



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:59 PM UTC

PDB ID : 8WVE / pdb_00008wve
Title : Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC
Authors : Furuike, Y.; Akiyama, S.
Deposited on : 2023-10-23
Resolution : 2.73 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

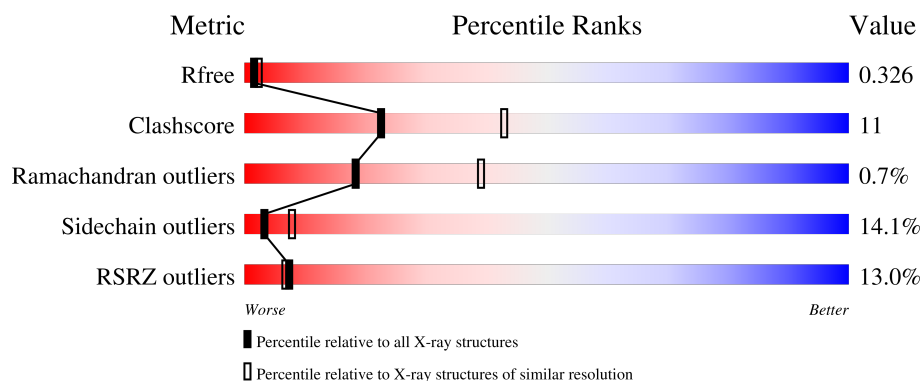
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	519	11% 66% 18% • 13%
1	B	519	11% 66% 18% • 13%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6562 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.

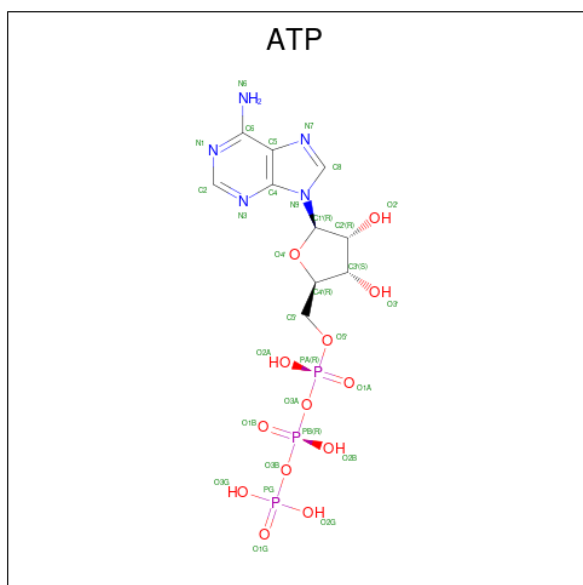
- Molecule 1 is a protein called Circadian clock oscillator protein KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3233	2050	566	603	14			
1	B	453	Total	C	N	O	S	0	0	0
			3173	2000	561	601	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	THR	SER	engineered mutation	UNP Q79PF4
A	432	VAL	THR	engineered mutation	UNP Q79PF4
B	431	THR	SER	engineered mutation	UNP Q79PF4
B	432	VAL	THR	engineered mutation	UNP Q79PF4

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		

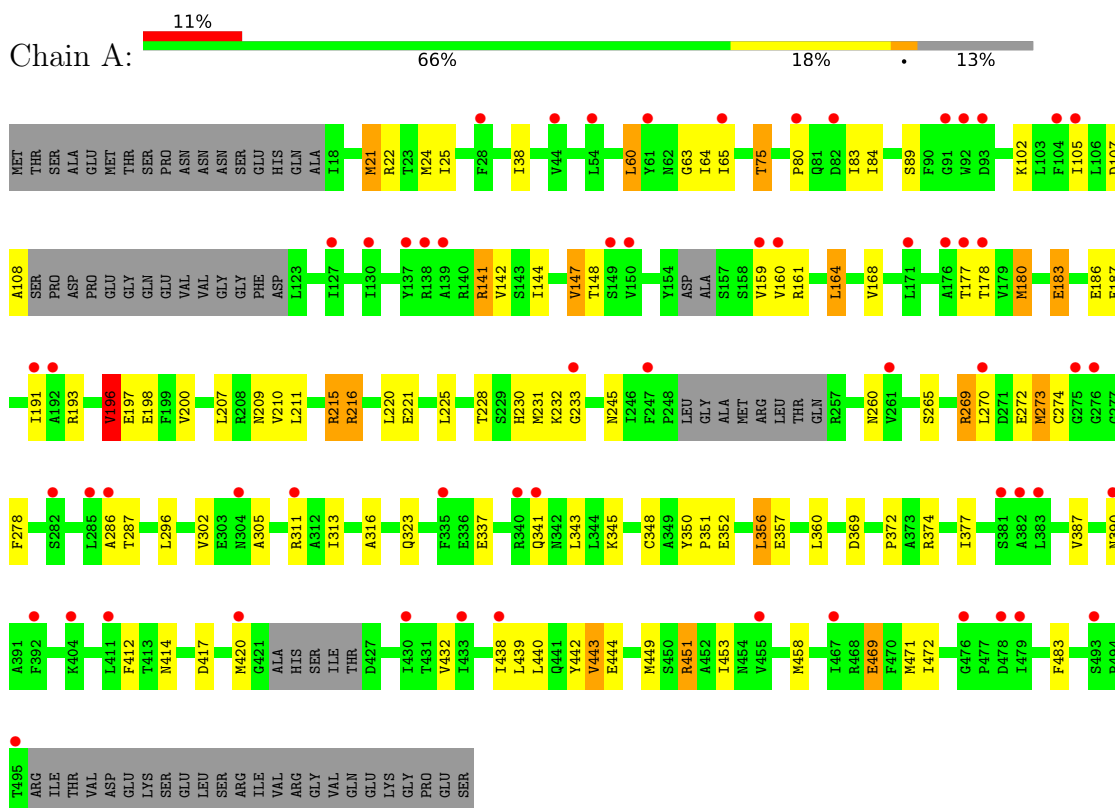
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	13	Total	O	0	0
			13	13		

