



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 PM UTC

PDB ID : 1A0I / pdb_00001a0i
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

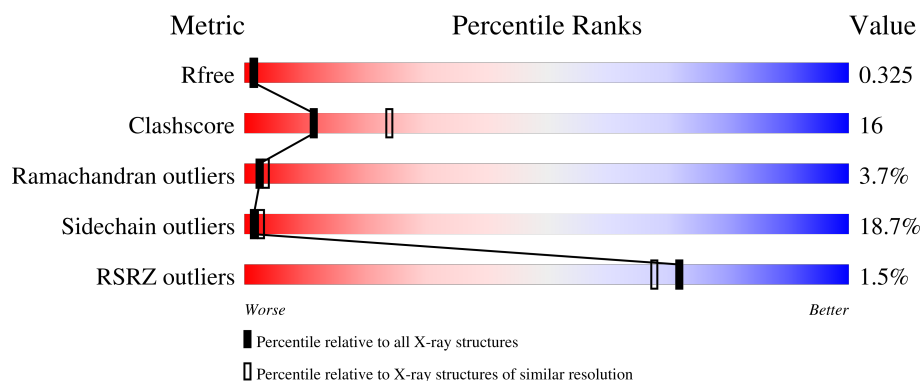
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	

2 Entry composition [i](#)

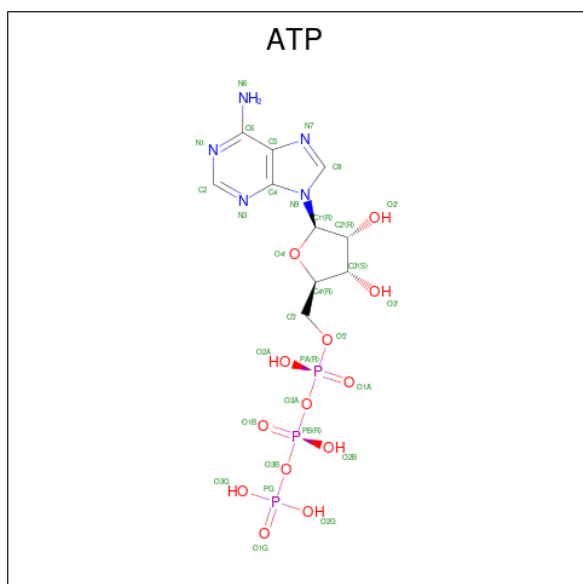
There are 3 unique types of molecules in this entry. The entry contains 2903 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	332	Total	C	N	O	S	0	0	0
			2679	1716	451	495	17			

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



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

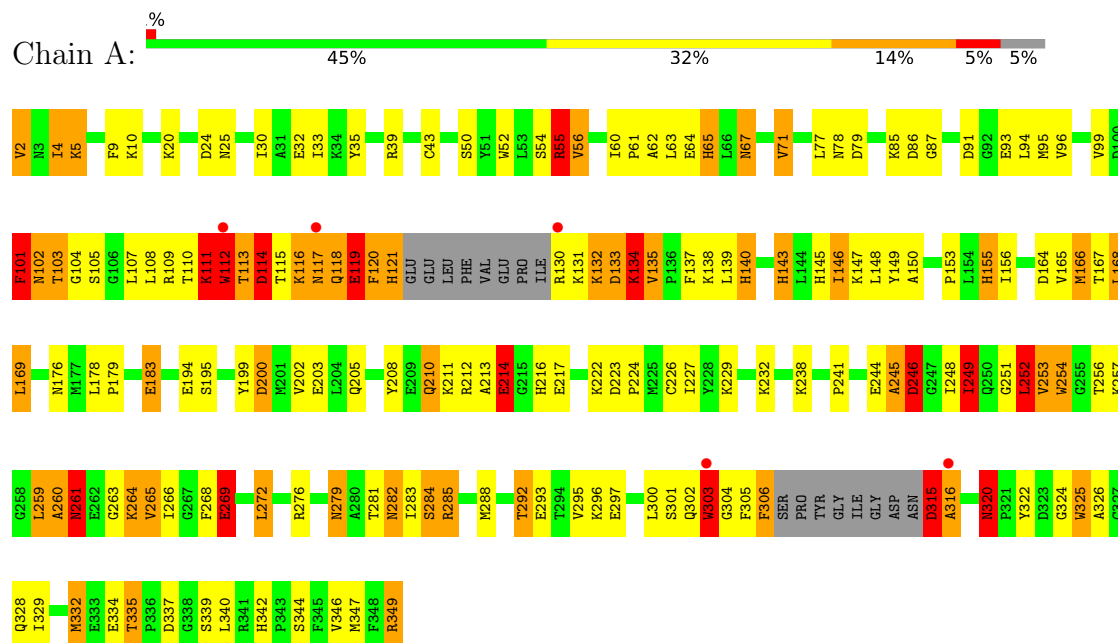
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	193	Total	O	0	0
			193	193		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA LIGASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	64.70Å 85.20Å 79.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 10.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.6 (10.00-2.60) 97.3 (10.00-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	689 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 95.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.02	10/2741 (0.4%)	2.10	99/3699 (2.7%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	ILE	CA-CB	7.01	1.63	1.54
1	A	140	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	265	VAL	CA-CB	5.91	1.62	1.54
1	A	155	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	342	HIS	CD2-NE2	-5.82	1.31	1.37
1	A	143	HIS	CD2-NE2	-5.82	1.31	1.37
1	A	65	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	253	VAL	CA-CB	5.60	1.61	1.54
1	A	121	HIS	CD2-NE2	-5.41	1.31	1.37
1	A	145	HIS	CD2-NE2	-5.14	1.32	1.37

