



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:38 AM UTC

PDB ID : 5GOZ / pdb_00005goz
Title : Crystal structure of ZIKV NS5 Methyltransferase in complex with GTP and SAH
Authors : Zhang, C.; Jin, T.
Deposited on : 2016-07-30
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

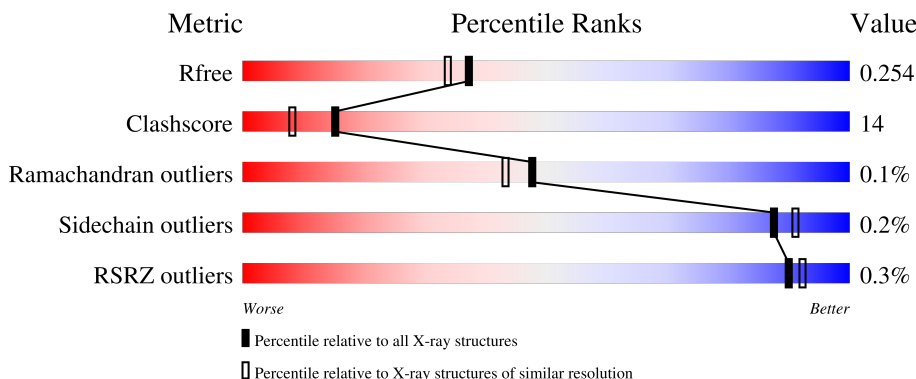
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	269	
1	B	269	
1	C	269	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6543 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.

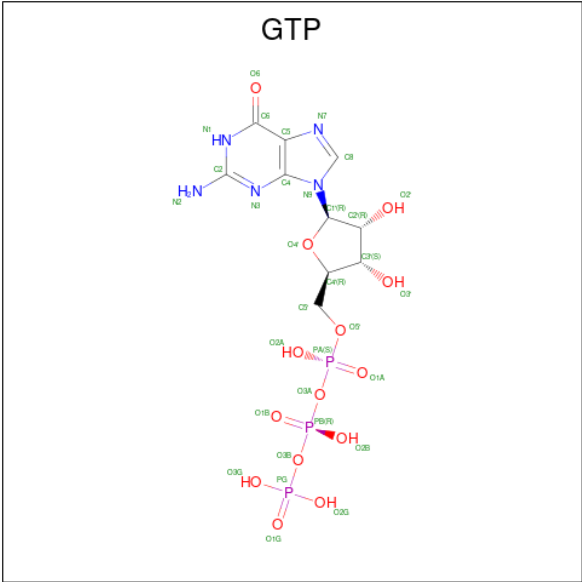
- Molecule 1 is a protein called RNA-directed RNA polymerase NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	2	0
			2057	1285	376	382	14			
1	B	261	Total	C	N	O	S	0	0	0
			2033	1271	368	380	14			
1	C	261	Total	C	N	O	S	0	0	0
			2033	1271	368	380	14			

There are 21 discrepancies between the modelled and reference sequences:

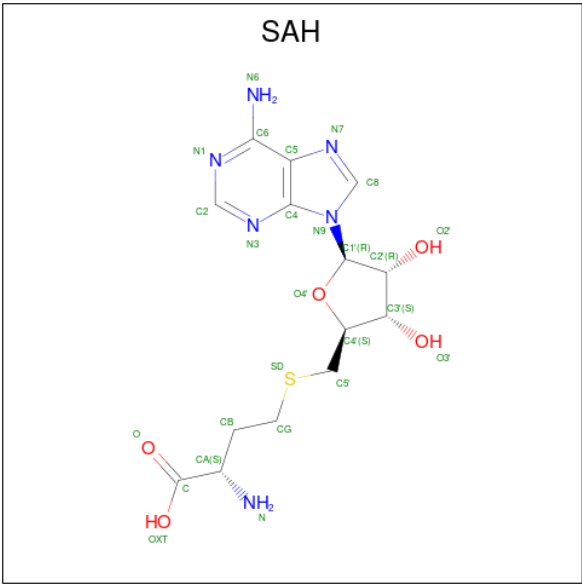
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP H9A910
A	1	SER	-	expression tag	UNP H9A910
A	2	VAL	-	expression tag	UNP H9A910
A	3	ASP	-	expression tag	UNP H9A910
A	266	ALA	-	expression tag	UNP H9A910
A	267	ALA	-	expression tag	UNP H9A910
A	268	SER	-	expression tag	UNP H9A910
B	0	GLY	-	expression tag	UNP H9A910
B	1	SER	-	expression tag	UNP H9A910
B	2	VAL	-	expression tag	UNP H9A910
B	3	ASP	-	expression tag	UNP H9A910
B	266	ALA	-	expression tag	UNP H9A910
B	267	ALA	-	expression tag	UNP H9A910
B	268	SER	-	expression tag	UNP H9A910
C	0	GLY	-	expression tag	UNP H9A910
C	1	SER	-	expression tag	UNP H9A910
C	2	VAL	-	expression tag	UNP H9A910
C	3	ASP	-	expression tag	UNP H9A910
C	266	ALA	-	expression tag	UNP H9A910
C	267	ALA	-	expression tag	UNP H9A910
C	268	SER	-	expression tag	UNP H9A910

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



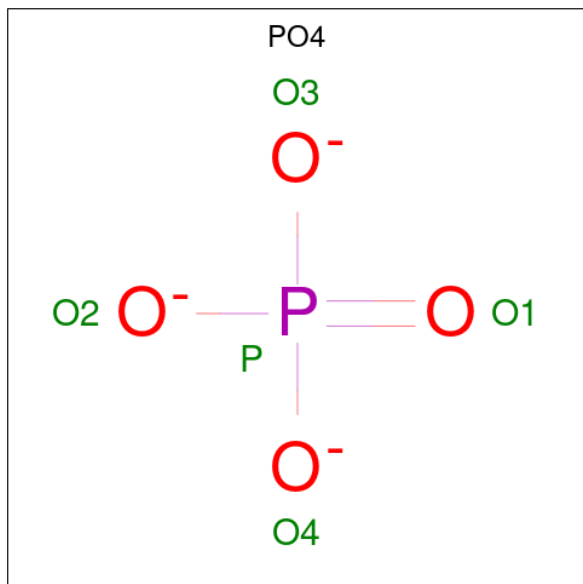
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



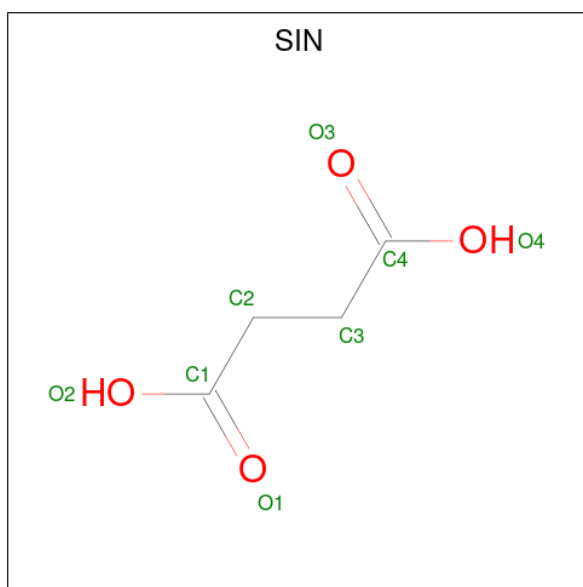
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



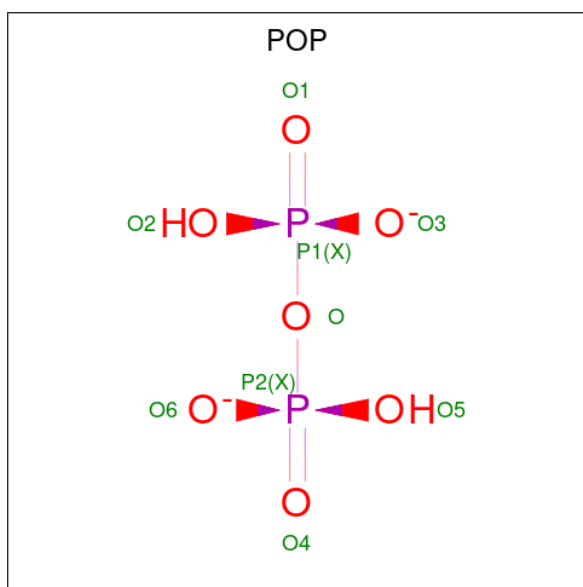
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		
5	C	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			9	7	2		

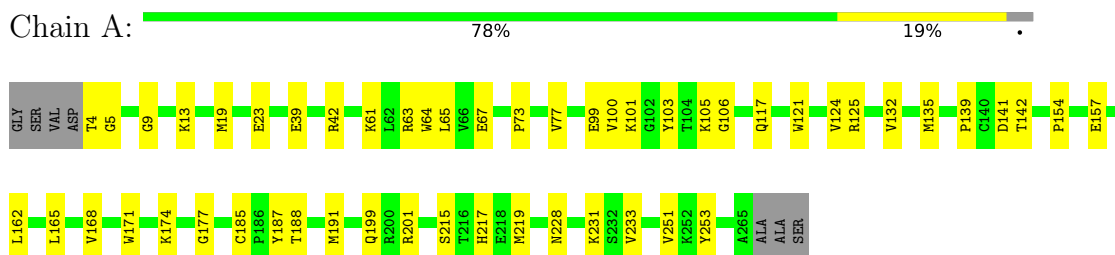
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	70	Total 70	O 70	0	0
7	B	54	Total 54	O 54	0	0
7	C	32	Total 32	O 32	0	0

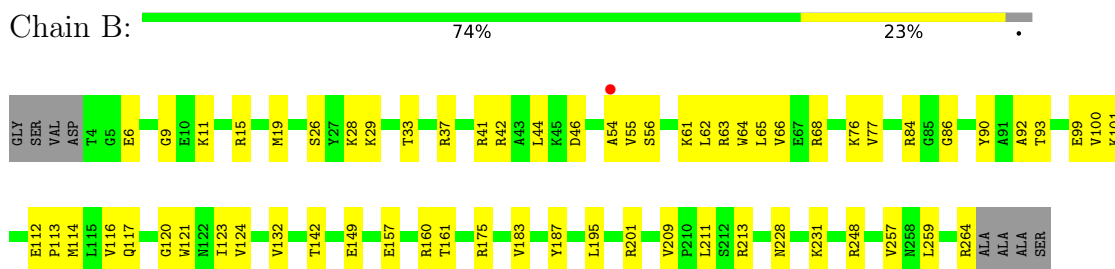
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