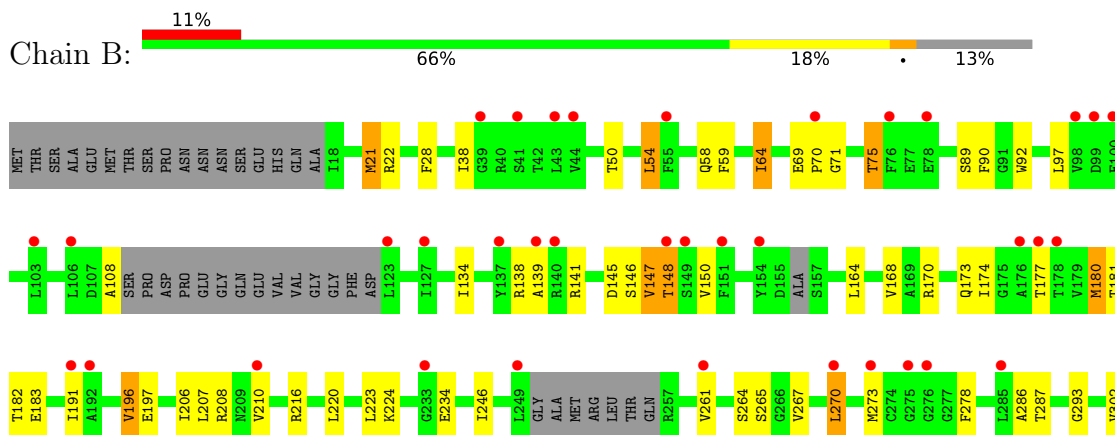
3 Residue-property plots

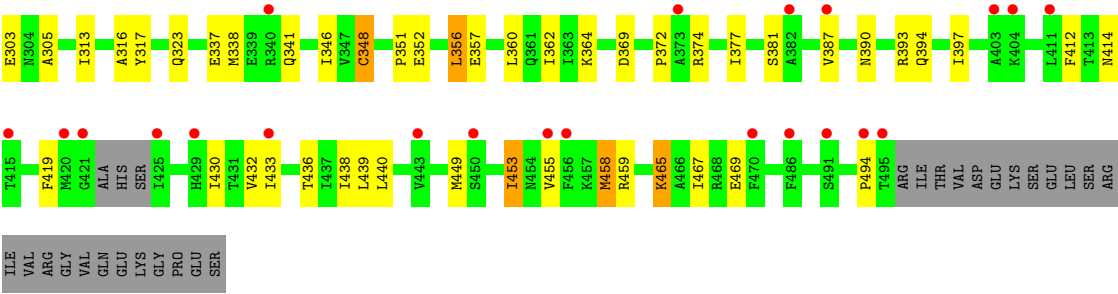
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Circadian clock oscillator protein KaiC



- Molecule 1: Circadian clock oscillator protein KaiC





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	94.19Å 94.19Å 179.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.14 – 2.73 47.14 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.14-2.73) 99.7 (47.14-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.280 , 0.338 0.280 , 0.326	Depositor DCC
R_{free} test set	1109 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6562	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.9736e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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, MG

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	0.46	0/3281	0.79	0/4449
1	B	0.46	0/3216	0.82	0/4370
All	All	0.46	0/6497	0.81	0/8819

There are no bond length outliers.

There are no bond angle outliers.

