



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:09 pm BST

PDB ID : 1TFW  
Title : How CCA is added to the 3' end of immature tRNA without the use of an oligonucleotide template  
Authors : Xiong, Y.; Steitz, T.A.  
Deposited on : 2004-05-27  
Resolution : 2.20 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.

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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

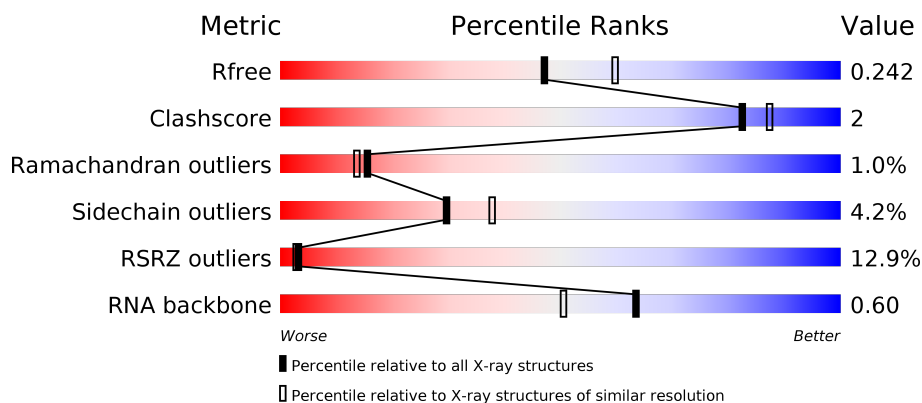
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)
RNA backbone	3102	1032 (2.60-1.80)

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	E	12	<div> <div>50%</div> <div> <div>67%</div> <div>33%</div> </div> </div>
2	G	13	<div> <div>15%</div> <div> <div>69%</div> <div>23%</div> <div>8%</div> </div> </div>
2	H	13	<div> <div>77%</div> <div>23%</div> </div>
2	I	13	<div> <div>15%</div> <div> <div>77%</div> <div>23%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	12	<div><div></div><div>67%</div><div></div><div>92%</div><div></div><div>8%</div></div>
4	J	13	<div><div></div><div>23%</div><div></div><div>46%</div><div></div><div>23%</div><div></div><div>15%</div><div></div><div>15%</div></div>
5	A	437	<div><div></div><div>5%</div><div></div><div>89%</div><div></div><div>9%</div><div></div><div>.</div></div>
5	B	437	<div><div></div><div>17%</div><div></div><div>92%</div><div></div><div>7%</div><div></div><div>.</div></div>
5	C	437	<div><div></div><div>5%</div><div></div><div>90%</div><div></div><div>9%</div><div></div><div>.</div></div>
5	D	437	<div><div></div><div>22%</div><div></div><div>92%</div><div></div><div>7%</div><div></div><div>.</div></div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17241 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 RNA chain called 5'-R(\*GP\*CP\*GP\*GP\*AP\*UP\*CP\*CP\*GP\*CP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	12	Total	C	N	O	P	0	0	0
			253	114	47	81	11			

- Molecule 2 is a RNA chain called 5'-R(\*GP\*CP\*GP\*GP\*AP\*UP\*CP\*CP\*GP\*CP\*AP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	13	Total	C	N	O	P	0	0	0
			273	123	50	88	12			
2	I	13	Total	C	N	O	P	0	0	0
			273	123	50	88	12			
2	G	13	Total	C	N	O	P	0	0	0
			273	123	50	88	12			

- Molecule 3 is a RNA chain called 5'-R(\*GP\*CP\*GP\*GP\*AP\*CP\*CP\*CP\*GP\*CP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			253	114	48	80	11			

- Molecule 4 is a RNA chain called 5'-R(\*CP\*GP\*CP\*GP\*GP\*AP\*UP\*CP\*CP\*GP\*CP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	13	Total	C	N	O	P	0	0	0
			273	123	50	88	12			

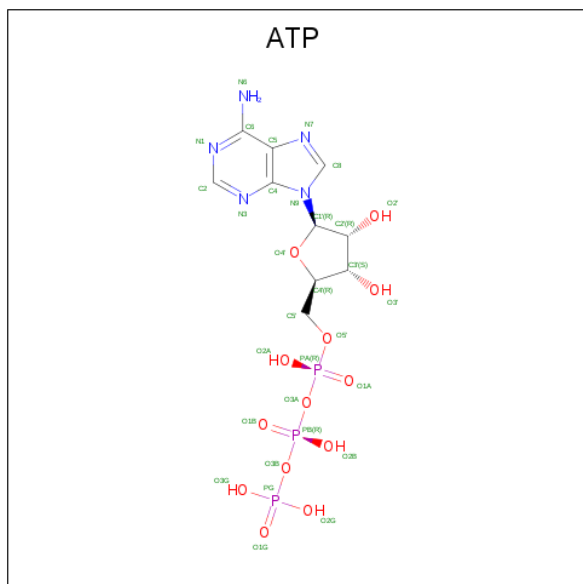
- Molecule 5 is a protein called tRNA nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			
5	B	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			
5	C	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			
5	D	437	Total	C	N	O	S	0	0	0
			3630	2333	632	652	13			

- 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	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

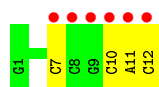
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	10	Total 10	O 10	0	0
8	H	14	Total 14	O 14	0	0
8	F	7	Total 7	O 7	0	0
8	I	7	Total 7	O 7	0	0
8	G	34	Total 34	O 34	0	0
8	J	41	Total 41	O 41	0	0
8	A	289	Total 289	O 289	0	0
8	B	211	Total 211	O 211	0	0
8	C	278	Total 278	O 278	0	0
8	D	168	Total 168	O 168	0	0

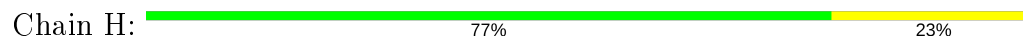
### 3 Residue-property plots [i](#)

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.

