



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:23 PM UTC

PDB ID : 1QL6 / pdb_00001ql6
Title : THE CATALYTIC MECHANISM OF PHOSPHORYLASE KINASE
PROBED BY MUTATIONAL STUDIES
Authors : Skamnaki, V.T.; Owen, D.J.; Noble, M.E.M.; Lowe, E.D.; Oikonomakos, N.G.;
Johnson, L.N.
Deposited on : 1999-08-24
Resolution : 2.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

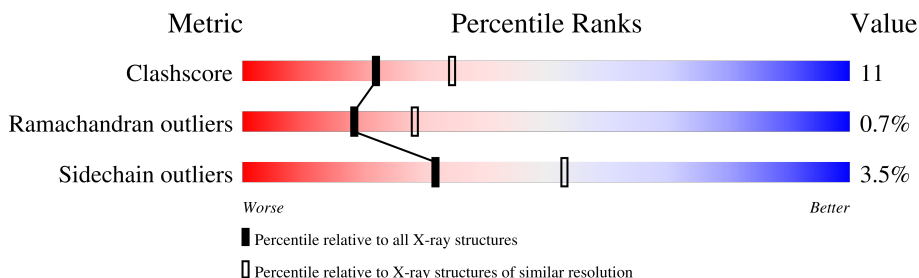
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	298	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2412 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.

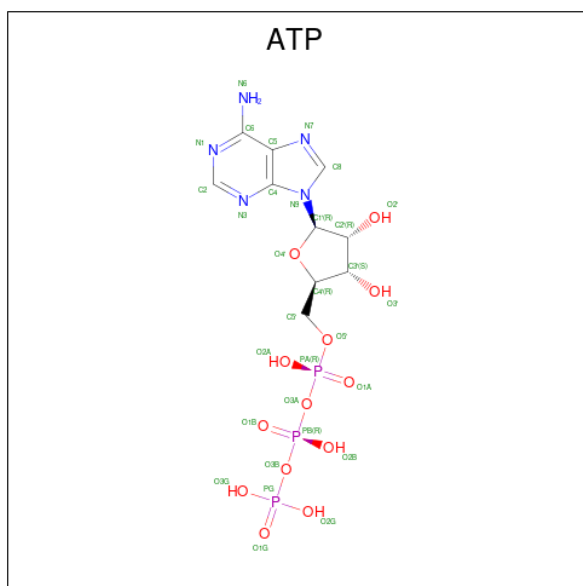
- Molecule 1 is a protein called PHOSPHORYLASE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	281	2270	1453	377	424	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	SER	GLU	engineered mutation	UNP P00518

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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		

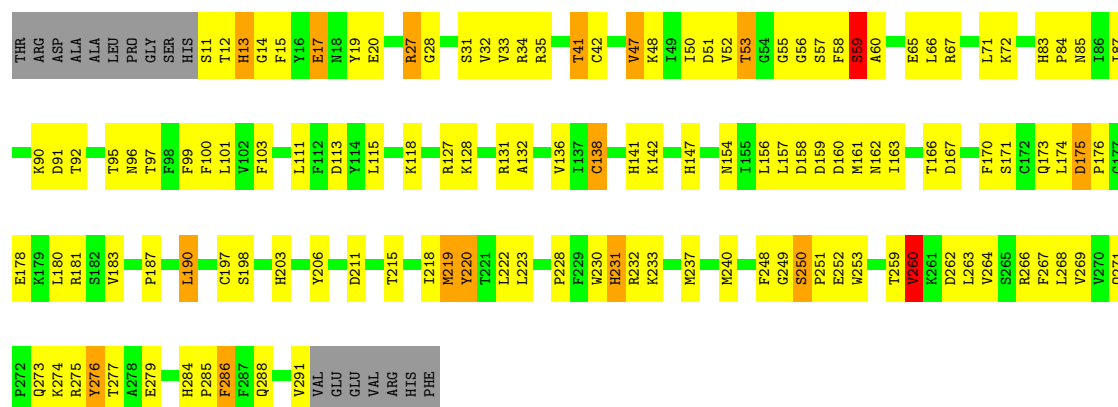
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: PHOSPHORYLASE KINASE

