Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 05:38 AM EDT

PDB ID	:	2Q0D
Title	:	Terminal uridylyl transferase 4 from Trypanosoma brucei with bound ATP
Authors	:	Stagno, J.; Luecke, H.
Deposited on	:	2007-05-21
Resolution	:	2.00 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:

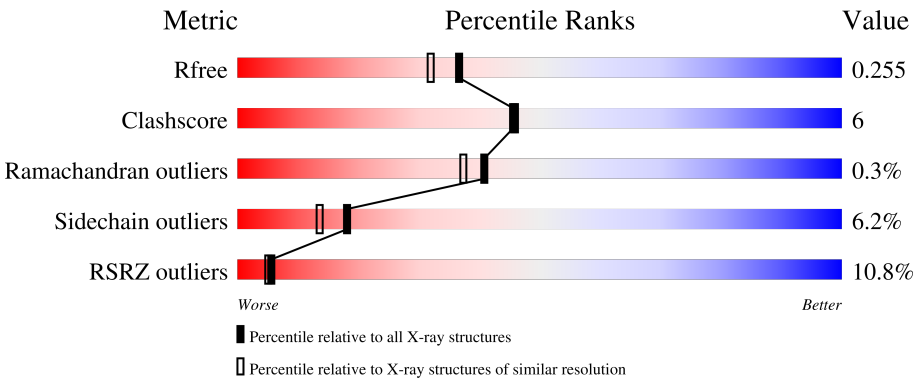
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	3% 79% 11% • 8%
1	B	353	17% 70% 19% • 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5460 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
			Total	C	N	O	S			
1	A	325	2590	1647	461	475	7	0	0	0
1	B	323	2573	1636	456	475	6	0	0	0

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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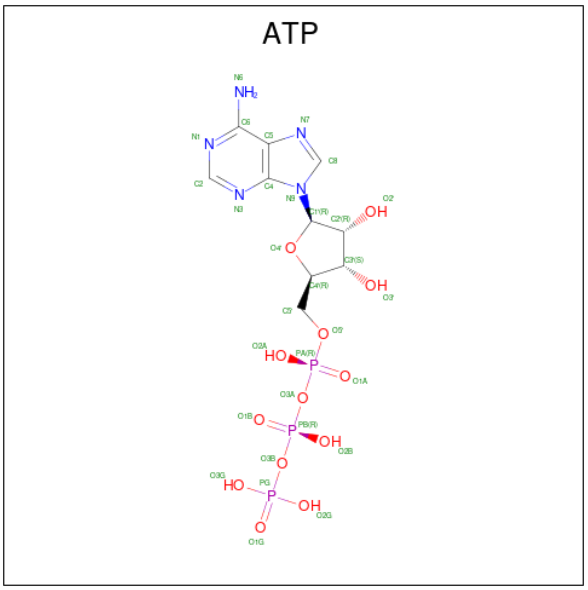
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q381M1
B	-13	HIS	-	expression tag	UNP Q381M1
B	-12	HIS	-	expression tag	UNP Q381M1
B	-11	HIS	-	expression tag	UNP Q381M1
B	-10	HIS	-	expression tag	UNP Q381M1
B	-9	SER	-	cloning artifact	UNP Q381M1
B	-8	SER	-	cloning artifact	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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	5	13	3	0	0

- Molecule 4 is water.

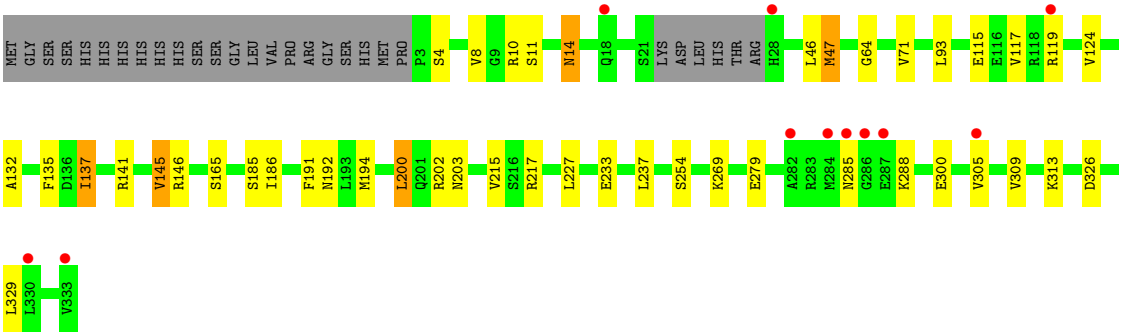
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	194	194	194	0	0
			Total	O		
4	B	70	70	70	0	0

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.