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	3233	0	2997	67	0
1	B	3173	0	2876	67	0
2	A	62	0	24	2	0
2	B	62	0	24	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	15	0	0	1	0
4	B	13	0	0	0	0
All	All	6562	0	5921	131	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 (131) 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:B:70:PRO:HB2	1:B:139:ALA:HB2	1.48	0.94
1:A:142:VAL:HB	1:A:178:THR:HG22	1.50	0.93
1:B:170:ARG:O	1:B:174:ILE:HD12	1.69	0.92
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.51	0.90
1:A:183:GLU:OE1	1:A:193:ARG:NH2	2.11	0.84
1:B:287:THR:HG22	1:B:414:ASN:HD22	1.50	0.76
1:B:316:ALA:HB3	1:B:348:CYS:HB3	1.67	0.75
1:A:420:MET:HG2	1:A:449:MET:HE1	1.68	0.75
1:A:21:MET:HE3	1:A:177:THR:HG21	1.69	0.74
1:B:148:THR:HG23	1:B:182:THR:HG23	1.73	0.70
1:B:337:GLU:O	1:B:341:GLN:HG3	1.93	0.68
1:B:356:LEU:CD2	1:B:387:VAL:HG11	2.23	0.67
1:B:305:ALA:HB2	1:B:374:ARG:HD3	1.77	0.67
1:B:440:LEU:CD2	1:B:453:ILE:HG13	2.25	0.67
1:B:21:MET:SD	1:B:141:ARG:NE	2.69	0.66
1:B:70:PRO:CB	1:B:139:ALA:HB2	2.25	0.66
1:A:215:ARG:HA	1:A:215:ARG:NE	2.12	0.63
1:A:64:ILE:HG21	1:A:102:LYS:HB3	1.82	0.61
1:A:211:LEU:HD21	1:B:234:GLU:OE1	2.00	0.61
1:A:442:TYR:HB3	1:A:449:MET:HE3	1.84	0.59
1:A:147:VAL:HG21	1:A:180:MET:HE2	1.84	0.59
1:B:207:LEU:HD21	1:B:220:LEU:HD12	1.83	0.59
1:A:420:MET:HE2	1:A:442:TYR:HB2	1.84	0.58
1:A:142:VAL:CB	1:A:178:THR:HG22	2.30	0.57
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.35	0.57
1:A:197:GLU:N	1:A:197:GLU:OE2	2.36	0.56
1:A:225:LEU:HB3	1:A:228:THR:HG23	1.87	0.56
1:A:442:TYR:HA	1:A:451:ARG:HA	1.88	0.56
1:B:70:PRO:O	1:B:139:ALA:HB1	2.07	0.55
1:B:147:VAL:HG21	1:B:180:MET:CE	2.37	0.55
1:A:311:ARG:HA	1:A:343:LEU:O	2.07	0.55
1:A:38:ILE:HA	1:A:177:THR:CG2	2.37	0.54
1:B:21:MET:HE3	1:B:177:THR:HG21	1.89	0.54
1:A:420:MET:CE	1:A:442:TYR:HB2	2.37	0.54
1:A:296:LEU:HD22	1:A:472:ILE:HD13	1.90	0.54
1:A:337:GLU:O	1:A:341:GLN:HG3	2.08	0.53
1:A:75:THR:HG22	1:A:107:ASP:HA	1.89	0.53
1:A:63:GLY:HA3	1:A:141:ARG:HD2	1.89	0.53
1:B:38:ILE:HA	1:B:177:THR:CG2	2.39	0.53
1:A:265:SER:HB3	1:A:278:PHE:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD21	1:A:220:LEU:HD12	1.91	0.52
1:B:191:ILE:HD12	1:B:206:ILE:HD11	1.92	0.52
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.91	0.51
1:B:147:VAL:O	1:B:150:VAL:HG12	2.11	0.51
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.91	0.51
1:B:21:MET:HB2	1:B:38:ILE:CD1	2.40	0.51
1:A:269:ARG:HH21	1:A:272:GLU:HB3	1.75	0.51
1:B:147:VAL:HG21	1:B:180:MET:HE2	1.93	0.51
1:B:54:LEU:HD22	1:B:90:PHE:CZ	2.46	0.50
1:B:197:GLU:OE2	1:B:197:GLU:N	2.43	0.50
1:B:164:LEU:CD2	1:B:197:GLU:HA	2.41	0.50
1:B:436:THR:OG1	1:B:458:MET:HE3	2.11	0.50
1:A:191:ILE:HD12	1:A:198:GLU:HG3	1.93	0.49
1:B:71:GLY:HA2	1:B:141:ARG:O	2.11	0.49
1:A:286:ALA:HA	1:A:438:ILE:O	2.12	0.49
1:B:267:VAL:HB	1:B:270:LEU:HB2	1.94	0.49
1:B:58:GLN:HG2	1:B:92:TRP:CH2	2.49	0.48
1:B:22:ARG:O	1:B:141:ARG:NH2	2.45	0.48
1:B:75:THR:O	1:B:108:ALA:HB3	2.14	0.48
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.48	0.48
1:A:21:MET:CE	1:A:177:THR:HG21	2.40	0.47
1:B:147:VAL:HG11	1:B:180:MET:HE1	1.97	0.47
1:A:89:SER:OG	2:A:601:ATP:N6	2.42	0.47
1:B:64:ILE:HG23	1:B:69:GLU:O	2.15	0.47
1:A:147:VAL:HG11	1:A:180:MET:HE1	1.95	0.47
1:B:59:PHE:O	1:B:141:ARG:NH1	2.48	0.47
1:A:420:MET:HE3	1:A:449:MET:CE	2.45	0.47
1:B:265:SER:HB3	1:B:278:PHE:CE2	2.50	0.46
1:A:147:VAL:HG21	1:A:180:MET:CE	2.44	0.46
1:A:160:VAL:O	1:A:164:LEU:HB2	2.16	0.46
1:A:274:CYS:HG	1:A:278:PHE:HE1	1.62	0.46
1:B:207:LEU:CD2	1:B:220:LEU:HD12	2.45	0.46
1:B:147:VAL:HG23	1:B:181:THR:O	2.15	0.46
1:A:232:LYS:NZ	4:A:702:HOH:O	2.48	0.46
1:A:225:LEU:HD12	1:A:230:HIS:HB3	1.96	0.46
1:B:89:SER:OG	2:B:601:ATP:N6	2.49	0.45
1:A:75:THR:O	1:A:108:ALA:HB3	2.17	0.45
1:B:317:TYR:HB3	1:B:351:PRO:HG3	1.98	0.45
1:B:264:SER:O	1:B:374:ARG:NH1	2.31	0.45
1:B:316:ALA:O	1:B:348:CYS:HA	2.17	0.45
1:B:21:MET:HG3	1:B:141:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASN:ND2	1:A:216:ARG:HG3	2.33	0.44
1:B:287:THR:CG2	1:B:414:ASN:HD22	2.23	0.44
1:B:390:ASN:O	1:B:394:GLN:HG3	2.18	0.44
1:A:469:GLU:CB	1:A:483:PHE:CZ	3.01	0.44
2:A:602:ATP:H3'	1:B:458:MET:O	2.18	0.44
1:B:54:LEU:C	1:B:54:LEU:HD12	2.43	0.44
1:A:449:MET:N	1:B:465:LYS:O	2.51	0.44
1:B:180:MET:HE2	1:B:180:MET:HB3	1.86	0.44
1:A:21:MET:SD	1:A:141:ARG:NE	2.91	0.43
1:A:269:ARG:O	1:A:273:MET:HG2	2.18	0.43
1:A:444:GLU:HG3	1:B:467:ILE:HD11	2.00	0.43
1:A:21:MET:HE1	1:A:177:THR:OG1	2.18	0.43
1:A:164:LEU:CD1	1:A:197:GLU:HA	2.48	0.43
1:B:134:ILE:O	1:B:138:ARG:N	2.50	0.43
1:A:440:LEU:CD2	1:A:453:ILE:HG13	2.49	0.43
1:B:21:MET:HB2	1:B:38:ILE:HD11	2.00	0.43
1:B:438:ILE:HD12	1:B:455:VAL:HG22	2.00	0.43
1:A:38:ILE:HA	1:A:177:THR:HG22	2.00	0.43
1:A:211:LEU:HD13	1:A:216:ARG:HD3	2.01	0.43
1:B:303:GLU:HG3	1:B:338:MET:HE1	2.00	0.43
1:A:80:PRO:O	1:A:84:ILE:HG13	2.19	0.43
1:A:180:MET:HE2	1:A:180:MET:HB3	1.86	0.43
1:A:287:THR:HA	1:A:414:ASN:O	2.19	0.43
1:A:142:VAL:HB	1:A:178:THR:CG2	2.35	0.42
1:A:220:LEU:C	1:A:220:LEU:HD23	2.43	0.42
1:A:221:GLU:HG3	1:A:233:GLY:C	2.44	0.42
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.93	0.42
1:B:377:ILE:HD12	1:B:412:PHE:CE1	2.54	0.42
1:B:28:PHE:HB2	1:B:246:ILE:HD12	2.00	0.42
1:B:164:LEU:HD21	1:B:197:GLU:HA	1.99	0.42
1:A:420:MET:HE3	1:A:449:MET:HE1	2.00	0.42
1:A:164:LEU:HD13	1:A:200:VAL:HB	2.01	0.42
1:A:265:SER:OG	1:A:270:LEU:HD23	2.20	0.42
1:A:313:ILE:HG13	1:A:372:PRO:HB3	2.02	0.42
1:B:286:ALA:HA	1:B:438:ILE:O	2.19	0.42
1:A:377:ILE:HD12	1:A:412:PHE:CE1	2.55	0.42
1:B:313:ILE:HG13	1:B:372:PRO:HB3	2.02	0.42
1:B:381:SER:HB3	1:B:414:ASN:OD1	2.20	0.42
1:A:305:ALA:HB2	1:A:374:ARG:HD2	2.02	0.41
1:B:449:MET:HE2	1:B:449:MET:HA	2.01	0.41
1:A:350:TYR:HA	1:A:351:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:VAL:HG21	1:A:483:PHE:CZ	2.56	0.41
1:B:393:ARG:O	1:B:397:ILE:HG12	2.21	0.41
1:B:145:ASP:HA	1:B:146:SER:HA	1.71	0.41
1:B:220:LEU:C	1:B:220:LEU:HD23	2.46	0.41
1:B:412:PHE:N	1:B:412:PHE:CD1	2.86	0.41
1:B:430:ILE:HA	1:B:433:ILE:HD13	2.03	0.41
1:B:206:ILE:HD11	1:B:223:LEU:HD22	2.03	0.41
1:A:316:ALA:HB3	1:A:348:CYS:SG	2.62	0.40
1:B:208:ARG:HG3	1:B:208:ARG:HH21	1.86	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	439/519 (85%)	409 (93%)	29 (7%)	1 (0%)	43	66
1	B	443/519 (85%)	406 (92%)	32 (7%)	5 (1%)	11	27
All	All	882/1038 (85%)	815 (92%)	61 (7%)	6 (1%)	18	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	97	LEU
1	B	494	PRO
1	B	196	VAL
1	B	419	PHE
1	A	196	VAL
1	B	293	GLY

