



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 03:01 AM UTC

PDB ID : 9F37 / pdb_00009f37
Title : Replication-like initiation state of influenza polymerase with GTP and CTP at respectively the -1 and +1 positions (strain A/little yellow-shouldered bat /Guatemala/060/2010/H17N10)
Authors : Cusack, S.; Drncova, P.
Deposited on : 2024-04-25
Resolution : 1.91 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

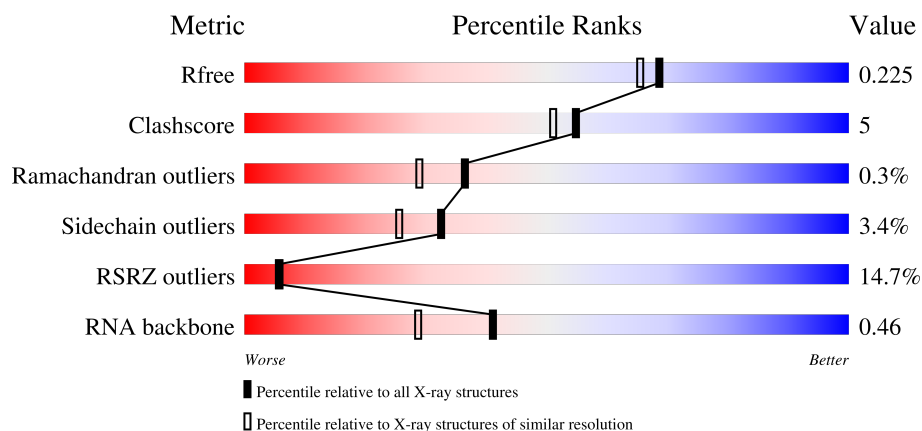
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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.



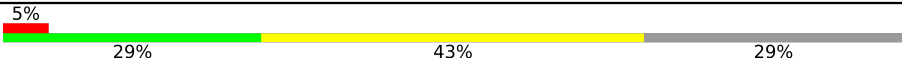
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)
RNA backbone	3983	1098 (2.30-1.50)

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	738	18% 81% 13% • 5%
2	B	776	4% 82% 11% • 5%
3	C	809	20% 76% 14% • 9%

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Mol	Chain	Length	Quality of chain
4	R	21	
5	V	16	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 19019 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	703	Total	C	N	O	S	0	7	0
			5795	3681	981	1095	38			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP H6QM92
A	-12	SER	-	expression tag	UNP H6QM92
A	-11	HIS	-	expression tag	UNP H6QM92
A	-10	HIS	-	expression tag	UNP H6QM92
A	-9	HIS	-	expression tag	UNP H6QM92
A	-8	HIS	-	expression tag	UNP H6QM92
A	-7	HIS	-	expression tag	UNP H6QM92
A	-6	HIS	-	expression tag	UNP H6QM92
A	-5	HIS	-	expression tag	UNP H6QM92
A	-4	HIS	-	expression tag	UNP H6QM92
A	-3	GLY	-	expression tag	UNP H6QM92
A	-2	SER	-	expression tag	UNP H6QM92
A	-1	GLY	-	expression tag	UNP H6QM92
A	0	SER	-	expression tag	UNP H6QM92
A	714	GLY	-	expression tag	UNP H6QM92
A	715	SER	-	expression tag	UNP H6QM92
A	716	GLY	-	expression tag	UNP H6QM92
A	717	SER	-	expression tag	UNP H6QM92
A	718	GLY	-	expression tag	UNP H6QM92
A	719	GLU	-	expression tag	UNP H6QM92
A	720	ASN	-	expression tag	UNP H6QM92
A	721	LEU	-	expression tag	UNP H6QM92
A	722	TYR	-	expression tag	UNP H6QM92
A	723	PHE	-	expression tag	UNP H6QM92
A	724	GLN	-	expression tag	UNP H6QM92

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	736	Total	C	N	O	S	0	9	0
			5931	3730	1049	1112	40			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP H6QM91
B	-7	SER	-	expression tag	UNP H6QM91
B	-6	GLY	-	expression tag	UNP H6QM91
B	-5	SER	-	expression tag	UNP H6QM91
B	-4	GLY	-	expression tag	UNP H6QM91
B	-3	SER	-	expression tag	UNP H6QM91
B	-2	GLY	-	expression tag	UNP H6QM91
B	-1	SER	-	expression tag	UNP H6QM91
B	0	GLY	-	expression tag	UNP H6QM91
B	757	GLY	-	expression tag	UNP H6QM91
B	758	SER	-	expression tag	UNP H6QM91
B	759	GLY	-	expression tag	UNP H6QM91
B	760	SER	-	expression tag	UNP H6QM91
B	761	GLY	-	expression tag	UNP H6QM91
B	762	GLU	-	expression tag	UNP H6QM91
B	763	ASN	-	expression tag	UNP H6QM91
B	764	LEU	-	expression tag	UNP H6QM91
B	765	TYR	-	expression tag	UNP H6QM91
B	766	PHE	-	expression tag	UNP H6QM91
B	767	GLN	-	expression tag	UNP H6QM91

