Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2025 – 03:35 PM EDT

PDB ID	:	2Q0E / pdb_00002q0e
Title	:	Terminal uridylyl transferase 4 from Trypanosoma brucei with bound GTP
Authors	:	Stagno, J.; Luecke, H.
Deposited on	:	2007-05-21
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

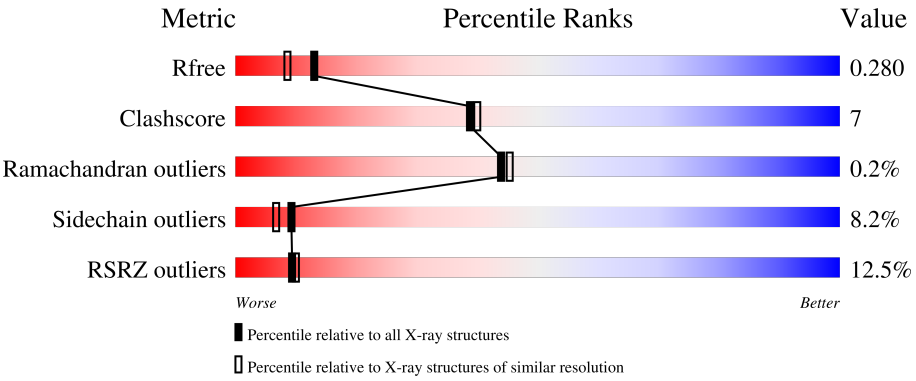
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.10 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	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	353	5% 73% 20% • 6%
1	B	353	18% 69% 15% • 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5372 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 uridylyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2643	1679	473	484	7			
1	B	308	Total	C	N	O	S	0	0	0
			2469	1578	437	447	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP Q381M1
A	-18	GLY	-	cloning artifact	UNP Q381M1
A	-17	SER	-	cloning artifact	UNP Q381M1
A	-16	SER	-	cloning artifact	UNP Q381M1
A	-15	HIS	-	expression tag	UNP Q381M1
A	-14	HIS	-	expression tag	UNP Q381M1
A	-13	HIS	-	expression tag	UNP Q381M1
A	-12	HIS	-	expression tag	UNP Q381M1
A	-11	HIS	-	expression tag	UNP Q381M1
A	-10	HIS	-	expression tag	UNP Q381M1
A	-9	SER	-	cloning artifact	UNP Q381M1
A	-8	SER	-	cloning artifact	UNP Q381M1
A	-7	GLY	-	cloning artifact	UNP Q381M1
A	-6	LEU	-	cloning artifact	UNP Q381M1
A	-5	VAL	-	cloning artifact	UNP Q381M1
A	-4	PRO	-	cloning artifact	UNP Q381M1
A	-3	ARG	-	cloning artifact	UNP Q381M1
A	-2	GLY	-	cloning artifact	UNP Q381M1
A	-1	SER	-	cloning artifact	UNP Q381M1
A	0	HIS	-	cloning artifact	UNP Q381M1
B	-19	MET	-	cloning artifact	UNP Q381M1
B	-18	GLY	-	cloning artifact	UNP Q381M1
B	-17	SER	-	cloning artifact	UNP Q381M1
B	-16	SER	-	cloning artifact	UNP Q381M1
B	-15	HIS	-	expression tag	UNP Q381M1

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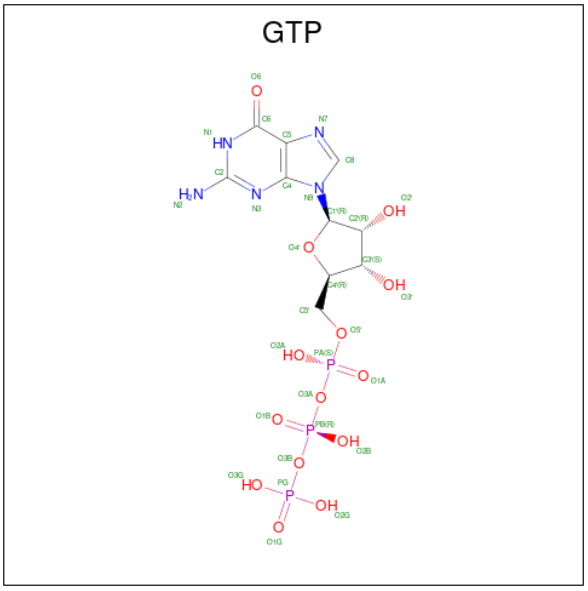
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q381M1
B	-13	HIS	-	expression tag	UNP Q381M1
B	-12	HIS	-	expression tag	UNP Q381M1
B	-11	HIS	-	expression tag	UNP Q381M1
B	-10	HIS	-	expression tag	UNP Q381M1
B	-9	SER	-	cloning artifact	UNP Q381M1
B	-8	SER	-	cloning artifact	UNP Q381M1
B	-7	GLY	-	cloning artifact	UNP Q381M1
B	-6	LEU	-	cloning artifact	UNP Q381M1
B	-5	VAL	-	cloning artifact	UNP Q381M1
B	-4	PRO	-	cloning artifact	UNP Q381M1
B	-3	ARG	-	cloning artifact	UNP Q381M1
B	-2	GLY	-	cloning artifact	UNP Q381M1
B	-1	SER	-	cloning artifact	UNP Q381M1
B	0	HIS	-	cloning artifact	UNP Q381M1