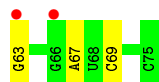
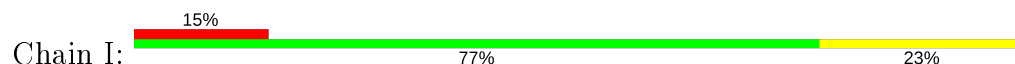
- Molecule 1: 5'-R(\*GP\*CP\*GP\*GP\*AP\*UP\*CP\*CP\*GP\*CP\*AP\*C)-3'



- Molecule 2: 5'-R(\*GP\*CP\*GP\*GP\*AP\*UP\*CP\*CP\*GP\*CP\*AP\*CP\*C)-3'



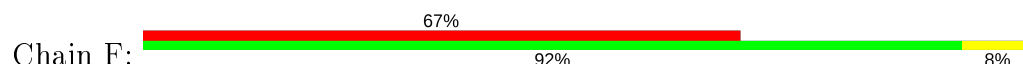
- Molecule 2: 5'-R(\*GP\*CP\*GP\*GP\*AP\*UP\*CP\*CP\*GP\*CP\*AP\*CP\*C)-3'



- Molecule 2: 5'-R(\*GP\*CP\*GP\*GP\*AP\*UP\*CP\*CP\*GP\*CP\*AP\*CP\*C)-3'



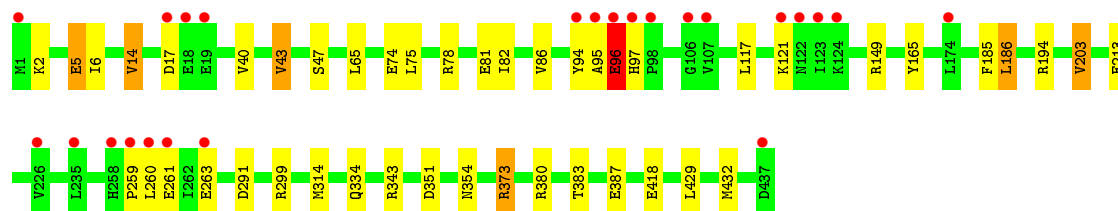
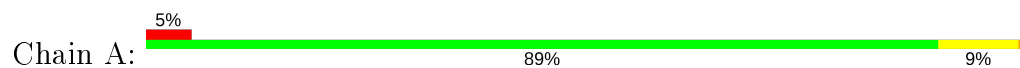
- Molecule 3: 5'-R(\*GP\*CP\*GP\*GP\*AP\*CP\*CP\*CP\*GP\*CP\*AP\*C)-3'



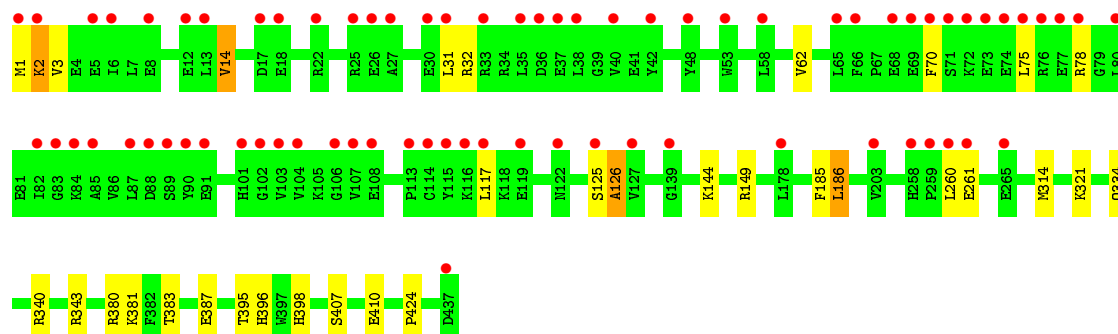
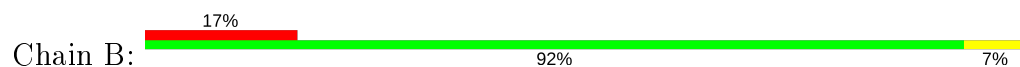
- Molecule 4: 5'-R(\*CP\*GP\*CP\*GP\*GP\*AP\*UP\*CP\*CP\*GP\*CP\*AP\*C)-3'



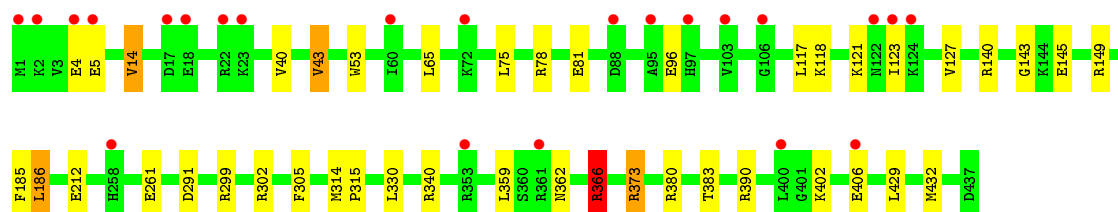
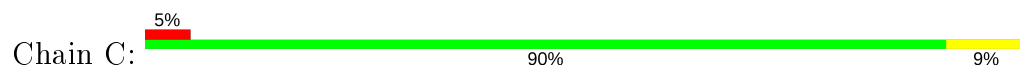
- Molecule 5: tRNA nucleotidyltransferase



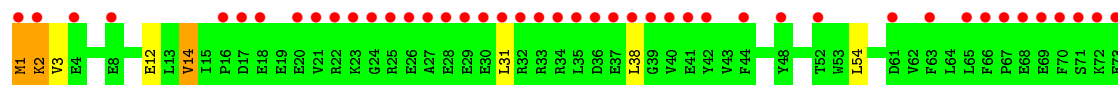
- Molecule 5: tRNA nucleotidyltransferase



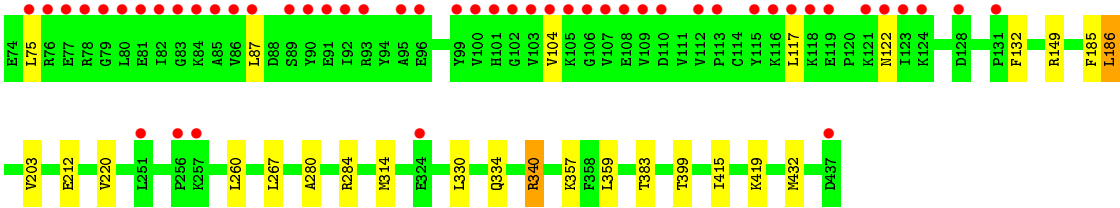
- Molecule 5: tRNA nucleotidyltransferase



