Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 11:49 PM JST

PDB ID	:	7DYE
Title	:	Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC
Authors	:	Furuike, Y.; Akiyama, S.
Deposited on	:	2021-01-21
Resolution	:	2.60 Å(reported)

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

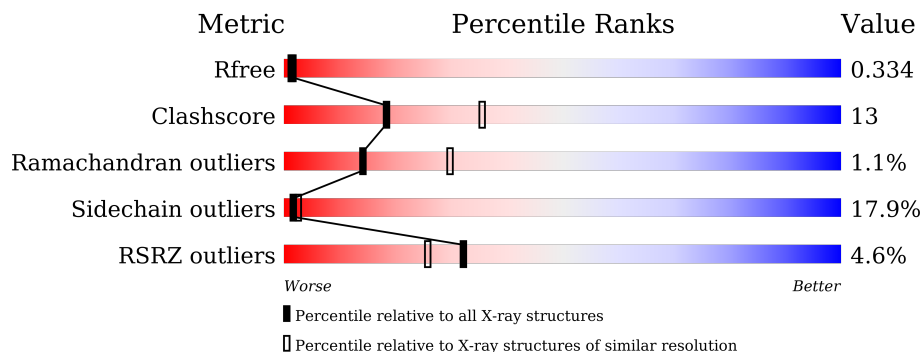|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.334
Clashscore		13
Ramachandran outliers		1.1%
Sidechain outliers		17.9%
RSRZ outliers		4.6%

Worse ————————————————— Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	4% / 64% 21% • 12%
1	B	519	4% / 61% 22% 5% 12%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6554 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 protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total 3189	C 2015	N 556	O 605	S 13	0	0	0
1	B	458	Total 3215	C 2014	N 579	O 608	S 14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
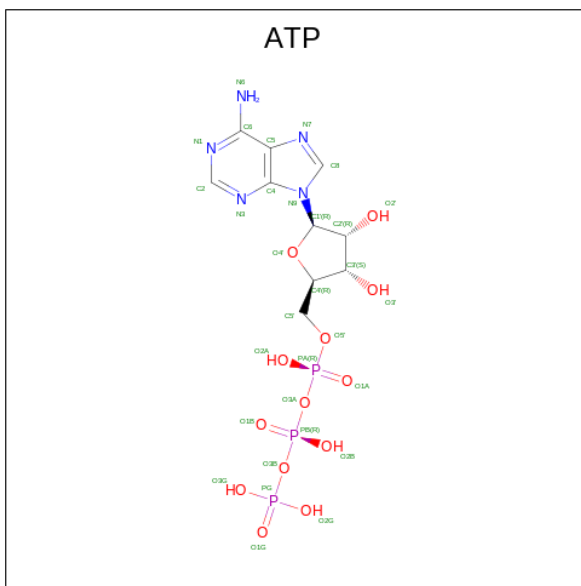
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: 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	9	Total	O	0	0
			9	9		
4	B	13	Total	O	0	0
			13	13		

3 Residue-property plots ⓘ

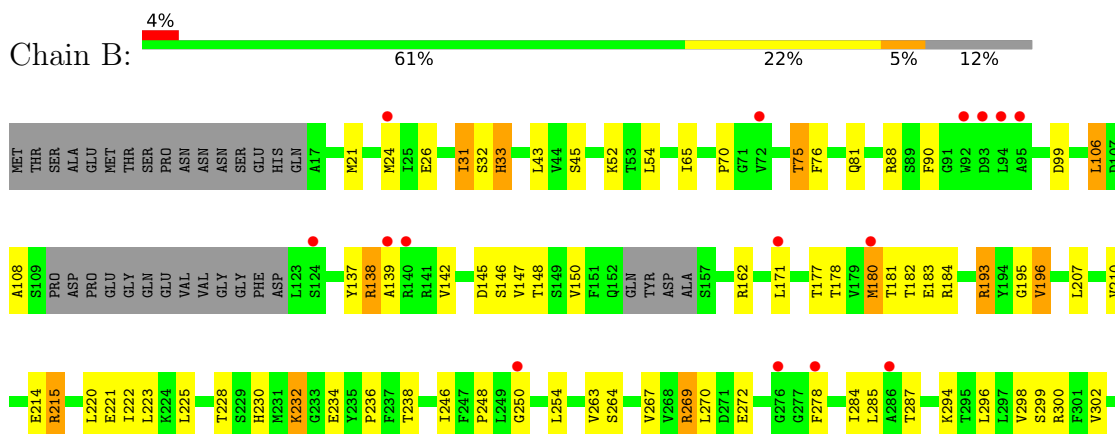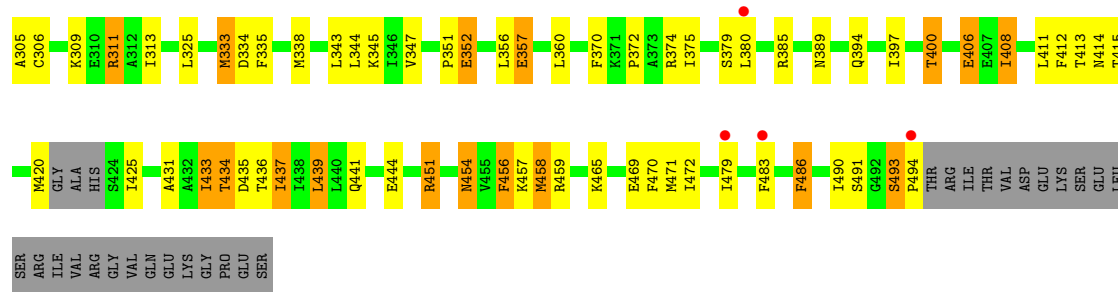These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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A305 C306 K309 E310 R311 A312 I313 L325 M333 D334 F335 M338 L343 L344 K345 I346 V347 P351 E352 L356 E357 L360 F370 K371 P372 A373 R374 I375 S379 L380 R385 N389 Q394 I397 T400 E406 E407 I408 L411 F412 T413 N414 T415

M420 GLY ALA HIS S424 I425 A431 A432 I433 T434 D435 T436 I437 I438 L439 L440 Q441 E444 R451 N454 V455 F456 K457 M458 R459 K465 E469 F470 M471 I472 I479 F483 F486 I490 S491 G492 S493 P494 THR ARG ILE THR VAL ASP GLU LYS SER GLU LEU

SER ARG ILE VAL ARG GLY VAL GLN GLU LYS GLY PRO GLU SER

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	94.91Å 94.91Å 276.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.50 – 2.60 47.45 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.50-2.60) 99.9 (47.45-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.279 , 0.337 0.279 , 0.334	Depositor DCC
R_{free} test set	1466 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	60.3	Xtriage
Anisotropy	0.898	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.038 for -h-k,k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6554	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, 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	0.69	0/3237	0.77	1/4400 (0.0%)
1	B	0.69	0/3261	0.76	0/4423
All	All	0.69	0/6498	0.77	1/8823 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	494	PRO	N-CA-CB	5.60	110.02	103.30

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	3189	0	2801	80	0
1	B	3215	0	2873	91	0
2	A	62	0	24	2	0
2	B	62	0	24	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	9	0	0	0	0
4	B	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6554	0	5722	163	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 13.

