Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2024 – 01:19 pm BST

PDB ID	:	9F37
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

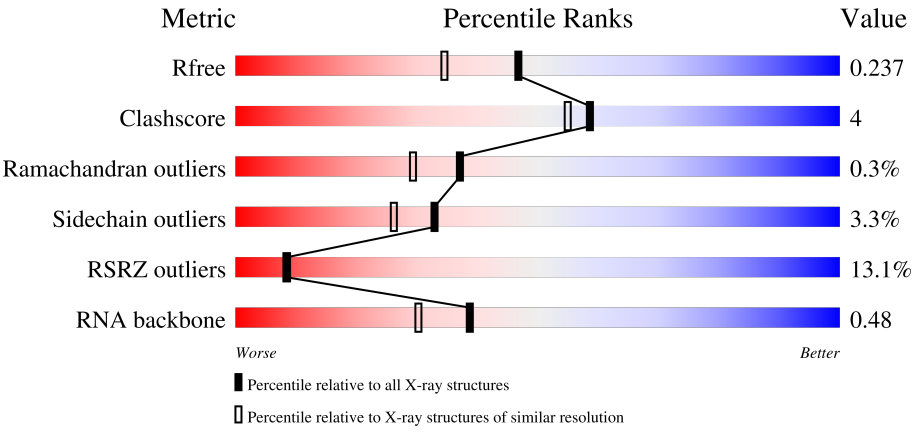
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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.



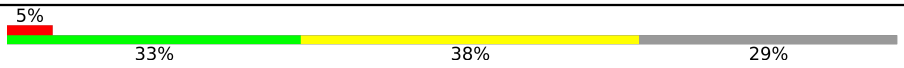
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)
RNA backbone	3690	1046 (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 <=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	17% 82% 12% • 5%
2	B	776	4% 83% 11% • 5%
3	C	809	17% 77% 13% • 9%

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	703	5795	3681	981	1095	38	0	7	0

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

Continued on next page...

Continued from previous page...

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

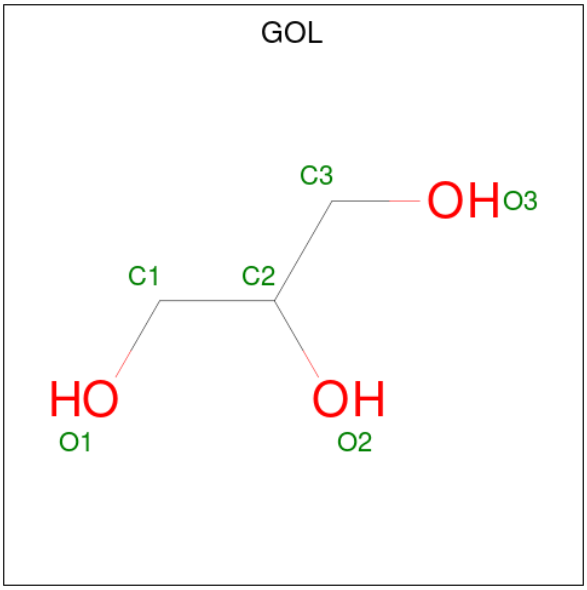
- Molecule 4 is a RNA chain called 3' end of the vRNA promoter.

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.

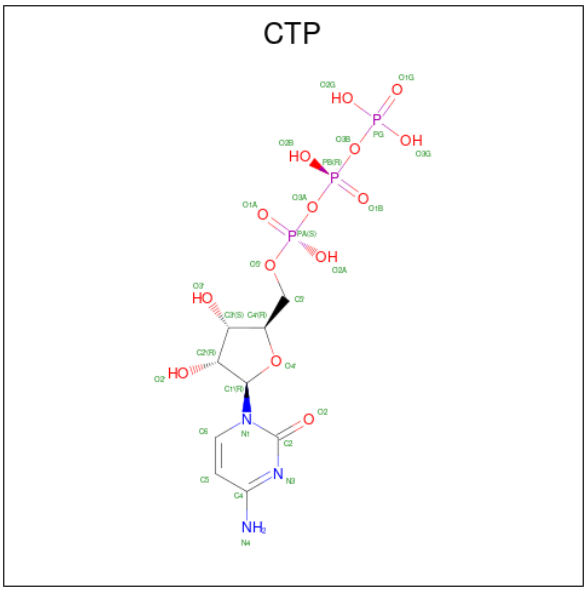
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	V	16	Total	C	N	O	P	0	0	0
			334	147	67	104	16			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



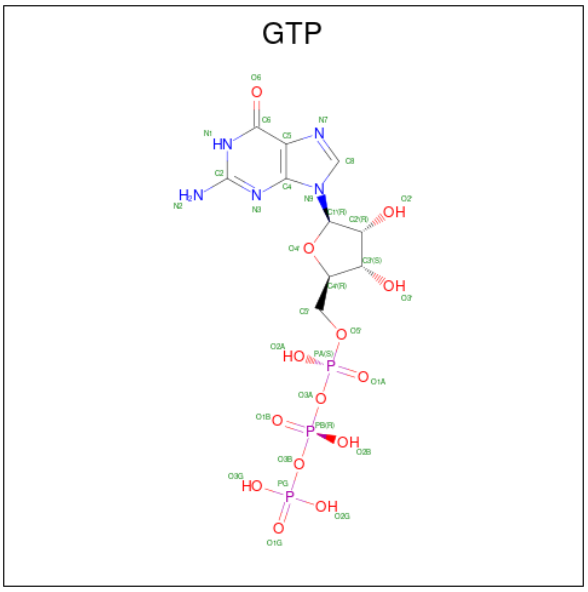
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

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



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

- Molecule 8 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

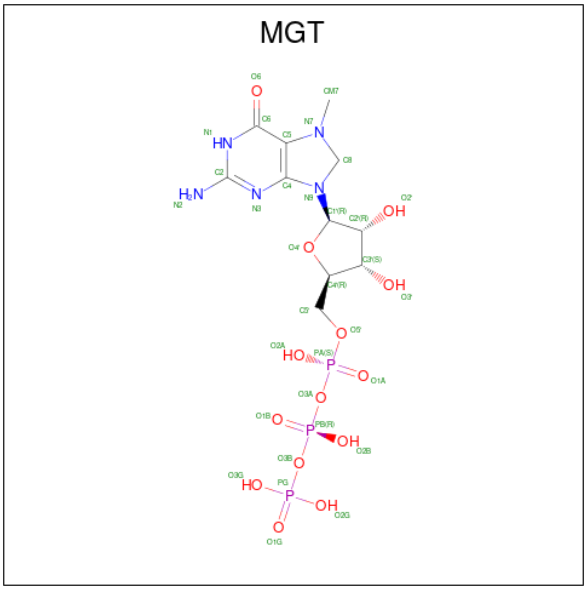


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

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

- Molecule 10 is 7N-METHYL-8-HYDROGUANOSINE-5'-TRIPHOSPHATE (three-letter code: 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 33 11 5 14 3	0	0

- Molecule 11 is water.

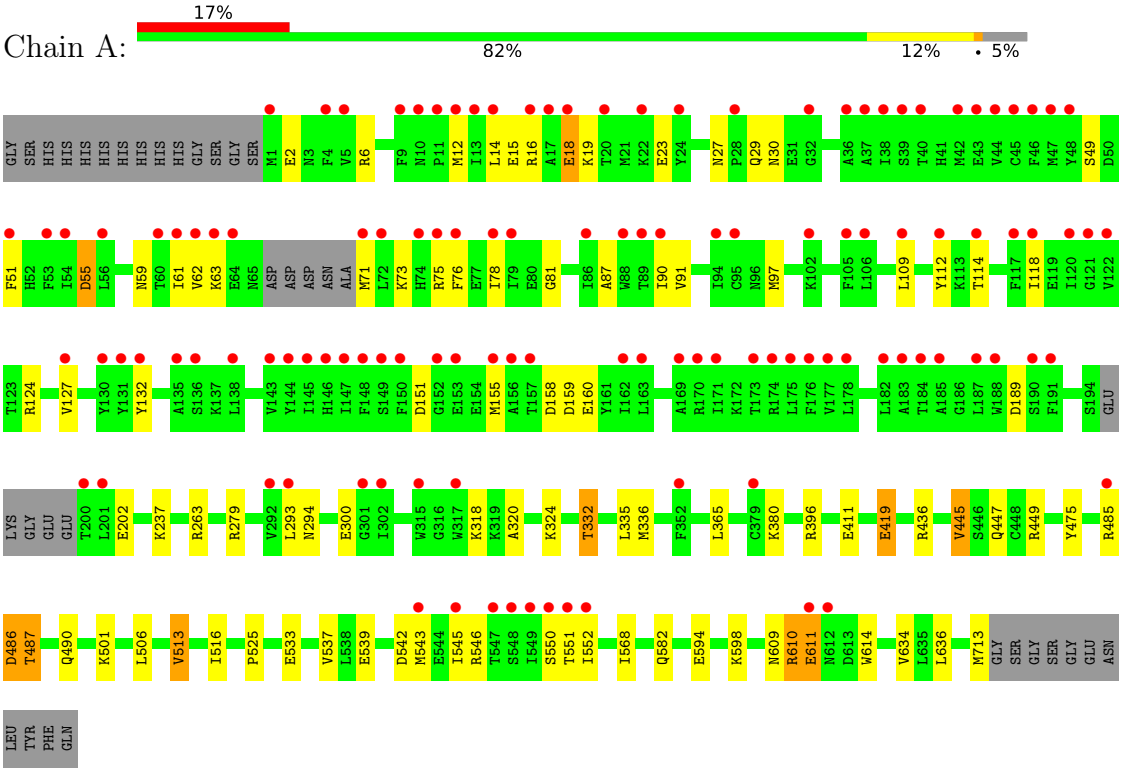
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	220	Total O 220 220	0	0
11	B	288	Total O 288 288	0	0
11	C	137	Total O 137 137	0	0
11	R	16	Total O 16 16	0	0
11	V	39	Total O 39 39	0	0

