



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:24 PM UTC

PDB ID : 4WTV / pdb_00004wtv
Title : Crystal structure of the phosphatidylinositol 4-kinase IIbeta
Authors : Klima, M.; Baumlova, A.; Chalupska, D.; Boura, E.
Deposited on : 2014-10-30
Resolution : 1.90 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

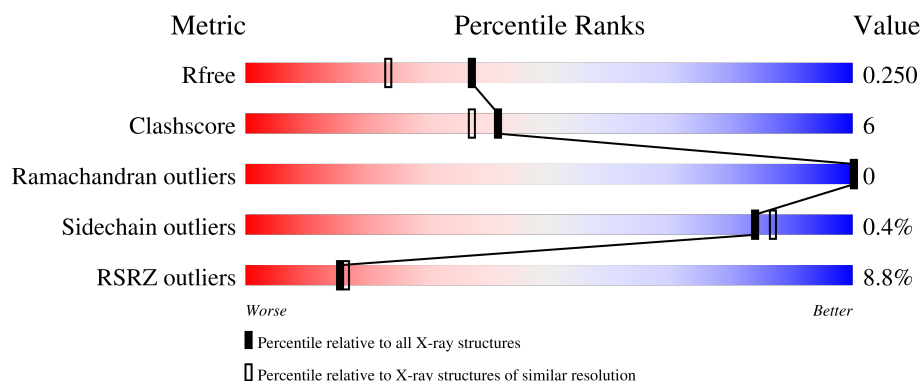
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	514	8% 75% 12% 13%
1	B	514	7% 72% 11% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7462 atoms, of which 48 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.

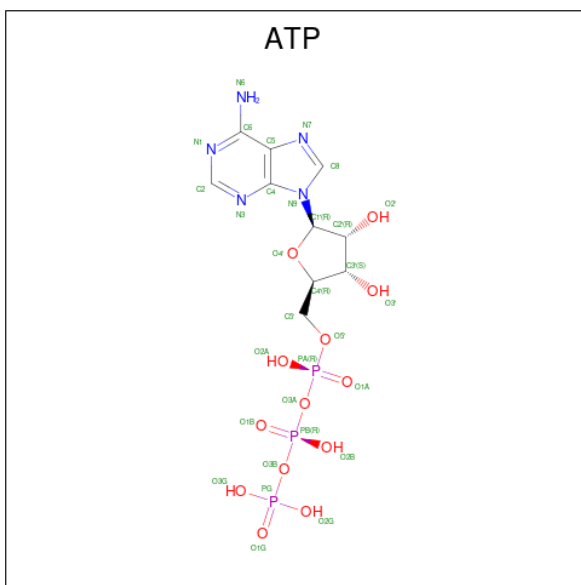
- Molecule 1 is a protein called Phosphatidylinositol 4-kinase type 2-beta,Endolysin,Phosphatidylinositol 4-kinase type 2-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	3	0
			3577	2310	601	655	11			
1	B	426	Total	C	N	O	S	0	3	0
			3434	2220	576	627	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1011	GLY	ARG	conflict	UNP P00720
A	1053	THR	CYS	conflict	UNP P00720
A	1096	ALA	CYS	conflict	UNP P00720
A	1136	ARG	ILE	conflict	UNP P00720
B	1011	GLY	ARG	conflict	UNP P00720
B	1053	THR	CYS	conflict	UNP P00720
B	1096	ALA	CYS	conflict	UNP P00720
B	1136	ARG	ILE	conflict	UNP P00720

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 86	C 20	H 24	N 10	O 26	P 6	0	1
2	B	1	Total 86	C 20	H 24	N 10	O 26	P 6	0	1

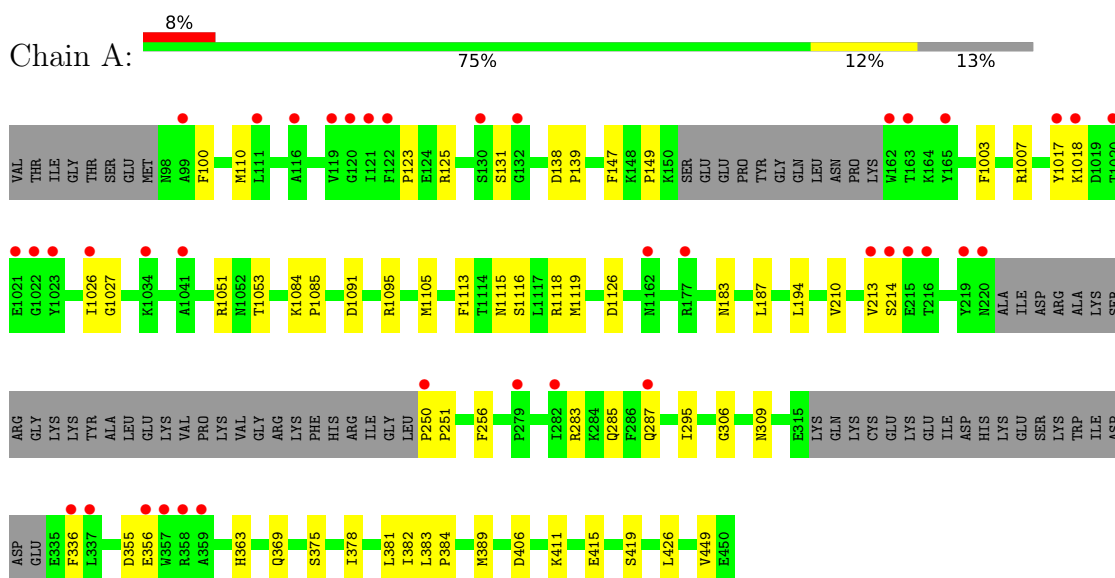
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	133	Total O 133 133	0	0
3	B	146	Total O 146 146	0	0