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	734	Total	C	N	O	S	0	2	0
			5828	3674	1034	1088	32			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP H6QM90
C	-7	SER	-	expression tag	UNP H6QM90
C	-6	GLY	-	expression tag	UNP H6QM90
C	-5	SER	-	expression tag	UNP H6QM90
C	-4	GLY	-	expression tag	UNP H6QM90
C	-3	SER	-	expression tag	UNP H6QM90
C	-2	GLY	-	expression tag	UNP H6QM90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP H6QM90
C	0	GLY	-	expression tag	UNP H6QM90
C	761	GLY	-	expression tag	UNP H6QM90
C	762	TRP	-	expression tag	UNP H6QM90
C	763	SER	-	expression tag	UNP H6QM90
C	764	HIS	-	expression tag	UNP H6QM90
C	765	PRO	-	expression tag	UNP H6QM90
C	766	GLN	-	expression tag	UNP H6QM90
C	767	PHE	-	expression tag	UNP H6QM90
C	768	GLU	-	expression tag	UNP H6QM90
C	769	LYS	-	expression tag	UNP H6QM90
C	770	GLY	-	expression tag	UNP H6QM90
C	771	GLY	-	expression tag	UNP H6QM90
C	772	GLY	-	expression tag	UNP H6QM90
C	773	SER	-	expression tag	UNP H6QM90
C	774	GLY	-	expression tag	UNP H6QM90
C	775	GLY	-	expression tag	UNP H6QM90
C	776	GLY	-	expression tag	UNP H6QM90
C	777	SER	-	expression tag	UNP H6QM90
C	778	GLY	-	expression tag	UNP H6QM90
C	779	GLY	-	expression tag	UNP H6QM90
C	780	SER	-	expression tag	UNP H6QM90
C	781	ALA	-	expression tag	UNP H6QM90
C	782	TRP	-	expression tag	UNP H6QM90
C	783	SER	-	expression tag	UNP H6QM90
C	784	HIS	-	expression tag	UNP H6QM90
C	785	PRO	-	expression tag	UNP H6QM90
C	786	GLN	-	expression tag	UNP H6QM90
C	787	PHE	-	expression tag	UNP H6QM90
C	788	GLU	-	expression tag	UNP H6QM90
C	789	LYS	-	expression tag	UNP H6QM90
C	790	GLY	-	expression tag	UNP H6QM90
C	791	ARG	-	expression tag	UNP H6QM90
C	792	SER	-	expression tag	UNP H6QM90
C	793	GLY	-	expression tag	UNP H6QM90
C	794	GLY	-	expression tag	UNP H6QM90
C	795	GLU	-	expression tag	UNP H6QM90
C	796	ASN	-	expression tag	UNP H6QM90
C	797	LEU	-	expression tag	UNP H6QM90
C	798	TYR	-	expression tag	UNP H6QM90
C	799	PHE	-	expression tag	UNP H6QM90
C	800	GLN	-	expression tag	UNP H6QM90

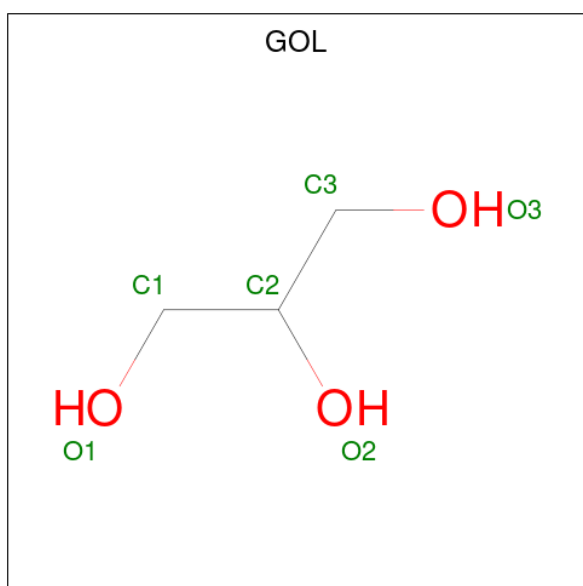
- Molecule 4 is a RNA chain called 3' end of the vRNA promoter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	15	Total	C	N	O	P	0	0	0
			305	138	45	108	14			

- Molecule 5 is a RNA chain called 5' end of the vRNA promoter.

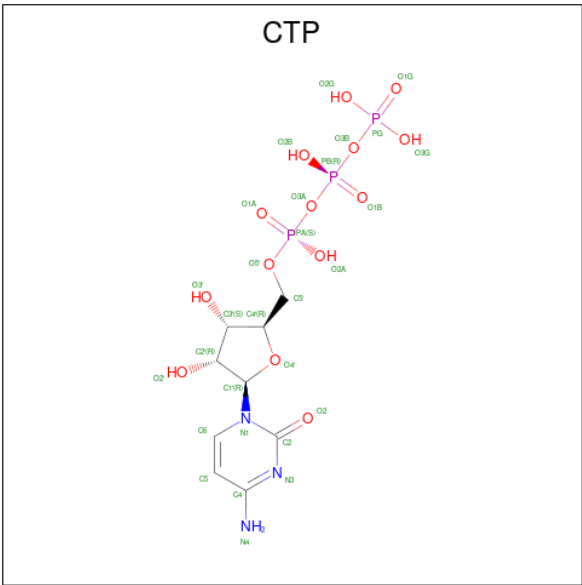
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	V	16	Total	C	N	O	P	0	0	0
			334	147	67	104	16			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



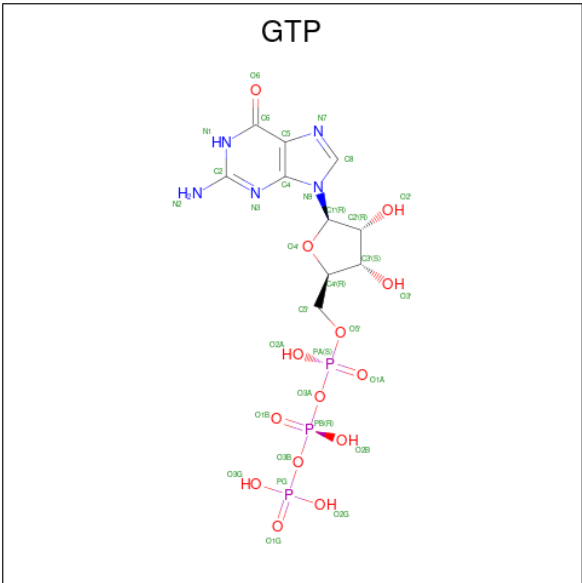
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	29	9	3	14	3	0	0

