



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:17 am GMT

PDB ID : 1A0I  
Title : ATP-DEPENDENT DNA LIGASE FROM BACTERIOPHAGE T7 COMPLEX WITH ATP  
Authors : Subramanya, H.S.; Doherty, A.J.; Ashford, S.R.; Wigley, D.B.  
Deposited on : 1997-12-01  
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

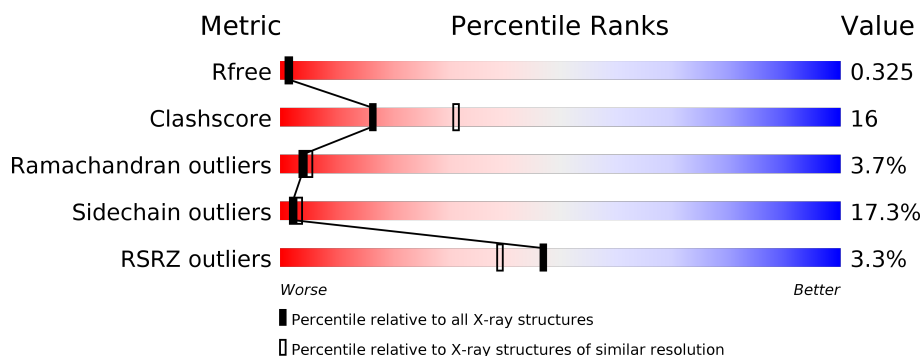
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	348	<div> <div>3%</div> <div>48%</div> <div>36%</div> <div>9%</div> <div>• 5%</div> </div>

## 2 Entry composition [i](#)

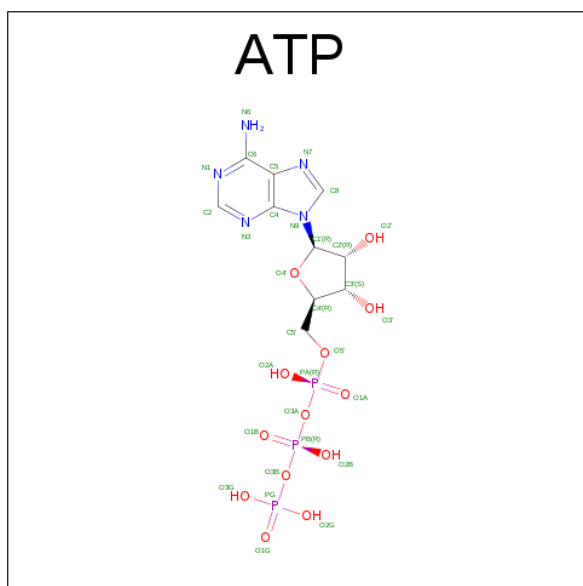
There are 3 unique types of molecules in this entry. The entry contains 2903 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	332	2679	1716	451	495	17	0	0	0

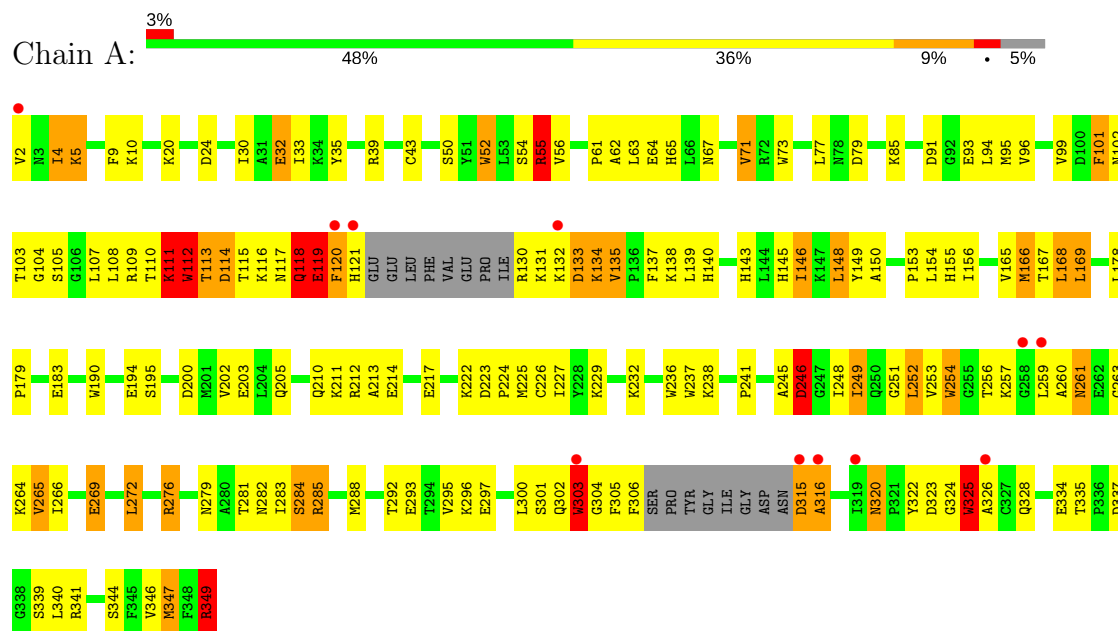
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