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.

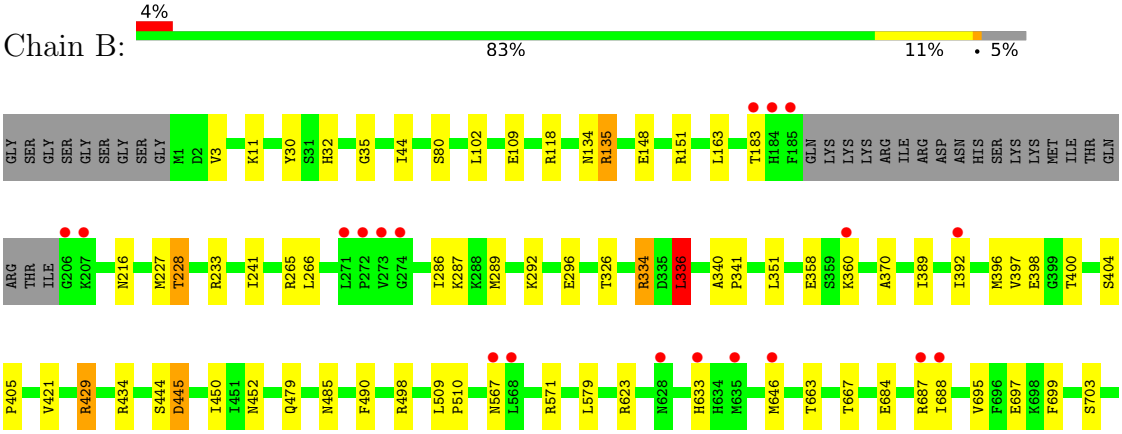
• Molecule 1: Polymerase acidic protein

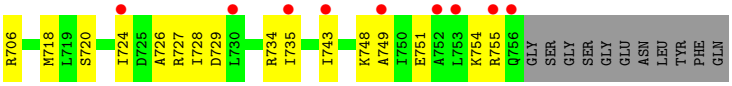
Chain A:



• Molecule 2: RNA-directed RNA polymerase catalytic subunit

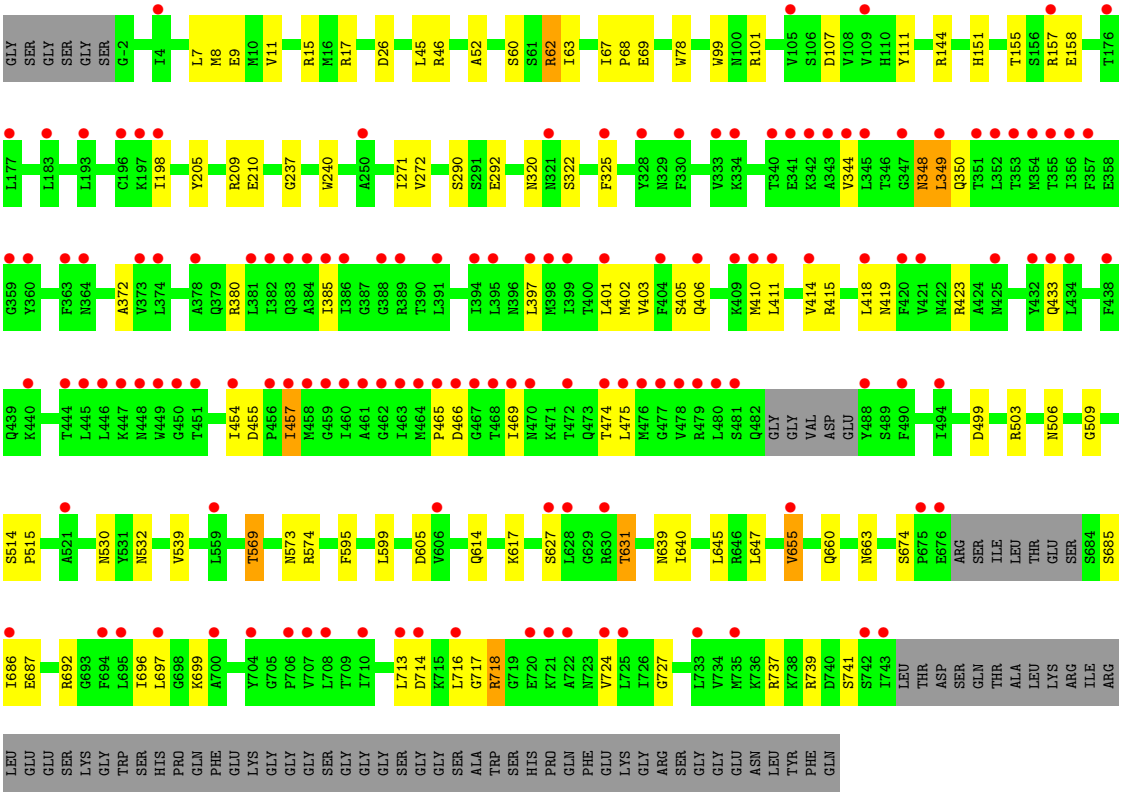
Chain B:





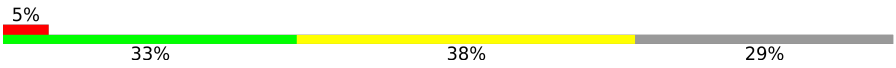
• Molecule 3: Polymerase basic protein 2

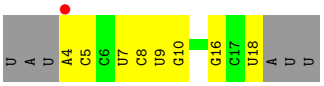
Chain C:



• Molecule 4: 3' end of the vRNA promoter

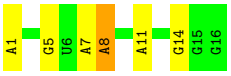
Chain R:





• Molecule 5: 5' end of the vRNA promoter

Chain V:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.34 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.189 , 0.232 0.197 , 0.237	Depositor DCC
R_{free} test set	7590 reflections (5.01%)	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)	0.37 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, CTP, MG, 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	0.38	0/5917	0.75	3/7966 (0.0%)
2	B	0.39	0/6048	0.76	3/8167 (0.0%)
3	C	0.36	0/5927	0.74	2/8000 (0.0%)
4	R	0.54	0/337	1.25	2/521 (0.4%)
5	V	0.77	1/375 (0.3%)	1.28	2/583 (0.3%)
All	All	0.39	1/18604 (0.0%)	0.78	12/25237 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	1	A	OP3-P	-8.35	1.51	1.61

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	V	8	A	O5'-P-OP1	-12.93	94.06	105.70
1	A	336	MET	CG-SD-CE	7.01	111.42	100.20
2	B	233	ARG	NE-CZ-NH2	-6.75	116.93	120.30
4	R	9	U	O5'-P-OP2	-6.17	100.15	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	336	LEU	CB-CG-CD1	5.67	120.64	111.00
4	R	18	U	C4'-C3'-O3'	5.50	124.00	113.00
1	A	543	MET	CG-SD-CE	5.23	108.58	100.20
2	B	623	ARG	NE-CZ-NH1	5.17	122.88	120.30
5	V	14	G	C4'-C3'-C2'	-5.14	97.46	102.60
3	C	423	ARG	CB-CA-C	-5.09	100.21	110.40
3	C	574	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	332	THR	CA-CB-OG1	-5.08	98.33	109.00

There are no chirality outliers.