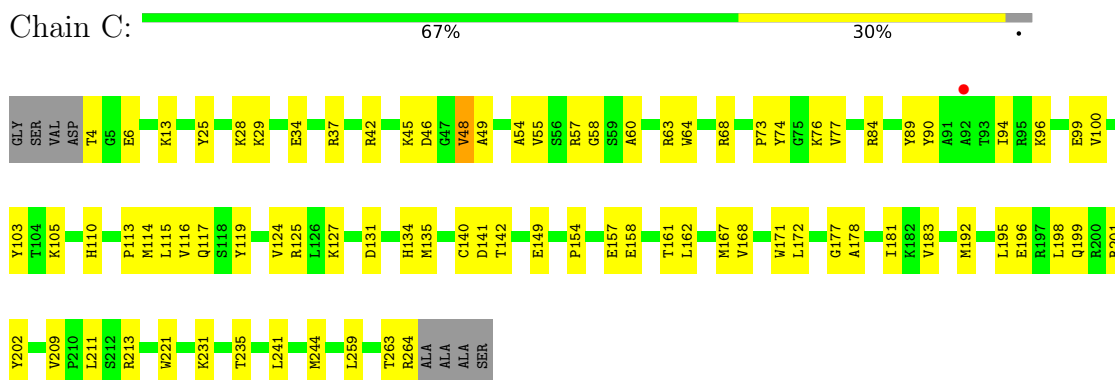
• Molecule 1: RNA-directed RNA polymerase NS5



• Molecule 1: RNA-directed RNA polymerase NS5



• Molecule 1: RNA-directed RNA polymerase NS5



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	123.79Å 123.79Å 120.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.52 – 2.05 40.52 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.52-2.05) 99.8 (40.52-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.236 , 0.263 0.236 , 0.254	Depositor DCC
R_{free} test set	1992 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.396 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6543	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1172e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SAH, GTP, SIN, POP

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	0.18	0/2100	0.33	0/2829
1	B	0.21	0/2073	0.43	0/2793
1	C	0.24	0/2073	0.47	0/2793
All	All	0.21	0/6246	0.41	0/8415

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2057	0	2066	36	0
1	B	2033	0	2034	58	0
1	C	2033	0	2036	79	0
2	A	32	0	12	1	0
2	B	32	0	12	1	0
2	C	64	0	24	4	0
3	A	26	0	19	1	0
3	B	26	0	19	1	0
3	C	26	0	19	1	0
4	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	0	0	0
4	C	5	0	0	1	0
5	B	16	0	8	1	0
5	C	8	0	4	2	0
6	C	9	0	0	0	0
7	A	70	0	0	2	0
7	B	54	0	0	1	0
7	C	32	0	0	1	0
All	All	6543	0	6253	172	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 14.

All (172) 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:B:175:ARG:HH12	1:B:201:ARG:NH1	1.30	1.25
1:B:175:ARG:NH1	1:B:201:ARG:NH1	2.08	1.01
1:C:96:LYS:HZ2	5:C:304:SIN:C4	1.86	0.88
1:B:175:ARG:HH12	1:B:201:ARG:HH11	1.21	0.84
1:C:76:LYS:HG3	1:C:140:CYS:HA	1.62	0.81
1:C:42:ARG:HH12	1:C:46:ASP:N	1.80	0.80
1:A:99:GLU:OE2	1:A:125:ARG:NH1	2.14	0.80
1:A:4:THR:HG22	1:A:5:GLY:H	1.47	0.77
1:B:175:ARG:NH1	1:B:201:ARG:HH12	1.81	0.74
1:C:37:ARG:NH1	1:C:54:ALA:O	2.19	0.74
1:C:100:VAL:HB	1:C:124:VAL:HG22	1.69	0.73
1:C:13:LYS:NZ	2:C:301:GTP:O3'	2.23	0.71
1:B:121:TRP:H	1:B:121:TRP:CD1	2.07	0.69
1:C:99:GLU:HG3	1:C:125:ARG:HH22	1.55	0.69
1:B:175:ARG:NH2	1:B:201:ARG:HH12	1.92	0.68
1:A:63:ARG:O	1:A:67:GLU:HG2	1.94	0.68
1:B:64:TRP:HE3	1:B:65:LEU:HD22	1.57	0.68
1:B:175:ARG:HH22	1:B:201:ARG:HH22	1.43	0.67
1:C:84:ARG:HD3	1:C:114:MET:SD	2.34	0.67
1:B:117:GLN:HE22	1:B:121:TRP:NE1	1.96	0.64
1:B:175:ARG:CZ	1:B:201:ARG:HH12	2.10	0.64
1:B:175:ARG:HH22	1:B:201:ARG:HH12	1.45	0.64
1:C:63:ARG:HD2	1:C:64:TRP:N	2.12	0.63
1:C:99:GLU:CG	1:C:125:ARG:HH22	2.12	0.62
1:C:60:ALA:O	1:C:63:ARG:NE	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ASN:HB3	1:B:231:LYS:HB3	1.82	0.61
1:C:89:TYR:HE2	1:C:116:VAL:HG22	1.65	0.61
1:B:175:ARG:HH22	1:B:201:ARG:NH2	1.98	0.61
1:B:92:ALA:HB1	1:B:120:GLY:O	2.00	0.61
1:A:13:LYS:HG2	1:A:154:PRO:HG3	1.83	0.61
1:C:84:ARG:HA	1:C:113:PRO:HA	1.82	0.61
1:B:175:ARG:HH22	1:B:201:ARG:NH1	2.00	0.60
1:A:139:PRO:HA	1:A:174:LYS:HB3	1.84	0.60
1:C:42:ARG:NH1	1:C:46:ASP:N	2.47	0.60
1:B:90:TYR:O	1:B:93:THR:OG1	2.20	0.60
1:B:77:VAL:HB	1:B:100:VAL:HG22	1.83	0.59
1:C:172:LEU:HB2	1:C:202:TYR:HE2	1.68	0.59
1:C:131:ASP:HB3	1:C:134:HIS:CE1	2.37	0.59
1:C:42:ARG:CZ	1:C:45:LYS:HB3	2.33	0.59
1:C:96:LYS:NZ	5:C:304:SIN:O3	2.34	0.58
1:B:42:ARG:O	1:B:46:ASP:HB3	2.04	0.58
1:B:175:ARG:CZ	1:B:201:ARG:NH1	2.67	0.57
1:A:99:GLU:CD	1:A:125:ARG:HH12	2.11	0.57
1:C:77:VAL:HG23	1:C:142:THR:OG1	2.05	0.57
1:B:259:LEU:H	1:B:259:LEU:HD12	1.69	0.57
1:C:89:TYR:CE2	1:C:116:VAL:HG22	2.39	0.57
1:C:28:LYS:HB2	1:C:28:LYS:HZ3	1.70	0.56
1:C:76:LYS:HG2	1:C:141:ASP:HB2	1.88	0.56
1:C:213:ARG:NH1	4:C:306:PO4:O2	2.38	0.56
1:A:201:ARG:NH2	5:B:304:SIN:H21	2.21	0.55
1:B:15:ARG:NH2	7:B:409:HOH:O	2.36	0.55
1:A:73:PRO:HA	1:A:142:THR:HG21	1.89	0.54
1:C:231:LYS:O	1:C:235:THR:HG22	2.06	0.54
1:C:158:GLU:O	1:C:162:LEU:HD22	2.08	0.54
1:C:49:ALA:HB1	1:C:117:GLN:N	2.23	0.54
1:A:19:MET:HE2	1:A:23:GLU:HG2	1.90	0.53
1:C:49:ALA:HB1	1:C:117:GLN:H	1.73	0.53
1:C:13:LYS:HG2	1:C:154:PRO:HG3	1.89	0.53
1:C:42:ARG:HH12	1:C:46:ASP:CA	2.20	0.53
1:C:76:LYS:CG	1:C:141:ASP:H	2.21	0.53
1:A:199:GLN:NE2	7:A:401:HOH:O	2.19	0.53
1:A:219:MET:HE1	1:A:233:VAL:HG22	1.91	0.53
1:C:28:LYS:HE3	2:C:301:GTP:O3G	2.09	0.53
1:C:77:VAL:HG12	1:C:99:GLU:O	2.09	0.53
1:A:61:LYS:NZ	7:A:413:HOH:O	2.39	0.52
1:B:117:GLN:HE22	1:B:121:TRP:CD1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:VAL:O	1:C:84:ARG:NH2	2.43	0.52
1:B:121:TRP:O	1:B:124:VAL:N	2.30	0.52
1:B:248:ARG:HD2	1:B:248:ARG:N	2.24	0.52
1:C:42:ARG:NH2	1:C:45:LYS:HB3	2.25	0.52
1:B:46:ASP:OD2	1:B:46:ASP:C	2.53	0.51
1:C:168:VAL:HG11	1:C:181:ILE:HG12	1.93	0.51
1:C:37:ARG:HD2	1:C:57:ARG:HG2	1.92	0.51
1:C:201:ARG:C	1:C:202:TYR:HD1	2.17	0.51
1:A:39:GLU:HA	1:A:42:ARG:HE	1.76	0.51
1:A:39:GLU:HA	1:A:42:ARG:NE	2.27	0.50
1:A:100:VAL:HB	1:A:124:VAL:HG22	1.93	0.50
1:B:77:VAL:HG22	1:B:142:THR:HB	1.94	0.49
1:A:228:ASN:HB3	1:A:231:LYS:HB3	1.94	0.49
1:B:28:LYS:HD2	1:B:213:ARG:NH1	2.28	0.49
1:B:19:MET:O	2:B:301:GTP:N2	2.44	0.49
1:C:142:THR:HA	1:C:178:ALA:O	2.13	0.49
1:C:135:MET:HE2	1:C:171:TRP:HH2	1.77	0.49
1:C:264:ARG:HA	1:C:264:ARG:HD2	1.63	0.49
1:B:26:SER:HB2	1:B:248:ARG:HG2	1.96	0.48
1:C:37:ARG:HH12	1:C:54:ALA:C	2.18	0.48
1:C:46:ASP:HB3	1:C:48:VAL:HG23	1.94	0.48
1:C:74:TYR:HB2	1:C:96:LYS:HG2	1.95	0.48
1:B:9:GLY:HA3	1:B:187:TYR:HB2	1.94	0.48
1:B:37:ARG:NH2	1:B:54:ALA:HB3	2.29	0.48
1:C:73:PRO:HA	1:C:142:THR:HG21	1.96	0.48
1:A:101:LYS:HE3	1:A:103:TYR:OH	2.14	0.47
1:A:4:THR:HG22	1:A:5:GLY:N	2.24	0.47
1:B:55:VAL:HG12	1:B:86:GLY:HA2	1.96	0.47
1:B:99:GLU:HA	1:B:123:ILE:HB	1.97	0.47
1:C:29:LYS:HE3	1:C:213:ARG:NH1	2.30	0.47
1:C:90:TYR:HD1	1:C:259:LEU:HD11	1.80	0.47
1:B:37:ARG:O	1:B:41:ARG:HD2	2.15	0.47
1:B:56:SER:HB3	1:B:84:ARG:HD2	1.97	0.47
1:B:149:GLU:HG3	1:B:160:ARG:NH2	2.31	0.46
1:A:105:LYS:HG2	1:A:106:GLY:O	2.15	0.46
1:B:62:LEU:O	1:B:66:VAL:HG23	2.15	0.46
1:B:175:ARG:HH22	1:B:201:ARG:CZ	2.27	0.46
1:C:28:LYS:HE3	2:C:301:GTP:PG	2.56	0.46
1:C:263:THR:O	1:C:264:ARG:HB2	2.16	0.46
1:C:28:LYS:HG3	1:C:29:LYS:HG3	1.98	0.46
1:B:157:GLU:O	1:B:161:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:VAL:HG11	1:B:195:LEU:HD11	1.98	0.46
1:A:77:VAL:HG22	1:A:142:THR:OG1	2.15	0.46
1:C:42:ARG:HE	1:C:42:ARG:C	2.25	0.45
1:A:132:VAL:HG13	3:A:302:SAH:H2	1.99	0.45
1:A:188:THR:OG1	1:A:191:MET:HG2	2.17	0.45
1:C:37:ARG:NH1	1:C:54:ALA:C	2.73	0.45
1:C:89:TYR:OH	1:C:115:LEU:HA	2.17	0.45
1:B:121:TRP:CD1	1:B:121:TRP:N	2.79	0.45
1:A:141:ASP:O	1:A:177:GLY:N	2.48	0.45
1:B:6:GLU:HG2	1:B:11:LYS:HG3	1.98	0.45
1:C:4:THR:N	1:C:6:GLU:OE1	2.50	0.45
1:C:141:ASP:O	1:C:177:GLY:N	2.50	0.44
1:C:58:GLY:HA3	3:C:303:SAH:O	2.16	0.44
1:C:172:LEU:HD13	1:C:202:TYR:HD2	1.82	0.44
1:C:149:GLU:OE2	2:C:302:GTP:O3G	2.36	0.44
1:C:172:LEU:HB2	1:C:202:TYR:CE2	2.51	0.44
1:C:119:TYR:OH	1:C:264:ARG:HG2	2.18	0.44
1:C:34:GLU:HG3	1:C:57:ARG:HH12	1.83	0.44
1:A:162:LEU:HB3	1:B:68:ARG:O	2.18	0.44
1:A:165:LEU:HA	1:A:168:VAL:HG22	1.99	0.43
1:B:264:ARG:HE	1:B:264:ARG:HB3	1.59	0.43
1:C:76:LYS:HG3	1:C:141:ASP:H	1.83	0.43
1:A:63:ARG:HD2	1:A:67:GLU:CD	2.42	0.43
1:C:192:MET:O	1:C:196:GLU:HG3	2.18	0.43
1:A:9:GLY:HA3	1:A:187:TYR:HB2	2.01	0.43
1:C:76:LYS:HG2	1:C:141:ASP:H	1.82	0.43
1:C:209:VAL:HG12	1:C:211:LEU:H	1.83	0.43
1:B:175:ARG:HD2	1:B:175:ARG:HA	1.68	0.43
1:C:68:ARG:NH1	7:C:406:HOH:O	2.40	0.43
1:B:55:VAL:HG23	1:B:116:VAL:HG21	2.02	0.42
1:B:175:ARG:NH2	1:B:201:ARG:NH1	2.57	0.42
1:C:183:VAL:HG11	1:C:195:LEU:HD11	2.01	0.42
1:C:25:TYR:HA	1:C:28:LYS:HD2	2.00	0.42
1:B:113:PRO:C	1:B:114:MET:HE2	2.45	0.42
1:C:73:PRO:HG2	1:C:94:ILE:HD12	2.00	0.42
1:B:33:THR:O	1:B:211:LEU:HA	2.19	0.42
1:C:42:ARG:NH1	1:C:46:ASP:CB	2.83	0.42
1:C:135:MET:HE2	1:C:171:TRP:CH2	2.55	0.42
1:C:167:MET:HE3	1:C:167:MET:HB3	1.91	0.42
1:A:157:GLU:HB3	1:A:185:CYS:HB2	2.02	0.42
1:B:11:LYS:HE2	1:B:11:LYS:HB3	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:NE	1:B:257:VAL:HB	2.34	0.42
1:A:217:HIS:O	1:A:217:HIS:ND1	2.51	0.42
1:B:132:VAL:HG13	3:B:302:SAH:H2	2.02	0.41
1:C:105:LYS:HD3	1:C:110:HIS:CD2	2.55	0.41
1:A:99:GLU:CG	1:A:125:ARG:HH12	2.33	0.41
1:A:64:TRP:CZ3	1:A:65:LEU:HD23	2.56	0.41
1:C:42:ARG:HH12	1:C:45:LYS:C	2.27	0.41
1:C:157:GLU:O	1:C:161:THR:OG1	2.33	0.41
1:C:162:LEU:HD22	1:C:162:LEU:H	1.85	0.41
1:A:215:SER:OG	2:A:301:GTP:O2B	2.23	0.41
1:B:29:LYS:HG2	1:B:213:ARG:HG2	2.02	0.41
1:B:41:ARG:C	1:B:44:LEU:H	2.28	0.41
1:B:61:LYS:HG3	1:B:209:VAL:HG11	2.01	0.41
1:C:201:ARG:HG2	1:C:202:TYR:CE1	2.55	0.41
1:B:76:LYS:NZ	1:B:101:LYS:HD3	2.36	0.41
1:A:77:VAL:HB	1:A:100:VAL:HG22	2.03	0.41
1:C:241:LEU:HD23	1:C:244:MET:HE2	2.02	0.41
1:A:251:VAL:HB	1:A:253:TYR:CZ	2.56	0.41
1:B:175:ARG:HH11	1:B:175:ARG:HD3	1.63	0.41
1:A:117:GLN:HB3	1:A:121:TRP:CD1	2.56	0.40
1:A:135:MET:HE3	1:A:171:TRP:CZ2	2.57	0.40
1:B:112:GLU:OE1	1:B:113:PRO:HD2	2.21	0.40
1:C:198:LEU:HB3	1:C:221:TRP:CH2	2.56	0.40
1:C:103:TYR:CE1	1:C:127:LYS:HE2	2.56	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	262/269 (97%)	254 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	259/269 (96%)	244 (94%)	15 (6%)	0	100	100
1	C	259/269 (96%)	245 (95%)	13 (5%)	1 (0%)	30	22
All	All	780/807 (97%)	743 (95%)	36 (5%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	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	219/221 (99%)	219 (100%)	0	100	100
1	B	217/221 (98%)	217 (100%)	0	100	100
1	C	217/221 (98%)	216 (100%)	1 (0%)	81	85
All	All	653/663 (98%)	652 (100%)	1 (0%)	87	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	199	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	B	98	GLN
1	B	199	GLN
1	B	217	HIS
1	C	72	GLN
1	C	134	HIS
1	C	217	HIS

