



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2022 – 12:05 AM JST

PDB ID : 7DYK
Title : Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC
Authors : Furuike, Y.; Akiyama, S.
Deposited on : 2021-01-22
Resolution : 2.99 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.27
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) : 2.27

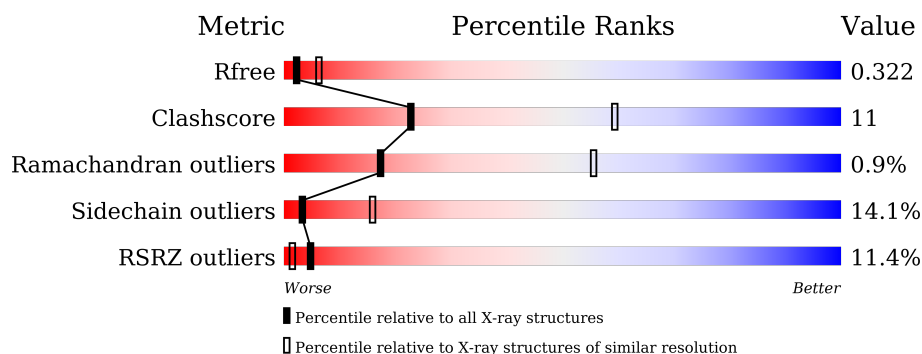
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	<div> <div>9%</div> <div>64%</div> <div>21%</div> <div>•</div> <div>12%</div> </div>
1	B	519	<div> <div>11%</div> <div>64%</div> <div>21%</div> <div>•</div> <div>12%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6705 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.

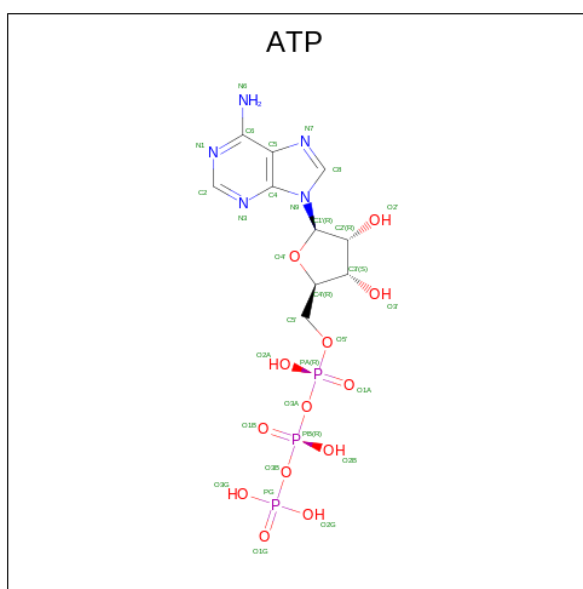
- Molecule 1 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3283	2074	575	621	13			
1	B	459	Total	C	N	O	S	0	0	0
			3281	2071	573	624	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	VAL	THR	conflict	UNP Q79PF4
B	432	VAL	THR	conflict	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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

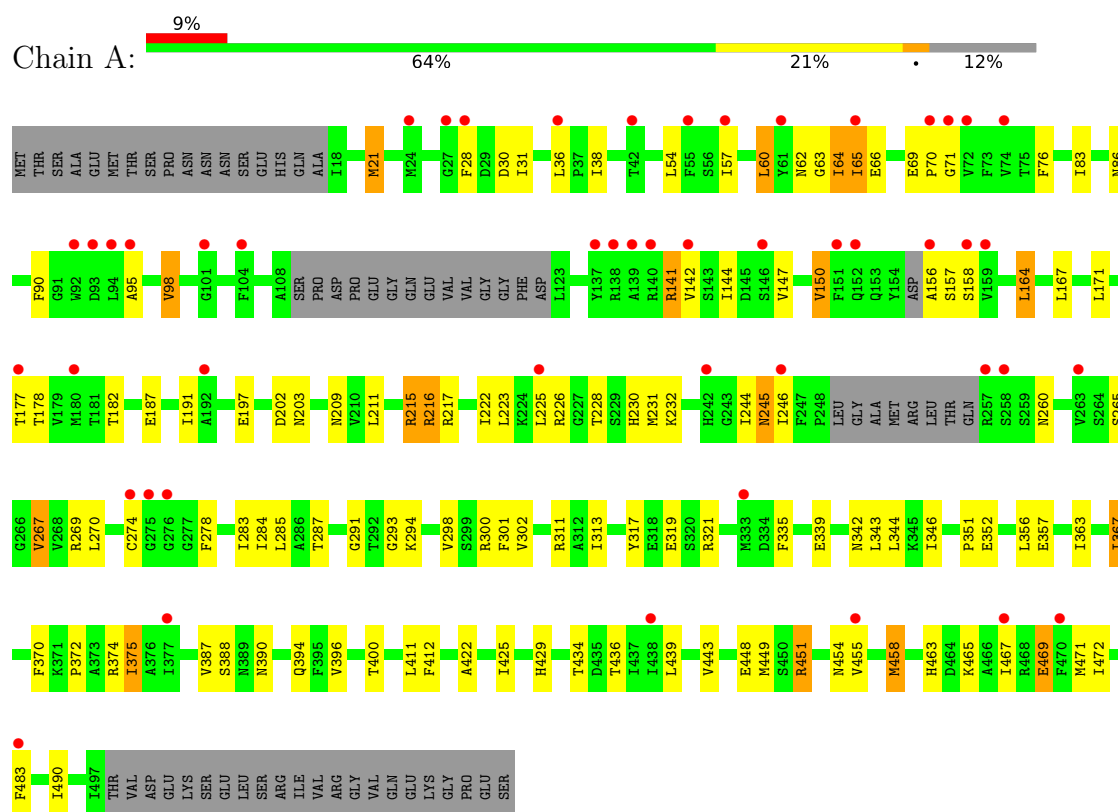
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	6	Total	O	0	0
			6	6		