- Molecule 5: tRNA nucleotidyltransferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.64Å 84.77Å 135.81Å 90.00° 104.66° 90.00°	Depositor
Resolution (Å)	47.70 – 2.20 47.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.70-2.20) 98.0 (47.66-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.192 , 0.242 0.198 , 0.242	Depositor DCC
$R_{free}$ test set	7348 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17241	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 7.30% 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

### 5.1 Standard geometry

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	E	0.67	0/282	1.21	1/438 (0.2%)
2	G	1.34	1/304 (0.3%)	1.61	3/472 (0.6%)
2	H	0.67	0/304	1.22	0/472
2	I	0.62	0/304	1.19	0/472
3	F	0.64	0/282	1.11	0/438
4	J	1.31	1/304 (0.3%)	1.74	11/472 (2.3%)
5	A	0.60	1/3713 (0.0%)	0.66	2/4987 (0.0%)
5	B	0.50	1/3713 (0.0%)	0.59	1/4987 (0.0%)
5	C	0.58	0/3713	0.68	7/4987 (0.1%)
5	D	0.47	0/3713	0.56	0/4987
All	All	0.60	4/16632 (0.0%)	0.76	25/22712 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7	U	O3'-P	11.74	1.75	1.61
5	B	387	GLU	CG-CD	6.82	1.62	1.51
4	J	65	G	C8-N7	5.27	1.34	1.30
5	A	387	GLU	CG-CD	5.14	1.59	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	299	ARG	NE-CZ-NH1	9.90	125.25	120.30
5	C	299	ARG	NE-CZ-NH2	-9.14	115.73	120.30
2	G	9	C	C2-N3-C4	8.15	123.97	119.90
4	J	61	C	N1-C2-O2	7.82	123.59	118.90
4	J	70	G	P-O3'-C3'	7.45	128.64	119.70
5	B	343	ARG	NE-CZ-NH2	-6.87	116.86	120.30
5	C	373	ARG	NE-CZ-NH1	6.77	123.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	302	ARG	NE-CZ-NH2	-6.75	116.92	120.30
4	J	69	C	O4'-C1'-N1	6.32	113.25	108.20
4	J	64	G	C8-N9-C4	-6.18	103.93	106.40
4	J	64	G	N9-C4-C5	6.05	107.82	105.40
4	J	64	G	N1-C6-O6	-5.95	116.33	119.90
4	J	61	C	N3-C2-O2	-5.94	117.75	121.90
4	J	65	G	N1-C6-O6	-5.82	116.41	119.90
2	G	9	C	N1-C2-O2	5.70	122.32	118.90
4	J	64	G	C5-C6-N1	5.61	114.30	111.50
1	E	10	C	O4'-C1'-N1	5.57	112.66	108.20
5	C	291	ASP	CB-CG-OD1	5.41	123.17	118.30
5	A	299	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	G	9	C	N3-C4-C5	-5.27	119.79	121.90
5	C	140	ARG	NE-CZ-NH2	-5.18	117.71	120.30
5	A	373	ARG	NE-CZ-NH1	5.18	122.89	120.30
4	J	65	G	C6-N1-C2	-5.16	122.00	125.10
5	C	366	ARG	NE-CZ-NH1	5.10	122.85	120.30
4	J	64	G	C6-N1-C2	-5.03	122.08	125.10

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	E	253	0	133	0	0
2	G	273	0	144	4	0
2	H	273	0	144	2	0
2	I	273	0	144	1	0
3	F	253	0	134	0	0
4	J	273	0	144	8	0
5	A	3630	0	3633	28	0
5	B	3630	0	3633	20	0
5	C	3630	0	3633	23	0
5	D	3630	0	3633	16	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
7	B	31	0	12	0	0
7	D	31	0	12	0	0
8	A	289	0	0	2	0
8	B	211	0	0	0	0
8	C	278	0	0	3	0
8	D	168	0	0	2	0
8	E	10	0	0	0	0
8	F	7	0	0	0	0
8	G	34	0	0	0	0
8	H	14	0	0	0	0
8	I	7	0	0	1	0
8	J	41	0	0	0	0
All	All	17241	0	15399	79	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 2.

