



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:24 pm BST

PDB ID : 3OVB  
Title : How the CCA-adding Enzyme Selects Adenine over Cytosine in Position 76 of tRNA  
Authors : Pan, B.C.; Xiong, Y.; Steitz, T.A.  
Deposited on : 2010-09-16  
Resolution : 1.95 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](mailto: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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

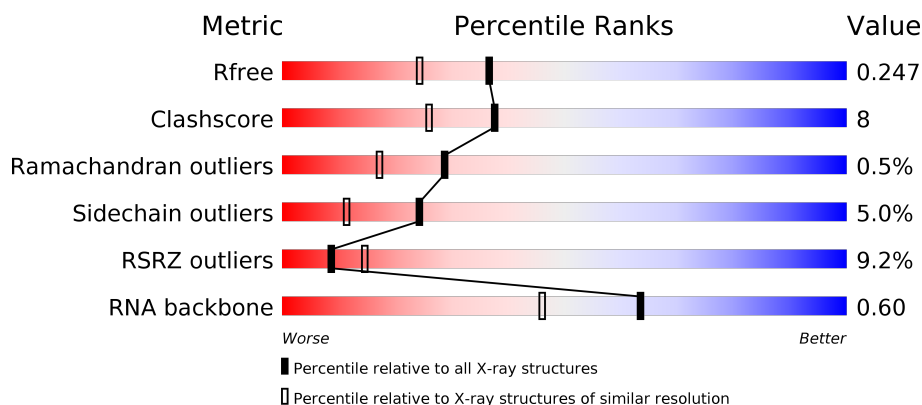
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)
RNA backbone	3102	1124 (2.50-1.42)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	441	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	B	441	<div> <div>16%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
2	C	35	<div> <div>3%</div> <div>51%</div> <div>37%</div> <div>11%</div> </div>
2	D	35	<div> <div>17%</div> <div>60%</div> <div>34%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	POP	B	602[A]	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9437 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 CCA-Adding Enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	1	0
			3666	2353	640	657	16			
1	B	437	Total	C	N	O	S	0	1	0
			3637	2337	633	654	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	CYS	-	EXPRESSION TAG	UNP O28126
A	439	CYS	-	EXPRESSION TAG	UNP O28126
A	440	CYS	-	EXPRESSION TAG	UNP O28126
A	441	GLN	-	EXPRESSION TAG	UNP O28126
B	438	CYS	-	EXPRESSION TAG	UNP O28126
B	439	CYS	-	EXPRESSION TAG	UNP O28126
B	440	CYS	-	EXPRESSION TAG	UNP O28126
B	441	GLN	-	EXPRESSION TAG	UNP O28126

- Molecule 2 is a RNA chain called RNA (35-MER).

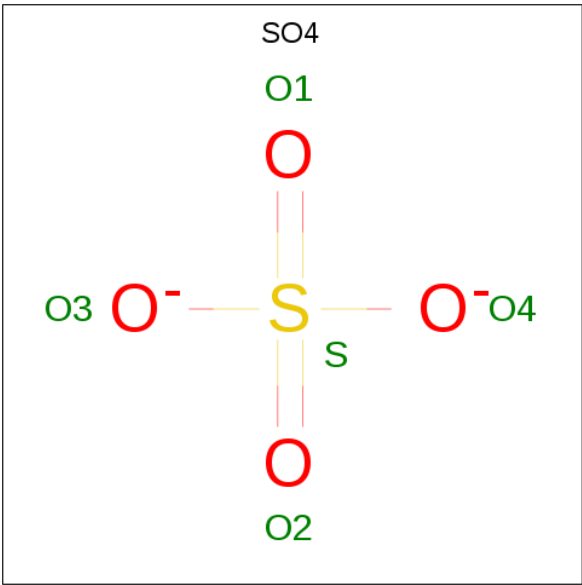
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	35	Total	C	N	O	P	0	2	0
			758	341	132	250	35			
2	D	35	Total	C	N	O	P	0	2	0
			758	341	132	250	35			

- 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
3	A	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	21	0
			31	10	5	13	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).

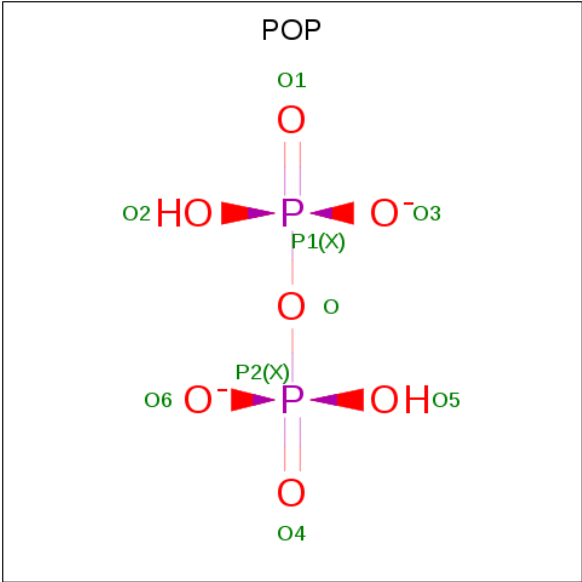


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $H_2O_7P_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	1
			9	7	2		
7	C	1	Total	O	P	0	1
			9	7	2		

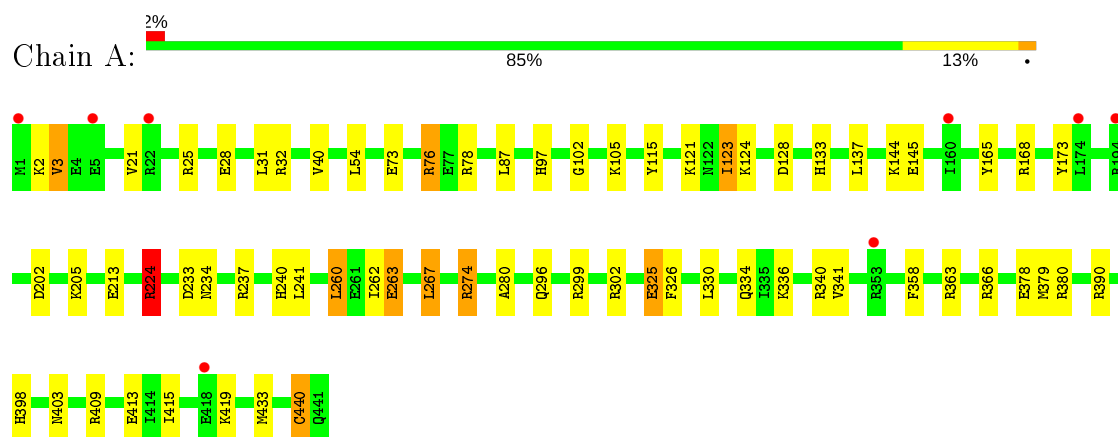
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	296	Total	O	0	0
			296	296		
8	B	122	Total	O	0	0
			122	122		
8	C	44	Total	O	0	0
			44	44		
8	D	13	Total	O	0	0
			13	13		

