



wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 02:28 PM EDT

PDB ID : 3JB0
EMDB ID: : EMD-6374
Title : Atomic model of cytoplasmic polyhedrosis virus with GTP
Authors : Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on : 2015-07-06
Resolution : 2.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

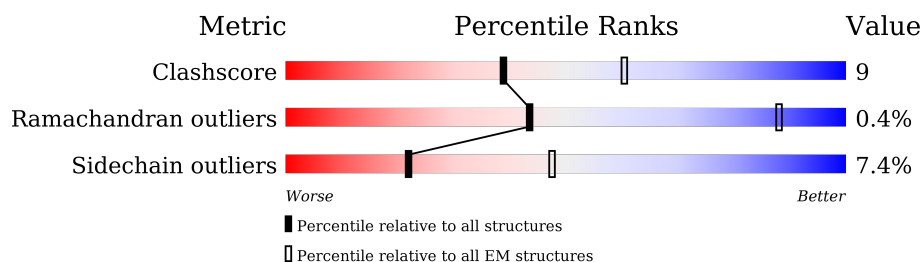
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY






The reported resolution of this entry is 2.90 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1058	
2	B	1333	
2	C	1333	
3	D	448	
3	E	448	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32276 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1057	Total	C	N	O	S	0	0
			8434	5345	1457	1587	45		

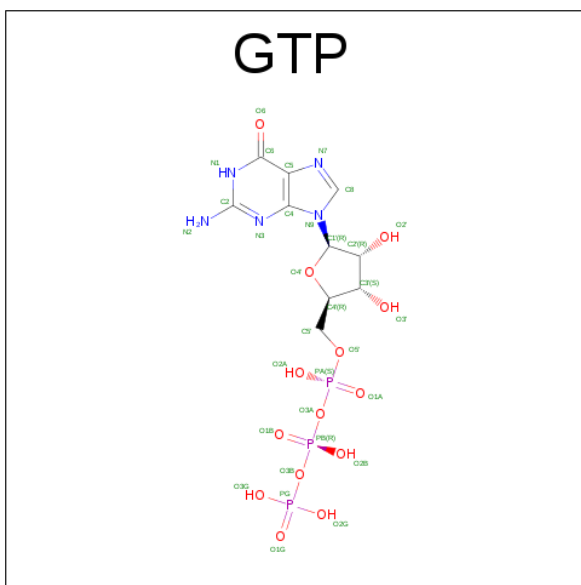
- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1191	Total	C	N	O	S	0	0
			9397	5937	1634	1789	37		
2	C	1250	Total	C	N	O	S	0	0
			9851	6219	1712	1882	38		

- Molecule 3 is a protein called Viral structural protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

