Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 12:03 AM JST

PDB ID	:	7DYI
Title	:	Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC
Authors	:	Furuike, Y.; Akiyama, S.
Deposited on	:	2021-01-21
Resolution	:	2.64 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 2.64 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.
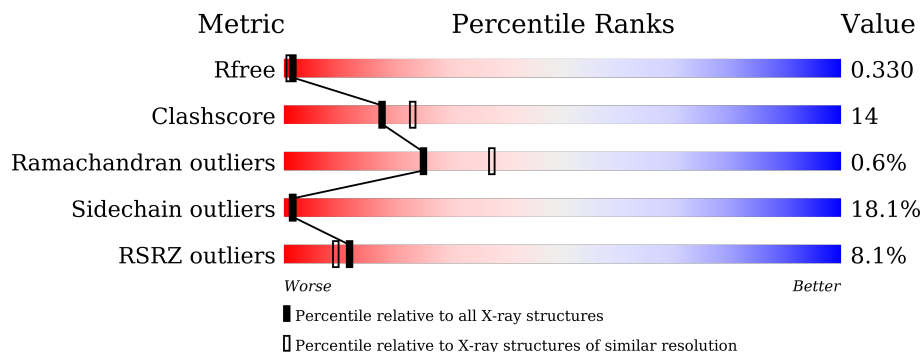
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	6% 63% 20% 5% 12%
1	B	519	8% 59% 24% 5% 12%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6669 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	456	Total 3243	C 2034	N 572	O 625	S 12	0	0	0
1	B	455	Total 3267	C 2052	N 580	O 623	S 12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	GLU	THR	engineered mutation	UNP Q79PF4
B	432	GLU	THR	engineered mutation	UNP Q79PF4

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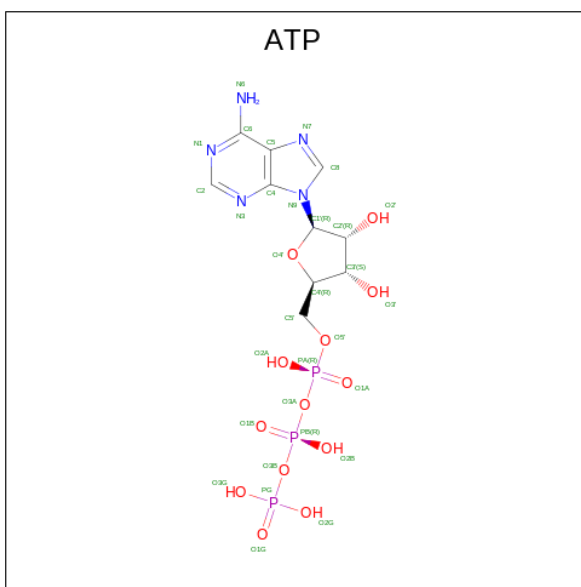
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	18	Total 18	O 18	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: Circadian clock protein kinase KaiC

Chain A:

• Molecule 1: Circadian clock protein kinase KaiC

Chain B:

GLN R257 S258 V261 S265 G266 V267 V268 R269 L270 C274 G275 G276 G277 F278 F279 K280 T287 T292 G293 K294 T295 L296 L297 V298 F301 V302 A305 C306 R311 A312 I313 A316 Y317 R321 A322 Q323 L324 L325 R326 N327 A328 Y329 F335 M338 L343 L344

K345 I346 V347 C348 P351 E352 L356 E357 D358 H359 L360 Q361 I362 E366 F370 K371 P372 A373 R374 I377 D378 S379 A382 R385 G386 V387 N390 R393 V399 T400 Q405 E406 L411 F412 T413 N414 D417 Q418 F419 M420 I425 S428 I433

L439 L440 V443 E444 I445 E448 M449 S450 R451 A452 I453 N454 V455 M458 H463 D464 K465 A466 I467 R468 E469 F470 M471 I472 S473 D474 K475 G476 P477 F483 I489 P494 T495 R496 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	P 63	Depositor
Cell constants a, b, c, α, β, γ	94.32Å 94.32Å 180.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.51 – 2.64 48.46 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.51-2.64) 99.8 (48.46-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.294 , 0.331 0.293 , 0.330	Depositor DCC
R_{free} test set	1339 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 72.1	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6669	wwPDB-VP
Average B, all atoms (Å^2)	70.0	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 51.68 % 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 5.4183e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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: 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	0.69	0/3293	0.75	0/4469
1	B	0.69	0/3318	0.75	0/4497
All	All	0.69	0/6611	0.75	0/8966

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	3243	0	2887	85	0
1	B	3267	0	2946	91	0
2	A	62	0	24	3	0
2	B	62	0	24	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	13	0	0	0	0
4	B	18	0	0	0	0
All	All	6669	0	5881	172	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 14.