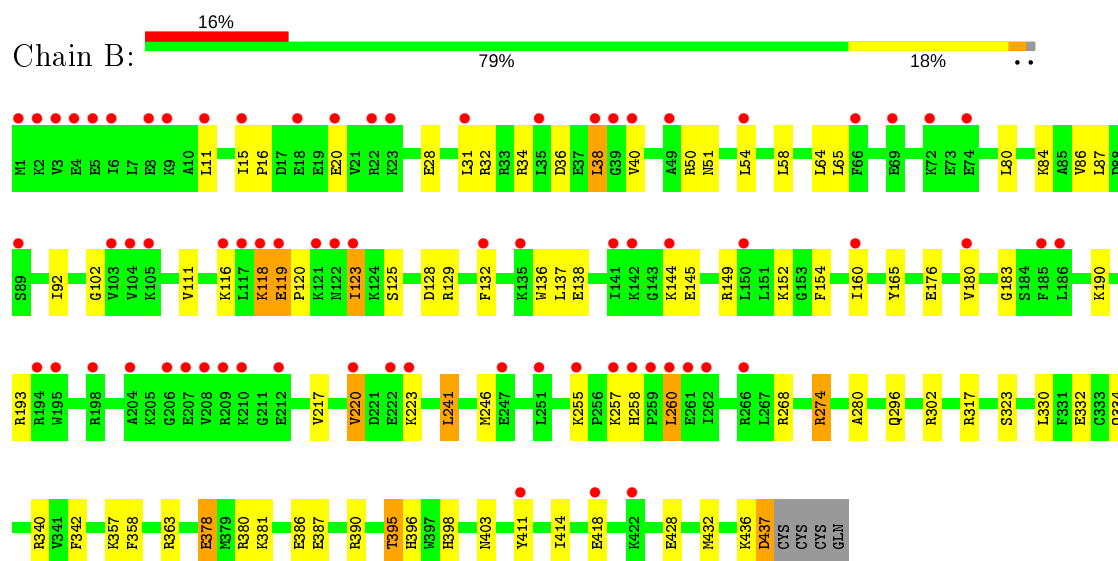
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: CCA-Adding Enzyme



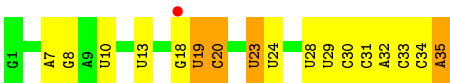
#### • Molecule 1: CCA-Adding Enzyme



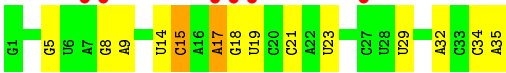
#### • Molecule 2: RNA (35-MER)







● Molecule 2: RNA (35-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.98 Å   215.83 Å   58.39 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	46.63 – 1.95 46.61 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.63-1.95) 98.0 (46.61-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 1.95 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.211   ,   0.248 0.211   ,   0.247	Depositor DCC
$R_{free}$ test set	5031 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9437	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, EDO, POP, SO4

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	0.62	1/3750 (0.0%)	0.77	11/5039 (0.2%)
1	B	0.48	0/3720	0.60	2/4998 (0.0%)
2	C	0.93	0/846	1.44	7/1315 (0.5%)
2	D	0.75	0/846	1.30	7/1315 (0.5%)
All	All	0.62	1/9162 (0.0%)	0.88	27/12667 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	CYS	CB-SG	-8.16	1.68	1.82

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ARG	NE-CZ-NH2	-13.14	113.73	120.30
2	D	17	A	C1'-O4'-C4'	-12.12	100.20	109.90
1	A	224	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	A	224	ARG	NE-CZ-NH2	-8.90	115.85	120.30
2	C	31	C	N1-C1'-C2'	8.61	125.20	114.00
1	A	274	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	A	78	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	A	390	ARG	NE-CZ-NH2	-7.16	116.72	120.30
2	C	24	U	O4'-C1'-N1	7.15	113.92	108.20
2	D	17	A	O4'-C1'-N9	6.80	113.64	108.20
1	A	390	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	D	17	A	C3'-C2'-C1'	-6.29	96.47	101.50
2	C	30	C	N1-C1'-C2'	6.26	122.14	114.00
1	A	299	ARG	NE-CZ-NH2	-6.10	117.25	120.30
2	D	17	A	P-O3'-C3'	5.88	126.76	119.70
2	D	14	U	O4'-C1'-N1	5.87	112.90	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	224	ARG	CD-NE-CZ	5.60	131.44	123.60
2	C	23	U	O4'-C1'-N1	5.29	112.43	108.20
2	C	13	U	O4'-C1'-N1	5.27	112.42	108.20
2	D	15	C	N3-C2-O2	-5.25	118.22	121.90
1	B	274	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	38	LEU	CA-CB-CG	5.23	127.33	115.30
2	C	10	U	O4'-C1'-N1	5.20	112.36	108.20
2	C	35[B]	A	C3'-C2'-C1'	-5.13	97.39	101.50
1	A	274	ARG	CG-CD-NE	-5.12	101.05	111.80
2	D	15	C	O4'-C1'-N1	5.07	112.25	108.20

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	3666	0	3663	61	0
1	B	3637	0	3636	70	0
2	C	758	0	385	8	0
2	D	758	0	386	10	0
3	A	31	0	5	2	0
3	B	31	0	7	1	0
3	C	31	0	12	0	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	A	16	0	24	5	1
5	B	4	0	6	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	9	0	0	4	0
7	C	9	0	0	2	0
8	A	296	0	0	6	3
8	B	122	0	0	4	0
8	C	44	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	13	0	0	1	0
All	All	9437	0	8124	131	3

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 8.