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.56 Å 68.17 Å 112.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	86.6 (20.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.240 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2412	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, SO4, 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	0/2322	2.17	92/3137 (2.9%)

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	GLY	N-CA-C	11.75	129.03	112.81
1	A	260	VAL	CB-CA-C	-11.39	96.51	112.22
1	A	275	ARG	CD-NE-CZ	9.99	138.38	124.40
1	A	34	ARG	NE-CZ-NH2	-9.21	110.91	119.20
1	A	267	PHE	N-CA-C	-9.07	102.34	113.41
1	A	103	PHE	CA-CB-CG	9.00	122.80	113.80
1	A	268	LEU	CA-C-N	8.72	134.46	123.12
1	A	268	LEU	C-N-CA	8.72	134.46	123.12
1	A	171	SER	CA-C-O	-8.25	112.07	121.81
1	A	127	ARG	NE-CZ-NH1	-8.16	113.34	121.50
1	A	170	PHE	CA-CB-CG	8.00	121.80	113.80
1	A	20	GLU	CA-C-O	7.62	124.24	119.29
1	A	220	TYR	CA-C-N	7.30	130.06	120.28
1	A	220	TYR	C-N-CA	7.30	130.06	120.28
1	A	173	GLN	CA-C-N	-7.24	111.21	122.87
1	A	173	GLN	C-N-CA	-7.24	111.21	122.87
1	A	260	VAL	N-CA-CB	7.16	121.31	110.58
1	A	127	ARG	NH1-CZ-NH2	7.14	128.59	119.30
1	A	53	THR	N-CA-C	-7.10	102.58	112.45
1	A	17	GLU	CB-CG-CD	6.99	124.47	112.60
1	A	175	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	35	ARG	N-CA-C	-6.82	100.38	110.48
1	A	34	ARG	CA-C-O	-6.79	113.50	121.44
1	A	215	THR	CA-C-N	6.75	127.43	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	THR	C-N-CA	6.75	127.43	119.94
1	A	262	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	90	LYS	CA-C-O	-6.69	111.85	119.41
1	A	286	PHE	CA-C-O	-6.63	112.77	120.20
1	A	178	GLU	CB-CG-CD	6.60	123.81	112.60
1	A	219	MET	CA-C-O	6.52	127.42	120.70
1	A	91	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	35	ARG	NE-CZ-NH1	-6.47	115.03	121.50
1	A	162	ASN	CB-CG-ND2	6.46	126.09	116.40
1	A	223	LEU	CA-C-O	-6.24	112.30	119.60
1	A	211	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	178	GLU	CA-CB-CG	6.19	126.49	114.10
1	A	19	TYR	CA-C-O	6.09	127.91	120.60
1	A	111	LEU	N-CA-C	-6.04	104.81	111.82
1	A	132	ALA	CA-C-O	-6.04	114.02	120.42
1	A	35	ARG	NH1-CZ-NH2	6.03	127.14	119.30