All (79) 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)
2:G:12:A:H61	4:J:61:C:N4	1.54	1.05
2:G:12:A:N6	4:J:61:C:H42	1.58	1.01
5:C:402:LYS:O	5:C:406:GLU:HG3	1.83	0.78
5:A:314:MET:CE	5:B:314:MET:HE3	2.19	0.72
5:C:406:GLU:HB3	8:C:438:HOH:O	1.89	0.72
5:C:14:VAL:HG13	5:C:149:ARG:HB3	1.72	0.71
5:A:314:MET:CE	5:B:314:MET:CE	2.69	0.71
5:C:314:MET:HE3	5:D:314:MET:CE	2.22	0.70
5:A:314:MET:HE2	5:B:314:MET:CE	2.23	0.68
5:A:314:MET:HE2	5:B:314:MET:HE3	1.76	0.68
5:C:314:MET:CE	5:D:314:MET:CE	2.71	0.68
5:D:14:VAL:HG13	5:D:149:ARG:HB3	1.78	0.65
5:C:402:LYS:O	5:C:406:GLU:CG	2.46	0.64
5:C:314:MET:CE	5:D:314:MET:HE3	2.30	0.60
5:B:395:THR:HG22	5:B:396:HIS:CD2	2.37	0.59
5:A:185:PHE:O	5:A:186:LEU:CB	2.48	0.59
5:A:14:VAL:HG13	5:A:149:ARG:HB3	1.85	0.58
5:C:366:ARG:HH11	5:C:366:ARG:HG3	1.68	0.57
5:B:31:LEU:HD21	5:B:62:VAL:HG21	1.85	0.57
4:J:70:G:O2'	4:J:71:C:H4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:69:C:H4'	5:A:291:ASP:OD2	2.06	0.56
5:A:40:VAL:HG21	5:A:82:ILE:HD13	1.88	0.56
2:G:12:A:H61	4:J:61:C:H42	0.75	0.56
5:B:14:VAL:HG13	5:B:149:ARG:HB3	1.89	0.55
5:B:125:SER:O	5:B:126:ALA:HB2	2.10	0.52
5:C:185:PHE:O	5:C:186:LEU:CB	2.58	0.52
5:C:314:MET:CE	5:D:314:MET:HE2	2.39	0.51
5:A:43:VAL:HG22	5:A:65:LEU:HD11	1.92	0.50
5:D:280:ALA:HB2	5:D:330:LEU:HD23	1.94	0.50
5:B:185:PHE:O	5:B:186:LEU:CB	2.59	0.50
5:C:390:ARG:NH1	8:C:697:HOH:O	2.44	0.50
5:D:203:VAL:HG23	8:D:1669:HOH:O	2.11	0.50
5:B:125:SER:O	5:B:126:ALA:CB	2.59	0.50
5:C:314:MET:HE3	5:D:314:MET:HE2	1.94	0.49
5:A:314:MET:HE3	5:B:314:MET:CE	2.41	0.49
5:A:5:GLU:HG2	5:A:6:ILE:N	2.27	0.49
5:A:43:VAL:CG2	5:A:65:LEU:HD11	2.42	0.49
2:G:14:C:C5	5:C:127:VAL:HG22	2.49	0.48
5:A:78:ARG:NH1	5:A:81:GLU:OE1	2.46	0.48
5:A:380:ARG:HH22	5:B:334:GLN:NE2	2.12	0.48
5:A:95:ALA:O	5:A:96:GLU:CG	2.62	0.47
5:A:74:GLU:O	5:A:78:ARG:HG2	2.14	0.47
5:C:143:GLY:N	5:C:145:GLU:OE1	2.47	0.47
5:B:1:MET:O	5:B:2:LYS:CB	2.63	0.47
5:B:185:PHE:O	5:B:186:LEU:HB3	2.15	0.46
5:B:125:SER:OG	5:B:126:ALA:N	2.48	0.46
5:D:340:ARG:HD2	8:D:1618:HOH:O	2.15	0.46
5:A:373:ARG:NH2	8:A:712:HOH:O	2.49	0.45
5:C:78:ARG:NH1	5:C:81:GLU:OE1	2.49	0.45
5:A:185:PHE:O	5:A:186:LEU:HB3	2.16	0.45
5:D:185:PHE:O	5:D:186:LEU:HB3	2.17	0.45
2:I:63:G:H3'	8:I:424:HOH:O	2.17	0.45
5:C:43:VAL:HG22	5:C:65:LEU:HD11	1.97	0.45
5:D:185:PHE:O	5:D:186:LEU:CB	2.63	0.44
2:H:68:U:H2'	2:H:69:C:C6	2.52	0.44
5:A:429:LEU:HD23	5:A:432:MET:CE	2.47	0.44
5:A:96:GLU:CG	5:A:97:HIS:H	2.30	0.44
5:B:321:LYS:NZ	5:B:424:PRO:O	2.51	0.44
5:B:407:SER:O	5:B:410:GLU:HG2	2.18	0.43
5:C:185:PHE:O	5:C:186:LEU:HB3	2.19	0.43
5:C:305:PHE:CE1	5:C:315:PRO:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:70:G:C2	5:A:95:ALA:HB3	2.53	0.43
5:D:1:MET:SD	5:D:2:LYS:N	2.91	0.43
5:C:429:LEU:HD23	5:C:432:MET:CE	2.48	0.43
5:A:95:ALA:O	5:A:96:GLU:HG2	2.19	0.42
5:A:334:GLN:NE2	5:B:380:ARG:HH22	2.17	0.42
5:C:366:ARG:HH11	5:C:366:ARG:CG	2.32	0.42
5:C:373:ARG:HD2	8:C:560:HOH:O	2.20	0.41
5:A:351:ASP:CG	5:A:354:ASN:HD22	2.22	0.41
4:J:70:G:N2	5:A:95:ALA:HB3	2.36	0.41
2:H:65:G:OP1	5:B:398:HIS:HD2	2.03	0.41
5:C:330:LEU:HB3	5:C:432:MET:HE1	2.01	0.41
4:J:68:C:H1'	5:A:165:TYR:CE1	2.56	0.41
5:C:380:ARG:HH22	5:D:334:GLN:NE2	2.18	0.41
5:D:132:PHE:CB	5:D:220:VAL:HG21	2.51	0.41
5:D:415:ILE:HG23	5:D:419:LYS:HD2	2.02	0.41
5:A:380:ARG:HH12	5:B:334:GLN:HE21	1.69	0.40
5:A:203:VAL:CG1	8:A:551:HOH:O	2.69	0.40
5:D:14:VAL:HG22	5:D:54:LEU:HD11	2.03	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	
5	A	435/437 (100%)	418 (96%)	12 (3%)	5 (1%)	14	12
5	B	435/437 (100%)	414 (95%)	15 (3%)	6 (1%)	11	8
5	C	435/437 (100%)	420 (97%)	12 (3%)	3 (1%)	22	22
5	D	435/437 (100%)	414 (95%)	17 (4%)	4 (1%)	17	16
All	All	1740/1748 (100%)	1666 (96%)	56 (3%)	18 (1%)	15	14

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	96	GLU
5	B	2	LYS
5	A	186	LEU
5	A	203	VAL
5	B	126	ALA
5	B	186	LEU
5	B	261	GLU
5	C	117	LEU
5	C	121	LYS
5	C	186	LEU
5	D	2	LYS
5	D	117	LEU
5	D	186	LEU
5	A	259	PRO
5	B	117	LEU
5	A	117	LEU
5	B	3	VAL
5	D	3	VAL

### 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	
5	A	387/387 (100%)	368 (95%)	19 (5%)	25	31
5	B	387/387 (100%)	377 (97%)	10 (3%)	46	58
5	C	387/387 (100%)	370 (96%)	17 (4%)	28	35
5	D	387/387 (100%)	368 (95%)	19 (5%)	25	31
All	All	1548/1548 (100%)	1483 (96%)	65 (4%)	30	38

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	2	LYS
5	A	5	GLU
5	A	14	VAL
5	A	17	ASP