All (163) 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:283:ILE:HG13	1:A:400:THR:HG23	1.50	0.94
1:A:70:PRO:O	1:A:139:ALA:HA	1.75	0.86
1:A:294:LYS:HE2	2:A:602:ATP:O1B	1.80	0.81
1:A:293:GLY:HA2	2:A:602:ATP:O2A	1.82	0.79
1:A:469:GLU:HB3	1:A:483:PHE:CZ	2.18	0.79
1:A:400:THR:HG21	1:A:433:ILE:HG22	1.65	0.78
1:A:435:ASP:HA	1:A:459:ARG:HD2	1.70	0.74
1:A:341:GLN:HE21	1:A:343:LEU:HD12	1.53	0.73
1:A:400:THR:HG21	1:A:433:ILE:CG2	2.17	0.73
1:B:493:SER:CB	1:B:494:PRO:CD	2.69	0.71
1:B:264:SER:O	1:B:374:ARG:NH2	2.17	0.70
1:A:440:LEU:HD23	1:A:453:ILE:HG13	1.73	0.70
1:B:493:SER:CB	1:B:494:PRO:HD3	2.23	0.69
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.74	0.68
1:B:269:ARG:O	1:B:269:ARG:NH1	2.26	0.68
1:A:372:PRO:HG2	1:A:375:ILE:HD11	1.73	0.68
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.75	0.67
1:B:70:PRO:HG2	1:B:138:ARG:CB	2.26	0.65
1:B:397:ILE:HD13	1:B:433:ILE:HD11	1.78	0.65
1:B:400:THR:HG21	1:B:433:ILE:HD13	1.79	0.64
1:A:284:ILE:HB	1:A:411:LEU:HD12	1.80	0.64
1:A:21:MET:CE	1:A:177:THR:CB	2.77	0.62
1:B:31:ILE:CD1	1:B:248:PRO:HB3	2.31	0.61
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.66	0.60
1:B:220:LEU:HD13	1:B:246:ILE:HD11	1.83	0.59
1:B:207:LEU:HD21	1:B:220:LEU:HD12	1.83	0.59
1:B:379:SER:HB3	1:B:413:THR:OG1	2.03	0.59
1:A:214:GLU:HB3	1:B:234:GLU:HB2	1.84	0.58
1:B:76:PHE:CE2	1:B:150:VAL:CB	2.86	0.58
1:B:400:THR:HG21	1:B:433:ILE:HG23	1.84	0.58
1:B:298:VAL:HG22	1:B:411:LEU:HD23	1.84	0.58
1:B:31:ILE:HD11	1:B:248:PRO:HB3	1.85	0.58
1:A:360:LEU:HD23	1:A:399:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LEU:HD12	1:B:230:HIS:HB3	1.85	0.57
1:A:70:PRO:HA	1:A:102:LYS:O	2.05	0.57
1:B:70:PRO:HB2	1:B:137:TYR:O	2.05	0.56
1:A:264:SER:O	1:A:374:ARG:NH2	2.37	0.56
1:A:187:GLU:HG3	1:A:208:ARG:HG2	1.88	0.55
1:B:352:GLU:OE1	1:B:385:ARG:NH1	2.39	0.55
1:B:439:LEU:HD23	1:B:454:ASN:ND2	2.21	0.55
1:B:313:ILE:HG13	1:B:372:PRO:HG3	1.88	0.55
1:B:309:LYS:HA	1:B:343:LEU:CD1	2.37	0.55
1:A:21:MET:HE1	1:A:177:THR:CB	2.37	0.55
1:B:451:ARG:NH2	2:B:602:ATP:O2'	2.40	0.53
1:A:451:ARG:HG2	1:A:451:ARG:NH1	2.23	0.53
1:B:52:LYS:HE2	2:B:601:ATP:O2B	2.08	0.53
1:B:54:LEU:HD13	1:B:90:PHE:CE1	2.43	0.53
1:A:438:ILE:HD12	1:A:455:VAL:HG22	1.90	0.52
1:B:32:SER:HB3	1:B:222:ILE:CD1	2.39	0.52
1:B:236:PRO:HG3	1:B:394:GLN:NE2	2.24	0.52
1:B:311:ARG:HB3	1:B:372:PRO:HA	1.91	0.52
1:A:469:GLU:CB	1:A:483:PHE:CZ	2.92	0.52
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.90	0.52
1:B:45:SER:HA	1:B:182:THR:O	2.10	0.52
1:A:31:ILE:HD12	1:A:248:PRO:HG3	1.92	0.51
1:A:43:LEU:HD11	1:A:182:THR:CB	2.40	0.51
1:A:97:LEU:HD23	1:A:97:LEU:N	2.25	0.51
1:A:419:PHE:CZ	1:B:425:ILE:HA	2.45	0.51
1:B:313:ILE:HG13	1:B:372:PRO:CG	2.40	0.51
1:B:75:THR:HG22	1:B:108:ALA:H	1.75	0.51
1:B:287:THR:HA	1:B:414:ASN:O	2.10	0.50
1:B:306:CYS:SG	1:B:344:LEU:HB2	2.52	0.50
1:A:299:SER:C	1:A:333:MET:HE1	2.31	0.50
1:A:353:SER:HA	1:B:250:GLY:HA2	1.93	0.50
1:B:351:PRO:HD2	1:B:385:ARG:NH1	2.27	0.50
1:A:193:ARG:NH2	1:B:195:GLY:O	2.42	0.49
1:A:197:GLU:N	1:A:197:GLU:OE2	2.44	0.49
1:B:434:THR:O	1:B:457:LYS:NZ	2.32	0.49
1:A:225:LEU:HD12	1:A:230:HIS:HB3	1.93	0.49
1:A:344:LEU:HD11	1:A:346:ILE:CG1	2.42	0.48
1:B:220:LEU:HD13	1:B:246:ILE:CD1	2.42	0.48
1:A:285:LEU:HB2	1:A:434:THR:HG21	1.96	0.48
1:A:211:LEU:HD21	1:B:234:GLU:OE1	2.13	0.48
1:A:24:MET:HE3	1:A:24:MET:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:O	1:A:325:LEU:HG	2.14	0.48
1:B:21:MET:HE3	1:B:177:THR:HG21	1.96	0.48
1:A:273:MET:SD	1:A:468:ARG:HD2	2.54	0.48
1:B:437:ILE:HG22	1:B:457:LYS:HB2	1.95	0.48
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.95	0.48
1:A:317:TYR:HB3	1:A:351:PRO:HG3	1.94	0.48
1:A:294:LYS:HZ1	1:A:415:THR:HG23	1.80	0.47
1:B:325:LEU:HD23	1:B:335:PHE:HB2	1.96	0.47
1:A:70:PRO:O	1:A:139:ALA:CA	2.57	0.47
1:B:284:ILE:HB	1:B:411:LEU:HD12	1.97	0.47