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ASP	N-CA-C	23.55	145.29	109.96
1	A	120	PHE	N-CA-C	22.93	140.12	110.53
1	A	284	SER	N-CA-C	14.16	129.66	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	THR	N-CA-C	13.42	131.32	108.23
1	A	56	VAL	N-CA-CB	-11.22	97.52	112.22
1	A	261	ASN	CA-CB-CG	10.57	123.17	112.60
1	A	67	ASN	OD1-CG-ND2	-10.30	112.30	122.60
1	A	119	GLU	N-CA-C	-9.92	89.66	110.80
1	A	316	ALA	N-CA-C	9.27	124.43	108.76
1	A	246	ASP	CA-CB-CG	8.87	121.47	112.60
1	A	118	GLN	N-CA-C	-8.63	95.14	109.46
1	A	120	PHE	N-CA-CB	-8.04	98.94	110.44
1	A	115	THR	CA-C-O	8.02	129.64	120.98
1	A	315	ASP	CA-CB-CG	7.97	120.58	112.60
1	A	103	THR	N-CA-C	-7.93	100.62	112.04
1	A	71	VAL	CB-CA-C	-7.82	100.05	112.16
1	A	9	PHE	CA-CB-CG	7.80	121.60	113.80
1	A	131	LYS	N-CA-C	7.70	120.91	109.59
1	A	116	LYS	N-CA-C	-7.57	101.19	110.88
1	A	133	ASP	CA-C-N	7.52	135.91	121.54
1	A	133	ASP	C-N-CA	7.52	135.91	121.54
1	A	4	ILE	CA-C-O	7.41	130.04	120.78
1	A	133	ASP	CA-C-O	7.25	129.15	120.81
1	A	306	PHE	CA-CB-CG	7.22	121.02	113.80
1	A	117	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	A	210	GLN	OE1-CD-NE2	-7.07	115.53	122.60
1	A	111	LYS	CA-C-N	6.99	134.89	121.54
1	A	111	LYS	C-N-CA	6.99	134.89	121.54
1	A	216	HIS	N-CA-C	-6.94	98.37	109.76
1	A	55	ARG	CA-CB-CG	6.87	127.85	114.10
1	A	102	ASN	CA-CB-CG	-6.70	105.90	112.60
1	A	265	VAL	N-CA-C	6.67	123.22	109.34
1	A	65	HIS	CA-CB-CG	6.62	120.42	113.80
1	A	217	GLU	CB-CG-CD	6.47	123.61	112.60
1	A	114	ASP	CA-CB-CG	-6.42	106.18	112.60
1	A	264	LYS	CA-C-N	6.41	133.50	121.97
1	A	264	LYS	C-N-CA	6.41	133.50	121.97
1	A	117	ASN	CA-C-N	6.39	131.20	122.19
1	A	117	ASN	C-N-CA	6.39	131.20	122.19
1	A	121	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	A	164	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	118	GLN	CA-C-O	-6.23	113.50	120.54
1	A	320	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	A	131	LYS	CA-C-O	6.15	127.71	120.58
1	A	342	HIS	CB-CG-CD2	-6.11	123.25	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	GLU	N-CA-C	-6.09	99.27	108.96
1	A	279	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	A	249	ILE	N-CA-C	-5.96	101.32	109.55
1	A	111	LYS	N-CA-C	-5.96	97.50	107.80
1	A	65	HIS	CB-CG-CD2	-5.96	123.46	131.20
1	A	303	TRP	CG-CD2-CE3	5.95	139.85	133.90
1	A	112	TRP	CB-CG-CD1	-5.91	118.03	126.90
1	A	253	VAL	N-CA-C	-5.91	99.96	108.53
1	A	254	TRP	N-CA-C	5.91	122.02	110.56
1	A	176	ASN	CB-CG-ND2	5.87	125.20	116.40
1	A	335	THR	CA-C-N	5.84	125.32	119.24
1	A	335	THR	C-N-CA	5.84	125.32	119.24
1	A	56	VAL	CB-CA-C	5.76	120.12	112.46
1	A	112	TRP	CG-CD2-CE3	5.74	139.64	133.90
1	A	244	GLU	CB-CG-CD	5.74	122.36	112.60
1	A	113	THR	N-CA-CB	-5.73	100.81	110.49
1	A	199	TYR	O-C-N	-5.69	114.87	122.49
1	A	78	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	292	THR	CA-C-O	-5.65	114.88	120.70
1	A	245	ALA	N-CA-C	5.62	115.66	108.24
1	A	210	GLN	CG-CD-NE2	5.58	124.77	116.40
1	A	87	GLY	N-CA-C	-5.57	106.05	112.29
1	A	121	HIS	CB-CG-ND1	5.55	131.03	122.70
1	A	119	GLU	CA-C-O	5.53	128.41	120.51
1	A	134	LYS	CA-CB-CG	-5.50	103.10	114.10
1	A	113	THR	CA-C-N	5.49	132.02	121.54
1	A	113	THR	C-N-CA	5.49	132.02	121.54
1	A	5	LYS	N-CA-C	-5.48	96.94	107.57
1	A	176	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	A	67	ASN	CB-CG-ND2	5.45	124.57	116.40
1	A	316	ALA	N-CA-CB	-5.43	101.41	110.80
1	A	320	ASN	CB-CG-ND2	5.42	124.53	116.40
1	A	133	ASP	N-CA-CB	-5.40	101.80	109.85
1	A	140	HIS	CB-CG-CD2	-5.37	124.21	131.20
1	A	214	GLU	N-CA-C	-5.35	106.06	112.59
1	A	95	MET	CG-SD-CE	-5.35	89.13	100.90
1	A	285	ARG	N-CA-CB	5.35	119.53	110.49
1	A	252	LEU	CA-C-N	-5.33	116.23	123.10
1	A	252	LEU	C-N-CA	-5.33	116.23	123.10
1	A	113	THR	CA-CB-CG2	5.31	119.53	110.50
1	A	101	PHE	N-CA-C	-5.29	102.46	110.28
1	A	86	ASP	CA-CB-CG	5.28	117.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	THR	CA-CB-OG1	-5.26	101.70	109.60
1	A	268	PHE	N-CA-C	5.22	117.62	109.52
1	A	320	ASN	CA-CB-CG	5.22	117.83	112.60
1	A	260	ALA	N-CA-C	5.22	121.92	110.80
1	A	117	ASN	N-CA-C	5.21	118.22	110.52
1	A	25	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	145	HIS	N-CA-C	-5.20	100.70	109.07
1	A	282	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	A	60	ILE	CA-C-N	5.12	126.24	119.84
1	A	60	ILE	C-N-CA	5.12	126.24	119.84
1	A	200	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	261	ASN	N-CA-C	5.04	121.54	110.80