1	A	206	TYR	CA-C-O	-6.03	114.59	121.58
1	A	219	MET	O-C-N	-6.03	115.58	122.09
1	A	115	LEU	CA-C-N	6.02	128.62	120.38
1	A	115	LEU	C-N-CA	6.02	128.62	120.38
1	A	175	ASP	N-CA-CB	5.99	117.34	109.55
1	A	269	VAL	CA-C-N	5.98	128.09	120.56
1	A	269	VAL	C-N-CA	5.98	128.09	120.56
1	A	13	HIS	N-CA-C	-5.94	104.50	110.97
1	A	92	THR	N-CA-CB	5.91	121.83	111.13
1	A	159	ASP	CA-C-O	-5.90	113.44	120.10
1	A	259	THR	CA-CB-OG1	-5.87	100.80	109.60
1	A	27	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	A	113	ASP	O-C-N	5.84	128.32	122.12
1	A	277	THR	CB-CA-C	-5.82	99.51	110.51
1	A	253	TRP	CA-C-N	5.80	128.05	120.28
1	A	253	TRP	C-N-CA	5.80	128.05	120.28
1	A	58	PHE	N-CA-C	5.70	120.00	111.96
1	A	141	HIS	CB-CA-C	5.64	121.50	110.67
1	A	215	THR	CB-CA-C	5.60	120.19	110.68
1	A	231	HIS	CA-CB-CG	-5.58	108.22	113.80
1	A	277	THR	N-CA-CB	5.58	118.90	110.42
1	A	173	GLN	N-CA-CB	5.58	119.50	110.41
1	A	90	LYS	O-C-N	5.57	130.26	122.36
1	A	101	LEU	CA-C-O	5.57	126.31	120.36
1	A	173	GLN	CA-CB-CG	5.53	125.16	114.10
1	A	136	VAL	CA-C-N	5.48	127.96	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	VAL	C-N-CA	5.48	127.96	120.46
1	A	28	GLY	N-CA-C	-5.46	102.99	111.12
1	A	31	SER	CA-C-O	5.45	127.56	121.40
1	A	162	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	99	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	113	ASP	CB-CA-C	-5.43	101.78	110.79
1	A	100	PHE	CA-C-N	-5.42	115.56	122.77
1	A	100	PHE	C-N-CA	-5.42	115.56	122.77
1	A	59	SER	N-CA-CB	5.42	119.64	110.49
1	A	167	ASP	N-CA-C	5.41	117.78	111.02
1	A	85	ASN	N-CA-CB	-5.40	102.39	110.91
1	A	131	ARG	CD-NE-CZ	5.30	131.82	124.40
1	A	248	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	128	LYS	O-C-N	5.18	128.05	122.15
1	A	65	GLU	N-CA-C	-5.13	105.77	112.23
1	A	197	CYS	CA-C-O	-5.13	115.41	120.90
1	A	190	LEU	N-CA-C	5.12	117.64	109.96
1	A	118	LYS	CA-C-N	5.11	131.17	121.97
1	A	118	LYS	C-N-CA	5.11	131.17	121.97
1	A	173	GLN	O-C-N	5.08	128.75	123.06
1	A	17	GLU	N-CA-C	-5.07	105.83	111.36
1	A	47	VAL	CA-C-N	-5.07	116.02	122.77
1	A	47	VAL	C-N-CA	-5.07	116.02	122.77
1	A	171	SER	O-C-N	5.06	128.62	122.85
1	A	147	HIS	O-C-N	-5.05	116.87	122.07
1	A	41	THR	CA-CB-OG1	5.03	117.15	109.60