All (131) 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:398:HIS:HB2	5:A:805:EDO:H11	1.24	1.19
1:B:274:ARG:NH1	1:B:332:GLU:OE2	1.83	1.10
1:B:395:THR:HG23	1:B:396:HIS:CD2	1.86	1.09
1:A:123:ILE:HG13	1:A:128:ASP:HB2	1.41	1.01
1:B:395:THR:CG2	1:B:396:HIS:HD2	1.75	1.00
1:B:395:THR:HG23	1:B:396:HIS:HD2	1.27	1.00
2:C:35[B]:A:H5"	7:C:601[B]:POP:O4	1.67	0.94
1:A:398:HIS:HB2	5:A:805:EDO:C1	1.99	0.93
1:A:296:GLN:HE22	1:A:403:ASN:HD22	1.20	0.88
1:B:274:ARG:HH12	1:B:332:GLU:CD	1.78	0.87
1:A:380:ARG:HH22	1:B:334:GLN:HE22	1.18	0.87
1:A:409:ARG:HD3	5:A:801:EDO:H12	1.59	0.83
1:A:334:GLN:HE22	1:B:380:ARG:HH22	1.27	0.83
1:A:415:ILE:CG2	1:A:419:LYS:HG3	2.07	0.82
1:B:136:TRP:HE3	1:B:137:LEU:HD12	1.46	0.80
1:B:296:GLN:HE22	1:B:403:ASN:HD22	1.33	0.77
7:B:602[A]:POP:O4	2:D:35[A]:A:O3'	2.03	0.76
1:A:325:GLU:HG2	1:A:326:PHE:CD1	2.20	0.76
2:D:15:C:H5	8:D:298:HOH:O	1.67	0.76
1:B:123:ILE:HG12	1:B:128:ASP:HB2	1.68	0.75
1:A:363:ARG:NH1	1:A:378:GLU:OE2	2.20	0.74
1:B:395:THR:CG2	1:B:396:HIS:CD2	2.58	0.74
7:B:602[A]:POP:O4	2:D:35[A]:A:C3'	2.36	0.74
1:B:358:PHE:O	1:B:363:ARG:NH2	2.19	0.74
1:A:123:ILE:CG1	1:A:128:ASP:HB2	2.16	0.73
1:A:224:ARG:HD2	8:A:455:HOH:O	1.88	0.73
1:B:274:ARG:NH1	1:B:332:GLU:CD	2.39	0.72
1:A:415:ILE:HG23	1:A:419:LYS:CG	2.19	0.72
1:B:268:ARG:NH1	1:B:418:GLU:HG2	2.03	0.72
1:B:436:LYS:O	1:B:437:ASP:HB2	1.87	0.72
1:A:263:GLU:H	1:A:263:GLU:CD	1.94	0.70
1:B:32:ARG:O	1:B:36:ASP:HB2	1.93	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:OE2	1:A:76:ARG:NH1	2.25	0.69
1:A:415:ILE:HG21	1:A:419:LYS:HG3	1.75	0.67
1:B:54:LEU:HD21	1:B:152:LYS:HB3	1.75	0.67
1:A:334:GLN:NE2	1:B:380:ARG:HH22	1.95	0.65
1:A:358:PHE:O	1:A:363:ARG:NH2	2.28	0.65
1:A:336:LYS:HD3	8:B:501:HOH:O	1.96	0.64
1:B:160:ILE:O	1:B:160:ILE:HG22	1.97	0.64
1:B:154:PHE:CZ	1:B:241:LEU:HD12	2.32	0.64
1:B:11:LEU:O	1:B:15:ILE:HG22	1.97	0.64
1:A:415:ILE:HG23	1:A:419:LYS:HG2	1.81	0.61
1:B:136:TRP:CE3	1:B:137:LEU:HD12	2.34	0.61
1:A:380:ARG:HH22	1:B:334:GLN:NE2	1.96	0.61
1:A:415:ILE:HG23	1:A:419:LYS:HG3	1.78	0.60
1:A:380:ARG:HH12	1:B:334:GLN:NE2	1.99	0.60
1:A:168:ARG:HD3	8:A:518:HOH:O	2.02	0.60
7:B:602[A]:POP:O4	2:D:35[A]:A:H3'	2.01	0.59
1:B:120:PRO:HG2	1:B:220:VAL:HG22	1.83	0.59
1:A:398:HIS:HD2	2:C:23:U:OP1	1.84	0.59
1:A:415:ILE:CG2	1:A:419:LYS:CG	2.78	0.58
1:A:398:HIS:CB	5:A:805:EDO:H11	2.17	0.58
1:B:132:PHE:HB3	1:B:220:VAL:HG21	1.85	0.58
1:A:280:ALA:HB2	1:A:330:LEU:HD23	1.86	0.57
1:B:160:ILE:O	1:B:160:ILE:CG2	2.51	0.57
1:B:280:ALA:HB2	1:B:330:LEU:HD23	1.86	0.57
1:B:357:LYS:HG2	2:D:15:C:H4'	1.88	0.56
1:B:193:ARG:HD3	1:B:246:MET:HG3	1.87	0.55
1:A:341:VAL:HG22	1:A:379:MET:SD	2.47	0.55
1:B:176:GLU:O	1:B:180:VAL:HG23	2.06	0.55
2:C:35[B]:A:O3'	7:C:601[B]:POP:O6	2.25	0.54
1:B:54:LEU:HD21	1:B:152:LYS:CB	2.38	0.54
1:A:380:ARG:NH2	1:B:334:GLN:HE22	1.96	0.54
1:A:123:ILE:HG13	1:A:128:ASP:CB	2.27	0.54
1:A:341:VAL:HG21	1:B:274:ARG:HG2	1.90	0.54
1:B:302:ARG:NH2	4:B:702:SO4:O4	2.41	0.54
1:B:395:THR:HG22	1:B:396:HIS:HD2	1.70	0.53
1:A:28:GLU:O	1:A:32:ARG:HG3	2.09	0.53
1:B:381:LYS:HE3	8:B:563:HOH:O	2.07	0.52
1:A:87:LEU:HD13	1:A:102:GLY:HA3	1.91	0.52
1:A:274:ARG:NH2	1:A:433:MET:O	2.43	0.52
1:A:413:GLU:OE1	1:A:415:ILE:HD11	2.09	0.51
1:A:173:TYR:HB2	3:A:501[A]:ATP:H2'	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ARG:HB3	1:B:86:VAL:HG22	1.92	0.51
1:B:387:GLU:OE2	1:B:390:ARG:NH1	2.44	0.51
1:A:202:ASP:OD2	1:A:205:LYS:HD2	2.11	0.51
1:B:386:GLU:HB3	1:B:414:ILE:HG21	1.91	0.51
1:B:50:ARG:NH1	1:B:176:GLU:OE2	2.44	0.51
1:A:234:ASN:ND2	1:A:237:ARG:HH11	2.09	0.51
1:B:136:TRP:HE3	1:B:137:LEU:CD1	2.21	0.50
1:A:260:LEU:HD11	1:A:440:CYS:HB3	1.93	0.49
1:A:380:ARG:HH12	1:B:334:GLN:HE21	1.60	0.49
1:A:165:TYR:CE1	2:C:32:A:H1'	2.46	0.49
1:A:260:LEU:HD11	1:A:440:CYS:CB	2.43	0.49
1:B:15:ILE:HD12	1:B:16:PRO:HD2	1.94	0.49
1:A:240:HIS:HD2	8:A:503:HOH:O	1.95	0.48
1:B:64:LEU:HD11	1:B:111:VAL:HG12	1.95	0.48
7:B:602[A]:POP:O4	2:D:35[A]:A:H5''	2.12	0.48
1:B:342:PHE:CZ	1:B:378:GLU:HB3	2.49	0.48
1:A:2:LYS:HE3	1:A:3:VAL:HG22	1.96	0.47
1:B:390:ARG:NH2	8:B:486:HOH:O	2.45	0.47
1:B:317:ARG:HB2	8:B:513:HOH:O	2.15	0.47
1:B:190:LYS:HG2	1:B:193:ARG:NH2	2.30	0.46
1:A:144:LYS:NZ	8:A:494:HOH:O	2.48	0.46
1:B:65:LEU:HD23	1:B:116:LYS:HG3	1.98	0.46
1:B:398:HIS:HD2	2:D:23:U:OP1	1.99	0.46
1:A:233:ASP:O	1:A:237:ARG:HG3	2.16	0.45
1:B:51:ASN:O	1:B:149:ARG:NH2	2.50	0.45
1:B:268:ARG:HH11	1:B:418:GLU:HG2	1.79	0.45
1:A:21:VAL:O	1:A:25:ARG:HG2	2.17	0.45
1:A:2:LYS:HA	1:A:2:LYS:HD2	1.69	0.45
1:B:274:ARG:NH1	1:B:332:GLU:OE1	2.45	0.45
2:C:33:C:H5''	2:C:34[B]:C:OP2	2.17	0.45
1:A:302:ARG:NH1	8:C:36:HOH:O	2.49	0.44
1:B:28:GLU:OE2	1:B:32:ARG:NH1	2.50	0.44
1:A:366:ARG:HE	1:B:436:LYS:HG2	1.82	0.44
1:A:115:TYR:CD1	1:A:124:LYS:HB3	2.53	0.44
1:B:165:TYR:CE1	2:D:32:A:H1'	2.52	0.44
1:A:133:HIS:ND1	3:A:501[A]:ATP:O2'	2.38	0.43
1:B:84:LYS:HD2	1:B:92:ILE:HD11	1.99	0.43
1:A:105:LYS:NZ	8:A:716:HOH:O	2.52	0.43
1:B:258:HIS:O	1:B:260:LEU:HD12	2.17	0.43
2:C:7:A:H2'	2:C:8:G:O4'	2.18	0.43
1:B:396:HIS:HE1	2:D:21:C:O2'	2.01	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:PRO:HG3	1:B:132:PHE:CG	2.53	0.43
1:A:73:GLU:CD	1:A:76:ARG:NH1	2.71	0.43
3:B:502[B]:ATP:O1A	2:D:34[B]:C:O3'	2.34	0.43
1:B:436:LYS:O	1:B:437:ASP:CB	2.64	0.43
1:B:296:GLN:HE22	1:B:403:ASN:ND2	2.09	0.42
1:A:262:ILE:HD13	1:A:267:LEU:HD13	2.00	0.42
1:A:165:TYR:CD1	2:C:32:A:H1'	2.54	0.42
1:A:334:GLN:HE21	1:B:380:ARG:HH12	1.67	0.42
1:A:334:GLN:NE2	1:B:380:ARG:HH12	2.17	0.42
1:B:118:LYS:O	1:B:119:GLU:HB2	2.19	0.41
2:C:19:U:H5''	2:C:20:C:H5	1.84	0.41
1:A:97:HIS:HD2	8:A:488:HOH:O	2.03	0.41
1:A:409:ARG:CD	5:A:801:EDO:H12	2.42	0.41
1:B:428:GLU:O	1:B:432:MET:HB2	2.21	0.41
1:B:342:PHE:CE2	1:B:378:GLU:HB3	2.56	0.40
1:B:87:LEU:HD13	1:B:102:GLY:HA3	2.02	0.40
1:B:144:LYS:HE3	1:B:183:GLY:HA2	2.02	0.40