- Molecule 8 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

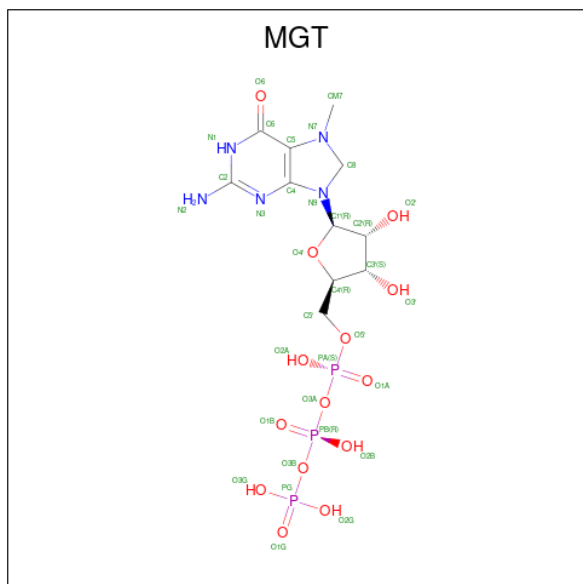


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	B	1	32	10	5	14	3	0	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total	Mg	0	0
			2	2		

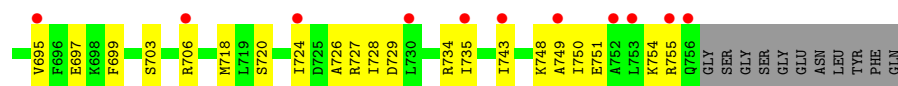
- Molecule 10 is 7N-METHYL-8-HYDROGUANOSINE-5'-TRIPHOSPHATE (CCD ID: MGT) (formula: $C_{11}H_{20}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



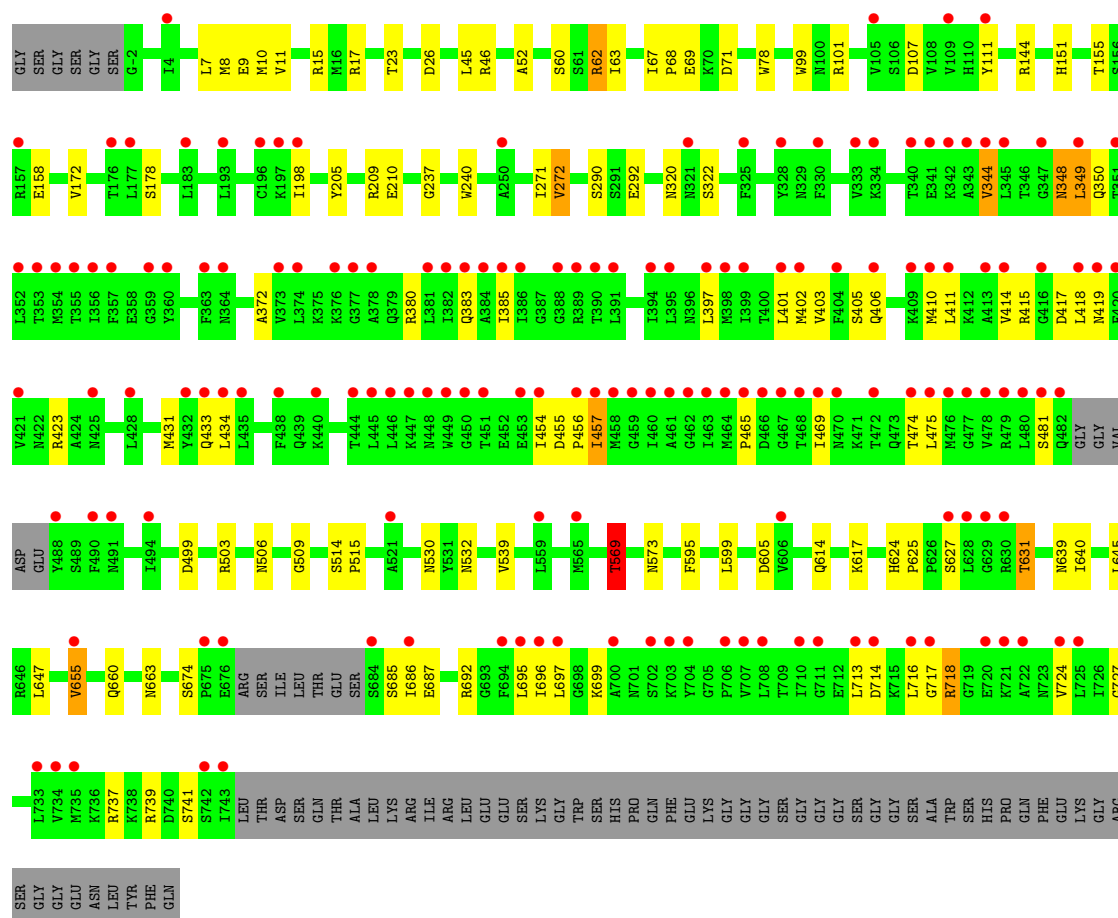
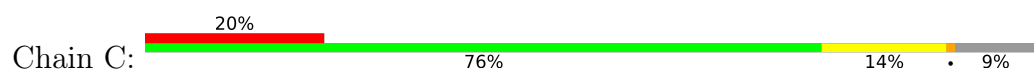
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	N	O	P	0	0
			33	11	5	14	3		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	220	Total	O	0	0
			220	220		
11	B	288	Total	O	0	0
			288	288		
11	C	137	Total	O	0	0
			137	137		
11	R	16	Total	O	0	0
			16	16		
11	V	39	Total	O	0	0
			39	39		