1:B:431:ALA:O	1:B:457:LYS:NZ	2.48	0.47
1:B:435:ASP:HA	1:B:459:ARG:HD2	1.96	0.47
1:A:31:ILE:HA	1:A:231:MET:SD	2.55	0.47
1:B:43:LEU:HD11	1:B:182:THR:OG1	2.15	0.47
1:A:209:ASN:ND2	1:A:216:ARG:HG3	2.29	0.47
1:A:430:ILE:C	1:A:430:ILE:HD12	2.35	0.46
1:B:147:VAL:HG11	1:B:180:MET:CE	2.45	0.46
1:B:207:LEU:CD2	1:B:220:LEU:HD12	2.45	0.46
1:A:60:LEU:HD22	1:A:141:ARG:HB2	1.98	0.46
1:A:375:ILE:O	1:A:410:GLY:HA2	2.15	0.46
1:A:63:GLY:HA3	1:A:141:ARG:HD2	1.98	0.46
1:B:294:LYS:NZ	1:B:415:THR:HG23	2.31	0.46
1:A:96:LYS:O	1:A:100:GLU:HG3	2.14	0.46
1:B:490:ILE:HG22	1:B:490:ILE:O	2.16	0.46
1:A:337:GLU:O	1:A:341:GLN:HG3	2.16	0.46
1:A:370:PHE:HD2	1:A:372:PRO:HG3	1.81	0.46
1:B:52:LYS:HE3	1:B:52:LYS:HB2	1.82	0.45
1:B:106:LEU:C	1:B:106:LEU:HD12	2.36	0.45
1:B:439:LEU:HD21	1:B:456:PHE:HB2	1.98	0.45
1:B:148:THR:CG2	1:B:193:ARG:HD2	2.46	0.45
1:A:444:GLU:HB2	1:A:449:MET:CE	2.47	0.45
1:A:379:SER:HB3	1:A:413:THR:OG1	2.16	0.45
1:B:311:ARG:HG2	1:B:370:PHE:CZ	2.52	0.45
1:A:299:SER:HB3	1:A:333:MET:HE2	1.98	0.45
1:B:267:VAL:HB	1:B:270:LEU:HB3	1.98	0.45
1:A:444:GLU:HB2	1:A:449:MET:HE1	1.98	0.44
1:A:455:VAL:HG11	1:A:463:HIS:HB2	2.00	0.44
1:B:344:LEU:C	1:B:344:LEU:HD13	2.37	0.44
1:B:309:LYS:HA	1:B:343:LEU:HD13	1.99	0.44
1:A:306:CYS:SG	1:A:344:LEU:HB2	2.57	0.44
1:A:344:LEU:C	1:A:344:LEU:HD13	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:PHE:CD1	1:B:284:ILE:HG13	2.53	0.44
1:A:440:LEU:CD2	1:A:453:ILE:HG13	2.44	0.44
1:B:21:MET:HE1	1:B:177:THR:HB	2.00	0.43
1:A:287:THR:HA	1:A:414:ASN:O	2.18	0.43
1:A:323:GLN:NE2	1:B:459:ARG:HD3	2.34	0.43
1:B:254:LEU:HD12	1:B:254:LEU:N	2.33	0.43
1:B:379:SER:HB2	1:B:413:THR:O	2.19	0.43
1:A:486:PHE:CD1	1:A:486:PHE:N	2.86	0.43
1:B:299:SER:C	1:B:333:MET:HE1	2.39	0.43
1:B:313:ILE:HD11	1:B:370:PHE:HB3	2.01	0.43
1:A:289:ALA:O	1:A:292:THR:OG1	2.24	0.43
1:B:238:THR:CG2	1:B:357:GLU:HB2	2.49	0.43
1:B:296:LEU:HD22	1:B:472:ILE:HD12	2.00	0.43
1:B:311:ARG:NH2	1:B:311:ARG:HB2	2.33	0.43
1:A:24:MET:HA	1:A:24:MET:CE	2.48	0.43
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.84	0.43
1:A:22:ARG:O	1:A:141:ARG:NH2	2.46	0.43
1:A:360:LEU:CD2	1:A:399:VAL:HG22	2.49	0.43
1:B:406:GLU:HB3	1:B:408:ILE:HD11	2.00	0.43
1:B:142:VAL:O	1:B:178:THR:HA	2.19	0.42
1:B:214:GLU:O	1:B:215:ARG:NH2	2.52	0.42
1:A:344:LEU:HD22	1:A:345:LYS:N	2.33	0.42
1:B:269:ARG:NH1	1:B:272:GLU:HB2	2.33	0.42
1:B:380:LEU:CD1	1:B:412:PHE:HB3	2.49	0.42
1:A:313:ILE:HG13	1:A:372:PRO:CG	2.49	0.42
1:A:440:LEU:HD23	1:A:453:ILE:CG1	2.46	0.42
1:A:449:MET:HA	1:A:449:MET:HE2	2.01	0.42
1:B:285:LEU:HD23	1:B:437:ILE:HD13	2.00	0.42
1:B:439:LEU:HD21	1:B:456:PHE:CG	2.54	0.42
1:A:400:THR:HG21	1:A:433:ILE:HG23	2.00	0.42
1:A:418:GLN:HA	1:B:425:ILE:CB	2.50	0.42
1:A:215:ARG:NH2	1:B:232:LYS:O	2.53	0.42
1:B:309:LYS:HA	1:B:343:LEU:HD11	2.01	0.42
1:B:479:ILE:HD12	1:B:479:ILE:N	2.34	0.42
1:B:412:PHE:CD1	1:B:412:PHE:N	2.88	0.42
1:B:436:THR:OG1	1:B:458:MET:HE2	2.20	0.42
1:A:73:PHE:O	1:A:106:LEU:N	2.53	0.41
1:A:209:ASN:O	1:A:216:ARG:NH1	2.52	0.41
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.89	0.41
1:A:344:LEU:HD11	1:A:346:ILE:HG13	2.02	0.41
1:B:379:SER:CB	1:B:413:THR:OG1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ASP:HA	1:B:146:SER:HA	1.85	0.41
1:A:406:GLU:HB3	1:A:408:ILE:CD1	2.51	0.41
1:B:439:LEU:CD2	1:B:456:PHE:HB2	2.51	0.41
1:A:300:ARG:NH1	1:A:475:LYS:O	2.48	0.41
1:B:263:VAL:HB	1:B:374:ARG:HH21	1.86	0.40
1:B:302:VAL:HG13	1:B:344:LEU:HD23	2.03	0.40
1:B:334:ASP:O	1:B:338:MET:HG3	2.21	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	450/519 (87%)	408 (91%)	38 (8%)	4 (1%)	17	35
1	B	450/519 (87%)	408 (91%)	36 (8%)	6 (1%)	12	24
All	All	900/1038 (87%)	816 (91%)	74 (8%)	10 (1%)	14	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ILE
1	A	489	ILE
1	B	139	ALA
1	B	493	SER
1	B	33	HIS
1	B	138	ARG
1	A	427	ASP
1	A	490	ILE
1	B	491	SER
1	B	196	VAL