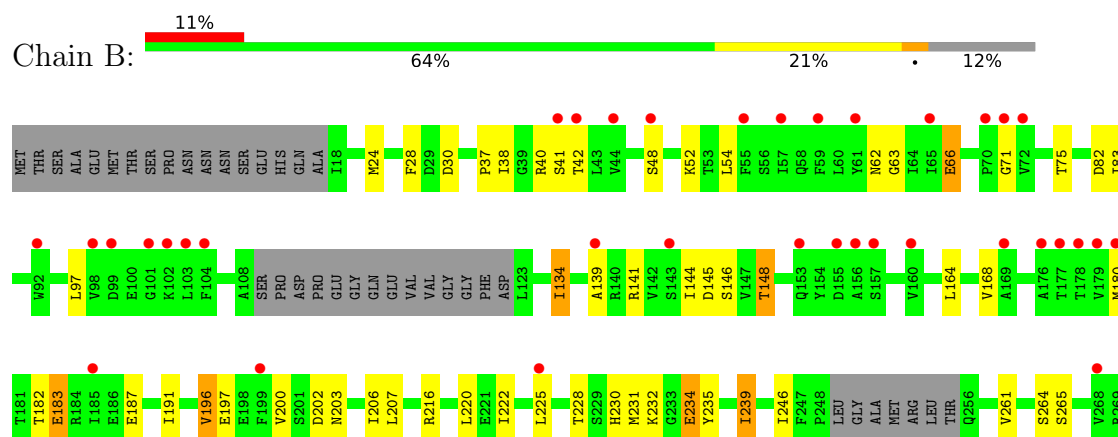
3 Residue-property plots [i](#)

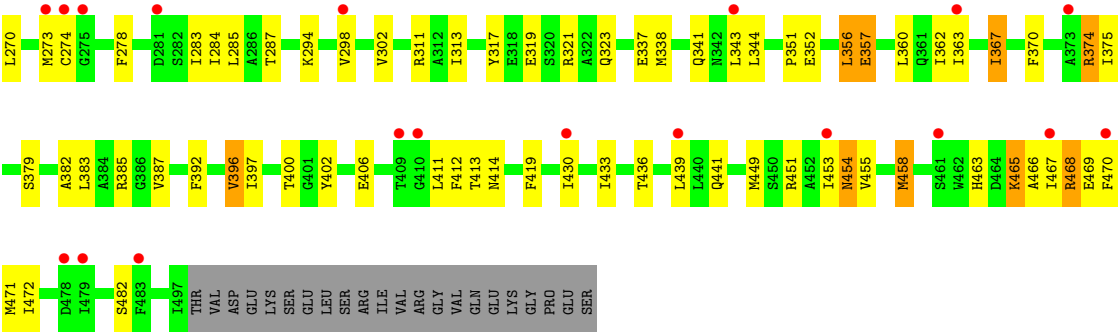
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Circadian clock protein kinase KaiC





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	94.85Å 94.85Å 180.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.55 – 2.99 48.55 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.55-2.99) 99.8 (48.55-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.274 , 0.328 0.272 , 0.322	Depositor DCC
R_{free} test set	881 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.796	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.063 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6705	wwPDB-VP
Average B, all atoms (Å ²)	72.0	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 53.02 % 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 4.4726e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0/3335	0.75	0/4526
1	B	0.69	0/3332	0.75	0/4527
All	All	0.69	0/6667	0.75	0/9053