All (172) 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:400:THR:HG21	1:B:433:ILE:HD11	1.18	1.11
1:A:316:ALA:HB3	1:A:348:CYS:HB3	1.47	0.94
1:B:400:THR:HG21	1:B:433:ILE:CD1	1.97	0.93
1:A:400:THR:HG21	1:A:433:ILE:HD11	1.47	0.93
1:B:400:THR:CG2	1:B:433:ILE:HD11	1.99	0.92
1:B:356:LEU:CD2	1:B:387:VAL:HG11	2.02	0.90
1:B:84:ILE:HG23	1:B:94:LEU:CB	2.03	0.88
1:A:356:LEU:HD21	1:A:387:VAL:HG11	1.60	0.84
1:B:469:GLU:HB2	1:B:483:PHE:CZ	2.20	0.76
1:B:356:LEU:HD21	1:B:387:VAL:HG11	1.66	0.76
1:B:220:LEU:HD13	1:B:246:ILE:HD11	1.70	0.74
1:A:60:LEU:CD2	1:A:141:ARG:HB3	2.18	0.73
1:B:93:ASP:O	1:B:97:LEU:HD23	1.92	0.69
1:B:191:ILE:HB	1:B:198:GLU:HG2	1.73	0.69
1:B:443:VAL:HG13	1:B:494:PRO:HG2	1.75	0.68
1:A:75:THR:HG22	1:A:107:ASP:HA	1.76	0.67
1:A:337:GLU:O	1:A:341:GLN:HG3	1.95	0.67
1:B:443:VAL:CG1	1:B:494:PRO:HG2	2.25	0.67
1:B:443:VAL:HG13	1:B:494:PRO:CG	2.26	0.66
1:B:70:PRO:HB2	1:B:139:ALA:HA	1.76	0.66
1:A:344:LEU:HD11	1:A:346:ILE:HG13	1.78	0.66
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.78	0.64
1:B:338:MET:HB2	1:B:344:LEU:HB3	1.80	0.63
1:A:306:CYS:SG	1:A:344:LEU:HB2	2.39	0.63
1:B:60:LEU:CD2	1:B:141:ARG:HB2	2.30	0.62
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.29	0.62
1:B:298:VAL:HA	1:B:411:LEU:HD23	1.82	0.61
1:B:225:LEU:HD12	1:B:230:HIS:HB3	1.82	0.60
1:A:400:THR:CG2	1:A:433:ILE:HD11	2.28	0.60
1:A:436:THR:HG23	1:A:458:MET:HG2	1.85	0.59
1:B:209:ASN:O	1:B:216:ARG:NH1	2.33	0.58
1:A:265:SER:HB3	1:A:278:PHE:CE1	2.38	0.58
1:B:267:VAL:HB	1:B:270:LEU:HB2	1.86	0.58
1:B:21:MET:HE1	1:B:177:THR:CB	2.33	0.57
1:B:306:CYS:SG	1:B:344:LEU:HB2	2.44	0.57
1:A:440:LEU:HD21	1:A:453:ILE:HG13	1.86	0.57
1:A:187:GLU:HG3	1:A:208:ARG:HG2	1.86	0.57
1:B:63:GLY:HA3	1:B:141:ARG:HD2	1.86	0.57
1:B:323:GLN:HE21	1:B:327:ASN:HD21	1.53	0.57
1:B:31:ILE:HA	1:B:231:MET:SD	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ALA:HB3	1:B:348:CYS:HB3	1.88	0.56
1:A:60:LEU:HD23	1:A:141:ARG:HB3	1.86	0.56
1:A:278:PHE:CD2	1:A:284:ILE:HD12	2.41	0.56
1:B:142:VAL:O	1:B:178:THR:HA	2.06	0.55
1:A:291:GLY:O	1:A:451:ARG:NH1	2.39	0.55
1:A:68:ASP:OD2	1:A:68:ASP:O	2.25	0.55
1:A:191:ILE:CG2	1:A:198:GLU:HG2	2.37	0.55
1:A:191:ILE:HG21	1:A:198:GLU:HG2	1.86	0.55
1:B:206:ILE:HD12	1:B:223:LEU:HB2	1.88	0.55
1:B:344:LEU:HD11	1:B:346:ILE:HG13	1.89	0.55
1:A:400:THR:HG21	1:A:433:ILE:CD1	2.28	0.54
1:A:316:ALA:O	1:A:348:CYS:HA	2.08	0.54
1:A:440:LEU:CD2	1:A:453:ILE:HG13	2.38	0.54
1:B:31:ILE:HD12	1:B:246:ILE:HG21	1.89	0.54
1:B:265:SER:HB3	1:B:278:PHE:CE1	2.43	0.54
1:B:45:SER:HB3	1:B:182:THR:OG1	2.08	0.53
1:B:316:ALA:O	1:B:348:CYS:HA	2.07	0.53
1:A:52:LYS:HB3	1:A:181:THR:HG23	1.91	0.53
1:A:75:THR:O	1:A:108:ALA:HB3	2.08	0.53
1:B:191:ILE:CB	1:B:198:GLU:HG2	2.39	0.53
1:B:440:LEU:CD2	1:B:453:ILE:HG13	2.38	0.52
1:A:265:SER:OG	1:A:270:LEU:HD12	2.10	0.52
1:A:204:VAL:HG11	1:A:223:LEU:HD12	1.91	0.52
1:B:458:MET:HB2	1:B:463:HIS:CD2	2.45	0.52
1:B:287:THR:HA	1:B:414:ASN:O	2.10	0.51
1:B:296:LEU:CD2	1:B:472:ILE:HD13	2.39	0.51
1:A:301:PHE:CZ	1:A:374:ARG:HD3	2.45	0.51
1:A:57:ILE:HD13	1:A:73:PHE:CE1	2.45	0.51
1:A:28:PHE:HB2	1:A:246:ILE:HD12	1.92	0.51
1:B:301:PHE:CZ	1:B:374:ARG:HD3	2.45	0.51
1:B:287:THR:HG21	1:B:425:ILE:CD1	2.40	0.51
1:B:338:MET:HB2	1:B:344:LEU:CB	2.40	0.51
1:B:21:MET:CE	1:B:177:THR:CB	2.88	0.51
1:B:261:VAL:HG12	1:B:280:LYS:CB	2.41	0.51
1:A:313:ILE:HG13	1:A:372:PRO:HB3	1.91	0.50
1:B:220:LEU:HD13	1:B:246:ILE:CD1	2.39	0.50
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.88	0.50
1:A:321:ARG:HH21	1:A:321:ARG:HG3	1.77	0.49
1:A:215:ARG:NH1	1:B:232:LYS:O	2.45	0.49
1:A:24:MET:HG3	1:A:66:GLU:HG3	1.94	0.49
1:B:469:GLU:HB2	1:B:483:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.76	0.49
1:A:204:VAL:HG12	1:A:223:LEU:HB2	1.94	0.48
1:B:400:THR:CB	1:B:433:ILE:HD11	2.43	0.48
1:A:18:ILE:HB	1:A:228:THR:HG23	1.96	0.48
1:A:344:LEU:C	1:A:344:LEU:HD13	2.34	0.48
1:A:287:THR:HA	1:A:414:ASN:O	2.13	0.48
2:A:601:ATP:PG	1:B:224:LYS:NZ	2.86	0.48
1:A:220:LEU:HD13	1:A:246:ILE:HD11	1.95	0.48
1:A:57:ILE:CD1	1:A:73:PHE:CE1	2.98	0.47
1:B:41:SER:HA	1:B:178:THR:O	2.14	0.47
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.80	0.46
1:A:311:ARG:NH1	1:A:370:PHE:O	2.46	0.46
1:A:298:VAL:HA	1:A:411:LEU:HD23	1.95	0.46
1:A:489:ILE:HA	1:A:494:PRO:HG3	1.97	0.46
1:B:433:ILE:C	1:B:433:ILE:HD13	2.36	0.46
1:A:344:LEU:CD1	1:A:346:ILE:HG13	2.44	0.46
1:B:311:ARG:HA	1:B:343:LEU:O	2.14	0.46
1:B:382:ALA:O	1:B:385:ARG:HG2	2.16	0.46
1:B:296:LEU:HD11	1:B:477:PRO:HD3	1.98	0.46
1:B:344:LEU:CD1	1:B:346:ILE:HG13	2.45	0.46
1:B:24:MET:HB2	1:B:62:ASN:HB3	1.98	0.46
1:B:321:ARG:O	1:B:325:LEU:HG	2.15	0.46
1:A:203:ASN:HB3	1:A:225:LEU:CD2	2.44	0.46
1:A:278:PHE:CG	1:A:284:ILE:HD12	2.50	0.46
1:B:417:ASP:N	1:B:417:ASP:OD1	2.49	0.46
1:A:214:GLU:HB3	1:B:234:GLU:HB2	1.97	0.45
1:B:134:ILE:O	1:B:138:ARG:N	2.50	0.45
1:B:147:VAL:HG21	1:B:180:MET:CE	2.46	0.45
1:B:425:ILE:HD13	1:B:425:ILE:N	2.31	0.45
1:A:237:PHE:HB2	1:A:246:ILE:HA	1.99	0.45
1:A:28:PHE:HB2	1:A:246:ILE:CD1	2.46	0.45
1:A:220:LEU:HD13	1:A:246:ILE:CD1	2.47	0.45
1:B:313:ILE:HD11	1:B:370:PHE:HB3	1.99	0.45
1:B:317:TYR:HB3	1:B:351:PRO:HG3	1.99	0.45
1:A:351:PRO:CD	1:A:385:ARG:HH11	2.29	0.45
2:A:601:ATP:O3G	1:B:224:LYS:NZ	2.50	0.45
1:A:395:PHE:O	1:A:399:VAL:HG23	2.18	0.44
1:B:464:ASP:OD2	1:B:468:ARG:NE	2.50	0.44
1:B:351:PRO:CD	1:B:385:ARG:HH21	2.31	0.44
1:B:146:SER:O	1:B:149:SER:OG	2.34	0.44
1:B:187:GLU:HG3	1:B:208:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:O	1:A:273:MET:HG3	2.18	0.44
1:B:489:ILE:HA	1:B:494:PRO:HG3	2.00	0.44
1:B:52:LYS:HB3	1:B:181:THR:HG23	1.99	0.43
1:A:278:PHE:HB3	1:A:284:ILE:HD11	2.00	0.43
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.99	0.43
1:B:102:LYS:HA	1:B:102:LYS:HD3	1.86	0.43
1:B:335:PHE:HA	1:B:338:MET:HG3	1.99	0.43
1:A:300:ARG:NH1	1:A:475:LYS:O	2.49	0.43
1:B:60:LEU:HD23	1:B:141:ARG:HB2	2.01	0.43
1:A:264:SER:HA	1:A:271:ASP:OD2	2.19	0.43
2:A:601:ATP:O1G	1:B:224:LYS:NZ	2.51	0.43
1:B:296:LEU:HD22	1:B:472:ILE:HD13	2.01	0.43
1:A:31:ILE:HA	1:A:231:MET:SD	2.59	0.42
1:A:211:LEU:HD21	1:B:234:GLU:OE1	2.18	0.42
1:B:445:ILE:O	1:B:448:GLU:HB2	2.19	0.42
1:A:45:SER:HA	1:A:182:THR:O	2.20	0.42
1:A:43:LEU:HD13	1:A:197:GLU:O	2.20	0.42
1:A:191:ILE:HG13	1:A:206:ILE:HD11	2.01	0.42
1:A:351:PRO:HG2	1:A:385:ARG:HE	1.84	0.42
1:A:21:MET:HE3	1:A:177:THR:HG21	2.01	0.42
1:B:235:TYR:HA	1:B:236:PRO:HD2	1.92	0.42
1:A:285:LEU:HB3	1:A:434:THR:HG21	2.00	0.42
1:B:390:ASN:HA	1:B:393:ARG:NH1	2.35	0.42
1:A:54:LEU:HD13	1:A:90:PHE:CE1	2.55	0.41
1:A:311:ARG:HA	1:A:343:LEU:O	2.20	0.41
1:A:350:TYR:HA	1:A:351:PRO:HD3	1.91	0.41
1:B:449:MET:HA	1:B:449:MET:CE	2.50	0.41
1:A:321:ARG:HH21	1:A:321:ARG:CG	2.31	0.41
1:B:37:PRO:HD2	1:B:203:ASN:ND2	2.34	0.41
1:B:204:VAL:HG11	1:B:223:LEU:HD12	2.02	0.41
1:B:269:ARG:HA	1:B:269:ARG:HD2	1.51	0.41
1:A:24:MET:HB2	1:A:62:ASN:HB3	2.01	0.41
1:A:278:PHE:CG	1:A:284:ILE:CD1	3.04	0.41
1:A:448:GLU:HA	1:B:466:ALA:HA	2.02	0.41
1:B:379:SER:HB3	1:B:413:THR:OG1	2.20	0.41
1:A:31:ILE:HD12	1:A:246:ILE:HG21	2.02	0.41
1:A:52:LYS:HB3	1:A:181:THR:CG2	2.50	0.41
1:A:379:SER:HB3	1:A:413:THR:OG1	2.20	0.41
1:B:313:ILE:HG13	1:B:372:PRO:HB3	2.01	0.41
1:A:225:LEU:HD12	1:A:230:HIS:HB3	2.03	0.41
1:B:245:ASN:HD22	1:B:245:ASN:HA	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:HB	1:A:198:GLU:HG2	2.02	0.41
1:A:133:ALA:HA	1:A:136:LYS:CB	2.50	0.40
1:A:31:ILE:CD1	1:A:246:ILE:HG21	2.52	0.40
1:A:68:ASP:O	1:A:68:ASP:CG	2.60	0.40
1:A:191:ILE:CB	1:A:198:GLU:HG2	2.51	0.40
1:A:319:GLU:HG2	1:A:323:GLN:HG2	2.04	0.40
1:A:454:ASN:HB2	1:A:467:ILE:HA	2.03	0.40
1:B:358:ASP:O	1:B:362:ILE:HG13	2.20	0.40
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.56	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	448/519 (86%)	409 (91%)	38 (8%)	1 (0%)	47	64
1	B	447/519 (86%)	412 (92%)	31 (7%)	4 (1%)	17	26
All	All	895/1038 (86%)	821 (92%)	69 (8%)	5 (1%)	25	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	428	SER
1	B	428	SER
1	B	26	GLU
1	B	420	MET
1	B	150	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	289/444 (65%)	238 (82%)	51 (18%)	2	1
1	B	296/444 (67%)	241 (81%)	55 (19%)	1	1
All	All	585/888 (66%)	479 (82%)	106 (18%)	1	1