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Mol	Chain	Res	Type
5	A	43	VAL
5	A	47	SER
5	A	75	LEU
5	A	86	VAL
5	A	94	TYR
5	A	96	GLU
5	A	121	LYS
5	A	194	ARG
5	A	213	GLU
5	A	260	LEU
5	A	261	GLU
5	A	263	GLU
5	A	343	ARG
5	A	383	THR
5	A	418	GLU
5	B	14	VAL
5	B	32	ARG
5	B	70	PHE
5	B	75	LEU
5	B	78	ARG
5	B	144	LYS
5	B	260	LEU
5	B	340	ARG
5	B	381	LYS
5	B	383	THR
5	C	4	GLU
5	C	5	GLU
5	C	14	VAL
5	C	40	VAL
5	C	43	VAL
5	C	53	TRP
5	C	75	LEU
5	C	96	GLU
5	C	118	LYS
5	C	123	ILE
5	C	212	GLU
5	C	261	GLU
5	C	340	ARG
5	C	359	LEU
5	C	362	ASN
5	C	366	ARG
5	C	383	THR

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Mol	Chain	Res	Type
5	D	1	MET
5	D	12	GLU
5	D	14	VAL
5	D	31	LEU
5	D	38	LEU
5	D	75	LEU
5	D	87	LEU
5	D	104	VAL
5	D	122	ASN
5	D	212	GLU
5	D	260	LEU
5	D	267	LEU
5	D	284	ARG
5	D	340	ARG
5	D	357	LYS
5	D	359	LEU
5	D	383	THR
5	D	399	THR
5	D	432	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	51	ASN
5	A	334	GLN
5	A	348	GLN
5	A	362	ASN
5	B	51	ASN
5	B	334	GLN
5	B	354	ASN
5	B	396	HIS
5	B	398	HIS
5	C	51	ASN
5	C	122	ASN
5	C	334	GLN
5	C	348	GLN
5	D	334	GLN
5	D	396	HIS
5	D	398	HIS

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	11/12 (91%)	3 (27%)	0
2	G	12/13 (92%)	1 (8%)	0
2	H	12/13 (92%)	0	0
2	I	12/13 (92%)	2 (16%)	0
3	F	11/12 (91%)	1 (9%)	0
4	J	12/13 (92%)	2 (16%)	1 (8%)
All	All	70/76 (92%)	9 (12%)	1 (1%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	7	C
1	E	11	A
1	E	12	C
3	F	12	C
2	I	67	A
2	I	69	C
2	G	14	C
4	J	69	C
4	J	71	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	J	70	G

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
7	ATP	B	1501	6	26,33,33	1.04	3 (11%)	31,52,52	1.27	3 (9%)
7	ATP	D	1502	6	26,33,33	0.95	2 (7%)	31,52,52	1.33	4 (12%)

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
7	ATP	B	1501	6	-	3/18/38/38	0/3/3/3
7	ATP	D	1502	6	-	2/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1501	ATP	C5-C4	2.70	1.48	1.40
7	D	1502	ATP	C5-C4	2.30	1.47	1.40
7	B	1501	ATP	C2-N3	2.24	1.35	1.32
7	B	1501	ATP	O4'-C1'	2.21	1.44	1.41
7	D	1502	ATP	O4'-C1'	2.19	1.44	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1502	ATP	N3-C2-N1	-4.18	122.14	128.68
7	B	1501	ATP	N3-C2-N1	-3.66	122.96	128.68
7	D	1502	ATP	PB-O3B-PG	-2.53	124.15	132.83
7	D	1502	ATP	C4-C5-N7	-2.29	107.01	109.40
7	B	1501	ATP	C4-C5-N7	-2.25	107.06	109.40
7	D	1502	ATP	C2-N1-C6	2.12	122.37	118.75
7	B	1501	ATP	C2-N1-C6	2.08	122.31	118.75

There are no chirality outliers.

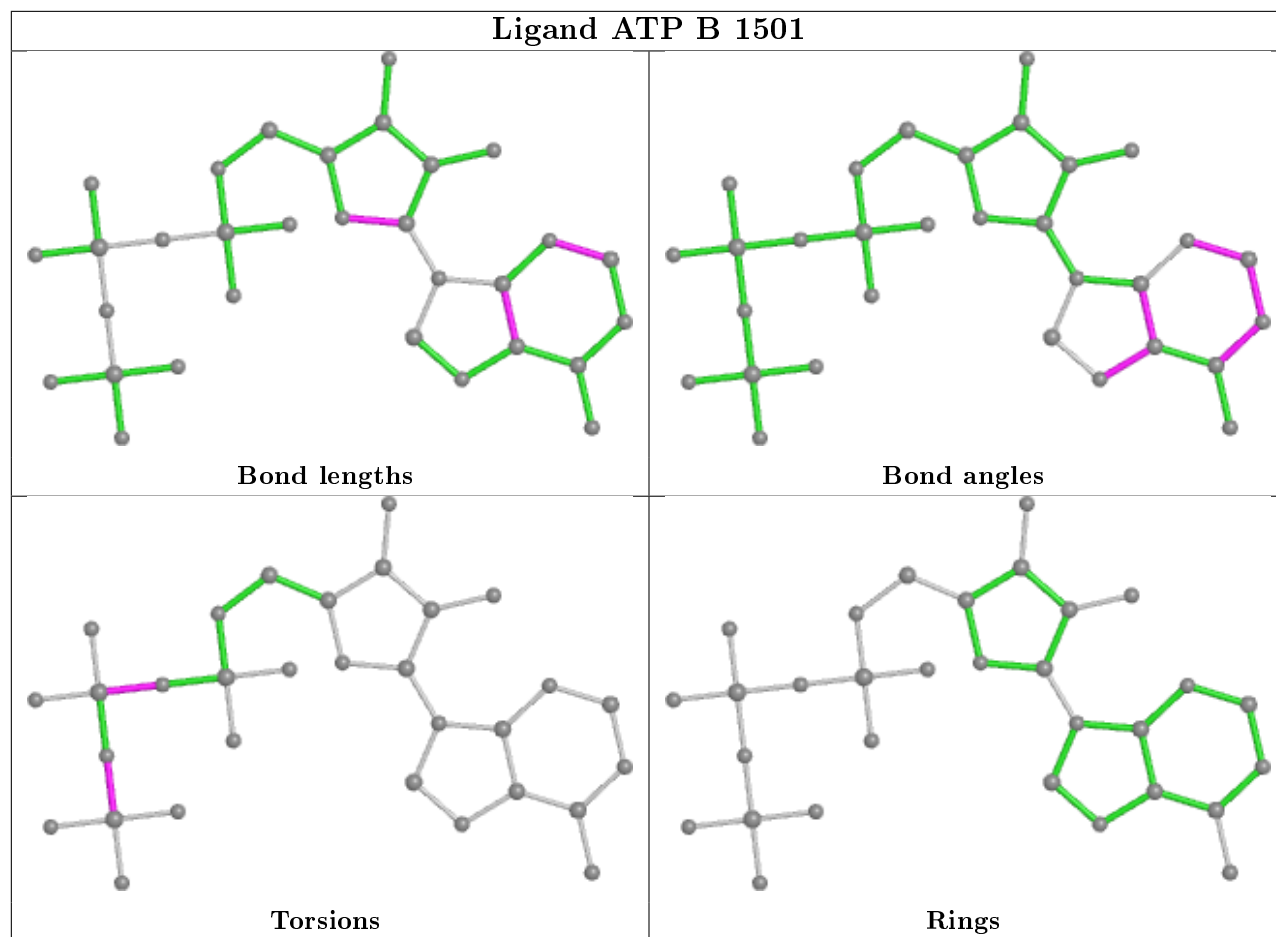
All (5) torsion outliers are listed below:

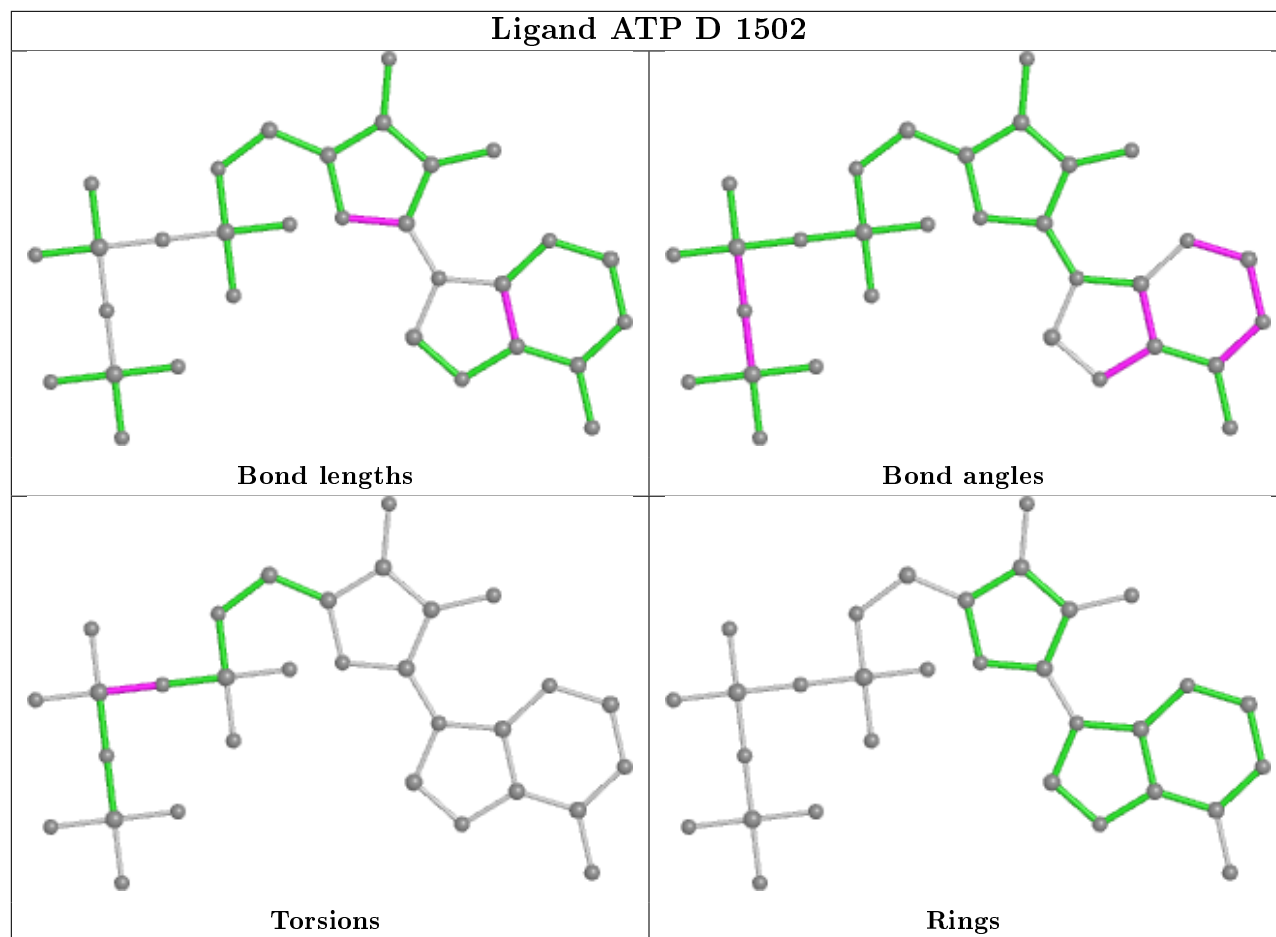
Mol	Chain	Res	Type	Atoms
7	B	1501	ATP	PB-O3B-PG-O3G
7	B	1501	ATP	PA-O3A-PB-O2B
7	D	1502	ATP	PA-O3A-PB-O2B
7	D	1502	ATP	PA-O3A-PB-O1B
7	B	1501	ATP	PB-O3B-PG-O1G