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	3283	0	3008	77	0
1	B	3281	0	3007	74	0
2	A	62	0	24	1	0
2	B	62	0	24	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	7	0	0	0	0
4	B	6	0	0	0	0
All	All	6705	0	6063	146	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 (146) 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:356:LEU:HD22	1:A:387:VAL:HG11	1.42	1.01
1:A:167:LEU:HD12	1:A:171:LEU:HD21	1.62	0.80
1:B:24:MET:HG3	1:B:66:GLU:HG2	1.65	0.78
1:B:468:ARG:HA	1:B:482:SER:HA	1.69	0.75
1:A:76:PHE:CE2	1:A:150:VAL:CB	2.73	0.72
1:B:317:TYR:HB3	1:B:351:PRO:HG3	1.70	0.72
1:A:283:ILE:HG13	1:A:400:THR:HG23	1.73	0.71
1:A:167:LEU:O	1:A:171:LEU:HD23	1.90	0.71
1:A:225:LEU:HB3	1:A:228:THR:CG2	2.23	0.69
1:A:225:LEU:HB3	1:A:228:THR:HG23	1.79	0.65
1:B:225:LEU:HB3	1:B:228:THR:HG23	1.78	0.65
1:A:63:GLY:HA3	1:A:141:ARG:HD2	1.79	0.64
1:B:54:LEU:CD2	1:B:239:ILE:HG12	2.29	0.63
1:B:458:MET:HB2	1:B:463:HIS:CD2	2.34	0.62
1:A:38:ILE:HA	1:A:177:THR:CG2	2.30	0.62
1:A:167:LEU:CD1	1:A:171:LEU:HD21	2.30	0.61
1:B:134:ILE:HA	1:B:139:ALA:HB3	1.83	0.61
1:A:191:ILE:HD13	1:A:223:LEU:HD22	1.82	0.60
1:A:57:ILE:HD11	1:A:83:ILE:HG23	1.84	0.59
1:B:164:LEU:CD2	1:B:197:GLU:HA	2.32	0.59
1:B:367:ILE:HD13	1:B:375:ILE:HG21	1.83	0.59
1:A:167:LEU:O	1:A:171:LEU:CD2	2.51	0.58
1:B:287:THR:HG22	1:B:414:ASN:HD22	1.68	0.58
1:B:451:ARG:HG3	1:B:470:PHE:CE1	2.39	0.58
1:B:63:GLY:HA3	1:B:141:ARG:HD2	1.85	0.58
1:B:436:THR:HG23	1:B:458:MET:HG2	1.86	0.57
1:A:62:ASN:HA	1:A:65:ILE:HG22	1.86	0.56
1:A:390:ASN:O	1:A:394:GLN:HG3	2.07	0.55
1:B:337:GLU:O	1:B:341:GLN:HG3	2.08	0.54
1:A:21:MET:HE3	1:A:177:THR:HG21	1.88	0.54
1:B:41:SER:CB	1:B:168:VAL:HG12	2.38	0.54
1:A:356:LEU:CD2	1:A:387:VAL:HG11	2.29	0.54
1:A:225:LEU:HD12	1:A:230:HIS:HB3	1.89	0.53
1:A:164:LEU:HD12	1:A:197:GLU:HG3	1.89	0.53
1:A:422:ALA:HB2	1:A:490:ILE:HD12	1.89	0.53
1:B:379:SER:O	1:B:383:LEU:HD12	2.09	0.53
1:A:291:GLY:O	1:A:451:ARG:NH1	2.41	0.53
1:B:284:ILE:HB	1:B:411:LEU:HD12	1.91	0.53
1:A:171:LEU:HD22	1:A:171:LEU:N	2.24	0.53
1:A:274:CYS:HG	1:A:278:PHE:HE1	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ILE:HD11	1:B:370:PHE:HB3	1.91	0.52
1:A:191:ILE:HD13	1:A:223:LEU:CD2	2.38	0.52
1:A:197:GLU:N	1:A:197:GLU:OE2	2.42	0.52
1:B:392:PHE:O	1:B:396:VAL:HG23	2.09	0.52
1:A:71:GLY:HA2	1:A:141:ARG:O	2.11	0.51
1:B:338:MET:HB3	1:B:344:LEU:HB3	1.93	0.51
1:A:211:LEU:HD21	1:B:234:GLU:OE1	2.11	0.50
1:A:215:ARG:NH2	1:B:232:LYS:O	2.44	0.50
1:A:313:ILE:HG13	1:A:372:PRO:HB3	1.92	0.50
1:B:363:ILE:O	1:B:367:ILE:HG13	2.11	0.50
1:B:148:THR:HG21	1:B:183:GLU:H	1.76	0.50
1:A:265:SER:HB3	1:A:278:PHE:CE2	2.46	0.50
1:A:28:PHE:CZ	1:A:36:LEU:HD21	2.47	0.49
1:A:367:ILE:HG23	1:A:372:PRO:HG2	1.94	0.49
1:B:148:THR:HG21	1:B:183:GLU:CG	2.43	0.49
1:A:317:TYR:HB3	1:A:351:PRO:HG3	1.93	0.49
1:B:225:LEU:HD12	1:B:230:HIS:HB3	1.95	0.49
1:A:167:LEU:HD12	1:A:171:LEU:CD2	2.40	0.49
1:B:62:ASN:O	1:B:66:GLU:HB2	2.12	0.49
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.95	0.49
1:B:396:VAL:HG21	1:B:430:ILE:CD1	2.43	0.49
1:A:209:ASN:O	1:A:216:ARG:NH2	2.46	0.49
1:A:335:PHE:O	1:A:339:GLU:HG3	2.13	0.48
1:A:54:LEU:CD2	1:A:244:ILE:HG12	2.43	0.48
1:B:273:MET:SD	1:B:468:ARG:HD2	2.52	0.48
1:A:294:LYS:HE2	2:A:602:ATP:O2B	2.14	0.48
1:B:294:LYS:HE2	2:B:602:ATP:O2B	2.13	0.48
1:B:311:ARG:HA	1:B:343:LEU:O	2.12	0.48
1:B:396:VAL:HG21	1:B:430:ILE:HD12	1.96	0.48
1:A:313:ILE:HD11	1:A:370:PHE:HB3	1.96	0.48
1:B:134:ILE:O	1:B:139:ALA:N	2.46	0.47
1:A:302:VAL:CG1	1:A:344:LEU:HD13	2.44	0.47
1:A:311:ARG:HA	1:A:343:LEU:O	2.13	0.47
1:A:449:MET:N	1:B:465:LYS:O	2.47	0.47
1:A:95:ALA:O	1:A:98:VAL:HG12	2.15	0.47
1:B:231:MET:HB3	1:B:235:TYR:OH	2.14	0.47
1:B:274:CYS:HG	1:B:278:PHE:HE1	1.60	0.47
1:B:225:LEU:HB3	1:B:228:THR:CG2	2.45	0.47
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.50	0.46
1:B:168:VAL:HG13	1:B:180:MET:HE1	1.97	0.46
1:A:301:PHE:CZ	1:A:374:ARG:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:THR:CG2	1:B:414:ASN:HD22	2.29	0.46
1:B:71:GLY:HA2	1:B:141:ARG:O	2.14	0.46
1:B:148:THR:HG21	1:B:183:GLU:HG3	1.96	0.46
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.98	0.46
1:B:42:THR:HA	1:B:203:ASN:HB2	1.98	0.46
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.98	0.46
1:B:28:PHE:HB2	1:B:246:ILE:HD12	1.98	0.45
1:B:468:ARG:HA	1:B:482:SER:CA	2.42	0.45
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.97	0.45
1:B:356:LEU:CD2	1:B:387:VAL:HG11	2.47	0.45
1:A:298:VAL:HA	1:A:411:LEU:HD23	1.98	0.45
1:B:207:LEU:N	1:B:207:LEU:HD23	2.31	0.45
1:B:363:ILE:CG2	1:B:367:ILE:HD11	2.47	0.44
1:A:436:THR:HG23	1:A:458:MET:HG2	2.00	0.44
1:B:191:ILE:HD12	1:B:206:ILE:HD11	2.00	0.44
1:B:419:PHE:O	1:B:441:GLN:NE2	2.40	0.44
1:A:448:GLU:HA	1:B:466:ALA:HA	1.99	0.44
1:B:382:ALA:O	1:B:385:ARG:HG3	2.17	0.44
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.85	0.43
1:A:64:ILE:HG22	1:A:69:GLU:C	2.39	0.43
1:B:298:VAL:HA	1:B:411:LEU:HD23	1.99	0.43
1:B:148:THR:HG22	1:B:182:THR:HA	2.00	0.43
1:B:164:LEU:HG	1:B:200:VAL:HG11	1.99	0.43
1:A:64:ILE:HG22	1:A:69:GLU:O	2.18	0.43
1:B:357:GLU:H	1:B:357:GLU:CD	2.20	0.43
1:A:367:ILE:HD13	1:A:375:ILE:HG21	2.00	0.43
1:A:363:ILE:O	1:A:367:ILE:HG13	2.18	0.43
1:B:207:LEU:HD22	1:B:220:LEU:HD12	2.01	0.43
1:B:264:SER:O	1:B:374:ARG:NH1	2.43	0.43
1:B:145:ASP:HA	1:B:146:SER:HA	1.70	0.43
1:B:164:LEU:HD21	1:B:197:GLU:HA	2.01	0.43
1:B:397:ILE:CD1	1:B:433:ILE:HD13	2.49	0.43
1:A:244:ILE:HG22	1:A:246:ILE:HG13	2.01	0.42
1:B:412:PHE:CD1	1:B:412:PHE:N	2.87	0.42
1:A:245:ASN:HD22	1:A:245:ASN:HA	1.56	0.42
1:B:402:TYR:O	1:B:406:GLU:HG2	2.20	0.42
1:A:54:LEU:HD13	1:A:90:PHE:CZ	2.54	0.42
1:A:156:ALA:O	1:A:158:SER:N	2.52	0.42
1:A:267:VAL:HB	1:A:270:LEU:CB	2.50	0.42
1:A:54:LEU:HD23	1:A:244:ILE:HG12	2.02	0.42
1:B:451:ARG:NH2	1:B:472:ILE:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HD12	1:A:246:ILE:HG21	2.02	0.42
1:A:287:THR:HG21	1:A:425:ILE:CG1	2.49	0.42
1:A:370:PHE:HB3	1:A:372:PRO:HD3	2.02	0.42
1:A:164:LEU:CD1	1:A:197:GLU:HA	2.50	0.41
1:A:191:ILE:CD1	1:A:223:LEU:CD2	2.98	0.41
1:A:211:LEU:HD13	1:A:216:ARG:HD3	2.01	0.41
1:B:285:LEU:HA	1:B:412:PHE:O	2.20	0.41
1:B:168:VAL:HG13	1:B:180:MET:CE	2.51	0.41
1:A:86:ASN:OD1	1:B:40:ARG:NH2	2.54	0.41
1:A:356:LEU:HD12	1:A:356:LEU:HA	1.85	0.41
1:B:265:SER:HB3	1:B:278:PHE:CE2	2.56	0.41
1:A:202:ASP:HA	1:A:226:ARG:NH1	2.35	0.41
1:A:454:ASN:HB2	1:A:467:ILE:HA	2.02	0.41
1:A:490:ILE:HD13	1:A:490:ILE:HA	1.92	0.41
1:B:455:VAL:HG11	1:B:463:HIS:HB2	2.03	0.41
1:A:203:ASN:HB3	1:A:225:LEU:CD2	2.50	0.41
1:B:37:PRO:HD2	1:B:203:ASN:ND2	2.36	0.41
1:B:164:LEU:HD22	1:B:197:GLU:HG3	2.03	0.41
1:B:396:VAL:HG11	1:B:430:ILE:HG23	2.03	0.41
1:B:454:ASN:HB2	1:B:467:ILE:HA	2.02	0.41
1:A:458:MET:HB2	1:A:463:HIS:CD2	2.55	0.40
1:A:285:LEU:HD12	1:A:412:PHE:O	2.21	0.40
1:A:142:VAL:O	1:A:178:THR:HA	2.21	0.40
1:A:287:THR:HG21	1:A:425:ILE:HG12	2.03	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	449/519 (86%)	404 (90%)	41 (9%)	4 (1%)	17 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	453/519 (87%)	409 (90%)	40 (9%)	4 (1%)	17	55
All	All	902/1038 (87%)	813 (90%)	81 (9%)	8 (1%)	17	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	SER
1	B	97	LEU
1	A	70	PRO
1	B	66	GLU
1	B	196	VAL
1	A	293	GLY
1	B	134	ILE
1	A	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	304/444 (68%)	259 (85%)	45 (15%)	3	14
1	B	305/444 (69%)	264 (87%)	41 (13%)	4	17
All	All	609/888 (69%)	523 (86%)	86 (14%)	3	16