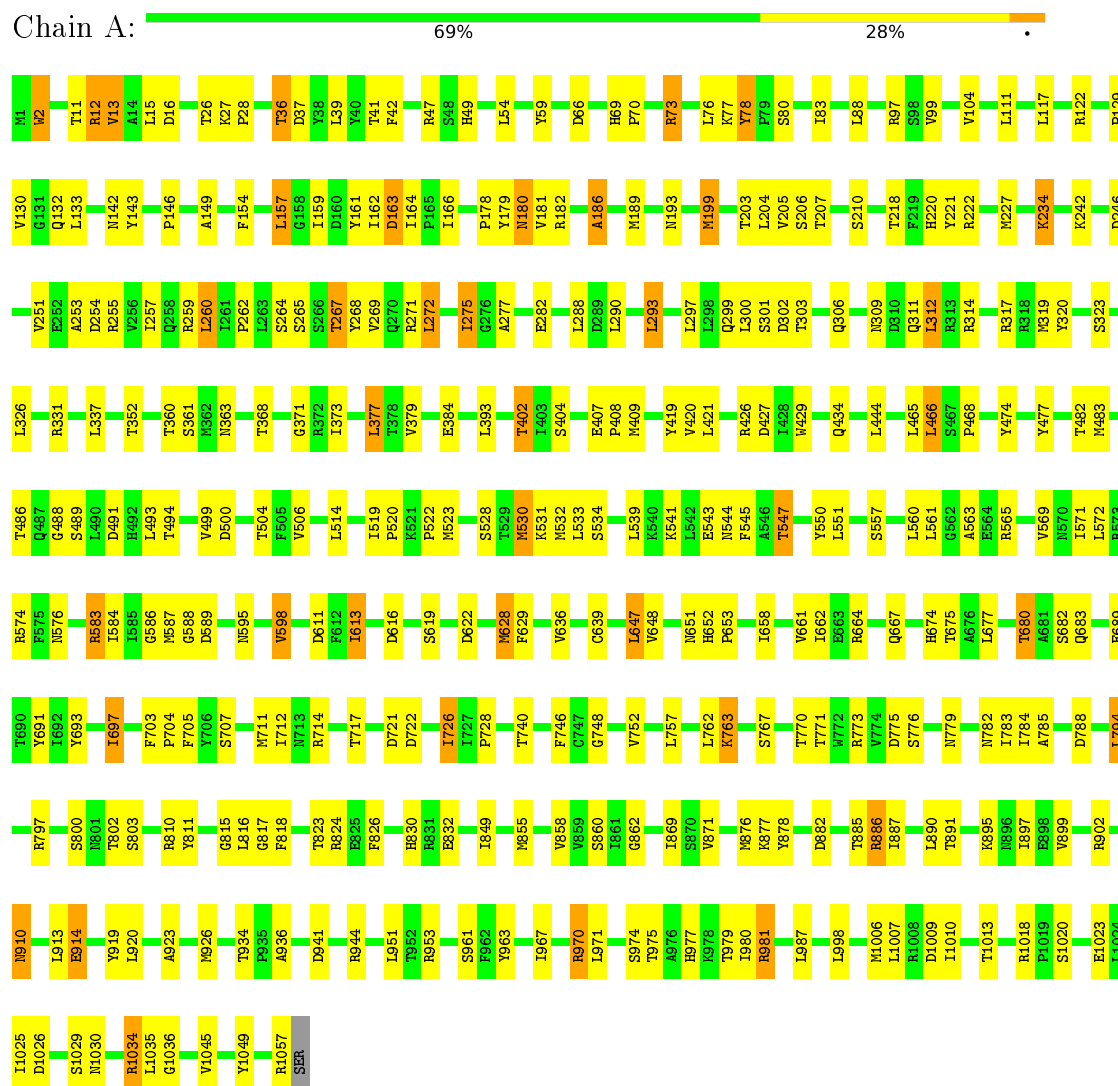


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

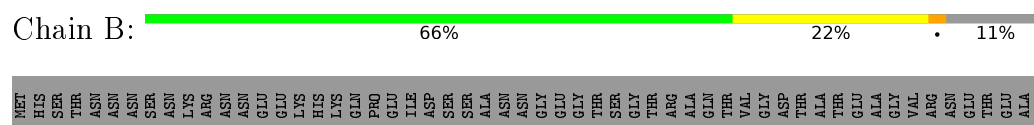
3 Residue-property plots

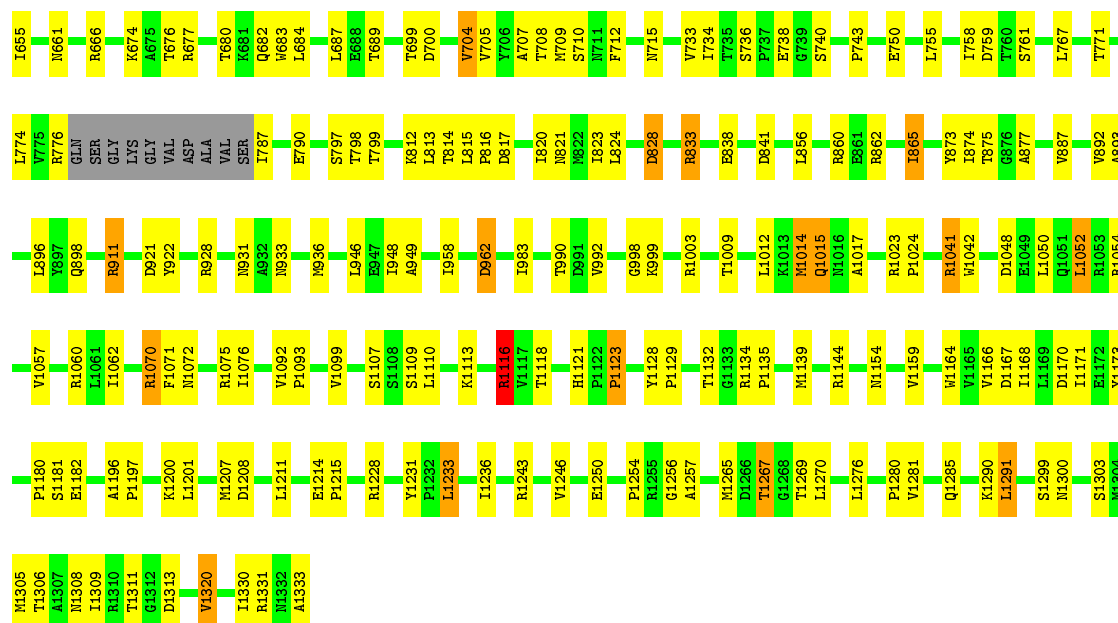
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. 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: Structural protein VP3