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Mol	Chain	Res	Type
1	C	238	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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	$\# Z > 2$
5	SIN	B	303	-	7,7,7	1.05	0	8,8,8	1.65	2 (25%)
2	GTP	A	301	-	33,34,34	3.73	20 (60%)	50,54,54	2.67	14 (28%)
2	GTP	C	301	-	33,34,34	3.60	20 (60%)	50,54,54	3.80	19 (38%)
5	SIN	C	304	-	7,7,7	1.04	0	8,8,8	1.63	2 (25%)
4	PO4	B	305	-	4,4,4	0.93	0	6,6,6	0.48	0
6	POP	C	305	-	6,8,8	0.75	0	12,13,13	0.87	0
4	PO4	C	306	-	4,4,4	0.98	0	6,6,6	0.45	0
3	SAH	C	303	-	27,28,28	1.09	4 (14%)	36,40,40	2.01	9 (25%)
2	GTP	B	301	-	33,34,34	3.73	19 (57%)	50,54,54	2.73	13 (26%)
4	PO4	A	304	-	4,4,4	0.95	0	6,6,6	0.45	0
2	GTP	C	302	-	33,34,34	3.82	19 (57%)	50,54,54	3.19	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SIN	B	304	-	7,7,7	1.01	0	8,8,8	1.84	2 (25%)
4	PO4	B	306	-	4,4,4	0.96	0	6,6,6	0.49	0
3	SAH	B	302	-	27,28,28	1.10	4 (14%)	36,40,40	2.03	9 (25%)
3	SAH	A	302	-	27,28,28	1.08	4 (14%)	36,40,40	2.02	9 (25%)
4	PO4	A	303	-	4,4,4	0.95	0	6,6,6	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SIN	B	303	-	-	3/5/5/5	-
2	GTP	A	301	-	-	9/22/38/38	0/3/3/3
2	GTP	C	301	-	-	1/22/38/38	0/3/3/3
5	SIN	C	304	-	-	1/5/5/5	-
6	POP	C	305	-	-	0/6/6/6	-
3	SAH	C	303	-	-	5/15/31/31	0/3/3/3
2	GTP	B	301	-	-	4/22/38/38	0/3/3/3
2	GTP	C	302	-	-	4/22/38/38	0/3/3/3
5	SIN	B	304	-	-	4/5/5/5	-
3	SAH	B	302	-	-	2/15/31/31	0/3/3/3
3	SAH	A	302	-	-	2/15/31/31	0/3/3/3