All (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
3	C	144	ARG	Sidechain
3	C	46	ARG	Sidechain
3	C	62	ARG	Sidechain

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	5795	0	5702	51	0
2	B	5931	0	5913	60	0
3	C	5828	0	5929	52	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	155	0

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

All (155) 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
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
2:B:148:GLU:HG3	11:B:904:HOH:O	1.86	0.74
3:C:414:VAL:O	3:C:415:ARG:NH1	2.26	0.69
3:C:271:ILE:HD11	3:C:515:PRO:HB2	1.74	0.69
2:B:228:THR:HG23	11:B:950:HOH:O	1.92	0.68
2:B:216:ASN:ND2	2:B:398:GLU:OE1	2.26	0.68
2:B:216:ASN:HB3	11:B:1164:HOH:O	1.94	0.67
1:A:411:GLU:HB2	1:A:449[B]:ARG:HH12	1.60	0.66
3:C:499:ASP:OD2	3:C:503:ARG:NH1	2.31	0.64
1:A:27:ASN:HB3	1:A:30:ASN:HB2	1.81	0.63
1:A:75:ARG:HD3	1:A:76:PHE:CE1	2.35	0.62
2:B:684:GLU:OE1	2:B:687:ARG:NH1	2.32	0.62
1:A:610:ARG:HH11	1:A:610:ARG:HB3	1.64	0.61
3:C:237:GLY:HA3	3:C:240:TRP:CE2	2.36	0.61
1:A:614:TRP:CD1	2:B:11:LYS:HD3	2.35	0.60
2:B:687:ARG:HD2	11:B:1152:HOH:O	2.00	0.60
3:C:402:MET:O	3:C:405:SER:OG	2.16	0.60
3:C:595:PHE:CE2	3:C:599:LEU:HD11	2.36	0.59
2:B:479:GLN:HG2	11:B:1039:HOH:O	2.03	0.59
2:B:571:ARG:NH1	3:C:52:ALA:O	2.32	0.58
3:C:713:LEU:O	3:C:716:LEU:HG	2.05	0.57
1:A:365:LEU:CD2	1:A:516:ILE:HD12	2.34	0.57
1:A:293:LEU:O	1:A:294:ASN:C	2.42	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:LYS:O	2:B:429:ARG:NH1	2.39	0.56
2:B:351:LEU:HD21	2:B:392[A]:ILE:HD11	1.87	0.56
2:B:109:GLU:OE2	2:B:265:ARG:NH2	2.37	0.56
2:B:699:PHE:CE2	2:B:718:MET:HE2	2.42	0.55
3:C:530:ASN:OD1	3:C:532[A]:ASN:ND2	2.39	0.55
2:B:35:GLY:HA3	2:B:228:THR:HG22	1.88	0.55
1:A:449[B]:ARG:HB2	1:A:449[B]:ARG:NH1	2.20	0.55
2:B:444[A]:SER:OG	2:B:445:ASP:N	2.39	0.54
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.89	0.53
1:A:2:GLU:OE2	1:A:6:ARG:NH2	2.37	0.53
3:C:717:GLY:O	3:C:718:ARG:C	2.46	0.53
2:B:228:THR:CG2	11:B:950:HOH:O	2.54	0.53
2:B:151:ARG:NE	11:B:904:HOH:O	2.36	0.52
1:A:447:GLN:OE1	1:A:487:THR:HG23	2.10	0.52
1:A:419:GLU:HG3	1:A:485:ARG:NH2	2.25	0.52
3:C:205:TYR:O	3:C:209:ARG:HG2	2.11	0.51
3:C:155:THR:OG1	3:C:158:GLU:OE1	2.26	0.51
2:B:336:LEU:HD12	2:B:336:LEU:O	2.10	0.51
1:A:71:MET:C	1:A:71:MET:SD	2.90	0.50
2:B:286:ILE:HD11	2:B:490:PHE:CE2	2.47	0.50
4:R:4:A:H3'	4:R:5:C:C6	2.47	0.50
1:A:2:GLU:HG3	1:A:29:GLN:HG3	1.94	0.50
3:C:474:THR:HG23	3:C:475:LEU:O	2.12	0.50
1:A:55:ASP:OD1	1:A:59:ASN:N	2.46	0.49
3:C:151:HIS:HA	3:C:210:GLU:O	2.11	0.49
3:C:344:VAL:HG13	3:C:411:LEU:HD13	1.95	0.49
4:R:10:G:N3	4:R:10:G:H2'	2.28	0.49
2:B:296:GLU:HA	3:C:727:GLY:HA2	1.94	0.49
3:C:663:ASN:O	3:C:674:SER:HB3	2.12	0.48
2:B:241:ILE:HD12	4:R:16:G:C8	2.49	0.48
2:B:720:SER:O	2:B:724:ILE:HD13	2.14	0.48
1:A:365:LEU:HG	1:A:516:ILE:HD11	1.94	0.47
2:B:684:GLU:O	2:B:688:ILE:HG12	2.13	0.47
2:B:434:ARG:HG2	2:B:434:ARG:HH11	1.79	0.47
1:A:16:ARG:HH11	1:A:81:GLY:HA3	1.79	0.47
1:A:486:ASP:OD2	1:A:490:GLN:HB2	2.14	0.47
3:C:631:THR:O	3:C:692:ARG:NH2	2.47	0.47
1:A:12:MET:CE	2:B:755:ARG:HH12	2.27	0.47
1:A:318:LYS:NZ	1:A:542:ASP:OD2	2.39	0.47
2:B:695:VAL:HG13	2:B:718:MET:HE1	1.95	0.47
4:R:4:A:H2'	4:R:5:C:O4'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:111:TYR:CD1	3:C:198:ILE:HD11	2.50	0.47
3:C:645:LEU:HD13	3:C:655:VAL:CG2	2.45	0.47
2:B:134:ASN:O	2:B:135:ARG:HD2	2.14	0.47
2:B:754:LYS:O	2:B:754:LYS:HG2	2.14	0.47
2:B:336:LEU:HD12	2:B:336:LEU:C	2.35	0.46
2:B:396:MET:HA	2:B:400:THR:O	2.15	0.46
2:B:289:MET:HG2	2:B:450:ILE:HG21	1.98	0.46
1:A:90:ILE:HG12	2:B:724:ILE:HG12	1.96	0.46
3:C:320:ASN:O	3:C:322:SER:N	2.48	0.46
3:C:7:LEU:O	3:C:11:VAL:HG23	2.15	0.46
3:C:372:ALA:HA	3:C:385:ILE:O	2.16	0.46
1:A:87:ALA:O	1:A:91:VAL:HG23	2.14	0.46
3:C:419:ASN:O	3:C:433:GLN:OE1	2.34	0.46
1:A:15:GLU:HG2	1:A:19:LYS:HE2	1.97	0.46
3:C:457:ILE:O	3:C:457:ILE:HG22	2.15	0.46
1:A:582:GLN:HB2	2:B:509:LEU:HD11	1.98	0.46
1:A:609:ASN:O	1:A:611:GLU:N	2.49	0.45
2:B:351:LEU:HB2	2:B:370:ALA:HB1	1.99	0.45
2:B:754:LYS:O	2:B:754:LYS:CG	2.64	0.45
3:C:687:GLU:HB2	3:C:696:ILE:HB	1.98	0.45
1:A:158:ASP:O	1:A:160:GLU:HG3	2.16	0.45
2:B:728:ILE:HG22	2:B:734:ARG:HH12	1.82	0.45
2:B:135:ARG:HH11	2:B:135:ARG:HG2	1.82	0.45
2:B:697:GLU:HG2	2:B:703:SER:OG	2.17	0.45
2:B:749:ALA:HB3	3:C:8:MET:CE	2.47	0.44
3:C:737:ARG:HH22	3:C:739:ARG:NH1	2.15	0.44
1:A:320:ALA:HB3	1:A:335:LEU:HD11	1.99	0.44
1:A:109:LEU:HB2	1:A:118:ILE:HB	2.00	0.44
1:A:263:ARG:HG3	1:A:713:MET:HE3	1.98	0.44
3:C:639:ASN:C	3:C:640:ILE:HD12	2.38	0.44
3:C:686:ILE:HA	3:C:696:ILE:O	2.18	0.44
2:B:397:VAL:HG23	11:B:1106:HOH:O	2.17	0.43
3:C:69:GLU:HB2	3:C:78:TRP:CZ2	2.53	0.43
3:C:569:THR:O	3:C:573:ASN:ND2	2.51	0.43
3:C:617:LYS:HD3	3:C:647:LEU:HD21	2.00	0.43
1:A:445:VAL:HG22	1:A:636:LEU:HD22	1.99	0.43
2:B:35:GLY:CA	2:B:228:THR:HG22	2.48	0.43
3:C:539:VAL:HG23	11:C:1095:HOH:O	2.18	0.43
1:A:78:ILE:HA	1:A:109:LEU:HD23	2.00	0.43
1:A:51:PHE:HB3	1:A:63:LYS:O	2.18	0.43
1:A:411:GLU:CB	1:A:449[B]:ARG:HH12	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:VAL:O	3:C:17:ARG:NH1	2.52	0.43
3:C:67:ILE:HB	3:C:68:PRO:HD2	1.99	0.43
3:C:414:VAL:HG11	3:C:418:LEU:HD23	2.00	0.43
3:C:617:LYS:CD	3:C:647:LEU:HD21	2.49	0.43
1:A:127:VAL:HG12	1:A:127:VAL:O	2.19	0.43
3:C:685:SER:HB2	3:C:697:LEU:O	2.18	0.43
1:A:14:LEU:O	1:A:18:GLU:HB2	2.18	0.42
2:B:509:LEU:N	2:B:510:PRO:CD	2.82	0.42
1:A:551:THR:O	1:A:552:ILE:HG23	2.19	0.42
2:B:266:LEU:HD13	2:B:421:VAL:HG11	2.02	0.42
2:B:102:LEU:HD13	2:B:265:ARG:HD3	2.01	0.42
3:C:350:GLN:NE2	3:C:418:LEU:O	2.50	0.42
1:A:634:VAL:HG22	2:B:3:VAL:HG11	2.00	0.42
3:C:403:VAL:HG13	3:C:410:MET:HE3	2.00	0.42
1:A:594:GLU:OE2	1:A:598:LYS:HE2	2.19	0.42
2:B:579:LEU:HD13	3:C:101:ARG:HB3	2.01	0.42
4:R:7:U:H2'	4:R:8:C:C6	2.54	0.42
1:A:112:TYR:CG	2:B:727:ARG:NH2	2.88	0.42
1:A:475:TYR:HA	1:A:501:LYS:O	2.20	0.42
3:C:506:ASN:OD1	3:C:509:GLY:N	2.51	0.42
1:A:546:ARG:HA	1:A:551:THR:HA	2.01	0.41
3:C:60:SER:O	3:C:63:ILE:HG22	2.19	0.41
3:C:605:ASP:OD2	3:C:741:SER:OG	2.32	0.41
1:A:320:ALA:HA	1:A:539:GLU:O	2.19	0.41
1:A:545:ILE:O	1:A:552:ILE:N	2.44	0.41
1:A:19:LYS:O	1:A:23:GLU:N	2.47	0.41
2:B:729:ASP:C	2:B:735:ILE:HG22	2.40	0.41
1:A:61:ILE:HG22	1:A:62:VAL:N	2.35	0.41
3:C:405:SER:O	3:C:406:GLN:HB2	2.21	0.41
2:B:726:ALA:HB2	2:B:743:ILE:HG21	2.03	0.41
3:C:397:LEU:O	3:C:401:LEU:HG	2.21	0.41
3:C:614:GLN:HA	3:C:614:GLN:OE1	2.20	0.41
1:A:568:ILE:HG12	2:B:30:TYR:CE1	2.55	0.41
2:B:44:ILE:HG13	2:B:392[B]:ILE:HD11	2.03	0.41
2:B:389:ILE:HA	2:B:392[A]:ILE:HG22	2.03	0.41
2:B:389:ILE:O	2:B:392[A]:ILE:HG22	2.21	0.41
2:B:633:HIS:HB3	2:B:667:THR:HG21	2.03	0.41
2:B:663:THR:HG21	3:C:99:TRP:CD1	2.56	0.41
3:C:348:ASN:O	3:C:349:LEU:HB2	2.21	0.41
3:C:713:LEU:HD21	3:C:724:VAL:HG22	2.03	0.41
2:B:404:SER:N	2:B:405:PRO:CD	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:PRO:HG3	1:A:537:VAL:HG21	2.03	0.40
2:B:326:THR:O	2:B:334:ARG:HD3	2.22	0.40
2:B:748:LYS:O	2:B:751:GLU:HB2	2.20	0.40
1:A:49:SER:HB2	1:A:76:PHE:HB2	2.02	0.40
3:C:45:LEU:HD23	3:C:45:LEU:C	2.42	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	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%)	25	17
All	All	2175/2323 (94%)	2080 (96%)	88 (4%)	7 (0%)	37	29