All (3) 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)
5:A:803:EDO:O1	8:A:481:HOH:O[4_444]	1.56	0.64
8:A:678:HOH:O	8:A:694:HOH:O[1_554]	1.86	0.34
8:A:729:HOH:O	8:A:734:HOH:O[4_544]	1.91	0.29

## 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	440/441 (100%)	432 (98%)	8 (2%)	0	<b>100</b> <b>100</b>

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	436/441 (99%)	419 (96%)	13 (3%)	4 (1%)	17	8
All	All	876/882 (99%)	851 (97%)	21 (2%)	4 (0%)	29	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	VAL
1	B	260	LEU
1	B	119	GLU
1	B	138	GLU

### 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 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	392/391 (100%)	375 (96%)	17 (4%)	29	16
1	B	388/391 (99%)	366 (94%)	22 (6%)	20	9
All	All	780/782 (100%)	741 (95%)	39 (5%)	24	11

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	31	LEU
1	A	40	VAL
1	A	54	LEU
1	A	76	ARG
1	A	121	LYS
1	A	123	ILE
1	A	137	LEU
1	A	145	GLU
1	A	213	GLU
1	A	224	ARG
1	A	241	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	260	LEU
1	A	263	GLU
1	A	267	LEU
1	A	325	GLU
1	A	340	ARG
1	B	20	GLU
1	B	31	LEU
1	B	38	LEU
1	B	58	LEU
1	B	80	LEU
1	B	118	LYS
1	B	123	ILE
1	B	125	SER
1	B	129	ARG
1	B	145	GLU
1	B	217	VAL
1	B	220	VAL
1	B	223	LYS
1	B	241	LEU
1	B	255	LYS
1	B	257	LYS
1	B	323	SER
1	B	340	ARG
1	B	378	GLU
1	B	395	THR
1	B	411	TYR
1	B	437	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	234	ASN
1	A	240	HIS
1	A	334	GLN
1	A	396	HIS
1	A	398	HIS
1	A	403	ASN
1	B	234	ASN
1	B	334	GLN
1	B	396	HIS
1	B	398	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	403	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	33/35 (94%)	5 (15%)	2 (6%)
2	D	33/35 (94%)	7 (21%)	2 (6%)
All	All	66/70 (94%)	12 (18%)	4 (6%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	18	G
2	C	19	U
2	C	20	C
2	C	28	U
2	C	29	U
2	D	5	G
2	D	8	G
2	D	9	A
2	D	17	A
2	D	18	G
2	D	19	U
2	D	29	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	18	G
2	C	19	U
2	D	17	A
2	D	19	U