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	30	ASP
1	A	60	LEU
1	A	64	ILE
1	A	65	ILE
1	A	66	GLU
1	A	98	VAL
1	A	141	ARG

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Mol	Chain	Res	Type
1	A	144	ILE
1	A	147	VAL
1	A	164	LEU
1	A	182	THR
1	A	187	GLU
1	A	215	ARG
1	A	216	ARG
1	A	217	ARG
1	A	222	ILE
1	A	231	MET
1	A	232	LYS
1	A	245	ASN
1	A	260	ASN
1	A	267	VAL
1	A	269	ARG
1	A	284	ILE
1	A	300	ARG
1	A	319	GLU
1	A	321	ARG
1	A	342	ASN
1	A	346	ILE
1	A	352	GLU
1	A	357	GLU
1	A	367	ILE
1	A	375	ILE
1	A	388	SER
1	A	396	VAL
1	A	429	HIS
1	A	434	THR
1	A	439	LEU
1	A	443	VAL
1	A	451	ARG
1	A	458	MET
1	A	465	LYS
1	A	469	GLU
1	A	471	MET
1	A	472	ILE
1	B	30	ASP
1	B	38	ILE
1	B	48	SER
1	B	52	LYS
1	B	75	THR

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Mol	Chain	Res	Type
1	B	82	ASP
1	B	83	ILE
1	B	144	ILE
1	B	148	THR
1	B	183	GLU
1	B	187	GLU
1	B	196	VAL
1	B	202	ASP
1	B	216	ARG
1	B	222	ILE
1	B	234	GLU
1	B	239	ILE
1	B	261	VAL
1	B	270	LEU
1	B	302	VAL
1	B	319	GLU
1	B	321	ARG
1	B	323	GLN
1	B	352	GLU
1	B	356	LEU
1	B	357	GLU
1	B	360	LEU
1	B	362	ILE
1	B	367	ILE
1	B	374	ARG
1	B	396	VAL
1	B	413	THR
1	B	439	LEU
1	B	449	MET
1	B	453	ILE
1	B	454	ASN
1	B	458	MET
1	B	465	LYS
1	B	468	ARG
1	B	469	GLU
1	B	471	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	A	245	ASN

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Mol	Chain	Res	Type
1	A	304	ASN
1	A	361	GLN
1	A	389	ASN
1	A	418	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	601	3	26,33,33	0.65	0	31,52,52	0.79	1 (3%)
2	ATP	B	601	3	26,33,33	0.65	0	31,52,52	0.75	1 (3%)
2	ATP	A	602	3	26,33,33	0.67	0	31,52,52	0.79	1 (3%)
2	ATP	B	602	3	26,33,33	0.66	0	31,52,52	0.74	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	A	601	3	-	3/18/38/38	0/3/3/3
2	ATP	B	601	3	-	7/18/38/38	0/3/3/3
2	ATP	A	602	3	-	5/18/38/38	0/3/3/3
2	ATP	B	602	3	-	0/18/38/38	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(°)	Ideal(°)
2	A	601	ATP	C5-C6-N6	2.34	123.90	120.35
2	B	601	ATP	C5-C6-N6	2.28	123.82	120.35
2	A	602	ATP	C5-C6-N6	2.13	123.59	120.35
2	B	602	ATP	C5-C6-N6	2.12	123.58	120.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	ATP	C5'-O5'-PA-O3A
2	A	602	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	C5'-O5'-PA-O2A
2	A	601	ATP	O4'-C4'-C5'-O5'
2	A	601	ATP	C3'-C4'-C5'-O5'
2	A	602	ATP	C3'-C4'-C5'-O5'
2	A	601	ATP	PA-O3A-PB-O2B
2	A	602	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	PB-O3B-PG-O1G
2	B	601	ATP	PA-O3A-PB-O1B
2	B	601	ATP	C5'-O5'-PA-O3A
2	B	601	ATP	O4'-C4'-C5'-O5'
2	A	602	ATP	PB-O3A-PA-O1A
2	B	601	ATP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