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	270/442 (61%)	227 (84%)	43 (16%)	2	4
1	B	279/442 (63%)	224 (80%)	55 (20%)	1	2
All	All	549/884 (62%)	451 (82%)	98 (18%)	2	2

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	31	ILE
1	A	103	LEU
1	A	106	LEU
1	A	135	GLN
1	A	150	VAL
1	A	180	MET
1	A	184	ARG
1	A	193	ARG
1	A	210	VAL
1	A	216	ARG
1	A	219	THR
1	A	223	LEU
1	A	258	SER
1	A	260	ASN
1	A	267	VAL
1	A	270	LEU
1	A	292	THR
1	A	300	ARG
1	A	330	SER
1	A	333	MET
1	A	352	GLU
1	A	356	LEU
1	A	357	GLU
1	A	360	LEU
1	A	361	GLN
1	A	364	LYS

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Mol	Chain	Res	Type
1	A	372	PRO
1	A	375	ILE
1	A	377	ILE
1	A	394	GLN
1	A	405	GLN
1	A	406	GLU
1	A	419	PHE
1	A	440	LEU
1	A	441	GLN
1	A	451	ARG
1	A	454	ASN
1	A	457	LYS
1	A	458	MET
1	A	465	LYS
1	A	483	PHE
1	A	486	PHE
1	B	24	MET
1	B	26	GLU
1	B	31	ILE
1	B	33	HIS
1	B	65	ILE
1	B	75	THR
1	B	81	GLN
1	B	88	ARG
1	B	99	ASP
1	B	106	LEU
1	B	162	ARG
1	B	171	LEU
1	B	180	MET
1	B	181	THR
1	B	183	GLU
1	B	184	ARG
1	B	193	ARG
1	B	196	VAL
1	B	210	VAL
1	B	215	ARG
1	B	221	GLU
1	B	223	LEU
1	B	228	THR
1	B	232	LYS
1	B	269	ARG
1	B	300	ARG

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Mol	Chain	Res	Type
1	B	311	ARG
1	B	333	MET
1	B	345	LYS
1	B	347	VAL
1	B	352	GLU
1	B	356	LEU
1	B	357	GLU
1	B	360	LEU
1	B	375	ILE
1	B	389	ASN
1	B	400	THR
1	B	406	GLU
1	B	408	ILE
1	B	420	MET
1	B	433	ILE
1	B	434	THR
1	B	437	ILE
1	B	439	LEU
1	B	441	GLN
1	B	444	GLU
1	B	451	ARG
1	B	454	ASN
1	B	456	PHE
1	B	458	MET
1	B	465	LYS
1	B	469	GLU
1	B	470	PHE
1	B	471	MET
1	B	486	PHE

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

Mol	Chain	Res	Type
1	A	33	HIS
1	A	209	ASN
1	A	341	GLN
1	A	368	ASN
1	A	441	GLN
1	B	209	ASN
1	B	260	ASN
1	B	341	GLN
1	B	454	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 monosaccharides 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	26,33,33	0.67	0	31,52,52	0.75	1 (3%)
2	ATP	A	601	3	26,33,33	0.65	0	31,52,52	0.79	1 (3%)
2	ATP	A	602	3	26,33,33	0.69	0	31,52,52	0.77	1 (3%)
2	ATP	B	601	3	26,33,33	0.65	0	31,52,52	0.79	1 (3%)

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	-	7/18/38/38	0/3/3/3
2	ATP	A	601	3	-	4/18/38/38	0/3/3/3
2	ATP	A	602	3	-	6/18/38/38	0/3/3/3
2	ATP	B	601	3	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	ATP	C5-C6-N6	2.25	123.77	120.35
2	B	602	ATP	C5-C6-N6	2.05	123.47	120.35
2	A	602	ATP	C5-C6-N6	2.04	123.45	120.35
2	B	601	ATP	C5-C6-N6	2.03	123.44	120.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O3A
2	A	601	ATP	C3'-C4'-C5'-O5'
2	A	602	ATP	C5'-O5'-PA-O3A
2	B	601	ATP	PB-O3B-PG-O2G
2	B	601	ATP	C5'-O5'-PA-O3A
2	B	602	ATP	C5'-O5'-PA-O1A
2	B	602	ATP	C3'-C4'-C5'-O5'
2	A	602	ATP	O4'-C4'-C5'-O5'
2	A	602	ATP	C3'-C4'-C5'-O5'
2	B	601	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	C3'-C4'-C5'-O5'
2	A	601	ATP	O4'-C4'-C5'-O5'
2	B	602	ATP	O4'-C4'-C5'-O5'
2	A	602	ATP	PA-O3A-PB-O1B
2	A	601	ATP	C5'-O5'-PA-O1A
2	A	602	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	C5'-O5'-PA-O1A
2	B	602	ATP	C5'-O5'-PA-O2A
2	A	602	ATP	PA-O3A-PB-O2B
2	B	602	ATP	PB-O3A-PA-O1A
2	B	601	ATP	PB-O3B-PG-O3G
2	B	602	ATP	C5'-O5'-PA-O3A
2	B	602	ATP	PB-O3A-PA-O2A