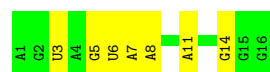
• Molecule 3: Polymerase basic protein 2



• Molecule 4: 3' end of the vRNA promoter



• Molecule 5: 5' end of the vRNA promoter



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.94Å 119.00Å 251.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.57 – 1.91 86.57 – 1.91	Depositor EDS
% Data completeness (in resolution range)	71.2 (86.57-1.91) 71.2 (86.57-1.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.189 , 0.232 (Not available) , 0.225	Depositor DCC
R_{free} test set	7590 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19019	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CTP, GTP, MGT, GOL

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	0.52	0/5917	1.00	8/7966 (0.1%)
2	B	0.55	0/6048	1.01	6/8167 (0.1%)
3	C	0.53	0/5927	1.00	5/8000 (0.1%)
4	R	0.54	0/337	1.23	5/521 (1.0%)
5	V	0.59	0/375	1.14	2/583 (0.3%)
All	All	0.53	0/18604	1.01	26/25237 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	3
3	C	0	3
All	All	0	8

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	18	U	C4'-C3'-O3'	9.73	124.00	109.40
4	R	18	U	C3'-C2'-O2'	-8.16	102.36	114.60
1	A	332	THR	CA-CB-OG1	-7.51	98.33	109.60
1	A	513	VAL	CB-CA-C	-6.53	102.04	110.98
3	C	569	THR	CA-CB-OG1	-6.20	100.30	109.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	ARG	Sidechain
1	A	436	ARG	Sidechain
2	B	334	ARG	Sidechain
2	B	429	ARG	Sidechain
2	B	498	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5795	0	5702	57	0
2	B	5931	0	5913	71	0
3	C	5828	0	5929	61	0
4	R	305	0	161	5	0
5	V	334	0	163	0	0
6	A	6	0	8	0	0
6	B	18	0	24	0	0
6	C	6	0	8	0	0
7	B	29	0	12	0	0
8	B	32	0	11	0	0
9	B	2	0	0	0	0
10	C	33	0	16	0	0
11	A	220	0	0	0	0
11	B	288	0	0	9	0
11	C	137	0	0	1	0
11	R	16	0	0	0	0
11	V	39	0	0	0	0
All	All	19019	0	17947	174	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 5.

The worst 5 of 174 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396[A]:ARG:NH2	1:A:533:GLU:OE1	2.04	0.90
1:A:365:LEU:HD21	1:A:516:ILE:HD12	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:LEU:HD11	1:A:513:VAL:HG22	1.63	0.80
2:B:287:LYS:HE2	11:B:1172:HOH:O	1.86	0.75
1:A:449[B]:ARG:HH11	1:A:449[B]:ARG:HB2	1.52	0.75

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	704/738 (95%)	666 (95%)	35 (5%)	3 (0%)	30	22
2	B	741/776 (96%)	716 (97%)	25 (3%)	0	100	100
3	C	730/809 (90%)	698 (96%)	28 (4%)	4 (0%)	24	16
All	All	2175/2323 (94%)	2080 (96%)	88 (4%)	7 (0%)	36	29

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	349	LEU
1	A	159	ASP
1	A	550	SER
3	C	718	ARG
1	A	155	MET

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	636/657 (97%)	612 (96%)	24 (4%)	29	21
2	B	653/676 (97%)	636 (97%)	17 (3%)	40	35
3	C	647/706 (92%)	621 (96%)	26 (4%)	28	20
All	All	1936/2039 (95%)	1869 (96%)	67 (4%)	32	24

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	481	SER
3	C	569	THR
3	C	699	LYS
2	B	1	MET
1	A	616	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	530	ASN
3	C	556	ASN
3	C	573	ASN
3	C	548	ASN
2	B	628	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	14/21 (66%)	0	0
5	V	14/16 (87%)	5 (35%)	1 (7%)
All	All	28/37 (75%)	5 (17%)	1 (3%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	V	5	G
5	V	6	U
5	V	7	A
5	V	8	A
5	V	11	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	V	5	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
6	GOL	B	801	-	5,5,5	0.13	0	5,5,5	0.44	0
8	GTP	B	805	9	33,34,34	0.64	0	50,54,54	0.91	2 (4%)
6	GOL	A	801	-	5,5,5	0.11	0	5,5,5	0.35	0
10	MGT	C	902	-	34,35,35	0.91	1 (2%)	45,56,56	0.83	1 (2%)
6	GOL	C	901	-	5,5,5	0.17	0	5,5,5	0.53	0
7	CTP	B	804	9	29,30,30	1.00	2 (6%)	43,47,47	0.65	0
6	GOL	B	802	-	5,5,5	0.15	0	5,5,5	0.47	0
6	GOL	B	803	-	5,5,5	0.25	0	5,5,5	0.57	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	801	-	-	2/4/4/4	-
8	GTP	B	805	9	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	801	-	-	2/4/4/4	-
10	MGT	C	902	-	-	8/22/50/50	0/3/3/3
6	GOL	C	901	-	-	2/4/4/4	-
7	CTP	B	804	9	-	2/22/38/38	0/2/2/2
6	GOL	B	802	-	-	0/4/4/4	-
6	GOL	B	803	-	-	3/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	902	MGT	C5-N7	3.53	1.40	1.35
7	B	804	CTP	PA-O3A	3.12	1.62	1.59
7	B	804	CTP	PB-O3A	2.76	1.62	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	902	MGT	C4-C5-N7	2.51	108.34	105.38
8	B	805	GTP	O2G-PG-O3B	2.29	112.31	104.64
8	B	805	GTP	O2B-PB-O3A	2.05	112.83	107.27