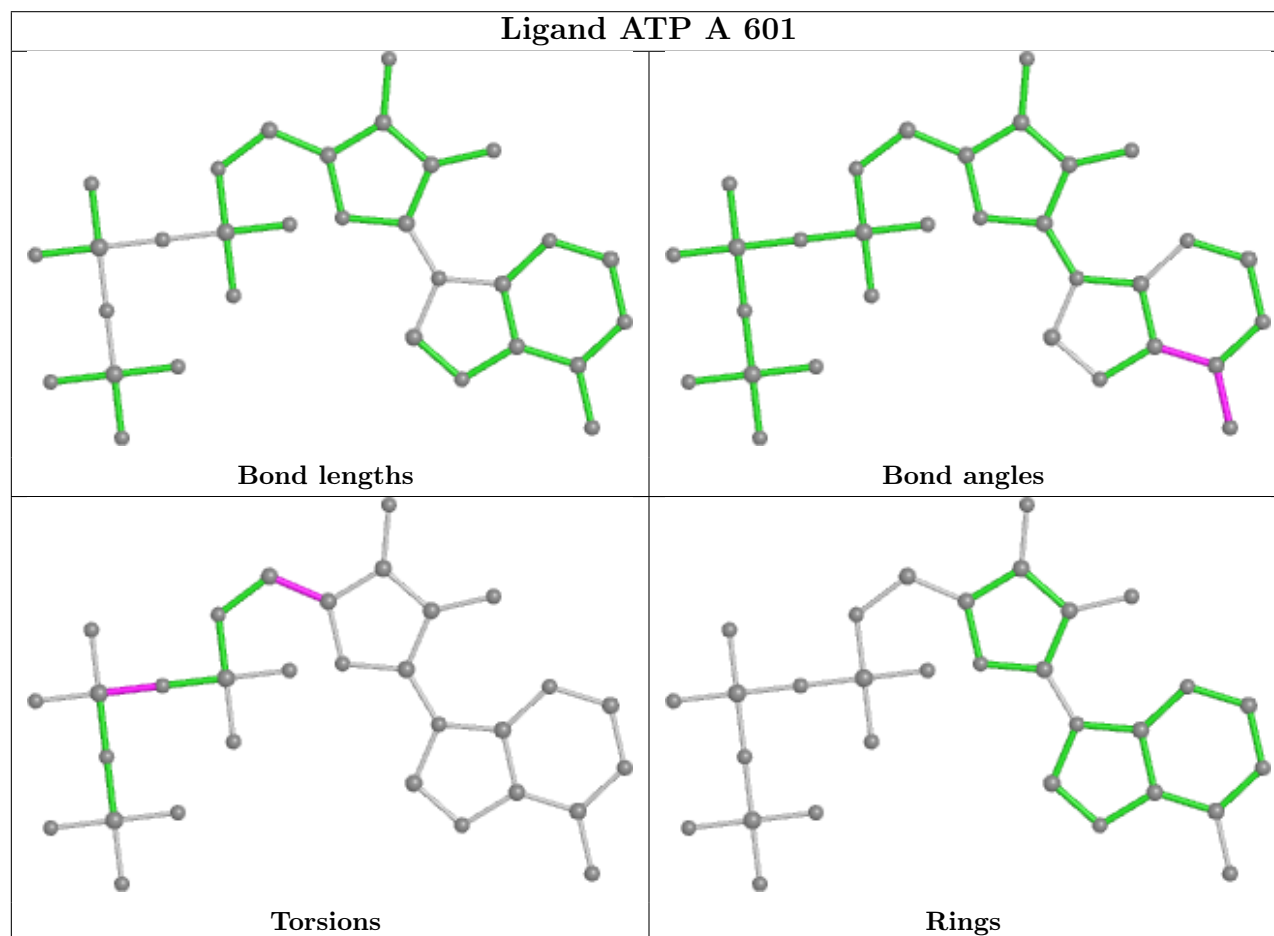
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	ATP	1	0