There are no ring outliers.
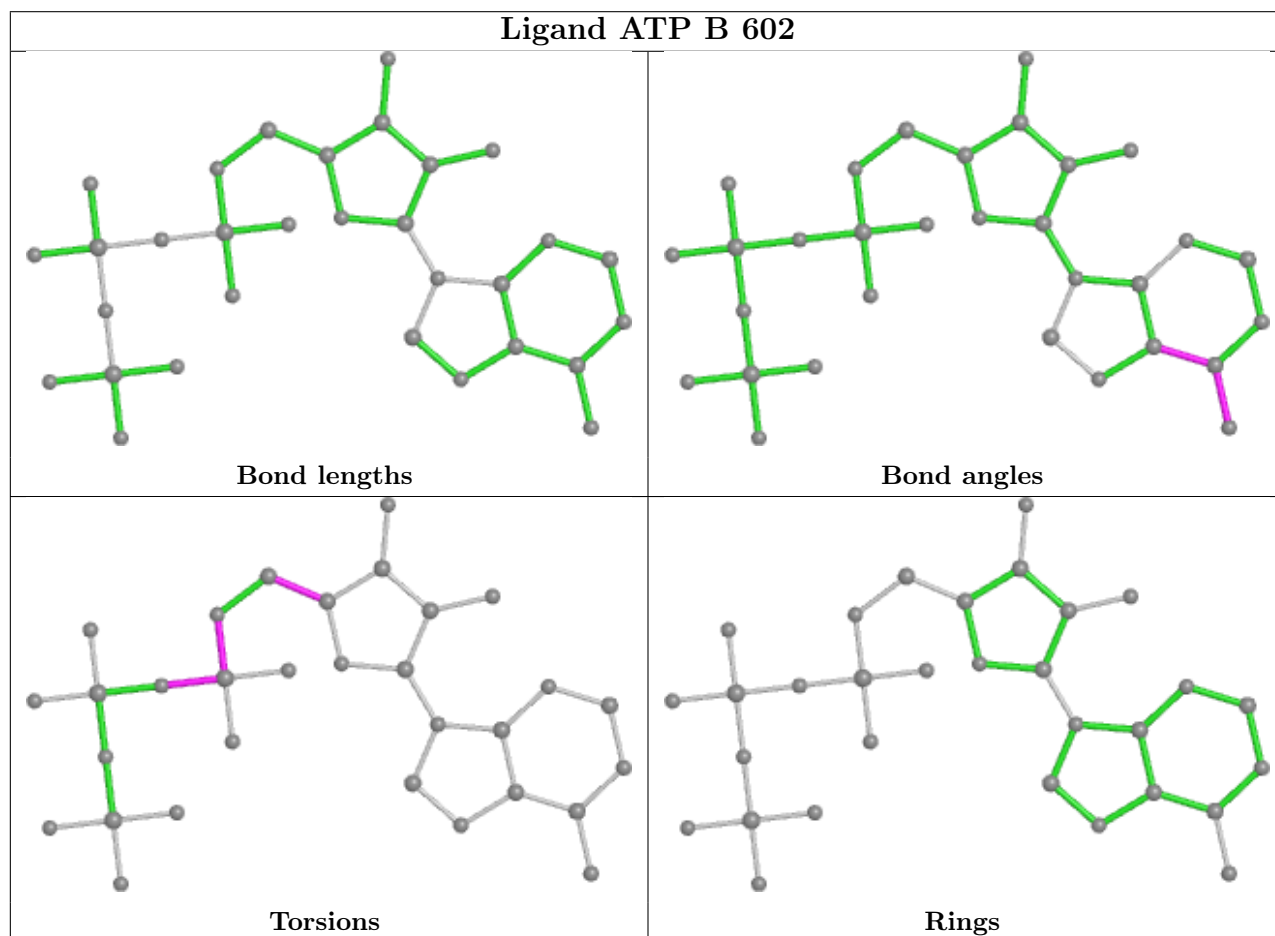
3 monomers are involved in 4 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	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 then 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.