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 4 is water.

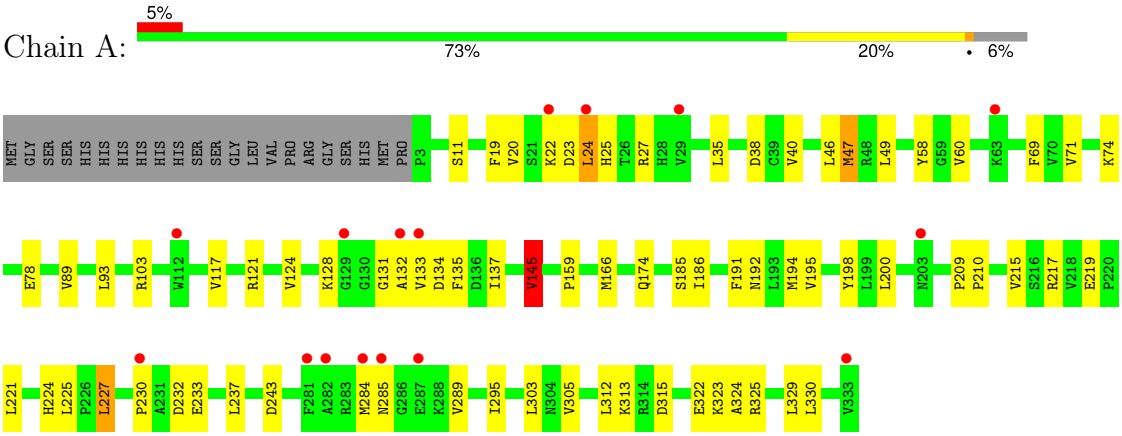
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	156	Total	O	0	0
			156	156		
4	B	70	Total	O	0	0
			70	70		

3 Residue-property plots (i)

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.