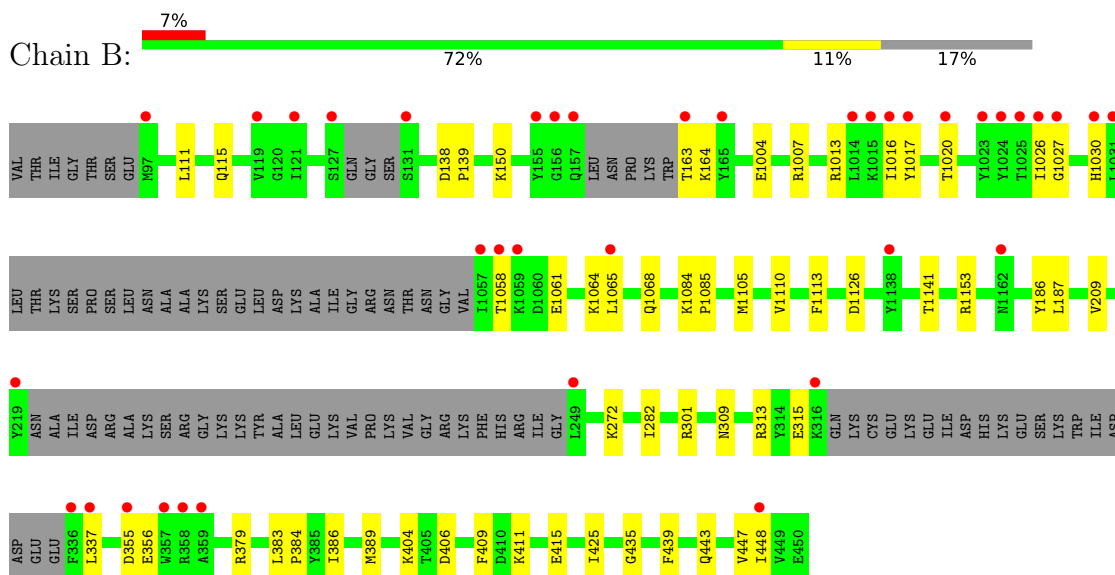
3 Residue-property plots

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 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: Phosphatidylinositol 4-kinase type 2-beta,Endolysin,Phosphatidylinositol 4-kinase type 2-beta



- Molecule 1: Phosphatidylinositol 4-kinase type 2-beta,Endolysin,Phosphatidylinositol 4-kinase type 2-beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.01Å 106.01Å 214.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.52 – 1.90 47.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.52-1.90) 100.0 (47.52-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.209 , 0.240 (Not available) , 0.250	Depositor DCC
R_{free} test set	4839 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7462	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/3661	0.74	2/4964 (0.0%)
1	B	0.48	0/3514	0.72	0/4763
All	All	0.48	0/7175	0.73	2/9727 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	250	PRO	CA-C-N	5.41	125.17	119.76
1	A	250	PRO	C-N-CA	5.41	125.17	119.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	309	ASN	Peptide
1	B	309	ASN	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	3577	0	3479	42	0
1	B	3434	0	3329	45	0
2	A	62	24	24	3	0
2	B	62	24	24	0	0
3	A	133	0	0	1	0
3	B	146	0	0	1	0
All	All	7414	48	6856	89	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 6.

All (89) 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:110:MET:HA	1:A:110:MET:HE2	1.48	0.96
1:A:213:VAL:HG22	1:A:251:PRO:HA	1.62	0.80
1:A:110:MET:HE1	1:A:256:PHE:CZ	2.19	0.75
1:B:282:ILE:HD11	1:B:337:LEU:HD13	1.67	0.74
1:B:163:THR:HG23	1:B:164:LYS:H	1.54	0.71
1:A:110:MET:HE1	1:A:256:PHE:CE1	2.26	0.71
1:B:164:LYS:O	1:B:1004:GLU:HG3	1.93	0.69
1:B:1004:GLU:OE2	1:B:1007:ARG:NH1	2.25	0.69
1:A:287[B]:GLN:OE1	1:A:369:GLN:HG2	1.93	0.69
1:A:1116:SER:HA	1:A:1119:MET:HE3	1.76	0.67
1:B:389:MET:HA	1:B:389:MET:HE2	1.76	0.66
1:A:213:VAL:HG22	1:A:251:PRO:CA	2.26	0.65
1:B:1126:ASP:OD2	1:B:1153:ARG:NH1	2.29	0.65
1:A:110:MET:HE2	1:A:110:MET:CA	2.25	0.64
1:A:110:MET:HA	1:A:110:MET:CE	2.27	0.63
1:A:1105:MET:HE1	1:A:1113:PHE:HE2	1.64	0.62
1:B:1105:MET:HE1	1:B:1113:PHE:HE2	1.63	0.62
1:B:1058:THR:HG22	1:B:1061:GLU:OE1	2.00	0.62
1:A:125:ARG:HG2	1:A:131:SER:HB2	1.82	0.61
1:B:1020:THR:HG21	1:B:1141:THR:HG22	1.81	0.61
1:B:209:VAL:HG22	3:B:1388:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ASP:O	1:B:356:GLU:HB2	1.99	0.60
1:A:138:ASP:HB2	1:A:139:PRO:HD2	1.85	0.58
1:B:1058:THR:HG23	1:B:1061:GLU:H	1.68	0.58
1:A:187:LEU:HD11	1:A:406:ASP:HB2	1.86	0.57
2:A:1201[A]:ATP:H5'2	2:A:1201[A]:ATP:C8	2.40	0.57
1:A:1084:LYS:HB3	1:A:1085:PRO:HD3	1.86	0.57
1:B:1084:LYS:HB3	1:B:1085:PRO:HD3	1.86	0.57
1:A:1113:PHE:HB3	1:A:1116:SER:HB2	1.87	0.56
1:B:150:LYS:HD2	1:B:186:TYR:CE2	2.39	0.56
1:A:1115:ASN:OD1	1:A:1118:ARG:NH2	2.39	0.56
1:A:125:ARG:NE	1:A:131:SER:OG	2.38	0.55
1:A:389:MET:HE2	1:A:389:MET:HA	1.88	0.55
1:A:285:GLN:OE1	1:A:336:PHE:HA	2.06	0.55
1:A:411:LYS:HE2	1:A:415:GLU:OE2	2.08	0.54
1:B:379:ARG:HH11	1:B:435:GLY:HA2	1.73	0.53
1:B:138:ASP:HB2	1:B:139:PRO:CD	2.39	0.53
1:B:1030:HIS:ND1	1:B:1065:LEU:HD22	2.25	0.52
2:A:1201[A]:ATP:H5'2	2:A:1201[A]:ATP:H8	1.75	0.52
1:A:1051:ARG:HH12	1:A:1053:THR:HA	1.75	0.52
1:B:1058:THR:CG2	1:B:1061:GLU:HB2	2.39	0.52
1:B:1064:LYS:O	1:B:1068:GLN:HG3	2.11	0.50
1:A:138:ASP:HB2	1:A:139:PRO:CD	2.42	0.50
1:B:163:THR:HG23	1:B:164:LYS:N	2.24	0.50
1:B:1105:MET:HE2	1:B:1110:VAL:HG22	1.93	0.50
1:A:147:PHE:CE2	1:A:149:PRO:HG3	2.47	0.49
1:B:1013:ARG:O	1:B:1027:GLY:HA2	2.13	0.49
1:B:187:LEU:HD11	1:B:406:ASP:HB2	1.95	0.49
1:A:306:GLY:HA2	1:A:363:HIS:HB2	1.95	0.48
1:B:313:ARG:NH2	1:B:315:GLU:OE2	2.46	0.48
1:B:1026:ILE:N	1:B:1026:ILE:HD12	2.29	0.48
1:B:404:LYS:HA	1:B:409:PHE:CD1	2.48	0.47
1:B:111:LEU:HG	1:B:115:GLN:NE2	2.29	0.47
1:A:355:ASP:O	1:A:356:GLU:HB2	2.15	0.47
1:B:1105:MET:HE2	1:B:1105:MET:HB2	1.66	0.46
1:B:411:LYS:HE2	1:B:415:GLU:OE2	2.15	0.46
1:B:439:PHE:O	1:B:443[A]:GLN:HG2	2.16	0.46
1:B:1105:MET:HE1	1:B:1113:PHE:CE2	2.49	0.46
1:B:389:MET:HE2	1:B:389:MET:CA	2.46	0.45
1:A:375:SER:O	1:A:378:ILE:HG22	2.16	0.45
1:B:1058:THR:HG23	1:B:1061:GLU:HB2	1.98	0.45
1:A:426:LEU:C	1:A:426:LEU:HD23	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:ILE:HG12	1:A:1027:GLY:N	2.32	0.44
1:B:282:ILE:CD1	1:B:337:LEU:HD13	2.41	0.44
1:B:1016:ILE:HG22	1:B:1017:TYR:N	2.32	0.44
1:B:386:ILE:HB	1:B:425:ILE:HG23	2.00	0.44
1:A:419:SER:HB2	1:A:449:VAL:O	2.18	0.44
1:B:447:VAL:HG12	1:B:448:ILE:N	2.33	0.43
1:A:1091:ASP:O	1:A:1095:ARG:HG3	2.18	0.43
1:A:295:ILE:HD13	1:A:382:ILE:HG13	2.01	0.43
1:B:1026:ILE:HG22	1:B:1027:GLY:N	2.33	0.43
1:B:1061:GLU:O	1:B:1065:LEU:HD12	2.18	0.43
1:B:404:LYS:HA	1:B:409:PHE:CG	2.53	0.43
1:A:125:ARG:CG	1:A:131:SER:HB2	2.49	0.42
1:A:123:PRO:HD2	1:A:214:SER:OG	2.19	0.42
1:A:194:LEU:C	1:A:194:LEU:HD23	2.44	0.42
1:B:1058:THR:HG22	1:B:1061:GLU:HB2	2.02	0.42
1:A:125:ARG:HG2	1:A:131:SER:CB	2.50	0.42
1:B:1105:MET:HE2	1:B:1110:VAL:CG2	2.49	0.41
1:A:283:ARG:NH2	1:A:287[A]:GLN:OE1	2.51	0.41
1:B:383:LEU:N	1:B:384:PRO:CD	2.83	0.41
1:B:411:LYS:O	1:B:415:GLU:HG2	2.20	0.41
1:A:100:PHE:HZ	1:A:210:VAL:HG12	1.86	0.41
1:A:1003:PHE:O	1:A:1007:ARG:HG3	2.21	0.41
1:A:383:LEU:N	1:A:384:PRO:CD	2.84	0.41
1:A:381:LEU:HD21	3:A:1385:HOH:O	2.20	0.41
2:A:1201[A]:ATP:O3G	1:B:272:LYS:NZ	2.37	0.40
1:A:1017:TYR:HD1	1:A:1018:LYS:O	2.05	0.40
1:A:1051:ARG:NH1	1:A:1053:THR:HA	2.37	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	442/514 (86%)	430 (97%)	12 (3%)	0	100	100
1	B	417/514 (81%)	403 (97%)	14 (3%)	0	100	100
All	All	859/1028 (84%)	833 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/448 (83%)	368 (100%)	2 (0%)	81	84
1	B	355/448 (79%)	354 (100%)	1 (0%)	86	88
All	All	725/896 (81%)	722 (100%)	3 (0%)	84	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1126	ASP
1	A	183	ASN
1	B	301	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	115	GLN
1	B	1139	ASN
1	B	1140	GLN
1	B	183	ASN
1	B	197	ASN
1	B	427	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are 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	1201[B]	-	32,33,33	1.84	6 (18%)	48,52,52	2.12	14 (29%)
2	ATP	A	1201[A]	-	32,33,33	2.20	10 (31%)	48,52,52	2.46	16 (33%)
2	ATP	B	1201[A]	-	32,33,33	2.62	10 (31%)	48,52,52	2.06	15 (31%)
2	ATP	B	1201[B]	-	32,33,33	2.20	11 (34%)	48,52,52	2.08	15 (31%)