### 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: DNA LIGASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.70Å 85.20Å 79.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 19.87 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.6 (10.00-2.60) 99.4 (19.87-2.61)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.24 (at 2.59Å)	Xtriage
Refinement program	X-PLOR 3.0	Depositor
R, $R_{free}$	0.222 , 0.341 0.213 , 0.325	Depositor DCC
$R_{free}$ test set	680 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 122.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2903	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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: 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	0.84	0/2741	1.72	64/3699 (1.7%)

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	2

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ASP	N-CA-C	12.70	145.29	111.00
1	A	349	ARG	NE-CZ-NH2	-10.81	114.90	120.30
1	A	120	PHE	N-CA-C	10.78	140.12	111.00
1	A	349	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	133	ASP	CA-C-N	-8.11	99.36	117.20
1	A	190	TRP	CD1-CG-CD2	7.92	112.64	106.30
1	A	119	GLU	N-CA-C	-7.90	89.66	111.00
1	A	119	GLU	CA-C-N	-7.71	100.23	117.20
1	A	115	THR	N-CA-C	7.53	131.32	111.00
1	A	236	TRP	CD1-CG-CD2	7.52	112.32	106.30
1	A	325	TRP	CD1-CG-CD2	7.42	112.24	106.30
1	A	237	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	A	190	TRP	CE2-CD2-CG	-7.09	101.62	107.30
1	A	303	TRP	CE2-CD2-CG	-7.02	101.68	107.30
1	A	73	TRP	CD1-CG-CD2	7.01	111.91	106.30
1	A	112	TRP	CD1-CG-CD2	7.01	111.91	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	MET	CG-SD-CE	-6.92	89.13	100.20
1	A	55	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	284	SER	N-CA-C	6.91	129.66	111.00
1	A	112	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	A	112	TRP	CB-CG-CD1	-6.90	118.03	127.00
1	A	285	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	303	TRP	CG-CD2-CE3	6.61	139.85	133.90
1	A	236	TRP	CE2-CD2-CG	-6.58	102.04	107.30
1	A	55	ARG	CA-CB-CG	6.57	127.85	113.40
1	A	237	TRP	CE2-CD2-CG	-6.56	102.05	107.30
1	A	246	ASP	CB-CG-OD1	6.54	124.18	118.30
1	A	120	PHE	N-CA-CB	-6.48	98.94	110.60
1	A	52	TRP	CD1-CG-CD2	6.43	111.44	106.30
1	A	112	TRP	CG-CD2-CE3	6.38	139.64	133.90
1	A	131	LYS	CA-C-N	-6.36	103.20	117.20
1	A	56	VAL	N-CA-CB	-6.35	97.52	111.50
1	A	52	TRP	CE2-CD2-CG	-6.24	102.31	107.30
1	A	115	THR	CA-C-N	-6.23	103.50	117.20
1	A	316	ALA	N-CA-CB	-6.21	101.41	110.10
1	A	32	GLU	OE1-CD-OE2	-6.18	115.89	123.30
1	A	73	TRP	CE2-CD2-CG	-6.16	102.37	107.30
1	A	4	ILE	CA-C-N	-6.16	103.66	117.20
1	A	325	TRP	CE2-CD2-CG	-6.10	102.42	107.30
1	A	71	VAL	CB-CA-C	-5.98	100.05	111.40
1	A	254	TRP	CD1-CG-CD2	5.94	111.05	106.30
1	A	217	GLU	OE1-CD-OE2	-5.92	116.19	123.30
1	A	276	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	A	118	GLN	N-CA-C	-5.87	95.14	111.00
1	A	225	MET	CG-SD-CE	-5.85	90.85	100.20
1	A	347	MET	CA-CB-CG	5.83	123.21	113.30
1	A	133	ASP	C-N-CA	5.68	135.91	121.70
1	A	190	TRP	CB-CG-CD1	-5.68	119.62	127.00
1	A	254	TRP	CE2-CD2-CG	-5.65	102.78	107.30
1	A	148	LEU	CA-CB-CG	5.58	128.13	115.30
1	A	303	TRP	CB-CG-CD1	-5.55	119.79	127.00
1	A	73	TRP	CB-CG-CD1	-5.34	120.05	127.00
1	A	303	TRP	CD1-CG-CD2	5.33	110.56	106.30
1	A	265	VAL	CA-C-N	-5.32	105.50	117.20
1	A	323	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	111	LYS	C-N-CA	5.27	134.89	121.70
1	A	190	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	A	237	TRP	CG-CD2-CE3	5.24	138.61	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	LYS	N-CA-C	-5.21	96.94	111.00
1	A	190	TRP	CG-CD2-CE3	5.20	138.58	133.90
1	A	341	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	113	THR	CA-CB-CG2	5.09	119.53	112.40
1	A	237	TRP	CB-CG-CD1	-5.04	120.45	127.00
1	A	111	LYS	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLU	Mainchain,Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2679	0	2637	85	0
2	A	31	0	10	1	0
3	A	193	0	0	6	0
All	All	2903	0	2647	85	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 16.