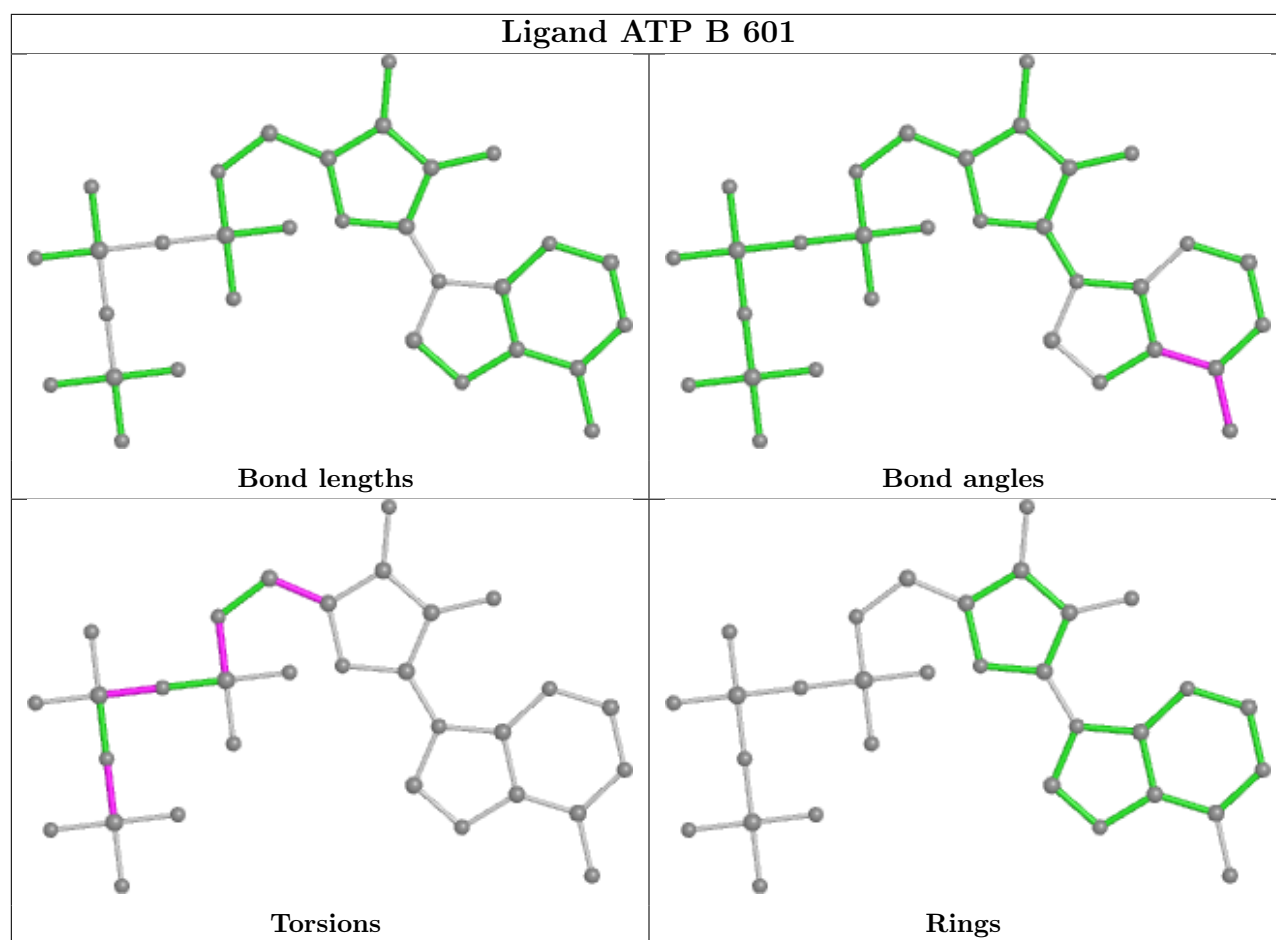
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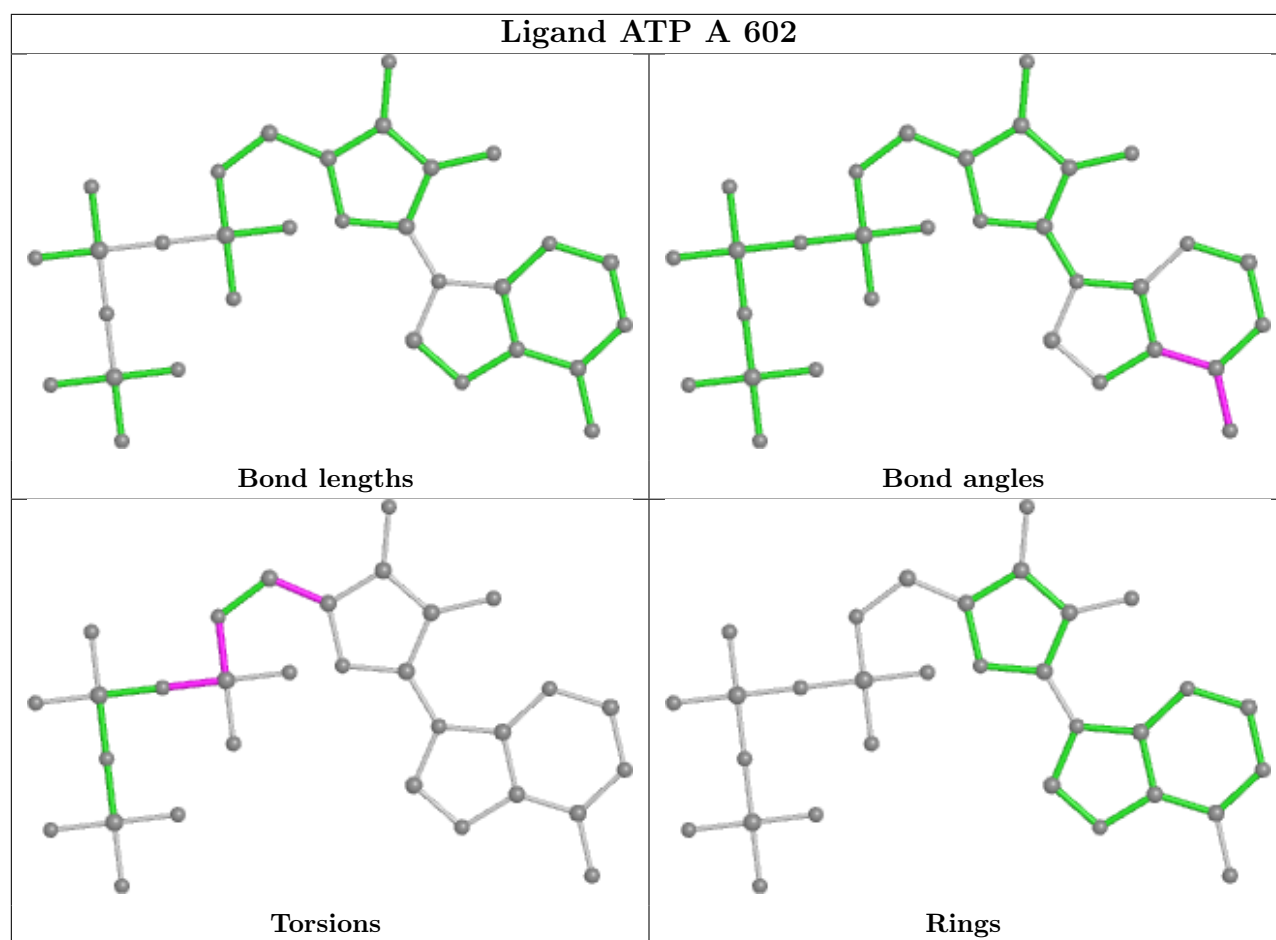
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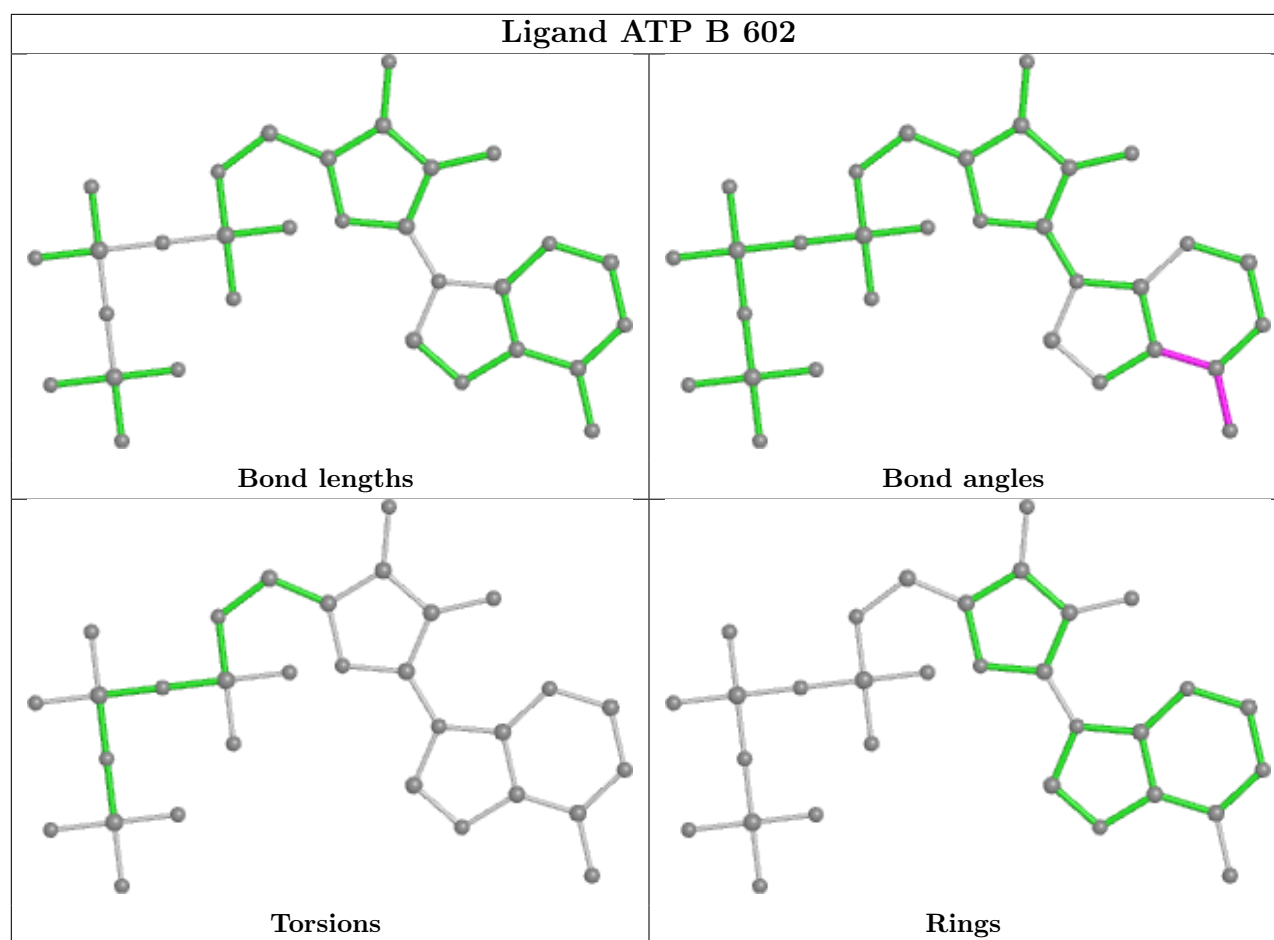
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	ATP	1	0