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	GTP	C2'-C3'	-10.69	1.24	1.53
2	B	301	GTP	C2'-C3'	-10.64	1.24	1.53
2	C	301	GTP	C2'-C3'	-10.59	1.24	1.53
2	C	302	GTP	C2'-C3'	-10.47	1.25	1.53
2	B	301	GTP	C4-N3	6.67	1.49	1.34
2	C	302	GTP	C4-N3	6.67	1.49	1.34
2	A	301	GTP	O4'-C4'	-6.58	1.30	1.45
2	C	301	GTP	O4'-C4'	-6.52	1.30	1.45
2	B	301	GTP	O4'-C4'	-6.48	1.30	1.45
2	A	301	GTP	C4-N3	6.43	1.49	1.34
2	C	302	GTP	O4'-C4'	-6.42	1.30	1.45
2	C	302	GTP	C3'-C4'	5.71	1.67	1.53
2	C	302	GTP	PA-O3A	5.67	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	GTP	C2-N3	5.65	1.46	1.33
2	C	301	GTP	C4-N3	5.62	1.47	1.34
2	C	301	GTP	C3'-C4'	5.55	1.67	1.53
2	C	302	GTP	PB-O3B	5.50	1.65	1.59
2	B	301	GTP	C3'-C4'	5.42	1.66	1.53
2	A	301	GTP	C3'-C4'	5.42	1.66	1.53
2	B	301	GTP	C2-N3	5.41	1.46	1.33
2	C	302	GTP	PB-O3A	5.38	1.65	1.59
2	A	301	GTP	PB-O3B	5.21	1.65	1.59
2	A	301	GTP	C2-N3	5.20	1.45	1.33
2	C	302	GTP	C1'-N9	-5.19	1.32	1.47
2	B	301	GTP	PB-O3B	5.14	1.65	1.59
2	C	301	GTP	C1'-N9	-5.11	1.33	1.47
2	A	301	GTP	C1'-N9	-4.89	1.33	1.47
2	A	301	GTP	PA-O3A	4.85	1.64	1.59
2	C	302	GTP	C2-N2	4.84	1.45	1.34
2	B	301	GTP	C2-N2	4.84	1.45	1.34
2	A	301	GTP	C2-N2	4.77	1.45	1.34
2	A	301	GTP	PB-O3A	4.77	1.64	1.59
2	B	301	GTP	C1'-N9	-4.74	1.34	1.47
2	B	301	GTP	PB-O3A	4.70	1.64	1.59
2	B	301	GTP	PA-O3A	4.65	1.64	1.59
2	C	301	GTP	C2-N3	4.62	1.44	1.33
2	C	301	GTP	PA-O3A	4.61	1.64	1.59
2	C	301	GTP	PB-O3B	4.54	1.64	1.59
2	C	301	GTP	C2-N2	4.30	1.44	1.34
2	C	301	GTP	PB-O3A	4.17	1.64	1.59
2	B	301	GTP	O4'-C1'	4.11	1.51	1.42
2	A	301	GTP	O4'-C1'	3.99	1.51	1.42
2	C	302	GTP	O4'-C1'	3.86	1.50	1.42
2	C	301	GTP	O4'-C1'	3.68	1.50	1.42
2	C	301	GTP	C4-N9	-3.16	1.30	1.38
2	C	302	GTP	O2'-C2'	3.10	1.50	1.43
2	A	301	GTP	O2'-C2'	2.95	1.50	1.43
2	B	301	GTP	O2'-C2'	2.94	1.50	1.43
2	B	301	GTP	C2-N1	2.94	1.44	1.37
2	C	301	GTP	O2'-C2'	2.91	1.50	1.43
2	C	302	GTP	C5-N7	-2.89	1.33	1.39
2	C	302	GTP	C2-N1	2.88	1.44	1.37
2	C	301	GTP	O6-C6	-2.88	1.18	1.23
2	A	301	GTP	C2-N1	2.85	1.44	1.37
2	B	301	GTP	C5-N7	-2.75	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	GTP	C5-N7	-2.69	1.33	1.39
2	A	301	GTP	C5-N7	-2.61	1.33	1.39
2	A	301	GTP	C5-C6	2.59	1.54	1.44
2	B	301	GTP	O6-C6	-2.57	1.18	1.23
2	A	301	GTP	C6-N1	2.55	1.43	1.38
2	C	301	GTP	C2-N1	2.54	1.43	1.37
3	C	303	SAH	C2-N3	2.53	1.38	1.33
3	C	303	SAH	C2-N1	2.50	1.38	1.33
2	C	301	GTP	C5-C6	2.50	1.53	1.44
2	B	301	GTP	C5-C6	2.48	1.53	1.44
2	B	301	GTP	C2'-C1'	2.48	1.61	1.53
3	A	302	SAH	C2-N1	2.47	1.38	1.33
3	B	302	SAH	C2-N1	2.46	1.38	1.33
2	C	302	GTP	C5-C6	2.46	1.53	1.44
2	A	301	GTP	O6-C6	-2.44	1.18	1.23
3	A	302	SAH	C2-N3	2.42	1.38	1.33
3	B	302	SAH	C2-N3	2.40	1.38	1.33
2	A	301	GTP	C2'-C1'	2.38	1.61	1.53
2	B	301	GTP	C6-N1	2.37	1.43	1.38
2	C	302	GTP	C2'-C1'	2.36	1.60	1.53
2	C	302	GTP	O6-C6	-2.35	1.19	1.23
2	C	302	GTP	C6-N1	2.33	1.43	1.38
3	B	302	SAH	OXT-C	-2.27	1.23	1.30
3	B	302	SAH	C8-N7	2.26	1.36	1.31
3	A	302	SAH	OXT-C	-2.26	1.23	1.30
2	C	301	GTP	C2'-C1'	2.26	1.60	1.53
3	C	303	SAH	OXT-C	-2.24	1.23	1.30
3	C	303	SAH	C8-N7	2.21	1.35	1.31
2	A	301	GTP	C4-N9	-2.21	1.32	1.38
3	A	302	SAH	C8-N7	2.19	1.35	1.31
2	C	301	GTP	O3'-C3'	2.15	1.48	1.43
2	A	301	GTP	O3'-C3'	2.07	1.48	1.43
2	C	302	GTP	O3'-C3'	2.06	1.48	1.43
2	B	301	GTP	O3'-C3'	2.04	1.48	1.43
2	C	301	GTP	C6-N1	2.03	1.42	1.38

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	302	GTP	C1'-N9-C8	-13.84	87.43	126.73
2	C	302	GTP	C1'-N9-C4	12.58	163.63	126.49
2	C	301	GTP	O2B-PB-O3B	-11.35	76.58	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	GTP	C1'-N9-C8	-11.19	94.93	126.73
2	C	301	GTP	O2B-PB-O3A	-10.88	77.88	107.27
2	A	301	GTP	C1'-N9-C8	-10.81	96.02	126.73
2	B	301	GTP	C1'-N9-C4	10.37	157.11	126.49
2	A	301	GTP	C1'-N9-C4	9.96	155.91	126.49
2	C	301	GTP	O3B-PB-O1B	-9.31	82.70	110.70
2	C	301	GTP	O3A-PB-O1B	-9.17	83.12	110.70
2	C	301	GTP	C1'-N9-C8	-9.13	100.81	126.73
2	C	301	GTP	C1'-N9-C4	8.58	151.82	126.49
3	B	302	SAH	N3-C2-N1	-5.59	120.11	128.58
3	A	302	SAH	N3-C2-N1	-5.52	120.23	128.58
3	C	303	SAH	N3-C2-N1	-5.43	120.36	128.58
2	C	302	GTP	C5-C4-N3	-5.35	119.87	128.39
2	B	301	GTP	C5-C4-N3	-4.88	120.63	128.39
2	C	302	GTP	C4'-O4'-C1'	-4.61	99.28	109.47
3	C	303	SAH	C5-C4-N3	-4.60	120.38	126.72
2	B	301	GTP	C2-N3-C4	4.55	120.13	112.30
3	A	302	SAH	C5-C4-N3	-4.50	120.52	126.72
2	A	301	GTP	C2-N3-C4	4.48	120.01	112.30
2	A	301	GTP	C5-C4-N3	-4.43	121.34	128.39
2	C	302	GTP	C2-N3-C4	4.43	119.92	112.30
2	C	301	GTP	O2B-PB-O1B	4.33	132.57	112.44
3	B	302	SAH	C5-C4-N3	-4.26	120.86	126.72
3	B	302	SAH	N9-C8-N7	-4.04	108.21	113.94
3	B	302	SAH	C5'-SD-CG	-3.96	90.50	102.26
3	A	302	SAH	N9-C8-N7	-3.92	108.38	113.94
3	C	303	SAH	N9-C8-N7	-3.85	108.47	113.94
3	A	302	SAH	C5'-SD-CG	-3.82	90.92	102.26
2	C	302	GTP	N9-C4-N3	3.62	133.19	125.95
3	A	302	SAH	C2-N3-C4	3.50	120.38	111.83
5	B	304	SIN	C2-C3-C4	-3.48	104.44	113.67
3	C	303	SAH	C5-N7-C8	3.48	108.92	103.45
2	C	301	GTP	C2-N3-C4	3.45	118.24	112.30
3	C	303	SAH	C2-N3-C4	3.45	120.25	111.83
3	B	302	SAH	C2-N3-C4	3.42	120.19	111.83
3	A	302	SAH	C5-N7-C8	3.42	108.83	103.45
3	B	302	SAH	C5-N7-C8	3.41	108.81	103.45
2	C	301	GTP	C5-C4-N3	-3.41	122.97	128.39
2	C	301	GTP	C2-N1-C6	-3.28	119.16	125.11
3	C	303	SAH	C5'-SD-CG	-3.20	92.77	102.26
2	C	301	GTP	N9-C8-N7	-3.19	107.49	113.40
2	A	301	GTP	N9-C8-N7	-3.18	107.51	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	GTP	C4'-O4'-C1'	-3.14	102.54	109.47
2	C	302	GTP	N9-C8-N7	-3.12	107.61	113.40
2	B	301	GTP	O4'-C1'-N9	3.11	115.40	108.36
2	C	301	GTP	O4'-C1'-N9	3.05	115.27	108.36
2	C	302	GTP	C2-N1-C6	-2.96	119.74	125.11
2	B	301	GTP	N9-C8-N7	-2.94	107.94	113.40
2	A	301	GTP	O4'-C1'-N9	2.89	114.91	108.36
2	B	301	GTP	C4'-O4'-C1'	-2.88	103.11	109.47
2	B	301	GTP	C2-N1-C6	-2.88	119.89	125.11
3	C	303	SAH	N3-C4-N9	2.84	132.00	127.17
3	A	302	SAH	N3-C4-N9	2.83	131.97	127.17
2	C	301	GTP	C5-C4-N9	2.82	110.69	105.66
2	A	301	GTP	C2-N1-C6	-2.80	120.04	125.11
3	B	302	SAH	OXT-C-O	-2.75	117.83	124.08
2	B	301	GTP	C5-C6-N1	2.71	120.15	113.25
3	C	303	SAH	OXT-C-O	-2.67	118.03	124.08
3	A	302	SAH	OXT-C-O	-2.66	118.04	124.08
2	C	301	GTP	C4'-O4'-C1'	-2.66	103.60	109.47
2	A	301	GTP	C5-C6-N1	2.64	119.96	113.25
3	C	303	SAH	C4-C5-N7	-2.61	107.59	110.58
2	C	301	GTP	C5-C6-N1	2.61	119.90	113.25
2	B	301	GTP	N9-C4-N3	2.59	131.14	125.95
3	B	302	SAH	N3-C4-N9	2.59	131.57	127.17
2	C	301	GTP	C6-C5-N7	2.57	134.97	130.29
3	B	302	SAH	C4-C5-N7	-2.55	107.67	110.58
2	C	302	GTP	C5-C6-N1	2.54	119.72	113.25
3	A	302	SAH	C4-C5-N7	-2.54	107.68	110.58
2	C	301	GTP	C4-C5-N7	-2.47	106.75	110.67
2	B	301	GTP	O6-C6-C5	-2.47	120.00	126.53
2	C	302	GTP	O6-C6-C5	-2.46	120.03	126.53
2	C	302	GTP	O4'-C1'-C2'	-2.42	101.44	106.62
2	C	301	GTP	C2'-C3'-C4'	2.34	107.14	102.61
2	C	302	GTP	O4'-C1'-N9	2.33	113.63	108.36
2	C	302	GTP	C2'-C3'-C4'	2.26	106.97	102.61
2	A	301	GTP	C8-N7-C5	2.22	108.21	104.26
5	B	304	SIN	O2-C1-C2	2.20	120.97	114.00
2	A	301	GTP	O6-C6-C5	-2.19	120.76	126.53
2	C	302	GTP	C8-N7-C5	2.18	108.15	104.26
5	C	304	SIN	O4-C4-C3	2.17	120.85	114.00
5	B	303	SIN	O4-C4-C3	2.17	120.84	114.00
5	B	303	SIN	O2-C1-C2	2.12	120.70	114.00
2	A	301	GTP	C3'-C2'-C1'	2.12	105.47	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	GTP	N2-C2-N1	2.11	121.22	116.76
2	B	301	GTP	C3'-C2'-C1'	2.11	105.45	101.46
5	C	304	SIN	O2-C1-C2	2.10	120.65	114.00
2	A	301	GTP	C4-C5-N7	-2.08	107.37	110.67
2	B	301	GTP	C8-N7-C5	2.08	107.96	104.26
2	C	301	GTP	O6-C6-C5	-2.02	121.20	126.53