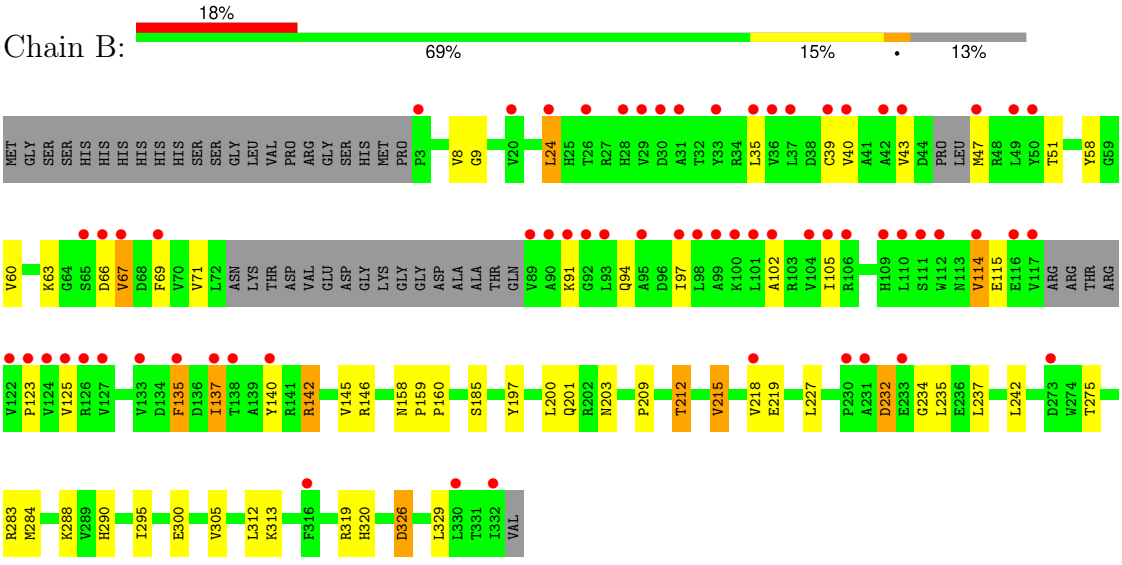
• Molecule 1: RNA uridylyl transferase

Chain A:



• Molecule 1: RNA uridylyl transferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.79Å 41.92Å 106.39Å 90.00° 93.34° 90.00°	Depositor
Resolution (Å)	45.60 – 2.10 45.60 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.60-2.10) 99.7 (45.60-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.280 0.230 , 0.280	Depositor DCC
R_{free} test set	2161 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5372	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.76	2/2702 (0.1%)	1.00	3/3666 (0.1%)
1	B	0.62	0/2524	0.90	2/3423 (0.1%)
All	All	0.70	2/5226 (0.0%)	0.95	5/7089 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	VAL	CA-CB	7.35	1.65	1.54
1	A	195	VAL	CA-CB	5.53	1.60	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	159	PRO	N-CA-C	5.97	117.99	110.70
1	A	221	LEU	CA-C-N	5.58	123.74	119.66
1	A	221	LEU	C-N-CA	5.58	123.74	119.66
1	B	159	PRO	N-CA-C	5.41	117.30	110.70
1	B	135	PHE	N-CA-C	5.02	116.82	109.24

There are no chirality outliers.

There are no planarity outliers.