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	457/519 (88%)	0.71	49 (10%) 6 2	46, 70, 101, 116	0
1	B	459/519 (88%)	0.74	55 (11%) 4 1	48, 71, 113, 124	0
All	All	916/1038 (88%)	0.72	104 (11%) 5 1	46, 70, 105, 124	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	ARG	6.0
1	A	94	LEU	5.4
1	B	176	ALA	5.4
1	A	71	GLY	5.3
1	A	95	ALA	5.3
1	A	276	GLY	5.3
1	A	275	GLY	5.0
1	B	98	VAL	5.0
1	B	178	THR	4.8
1	B	177	THR	4.6
1	A	92	TRP	4.6
1	A	139	ALA	4.4
1	B	155	ASP	4.4
1	A	72	VAL	4.2
1	A	177	THR	4.0
1	B	180	MET	4.0
1	A	57	ILE	3.9
1	B	71	GLY	3.8
1	A	101	GLY	3.7
1	B	61	TYR	3.7
1	B	479	ILE	3.7
1	A	61	TYR	3.5
1	A	483	PHE	3.4
1	A	24	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	72	VAL	3.3
1	B	55	PHE	3.2
1	A	263	VAL	3.2
1	A	74	VAL	3.2
1	B	99	ASP	3.1
1	B	156	ALA	3.1
1	A	104	PHE	3.1
1	B	42	THR	3.1
1	B	373	ALA	3.0
1	B	470	PHE	2.9
1	A	140	ARG	2.9
1	B	48	SER	2.9
1	A	156	ALA	2.9
1	B	101	GLY	2.9
1	B	275	GLY	2.9
1	A	225	LEU	2.9
1	B	274	CYS	2.9
1	B	44	VAL	2.8
1	B	179	VAL	2.8
1	A	180	MET	2.7
1	B	225	LEU	2.7
1	B	483	PHE	2.7
1	A	151	PHE	2.6
1	B	461	SER	2.6
1	B	343	LEU	2.6
1	B	157	SER	2.6
1	B	70	PRO	2.6
1	A	28	PHE	2.6
1	A	438	ILE	2.6
1	B	92	TRP	2.6
1	B	169	ALA	2.6
1	A	470	PHE	2.6
1	A	152	GLN	2.6
1	B	143	SER	2.6
1	A	377	ILE	2.5
1	A	455	VAL	2.5
1	A	246	ILE	2.5
1	B	409	THR	2.5
1	A	93	ASP	2.5
1	A	159	VAL	2.5
1	A	137	TYR	2.5
1	B	467	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	65	ILE	2.4
1	A	274	CYS	2.4
1	B	57	ILE	2.4
1	B	478	ASP	2.4
1	B	65	ILE	2.3
1	A	242	HIS	2.3
1	B	185	ILE	2.3
1	B	102	LYS	2.3
1	A	192	ALA	2.3
1	A	55	PHE	2.3
1	A	333	MET	2.3
1	B	103	LEU	2.3
1	A	258	SER	2.3
1	B	273	MET	2.3
1	B	410	GLY	2.3
1	B	430	ILE	2.3
1	B	59	PHE	2.3
1	A	467	ILE	2.2
1	A	142	VAL	2.2
1	B	298	VAL	2.2
1	B	199	PHE	2.2
1	B	453	ILE	2.2
1	B	268	VAL	2.2
1	A	27	GLY	2.1
1	A	146	SER	2.1
1	B	439	LEU	2.1
1	B	41	SER	2.1
1	A	36	LEU	2.1
1	B	363	ILE	2.1
1	B	153	GLN	2.1
1	B	139	ALA	2.1
1	B	160	VAL	2.1
1	A	70	PRO	2.1
1	A	158	SER	2.1
1	B	281	ASP	2.1
1	B	104	PHE	2.0
1	A	257	ARG	2.0
1	A	42	THR	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