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	1201[B]	-	-	5/22/38/38	0/3/3/3
2	ATP	A	1201[A]	-	-	9/22/38/38	0/3/3/3
2	ATP	B	1201[A]	-	-	2/22/38/38	0/3/3/3
2	ATP	B	1201[B]	-	-	3/22/38/38	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201[A]	ATP	PB-O3A	8.81	1.69	1.59
2	B	1201[A]	ATP	PA-O3A	6.17	1.66	1.59
2	A	1201[A]	ATP	C5-N7	-5.57	1.28	1.39
2	B	1201[B]	ATP	PB-O3B	-5.54	1.53	1.59
2	A	1201[A]	ATP	PB-O3B	-5.25	1.53	1.59
2	A	1201[B]	ATP	C5-N7	-4.67	1.30	1.39
2	B	1201[B]	ATP	PA-O3A	-4.66	1.54	1.59
2	B	1201[A]	ATP	C5-N7	-4.53	1.30	1.39
2	B	1201[B]	ATP	C5-N7	-4.44	1.31	1.39
2	A	1201[A]	ATP	PA-O3A	4.24	1.64	1.59
2	B	1201[A]	ATP	C4-N9	-4.00	1.29	1.37
2	A	1201[B]	ATP	C8-N9	-3.83	1.31	1.37
2	B	1201[B]	ATP	C4-N9	-3.78	1.29	1.37
2	B	1201[A]	ATP	C8-N9	-3.65	1.31	1.37
2	A	1201[A]	ATP	C4-N9	-3.62	1.30	1.37
2	B	1201[B]	ATP	C8-N9	-3.54	1.31	1.37
2	A	1201[B]	ATP	C4-N9	-3.38	1.30	1.37
2	A	1201[A]	ATP	C8-N9	-3.14	1.32	1.37
2	A	1201[A]	ATP	O5'-C5'	-2.98	1.33	1.44
2	A	1201[B]	ATP	PA-O3A	-2.97	1.56	1.59
2	A	1201[B]	ATP	C5-C4	2.69	1.43	1.39
2	B	1201[B]	ATP	PG-O2G	-2.59	1.45	1.54
2	A	1201[A]	ATP	C5-C4	2.55	1.43	1.39
2	B	1201[A]	ATP	PG-O3G	-2.51	1.45	1.54
2	B	1201[A]	ATP	PG-O2G	-2.49	1.45	1.54
2	A	1201[B]	ATP	PB-O3B	-2.45	1.56	1.59
2	B	1201[B]	ATP	PA-O2A	-2.42	1.44	1.55
2	A	1201[A]	ATP	PA-O2A	-2.39	1.44	1.55
2	A	1201[A]	ATP	O4'-C4'	-2.36	1.39	1.45
2	B	1201[B]	ATP	C5-C4	2.35	1.43	1.39
2	B	1201[B]	ATP	PB-O3A	2.34	1.62	1.59
2	B	1201[A]	ATP	C5-C4	2.34	1.43	1.39
2	B	1201[B]	ATP	PG-O3G	-2.31	1.46	1.54
2	B	1201[A]	ATP	PA-O2A	-2.29	1.44	1.55
2	B	1201[A]	ATP	PB-O3B	-2.09	1.57	1.59
2	A	1201[A]	ATP	PG-O3G	-2.09	1.47	1.54
2	B	1201[B]	ATP	PB-O2B	-2.01	1.46	1.55

