



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:52 AM UTC

PDB ID : 8WV8 / pdb_00008wv8
Title : Crystal Structure of Cyanobacterial Circadian Clock Protein KaiC
Authors : Furuike, Y.; Akiyama, S.
Deposited on : 2023-10-23
Resolution : 2.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

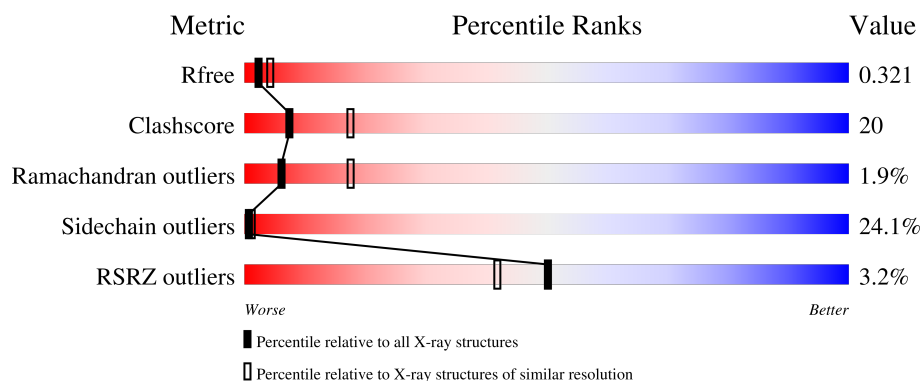
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	
1	B	519	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6654 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

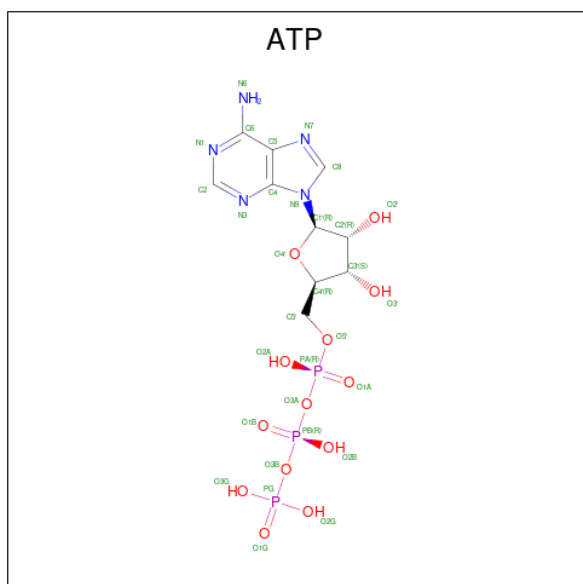
- Molecule 1 is a protein called Circadian clock oscillator protein KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3272	2070	572	616	14			
1	B	455	Total	C	N	O	S	0	0	0
			3238	2042	569	612	15			

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



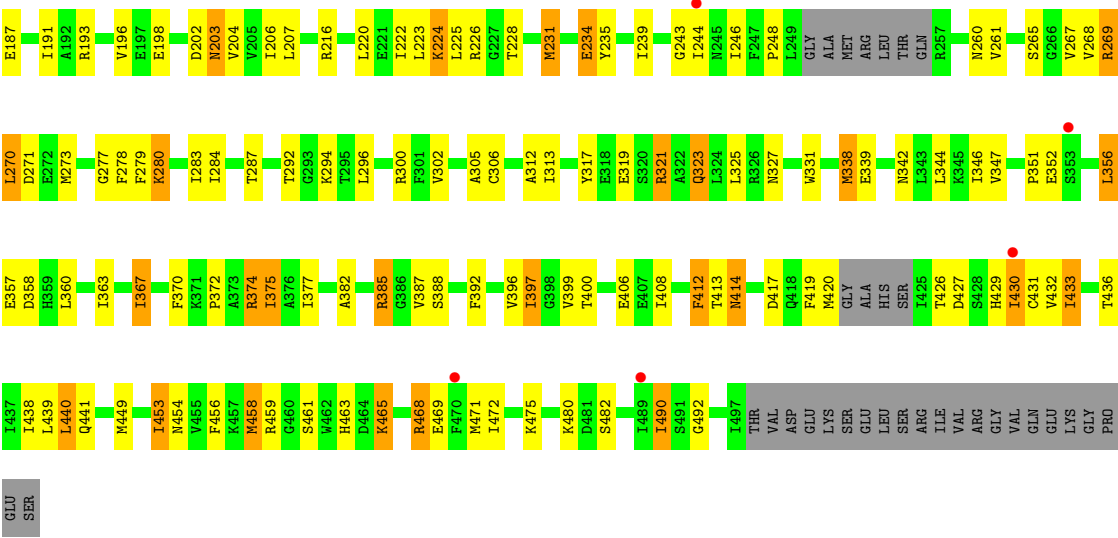
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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	9	Total	O	0	0
			9	9		