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	26	GLU
1	A	30	ASP
1	A	40	ARG
1	A	43	LEU
1	A	48	SER
1	A	57	ILE
1	A	68	ASP
1	A	97	LEU
1	A	143	SER
1	A	183	GLU
1	A	184	ARG
1	A	187	GLU
1	A	193	ARG
1	A	196	VAL
1	A	198	GLU
1	A	210	VAL
1	A	221	GLU
1	A	222	ILE
1	A	223	LEU
1	A	224	LYS
1	A	237	PHE
1	A	264	SER
1	A	270	LEU
1	A	271	ASP
1	A	284	ILE
1	A	287	THR

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Mol	Chain	Res	Type
1	A	294	LYS
1	A	302	VAL
1	A	321	ARG
1	A	333	MET
1	A	335	PHE
1	A	342	ASN
1	A	347	VAL
1	A	348	CYS
1	A	356	LEU
1	A	385	ARG
1	A	397	ILE
1	A	405	GLN
1	A	406	GLU
1	A	413	THR
1	A	417	ASP
1	A	433	ILE
1	A	451	ARG
1	A	453	ILE
1	A	454	ASN
1	A	457	LYS
1	A	458	MET
1	A	465	LYS
1	A	469	GLU
1	A	487	GLU
1	B	21	MET
1	B	26	GLU
1	B	30	ASP
1	B	40	ARG
1	B	66	GLU
1	B	81	GLN
1	B	83	ILE
1	B	84	ILE
1	B	106	LEU
1	B	141	ARG
1	B	147	VAL
1	B	159	VAL
1	B	184	ARG
1	B	187	GLU
1	B	193	ARG
1	B	196	VAL
1	B	198	GLU
1	B	210	VAL

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Mol	Chain	Res	Type
1	B	211	LEU
1	B	219	THR
1	B	221	GLU
1	B	223	LEU
1	B	224	LYS
1	B	239	ILE
1	B	245	ASN
1	B	267	VAL
1	B	269	ARG
1	B	270	LEU
1	B	287	THR
1	B	292	THR
1	B	294	LYS
1	B	302	VAL
1	B	321	ARG
1	B	338	MET
1	B	347	VAL
1	B	348	CYS
1	B	352	GLU
1	B	356	LEU
1	B	360	LEU
1	B	361	GLN
1	B	366	GLU
1	B	399	VAL
1	B	405	GLN
1	B	406	GLU
1	B	413	THR
1	B	417	ASP
1	B	418	GLN
1	B	433	ILE
1	B	451	ARG
1	B	453	ILE
1	B	454	ASN
1	B	458	MET
1	B	465	LYS
1	B	472	ILE
1	B	483	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS

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Mol	Chain	Res	Type
1	A	209	ASN
1	A	341	GLN
1	A	414	ASN
1	B	209	ASN
1	B	245	ASN
1	B	323	GLN
1	B	341	GLN
1	B	361	GLN
1	B	389	ASN
1	B	414	ASN
1	B	418	GLN

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	601	3	26,33,33	0.67	0	31,52,52	0.71	1 (3%)
2	ATP	A	601	3	26,33,33	0.65	0	31,52,52	0.79	1 (3%)

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	ATP	A	602	3	26,33,33	0.65	0	31,52,52	0.74	1 (3%)
2	ATP	B	602	3	26,33,33	0.67	0	31,52,52	0.71	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	601	3	-	9/18/38/38	0/3/3/3
2	ATP	A	601	3	-	2/18/38/38	0/3/3/3
2	ATP	A	602	3	-	1/18/38/38	0/3/3/3
2	ATP	B	602	3	-	1/18/38/38	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	602	ATP	C5-C6-N6	2.30	123.84	120.35
2	A	601	ATP	C5-C6-N6	2.28	123.81	120.35
2	B	601	ATP	C5-C6-N6	2.23	123.74	120.35
2	B	602	ATP	C5-C6-N6	2.16	123.64	120.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	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 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 601