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201[A]	ATP	O2A-PA-O3A	8.91	131.35	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201[B]	ATP	C5-C4-N3	-6.18	118.21	126.72
2	A	1201[A]	ATP	C5-C4-N3	-6.18	118.21	126.72
2	A	1201[B]	ATP	C5-C4-N3	-6.08	118.35	126.72
2	B	1201[A]	ATP	C5-C4-N3	-5.96	118.51	126.72
2	B	1201[B]	ATP	N3-C4-N9	5.32	136.22	127.17
2	A	1201[B]	ATP	N3-C4-N9	5.29	136.16	127.17
2	B	1201[A]	ATP	N3-C4-N9	5.25	136.10	127.17
2	A	1201[A]	ATP	N3-C4-N9	5.07	135.78	127.17
2	A	1201[B]	ATP	O3G-PG-O3B	-4.96	88.00	104.64
2	B	1201[A]	ATP	O2B-PB-O3B	-4.50	95.12	107.27
2	B	1201[B]	ATP	O2G-PG-O3B	-4.26	90.36	104.64
2	A	1201[B]	ATP	O2G-PG-O3B	3.92	117.79	104.64
2	B	1201[B]	ATP	C2-N3-C4	3.88	121.31	111.83
2	B	1201[A]	ATP	C2-N3-C4	3.74	120.95	111.83
2	A	1201[B]	ATP	C2-N3-C4	3.60	120.63	111.83
2	A	1201[A]	ATP	O2B-PB-O3B	3.56	116.89	107.27
2	A	1201[A]	ATP	C2-N3-C4	3.42	120.19	111.83
2	B	1201[B]	ATP	O3A-PA-O1A	-3.36	100.61	110.70
2	A	1201[A]	ATP	O3A-PA-O1A	-3.28	100.84	110.70
2	A	1201[B]	ATP	O3G-PG-O1G	3.18	123.21	110.83
2	A	1201[B]	ATP	N3-C2-N1	-3.13	123.85	128.58
2	B	1201[A]	ATP	O2B-PB-O3A	3.08	115.59	107.27
2	A	1201[A]	ATP	O3G-PG-O2G	3.07	119.31	107.80
2	A	1201[A]	ATP	N3-C2-N1	-3.05	123.96	128.58
2	A	1201[B]	ATP	C4-N9-C8	3.05	108.94	105.74
2	B	1201[A]	ATP	C4-N9-C8	2.98	108.87	105.74
2	A	1201[B]	ATP	C4-C5-N7	-2.90	107.26	110.58
2	B	1201[B]	ATP	N3-C2-N1	-2.88	124.23	128.58
2	B	1201[B]	ATP	O2B-PB-O3A	2.84	114.94	107.27
2	B	1201[A]	ATP	N3-C2-N1	-2.81	124.32	128.58
2	B	1201[A]	ATP	N6-C6-N1	2.81	124.64	118.38
2	B	1201[B]	ATP	N6-C6-N1	2.80	124.62	118.38
2	B	1201[B]	ATP	O2G-PG-O1G	2.77	121.61	110.83
2	A	1201[A]	ATP	N6-C6-N1	2.76	124.52	118.38
2	B	1201[B]	ATP	O3B-PG-O1G	-2.73	96.69	111.04
2	B	1201[B]	ATP	C4-N9-C8	2.71	108.58	105.74
2	A	1201[B]	ATP	O3B-PG-O1G	-2.68	96.96	111.04
2	A	1201[A]	ATP	O3B-PB-O1B	-2.68	102.66	110.70
2	B	1201[B]	ATP	C5-C6-N6	-2.67	116.68	123.29
2	B	1201[A]	ATP	O3B-PB-O1B	-2.66	102.71	110.70
2	B	1201[A]	ATP	C5-C6-N6	-2.61	116.81	123.29
2	A	1201[A]	ATP	C4-C5-N7	-2.43	107.80	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201[B]	ATP	C5-N7-C8	2.43	107.26	103.45
2	A	1201[A]	ATP	O3G-PG-O3B	-2.43	96.50	104.64
2	A	1201[A]	ATP	O4'-C1'-N9	2.41	112.72	108.09
2	B	1201[A]	ATP	O2A-PA-O3A	2.39	113.74	107.27
2	B	1201[B]	ATP	O2A-PA-O3A	2.37	113.67	107.27
2	A	1201[A]	ATP	O5'-C5'-C4'	2.29	116.78	108.99
2	B	1201[A]	ATP	O2B-PB-O1B	2.22	122.79	112.44
2	B	1201[A]	ATP	O2G-PG-O3B	-2.22	97.18	104.64
2	A	1201[B]	ATP	O3B-PB-O1B	-2.22	104.02	110.70
2	A	1201[A]	ATP	C5-C6-N6	-2.22	117.80	123.29
2	B	1201[B]	ATP	C4-C5-N7	-2.19	108.07	110.58
2	B	1201[A]	ATP	C4-C5-N7	-2.18	108.08	110.58
2	B	1201[B]	ATP	O3G-PG-O2G	2.16	115.90	107.80
2	A	1201[A]	ATP	C5-N7-C8	2.10	106.76	103.45
2	A	1201[B]	ATP	O3G-PG-O2G	2.05	115.50	107.80
2	A	1201[B]	ATP	N9-C8-N7	-2.03	111.05	113.94
2	B	1201[A]	ATP	O3G-PG-O2G	2.01	115.34	107.80

There are no chirality outliers.