All (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
3	C	457	ILE
3	C	465	PRO

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%)	614 (96%)	22 (4%)	31	24
2	B	653/676 (97%)	636 (97%)	17 (3%)	41	36
3	C	647/706 (92%)	623 (96%)	24 (4%)	29	22
All	All	1936/2039 (95%)	1873 (97%)	63 (3%)	33	26

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	55	ASP
1	A	73	LYS
1	A	97	MET
1	A	114	THR
1	A	124	ARG
1	A	132	TYR
1	A	151	ASP
1	A	189	ASP
1	A	202	GLU
1	A	237	LYS
1	A	300	GLU
1	A	324	LYS
1	A	332	THR
1	A	380	LYS
1	A	419	GLU
1	A	445	VAL
1	A	486	ASP
1	A	487	THR
1	A	513	VAL
1	A	610	ARG
1	A	611	GLU
2	B	32	HIS
2	B	80	SER
2	B	118	ARG
2	B	135	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	163	LEU
2	B	183	THR
2	B	227	MET
2	B	228	THR
2	B	336	LEU
2	B	358	GLU
2	B	360	LYS
2	B	445	ASP
2	B	452	ASN
2	B	485	ASN
2	B	567	ASN
2	B	646	MET
2	B	706	ARG
3	C	9	GLU
3	C	15	ARG
3	C	26	ASP
3	C	62	ARG
3	C	107	ASP
3	C	157	ARG
3	C	272	VAL
3	C	290	SER
3	C	292	GLU
3	C	325	PHE
3	C	348	ASN
3	C	380	ARG
3	C	454	ILE
3	C	455	ASP
3	C	466	ASP
3	C	469	ILE
3	C	514	SER
3	C	569	THR
3	C	627	SER
3	C	631	THR
3	C	655	VAL
3	C	660	GLN
3	C	699	LYS
3	C	714	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	96	ASN
1	A	582	GLN
3	C	497	ASN
3	C	573	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	14/21 (66%)	0	0
5	V	14/16 (87%)	3 (21%)	1 (7%)
All	All	28/37 (75%)	3 (10%)	1 (3%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
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	803	-	5,5,5	0.25	0	5,5,5	0.56	0
6	GOL	C	901	-	5,5,5	0.17	0	5,5,5	0.52	0
6	GOL	A	801	-	5,5,5	0.11	0	5,5,5	0.35	0
8	GTP	B	805	9	26,34,34	0.96	1 (3%)	32,54,54	1.01	2 (6%)
10	MGT	C	902	-	30,35,35	0.96	1 (3%)	42,56,56	0.88	2 (4%)
6	GOL	B	801	-	5,5,5	0.13	0	5,5,5	0.43	0
7	CTP	B	804	9	26,30,30	0.61	0	39,47,47	0.61	0
6	GOL	B	802	-	5,5,5	0.15	0	5,5,5	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
6	GOL	B	803	-	-	3/4/4/4	-
6	GOL	C	901	-	-	2/4/4/4	-
6	GOL	A	801	-	-	2/4/4/4	-
8	GTP	B	805	9	-	7/18/38/38	0/3/3/3
10	MGT	C	902	-	-	9/22/50/50	0/3/3/3
6	GOL	B	801	-	-	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	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	902	MGT	C5-N7	3.88	1.40	1.35
8	B	805	GTP	C5-C6	-2.32	1.42	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	805	GTP	O2G-PG-O3B	2.29	112.31	104.64
10	C	902	MGT	PB-O3B-PG	-2.12	125.55	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	805	GTP	O6-C6-C5	2.10	128.47	124.37
10	C	902	MGT	C4-C5-N7	2.03	108.34	105.53

There are no chirality outliers.