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	86	0
2	A	31	0	10	1	0
3	A	193	0	0	6	0
All	All	2903	0	2647	86	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 (86) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:39:ARG:NH1	2:A:1:ATP:H3'	2.21	0.56
1:A:249:ILE:HD12	1:A:251:GLY:H	1.71	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:99:VAL:HB	1:A:103:THR:HB	1.93	0.50
1:A:300:LEU:HD22	1:A:303:TRP:CE3	2.46	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:20:LYS:NZ	1:A:24:ASP:OD1	2.46	0.49
1:A:153:PRO:HG2	1:A:156:ILE:HD12	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:65:HIS:HB3	1:A:138:LYS:HD2	2.00	0.44
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: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:101:PHE:O	1:A:102:ASN:HB2	2.18	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:208:TYR:CZ	1:A:332:MET:HE1	2.54	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:54:SER:HB2	3:A:366:HOH:O	2.20	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: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:10:LYS:O	1:A:232:LYS:HA	2.20	0.41
1:A:104:GLY:O	1:A:107:LEU:HB2	2.20	0.41
1:A:55:ARG:NH2	3:A:459:HOH:O	2.53	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: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:52:TRP:HB2	1:A:67:ASN:HD21	1.86	0.40
1:A:167:THR:HB	1:A:224:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:O	1:A:111:LYS:HD2	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%)	2 3