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 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	E	12/12 (100%)	1.69	6 (50%) 0 0	46, 50, 65, 73	0
2	G	13/13 (100%)	1.34	2 (15%) 2 1	41, 48, 85, 99	0
2	H	13/13 (100%)	0.71	0 100 100	43, 50, 58, 64	0
2	I	13/13 (100%)	1.01	2 (15%) 2 1	42, 49, 64, 65	0
3	F	12/12 (100%)	2.75	8 (66%) 0 0	50, 54, 64, 72	0
4	J	13/13 (100%)	1.13	3 (23%) 0 0	26, 37, 99, 105	0
5	A	437/437 (100%)	0.63	24 (5%) 25 24	38, 48, 64, 76	0
5	B	437/437 (100%)	1.00	73 (16%) 1 1	37, 48, 58, 69	0
5	C	437/437 (100%)	0.59	23 (5%) 26 25	40, 48, 63, 75	0
5	D	437/437 (100%)	1.25	94 (21%) 0 0	40, 48, 57, 70	0
All	All	1824/1824 (100%)	0.89	235 (12%) 3 3	26, 48, 62, 105	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	40	VAL	11.6
5	A	1	MET	9.1
5	D	31	LEU	9.1
5	B	70	PHE	8.6
5	D	118	LYS	7.8
5	D	85	ALA	7.4
5	D	33	ARG	7.1
5	D	22	ARG	6.9
5	B	66	PHE	6.9
5	C	1	MET	6.8
5	B	1	MET	6.8
5	B	89	SER	6.6
5	D	39	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
5	D	103	VAL	6.6
5	A	94	TYR	6.5
5	D	1	MET	6.4
5	D	66	PHE	6.2
5	D	70	PHE	6.0
5	D	63	PHE	6.0
5	B	69	GLU	5.9
5	D	42	TYR	5.8
5	A	123	ILE	5.8
5	B	115	TYR	5.8
5	B	103	VAL	5.7
5	D	30	GLU	5.6
5	B	35	LEU	5.6
5	B	258	HIS	5.6
5	D	38	LEU	5.5
5	D	91	GLU	5.4
5	D	437	ASP	5.4
5	D	121	LYS	5.3
3	F	12	C	5.3
5	D	115	TYR	5.2
5	D	80	LEU	5.2
5	D	117	LEU	5.2
5	D	78	ARG	5.1
5	B	80	LEU	5.0
5	B	17	ASP	5.0
5	D	106	GLY	5.0
5	D	104	VAL	4.9
5	D	17	ASP	4.7
5	D	107	VAL	4.7
5	D	76	ARG	4.7
5	B	102	GLY	4.6
5	A	95	ALA	4.6
5	B	33	ARG	4.5
5	D	84	LYS	4.5
5	A	98	PRO	4.5
5	D	73	GLU	4.5
5	A	96	GLU	4.5
5	A	261	GLU	4.5
5	D	79	GLY	4.4
5	B	259	PRO	4.4
5	B	71	SER	4.4
5	D	35	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
5	D	83	GLY	4.3
5	C	124	LYS	4.3
5	D	20	GLU	4.3
5	B	68	GLU	4.3
5	A	259	PRO	4.3
5	D	26	GLU	4.3
5	B	42	TYR	4.2
5	B	5	GLU	4.2
5	D	92	ILE	4.2
5	D	48	TYR	4.2
5	D	25	ARG	4.2
5	D	37	GLU	4.2
3	F	11	A	4.1
3	F	7	C	4.1
5	B	13	LEU	4.1
5	B	116	LYS	4.0
5	D	101	HIS	4.0
5	B	75	LEU	4.0
5	A	18	GLU	4.0
5	B	106	GLY	3.9
4	J	73	C	3.9
2	G	2	G	3.9
2	G	14	C	3.9
3	F	6	C	3.8
5	D	122	ASN	3.8
3	F	10	C	3.8
5	B	104	VAL	3.8
5	D	77	GLU	3.8
3	F	9	G	3.7
5	B	12	GLU	3.7
5	B	73	GLU	3.7
5	D	24	GLY	3.7
5	C	122	ASN	3.7
5	B	48	TYR	3.7
5	D	71	SER	3.7
5	B	26	GLU	3.6
5	D	112	VAL	3.7
5	D	86	VAL	3.6
5	A	122	ASN	3.6
5	B	91	GLU	3.6
5	B	119	GLU	3.6
1	E	11	A	3.6

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Mol	Chain	Res	Type	RSRZ
5	B	117	LEU	3.6
5	B	37	GLU	3.5
5	C	123	ILE	3.5
5	D	102	GLY	3.5
5	D	29	GLU	3.5
5	D	72	LYS	3.5
5	B	78	ARG	3.5
5	C	23	LYS	3.4
5	A	106	GLY	3.4
5	D	16	PRO	3.4
2	I	66	G	3.4
5	A	17	ASP	3.4
5	D	96	GLU	3.4
5	A	437	ASP	3.4
5	B	27	ALA	3.4
5	B	72	LYS	3.4
5	B	114	CYS	3.3
5	D	119	GLU	3.3
5	D	21	VAL	3.3
1	E	10	C	3.3
5	D	69	GLU	3.3
5	B	65	LEU	3.3
5	D	95	ALA	3.2
5	B	85	ALA	3.2
5	C	18	GLU	3.2
5	D	36	ASP	3.2
1	E	12	C	3.2
5	D	108	GLU	3.2
5	D	90	TYR	3.2
5	D	81	GLU	3.2
5	B	6	ILE	3.1
5	D	44	PHE	3.1
5	B	76	ARG	3.1
5	B	18	GLU	3.1
5	B	260	LEU	3.1
5	D	18	GLU	3.1
5	D	123	ILE	3.1
5	D	2	LYS	3.1
5	D	68	GLU	3.1
5	C	17	ASP	3.0
5	B	107	VAL	3.0
5	D	34	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
5	B	2	LYS	3.0
5	B	437	ASP	3.0
5	A	260	LEU	3.0
5	D	116	LYS	3.0
5	B	30	GLU	3.0
1	E	9	G	2.9
5	C	5	GLU	2.9
5	D	23	LYS	2.9
5	D	82	ILE	2.9
5	D	110	ASP	2.9
5	C	22	ARG	2.9
3	F	8	C	2.9
5	B	261	GLU	2.9
5	D	4	GLU	2.9
5	D	124	LYS	2.8
5	A	258	HIS	2.8
5	A	97	HIS	2.8
5	D	67	PRO	2.8
1	E	8	C	2.8
5	D	65	LEU	2.8
5	D	75	LEU	2.8
5	C	406	GLU	2.8
5	B	84	LYS	2.8
5	C	95	ALA	2.7
1	E	7	C	2.7
5	B	40	VAL	2.7
5	D	27	ALA	2.7
5	B	90	TYR	2.7
5	C	103	VAL	2.7
5	D	93	ARG	2.6
5	C	2	LYS	2.6
5	A	19	GLU	2.6
5	B	203	VAL	2.6
5	C	60	ILE	2.6
5	B	122	ASN	2.6
5	D	324	GLU	2.6
5	B	31	LEU	2.5
5	A	121	LYS	2.5
5	D	109	VAL	2.5
5	D	105	LYS	2.5
5	D	32	ARG	2.5
5	B	53	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
4	J	71	C	2.5
5	C	106	GLY	2.5
5	C	400	LEU	2.5
5	D	87	LEU	2.5
5	B	8	GLU	2.4
5	D	113	PRO	2.4
4	J	61	C	2.4
5	D	100	VAL	2.4
5	A	124	LYS	2.4
5	B	25	ARG	2.4
5	D	128	ASP	2.4
5	C	97	HIS	2.3
5	C	88	ASP	2.3
5	B	38	LEU	2.3
5	B	139	GLY	2.3
5	D	99	TYR	2.3
5	B	74	GLU	2.3
5	D	52	THR	2.3
5	D	257	LYS	2.3
5	B	108	GLU	2.3
5	B	88	ASP	2.3
5	B	87	LEU	2.3
3	F	5	A	2.2
5	B	83	GLY	2.2
5	B	36	ASP	2.2
5	B	77	GLU	2.2
5	B	22	ARG	2.2
5	D	131	PRO	2.2
5	B	178	LEU	2.2
5	C	72	LYS	2.2
5	A	174	LEU	2.2
5	D	89	SER	2.2
5	D	256	PRO	2.2
5	D	61	ASP	2.1
5	A	263	GLU	2.1
5	B	101	HIS	2.1
5	A	107	VAL	2.1
5	D	251	LEU	2.1
5	B	127	VAL	2.1
5	B	58	LEU	2.1
5	D	28	GLU	2.1
5	A	226	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
5	B	82	ILE	2.1
5	C	4	GLU	2.1
5	D	8	GLU	2.0
5	D	41	GLU	2.0
5	C	258	HIS	2.0
5	C	353	ARG	2.0
5	B	125	SER	2.0
5	B	113	PRO	2.0
5	A	235	LEU	2.0
2	I	63	G	2.0
5	B	265	GLU	2.0
5	C	361	ARG	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](#)