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	299/444 (67%)	253 (85%)	46 (15%)	2	6
1	B	283/444 (64%)	247 (87%)	36 (13%)	4	10
All	All	582/888 (66%)	500 (86%)	82 (14%)	3	8

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	22	ARG
1	A	24	MET
1	A	25	ILE
1	A	60	LEU
1	A	65	ILE
1	A	75	THR
1	A	83	ILE
1	A	105	ILE
1	A	141	ARG
1	A	144	ILE
1	A	147	VAL
1	A	148	THR
1	A	159	VAL
1	A	164	LEU
1	A	168	VAL
1	A	180	MET
1	A	183	GLU
1	A	186	GLU
1	A	187	GLU
1	A	196	VAL
1	A	210	VAL
1	A	215	ARG
1	A	216	ARG
1	A	231	MET
1	A	245	ASN
1	A	260	ASN

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Mol	Chain	Res	Type
1	A	269	ARG
1	A	273	MET
1	A	302	VAL
1	A	323	GLN
1	A	345	LYS
1	A	352	GLU
1	A	356	LEU
1	A	357	GLU
1	A	360	LEU
1	A	369	ASP
1	A	390	ASN
1	A	417	ASP
1	A	432	VAL
1	A	439	LEU
1	A	443	VAL
1	A	451	ARG
1	A	458	MET
1	A	469	GLU
1	A	471	MET
1	B	21	MET
1	B	50	THR
1	B	54	LEU
1	B	64	ILE
1	B	75	THR
1	B	147	VAL
1	B	148	THR
1	B	168	VAL
1	B	173	GLN
1	B	180	MET
1	B	183	GLU
1	B	196	VAL
1	B	210	VAL
1	B	216	ARG
1	B	224	LYS
1	B	261	VAL
1	B	270	LEU
1	B	273	MET
1	B	302	VAL
1	B	323	GLN
1	B	346	ILE
1	B	348	CYS
1	B	352	GLU

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Mol	Chain	Res	Type
1	B	356	LEU
1	B	357	GLU
1	B	360	LEU
1	B	362	ILE
1	B	364	LYS
1	B	369	ASP
1	B	432	VAL
1	B	439	LEU
1	B	453	ILE
1	B	458	MET
1	B	459	ARG
1	B	465	LYS
1	B	469	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	209	ASN
1	A	245	ASN
1	A	323	GLN
1	A	327	ASN
1	A	341	GLN
1	A	361	GLN
1	B	203	ASN
1	B	359	HIS
1	B	414	ASN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	B	602	3	32,33,33	0.55	0	48,52,52	0.57	0
2	ATP	B	601	3	32,33,33	0.51	0	48,52,52	0.61	0
2	ATP	A	601	3	32,33,33	0.52	0	48,52,52	0.54	0
2	ATP	A	602	3	32,33,33	0.52	0	48,52,52	0.58	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	B	602	3	-	0/22/38/38	0/3/3/3
2	ATP	B	601	3	-	2/22/38/38	0/3/3/3
2	ATP	A	601	3	-	7/22/38/38	0/3/3/3
2	ATP	A	602	3	-	1/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O1A
2	A	601	ATP	C5'-O5'-PA-O2A
2	A	601	ATP	C5'-O5'-PA-O3A
2	A	601	ATP	C3'-C4'-C5'-O5'
2	A	601	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	PA-O3A-PB-O1B
2	A	601	ATP	PA-O3A-PB-O2B