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 602

Bond lengths

Bond angles

Torsions

Rings
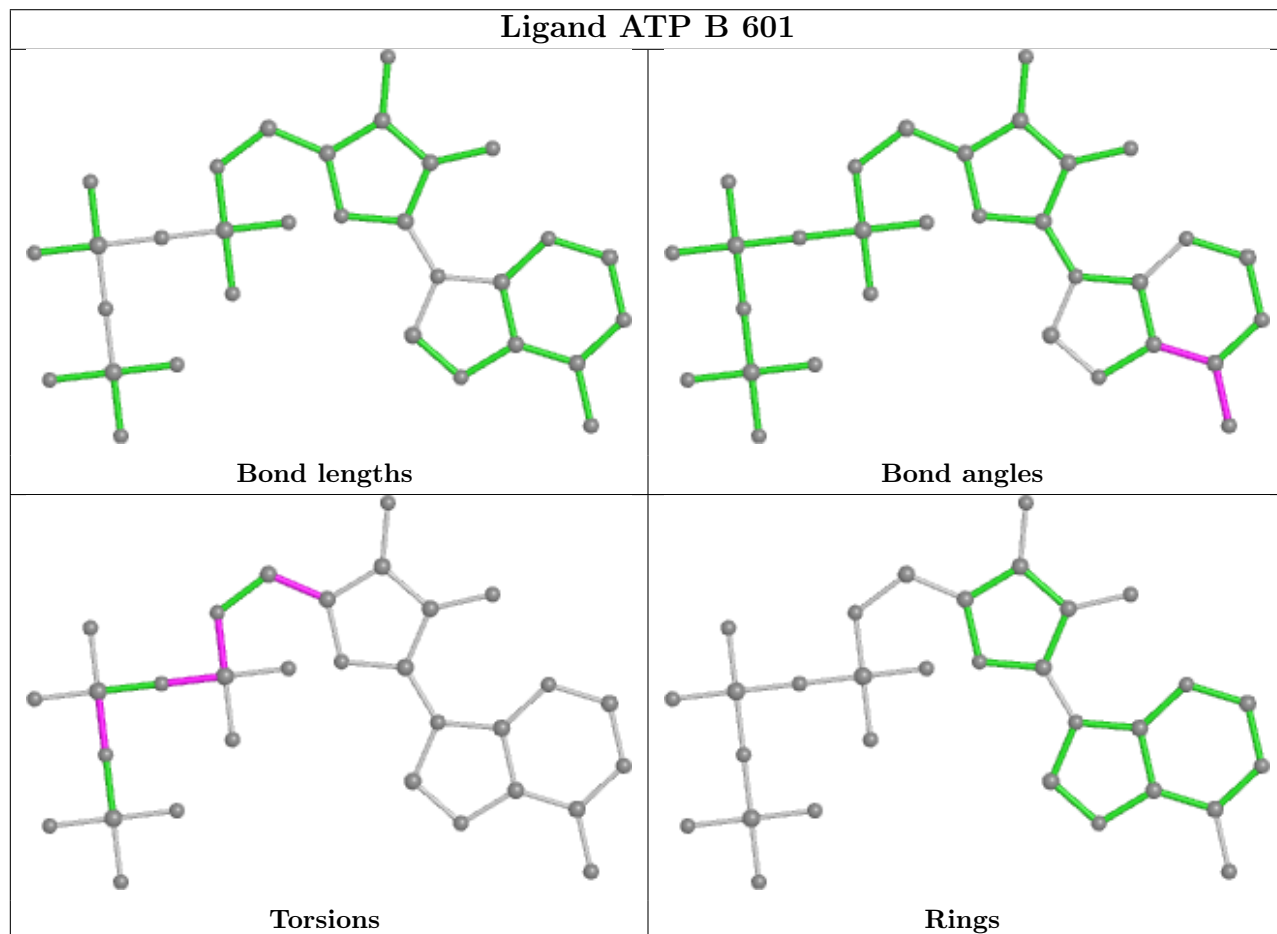