All (19) torsion outliers are listed below:

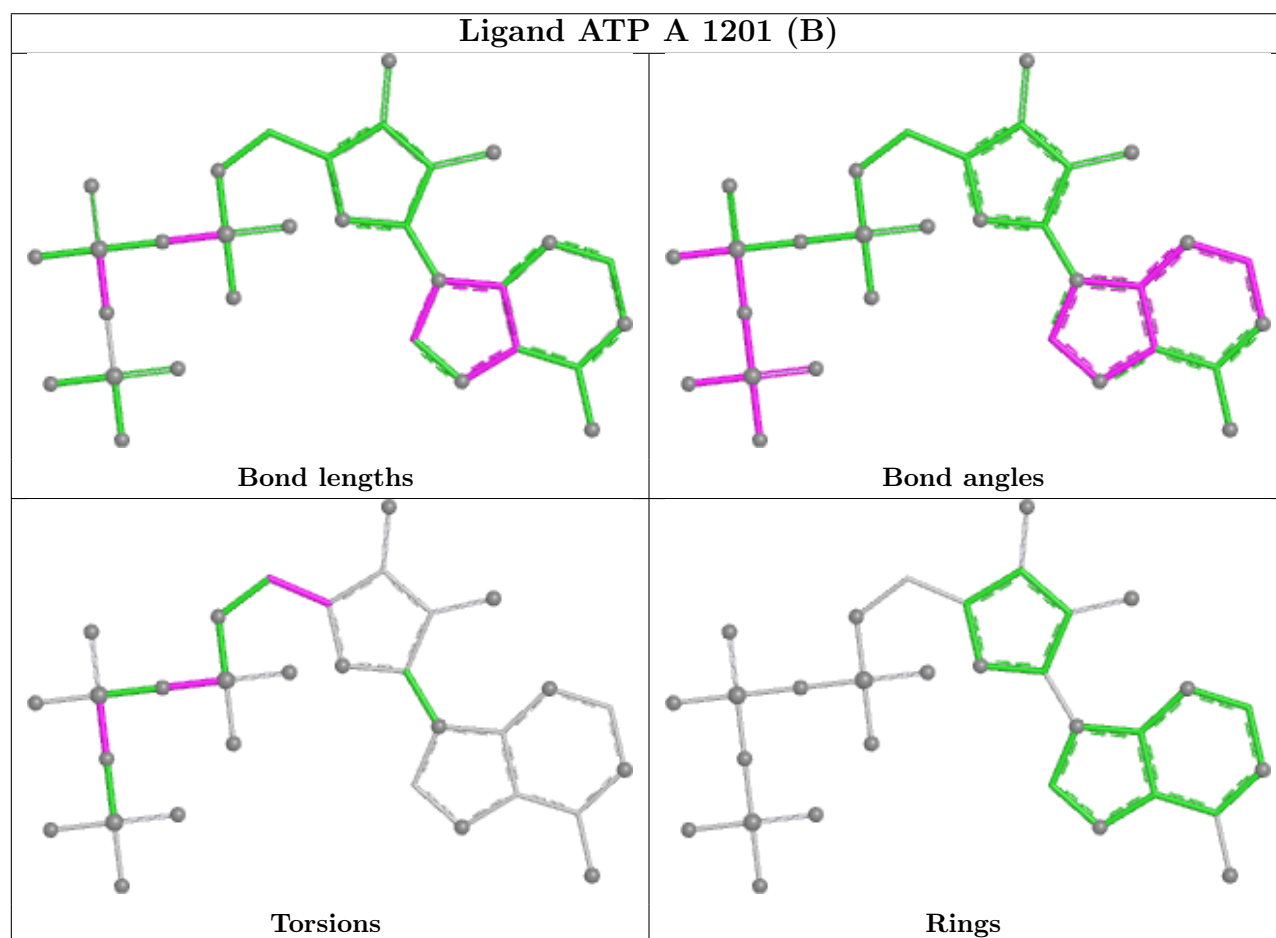
Mol	Chain	Res	Type	Atoms
2	A	1201[A]	ATP	C5'-O5'-PA-O2A
2	A	1201[A]	ATP	C5'-O5'-PA-O3A
2	B	1201[B]	ATP	PB-O3B-PG-O3G
2	A	1201[A]	ATP	O4'-C4'-C5'-O5'
2	A	1201[A]	ATP	C3'-C4'-C5'-O5'
2	A	1201[B]	ATP	O4'-C4'-C5'-O5'
2	A	1201[A]	ATP	PG-O3B-PB-O1B
2	A	1201[A]	ATP	PA-O3A-PB-O1B
2	A	1201[A]	ATP	PB-O3A-PA-O2A
2	A	1201[B]	ATP	PG-O3B-PB-O1B
2	A	1201[A]	ATP	C5'-O5'-PA-O1A
2	A	1201[A]	ATP	PA-O3A-PB-O2B
2	A	1201[B]	ATP	PB-O3A-PA-O2A
2	A	1201[B]	ATP	C3'-C4'-C5'-O5'
2	B	1201[B]	ATP	PB-O3B-PG-O1G
2	B	1201[B]	ATP	PB-O3B-PG-O2G
2	B	1201[A]	ATP	PA-O3A-PB-O2B
2	B	1201[A]	ATP	O4'-C4'-C5'-O5'
2	A	1201[B]	ATP	PG-O3B-PB-O2B