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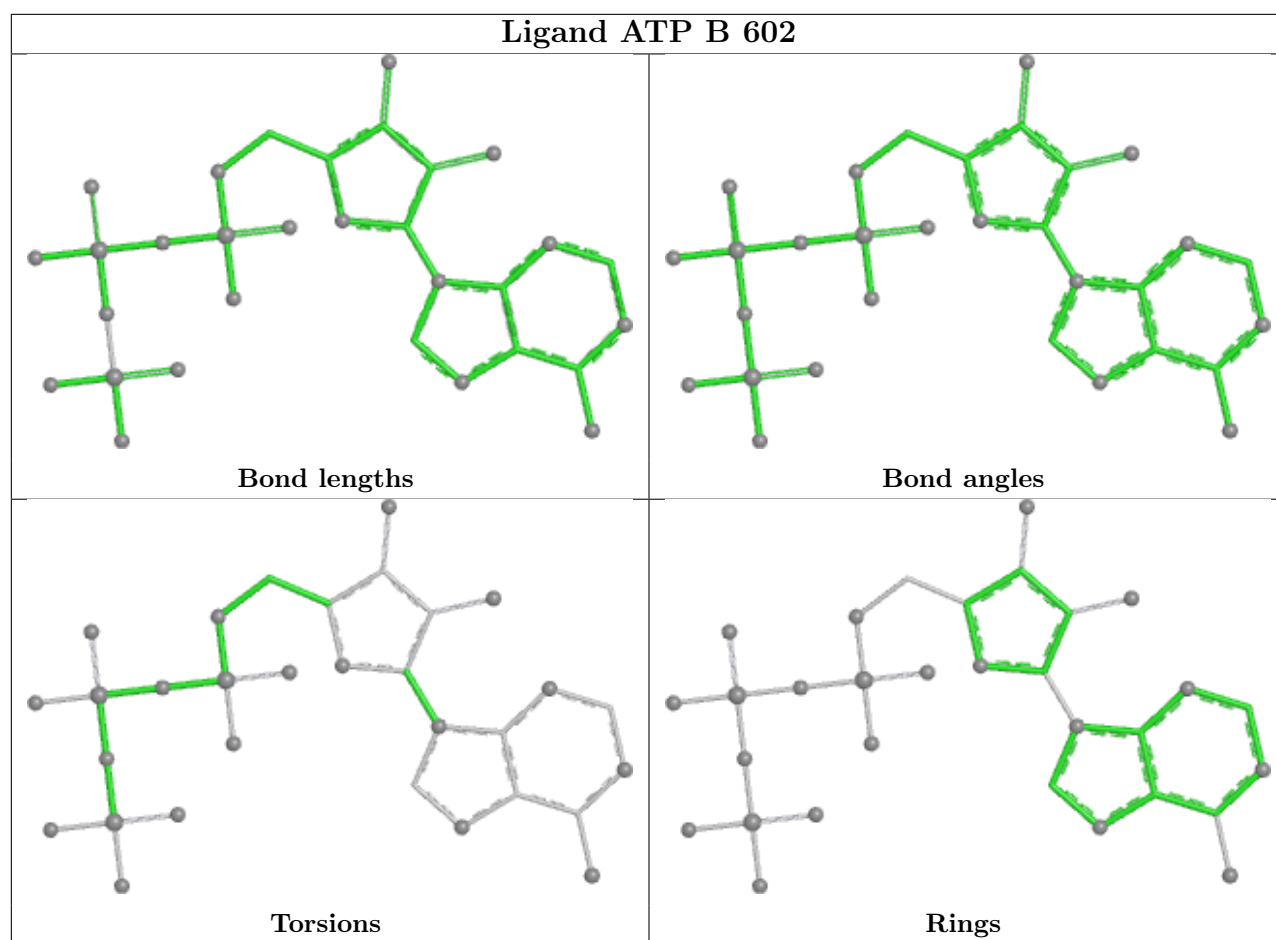
Mol	Chain	Res	Type	Atoms
2	A	602	ATP	PA-O3A-PB-O2B
2	A	601	ATP	PA-O3A-PB-O1B
2	B	601	ATP	PA-O3A-PB-O2B

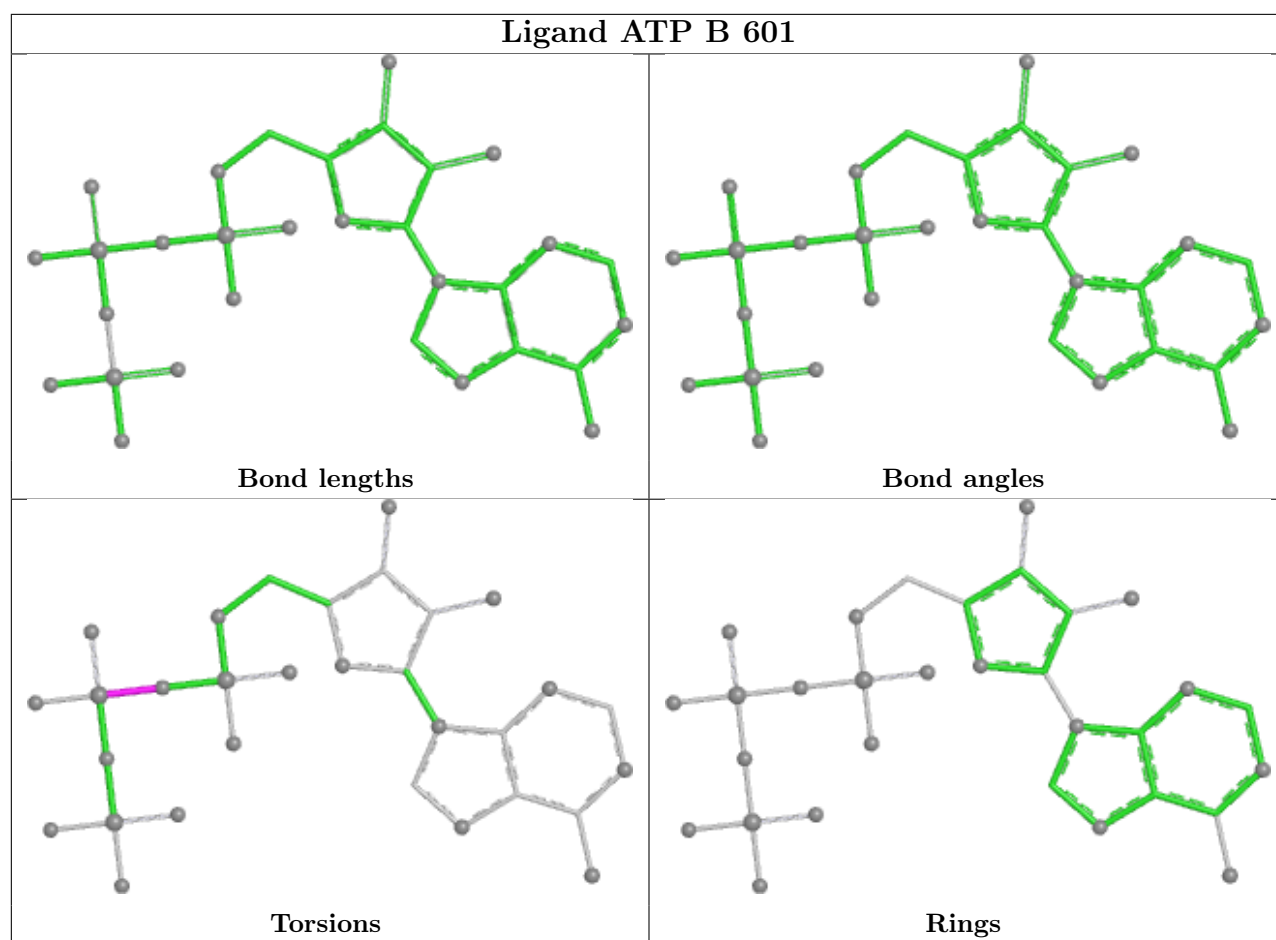
There are no ring outliers.