Ligand ATP B 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 601

Bond lengths

Bond angles

Torsions

Rings
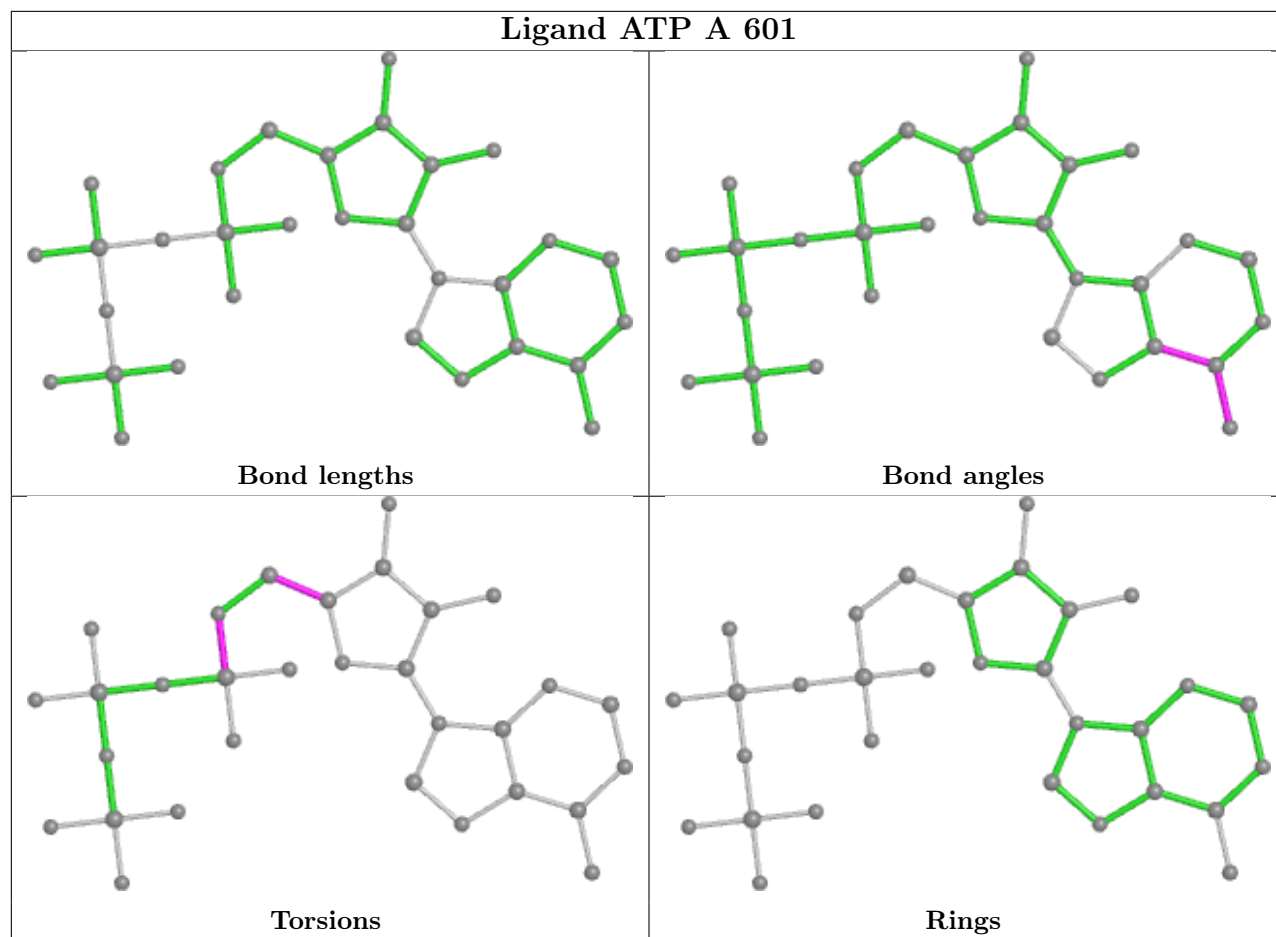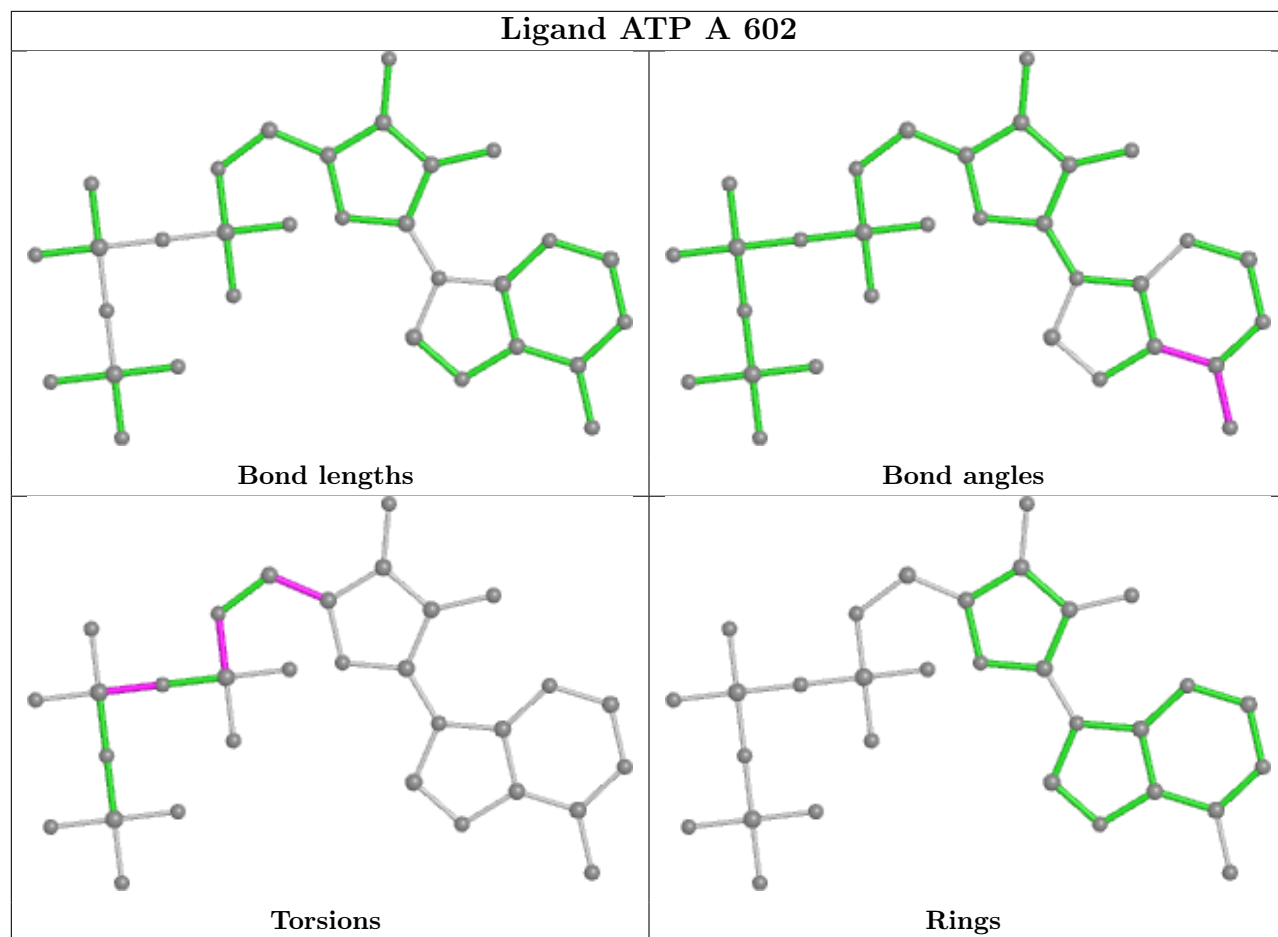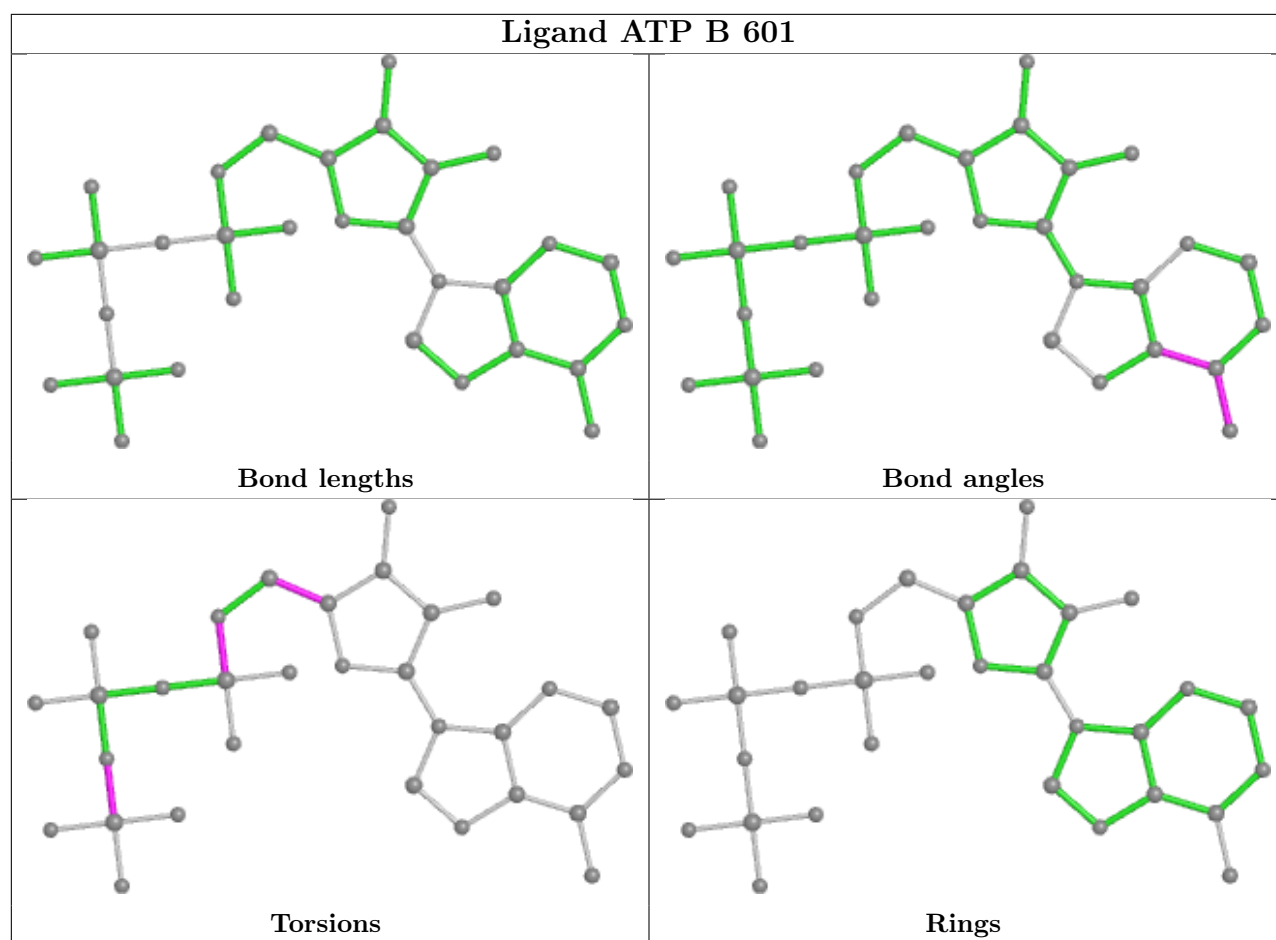
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	458/519 (88%)	0.26	23 (5%)	28	23	34, 54, 84, 99	0
1	B	458/519 (88%)	0.31	19 (4%)	37	30	38, 55, 87, 101	0
All	All	916/1038 (88%)	0.29	42 (4%)	32	26	34, 54, 86, 101	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	ALA	6.1
1	B	139	ALA	5.2
1	A	94	LEU	4.3
1	A	92	TRP	3.7
1	A	486	PHE	3.5
1	B	95	ALA	3.3
1	B	140	ARG	3.2
1	B	180	MET	3.2
1	B	276	GLY	3.1
1	A	180	MET	3.0
1	B	94	LEU	3.0
1	A	148	THR	2.9
1	A	137	TYR	2.9
1	B	286	ALA	2.6
1	A	491	SER	2.6
1	B	494	PRO	2.5
1	B	24	MET	2.5
1	A	377	ILE	2.5
1	B	92	TRP	2.5
1	A	139	ALA	2.4
1	B	483	PHE	2.4
1	A	61	TYR	2.4
1	A	250	GLY	2.4
1	A	490	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	93	ASP	2.3