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%)	235 (81%)	54 (19%)	1 3

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	55	ARG
1	A	56	VAL
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	114	ASP
1	A	116	LYS
1	A	117	ASN
1	A	121	HIS
1	A	132	LYS
1	A	133	ASP
1	A	134	LYS
1	A	135	VAL
1	A	146	ILE
1	A	147	LYS
1	A	148	LEU
1	A	149	TYR
1	A	166	MET
1	A	168	LEU
1	A	169	LEU
1	A	178	LEU
1	A	183	GLU
1	A	195	SER
1	A	203	GLU
1	A	205	GLN
1	A	214	GLU
1	A	238	LYS
1	A	246	ASP

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Mol	Chain	Res	Type
1	A	249	ILE
1	A	252	LEU
1	A	253	VAL
1	A	257	LYS
1	A	259	LEU
1	A	261	ASN
1	A	269	GLU
1	A	272	LEU
1	A	293	GLU
1	A	297	GLU
1	A	301	SER
1	A	306	PHE
1	A	315	ASP
1	A	320	ASN
1	A	325	TRP
1	A	329	ILE
1	A	332	MET
1	A	344	SER
1	A	347	MET
1	A	349	ARG

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

Mol	Chain	Res	Type
1	A	25	ASN
1	A	41	ASN
1	A	67	ASN
1	A	118	GLN
1	A	143	HIS
1	A	171	GLN
1	A	176	ASN
1	A	250	GLN
1	A	279	ASN
1	A	282	ASN
1	A	328	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	32,33,33	2.70	7 (21%)	48,52,52	3.07	17 (35%)

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	-	-	5/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ATP	PA-O3A	-8.80	1.50	1.59
2	A	1	ATP	PB-O3A	-8.02	1.50	1.59
2	A	1	ATP	C6-N6	5.02	1.47	1.34
2	A	1	ATP	C8-N7	4.35	1.40	1.31
2	A	1	ATP	C2-N1	3.13	1.39	1.33
2	A	1	ATP	C5-C4	-2.67	1.34	1.39
2	A	1	ATP	C2-N3	2.53	1.38	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ATP	C6-C5-C4	9.97	130.79	117.18
2	A	1	ATP	C5-C4-N3	-7.53	116.34	126.72
2	A	1	ATP	C6-C5-N7	-7.45	117.72	132.09
2	A	1	ATP	O4'-C1'-N9	5.76	119.15	108.09
2	A	1	ATP	O4'-C4'-C3'	4.99	115.05	105.15
2	A	1	ATP	N3-C4-N9	4.69	135.15	127.17
2	A	1	ATP	C2'-C1'-N9	4.48	124.42	113.30
2	A	1	ATP	O2'-C2'-C1'	4.17	124.47	110.10
2	A	1	ATP	O3G-PG-O3B	3.65	116.88	104.64
2	A	1	ATP	C5'-C4'-C3'	3.60	128.17	115.21
2	A	1	ATP	O3'-C3'-C4'	3.29	120.52	111.08
2	A	1	ATP	N9-C8-N7	-3.27	109.29	113.94
2	A	1	ATP	C4'-O4'-C1'	-3.17	102.46	109.47
2	A	1	ATP	O4'-C1'-C2'	2.83	112.67	106.62
2	A	1	ATP	C5-C4-N9	2.45	108.48	105.81
2	A	1	ATP	O2B-PB-O3B	2.10	112.95	107.27
2	A	1	ATP	O2G-PG-O3B	2.03	111.44	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	ATP	C3'-C4'-C5'-O5'
2	A	1	ATP	PB-O3B-PG-O1G
2	A	1	ATP	PA-O3A-PB-O1B
2	A	1	ATP	C4'-C5'-O5'-PA
2	A	1	ATP	O4'-C1'-N9-C8