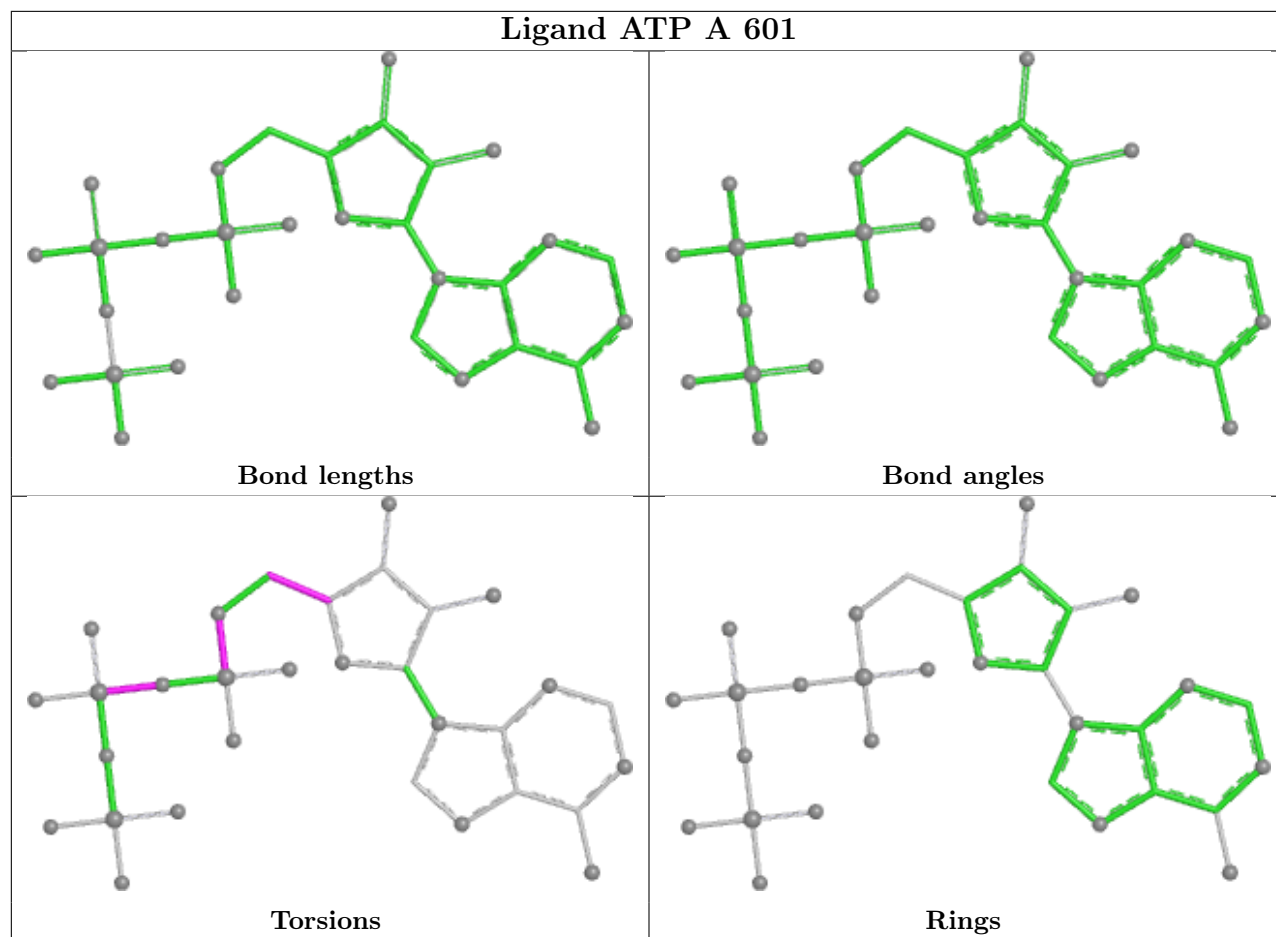
3 monomers are involved in 3 short contacts:

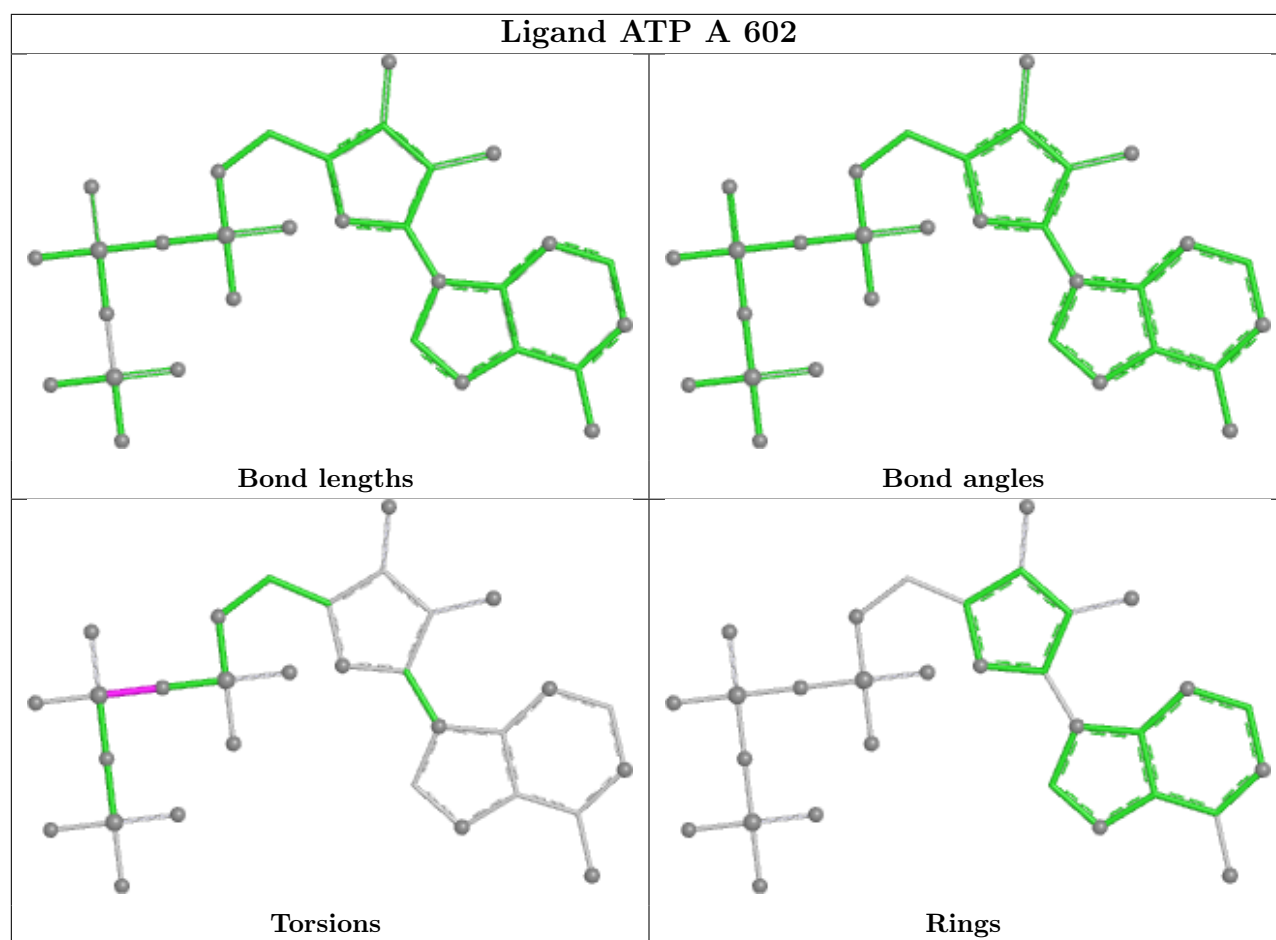
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	ATP	1	0
2	A	601	ATP	1	0
2	A	602	ATP	1	0