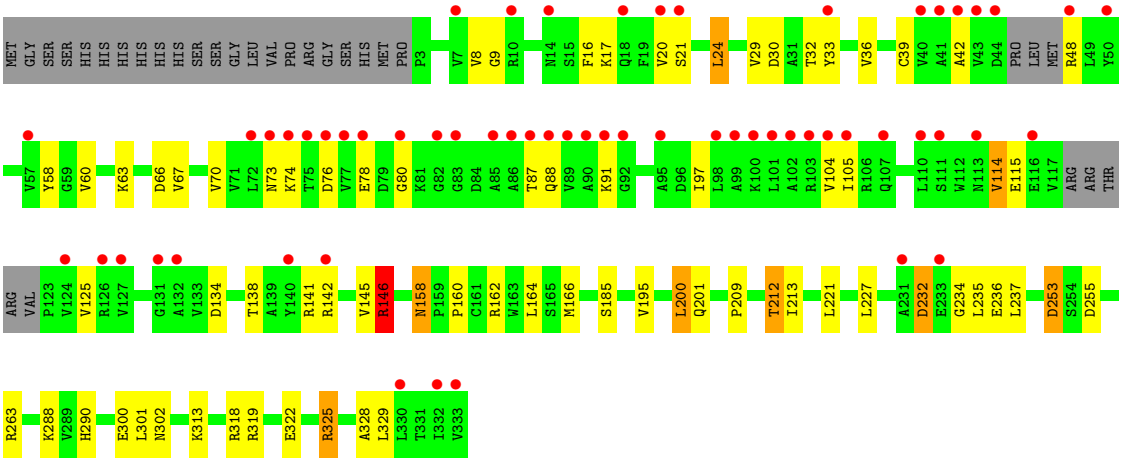
• Molecule 1: RNA uridylyl transferase

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	80.19Å 41.97Å 106.42Å 90.00° 94.01° 90.00°	Depositor
Resolution (Å)	35.38 – 2.00 35.39 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.38-2.00) 99.5 (35.39-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.254 0.219 , 0.255	Depositor DCC
R_{free} test set	2473 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.7	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	5460	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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 (i)

5.1 Standard geometry (i)

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

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	0.78	1/2647 (0.0%)	0.81	1/3591 (0.0%)
1	B	0.59	0/2629	0.75	5/3564 (0.1%)
All	All	0.69	1/5276 (0.0%)	0.78	6/7155 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	VAL	CB-CG2	5.59	1.64	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	263	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	B	263	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	B	146	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	253	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	200	LEU	CA-CB-CG	5.74	128.51	115.30
1	B	200	LEU	CA-CB-CG	5.65	128.30	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	ARG	Peptide

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	2590	0	2591	32	1
1	B	2573	0	2564	34	0
2	A	2	0	0	0	0
3	A	31	0	12	0	0
4	A	194	0	0	4	1
4	B	70	0	0	2	0
All	All	5460	0	5167	66	1

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 6.