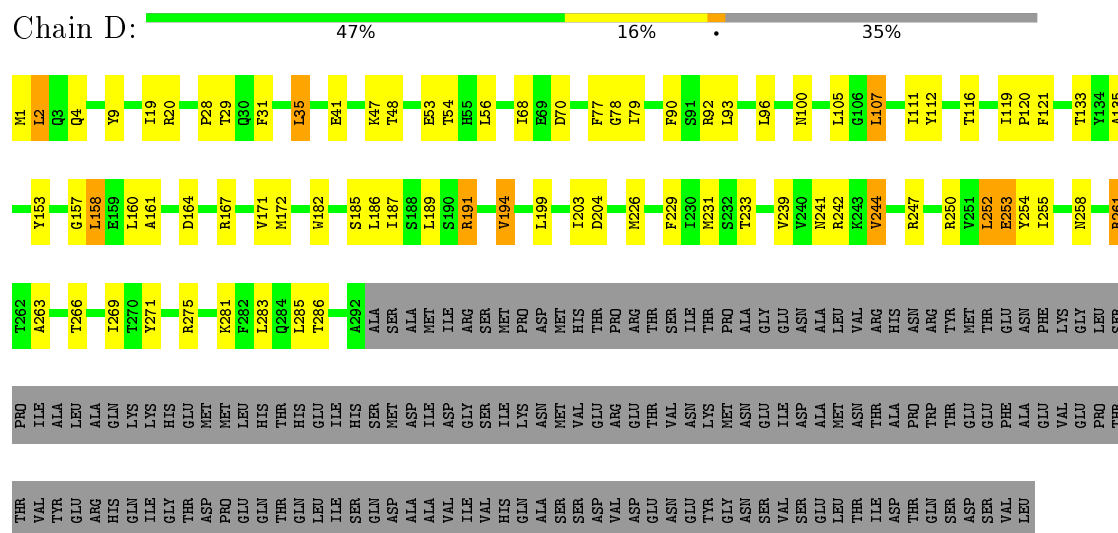


- Molecule 2: Capsid protein VP1

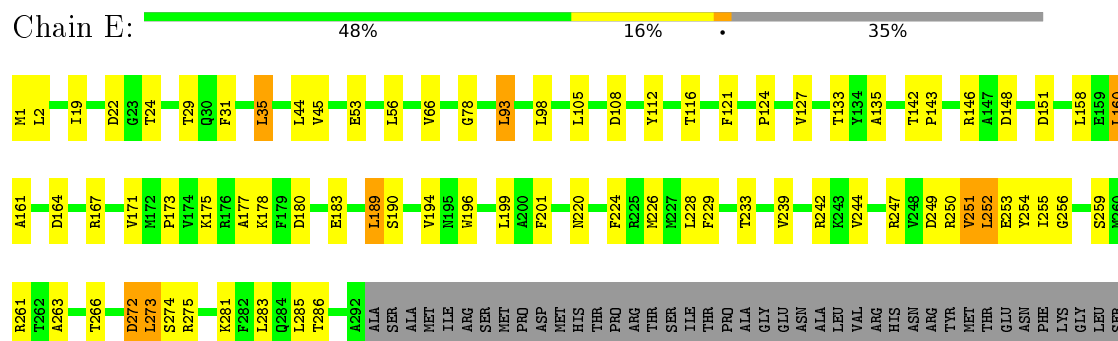




• Molecule 3: Viral structural protein 5



• Molecule 3: Viral structural protein 5



THR	PRO
VAL	ILE
TYR	ALA
GLU	LEU
ARG	ALA
HIS	GLN
GLN	LYS
ILE	LYS
GLY	HIS
THR	GLU
ASP	MET
PRO	MET
GLU	LEU
GLN	HIS
THR	THR
GLN	HIS
LEU	GLU
ILE	ILE
SER	HIS
GLN	SER
ASP	MET
ALA	ASP
ALA	ILE
VAL	ASP
ILE	GLY
VAL	SER
HIS	ILE
GLN	LYS
ALA	ASN
SER	MET
SER	VAL
ASP	GLU
VAL	ARG
ASP	GLU
GLU	THR
ASN	VAL
GLU	ASN
TYR	LYS
GLY	MET
ASN	ASN
SER	GLU
VAL	ILE
SER	ASP
GLU	ALA
LEU	MET
THR	ASN
ILE	THR
ASP	ALA
THR	PRO
GLN	TRP
SER	THR
ASP	GLU
SER	GLU
VAL	PHE
LEU	ALA
	GLU
	VAL
	GLU
	PRO
	THR

THR
VAL
TYR
GLU
ARG
HIS
GLN
ILE
GLY
THR
ASP
PRO
GLU
GLN
THR
GLN
LEU
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VAL
LEU

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	71946	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.28	0/8619	0.50	4/11737 (0.0%)
2	B	0.35	0/9590	0.55	0/13056
2	C	0.34	0/10052	0.56	1/13687 (0.0%)
3	D	0.33	0/2327	0.54	0/3163
3	E	0.31	0/2327	0.52	0/3163
All	All	0.33	0/32915	0.54	5/44806 (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
2	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ALA	C-N-CD	-8.43	102.05	120.60
1	A	78	TYR	C-N-CD	-6.39	106.53	120.60
1	A	186	ALA	C-N-CA	5.95	147.00	122.00
2	C	1116	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	78	TYR	C-N-CA	5.08	143.36	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	384	MET	Peptide

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	8434	0	8399	183	0
2	B	9397	0	9315	180	0
2	C	9851	0	9762	180	0
3	D	2281	0	2282	44	0
3	E	2281	0	2282	45	0
4	A	32	0	12	2	0
All	All	32276	0	32052	608	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 9.

The worst 5 of 608 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:111:LEU:HD13	1:A:142:ASN:HB3	1.60	0.84