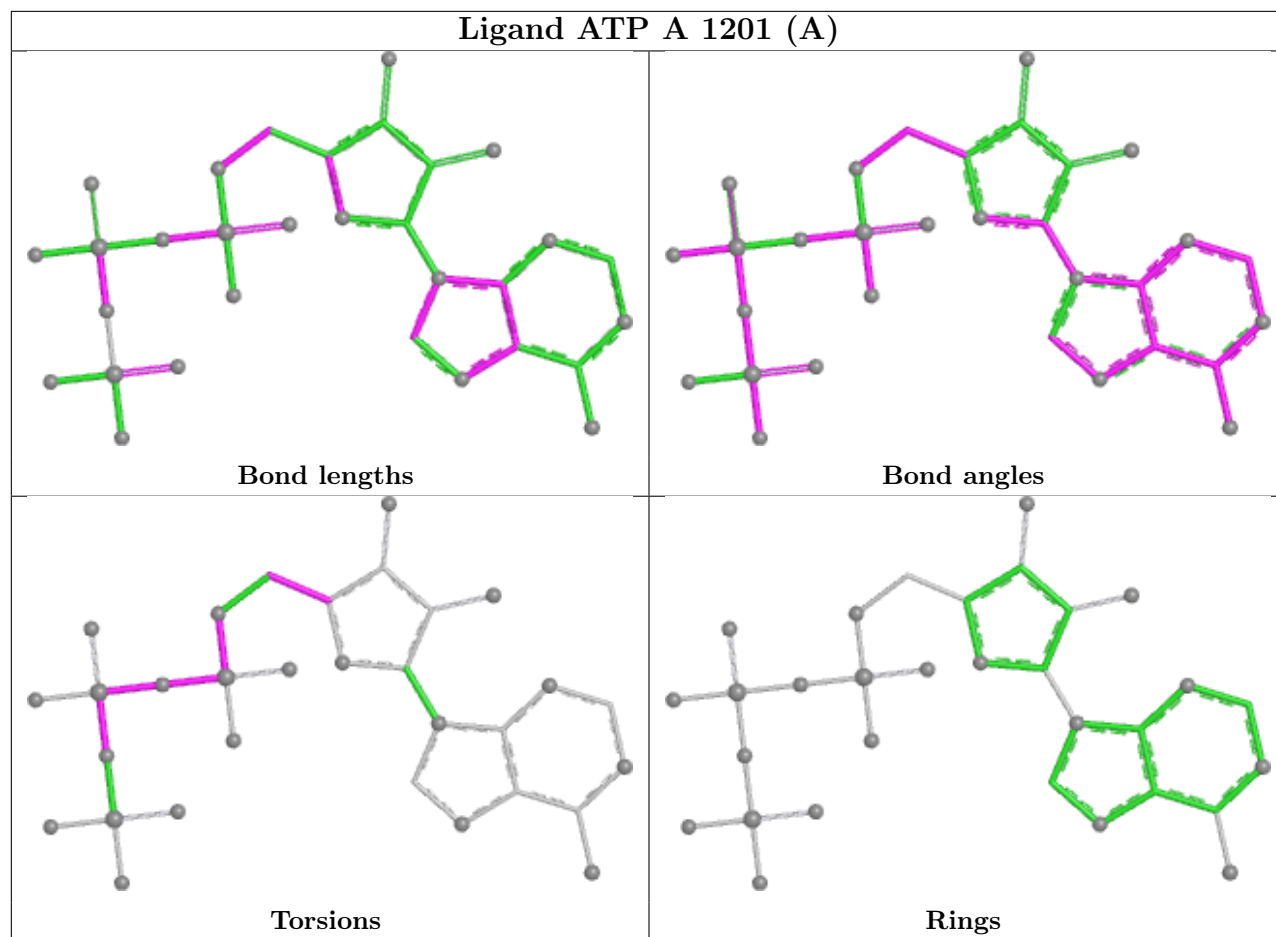
There are no ring outliers.

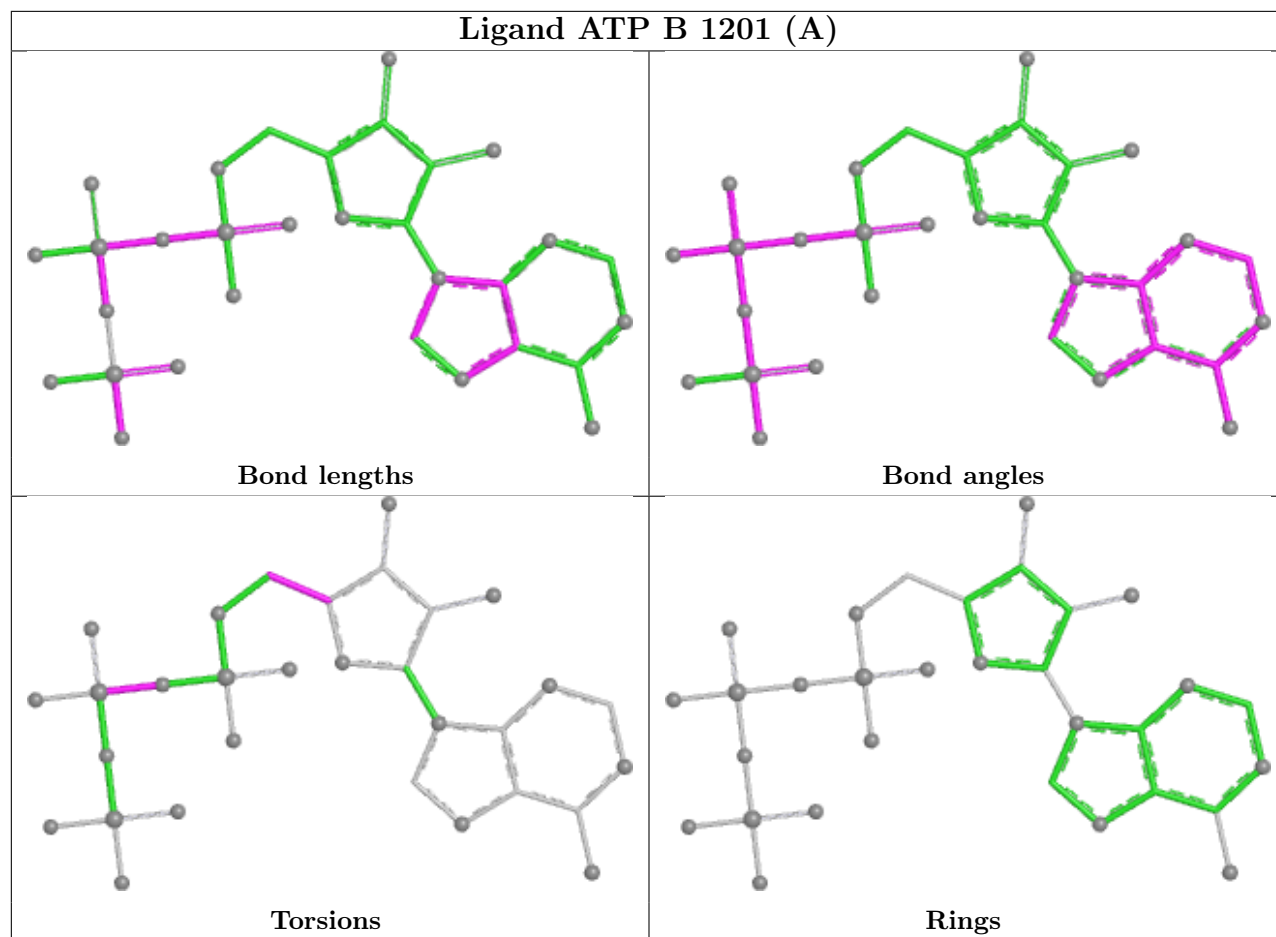
1 monomer is involved in 3 short contacts:

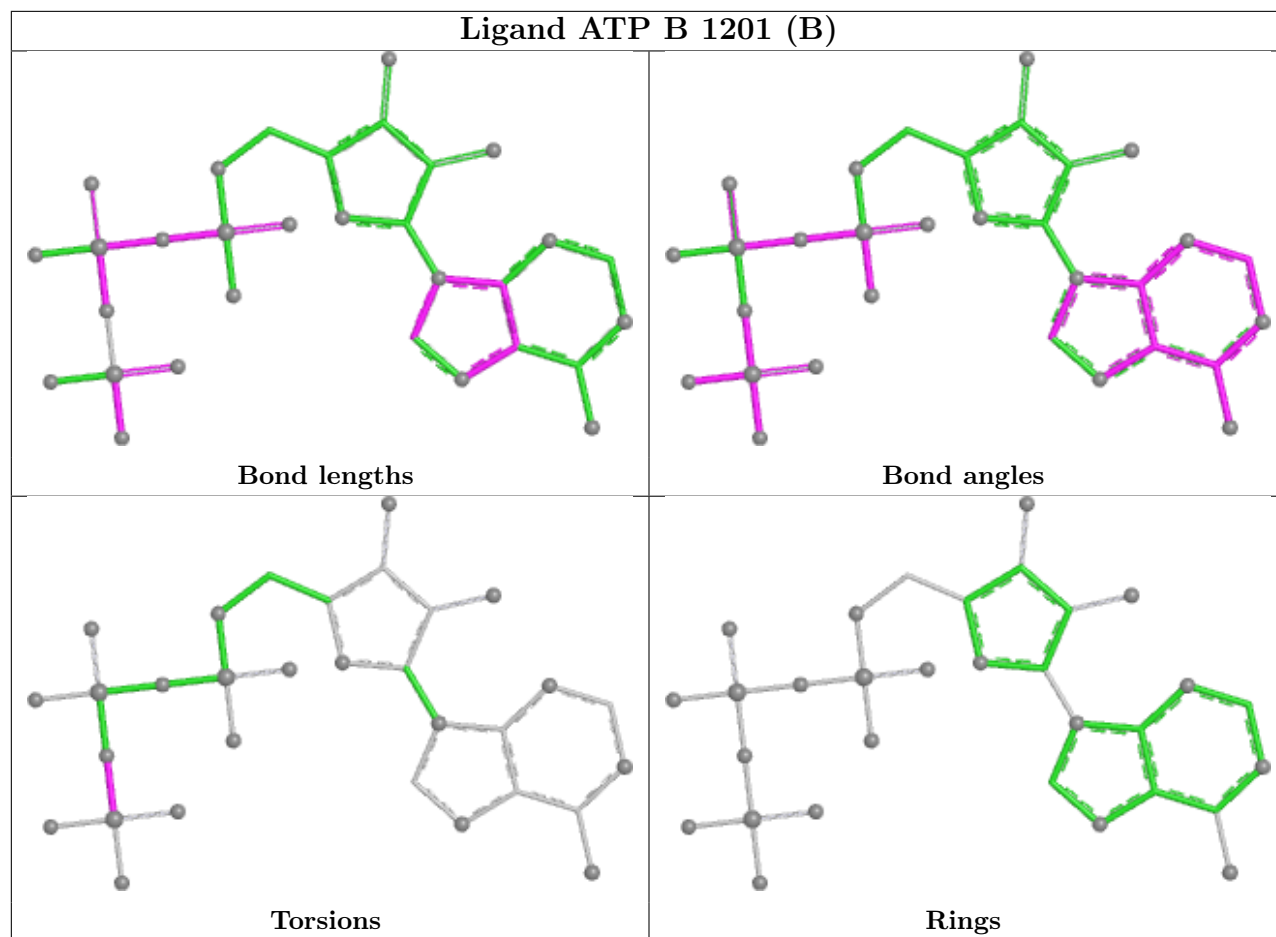
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201[A]	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	447/514 (86%)	0.70	39 (8%)	16 17	15, 40, 66, 84	3 (0%)
1	B	426/514 (82%)	0.64	38 (8%)	15 16	14, 39, 72, 89	3 (0%)
All	All	873/1028 (84%)	0.67	77 (8%)	15 16	14, 39, 69, 89	6 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	TRP	8.3
1	B	1024	TYR	6.6
1	B	1026	ILE	6.4
1	B	357	TRP	5.8
1	A	220	ASN	5.2
1	A	1023	TYR	4.8
1	A	250	PRO	4.6
1	B	336	PHE	4.6
1	B	1023	TYR	4.4
1	B	358	ARG	4.4
1	B	1016	ILE	4.3
1	A	162	TRP	4.2
1	B	1031	LEU	4.1
1	B	1057	ILE	4.1
1	B	127	SER	3.8
1	B	1014	LEU	3.7
1	A	336	PHE	3.7
1	B	155	TYR	3.6
1	B	1027	GLY	3.6
1	A	1020	THR	3.6
1	B	1025	THR	3.5
1	B	1020	THR	3.3
1	A	358	ARG	3.3
1	B	316	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	131	SER	3.2
1	B	163	THR	3.1
1	A	132	GLY	3.1
1	A	337	LEU	2.9
1	B	156	GLY	2.9
1	B	355	ASP	2.9
1	A	215	GLU	2.9
1	A	99	ALA	2.8
1	A	359	ALA	2.7
1	A	122	PHE	2.7
1	A	1018	LYS	2.7
1	B	119	VAL	2.7
1	A	219	TYR	2.7
1	B	121	ILE	2.7
1	B	1059	LYS	2.7
1	B	1138	TYR	2.7
1	A	1021	GLU	2.7
1	B	1065	LEU	2.6
1	B	1030	HIS	2.6
1	A	1017	TYR	2.6
1	B	337	LEU	2.6
1	B	359	ALA	2.6
1	B	1017	TYR	2.5
1	A	287[A]	GLN	2.5
1	A	177	ARG	2.4
1	B	97	MET	2.4
1	B	1058	THR	2.4
1	B	157	GLN	2.4
1	A	130	SER	2.4
1	B	1015	LYS	2.4
1	A	165	TYR	2.4
1	B	219	TYR	2.3
1	A	163	THR	2.3
1	A	282	ILE	2.3
1	A	279	PRO	2.3
1	A	1026	ILE	2.3
1	A	213	VAL	2.3
1	A	116	ALA	2.2
1	A	1022	GLY	2.2
1	A	1041	ALA	2.2
1	B	249	LEU	2.2
1	A	120	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	214	SER	2.2
1	A	111	LEU	2.2
1	A	1034	LYS	2.2
1	A	1162	ASN	2.1
1	B	165	TYR	2.1
1	B	448	ILE	2.1
1	A	216	THR	2.1
1	A	356	GLU	2.1
1	B	1162	ASN	2.1
1	A	121	ILE	2.0
1	A	119	VAL	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](#)