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	2643	0	2647	38	0
1	B	2469	0	2471	31	0
2	A	2	0	0	0	0
3	A	32	0	12	3	0
4	A	156	0	0	5	0
4	B	70	0	0	1	0
All	All	5372	0	5130	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (69) 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:219:GLU:HG3	4:A:654:HOH:O	1.71	0.89
1:A:185:SER:HB3	1:A:313:LYS:HD3	1.61	0.82
1:A:303:LEU:HD21	3:A:501:GTP:HN21	1.46	0.80
1:A:24:LEU:H	1:A:24:LEU:HD23	1.49	0.76
1:A:191:PHE:HA	1:A:194:MET:HE3	1.73	0.70
1:B:232:ASP:HB3	1:B:235:LEU:H	1.57	0.69
1:B:185:SER:HB3	1:B:313:LYS:HD3	1.73	0.68
1:A:230:PRO:HB3	4:A:565:HOH:O	1.94	0.68
1:A:47:MET:HG2	1:A:71:VAL:HG13	1.74	0.68
1:A:40:VAL:HG13	1:A:47:MET:HE3	1.77	0.66
1:B:125:VAL:HB	1:B:137:ILE:HG22	1.78	0.65
1:A:25:HIS:ND1	1:A:27:ARG:HB2	2.14	0.62
3:A:501:GTP:N2	4:A:548:HOH:O	2.32	0.62
1:A:103:ARG:NH2	1:B:203:ASN:OD1	2.34	0.61
1:B:39:CYS:SG	1:B:105:ILE:HG22	2.41	0.60
1:A:35:LEU:O	1:A:38:ASP:HB2	2.03	0.59
1:B:142:ARG:HD3	1:B:142:ARG:H	1.68	0.58
1:A:25:HIS:HA	1:A:224:HIS:CD2	2.40	0.56
1:A:47:MET:SD	1:A:71:VAL:CG1	2.95	0.55
1:B:24:LEU:HB3	1:B:60:VAL:HB	1.90	0.54
1:B:40:VAL:HG13	1:B:47:MET:HE3	1.89	0.54
1:B:215:VAL:HA	1:B:218:VAL:HG22	1.91	0.53
1:A:121:ARG:HB2	1:A:285:ASN:HD21	1.73	0.53
1:A:135:PHE:HE1	1:A:137:ILE:HD11	1.73	0.53
1:A:89:VAL:HG13	4:A:590:HOH:O	2.08	0.53
1:A:312:LEU:O	1:A:315:ASP:HB3	2.09	0.52
1:B:209:PRO:O	1:B:212:THR:HB	2.11	0.51
1:B:288:LYS:HE3	1:B:290:HIS:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:CE1	1:A:166:MET:HE1	2.47	0.50
1:B:9:GLY:HA3	1:B:234:GLY:O	2.10	0.50
1:B:67:VAL:HG12	1:B:135:PHE:HB3	1.92	0.50
1:B:326:ASP:N	1:B:326:ASP:OD1	2.43	0.50
1:A:232:ASP:O	1:A:233:GLU:HB2	2.11	0.50
1:A:24:LEU:HD23	1:A:24:LEU:N	2.22	0.49
1:B:197:TYR:O	1:B:201:GLN:HG2	2.12	0.49
1:B:319:ARG:HH12	1:B:320:HIS:CE1	2.31	0.49
1:B:283:ARG:NH1	1:B:284:MET:HE2	2.27	0.49
1:B:288:LYS:HE3	1:B:290:HIS:CE1	2.47	0.49
1:A:217:ARG:HD3	4:A:639:HOH:O	2.14	0.48
1:A:303:LEU:CD2	3:A:501:GTP:HN21	2.23	0.48
1:B:158:ASN:HD22	1:B:160:PRO:HD2	1.77	0.48
1:A:58:TYR:HB3	1:A:60:VAL:HG22	1.96	0.47
1:A:24:LEU:CD1	1:A:227:LEU:H	2.28	0.47
1:A:324:ALA:HB1	1:A:329:LEU:HD23	1.96	0.46
1:B:69:PHE:HB2	1:B:137:ILE:HG12	1.95	0.46
1:B:8:VAL:HG21	1:B:242:LEU:HD21	1.98	0.46
1:A:145:VAL:HG22	1:A:215:VAL:HG22	1.98	0.45
1:B:94:GLN:HE21	1:B:140:TYR:HB2	1.81	0.45
1:A:322:GLU:HG2	1:A:325:ARG:NH2	2.31	0.44
1:A:47:MET:SD	1:A:71:VAL:HG11	2.56	0.44
1:B:142:ARG:HD3	1:B:142:ARG:N	2.32	0.43
1:B:94:GLN:HB3	1:B:123:PRO:HG2	2.01	0.43
1:B:142:ARG:H	1:B:142:ARG:CD	2.30	0.43
1:B:102:ALA:HA	1:B:105:ILE:HG12	2.01	0.42
1:B:295:ILE:HB	1:B:305:VAL:HB	2.01	0.42
1:A:198:TYR:OH	1:A:243:ASP:HB3	2.20	0.42
1:B:115:GLU:O	1:B:125:VAL:HG13	2.19	0.42
1:B:58:TYR:HB3	1:B:60:VAL:HG22	2.01	0.41
1:A:117:VAL:HB	1:A:124:VAL:HG13	2.01	0.41
1:B:275:THR:HB	4:B:364:HOH:O	2.20	0.41
1:A:209:PRO:HA	1:A:210:PRO:HD3	1.93	0.41
1:A:315:ASP:OD1	1:A:315:ASP:C	2.64	0.41
1:A:74:LYS:O	1:A:78:GLU:HG3	2.21	0.41
1:A:192:ASN:HD22	1:A:192:ASN:HA	1.70	0.41
1:A:131:GLY:C	1:A:133:VAL:N	2.80	0.40
1:A:49:LEU:HD11	1:A:69:PHE:HB3	2.02	0.40
1:A:295:ILE:HB	1:A:305:VAL:HB	2.03	0.40
1:B:114:VAL:HG22	1:B:114:VAL:O	2.21	0.40
1:A:186:ILE:HB	1:A:191:PHE:CE2	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	329/353 (93%)	319 (97%)	9 (3%)	1 (0%)	37 37
1	B	300/353 (85%)	294 (98%)	6 (2%)	0	100 100
All	All	629/706 (89%)	613 (98%)	15 (2%)	1 (0%)	44 45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ALA

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	290/309 (94%)	270 (93%)	20 (7%)	13 10
1	B	272/309 (88%)	246 (90%)	26 (10%)	7 4
All	All	562/618 (91%)	516 (92%)	46 (8%)	9 7