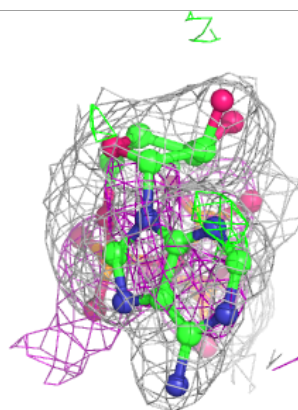
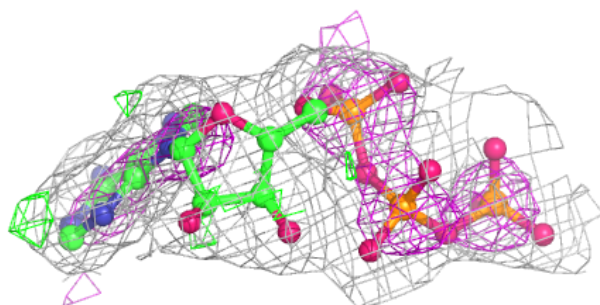
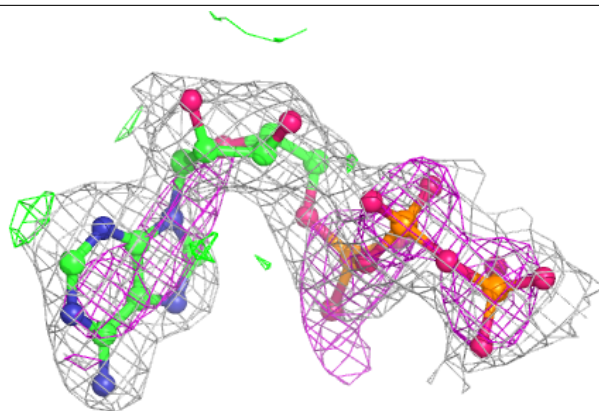
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	MG	D	1602	1/1	0.84	0.16	68,68,68,68	0
7	ATP	B	1501	31/31	0.86	0.21	63,71,73,77	0
7	ATP	D	1502	31/31	0.86	0.23	81,87,93,93	0
6	MG	B	1601	1/1	0.95	0.12	73,73,73,73	0

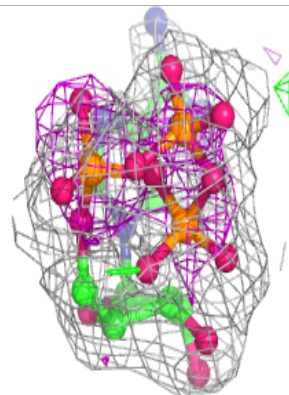
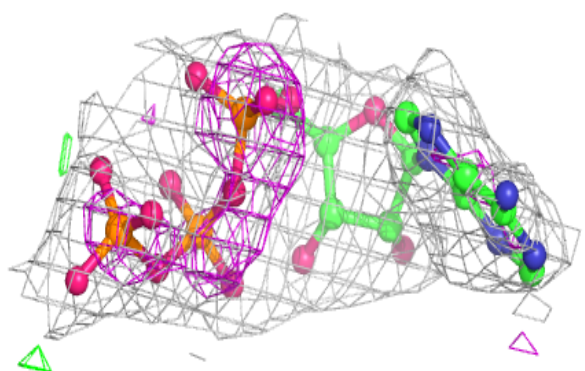
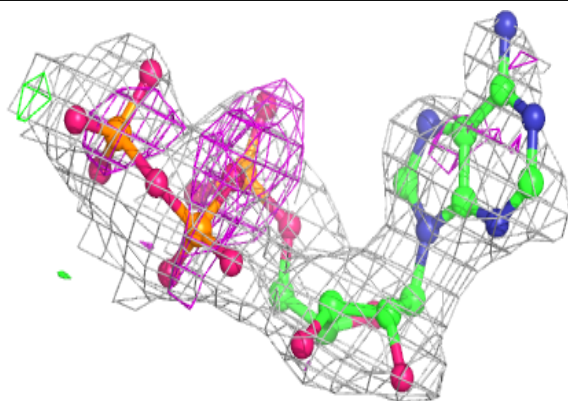
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP B 1501:**

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 D 1502:**

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)



## 6.5 Other polymers

There are no such residues in this entry.