1	B	171	LEU	2.3
1	A	297	LEU	2.3
1	B	479	ILE	2.3
1	B	124	SER	2.3
1	A	456	PHE	2.2
1	A	266	GLY	2.2
1	A	470	PHE	2.2
1	A	380	LEU	2.2
1	A	276	GLY	2.2
1	B	278	PHE	2.1
1	A	37	PRO	2.1
1	B	380	LEU	2.1
1	A	251	ALA	2.1
1	B	250	GLY	2.0
1	A	144	ILE	2.0
1	A	167	LEU	2.0
1	B	72	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	MG	A	603	1/1	0.89	0.22	47,47,47,47	0
3	MG	B	603	1/1	0.90	0.21	43,43,43,43	0
3	MG	A	604	1/1	0.91	0.26	54,54,54,54	0
2	ATP	A	601	31/31	0.94	0.16	47,49,51,51	0
2	ATP	B	601	31/31	0.94	0.15	51,53,56,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	ATP	B	602	31/31	0.94	0.14	34,36,39,40	0
2	ATP	A	602	31/31	0.96	0.12	34,37,38,39	0
3	MG	B	604	1/1	0.99	0.28	56,56,56,56	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.
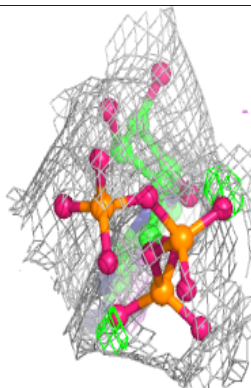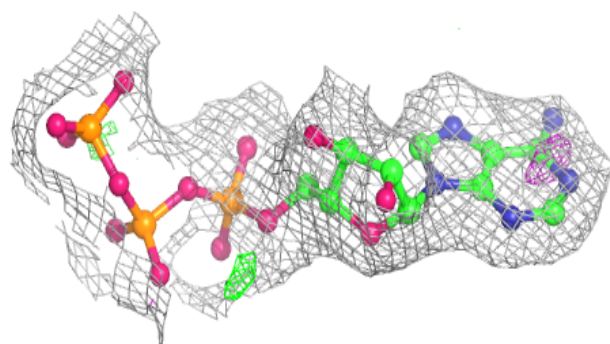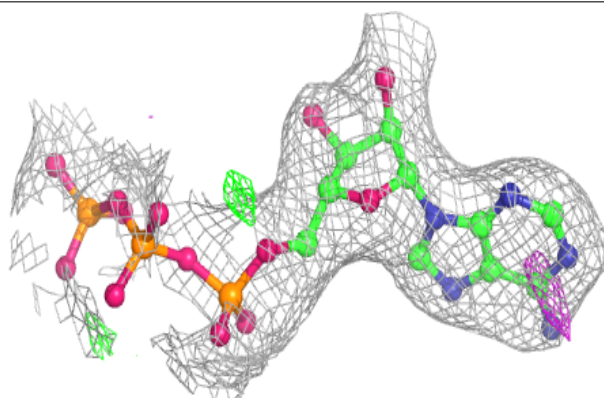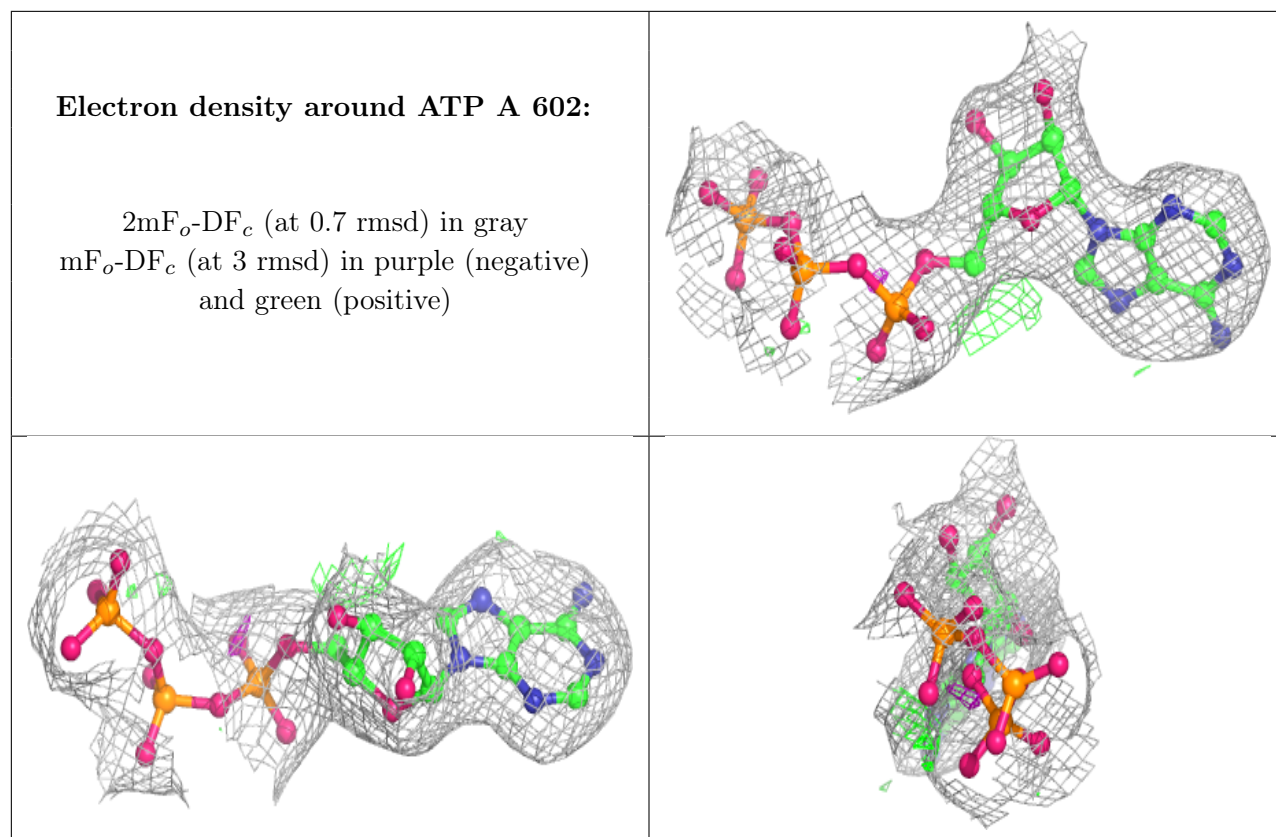