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

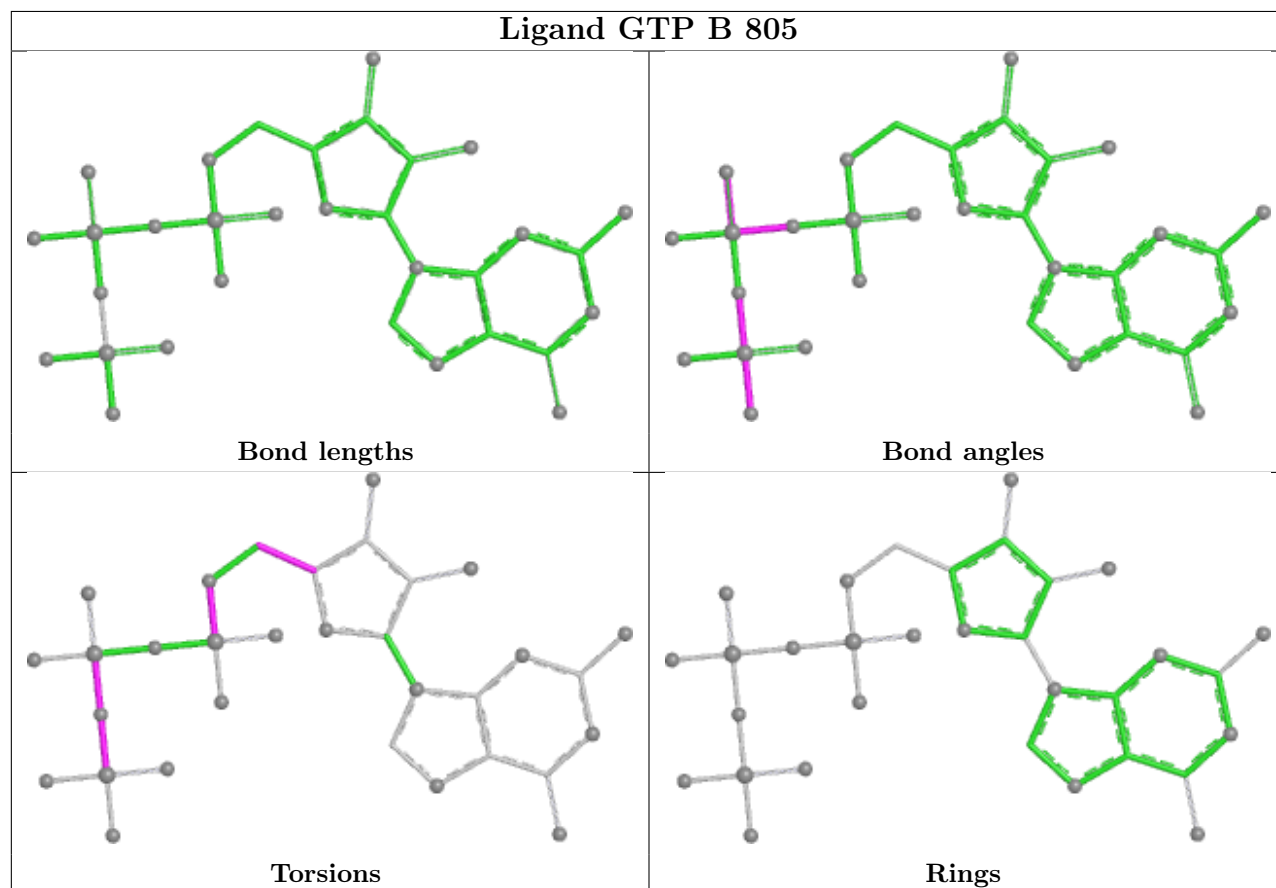
Mol	Chain	Res	Type	Atoms
6	A	801	GOL	O1-C1-C2-C3
6	B	801	GOL	O1-C1-C2-C3
6	B	803	GOL	O1-C1-C2-C3
8	B	805	GTP	C5'-O5'-PA-O3A
8	B	805	GTP	C5'-O5'-PA-O2A