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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[A]	6	26,33,33	1.09	1 (3%)	31,52,52	1.41	3 (9%)
5	EDO	A	804	-	3,3,3	0.40	0	2,2,2	0.50	0
5	EDO	A	805	-	3,3,3	0.38	0	2,2,2	0.62	0
5	EDO	B	802	-	3,3,3	0.49	0	2,2,2	0.34	0
4	SO4	A	701	-	4,4,4	0.20	0	6,6,6	0.13	0
3	ATP	C	851	-	26,33,33	1.03	2 (7%)	31,52,52	1.39	5 (16%)
7	POP	C	601[B]	-	6,8,8	0.69	0	13,13,13	1.31	1 (7%)
5	EDO	A	801	-	3,3,3	0.48	0	2,2,2	0.26	0
4	SO4	B	702	-	4,4,4	0.16	0	6,6,6	0.12	0
7	POP	B	602[A]	-	6,8,8	0.67	0	13,13,13	1.27	2 (15%)
5	EDO	A	803	-	3,3,3	0.38	0	2,2,2	0.26	0
3	ATP	B	502[B]	6	26,33,33	1.01	2 (7%)	31,52,52	1.38	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[A]	6	-	4/18/38/38	0/3/3/3
5	EDO	A	804	-	-	0/1/1/1	-
5	EDO	A	805	-	-	1/1/1/1	-
5	EDO	B	802	-	-	1/1/1/1	-
3	ATP	C	851	-	-	6/18/38/38	0/3/3/3
7	POP	C	601[B]	-	-	2/6/6/6	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	801	-	-	0/1/1/1	-
7	POP	B	602[A]	-	-	0/6/6/6	-
5	EDO	A	803	-	-	1/1/1/1	-
3	ATP	B	502[B]	6	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	851	ATP	C5-C4	2.81	1.48	1.40
3	B	502[B]	ATP	C5-C4	2.73	1.48	1.40
3	A	501[A]	ATP	C5-C4	2.63	1.47	1.40
3	C	851	ATP	C2-N3	2.23	1.35	1.32
3	B	502[B]	ATP	C2-N3	2.01	1.35	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501[A]	ATP	N3-C2-N1	-3.76	122.80	128.68
3	B	502[B]	ATP	N3-C2-N1	-3.45	123.29	128.68
3	C	851	ATP	N3-C2-N1	-3.33	123.47	128.68
3	A	501[A]	ATP	C4-C5-N7	-3.31	105.95	109.40
3	C	851	ATP	PA-O3A-PB	-3.00	122.53	132.83
7	C	601[B]	POP	P2-O-P1	-2.97	122.62	132.83
3	B	502[B]	ATP	PA-O3A-PB	-2.91	122.85	132.83
3	C	851	ATP	C3'-C2'-C1'	2.86	105.28	100.98
3	B	502[B]	ATP	C3'-C2'-C1'	2.84	105.26	100.98
7	B	602[A]	POP	P2-O-P1	-2.74	123.43	132.83
3	C	851	ATP	C4-C5-N7	-2.63	106.66	109.40
3	B	502[B]	ATP	C4-C5-N7	-2.62	106.67	109.40
3	A	501[A]	ATP	C2-N1-C6	2.35	122.77	118.75
3	B	502[B]	ATP	PB-O3B-PG	-2.18	125.35	132.83
3	C	851	ATP	PB-O3B-PG	-2.06	125.75	132.83
7	B	602[A]	POP	O5-P2-O	2.06	111.54	104.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501[A]	ATP	C5'-O5'-PA-O1A
3	C	851	ATP	C5'-O5'-PA-O1A
7	C	601[B]	POP	P1-O-P2-O5

*Continued on next page...*

*Continued from previous page...*

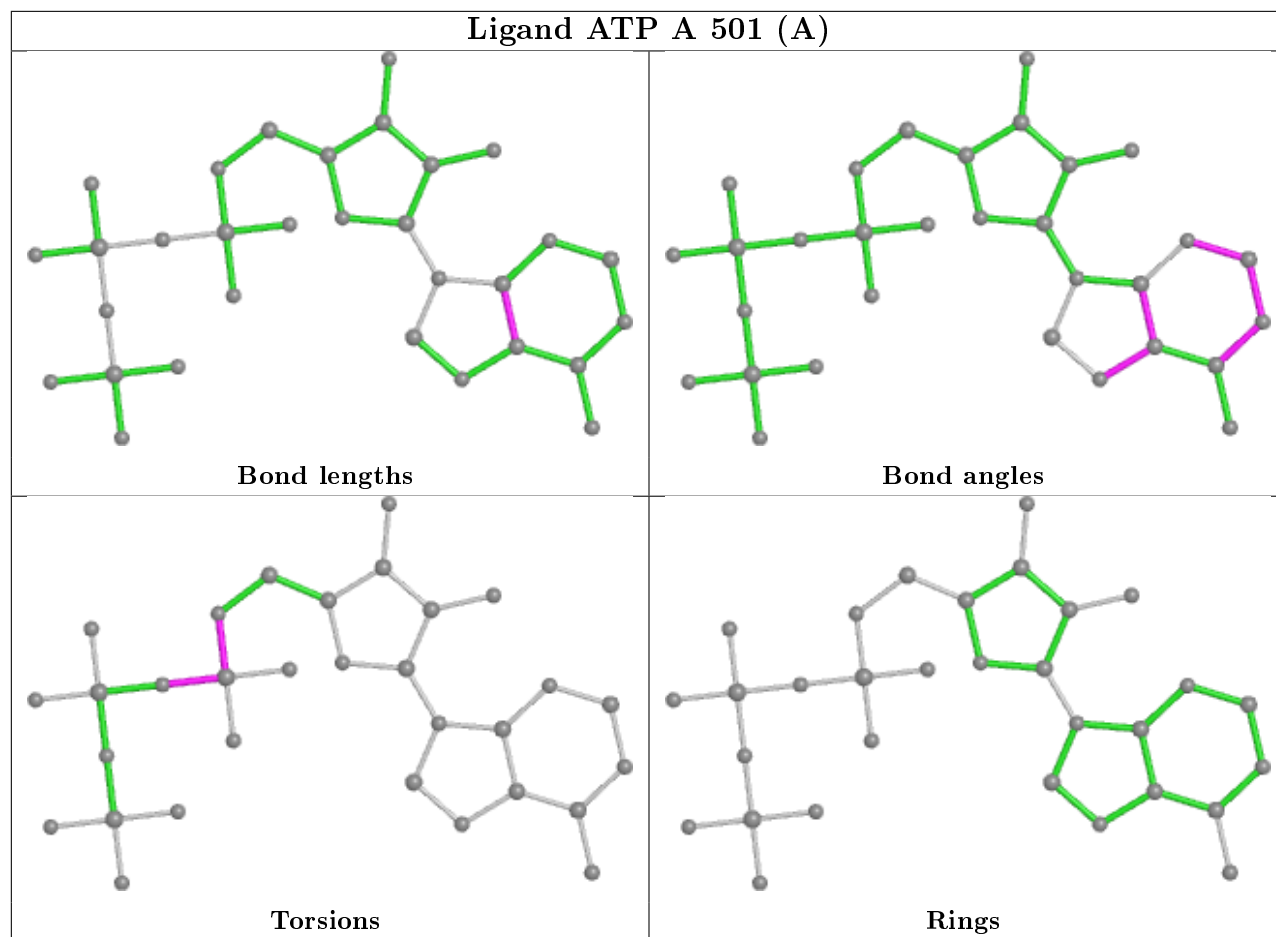
Mol	Chain	Res	Type	Atoms
3	B	502[B]	ATP	PB-O3A-PA-O5'
3	B	502[B]	ATP	C5'-O5'-PA-O1A
3	C	851	ATP	C3'-C4'-C5'-O5'
3	C	851	ATP	O4'-C4'-C5'-O5'
3	A	501[A]	ATP	PB-O3A-PA-O5'
3	C	851	ATP	C4'-C5'-O5'-PA
3	A	501[A]	ATP	C5'-O5'-PA-O3A
3	C	851	ATP	C5'-O5'-PA-O3A
3	B	502[B]	ATP	C5'-O5'-PA-O3A
3	A	501[A]	ATP	C5'-O5'-PA-O2A
3	C	851	ATP	C5'-O5'-PA-O2A
3	B	502[B]	ATP	C5'-O5'-PA-O2A
7	C	601[B]	POP	P1-O-P2-O4
5	B	802	EDO	O1-C1-C2-O2
5	A	803	EDO	O1-C1-C2-O2
5	A	805	EDO	O1-C1-C2-O2