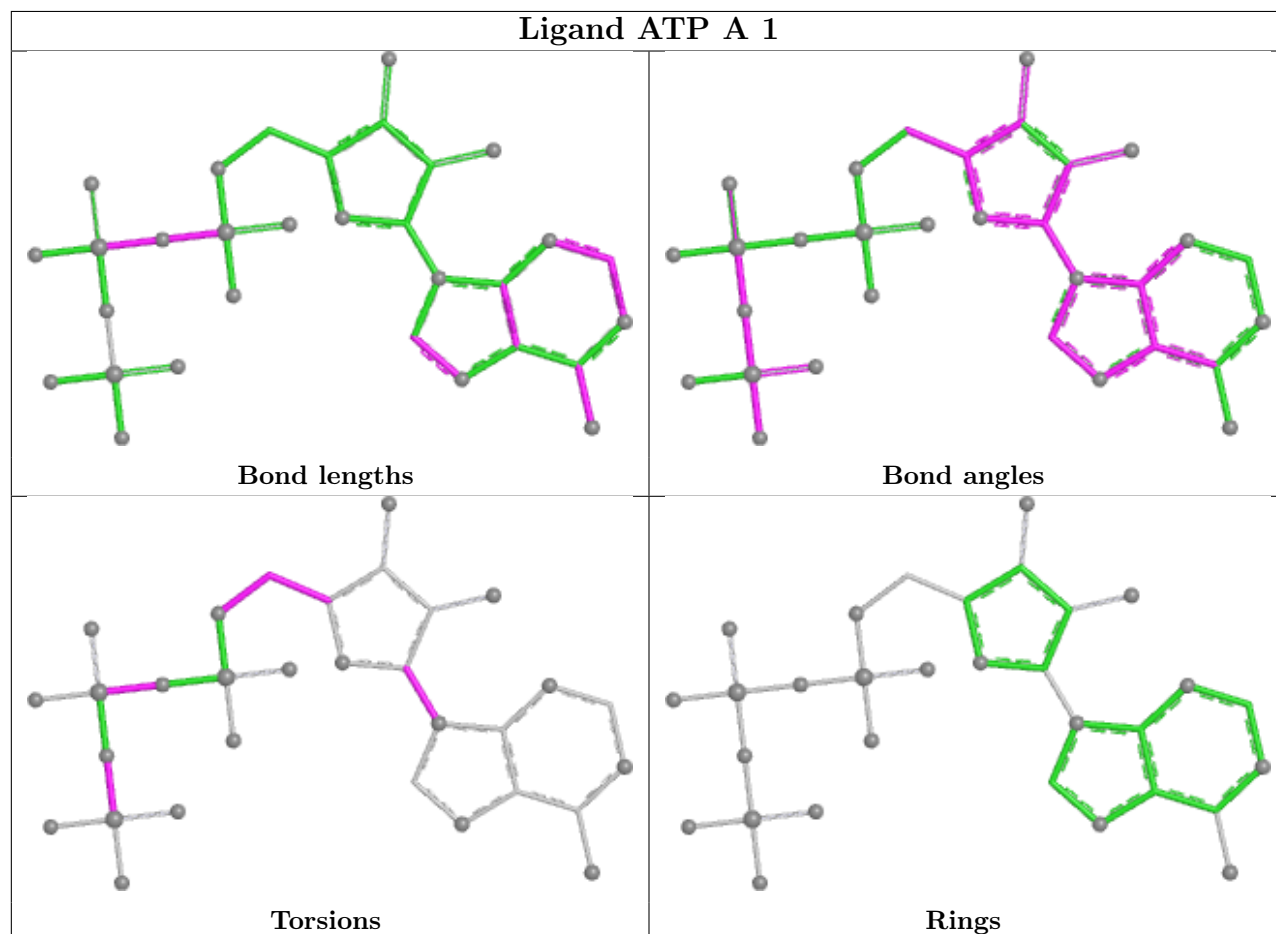
There are no ring outliers.