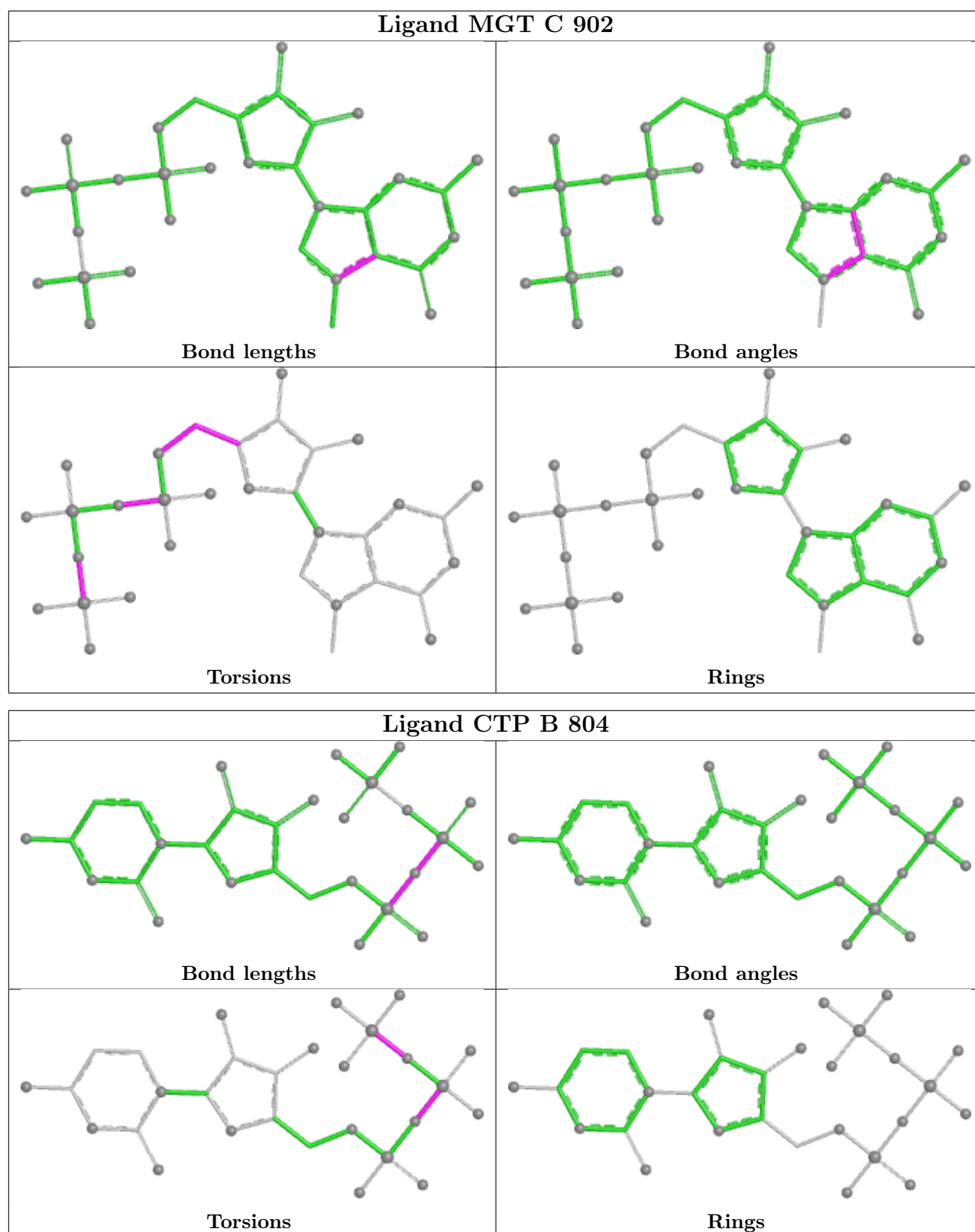
There are no ring outliers.

No monomer is involved in short contacts.

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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	703/738 (95%)	0.83	134 (19%) 3 3	13, 43, 129, 162	7 (0%)
2	B	736/776 (94%)	0.11	31 (4%) 40 43	14, 34, 71, 130	9 (1%)
3	C	734/809 (90%)	1.11	159 (21%) 2 2	16, 51, 110, 132	2 (0%)
4	R	15/21 (71%)	-0.01	1 (6%) 24 25	34, 43, 83, 98	0
5	V	16/16 (100%)	-0.44	0 100 100	27, 32, 73, 104	0
All	All	2204/2360 (93%)	0.67	325 (14%) 6 6	13, 42, 114, 162	18 (0%)

The worst 5 of 325 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	463	ILE	7.8
3	C	480	LEU	7.8
1	A	549	ILE	7.0
3	C	461	ALA	6.5
3	C	462	GLY	6.5

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.

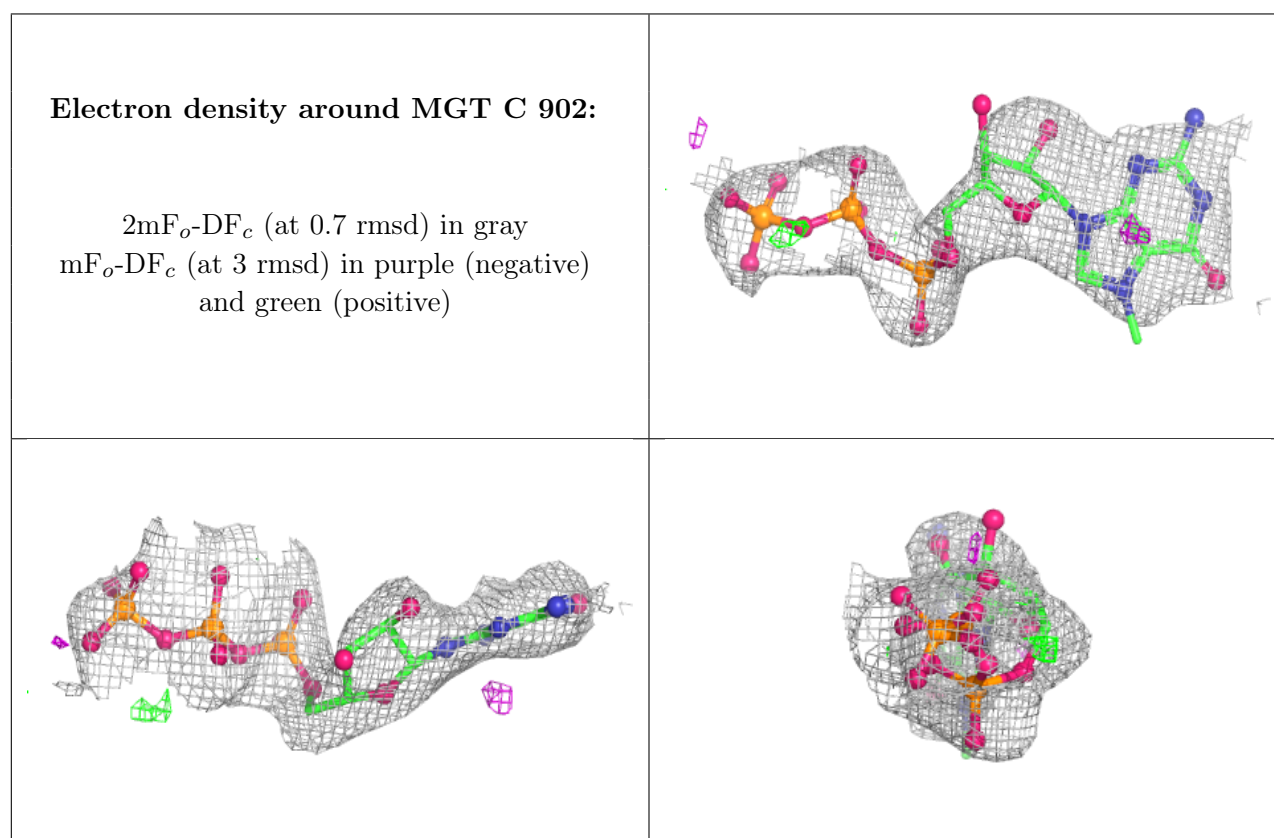
6.4 Ligands [i](#)

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.