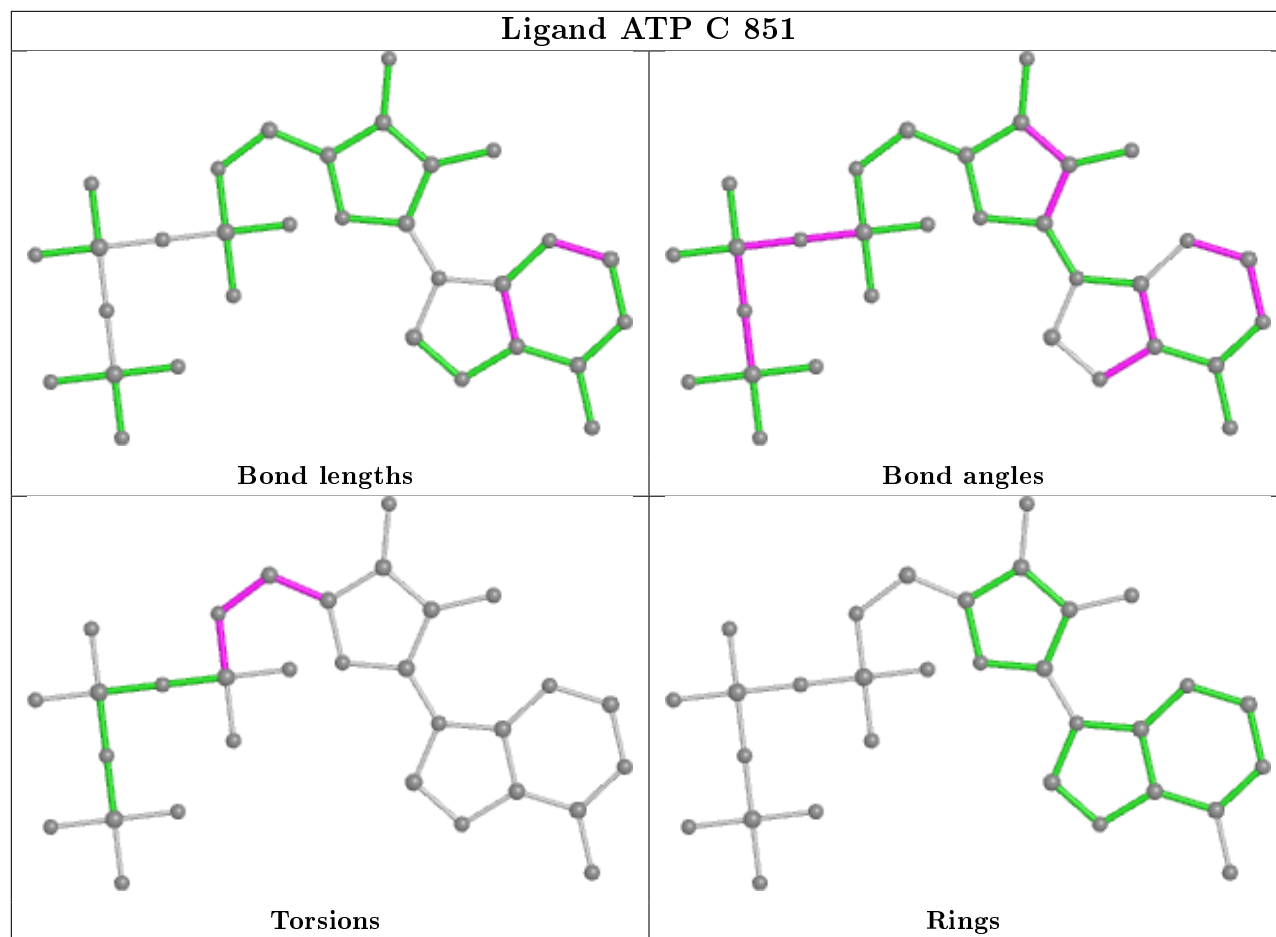
There are no ring outliers.