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	2270	0	2253	49	0
2	A	31	0	12	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
5	A	104	0	0	1	0
All	All	2412	0	2265	49	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 11.

All (49) 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:250:SER:HB3	1:A:251:PRO:CD	1.99	0.92
1:A:250:SER:HB3	1:A:251:PRO:HD3	1.49	0.91
1:A:230:TRP:HA	1:A:237:MET:HE2	1.60	0.83
1:A:219:MET:HE2	1:A:264:VAL:HG23	1.67	0.73
1:A:175:ASP:HB3	1:A:176:PRO:HD2	1.72	0.70
1:A:12:THR:OG1	1:A:95:THR:HG21	1.93	0.69
1:A:219:MET:HG2	1:A:264:VAL:HG22	1.73	0.69
1:A:11:SER:OG	1:A:95:THR:HG22	1.93	0.68
1:A:250:SER:CB	1:A:251:PRO:CD	2.72	0.67
1:A:260:VAL:HG13	1:A:286:PHE:CE1	2.30	0.67
1:A:284:HIS:CG	1:A:285:PRO:HD2	2.35	0.61
1:A:154:ASN:O	1:A:166:THR:HG22	2.03	0.59
1:A:251:PRO:HD2	1:A:252:GLU:OE1	2.02	0.59
1:A:138:CYS:O	1:A:142:LYS:HG3	2.04	0.58
1:A:33:VAL:HG22	1:A:48:LYS:HB2	1.86	0.57
1:A:218:ILE:O	1:A:222:LEU:HG	2.07	0.55
1:A:72:LYS:HG2	5:A:409:HOH:O	2.06	0.55
1:A:219:MET:HE2	1:A:264:VAL:CG2	2.37	0.55
1:A:181:ARG:NH2	1:A:203:HIS:O	2.39	0.54
1:A:175:ASP:HB3	1:A:176:PRO:CD	2.38	0.54
1:A:41:THR:O	1:A:42:CYS:HB2	2.08	0.53
1:A:59:SER:O	1:A:60:ALA:C	2.51	0.53
1:A:48:LYS:HE2	1:A:50:ILE:HD11	1.91	0.53
1:A:52:VAL:HG22	1:A:97:THR:O	2.11	0.51
1:A:13:HIS:O	1:A:17:GLU:N	2.37	0.51
1:A:156:LEU:O	1:A:163:ILE:HA	2.10	0.50
1:A:230:TRP:O	1:A:240:MET:HE1	2.12	0.50
1:A:51:ASP:OD2	1:A:55:GLY:N	2.43	0.50
1:A:15:PHE:CZ	1:A:47:VAL:HG21	2.48	0.48
1:A:231:HIS:ND1	1:A:232:ARG:N	2.62	0.48
1:A:174:LEU:HD21	1:A:180:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:O	1:A:276:TYR:HB2	2.14	0.47
1:A:187:PRO:HA	1:A:190:LEU:HD12	1.97	0.46
1:A:219:MET:HE1	1:A:263:LEU:HD23	1.98	0.45
1:A:138:CYS:SG	1:A:279:GLU:HG2	2.55	0.45
1:A:271:GLN:OE1	1:A:273:GLN:OE1	2.36	0.44
1:A:83:HIS:CG	1:A:84:PRO:HD2	2.52	0.44
1:A:87:ILE:HD12	1:A:87:ILE:HA	1.74	0.43
1:A:53:THR:HG22	1:A:56:GLY:H	1.83	0.43
1:A:27:ARG:HG2	1:A:32:VAL:HG22	2.00	0.43
1:A:233:LYS:HB3	1:A:233:LYS:HE2	1.83	0.43
1:A:158:ASP:OD1	1:A:158:ASP:C	2.61	0.42
1:A:183:VAL:HG21	1:A:198:SER:HB3	2.01	0.42
1:A:220:TYR:CD1	1:A:228:PRO:HD3	2.55	0.42
1:A:285:PRO:HA	1:A:288:GLN:HG2	2.02	0.42
1:A:67:ARG:CZ	1:A:71:LEU:HD11	2.50	0.41
1:A:13:HIS:O	1:A:14:GLY:C	2.64	0.41
1:A:271:GLN:HB3	1:A:273:GLN:OE1	2.20	0.41
1:A:157:LEU:HD13	1:A:161:MET:CE	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	279/298 (94%)	262 (94%)	15 (5%)	2 (1%)	18 28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	SER
1	A	250	SER

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	254/268 (95%)	245 (96%)	9 (4%)	32 53

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	66	LEU
1	A	96	ASN
1	A	138	CYS
1	A	160	ASP
1	A	260	VAL
1	A	274	LYS
1	A	276	TYR
1	A	291	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	289	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 oligosaccharides in this entry.

5.6 Ligand geometry

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
2	ATP	A	301	3	32,33,33	1.65	5 (15%)	48,52,52	1.88	11 (22%)
4	SO4	A	304	-	4,4,4	0.74	0	6,6,6	0.31	0

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	301	3	-	2/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ATP	C5-N7	-4.40	1.31	1.39
2	A	301	ATP	PB-O3B	3.33	1.63	1.59
2	A	301	ATP	C2-N1	3.22	1.39	1.33
2	A	301	ATP	PA-O3A	-2.78	1.56	1.59
2	A	301	ATP	C2-N3	-2.33	1.29	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	ATP	C4-N9-C8	-6.21	99.22	105.74
2	A	301	ATP	O4'-C1'-N9	4.97	117.64	108.09
2	A	301	ATP	O3A-PA-O1A	3.93	122.53	110.70
2	A	301	ATP	C4-N9-C1'	3.52	134.86	126.63
2	A	301	ATP	N9-C8-N7	3.49	118.89	113.94
2	A	301	ATP	O3'-C3'-C2'	2.45	119.66	111.82
2	A	301	ATP	O2B-PB-O3B	2.36	113.64	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	ATP	O2A-PA-O3A	2.36	113.64	107.27
2	A	301	ATP	N3-C2-N1	-2.33	125.06	128.58
2	A	301	ATP	C5-C4-N3	-2.20	123.69	126.72
2	A	301	ATP	O3B-PB-O1B	-2.11	104.36	110.70

There are no chirality outliers.