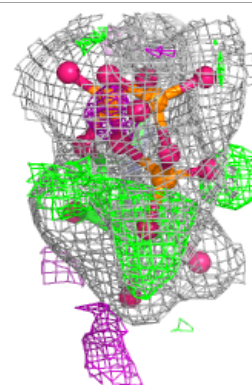
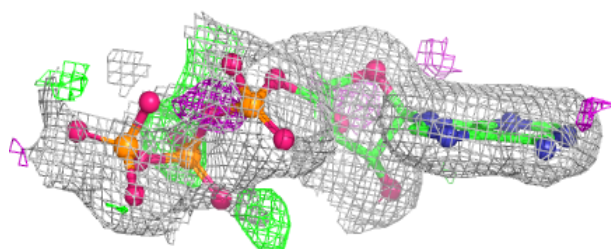
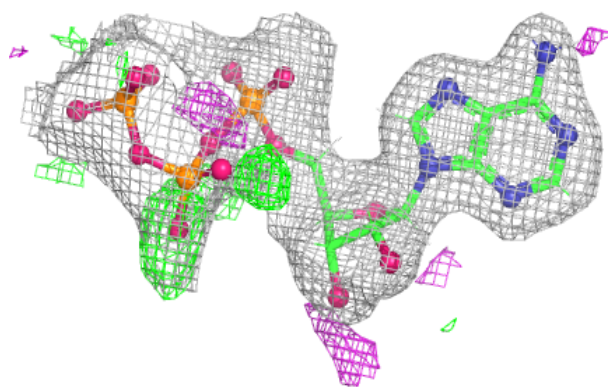
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1201[A]	31/31	0.63	0.15	32,45,58,61	43
2	ATP	A	1201[B]	31/31	0.63	0.15	32,44,57,61	43
2	ATP	B	1201[A]	31/31	0.85	0.09	32,42,51,56	43
2	ATP	B	1201[B]	31/31	0.85	0.09	32,42,52,58	43

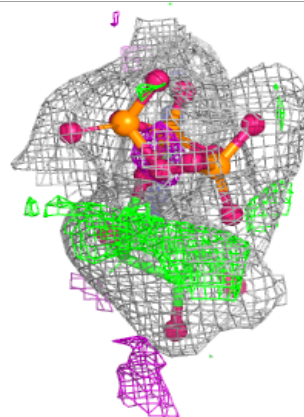
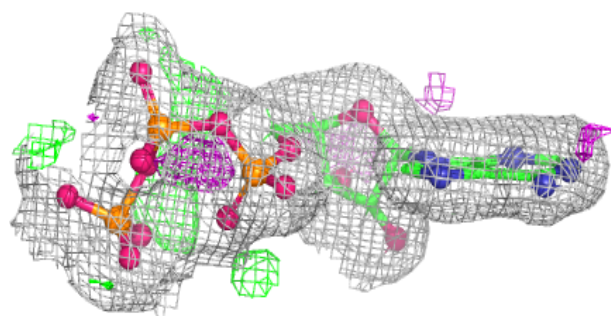
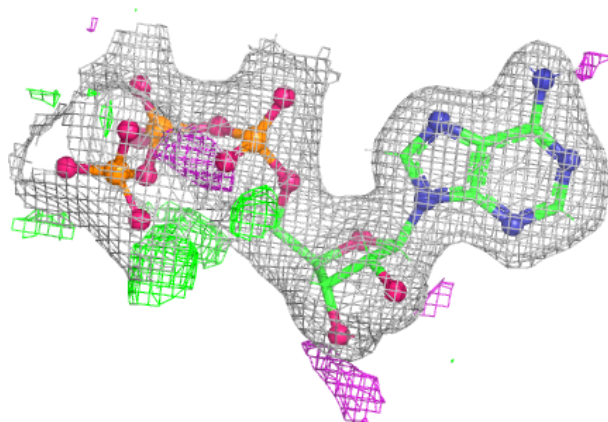
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 1201 (A):

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

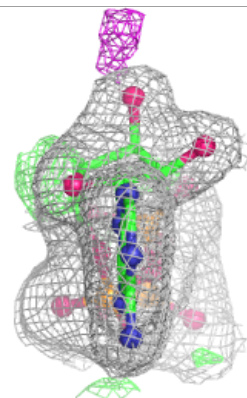
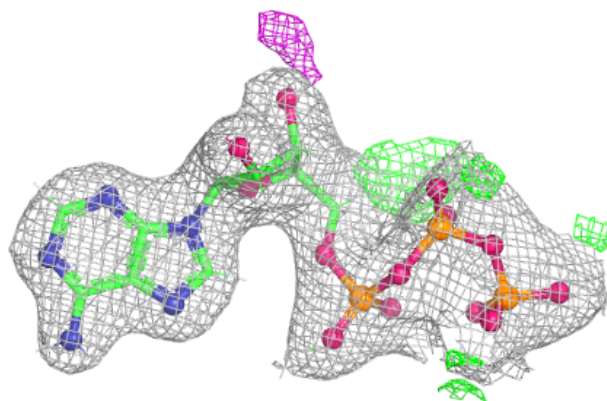
**Electron density around ATP A 1201 (B):**

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

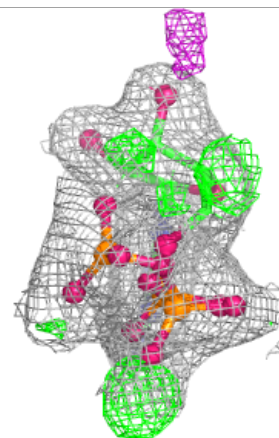
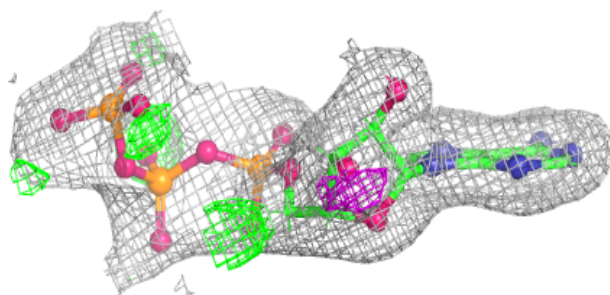
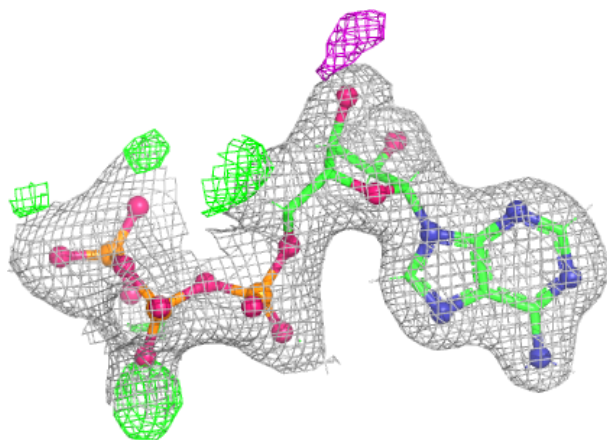


Electron density around ATP B 1201 (A):

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

**Electron density around ATP B 1201 (B):**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.