All (66) 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:191:PHE:HA	1:A:194:MET:HE3	1.61	0.81
1:A:47:MET:HG2	1:A:71:VAL:HG13	1.70	0.74
1:A:135:PHE:HE1	1:A:137:ILE:HD11	1.56	0.71
1:A:329:LEU:O	4:A:683:HOH:O	2.07	0.71
1:B:158:ASN:HD22	1:B:160:PRO:HD2	1.56	0.71
1:A:47:MET:HG2	1:A:71:VAL:CG1	2.21	0.70
1:B:209:PRO:O	1:B:212:THR:HB	1.95	0.66
1:A:64:GLY:O	4:A:667:HOH:O	2.15	0.64
1:A:185:SER:HB3	1:A:313:LYS:HD3	1.84	0.60
1:B:39:CYS:SG	1:B:105:ILE:HG22	2.43	0.58
1:A:115:GLU:OE2	4:A:691:HOH:O	2.17	0.58
1:A:146:ARG:HG3	1:A:215:VAL:HG23	1.88	0.56
1:B:58:TYR:HB3	1:B:60:VAL:HG22	1.88	0.56
1:A:279:GLU:HB3	1:A:288:LYS:HE2	1.88	0.56
1:B:318:ARG:HD3	4:B:393:HOH:O	2.07	0.55
1:B:162:ARG:O	1:B:166:MET:HG3	2.07	0.54
1:B:185:SER:HB3	1:B:313:LYS:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ARG:NH1	1:B:213:ILE:O	2.37	0.54
1:A:165:SER:OG	1:A:192:ASN:ND2	2.41	0.53
1:B:232:ASP:HB3	1:B:235:LEU:H	1.72	0.53
1:A:10:ARG:HG2	1:A:233:GLU:HG3	1.91	0.52
1:A:117:VAL:HB	1:A:124:VAL:HG13	1.91	0.51
1:A:4:SER:O	1:A:8:VAL:HG23	2.11	0.51
1:B:16:PHE:O	1:B:20:VAL:HG23	2.11	0.50
1:B:74:LYS:O	1:B:78:GLU:HG3	2.10	0.50
1:A:233:GLU:HG3	1:A:233:GLU:O	2.11	0.50
1:B:24:LEU:HB3	1:B:60:VAL:HB	1.93	0.49
1:A:47:MET:SD	1:A:71:VAL:HG11	2.52	0.49
1:B:9:GLY:HA3	1:B:234:GLY:O	2.13	0.49
1:A:135:PHE:CE1	1:A:137:ILE:HD11	2.43	0.49
1:B:29:VAL:HG22	1:B:67:VAL:HG21	1.95	0.48
1:A:10:ARG:O	1:A:14:ASN:HB3	2.13	0.48
1:A:186:ILE:HG21	1:A:194:MET:HE1	1.96	0.48
1:A:145:VAL:HG22	1:A:215:VAL:HG22	1.94	0.48
1:B:142:ARG:O	1:B:145:VAL:HG22	2.14	0.48
1:B:42:ALA:HB3	1:B:104:VAL:HG11	1.96	0.48
1:B:73:ASN:HB2	1:B:76:ASP:CG	2.35	0.47
1:A:186:ILE:HG21	1:A:194:MET:CE	2.45	0.47
1:B:322:GLU:O	1:B:325:ARG:HD2	2.15	0.47
1:B:48:ARG:HG3	1:B:74:LYS:HE2	1.96	0.47
1:B:30:ASP:HA	1:B:221:LEU:HD21	1.96	0.46
1:B:88:GLN:HA	1:B:91:LYS:HG2	1.97	0.46
1:B:76:ASP:O	1:B:142:ARG:HD3	2.15	0.46
1:B:8:VAL:HG22	1:B:328:ALA:HB2	1.97	0.46
1:A:146:ARG:HG3	1:A:215:VAL:CG2	2.45	0.46
1:A:254:SER:O	1:A:269:LYS:HE3	2.15	0.46
1:B:32:THR:O	1:B:36:VAL:HG23	2.17	0.45
1:A:141:ARG:NH2	1:A:300:GLU:OE2	2.48	0.45
1:A:185:SER:HB2	1:A:309:VAL:HG22	1.97	0.45
1:A:202:ARG:O	1:A:203:ASN:HB2	2.17	0.45
1:B:70:VAL:HG23	1:B:138:THR:HG23	1.98	0.45
1:A:192:ASN:HD22	1:A:192:ASN:HA	1.56	0.44
1:B:58:TYR:CB	1:B:60:VAL:HG22	2.47	0.44
1:A:145:VAL:CG2	1:A:215:VAL:HG22	2.48	0.43
1:B:115:GLU:O	1:B:125:VAL:HG13	2.19	0.43
1:A:47:MET:SD	1:A:71:VAL:CG1	3.07	0.43
1:A:141:ARG:HD2	4:A:631:HOH:O	2.17	0.43
1:B:33:TYR:CD2	1:B:221:LEU:HD22	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HG22	1:B:114:VAL:O	2.20	0.42
1:B:201:GLN:NE2	4:B:346:HOH:O	2.53	0.41
1:A:10:ARG:HG2	1:A:233:GLU:CG	2.51	0.41
1:B:253:ASP:OD1	1:B:255:ASP:HB2	2.20	0.41
1:B:17:LYS:HD3	1:B:17:LYS:HA	1.74	0.41
1:A:47:MET:CG	1:A:71:VAL:CG1	2.96	0.41
1:B:164:LEU:HD23	1:B:195:VAL:HG13	2.03	0.40
1:B:288:LYS:HE3	1:B:290:HIS:NE2	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:NH2	4:A:678:HOH:O[1_545]	2.19	0.01