All (85) 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:264:LYS:HD3	1:A:292:THR:HG21	1.53	0.91
1:A:322:TYR:HA	1:A:325:TRP:HE3	1.37	0.89
1:A:320:ASN:HD21	1:A:322:TYR:HB2	1.44	0.82
1:A:2:VAL:HG22	1:A:5:LYS:HB2	1.63	0.79
1:A:62:ALA:HB1	1:A:139:LEU:HB2	1.66	0.76
1:A:226:CYS:SG	1:A:229:LYS:HE3	2.28	0.74
1:A:302:GLN:OE1	1:A:316:ALA:HB1	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:TYR:HA	1:A:325:TRP:CE3	2.23	0.72
1:A:246:ASP:HB3	1:A:349:ARG:HH12	1.57	0.70
1:A:248:ILE:HD12	1:A:324:GLY:HA2	1.78	0.64
1:A:211:LYS:HA	1:A:214:GLU:HG3	1.80	0.63
1:A:109:ARG:NH1	3:A:497:HOH:O	2.34	0.60
1:A:52:TRP:H	1:A:67:ASN:ND2	2.00	0.60
1:A:52:TRP:H	1:A:67:ASN:HD21	1.51	0.59
1:A:245:ALA:O	1:A:328:GLN:HA	2.03	0.57
1:A:322:TYR:O	1:A:325:TRP:HB2	2.04	0.57
1:A:249:ILE:HG23	1:A:325:TRP:O	2.04	0.57
1:A:264:LYS:CD	1:A:292:THR:HG21	2.30	0.56
1:A:300:LEU:HD22	1:A:303:TRP:HE3	1.71	0.56
1:A:30:ILE:HB	1:A:222:LYS:HB2	1.87	0.56
1:A:249:ILE:HD12	1:A:251:GLY:H	1.71	0.56
1:A:39:ARG:NH1	2:A:1:ATP:H3'	2.21	0.56
1:A:248:ILE:HA	1:A:326:ALA:HA	1.88	0.55
1:A:256:THR:HB	1:A:260:ALA:HB3	1.89	0.54
1:A:269:GLU:HA	1:A:279:ASN:HD22	1.73	0.53
1:A:320:ASN:ND2	1:A:322:TYR:HB2	2.19	0.53
1:A:212:ARG:HH12	1:A:241:PRO:HG2	1.73	0.52
1:A:168:LEU:HB2	3:A:410:HOH:O	2.08	0.52
1:A:296:LYS:O	1:A:300:LEU:HG	2.11	0.50
1:A:300:LEU:HD22	1:A:303:TRP:CE3	2.46	0.50
1:A:99:VAL:HB	1:A:103:THR:HB	1.93	0.50
1:A:272:LEU:HD21	1:A:340:LEU:HD22	1.93	0.50
1:A:284:SER:HB3	3:A:533:HOH:O	2.11	0.50
1:A:179:PRO:O	1:A:183:GLU:HB2	2.13	0.49
1:A:104:GLY:O	1:A:108:LEU:HG	2.11	0.49
1:A:96:VAL:HG13	1:A:143:HIS:HB3	1.95	0.49
1:A:153:PRO:HG2	1:A:156:ILE:HD12	1.95	0.49
1:A:20:LYS:NZ	1:A:24:ASP:OD1	2.46	0.49
1:A:165:VAL:HG13	1:A:169:LEU:HB3	1.95	0.49
1:A:254:TRP:HE3	1:A:264:LYS:HA	1.78	0.49
1:A:281:THR:O	1:A:283:ILE:HG23	2.14	0.48
1:A:223:ASP:HB3	1:A:226:CYS:HB2	1.95	0.47
1:A:112:TRP:HA	1:A:135:VAL:O	2.14	0.47