8 monomers are involved in 16 short contacts:

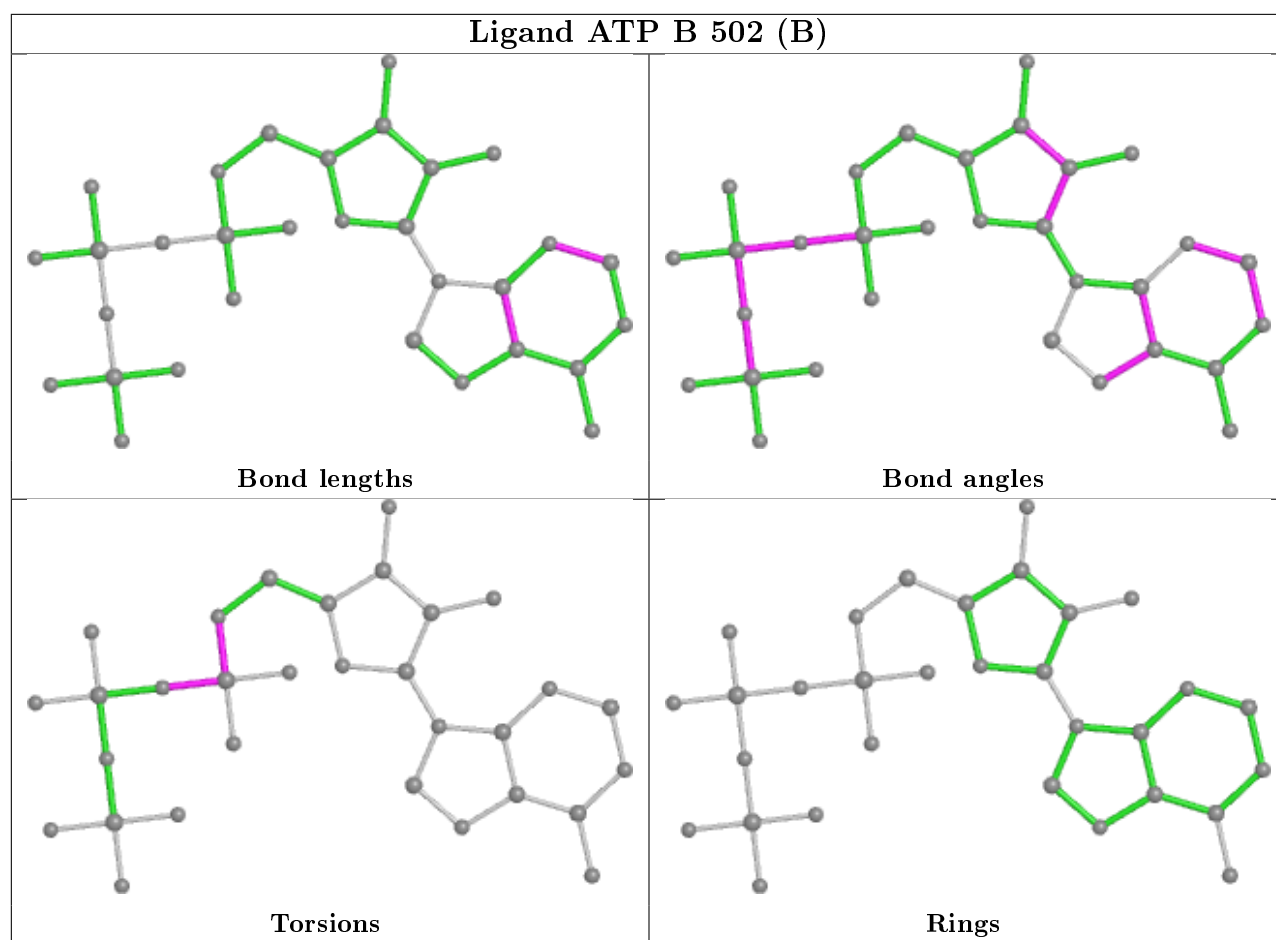
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501[A]	ATP	2	0
5	A	805	EDO	3	0
7	C	601[B]	POP	2	0
5	A	801	EDO	2	0
4	B	702	SO4	1	0
7	B	602[A]	POP	4	0
5	A	803	EDO	0	1
3	B	502[B]	ATP	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	441/441 (100%)	0.40	8 (1%) 68 76	19, 29, 51, 84	1 (0%)
1	B	437/441 (99%)	0.98	72 (16%) 1 2	23, 56, 113, 141	0
2	C	35/35 (100%)	0.33	1 (2%) 51 60	15, 56, 86, 100	1 (2%)
2	D	35/35 (100%)	0.94	6 (17%) 1 2	40, 71, 142, 157	1 (2%)
All	All	948/952 (99%)	0.69	87 (9%) 9 14	15, 38, 107, 157	3 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	LEU	12.2
1	B	3	VAL	9.6
2	D	18	G	7.5
1	B	1	MET	7.0
1	B	38	LEU	6.8
1	B	6	ILE	6.7
1	B	258	HIS	6.0
1	B	262	ILE	5.7
2	C	18	G	5.7
1	B	261	GLU	5.7
1	B	118	LYS	5.4
1	B	31	LEU	5.2
1	B	5	GLU	4.9
1	B	204	ALA	4.4
1	B	39	GLY	4.2
1	B	116	LYS	4.0
1	B	135	LYS	3.9
1	B	8	GLU	3.9
1	B	9	LYS	3.9
1	B	122	ASN	3.9
2	D	19	U	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	251	LEU	3.8
1	B	180	VAL	3.7
1	B	247	GLU	3.7
1	B	123	ILE	3.6
1	A	22	ARG	3.6
1	B	207	GLU	3.5
1	B	206	GLY	3.4
1	A	418	GLU	3.4
1	B	121	LYS	3.3
1	B	259	PRO	3.3
1	B	2	LYS	3.3
1	B	20	GLU	3.3
1	A	1	MET	3.3
1	B	74	GLU	3.2
1	B	18	GLU	3.2
2	D	17	A	3.2
1	B	35	LEU	3.1
1	B	66	PHE	3.1
1	B	22	ARG	3.1
2	D	7	A	3.0
1	B	119	GLU	3.0
1	B	104	VAL	2.9
1	B	212	GLU	2.9
1	B	418	GLU	2.9
1	B	186	LEU	2.9
1	A	194	ARG	2.8
1	B	160	ILE	2.8
1	B	15	ILE	2.8
1	B	105	LYS	2.7
1	B	11	LEU	2.7
1	B	40	VAL	2.7
1	B	132	PHE	2.7
1	B	49	ALA	2.6
1	B	210	LYS	2.6
1	B	257	LYS	2.6
1	B	208	VAL	2.6
1	B	89	SER	2.5
1	B	195	TRP	2.5
1	B	220	VAL	2.5
1	B	69	GLU	2.5
1	A	5	GLU	2.5
1	B	222	GLU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	198	ARG	2.5
1	B	422	LYS	2.4
1	B	103	VAL	2.4
1	B	142	LYS	2.4
1	B	117	LEU	2.3
1	B	23	LYS	2.3
1	B	209	ARG	2.3
1	A	353	ARG	2.3
1	B	266	ARG	2.3
1	B	141	ILE	2.3
1	B	150	LEU	2.3
1	B	223	LYS	2.2
1	A	160	ILE	2.2
2	D	8	G	2.2
1	B	194	ARG	2.2
1	B	255	LYS	2.2
1	B	411	TYR	2.2
1	B	72	LYS	2.2
1	B	54	LEU	2.1
1	A	174	LEU	2.1
1	B	4	GLU	2.1
1	B	185	PHE	2.1
2	D	27	C	2.1
1	B	144	LYS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