2:B:709:MET:O	2:B:715:ASN:ND2	2.13	0.82
2:B:491:ASN:HD22	2:B:756:THR:HG21	1.44	0.82
2:B:461:ARG:HH21	2:B:504:ASP:HB2	1.48	0.79
1:A:255:ARG:NH2	4:A:1101:GTP:O2A	2.15	0.79

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1055/1058 (100%)	1012 (96%)	40 (4%)	3 (0%)	46	79
2	B	1187/1333 (89%)	1145 (96%)	39 (3%)	3 (0%)	46	79
2	C	1246/1333 (94%)	1197 (96%)	41 (3%)	8 (1%)	30	67
3	D	290/448 (65%)	281 (97%)	8 (3%)	1 (0%)	46	79
3	E	290/448 (65%)	284 (98%)	6 (2%)	0	100	100
All	All	4068/4620 (88%)	3919 (96%)	134 (3%)	15 (0%)	43	74

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
2	B	1035	ILE
2	C	288	THR
2	C	1267	THR
1	A	483	MET

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 PDB entries followed by that with respect to all EM entries.

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	942/943 (100%)	849 (90%)	93 (10%)	10	29
2	B	1038/1153 (90%)	980 (94%)	58 (6%)	26	60
2	C	1089/1153 (94%)	1018 (94%)	71 (6%)	21	52
3	D	240/379 (63%)	219 (91%)	21 (9%)	12	35
3	E	240/379 (63%)	220 (92%)	20 (8%)	14	38
All	All	3549/4007 (89%)	3286 (93%)	263 (7%)	22	44

5 of 263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	643	THR

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Mol	Chain	Res	Type
2	B	1317	VAL
3	E	2	LEU
2	B	755	LEU
2	B	946	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1138	HIS
2	C	1138	HIS
2	C	156	GLN
1	A	595	ASN
2	B	1332	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
4	GTP	A	1101	-	26,34,34	0.93	1 (3%)	29,54,54	1.56	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	1101	-	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	GTP	C6-N1	2.89	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101	GTP	N3-C2-N1	-5.22	120.46	127.56
4	A	1101	GTP	C5-C6-N1	-3.17	119.38	123.52
4	A	1101	GTP	C6-N1-C2	3.25	119.69	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	GTP	2	0

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.