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GTP	PB-O3A-PA-O5'
2	A	301	GTP	C5'-O5'-PA-O3A
2	A	301	GTP	C5'-O5'-PA-O1A
2	A	301	GTP	C5'-O5'-PA-O2A
2	A	301	GTP	O4'-C4'-C5'-O5'
2	B	301	GTP	O4'-C4'-C5'-O5'
2	C	302	GTP	C5'-O5'-PA-O3A
3	C	303	SAH	N-CA-CB-CG
5	B	304	SIN	C1-C2-C3-C4
2	B	301	GTP	C3'-C4'-C5'-O5'
5	C	304	SIN	C1-C2-C3-C4
2	A	301	GTP	C3'-C4'-C5'-O5'
2	B	301	GTP	PG-O3B-PB-O3A
3	A	302	SAH	C2'-C1'-N9-C8
3	B	302	SAH	C2'-C1'-N9-C8
3	C	303	SAH	C2'-C1'-N9-C8
2	A	301	GTP	PA-O3A-PB-O1B
2	C	302	GTP	C5'-O5'-PA-O1A
3	C	303	SAH	CB-CG-SD-C5'
3	C	303	SAH	C-CA-CB-CG
2	C	302	GTP	PB-O3A-PA-O1A
5	B	303	SIN	O2-C1-C2-C3
5	B	303	SIN	O1-C1-C2-C3
3	A	302	SAH	O4'-C1'-N9-C8
3	B	302	SAH	O4'-C1'-N9-C8
2	C	302	GTP	C2'-C1'-N9-C4
2	A	301	GTP	PG-O3B-PB-O2B
2	B	301	GTP	PG-O3B-PB-O1B
5	B	304	SIN	C2-C3-C4-O4
5	B	304	SIN	C2-C3-C4-O3
3	C	303	SAH	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
5	B	303	SIN	C2-C3-C4-O4
5	B	304	SIN	O2-C1-C2-C3
2	A	301	GTP	PA-O3A-PB-O2B
2	C	301	GTP	PG-O3B-PB-O1B

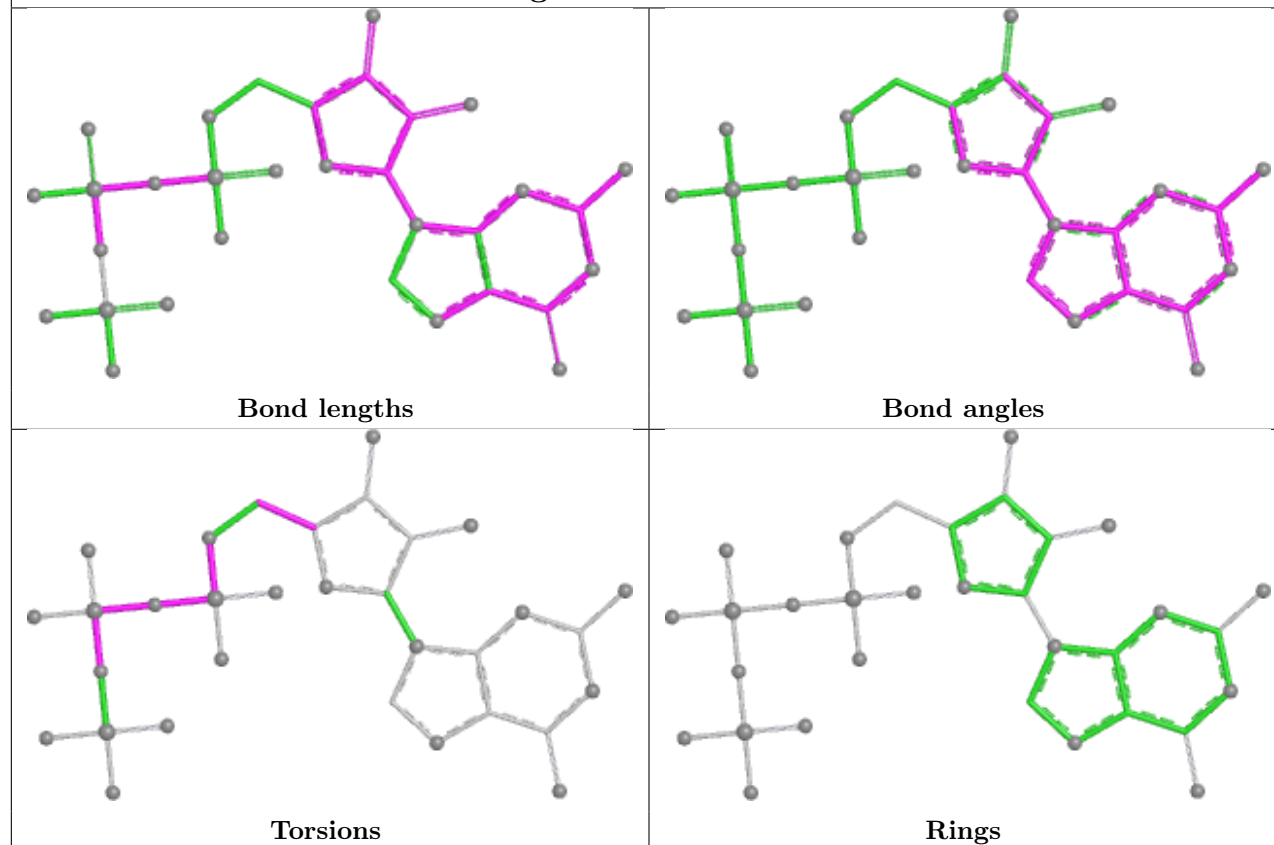
There are no ring outliers.

10 monomers are involved in 13 short contacts:

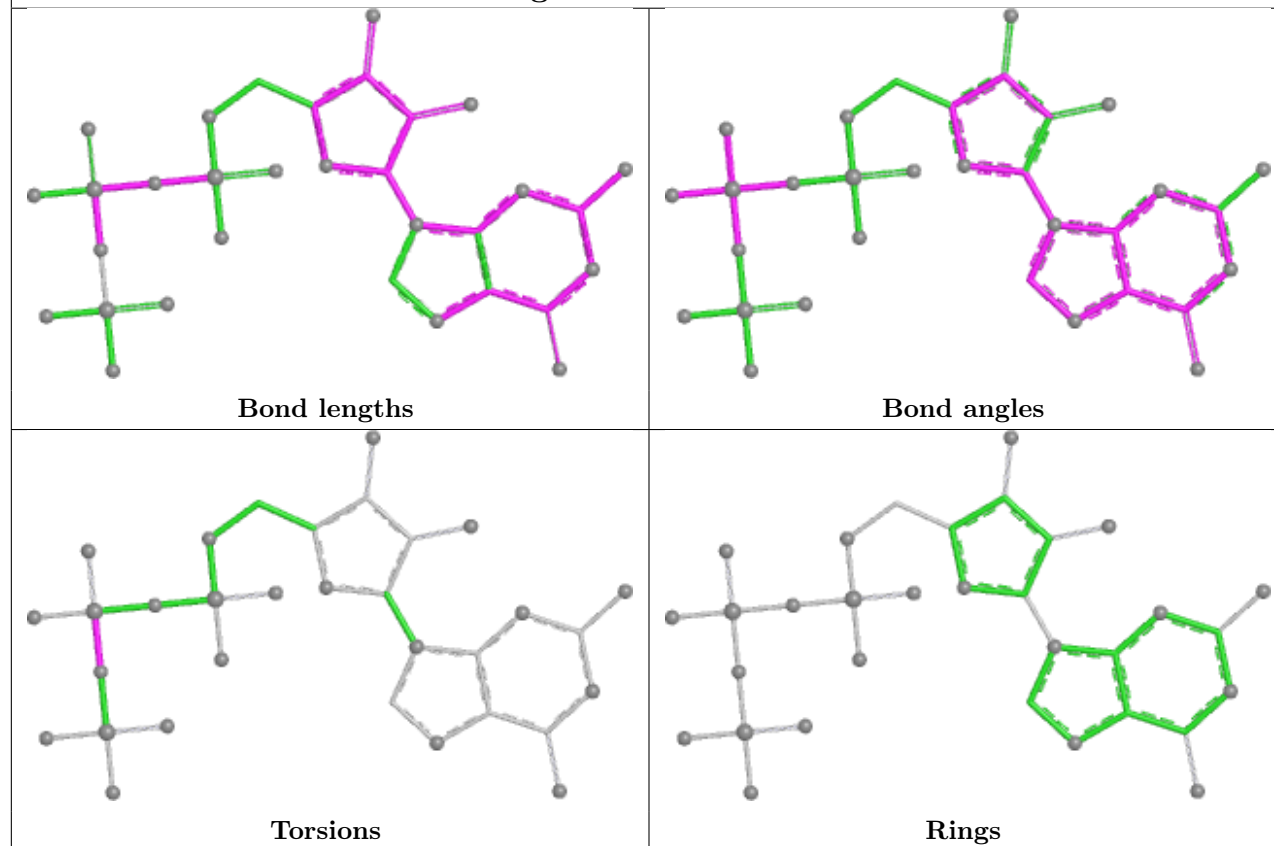
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GTP	1	0
2	C	301	GTP	3	0
5	C	304	SIN	2	0
4	C	306	PO4	1	0
3	C	303	SAH	1	0
2	B	301	GTP	1	0
2	C	302	GTP	1	0
5	B	304	SIN	1	0
3	B	302	SAH	1	0
3	A	302	SAH	1	0

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.