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	321/353 (91%)	313 (98%)	7 (2%)	1 (0%)	41	37
1	B	317/353 (90%)	308 (97%)	8 (2%)	1 (0%)	41	37
All	All	638/706 (90%)	621 (97%)	15 (2%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ALA
1	B	80	GLY

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	284/309 (92%)	272 (96%)	12 (4%)	30 27
1	B	282/309 (91%)	259 (92%)	23 (8%)	11 7
All	All	566/618 (92%)	531 (94%)	35 (6%)	18 13

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	14	ASN
1	A	46	LEU
1	A	47	MET
1	A	93	LEU
1	A	137	ILE
1	A	145	VAL
1	A	200	LEU
1	A	227	LEU
1	A	237	LEU
1	A	285	ASN
1	A	326	ASP
1	B	21	SER
1	B	24	LEU
1	B	63	LYS
1	B	66	ASP
1	B	87	THR
1	B	97	ILE
1	B	114	VAL
1	B	134	ASP
1	B	141	ARG
1	B	146	ARG
1	B	158	ASN
1	B	200	LEU
1	B	212	THR
1	B	227	LEU
1	B	232	ASP

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Mol	Chain	Res	Type
1	B	236	GLU
1	B	237	LEU
1	B	300	GLU
1	B	301	LEU
1	B	302	ASN
1	B	319	ARG
1	B	325	ARG
1	B	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	240	GLN
1	A	285	ASN
1	B	14	ASN
1	B	113	ASN
1	B	158	ASN
1	B	192	ASN
1	B	201	GLN
1	B	224	HIS
1	B	240	GLN
1	B	262	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 monosaccharides 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	ATP	A	501	2	26,33,33	1.29	4 (15%)	31,52,52	1.37	5 (16%)

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	ATP	A	501	2	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	ATP	O4'-C1'	3.09	1.45	1.41
3	A	501	ATP	C5-C4	2.86	1.48	1.40
3	A	501	ATP	C2-N3	2.34	1.35	1.32
3	A	501	ATP	C2'-C1'	-2.08	1.50	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	ATP	N3-C2-N1	-3.48	123.25	128.68
3	A	501	ATP	C3'-C2'-C1'	2.91	105.36	100.98
3	A	501	ATP	C4-C5-N7	-2.27	107.03	109.40
3	A	501	ATP	O3G-PG-O1G	2.07	118.80	110.68
3	A	501	ATP	O3B-PG-O1G	-2.06	99.74	111.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ATP	PB-O3B-PG-O3G
3	A	501	ATP	PB-O3B-PG-O1G