1:A:335:THR:HB	1:A:339:SER:HB2	1.95	0.47
1:A:269:GLU:HA	1:A:279:ASN:ND2	2.30	0.47
1:A:153:PRO:HB2	1:A:155:HIS:CE1	2.50	0.46
1:A:10:LYS:HB2	1:A:232:LYS:HA	1.97	0.46
1:A:79:ASP:O	1:A:85:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:MET:HA	1:A:227:ILE:HA	1.99	0.45
1:A:328:GLN:HE21	1:A:346:VAL:HB	1.81	0.45
1:A:119:GLU:N	1:A:120:PHE:HA	2.31	0.44
1:A:140:HIS:HB3	1:A:143:HIS:CD2	2.53	0.44
1:A:65:HIS:HB3	1:A:138:LYS:HD2	2.00	0.44
1:A:101:PHE:O	1:A:102:ASN:HB2	2.18	0.44
1:A:61:PRO:HB3	1:A:111:LYS:HB3	2.00	0.44
1:A:252:LEU:HD21	1:A:295:VAL:HG21	1.99	0.44
1:A:276:ARG:NH1	1:A:337:ASP:O	2.48	0.44
1:A:33:ILE:HD12	1:A:194:GLU:OE1	2.19	0.43
1:A:263:GLY:O	1:A:264:LYS:HG3	2.19	0.43
1:A:35:TYR:HB2	1:A:93:GLU:HG3	2.01	0.43
1:A:32:GLU:OE1	1:A:222:LYS:NZ	2.51	0.43
1:A:200:ASP:OD1	1:A:202:VAL:HB	2.18	0.43
1:A:210:GLN:O	1:A:213:ALA:HB3	2.19	0.42
1:A:328:GLN:HB2	1:A:349:ARG:HD3	2.01	0.42
1:A:254:TRP:CE3	1:A:264:LYS:HA	2.54	0.42
1:A:43:CYS:O	1:A:50:SER:HA	2.19	0.42
1:A:254:TRP:O	1:A:266:ILE:HG23	2.19	0.42
1:A:315:ASP:OD1	1:A:315:ASP:N	2.52	0.42
1:A:54:SER:HB2	3:A:366:HOH:O	2.20	0.42
1:A:65:HIS:CD2	1:A:118:GLN:HE21	2.38	0.42
1:A:91:ASP:HB3	1:A:150:ALA:HB3	2.01	0.42
1:A:130:ARG:O	1:A:132:LYS:HG2	2.20	0.42
1:A:266:ILE:HA	1:A:288:MET:HG2	2.02	0.42
1:A:104:GLY:O	1:A:107:LEU:HB2	2.20	0.41
1:A:10:LYS:O	1:A:232:LYS:HA	2.20	0.41
1:A:109:ARG:HH11	1:A:109:ARG:HG3	1.86	0.41
1:A:251:GLY:HA3	1:A:269:GLU:HB2	2.03	0.41
1:A:55:ARG:NH2	3:A:459:HOH:O	2.53	0.41
1:A:20:LYS:HG2	3:A:357:HOH:O	2.20	0.41
1:A:94:LEU:HD23	1:A:146:ILE:HD13	2.03	0.41
1:A:167:THR:HB	1:A:224:PRO:HA	2.03	0.40
1:A:52:TRP:HB2	1:A:67:ASN:HD21	1.86	0.40
1:A:111:LYS:HD2	1:A:111:LYS:O	2.21	0.40
1:A:113:THR:HA	1:A:137:PHE:HB2	2.04	0.40
1:A:334:GLU:HG3	1:A:340:LEU:HD12	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
1	A	326/348 (94%)	285 (87%)	29 (9%)	12 (4%)	<b>4</b> <b>5</b>