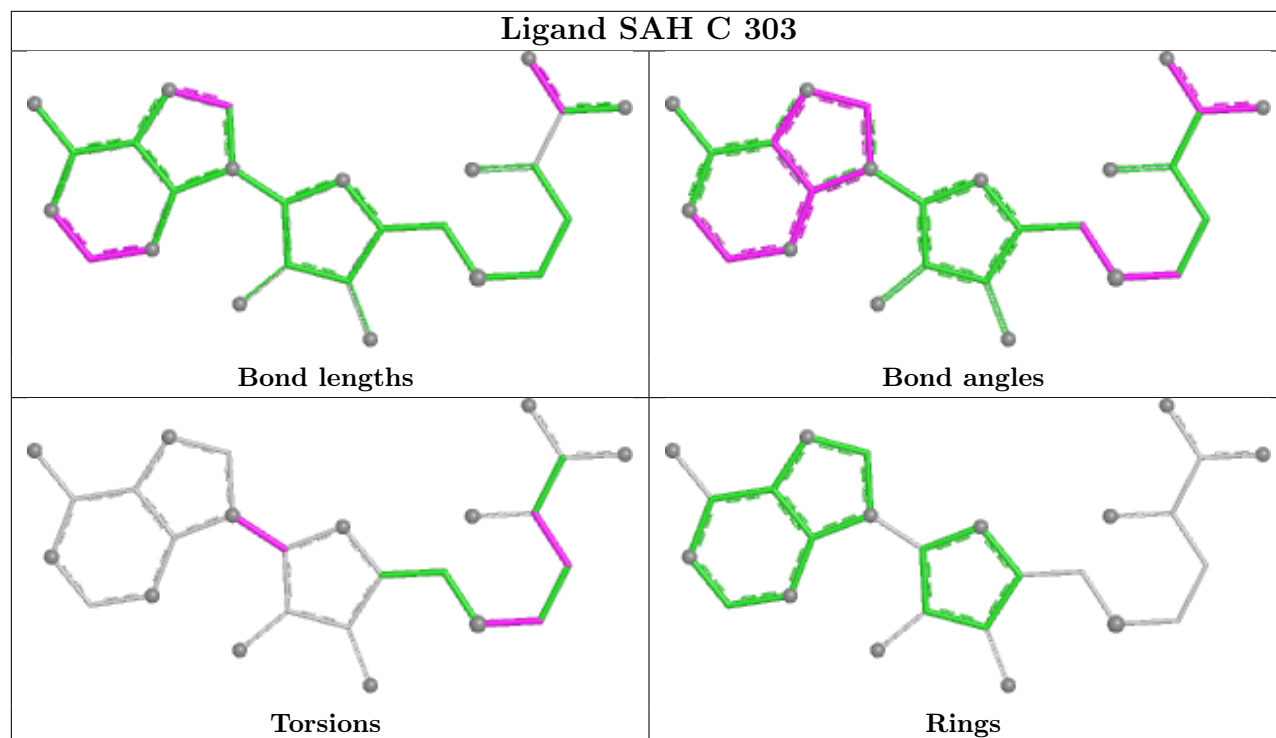
Ligand GTP A 301



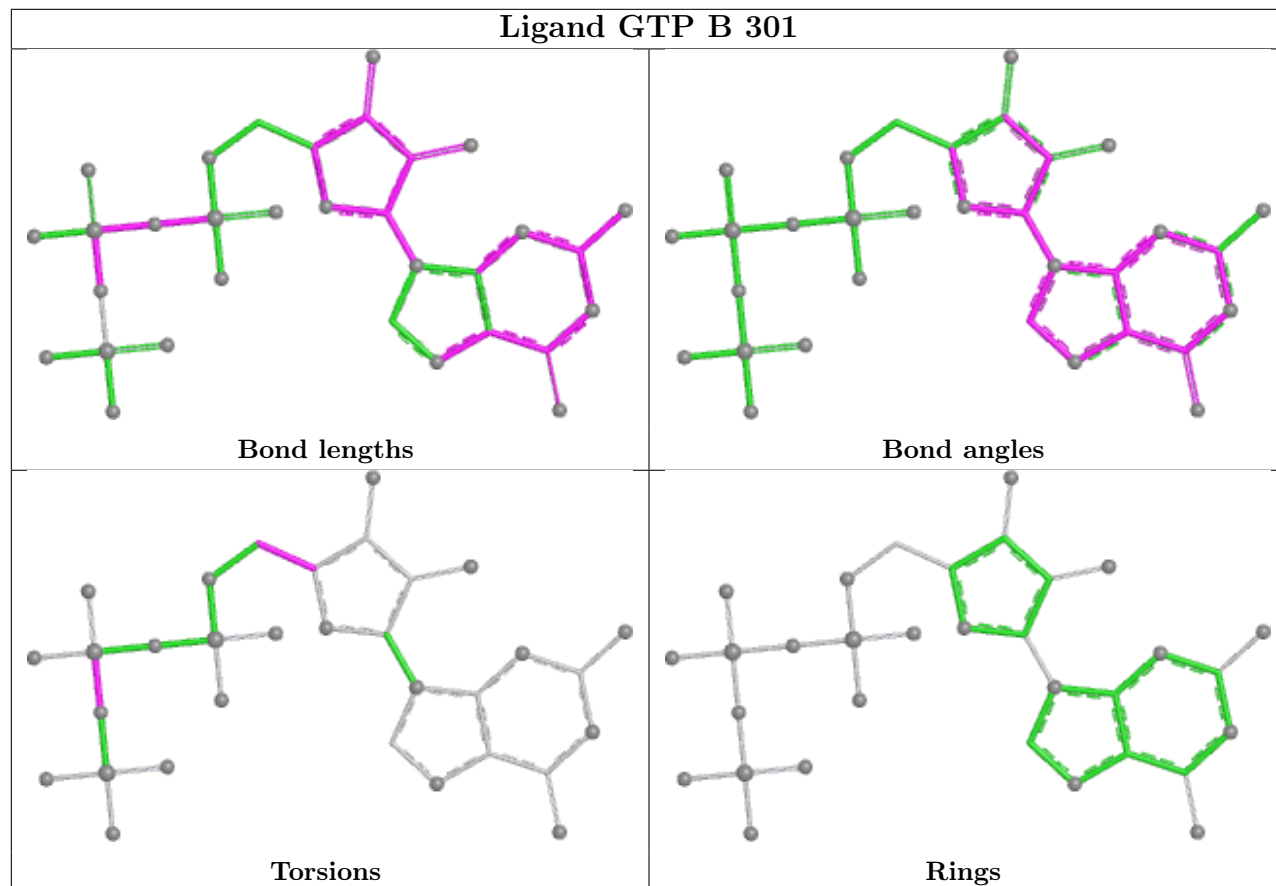
Ligand GTP C 301

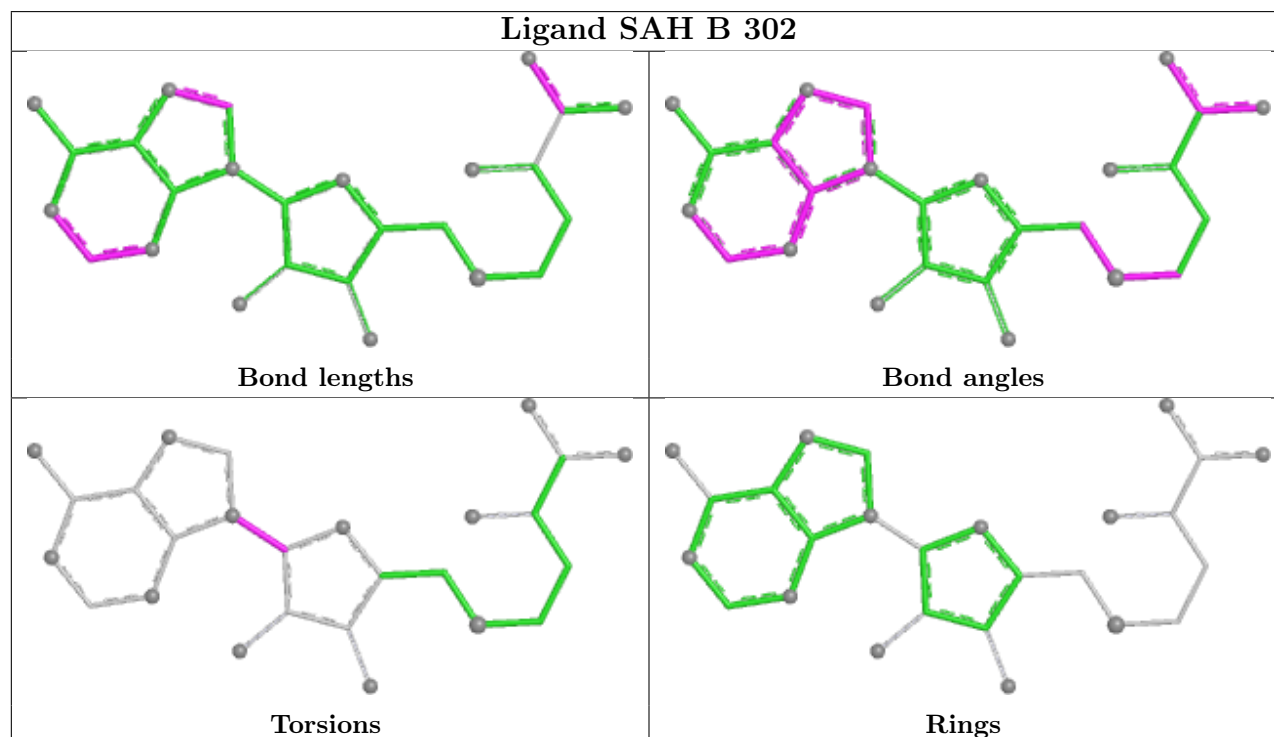
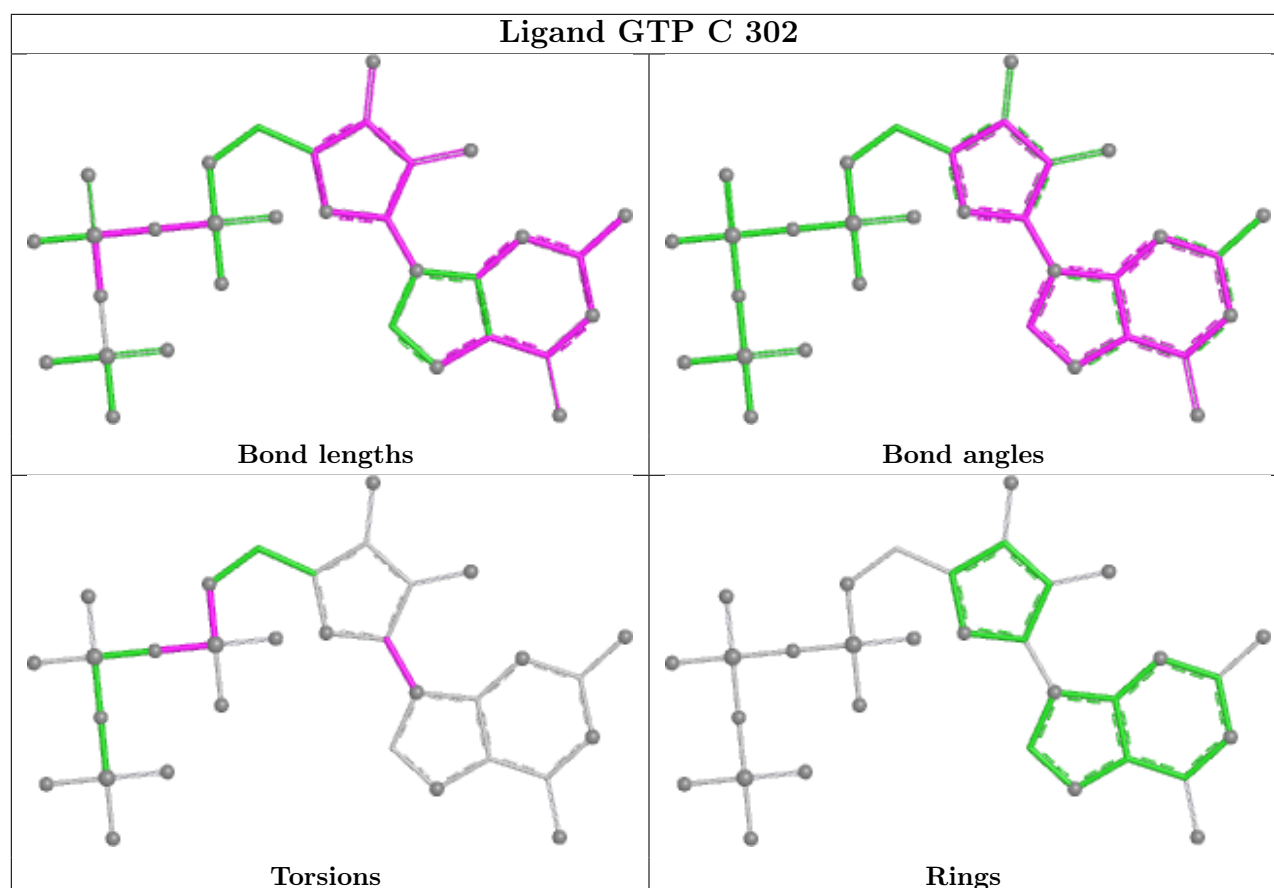