All (27) 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
10	C	902	MGT	PB-O3B-PG-O3G
10	C	902	MGT	O4'-C4'-C5'-O5'
10	C	902	MGT	C3'-C4'-C5'-O5'
6	C	901	GOL	O1-C1-C2-C3
6	A	801	GOL	O1-C1-C2-O2
6	B	803	GOL	O1-C1-C2-O2
6	C	901	GOL	O1-C1-C2-O2
10	C	902	MGT	C4'-C5'-O5'-PA
8	B	805	GTP	PB-O3B-PG-O3G
10	C	902	MGT	PB-O3B-PG-O2G
6	B	801	GOL	O1-C1-C2-O2
6	B	803	GOL	O2-C2-C3-O3
10	C	902	MGT	C5'-O5'-PA-O3A
10	C	902	MGT	PB-O3A-PA-O2A
8	B	805	GTP	PG-O3B-PB-O1B
8	B	805	GTP	O4'-C4'-C5'-O5'
10	C	902	MGT	PB-O3B-PG-O1G
7	B	804	CTP	PB-O3B-PG-O2G
8	B	805	GTP	PB-O3B-PG-O2G
7	B	804	CTP	PA-O3A-PB-O2B
10	C	902	MGT	PB-O3A-PA-O1A
8	B	805	GTP	C3'-C4'-C5'-O5'

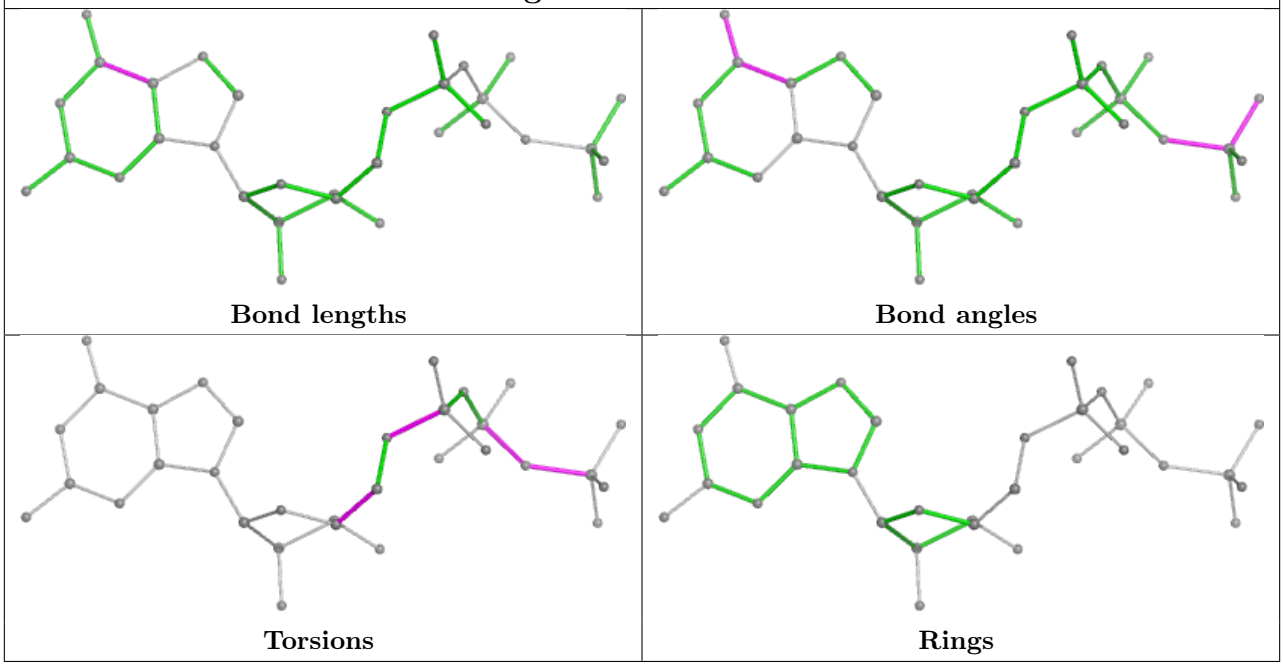
There are no ring outliers.

No monomer is involved in short contacts.

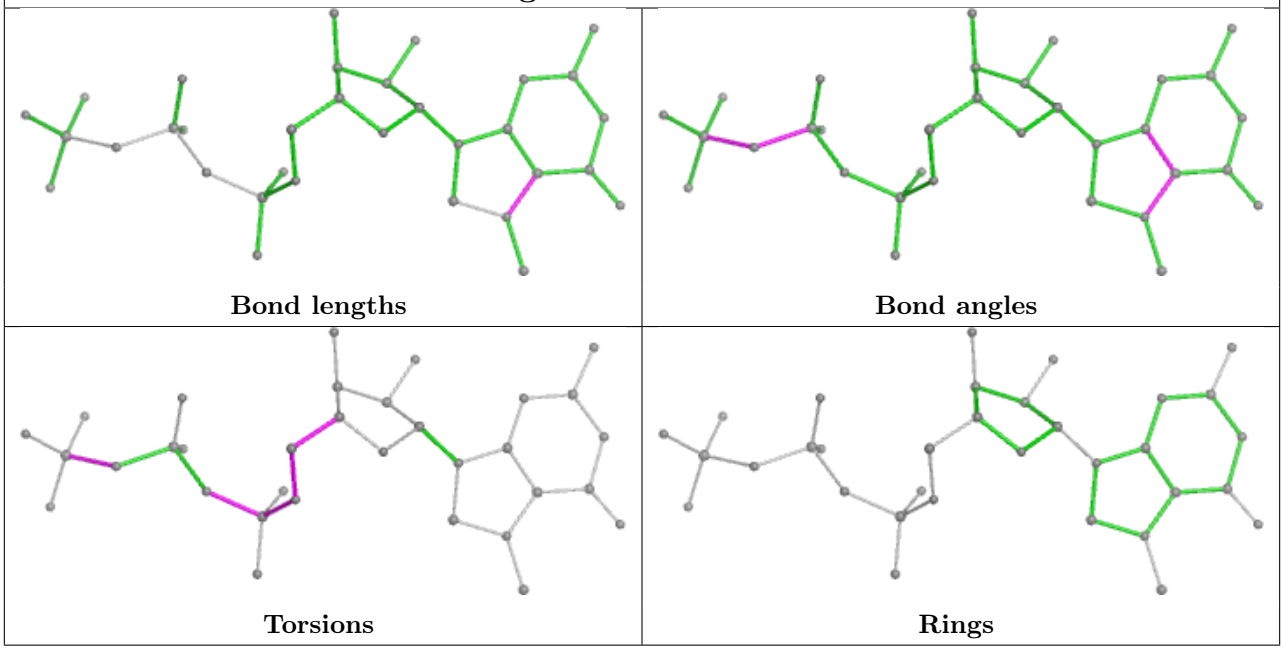
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