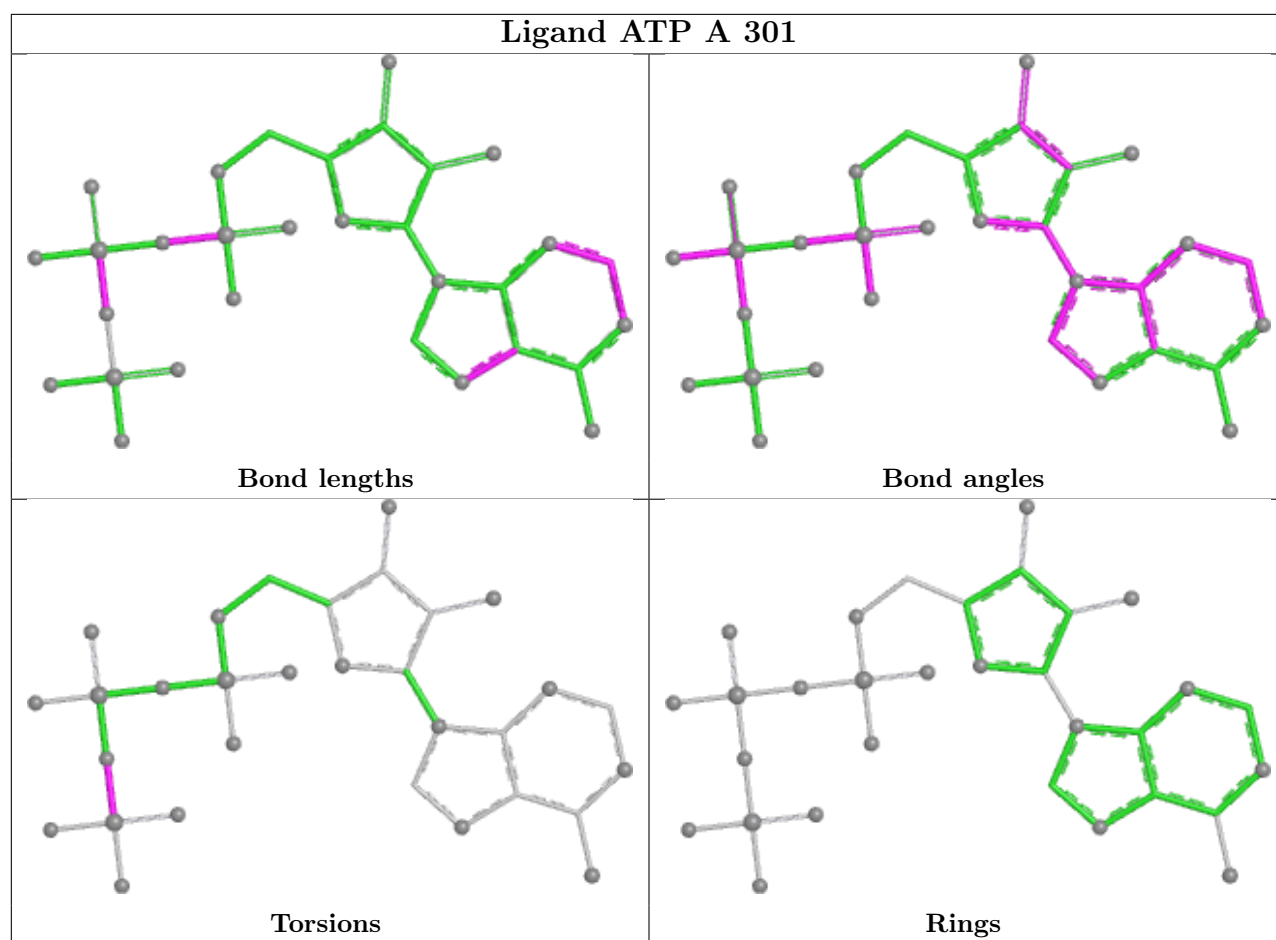
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ATP	PB-O3B-PG-O2G
2	A	301	ATP	PB-O3B-PG-O3G

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.