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	20	VAL

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Mol	Chain	Res	Type
1	A	22	LYS
1	A	23	ASP
1	A	24	LEU
1	A	46	LEU
1	A	47	MET
1	A	93	LEU
1	A	128	LYS
1	A	134	ASP
1	A	145	VAL
1	A	174	GLN
1	A	200	LEU
1	A	225	LEU
1	A	227	LEU
1	A	237	LEU
1	A	284	MET
1	A	289	VAL
1	A	323	LYS
1	A	330	LEU
1	B	24	LEU
1	B	35	LEU
1	B	43	VAL
1	B	51	THR
1	B	63	LYS
1	B	66	ASP
1	B	67	VAL
1	B	71	VAL
1	B	91	LYS
1	B	97	ILE
1	B	114	VAL
1	B	137	ILE
1	B	142	ARG
1	B	145	VAL
1	B	146	ARG
1	B	200	LEU
1	B	212	THR
1	B	215	VAL
1	B	219	GLU
1	B	227	LEU
1	B	232	ASP
1	B	237	LEU
1	B	300	GLU
1	B	312	LEU

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Mol	Chain	Res	Type
1	B	326	ASP
1	B	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	192	ASN
1	A	203	ASN
1	A	246	HIS
1	A	285	ASN
1	A	292	GLN
1	B	94	GLN
1	B	107	GLN
1	B	158	ASN
1	B	174	GLN
1	B	201	GLN
1	B	224	HIS
1	B	250	HIS
1	B	302	ASN
1	B	320	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GTP	A	501	2	29,34,34	1.17	3 (10%)	35,54,54	1.75	8 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	A	501	2	-	7/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GTP	C5-C6	-3.43	1.40	1.47
3	A	501	GTP	C2-N3	2.31	1.38	1.33
3	A	501	GTP	PB-O3B	2.21	1.61	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	GTP	O4'-C1'-N9	5.10	115.50	108.75
3	A	501	GTP	C8-N7-C5	3.72	108.89	102.55
3	A	501	GTP	C2-N1-C6	-3.49	118.72	125.11
3	A	501	GTP	C4'-O4'-C1'	3.36	113.00	109.92
3	A	501	GTP	C5-C6-N1	3.04	119.88	114.07
3	A	501	GTP	N2-C2-N1	2.58	122.20	116.76
3	A	501	GTP	O3G-PG-O3B	2.15	111.86	104.64
3	A	501	GTP	O6-C6-C5	-2.09	120.17	124.32

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GTP	PB-O3B-PG-O3G
3	A	501	GTP	O4'-C4'-C5'-O5'
3	A	501	GTP	PB-O3B-PG-O1G
3	A	501	GTP	PB-O3B-PG-O2G
3	A	501	GTP	PB-O3A-PA-O1A
3	A	501	GTP	PB-O3A-PA-O2A
3	A	501	GTP	C3'-C4'-C5'-O5'

