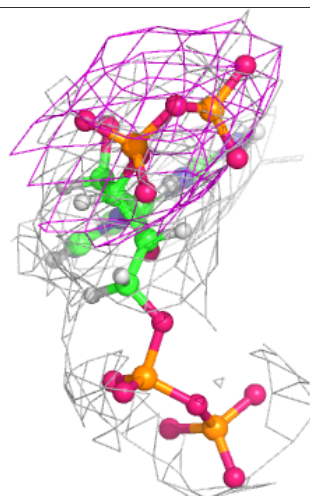
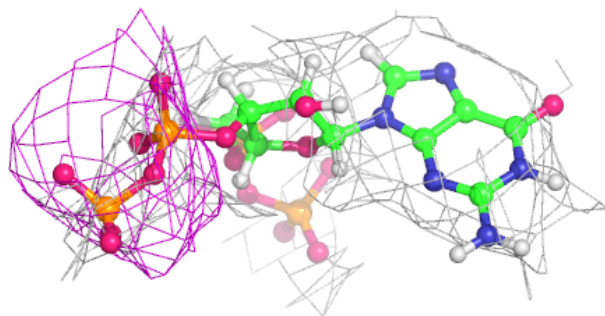
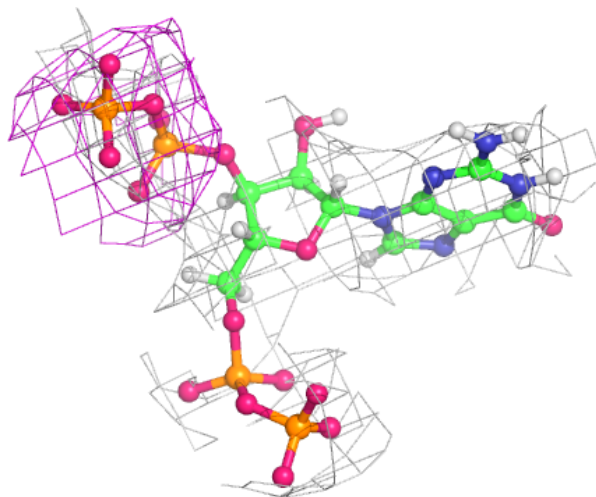
**Electron density around GMP A 503:**

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



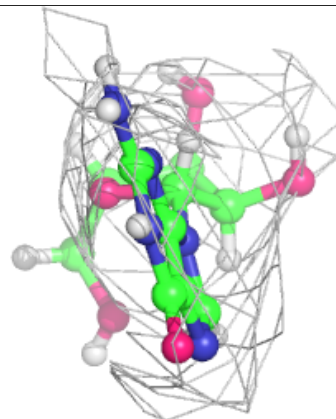
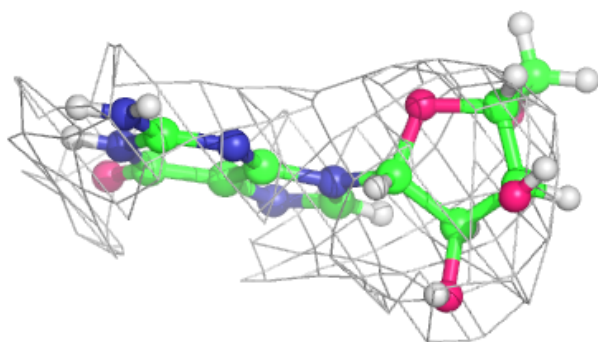
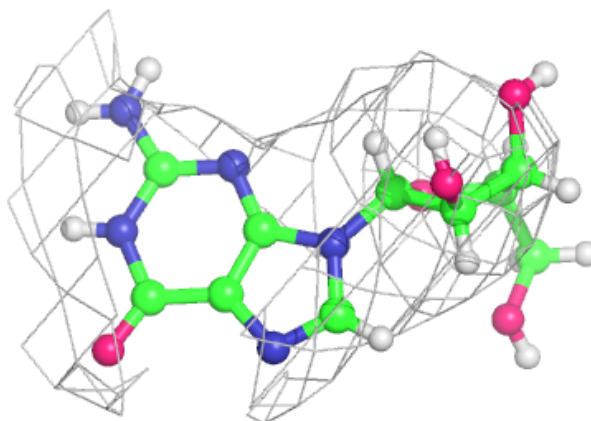
Electron density around G4P F 501:

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



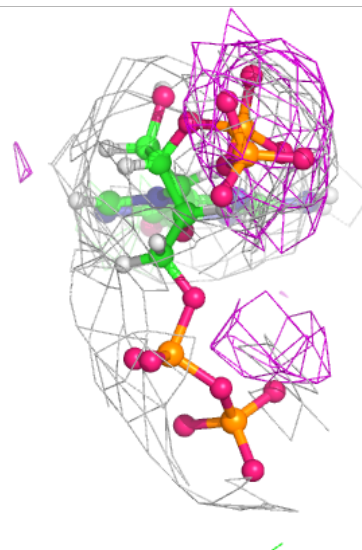
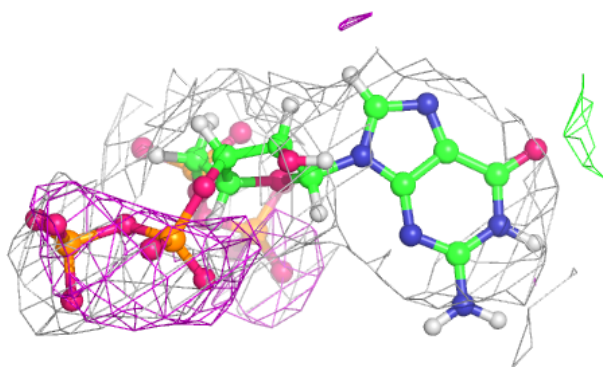
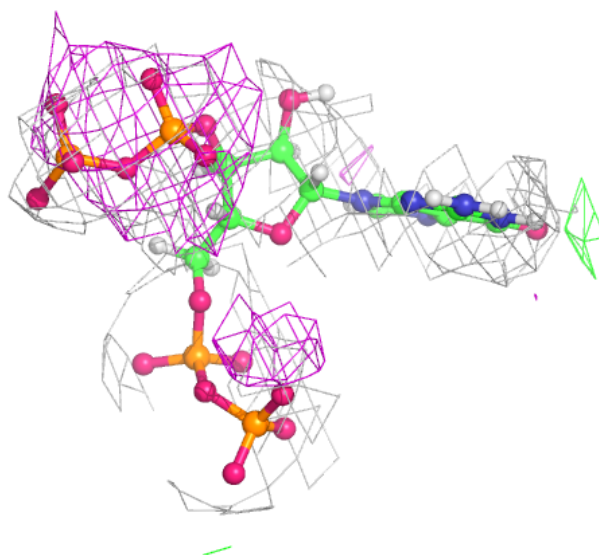
Electron density around GMP E 503:

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



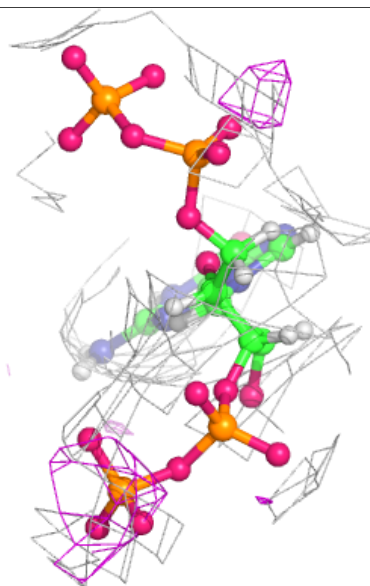
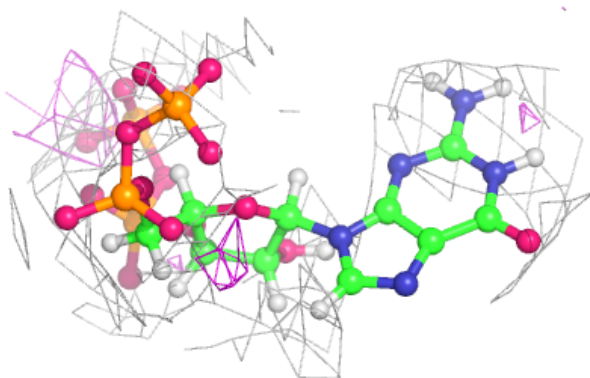
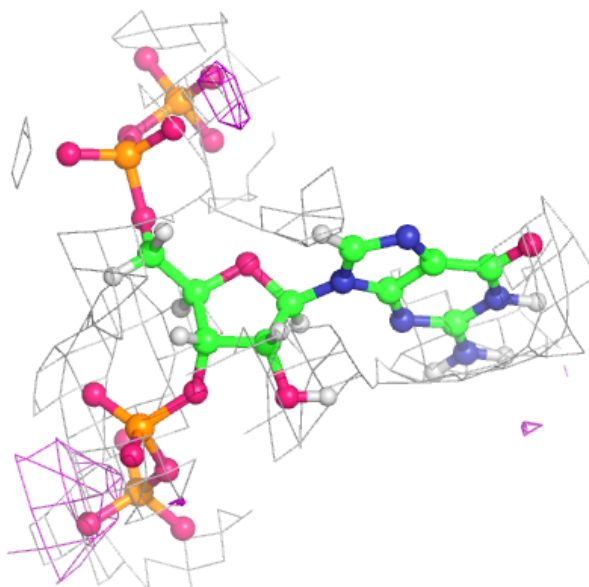
Electron density around G4P H 501:

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



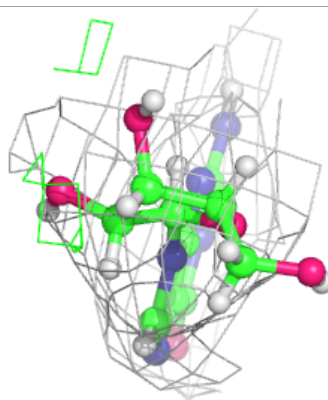
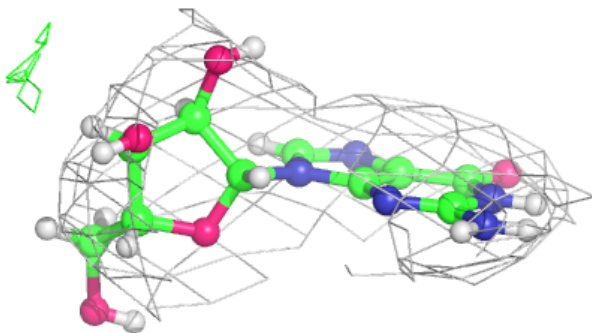
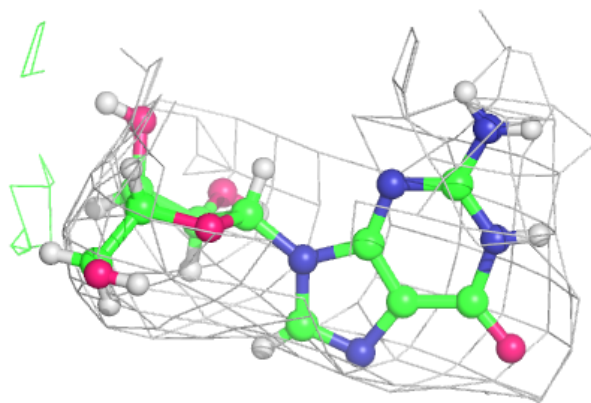
Electron density around G4P G 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



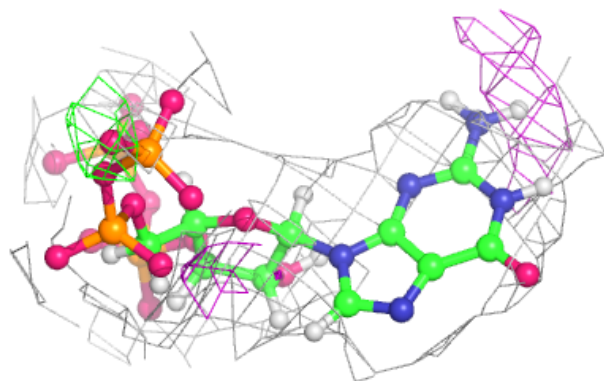
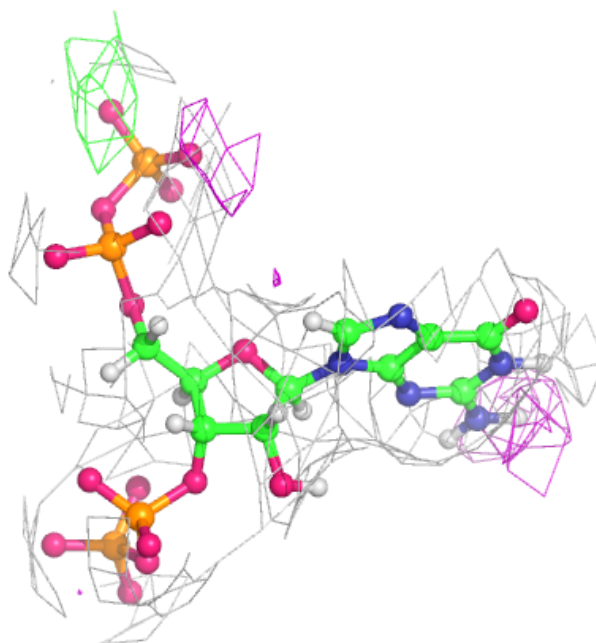
Electron density around GMP F 502:

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



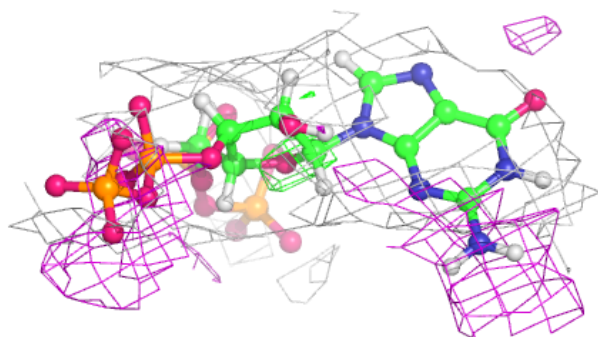
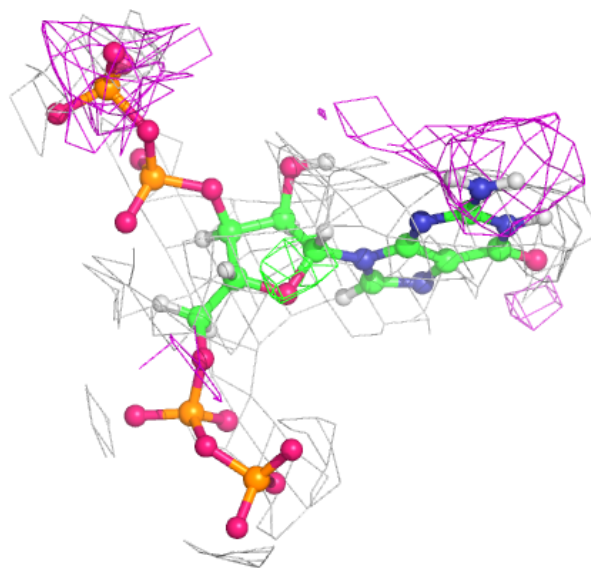
Electron density around G4P A 501:

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



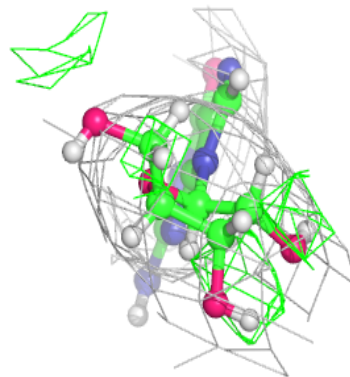
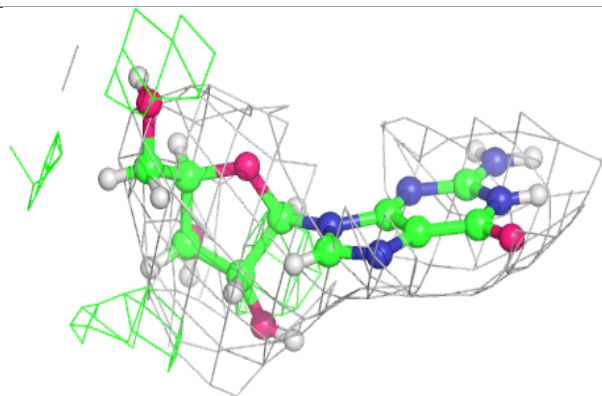
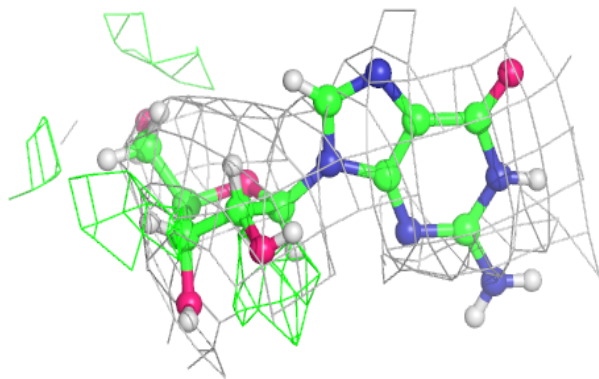
Electron density around G4P E 501:

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



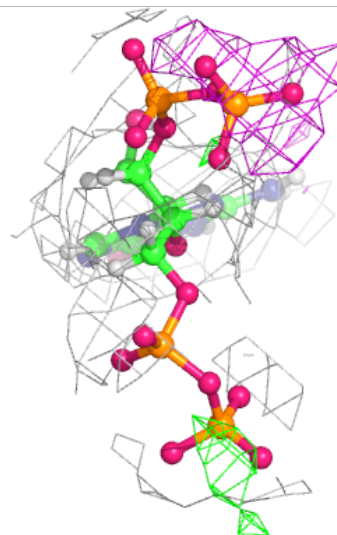
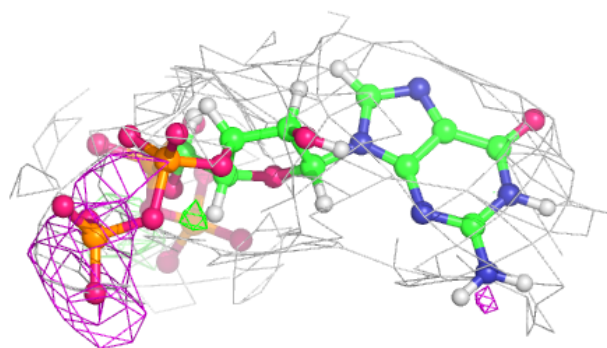
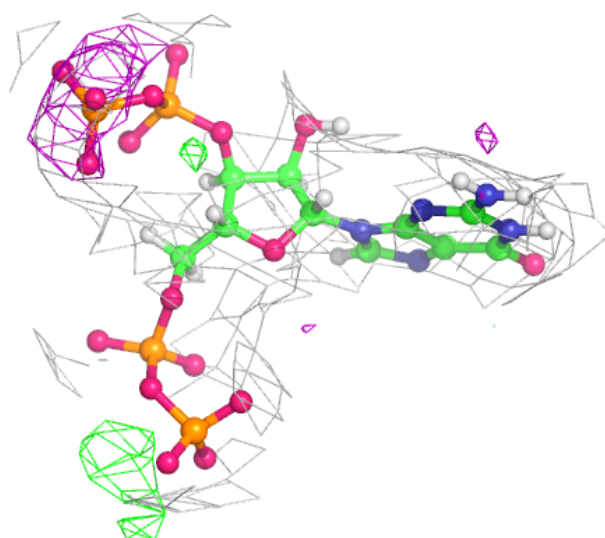
Electron density around GMP E 502:

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



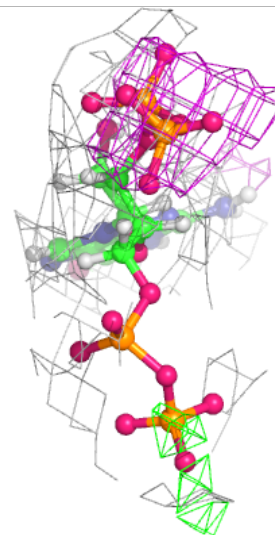
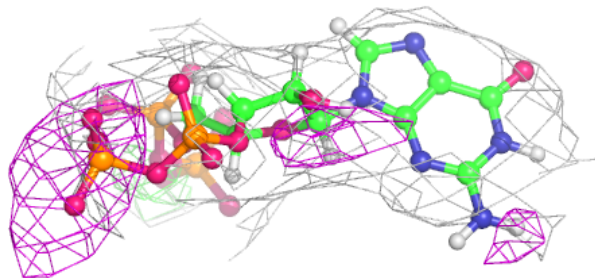
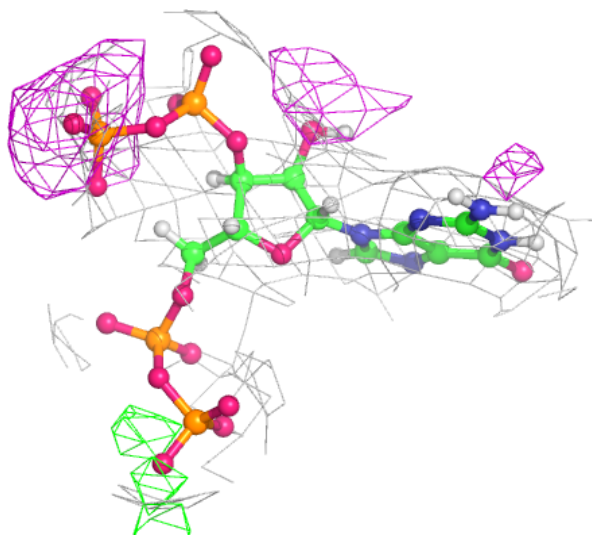
Electron density around G4P D 501:

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



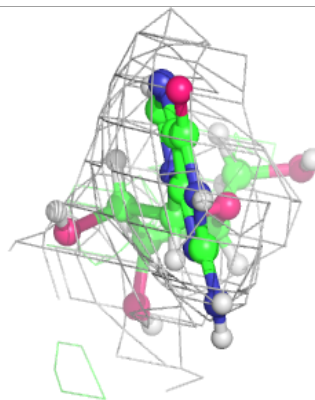
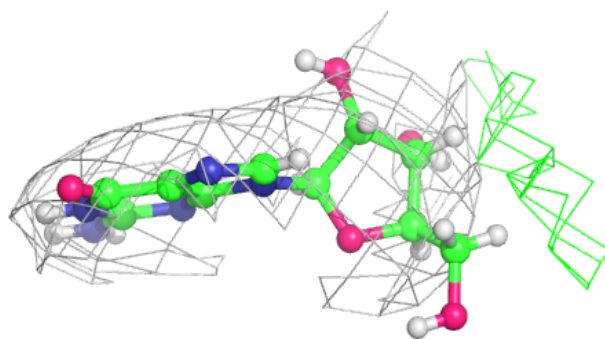
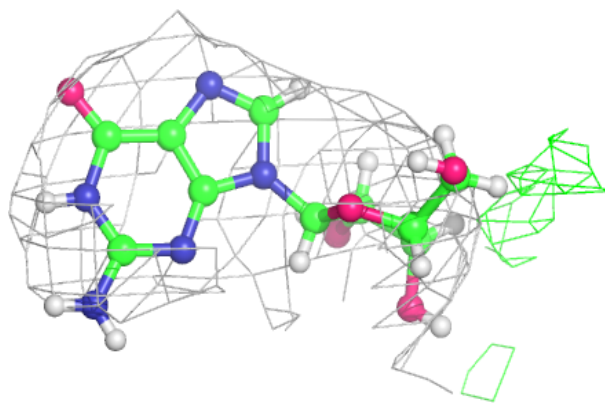
Electron density around G4P C 501:

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



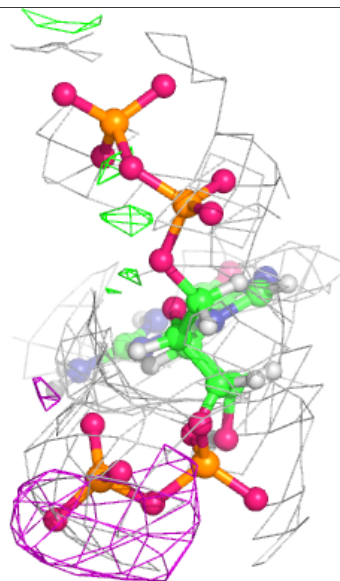
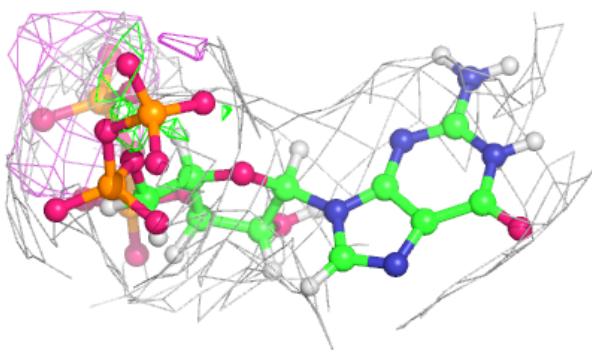
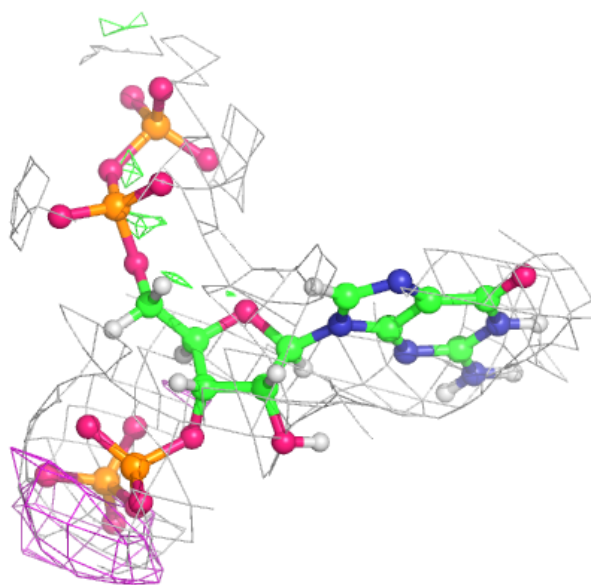
Electron density around GMP D 502:

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



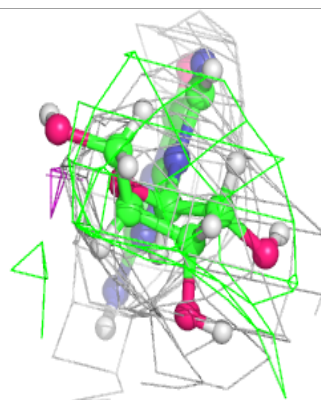
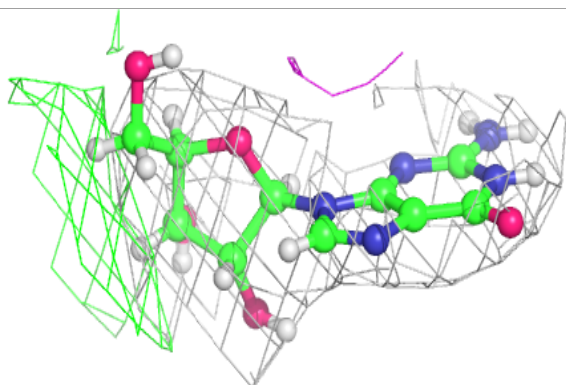
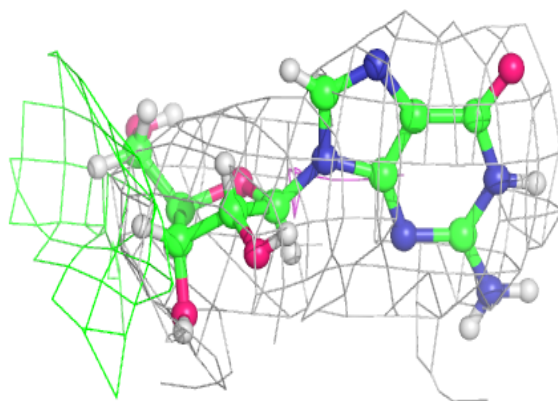
Electron density around G4P B 501:

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

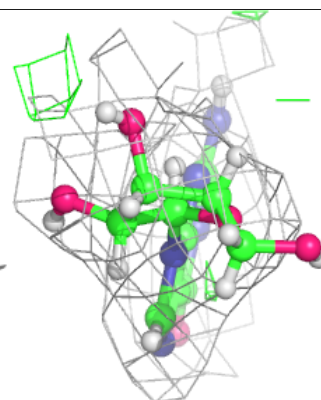
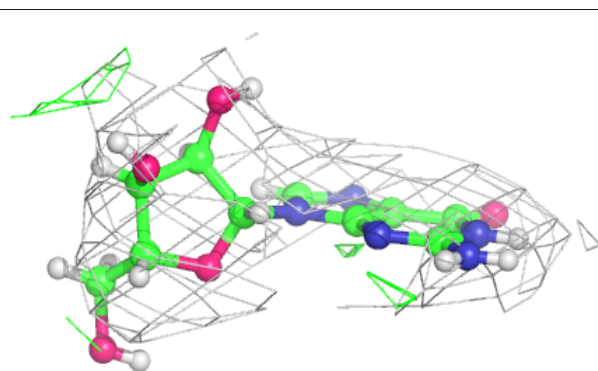
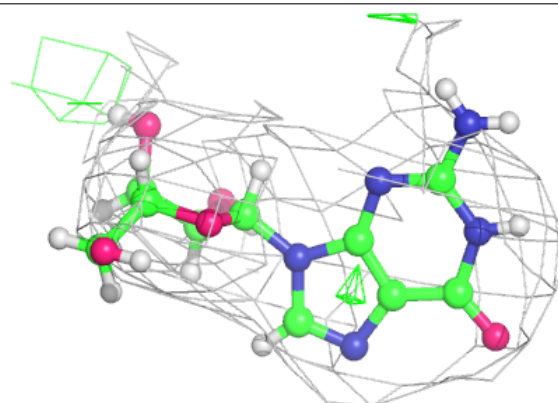