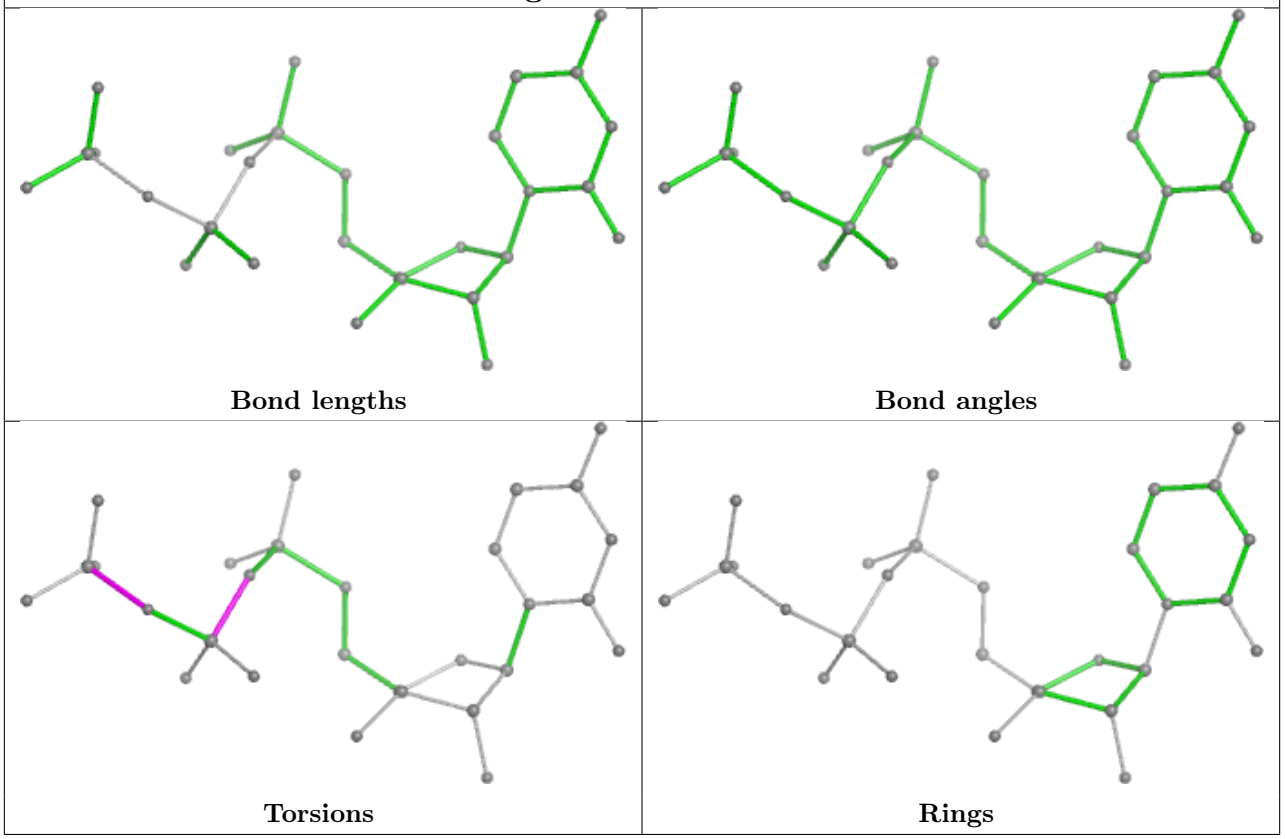
Ligand GTP B 805



Ligand MGT C 902



Ligand CTP B 804



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	703/738 (95%)	0.68	122 (17%) 5 4	13, 43, 129, 162	7 (0%)
2	B	736/776 (94%)	-0.01	28 (3%) 44 46	14, 34, 71, 130	9 (1%)
3	C	734/809 (90%)	0.95	137 (18%) 4 4	16, 51, 110, 132	2 (0%)
4	R	15/21 (71%)	-0.16	1 (6%) 25 26	34, 43, 83, 98	0
5	V	16/16 (100%)	-0.60	0 100 100	27, 32, 73, 104	0
All	All	2204/2360 (93%)	0.53	288 (13%) 8 8	13, 42, 114, 162	18 (0%)

All (288) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	463	ILE	7.4
3	C	480	LEU	7.3
1	A	549	ILE	6.6
3	C	462	GLY	6.0
3	C	461	ALA	6.0
3	C	469	ILE	5.6
3	C	478	VAL	5.6
1	A	171	ILE	5.5
1	A	315	TRP	5.4
3	C	445	LEU	5.1
1	A	62	VAL	5.0
3	C	460	ILE	4.8
3	C	722	ALA	4.8
3	C	352	LEU	4.7
3	C	411	LEU	4.7
1	A	138	LEU	4.6
1	A	51	PHE	4.5
1	A	48	TYR	4.5
1	A	152	GLY	4.5
3	C	628	LEU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	185	PHE	4.5
1	A	14	LEU	4.4
1	A	13	ILE	4.4
3	C	391	LEU	4.3
1	A	176	PHE	4.3
3	C	454	ILE	4.3
1	A	56	LEU	4.2
3	C	449	TRP	4.2
2	B	735	ILE	4.2
1	A	46	PHE	4.1
3	C	432	TYR	4.1
1	A	121	GLY	4.1
3	C	477	GLY	4.0
3	C	374	LEU	4.0
2	B	272	PRO	4.0
3	C	360	TYR	4.0
1	A	117	PHE	4.0
3	C	488	TYR	3.9
1	A	45	CYS	3.9
1	A	175	LEU	3.9
3	C	743	ILE	3.9
1	A	72	LEU	3.8
1	A	552	ILE	3.8
3	C	349	LEU	3.8
2	B	183	THR	3.8
3	C	446	LEU	3.8
1	A	38	ILE	3.8
1	A	191	PHE	3.8
3	C	733	LEU	3.8
1	A	118	ILE	3.8
1	A	122	VAL	3.7
1	A	143	VAL	3.7
1	A	94	ILE	3.7
3	C	177	LEU	3.6
3	C	708	LEU	3.6
2	B	756	GLN	3.6
2	B	274	GLY	3.6
1	A	79	ILE	3.6
1	A	156	ALA	3.6
1	A	44	VAL	3.6
1	A	40	THR	3.6
3	C	356	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	11	PRO	3.6
3	C	450	GLY	3.6
1	A	182	LEU	3.5
3	C	345	LEU	3.5
3	C	351	THR	3.5
1	A	76	PHE	3.5
1	A	109	LEU	3.5
3	C	713	LEU	3.5
1	A	548	SER	3.5
3	C	470	ASN	3.5
1	A	4	PHE	3.4
3	C	468	THR	3.4
1	A	12	MET	3.4
1	A	163	LEU	3.4
3	C	475	LEU	3.4
1	A	144	TYR	3.4
1	A	148	PHE	3.4
3	C	490	PHE	3.4
1	A	187	LEU	3.4
3	C	721	LYS	3.4
1	A	150	PHE	3.4
3	C	420	PHE	3.4
2	B	206	GLY	3.4
3	C	381	LEU	3.4
3	C	675	PRO	3.4
3	C	457	ILE	3.4
2	B	724	ILE	3.3
3	C	459	GLY	3.3
2	B	730	LEU	3.3
3	C	378	ALA	3.3
3	C	464	MET	3.3
1	A	132	TYR	3.3
1	A	545	ILE	3.2
1	A	42	MET	3.2
3	C	458	MET	3.2
3	C	384	ALA	3.2
3	C	344	VAL	3.2
3	C	725	LEU	3.2
1	A	20	THR	3.2
3	C	695	LEU	3.1
1	A	1	MET	3.1
1	A	149	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	706	PRO	3.1
1	A	162	ILE	3.1
1	A	112	TYR	3.1
1	A	185	ALA	3.1
2	B	271	LEU	3.1
3	C	414	VAL	3.1
3	C	472	THR	3.1
3	C	196	CYS	3.0
1	A	612	ASN	3.0
1	A	71	MET	3.0
1	A	293	LEU	3.0
1	A	28	PRO	3.0
3	C	385	ILE	3.0
3	C	394	ILE	3.0
3	C	357	PHE	3.0
1	A	200	THR	3.0
3	C	418	LEU	3.0
3	C	676	GLU	3.0
3	C	559	LEU	3.0
3	C	333	VAL	3.0
1	A	201	LEU	2.9
2	B	273	VAL	2.9
3	C	707	VAL	2.9
3	C	342	LYS	2.9
1	A	120	ILE	2.9
3	C	399	ILE	2.9
1	A	155	MET	2.9
1	A	178	LEU	2.8
1	A	90	ILE	2.8
3	C	710	ILE	2.8
3	C	193	LEU	2.8
3	C	476	MET	2.8
1	A	130	TYR	2.8
3	C	465	PRO	2.8
1	A	5	VAL	2.8
3	C	451	THR	2.8
1	A	317	TRP	2.8
1	A	146	HIS	2.8
3	C	382	ILE	2.8
2	B	635	MET	2.8
3	C	398	MET	2.8
3	C	409	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	397	LEU	2.8
1	A	105	PHE	2.8
3	C	438	PHE	2.8
3	C	433	GLN	2.8
1	A	61	ILE	2.8
2	B	392[A]	ILE	2.8
1	A	190	SER	2.8
1	A	53	PHE	2.7
3	C	474	THR	2.7
3	C	386	ILE	2.7
3	C	686	ILE	2.7
1	A	147	ILE	2.7
1	A	9	PHE	2.7
3	C	334	LYS	2.7
3	C	421	VAL	2.7
1	A	89	THR	2.7
3	C	383	GLN	2.7
1	A	47	MET	2.7
1	A	157	THR	2.6
3	C	448	ASN	2.6
1	A	37	ALA	2.6
3	C	742	SER	2.6
3	C	494	ILE	2.6
3	C	630	ARG	2.6
1	A	10	ASN	2.6
1	A	188	TRP	2.6
2	B	207	LYS	2.6
3	C	735	MET	2.6
3	C	183	LEU	2.6
1	A	131	TYR	2.6
3	C	197	LYS	2.6
3	C	456	PRO	2.6
1	A	86	ILE	2.6
2	B	753	LEU	2.5
1	A	32	GLY	2.5
1	A	301	GLY	2.5
3	C	410	MET	2.5
3	C	466	ASP	2.5
1	A	127	VAL	2.5
3	C	105	VAL	2.5
3	C	328	TYR	2.5
3	C	481	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	60	THR	2.5
1	A	184	THR	2.5
2	B	633	HIS	2.5
4	R	4	A	2.5
2	B	752	ALA	2.5
3	C	404	PHE	2.5
1	A	24	TYR	2.5
3	C	627	SER	2.5
3	C	467	GLY	2.5
1	A	36	ALA	2.5
1	A	169	ALA	2.5
2	B	184	HIS	2.4
3	C	330	PHE	2.4
1	A	551	THR	2.4
3	C	198	ILE	2.4
3	C	157	ARG	2.4
1	A	292	VAL	2.4
3	C	109	VAL	2.4
3	C	373	VAL	2.4
3	C	340	THR	2.4
3	C	354	MET	2.3
1	A	611	GLU	2.3
3	C	694	PHE	2.3
3	C	389	ARG	2.3
3	C	444	THR	2.3
3	C	440	LYS	2.3
1	A	39	SER	2.3
1	A	16	ARG	2.3
2	B	687	ARG	2.3
3	C	353	THR	2.3
2	B	646	MET	2.3
3	C	4	ILE	2.3
1	A	75	ARG	2.3
1	A	174	ARG	2.3
3	C	325	PHE	2.3
3	C	720	GLU	2.3
1	A	550	SER	2.3
3	C	395	LEU	2.3
3	C	716	LEU	2.3
2	B	749	ALA	2.2
3	C	700	ALA	2.2
1	A	74	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	401	LEU	2.2
1	A	183	ALA	2.2
1	A	302	ILE	2.2
3	C	359	GLY	2.2
1	A	63	LYS	2.2
2	B	360	LYS	2.2
3	C	425	ASN	2.2
3	C	406	GLN	2.2
3	C	479	ARG	2.2
1	A	22	LYS	2.2
3	C	321	ASN	2.2
1	A	543	MET	2.2
1	A	43	GLU	2.2
3	C	606	VAL	2.2
3	C	347	GLY	2.2
3	C	363	PHE	2.2
1	A	106	LEU	2.2
1	A	78	ILE	2.2
3	C	355	THR	2.1
1	A	177	VAL	2.1
3	C	388	GLY	2.1
1	A	153	GLU	2.1
3	C	250	ALA	2.1
2	B	755	ARG	2.1
1	A	54	ILE	2.1
1	A	547	THR	2.1
3	C	176	THR	2.1
1	A	102	LYS	2.1
1	A	18	GLU	2.1
2	B	567	ASN	2.1
1	A	352	PHE	2.1
2	B	568	LEU	2.1
3	C	434	LEU	2.1
1	A	145	ILE	2.1
2	B	743	ILE	2.1
1	A	114	THR	2.1
3	C	447	LYS	2.1
1	A	17	ALA	2.1
1	A	135	ALA	2.1
3	C	714	ASP	2.1
1	A	136	SER	2.1
1	A	173	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	364	ASN	2.1
1	A	170	ARG	2.1
1	A	485	ARG	2.1
1	A	95	CYS	2.0
1	A	379	CYS	2.0
3	C	655	VAL	2.0
3	C	724	VAL	2.0
3	C	521	ALA	2.0
2	B	628	ASN	2.0
2	B	688	ILE	2.0
3	C	704	TYR	2.0
1	A	88	TRP	2.0
1	A	64	GLU	2.0
3	C	341	GLU	2.0
3	C	343	ALA	2.0
3	C	697	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	0.94	0.10	35,42,46,49	0