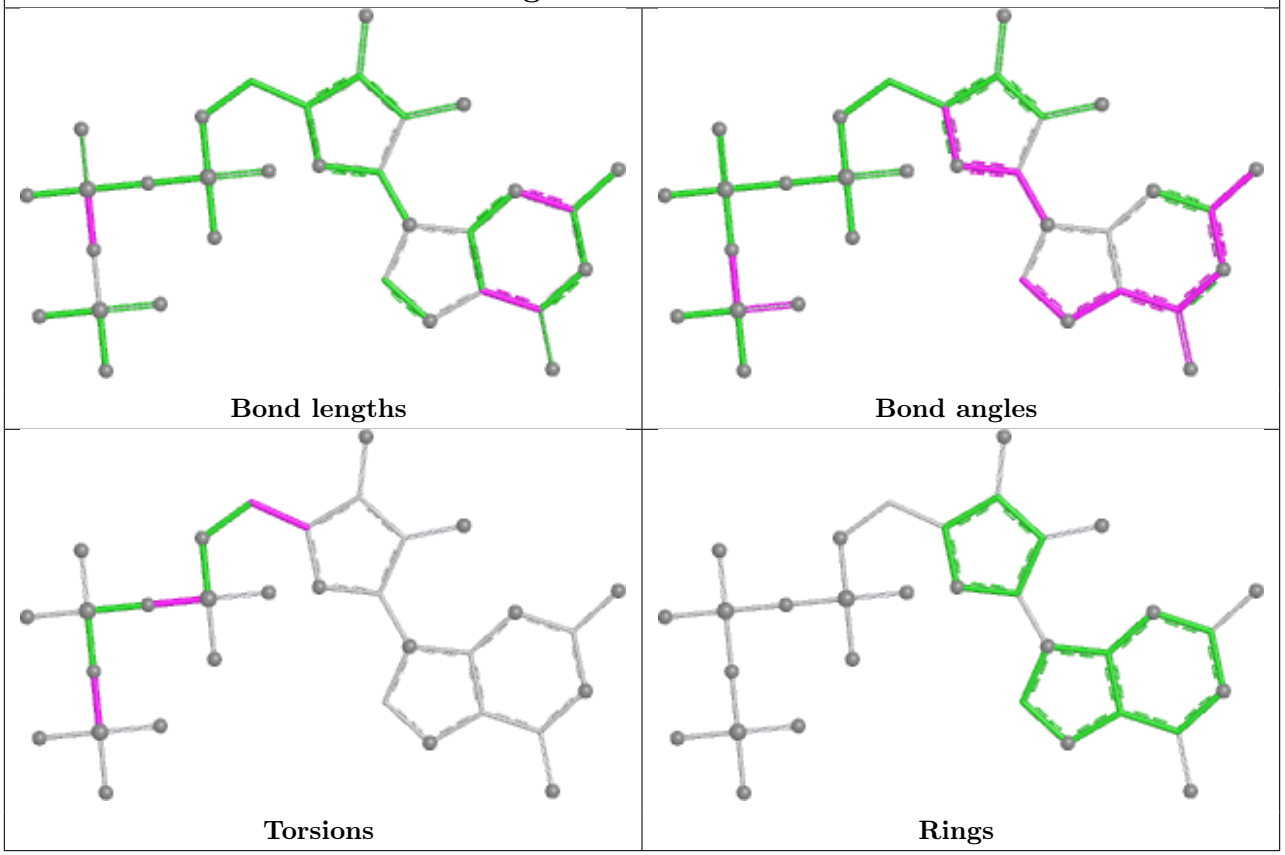
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GTP	3	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 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 A 501



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

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	331/353 (93%)	0.33	16 (4%) 36 38	16, 31, 52, 63	0
1	B	308/353 (87%)	1.02	64 (20%) 3 3	22, 44, 82, 85	0
All	All	639/706 (90%)	0.67	80 (12%) 9 10	16, 36, 76, 85	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	89	VAL	5.5
1	B	117	VAL	5.4
1	B	105	ILE	5.0
1	A	24	LEU	4.8
1	A	284	MET	4.6
1	B	124	VAL	4.4
1	B	43	VAL	4.2
1	A	129	GLY	4.2
1	B	40	VAL	4.2
1	A	333	VAL	4.1
1	B	93	LEU	4.1
1	B	90	ALA	4.0
1	B	133	VAL	4.0
1	B	3	PRO	3.8
1	B	102	ALA	3.5
1	B	110	LEU	3.5
1	B	97	ILE	3.3
1	B	101	LEU	3.3
1	B	114	VAL	3.3
1	A	285	ASN	3.2
1	B	135	PHE	3.1
1	B	35	LEU	3.1
1	B	49	LEU	3.1
1	A	282	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	104	VAL	3.0
1	B	127	VAL	3.0
1	B	33	TYR	2.9
1	B	137	ILE	2.9
1	B	112	TRP	2.8
1	B	99	ALA	2.8
1	B	126	ARG	2.8
1	B	91	LYS	2.8
1	A	281	PHE	2.8
1	B	330	LEU	2.7
1	B	67	VAL	2.7
1	B	92	GLY	2.7
1	B	42	ALA	2.6
1	B	37	LEU	2.6
1	B	231	ALA	2.6
1	B	316	PHE	2.6
1	A	63	LYS	2.5
1	B	24	LEU	2.5
1	B	47	MET	2.5
1	B	98	LEU	2.5
1	B	95	ALA	2.5
1	B	218	VAL	2.5
1	B	230	PRO	2.4
1	B	138	THR	2.4
1	B	125	VAL	2.4
1	B	50	TYR	2.4
1	B	332	ILE	2.4
1	B	36	VAL	2.4
1	B	100	LYS	2.3
1	B	109	HIS	2.3
1	B	20	VAL	2.3
1	B	29	VAL	2.3
1	B	65	SER	2.3
1	B	111	SER	2.3
1	B	30	ASP	2.3
1	B	233	GLU	2.3
1	A	132	ALA	2.3
1	A	29	VAL	2.3
1	B	123	PRO	2.2
1	B	31	ALA	2.2
1	B	28	HIS	2.2
1	A	287	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	133	VAL	2.2
1	B	26	THR	2.1
1	A	112	TRP	2.1
1	B	116	GLU	2.1
1	B	106	ARG	2.1
1	B	69	PHE	2.1
1	B	66	ASP	2.1
1	B	273	ASP	2.1
1	A	230	PRO	2.0
1	A	22	LYS	2.0
1	A	203	ASN	2.0
1	B	140	TYR	2.0
1	B	39	CYS	2.0
1	B	122	VAL	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)