Electron density around GMP A 502:

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

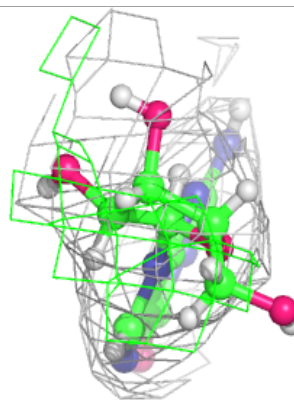
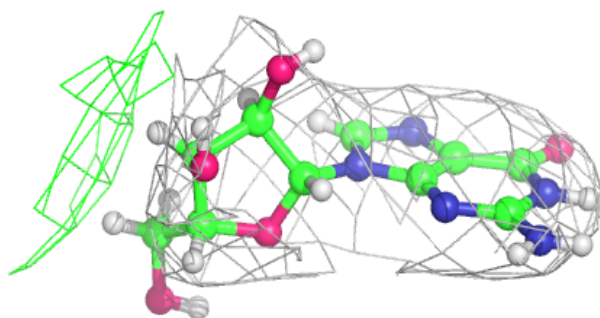
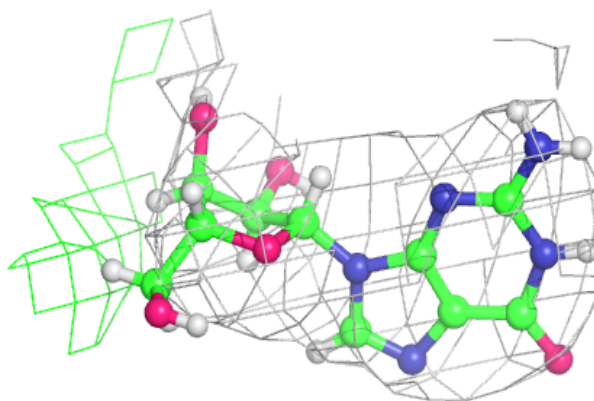
**Electron density around GMP B 502:**

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

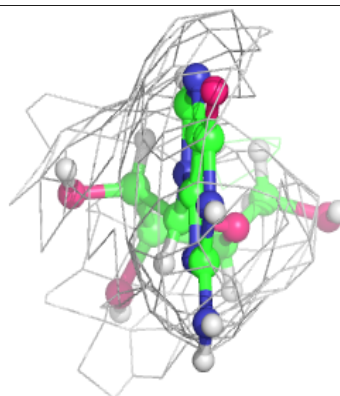
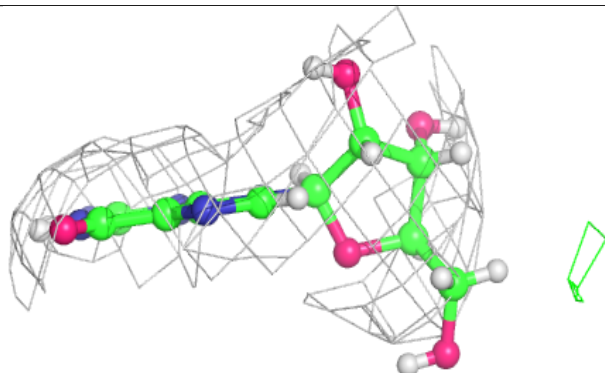
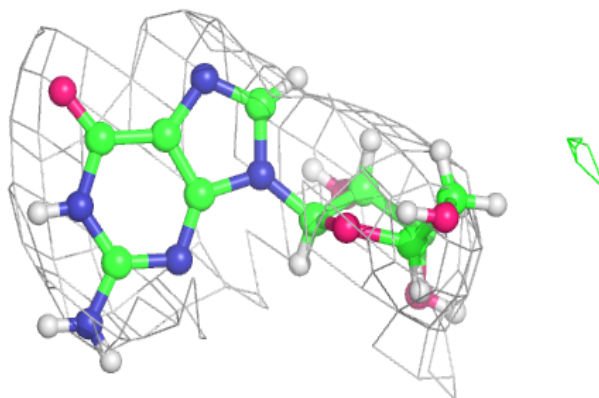


Electron density around GMP C 502:

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

**Electron density around GMP H 502:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.