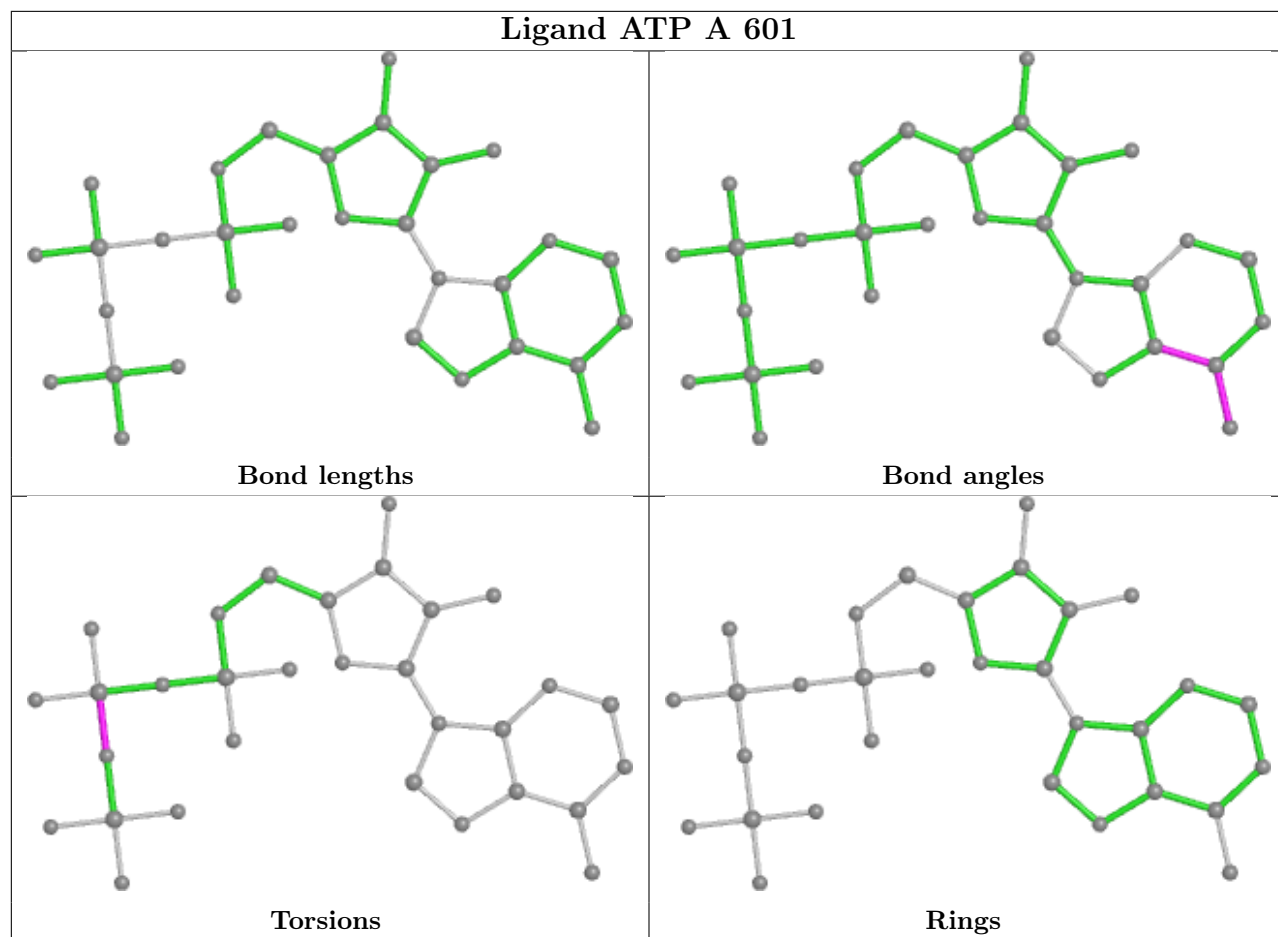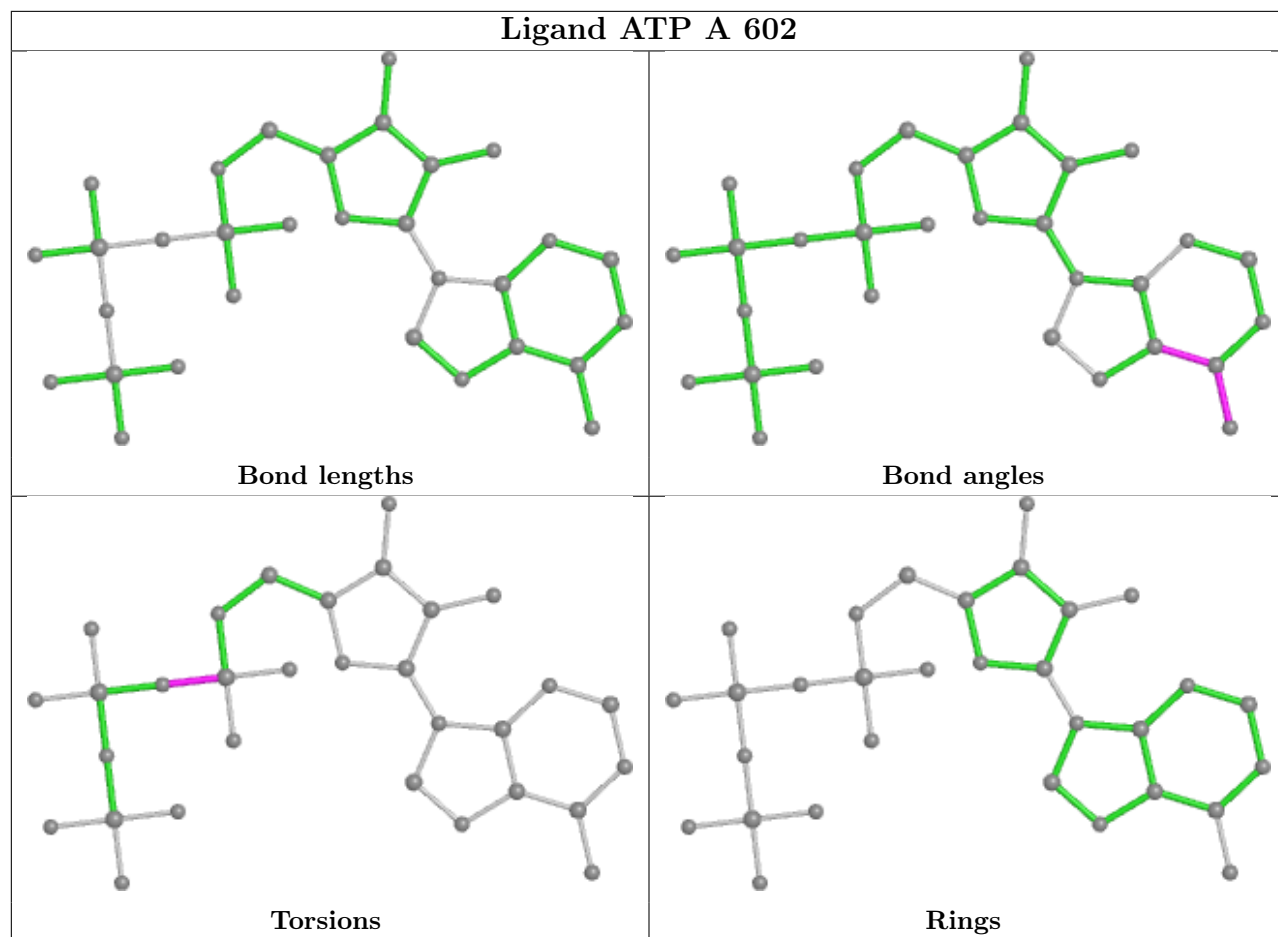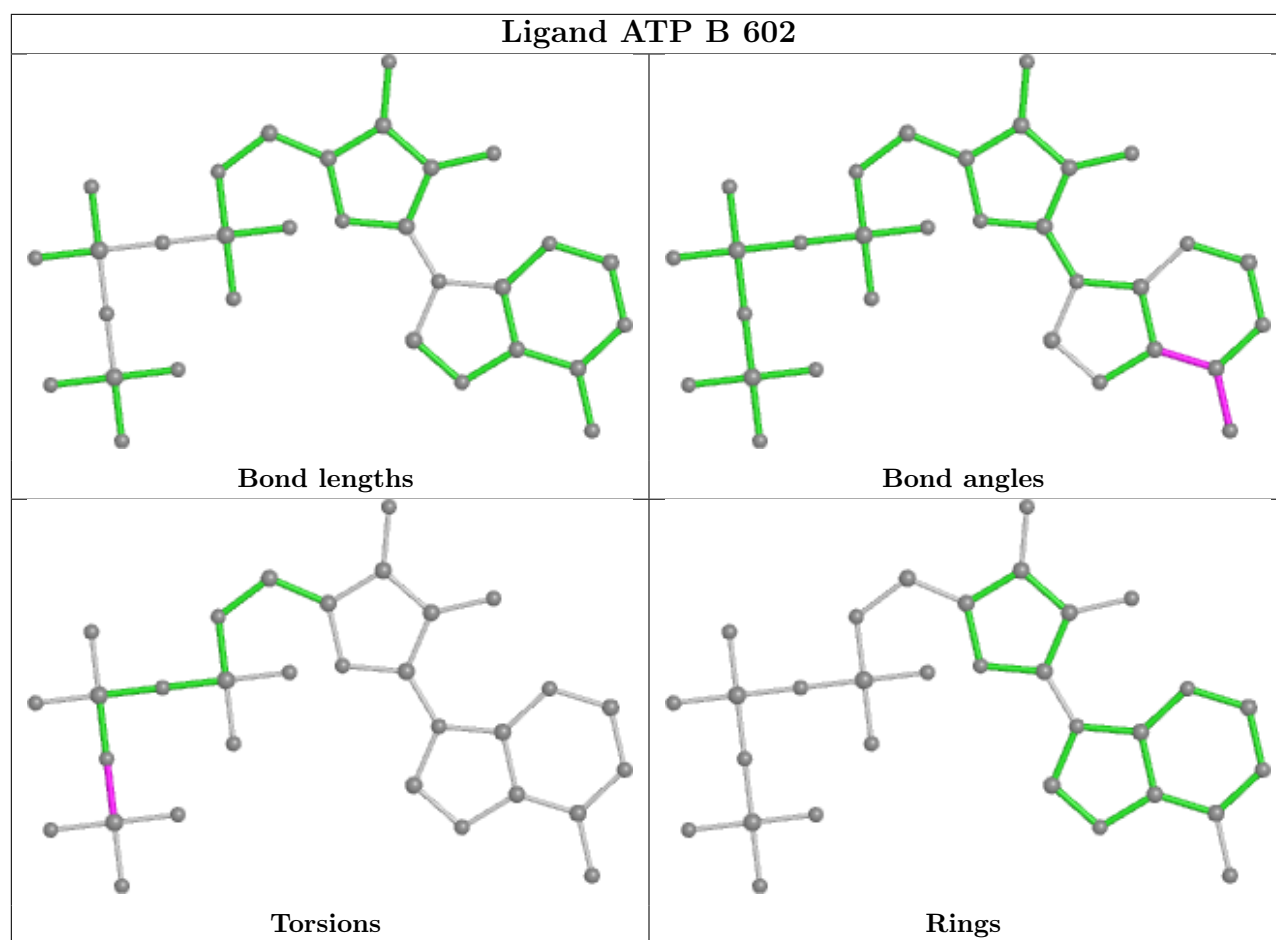
5.7 Other polymers ⓘ