Electron density around ATP A 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
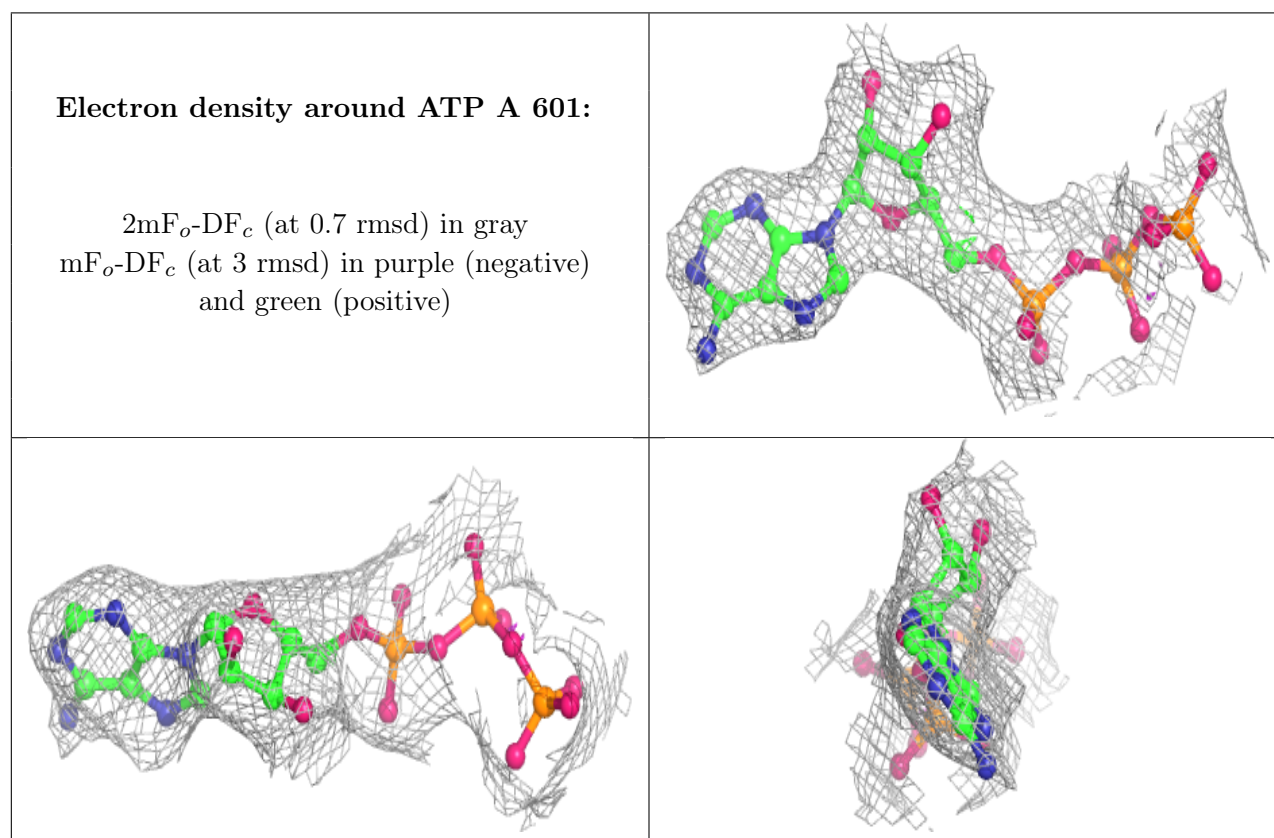
Electron density around ATP B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
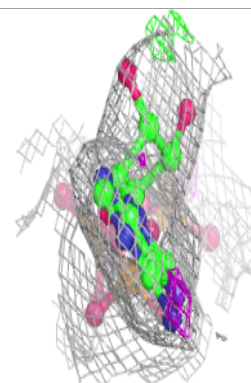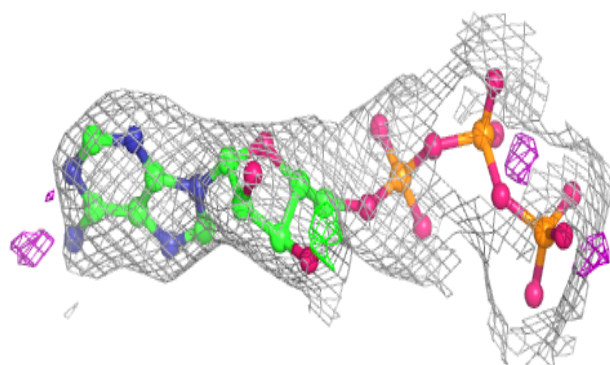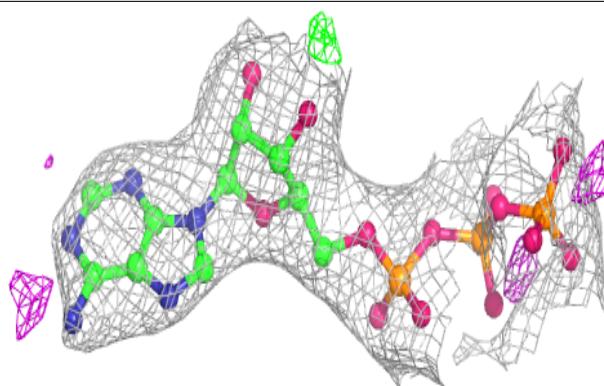
Electron density around ATP B 602:

$2mF_o$-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)

6.5 Other polymers ⓘ

There are no such residues in this entry.