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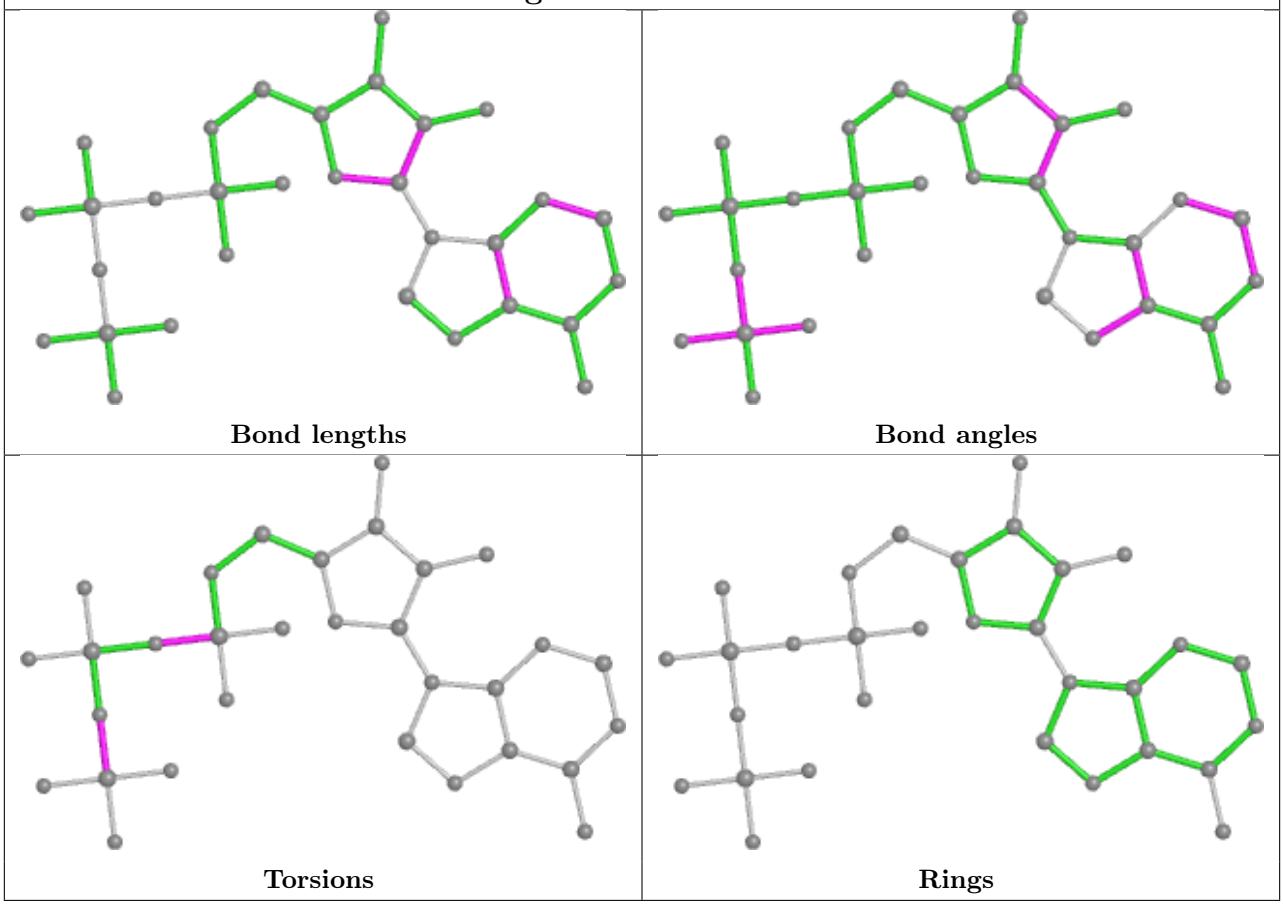
Mol	Chain	Res	Type	Atoms
3	A	501	ATP	PB-O3A-PA-O2A

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 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 ATP A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	325/353 (92%)	0.08	11 (3%)	45	44	13, 24, 47, 64	0
1	B	323/353 (91%)	0.93	59 (18%)	1	1	19, 41, 86, 91	0
All	All	648/706 (91%)	0.50	70 (10%)	5	5	13, 31, 79, 91	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	ILE	11.3
1	B	90	ALA	8.5
1	A	333	VAL	8.0
1	B	86	ALA	7.3
1	B	101	LEU	6.5
1	B	87	THR	6.4
1	B	111	SER	6.0
1	B	89	VAL	5.8
1	B	333	VAL	5.2
1	B	88	GLN	5.2
1	B	95	ALA	5.1
1	A	285	ASN	4.7
1	B	110	LEU	4.5
1	B	78	GLU	4.3
1	B	124	VAL	4.2
1	B	85	ALA	4.2
1	A	28	HIS	4.1
1	B	21	SER	3.9
1	B	99	ALA	3.9
1	B	131	GLY	3.9
1	B	7	VAL	3.9
1	B	43	VAL	3.8
1	B	40	VAL	3.7
1	B	91	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	286	GLY	3.6
1	B	103	ARG	3.6
1	B	102	ALA	3.6
1	B	92	GLY	3.6
1	B	113	ASN	3.5
1	B	48	ARG	3.5
1	B	75	THR	3.5
1	A	119	ARG	3.3
1	B	100	LYS	3.2
1	B	76	ASP	3.2
1	B	74	LYS	3.2
1	A	287	GLU	3.0
1	B	132	ALA	3.0
1	B	41	ALA	3.0
1	B	82	GLY	2.9
1	B	77	VAL	2.8
1	B	231	ALA	2.8
1	B	50	TYR	2.8
1	B	73	ASN	2.8
1	B	233	GLU	2.8
1	B	107	GLN	2.8
1	B	42	ALA	2.7
1	A	18	GLN	2.7
1	B	83	GLY	2.7
1	B	140	TYR	2.6
1	B	44	ASP	2.6
1	B	57	VAL	2.6
1	B	116	GLU	2.5
1	B	33	TYR	2.5
1	B	98	LEU	2.5
1	A	284	MET	2.5
1	B	126	ARG	2.5
1	A	282	ALA	2.4
1	B	332	ILE	2.4
1	B	18	GLN	2.3
1	B	330	LEU	2.3
1	B	20	VAL	2.2
1	B	10	ARG	2.2
1	B	104	VAL	2.2
1	B	127	VAL	2.2
1	B	14	ASN	2.2
1	B	80	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	72	LEU	2.1
1	B	142	ARG	2.1
1	A	305	VAL	2.1
1	A	330	LEU	2.1