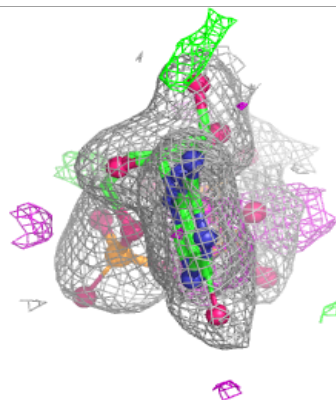
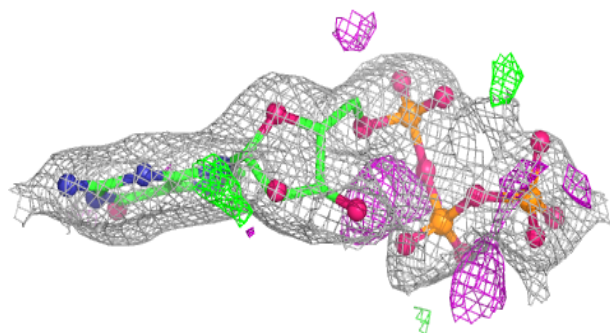
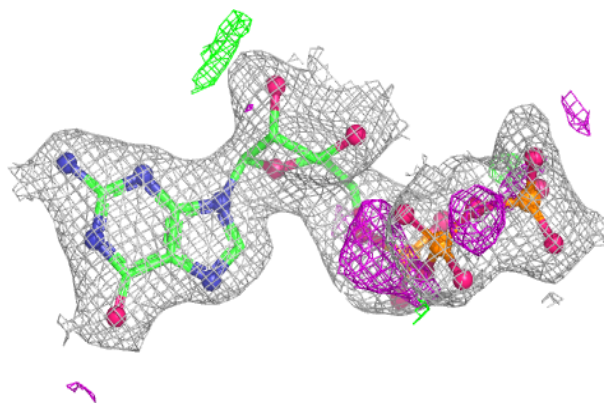
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	B	803	6/6	0.77	0.20	46,59,61,64	0
6	GOL	B	801	6/6	0.82	0.20	34,60,66,68	0
10	MGT	C	902	33/33	0.83	0.12	79,91,111,113	0
6	GOL	C	901	6/6	0.88	0.14	48,55,59,60	0
8	GTP	B	805	32/32	0.89	0.10	37,44,87,93	0
6	GOL	A	801	6/6	0.93	0.09	33,36,39,44	0
6	GOL	B	802	6/6	0.93	0.10	35,42,46,49	0
9	MG	B	806	1/1	0.98	0.09	35,35,35,35	0
7	CTP	B	804	29/29	0.98	0.06	28,33,38,40	0
9	MG	B	807	1/1	0.99	0.02	24,24,24,24	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



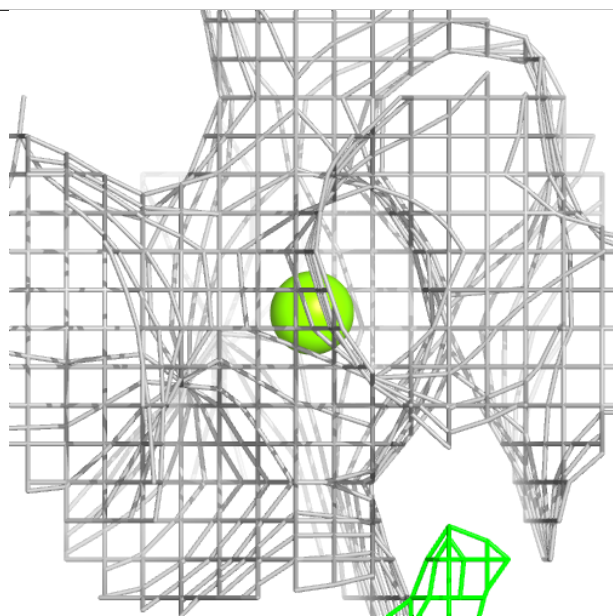
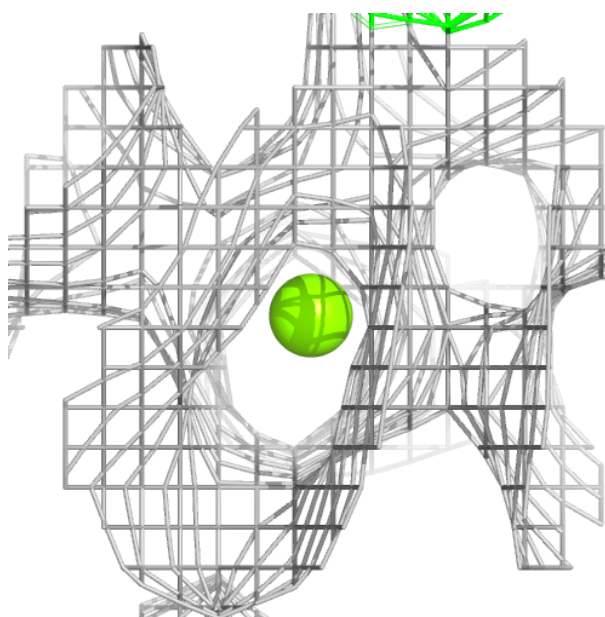
Electron density around GTP B 805:

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



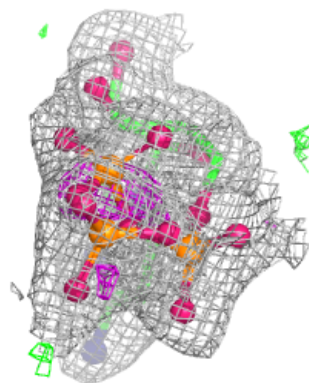
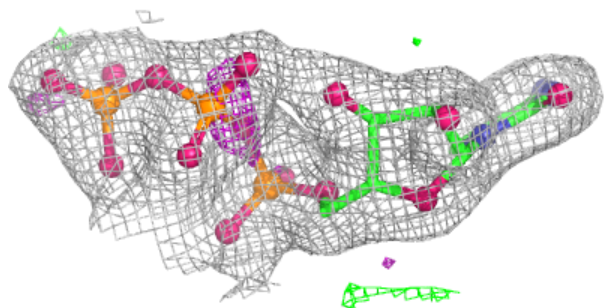
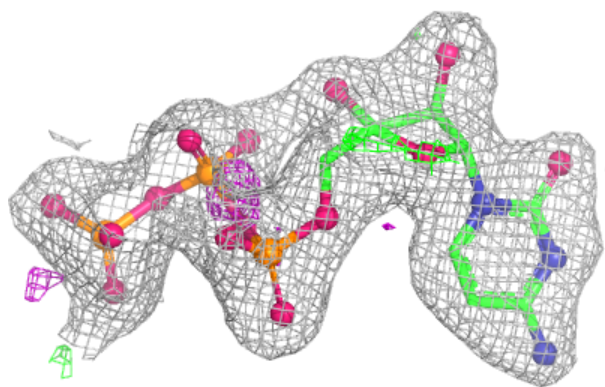
Electron density around MG B 806:

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



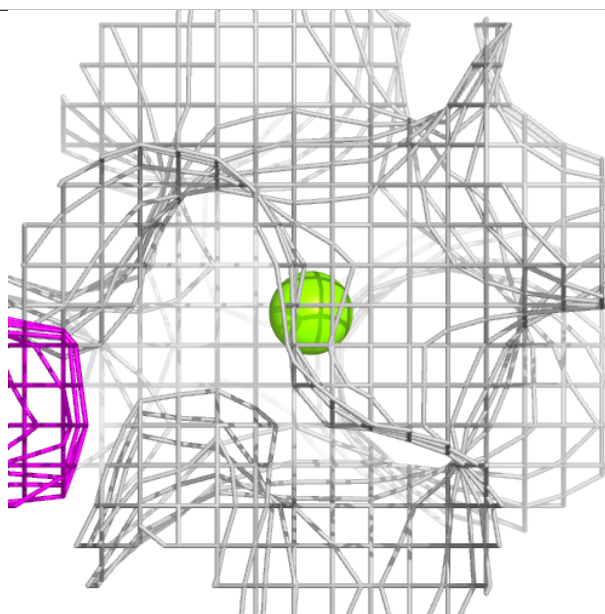
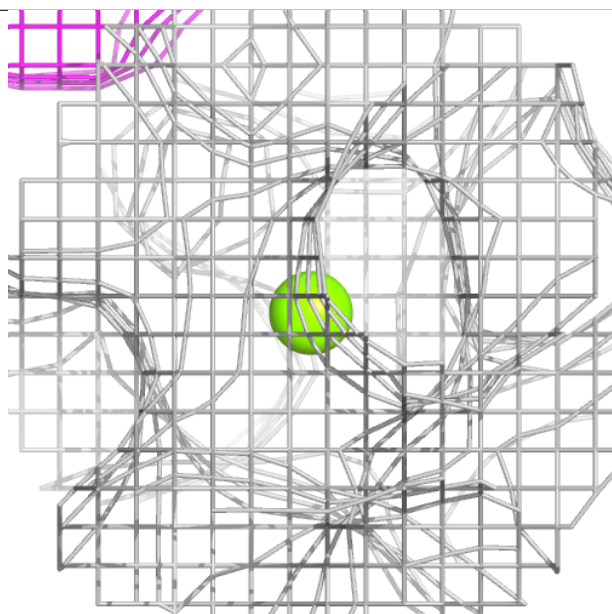
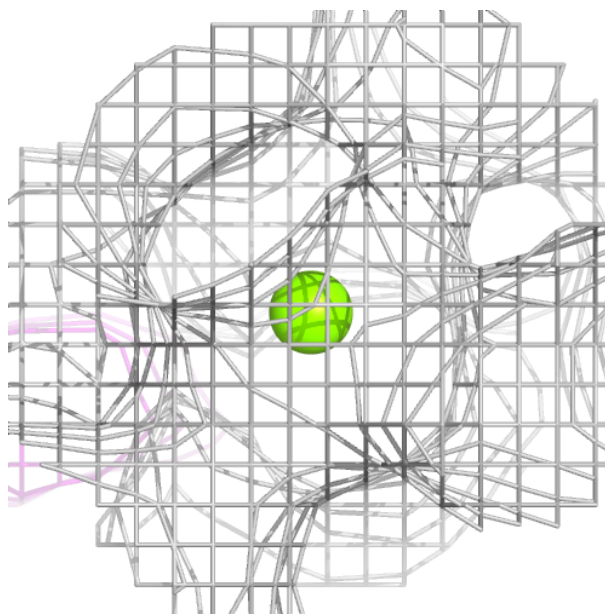
Electron density around CTP B 804:

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



Electron density around MG B 807:

$2mF_o-DF_c$ (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.