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	456/519 (87%)	0.57	32 (7%)	16	13	45, 69, 103, 134	0
1	B	455/519 (87%)	0.58	42 (9%)	9	7	45, 68, 101, 115	0
All	All	911/1038 (87%)	0.58	74 (8%)	12	9	45, 69, 103, 134	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	PHE	8.2
1	B	142	VAL	7.9
1	B	276	GLY	6.4
1	B	171	LEU	5.1
1	B	94	LEU	5.0
1	A	276	GLY	4.7
1	A	275	GLY	4.5
1	B	275	GLY	4.4
1	B	139	ALA	4.3
1	A	95	ALA	4.2
1	B	104	PHE	4.0
1	B	455	VAL	4.0
1	B	180	MET	4.0
1	A	146	SER	3.8
1	B	475	LYS	3.8
1	B	494	PRO	3.7
1	A	331	TRP	3.6
1	B	95	ALA	3.6
1	A	94	LEU	3.5
1	B	72	VAL	3.4
1	B	274	CYS	3.3
1	A	144	ILE	3.3
1	B	109	SER	3.3
1	A	176	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	176	ALA	3.2
1	A	97	LEU	3.1
1	B	76	PHE	3.0
1	B	258	SER	3.0
1	A	77	GLU	2.9
1	B	61	TYR	2.9
1	A	197	GLU	2.9
1	A	91	GLY	2.8
1	B	74	VAL	2.8
1	A	181	THR	2.8
1	B	225	LEU	2.7
1	A	168	VAL	2.6
1	A	307	ALA	2.6
1	B	57	ILE	2.5
1	A	75	THR	2.5
1	B	476	GLY	2.5
1	A	477	PRO	2.5
1	B	167	LEU	2.5
1	B	474	ASP	2.5
1	B	151	PHE	2.4
1	A	478	ASP	2.4
1	A	54	LEU	2.4
1	A	139	ALA	2.3
1	A	271	ASP	2.3
1	B	157	SER	2.3
1	A	274	CYS	2.3
1	B	41	SER	2.3
1	B	228	THR	2.3
1	B	92	TRP	2.3
1	B	77	GLU	2.3
1	B	377	ILE	2.3
1	B	443	VAL	2.3
1	B	24	MET	2.2
1	A	248	PRO	2.2
1	B	145	ASP	2.2
1	B	329	TYR	2.2
1	A	494	PRO	2.2
1	A	273	MET	2.2
1	A	194	TYR	2.2
1	B	439	LEU	2.2
1	A	474	ASP	2.1
1	A	148	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	2.1
1	B	470	PHE	2.1
1	B	147	VAL	2.1
1	B	80	PRO	2.1
1	A	23	THR	2.1
1	A	355	GLY	2.0
1	B	97	LEU	2.0
1	B	246	ILE	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
2	ATP	A	601	31/31	0.93	0.17	60,64,70,72	0
2	ATP	B	601	31/31	0.93	0.18	58,61,63,63	0
2	ATP	A	602	31/31	0.94	0.18	50,52,70,70	0
2	ATP	B	602	31/31	0.94	0.19	48,50,64,64	0
3	MG	B	603	1/1	0.94	0.18	49,49,49,49	0
3	MG	A	604	1/1	0.97	0.10	38,38,38,38	0
3	MG	A	603	1/1	0.97	0.06	44,44,44,44	0
3	MG	B	604	1/1	0.99	0.14	40,40,40,40	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:

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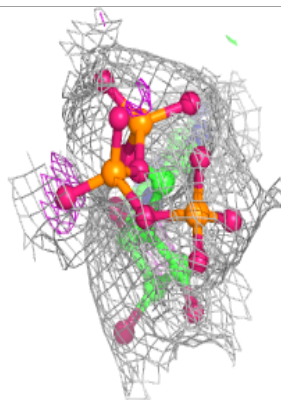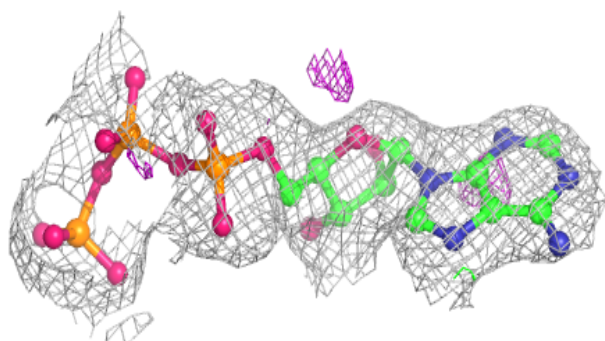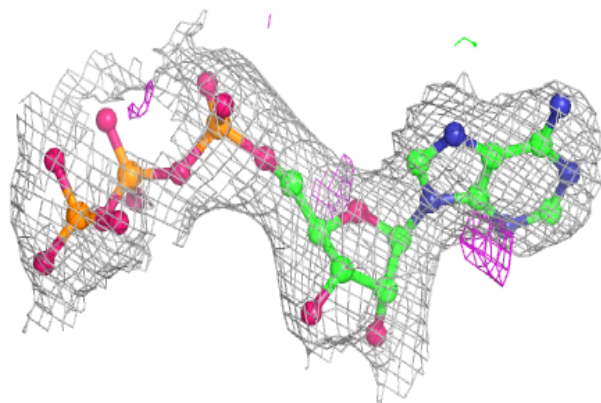mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
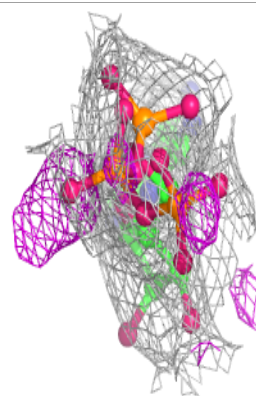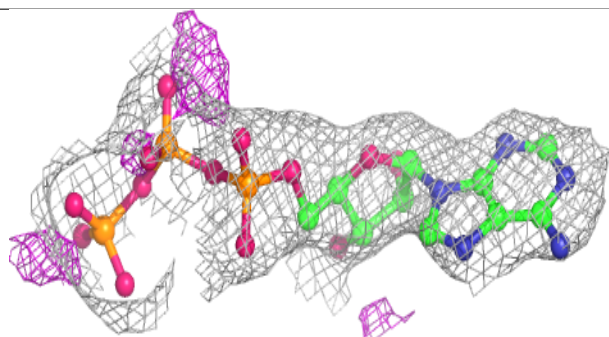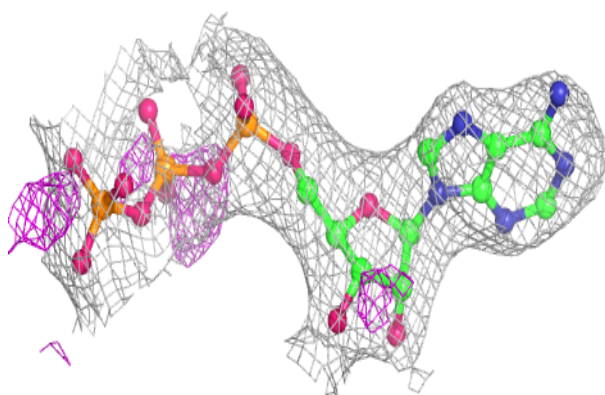
Electron density around ATP B 601:

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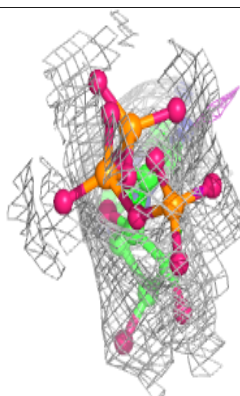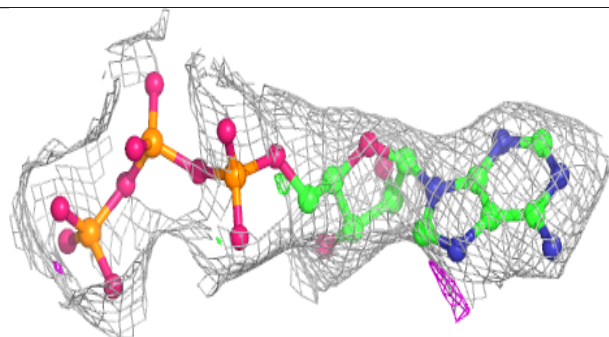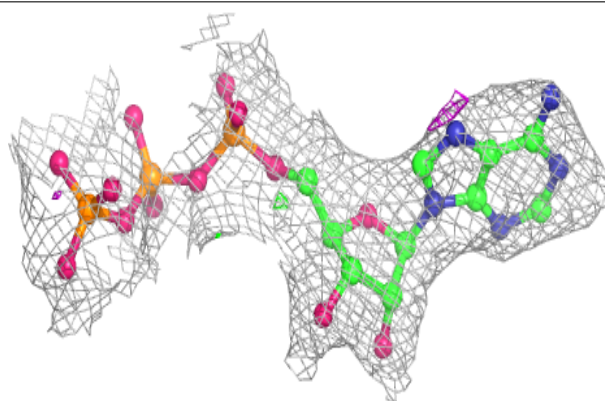
Electron density around ATP A 602:

$2mF_o\text{-}DF_c$ (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 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
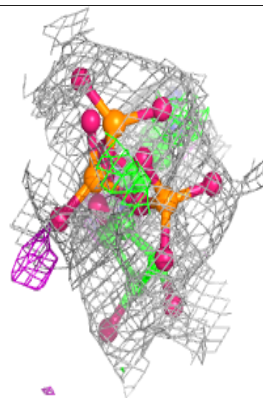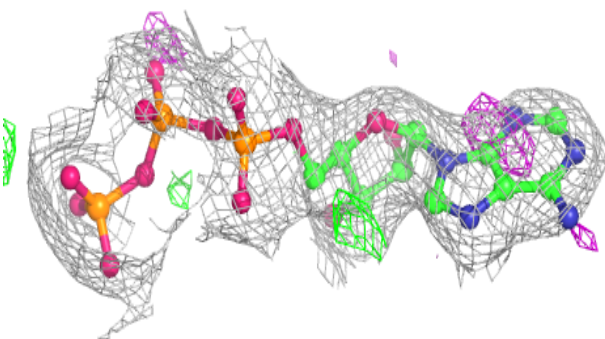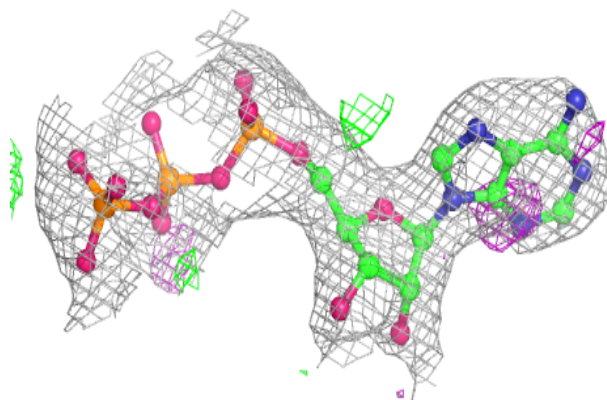
6.5 Other polymers (i)

There are no such residues in this entry.