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 ⓘ

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	449/519 (86%)	1.14	59 (13%) 7 7	47, 69, 106, 117	0
1	B	453/519 (87%)	1.16	58 (12%) 7 7	45, 69, 116, 133	0
All	All	902/1038 (86%)	1.15	117 (12%) 7 7	45, 69, 110, 133	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	TYR	5.0
1	B	98	VAL	4.9
1	A	276	GLY	4.6
1	B	140	ARG	4.5
1	B	373	ALA	4.4
1	B	470	PHE	4.4
1	A	139	ALA	4.1
1	B	106	LEU	4.0
1	A	138	ARG	4.0
1	A	275	GLY	3.9
1	B	450	SER	3.7
1	B	151	PHE	3.6
1	B	261	VAL	3.6
1	B	276	GLY	3.5
1	B	99	ASP	3.5
1	B	443	VAL	3.5
1	A	178	THR	3.4
1	A	404	LYS	3.3
1	A	91	GLY	3.3
1	B	275	GLY	3.2
1	B	491	SER	3.2
1	A	433	ILE	3.2
1	B	55	PHE	3.1
1	B	233	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	154	TYR	3.1
1	B	421	GLY	3.0
1	A	137	TYR	3.0
1	B	178	THR	2.9
1	A	92	TRP	2.8
1	B	41	SER	2.8
1	A	467	ILE	2.8
1	B	495	THR	2.8
1	A	127	ILE	2.8
1	B	249	LEU	2.8
1	A	176	ALA	2.8
1	B	44	VAL	2.7
1	A	493	SER	2.7
1	A	286	ALA	2.7
1	A	383	LEU	2.7
1	B	139	ALA	2.7
1	A	93	ASP	2.7
1	A	285	LEU	2.7
1	A	65	ILE	2.6
1	B	433	ILE	2.6
1	A	192	ALA	2.6
1	A	261	VAL	2.6
1	B	148	THR	2.6
1	B	415	THR	2.6
1	A	191	ILE	2.6
1	A	382	ALA	2.6
1	B	76	PHE	2.6
1	B	494	PRO	2.6
1	B	191	ILE	2.6
1	B	425	ILE	2.5
1	B	177	THR	2.5
1	A	171	LEU	2.5
1	B	70	PRO	2.5
1	A	150	VAL	2.5
1	B	210	VAL	2.5
1	B	455	VAL	2.5
1	B	192	ALA	2.5
1	A	270	LEU	2.4
1	A	430	ILE	2.4
1	A	282	SER	2.4
1	A	54	LEU	2.4
1	B	39	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	335	PHE	2.4
1	A	105	ILE	2.4
1	A	411	LEU	2.3
1	A	80	PRO	2.3
1	B	149	SER	2.3
1	B	270	LEU	2.3
1	A	476	GLY	2.3
1	B	285	LEU	2.3
1	B	404	LYS	2.3
1	B	100	GLU	2.3
1	A	149	SER	2.3
1	A	478	ASP	2.2
1	A	392	PHE	2.2
1	B	176	ALA	2.2
1	B	403	ALA	2.2
1	B	123	LEU	2.2
1	B	411	LEU	2.2
1	B	273	MET	2.2
1	B	456	PHE	2.2
1	A	340	ARG	2.2
1	A	304	ASN	2.2
1	B	103	LEU	2.2
1	B	420	MET	2.2
1	A	479	ILE	2.2
1	A	233	GLY	2.2
1	B	43	LEU	2.2
1	A	104	PHE	2.2
1	A	247	PHE	2.2
1	B	486	PHE	2.2
1	A	420	MET	2.1
1	A	160	VAL	2.1
1	B	382	ALA	2.1
1	A	390	ASN	2.1
1	B	137	TYR	2.1
1	A	44	VAL	2.1
1	A	381	SER	2.1
1	A	311	ARG	2.1
1	A	177	THR	2.1
1	A	341	GLN	2.1
1	B	127	ILE	2.1
1	A	495	THR	2.1
1	A	28	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	82	ASP	2.0
1	B	78	GLU	2.0
1	B	340	ARG	2.0
1	B	429	HIS	2.0
1	A	159	VAL	2.0
1	A	130	ILE	2.0
1	A	438	ILE	2.0
1	A	455	VAL	2.0
1	B	387	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](#)