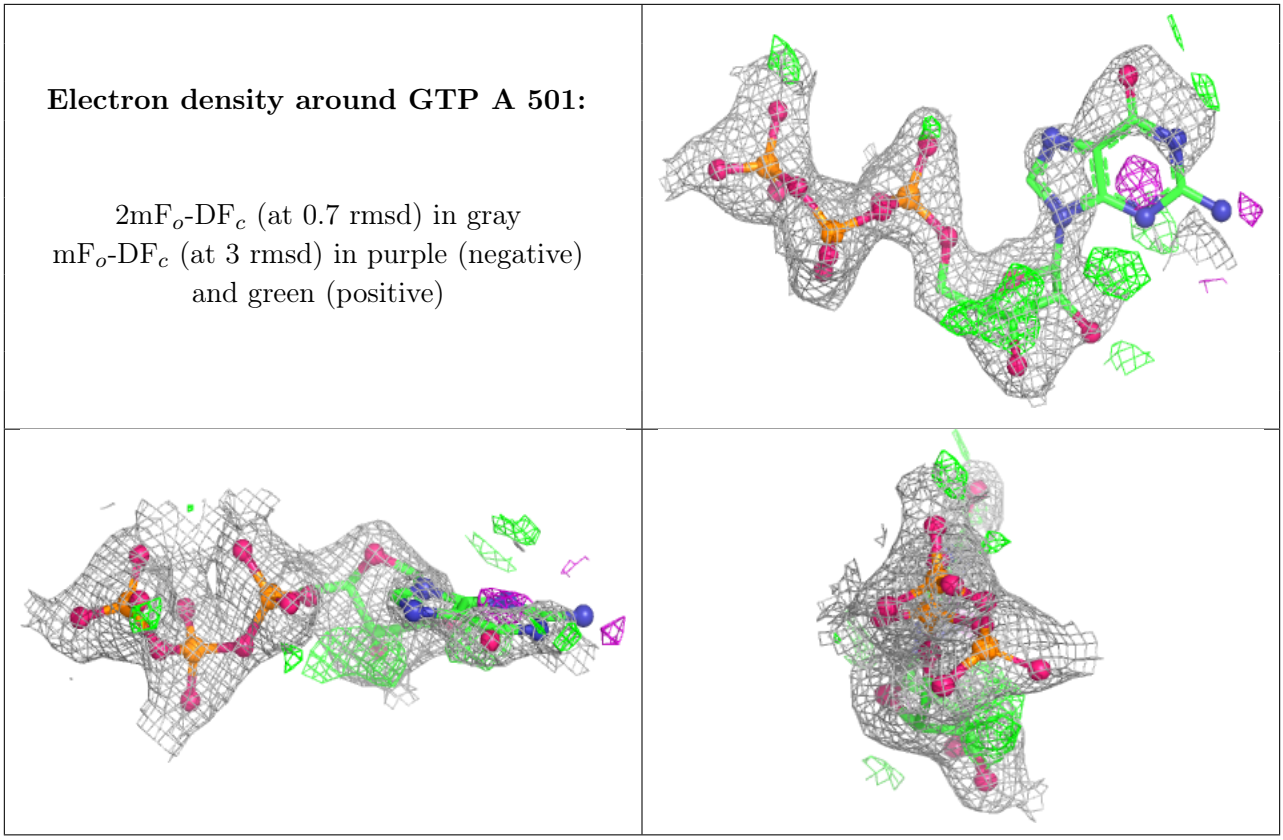
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	GTP	A	501	32/32	0.89	0.15	20,27,37,38	32
2	MG	A	402	1/1	0.93	0.09	23,23,23,23	1
2	MG	A	401	1/1	0.98	0.12	13,13,13,13	1

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 A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.