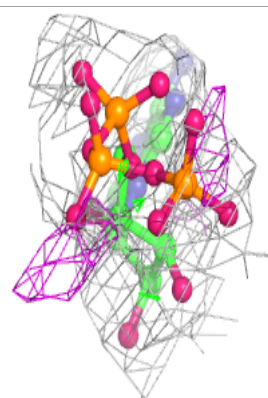
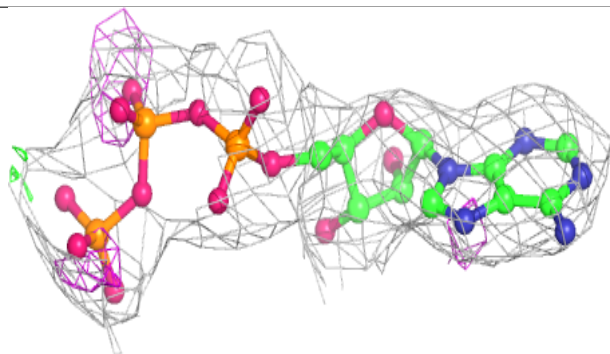
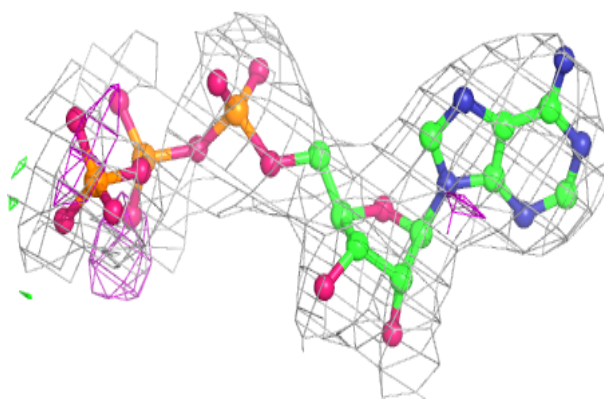
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	604	1/1	0.92	0.12	47,47,47,47	0
3	MG	B	603	1/1	0.92	0.11	45,45,45,45	0
2	ATP	A	602	31/31	0.93	0.18	49,52,66,67	0
2	ATP	B	601	31/31	0.93	0.19	70,76,84,85	0
2	ATP	B	602	31/31	0.94	0.18	53,55,64,65	0
2	ATP	A	601	31/31	0.95	0.18	58,71,83,87	0
3	MG	A	603	1/1	0.98	0.09	36,36,36,36	0
3	MG	B	604	1/1	0.98	0.12	35,35,35,35	0

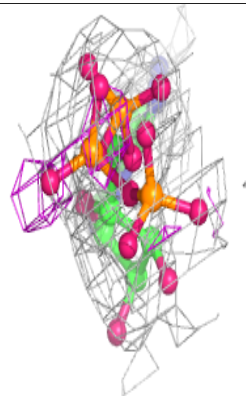
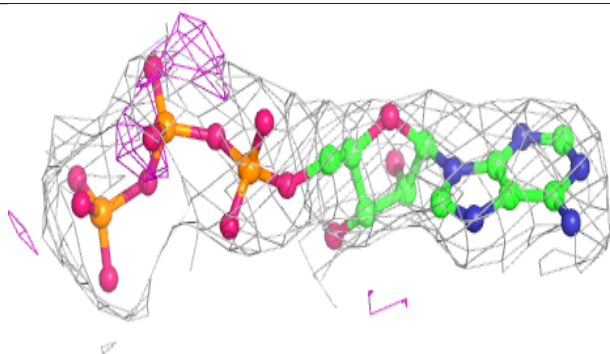
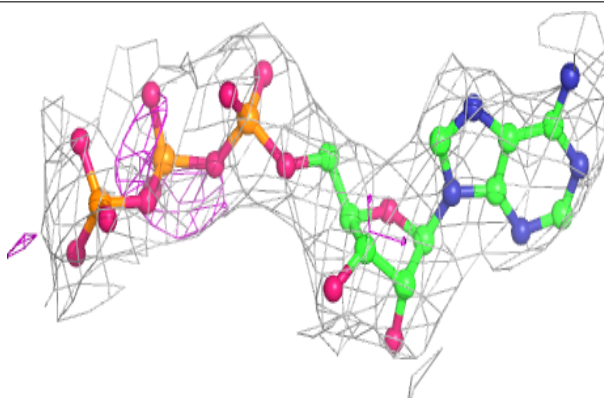
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 602:

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

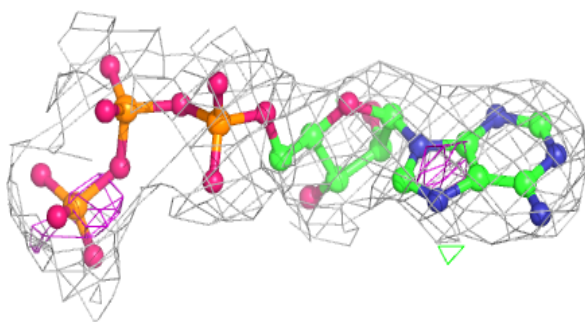
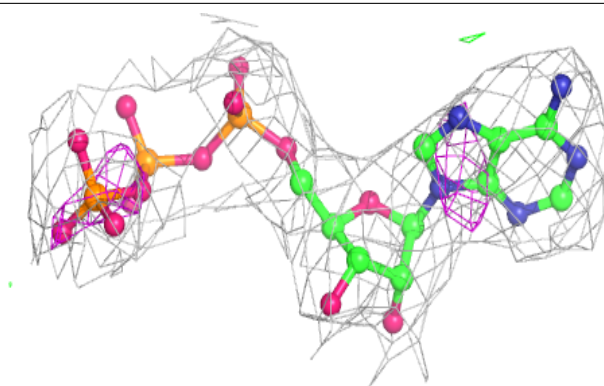
**Electron density around ATP B 601:**

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

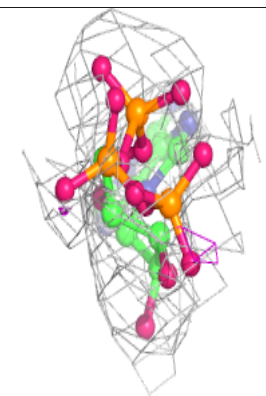
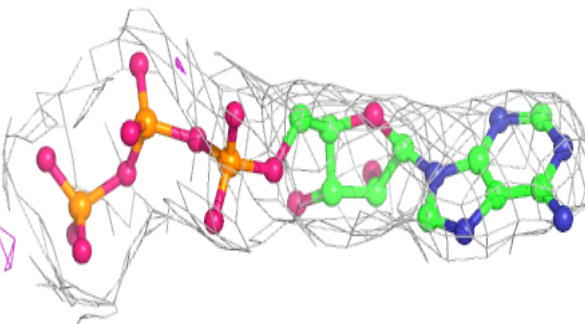
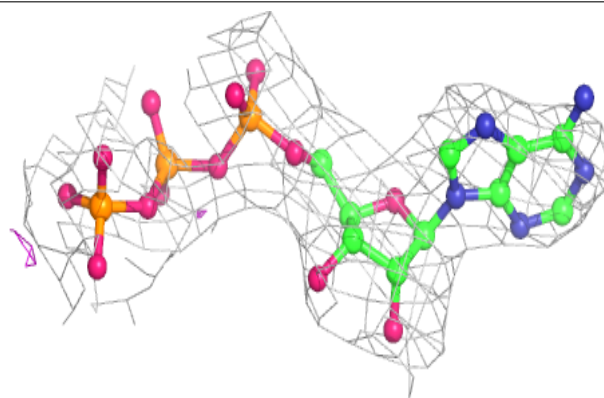


Electron density around ATP B 602:

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

**Electron density around ATP A 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.