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)

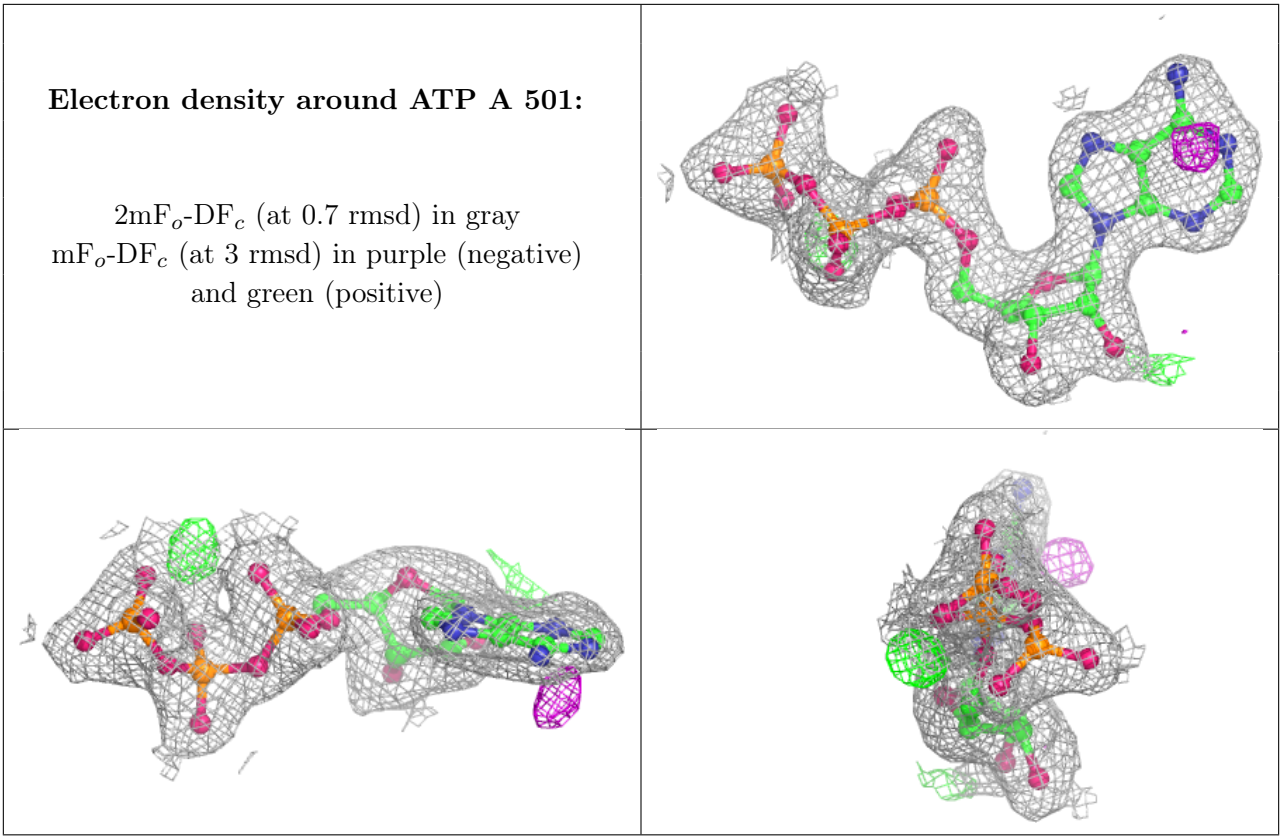
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	402	1/1	0.96	0.19	19,19,19,19	0
3	ATP	A	501	31/31	0.98	0.12	17,22,33,35	0
2	MG	A	401	1/1	1.00	0.23	10,10,10,10	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 ATP 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.