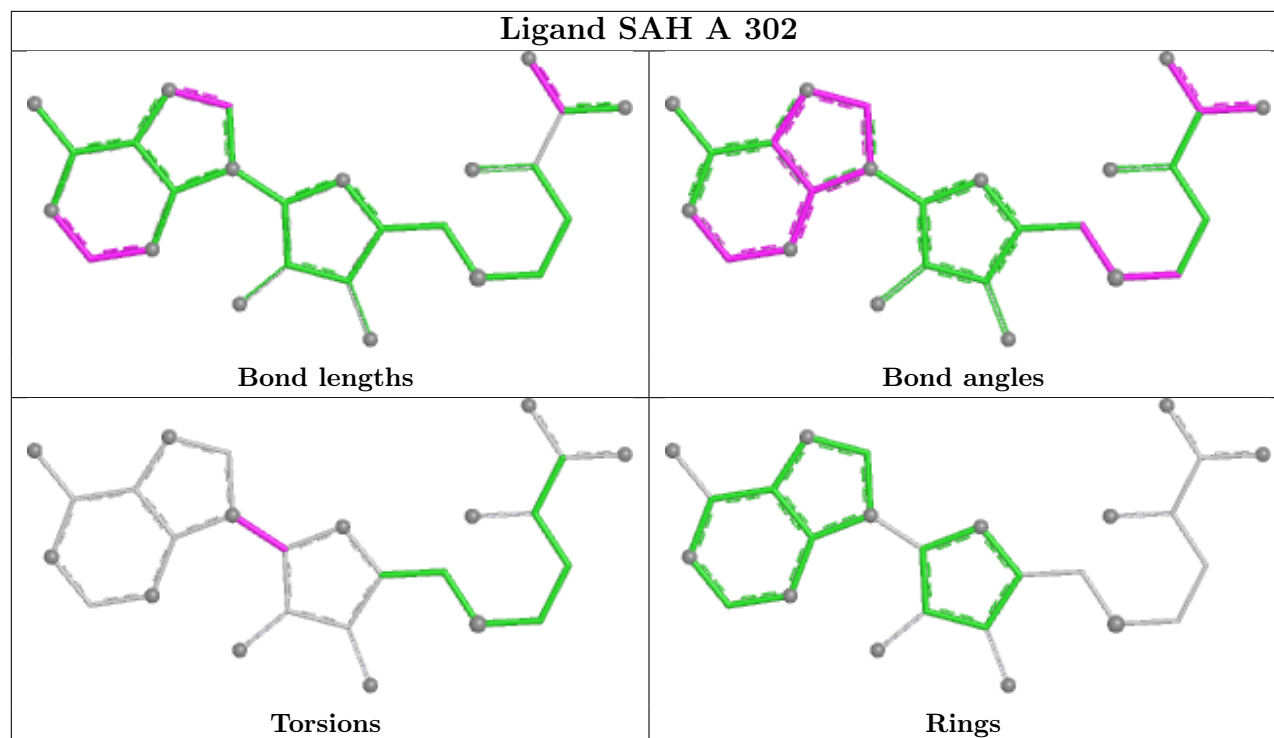
Ligand SAH C 303



Ligand GTP B 301







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	262/269 (97%)	-0.57	0	100 100	22, 46, 68, 94	2 (0%)
1	B	261/269 (97%)	-0.20	1 (0%)	88 90	32, 54, 94, 129	0
1	C	261/269 (97%)	0.07	1 (0%)	88 90	35, 61, 84, 111	0
All	All	784/807 (97%)	-0.23	2 (0%)	90 92	22, 52, 83, 129	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	ALA	2.8
1	C	92	ALA	2.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

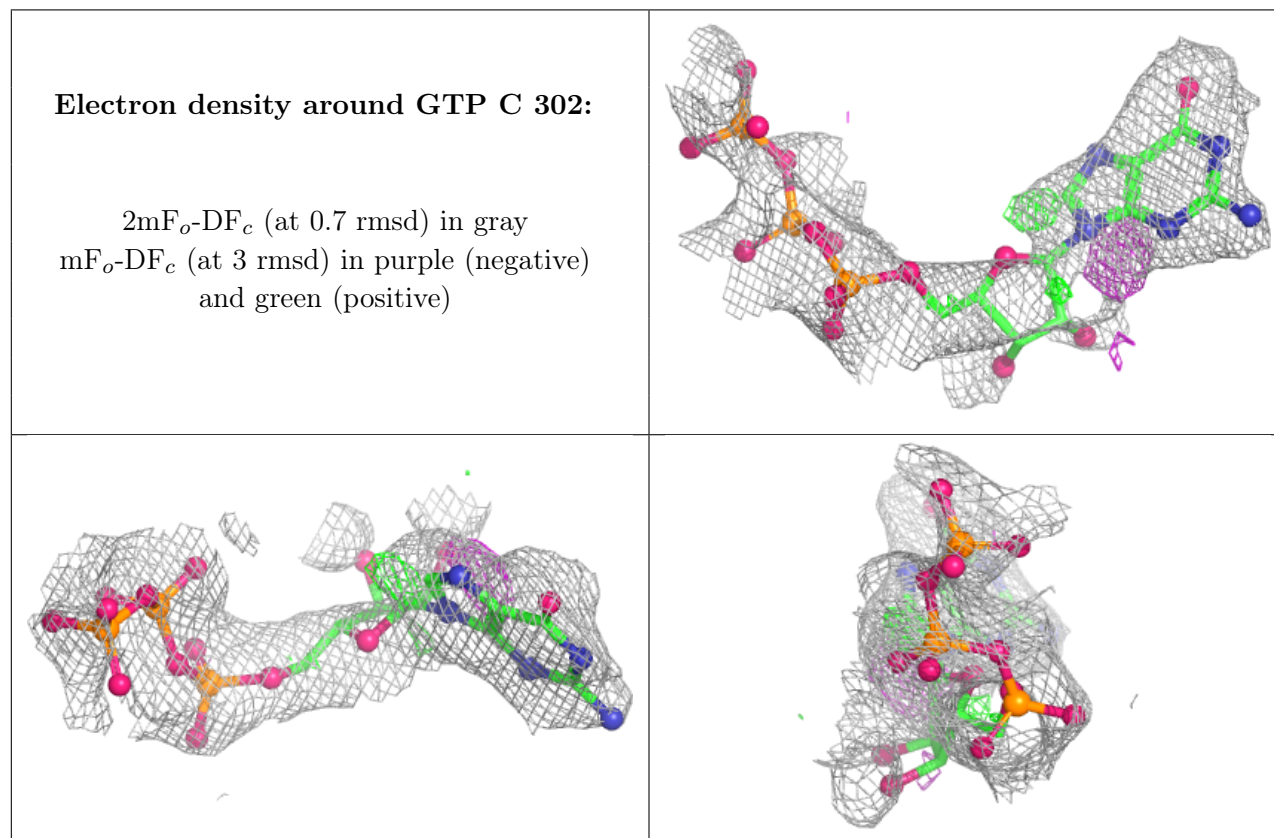
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SIN	C	304	8/8	0.88	0.13	82,83,86,86	0

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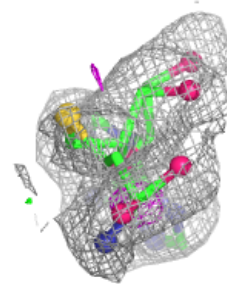
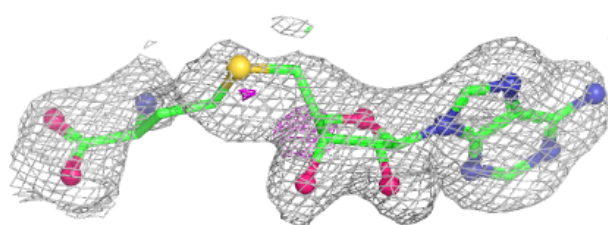
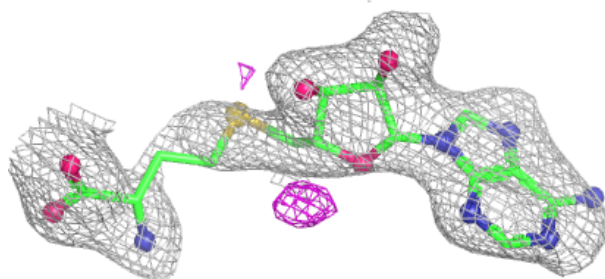
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GTP	C	302	32/32	0.91	0.13	73,99,133,135	0
4	PO4	C	306	5/5	0.94	0.08	96,97,97,97	0
6	POP	C	305	9/9	0.94	0.11	92,94,95,96	0
5	SIN	B	304	8/8	0.95	0.10	73,78,82,84	0
4	PO4	B	305	5/5	0.95	0.07	81,93,95,96	0
5	SIN	B	303	8/8	0.95	0.08	75,78,79,79	0
3	SAH	B	302	26/26	0.97	0.07	58,63,75,84	0
3	SAH	C	303	26/26	0.97	0.08	51,77,79,80	0
4	PO4	A	304	5/5	0.97	0.06	90,91,92,92	0
2	GTP	C	301	32/32	0.97	0.07	46,62,145,148	0
4	PO4	B	306	5/5	0.97	0.06	75,77,80,81	0
2	GTP	B	301	32/32	0.98	0.06	36,42,101,106	0
3	SAH	A	302	26/26	0.98	0.05	48,55,65,74	0
2	GTP	A	301	32/32	0.99	0.05	36,45,103,108	0
4	PO4	A	303	5/5	0.99	0.05	64,65,66,66	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.