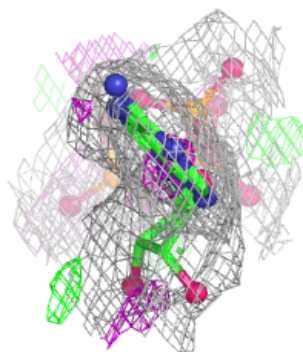
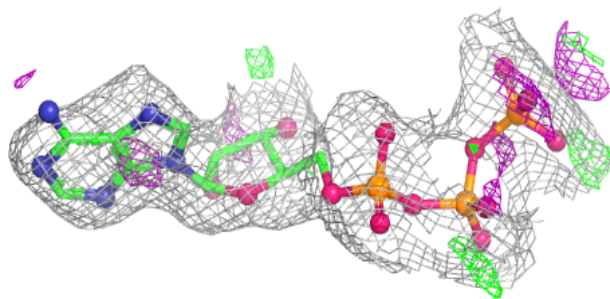
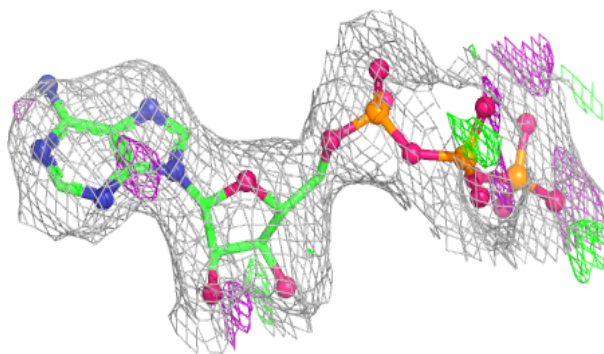
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	602	31/31	0.85	0.13	51,55,66,69	0
2	ATP	A	602	31/31	0.87	0.11	52,54,69,71	0
2	ATP	B	601	31/31	0.89	0.09	60,64,68,68	0
2	ATP	A	601	31/31	0.91	0.10	61,66,69,69	0
3	MG	B	604	1/1	0.91	0.10	44,44,44,44	0
3	MG	B	603	1/1	0.95	0.07	57,57,57,57	0
3	MG	A	603	1/1	0.95	0.11	65,65,65,65	0
3	MG	A	604	1/1	0.97	0.07	55,55,55,55	0

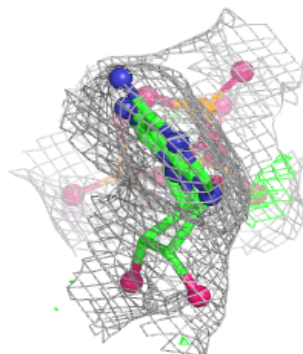
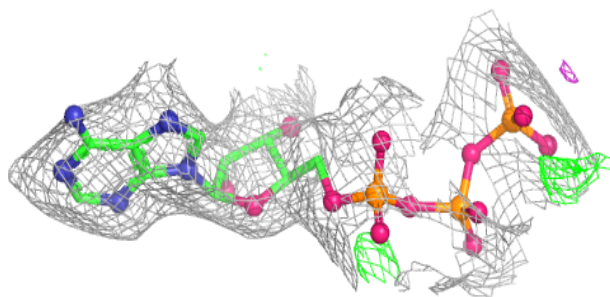
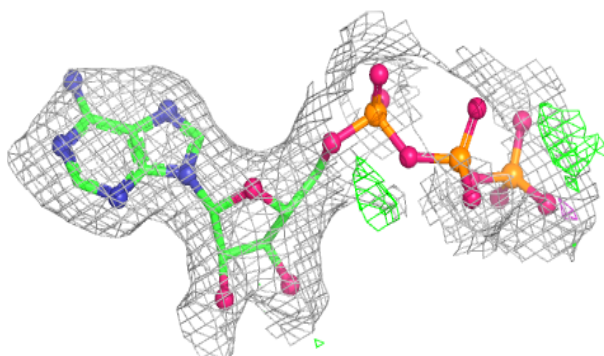
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 602:

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

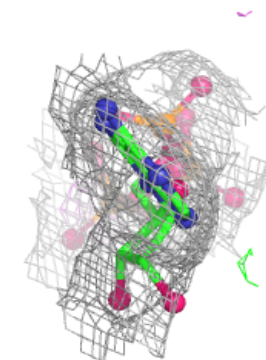
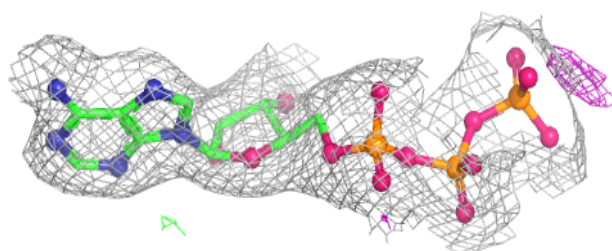
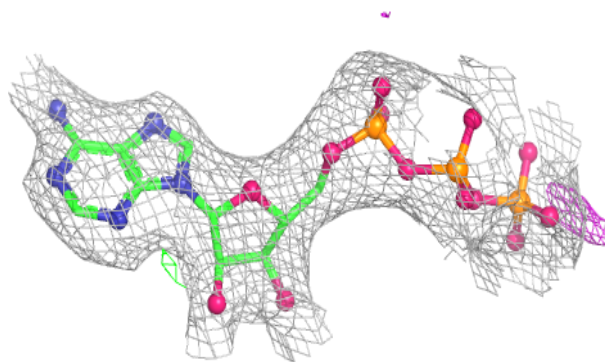
**Electron density around ATP A 602:**

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

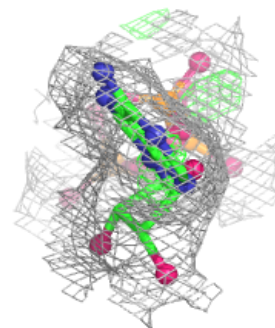
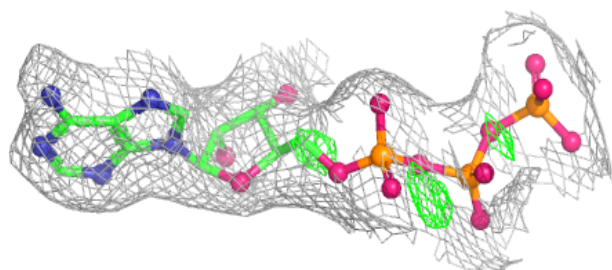
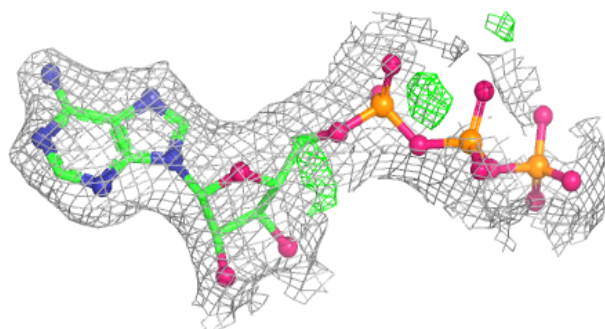


Electron density around ATP B 601:

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

**Electron density around ATP A 601:**

$2mF_o-DF_c$ (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.