Continued on next page...

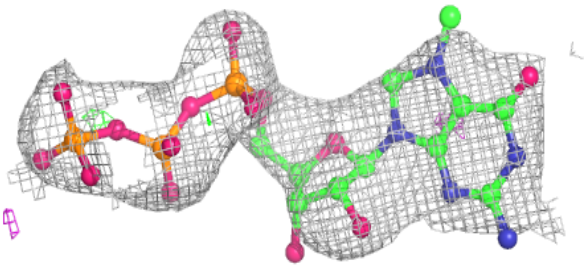
Continued from previous page...

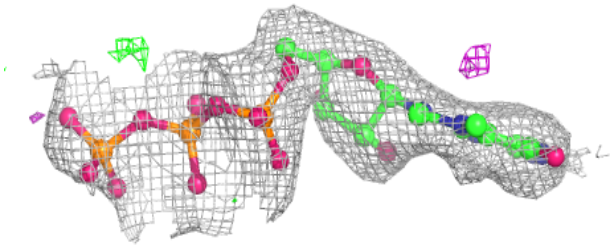
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MG	B	806	1/1	0.98	0.09	35,35,35,35	0
7	CTP	B	804	29/29	0.98	0.06	28,33,38,40	0
9	MG	B	807	1/1	0.99	0.02	24,24,24,24	0

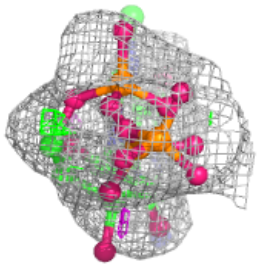
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGT C 902:

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

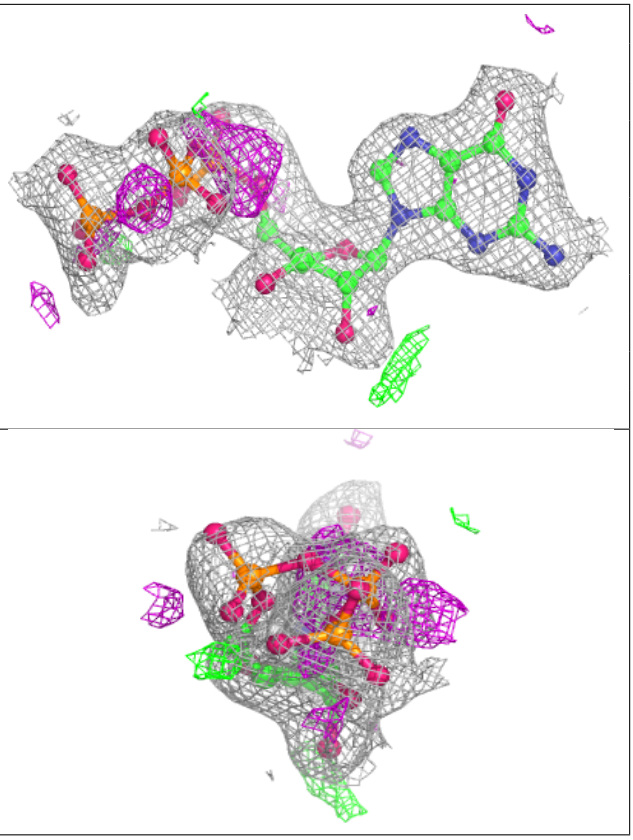


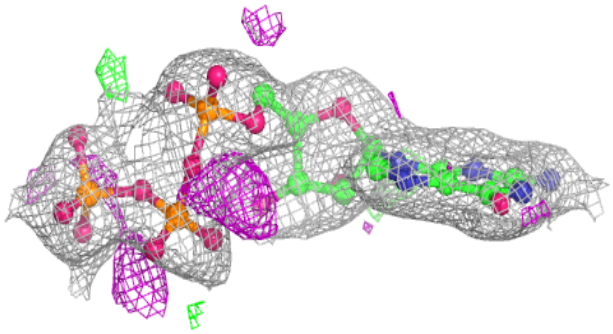




Electron density around GTP B 805:

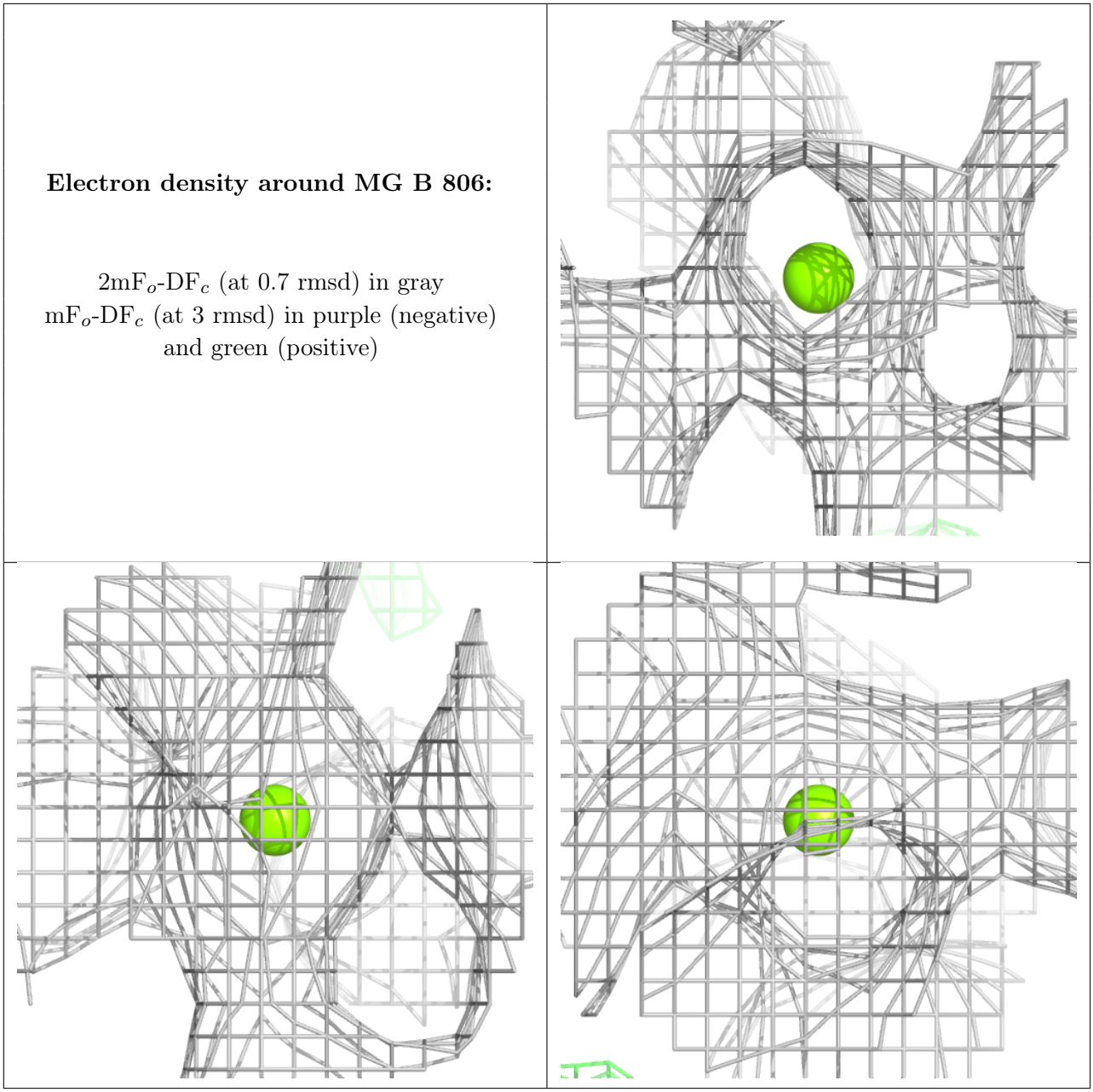
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





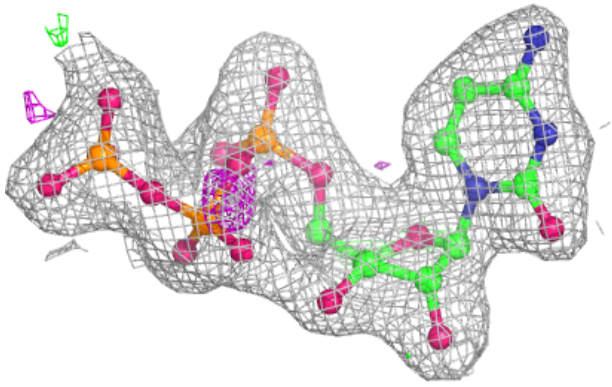
Electron density around MG B 806:

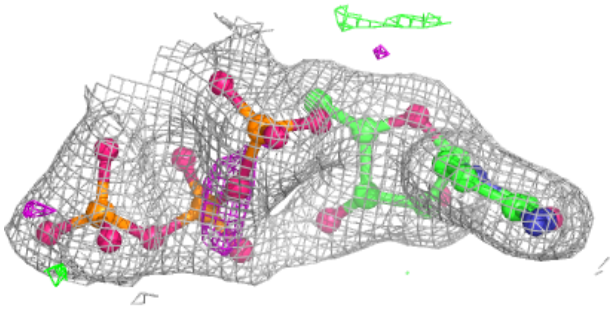
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

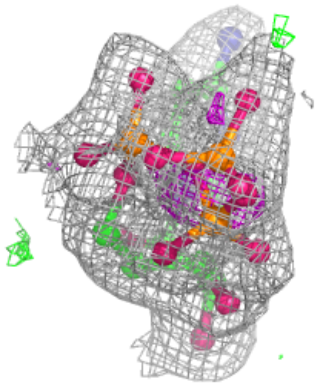


Electron density around CTP B 804:

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

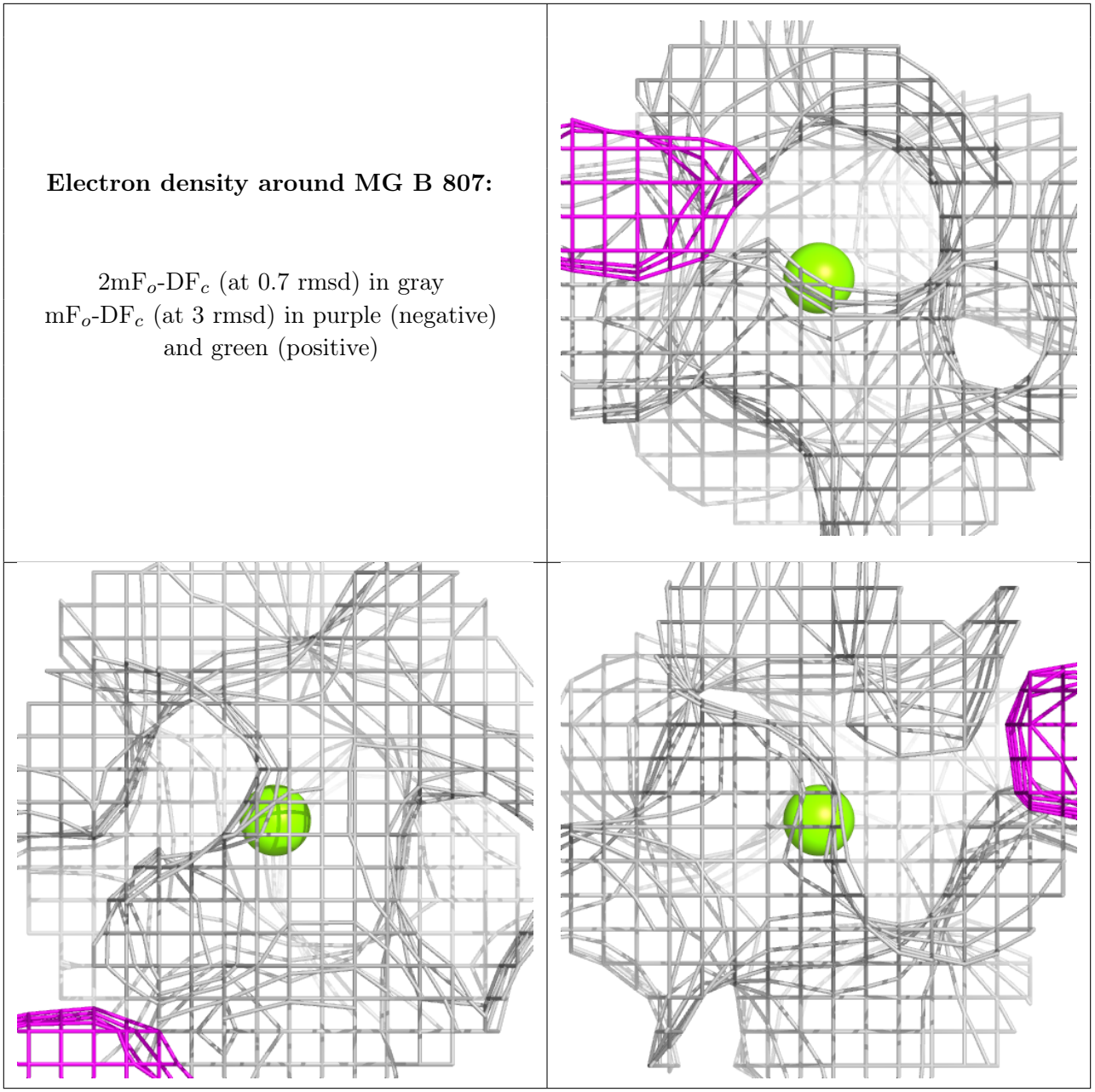






Electron density around MG B 807:

$2mF_o$-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 (i)

There are no such residues in this entry.