1 monomer is involved in 1 short contact:

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	332/348 (95%)	-0.27	5 (1%) 72 68	4, 25, 75, 134	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	ALA	2.9
1	A	303	TRP	2.6
1	A	117	ASN	2.3
1	A	112	TRP	2.1
1	A	130	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 oligosaccharides in this entry.

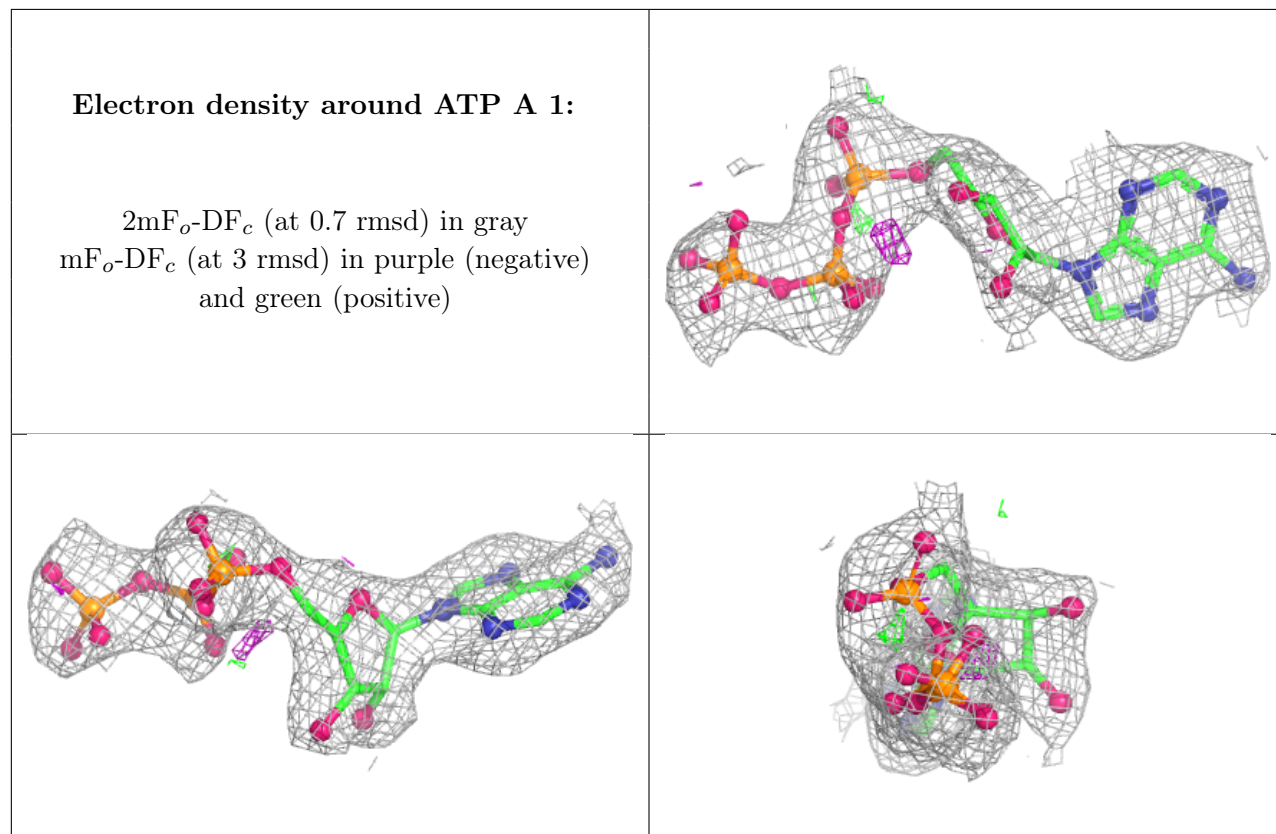
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ATP	A	1	31/31	0.92	0.10	2,39,98,105	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.