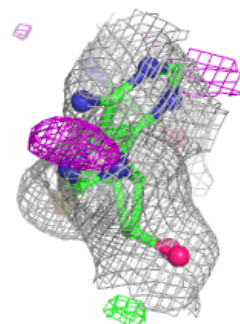
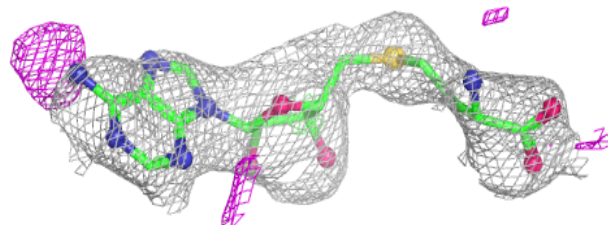
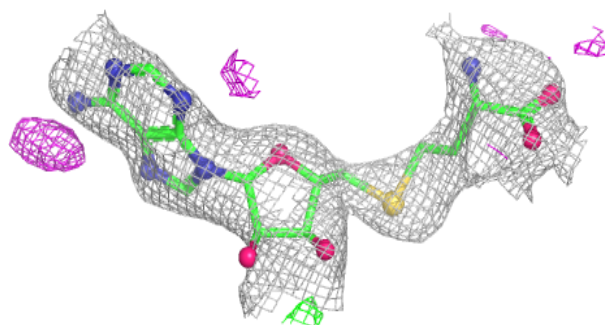


Electron density around SAH B 302:

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

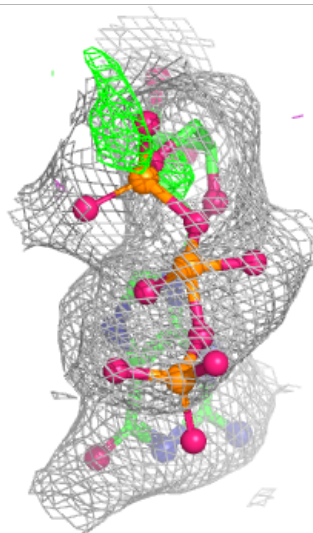
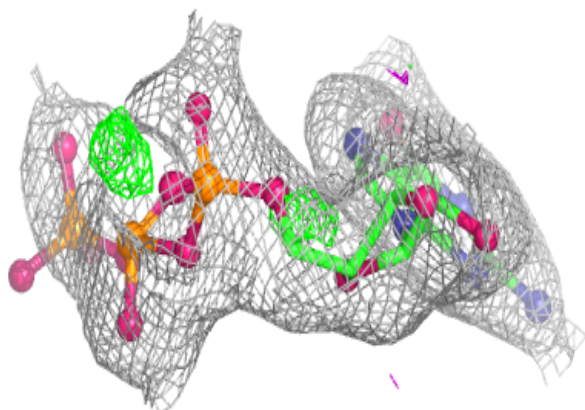
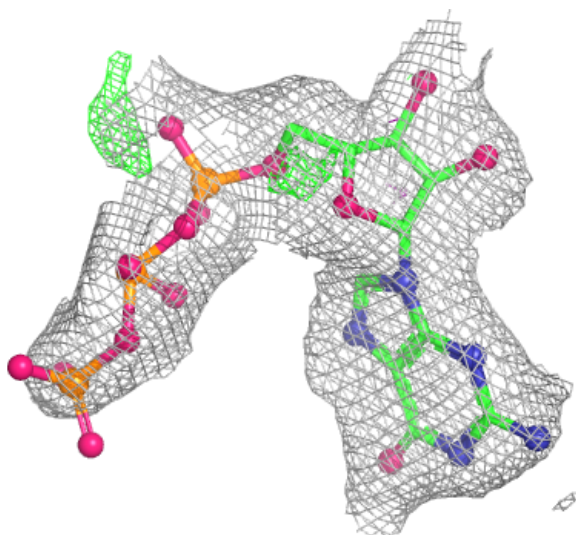
**Electron density around SAH C 303:**

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



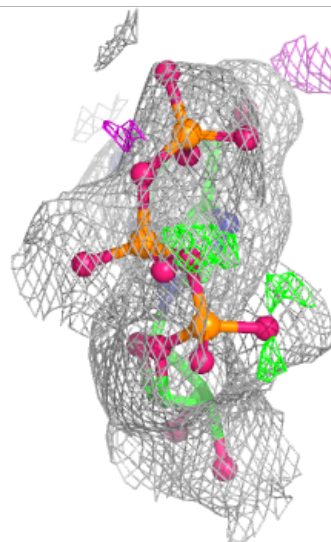
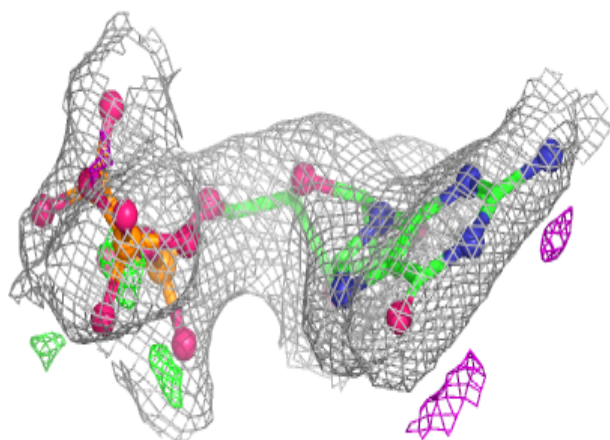
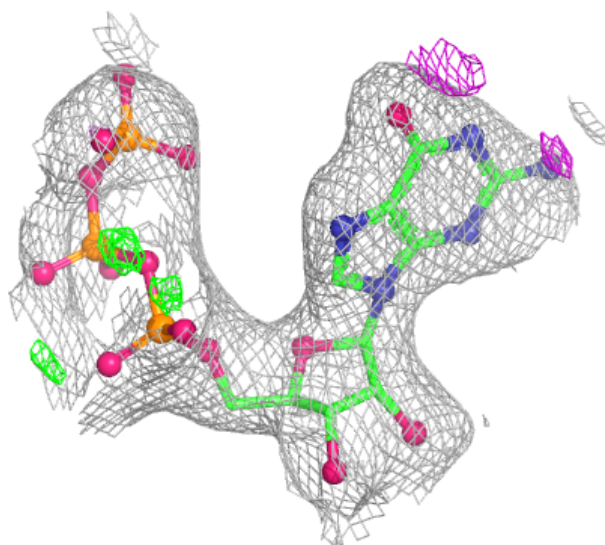
Electron density around GTP C 301:

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



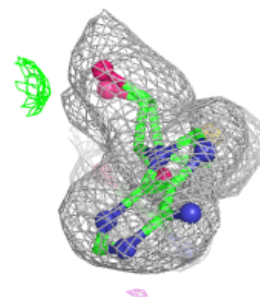
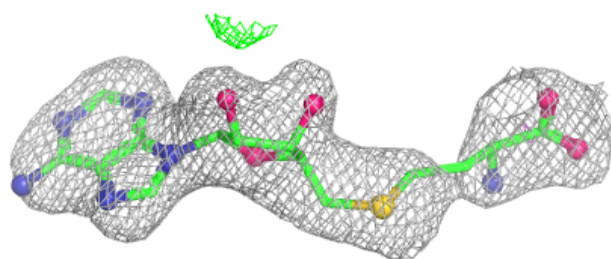
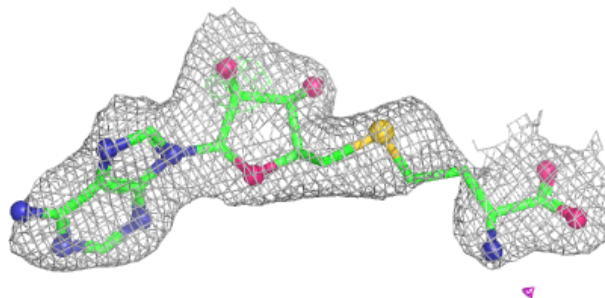
Electron density around GTP B 301:

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



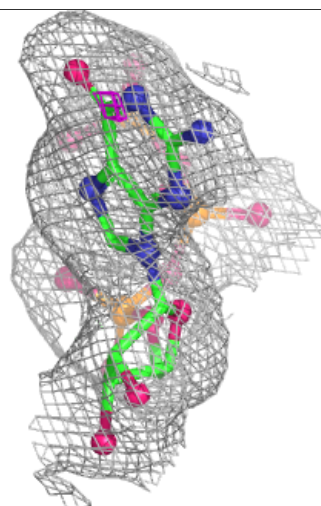
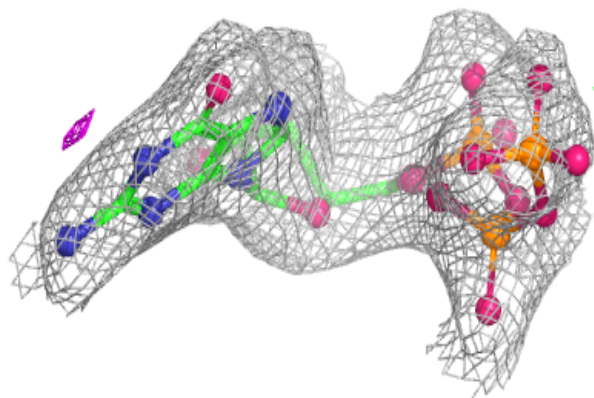
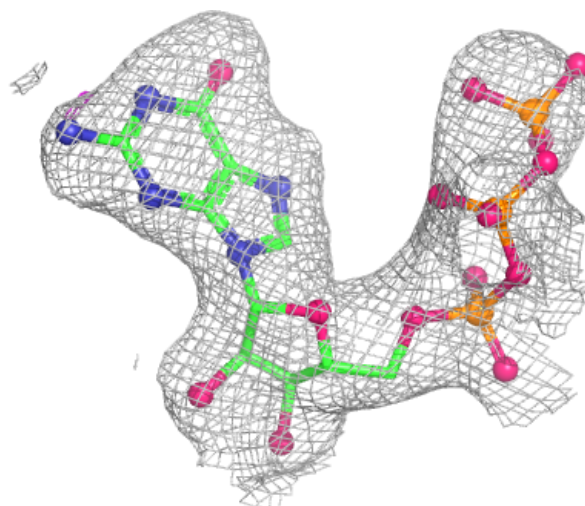
Electron density around SAH A 302:

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



Electron density around GTP 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.