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	TRP
1	A	134	LYS
1	A	261	ASN
1	A	282	ASN
1	A	285	ARG
1	A	303	TRP
1	A	4	ILE
1	A	114	ASP
1	A	259	LEU
1	A	265	VAL
1	A	305	PHE
1	A	304	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	289/303 (95%)	239 (83%)	50 (17%)	<b>2</b> <b>3</b>

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	55	ARG
1	A	63	LEU
1	A	64	GLU
1	A	71	VAL
1	A	77	LEU
1	A	101	PHE
1	A	105	SER
1	A	110	THR
1	A	111	LYS
1	A	112	TRP
1	A	114	ASP
1	A	116	LYS
1	A	117	ASN
1	A	118	GLN
1	A	121	HIS
1	A	133	ASP
1	A	134	LYS
1	A	135	VAL
1	A	145	HIS
1	A	146	ILE
1	A	148	LEU
1	A	149	TYR
1	A	154	LEU
1	A	166	MET
1	A	168	LEU
1	A	169	LEU
1	A	178	LEU
1	A	195	SER
1	A	203	GLU
1	A	205	GLN
1	A	238	LYS
1	A	246	ASP
1	A	249	ILE
1	A	252	LEU
1	A	253	VAL
1	A	257	LYS
1	A	261	ASN
1	A	269	GLU
1	A	272	LEU
1	A	293	GLU
1	A	297	GLU
1	A	301	SER

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Mol	Chain	Res	Type
1	A	306	PHE
1	A	315	ASP
1	A	320	ASN
1	A	325	TRP
1	A	344	SER
1	A	347	MET
1	A	349	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	67	ASN
1	A	118	GLN
1	A	143	HIS
1	A	216	HIS
1	A	243	ASN
1	A	250	GLN
1	A	279	ASN
1	A	328	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ATP	A	1	-	27,33,33	1.60	6 (22%)	25,52,52	2.43	7 (28%)

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
2	ATP	A	1	-	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ATP	C5-C4	-2.74	1.34	1.40
2	A	1	ATP	O4'-C1'	2.29	1.44	1.41
2	A	1	ATP	C8-N7	2.86	1.40	1.34
2	A	1	ATP	C2-N1	2.98	1.39	1.33
2	A	1	ATP	C6-N6	3.16	1.47	1.34
2	A	1	ATP	C2-N3	3.75	1.38	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ATP	C4'-O4'-C1'	-6.87	102.46	109.77
2	A	1	ATP	C1'-N9-C4	-2.31	122.65	126.64
2	A	1	ATP	C4-C5-N7	2.13	111.47	109.41
2	A	1	ATP	O3'-C3'-C4'	3.23	120.52	111.09
2	A	1	ATP	C5'-C4'-C3'	3.38	128.17	115.29
2	A	1	ATP	O2'-C2'-C1'	4.11	124.47	111.61
2	A	1	ATP	O4'-C4'-C3'	4.97	115.05	105.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ATP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 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, 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	332/348 (95%)	-0.41	11 (3%) 47 39	4, 25, 75, 134	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	GLY	6.9
1	A	316	ALA	5.2
1	A	121	HIS	3.7
1	A	315	ASP	3.6
1	A	2	VAL	3.5
1	A	259	LEU	3.3
1	A	120	PHE	2.8
1	A	132	LYS	2.7
1	A	319	ILE	2.2
1	A	326	ALA	2.1
1	A	303	TRP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.



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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ATP	A	1	31/31	0.95	0.12	-0.26	2,39,98,105	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.