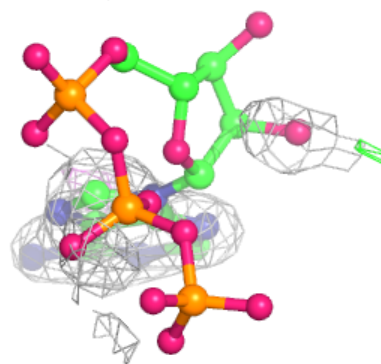
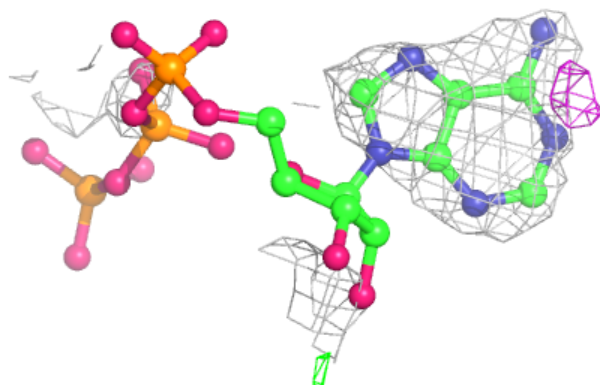
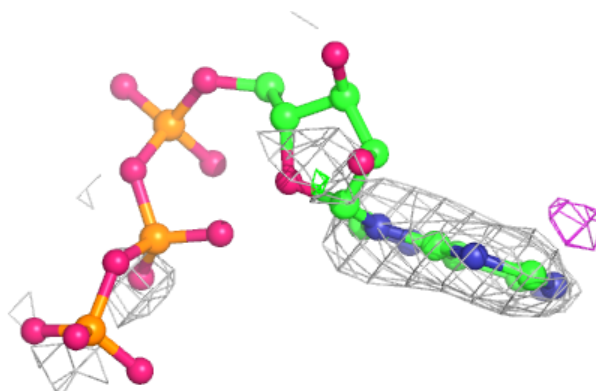
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	B	802	4/4	0.73	0.30	58,59,61,62	0
5	EDO	A	805	4/4	0.82	0.50	56,57,58,60	0
5	EDO	A	801	4/4	0.86	0.35	39,41,42,44	0
3	ATP	C	851	31/31	0.87	0.32	48,51,69,69	21
3	ATP	B	502[B]	31/31	0.92	0.12	49,51,55,55	31
5	EDO	A	804	4/4	0.92	0.17	50,50,50,51	0
6	MG	B	902	1/1	0.93	0.10	62,62,62,62	0
4	SO4	A	701	5/5	0.95	0.12	53,53,54,55	0
7	POP	B	602[A]	9/9	0.96	0.11	64,64,65,65	9
5	EDO	A	803	4/4	0.96	0.13	29,31,33,34	0
4	SO4	B	702	5/5	0.96	0.07	66,66,66,66	0
6	MG	A	901	1/1	0.98	0.11	39,39,39,39	0
3	ATP	A	501[A]	31/31	0.98	0.14	12,21,24,25	31
7	POP	C	601[B]	9/9	0.98	0.11	64,64,64,64	9

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.

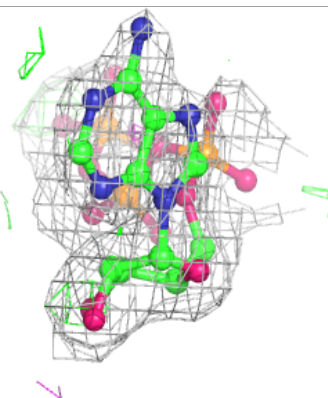
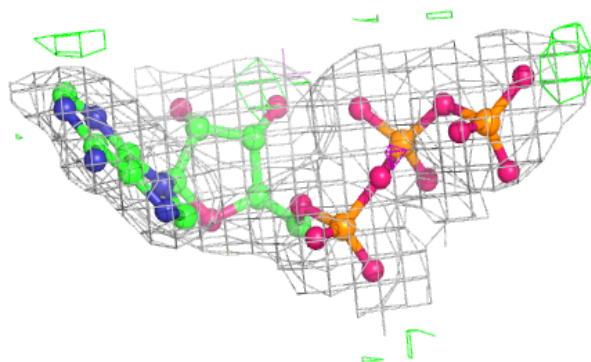
#### Electron density around ATP C 851:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

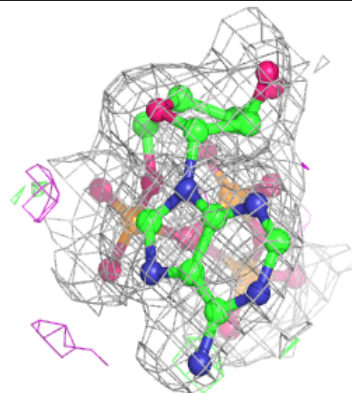
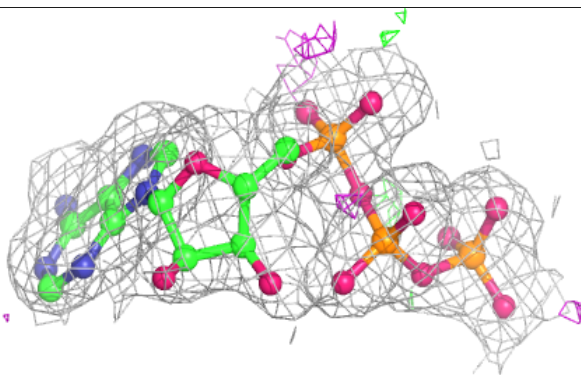
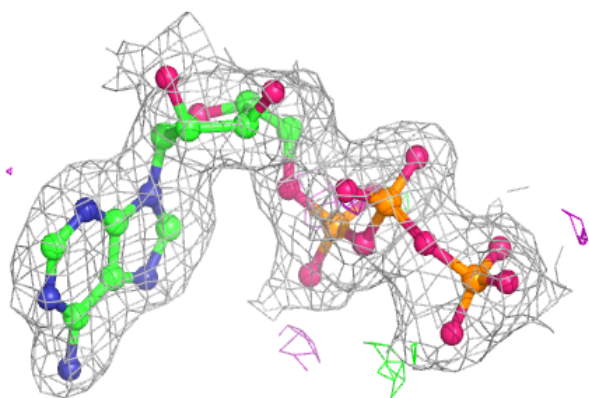


**Electron density around ATP B 502 (B):**

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

**Electron density around ATP A 501 (A):**

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



## 6.5 Other polymers

There are no such residues in this entry.