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	95.19Å 95.19Å 184.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.22 – 2.93 49.22 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.22-2.93) 99.8 (49.22-2.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.276 , 0.335 0.275 , 0.321	Depositor DCC
R_{free} test set	939 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 85.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6654	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.86 % 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 8.1009e-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: 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	1.05	0/3322	1.48	0/4508
1	B	1.05	0/3286	1.49	0/4460
All	All	1.05	0/6608	1.48	0/8968

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	3272	0	2988	135	1
1	B	3238	0	2949	134	1
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	7	0	0	0	0
4	B	9	0	0	0	0
All	All	6654	0	5985	258	1

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 20.

All (258) 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:313:ILE:CG1	1:A:372:PRO:HG2	1.75	1.16
1:A:356:LEU:CD2	1:A:387:VAL:HG11	1.82	1.08
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.39	1.02
1:B:356:LEU:CD2	1:B:387:VAL:HG11	1.96	0.95
1:A:313:ILE:HG13	1:A:372:PRO:HG2	1.43	0.94
1:A:313:ILE:HG12	1:A:372:PRO:HG2	1.50	0.89
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.54	0.88
1:B:25:ILE:HD13	1:B:58:GLN:HE21	1.39	0.85
1:B:25:ILE:HD13	1:B:58:GLN:NE2	1.94	0.83
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.60	0.82
1:B:134:ILE:HA	1:B:139:ALA:CB	2.12	0.79
1:B:134:ILE:HA	1:B:139:ALA:HB2	1.64	0.78
1:A:25:ILE:HG23	1:A:244:ILE:CG2	2.16	0.76
1:A:167:LEU:HD12	1:A:171:LEU:HD12	1.69	0.74
1:A:445:ILE:HD13	1:A:494:PRO:HG3	1.69	0.74
1:B:203:ASN:HB3	1:B:225:LEU:CD2	2.17	0.74
1:B:420:MET:HA	1:B:441:GLN:HE22	1.53	0.74
1:A:356:LEU:HD22	1:A:387:VAL:CG1	2.17	0.74
1:B:170:ARG:O	1:B:174:ILE:HD12	1.87	0.74
1:B:287:THR:HG22	1:B:414:ASN:ND2	2.04	0.73
1:B:420:MET:HA	1:B:441:GLN:NE2	2.04	0.73
1:A:22:ARG:O	1:A:141:ARG:NH2	2.22	0.72
1:A:60:LEU:HD12	1:A:141:ARG:HB2	1.70	0.72
1:A:48:SER:OG	1:B:224:LYS:NZ	2.22	0.72
1:A:37:PRO:CD	1:A:225:LEU:HD22	2.22	0.70
1:B:191:ILE:HG21	1:B:198:GLU:HB3	1.73	0.70
1:A:169:ALA:O	1:A:173:GLN:HG3	1.92	0.70
1:A:25:ILE:CG2	1:A:244:ILE:HG21	2.21	0.69
1:B:356:LEU:HD21	1:B:387:VAL:HG11	1.74	0.69
1:A:71:GLY:HA2	1:A:141:ARG:O	1.93	0.69
1:B:305:ALA:HB2	1:B:374:ARG:HD3	1.76	0.68
1:B:338:MET:HB3	1:B:344:LEU:HB3	1.74	0.68
1:B:287:THR:HG22	1:B:414:ASN:HD22	1.57	0.68
1:A:420:MET:HG2	1:A:492:GLY:HA2	1.75	0.67
1:A:432:VAL:O	1:A:459:ARG:NH2	2.26	0.67
1:A:225:LEU:HB3	1:A:228:THR:CG2	2.25	0.67
2:A:601:ATP:O3G	1:B:224:LYS:NZ	2.23	0.67
1:A:296:LEU:HD23	1:A:472:ILE:HD12	1.76	0.66
1:A:25:ILE:HG23	1:A:244:ILE:HG21	1.74	0.66
1:A:89:SER:CB	2:A:601:ATP:HN61	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PRO:HD3	1:A:225:LEU:HD22	1.78	0.66
1:A:225:LEU:HB3	1:A:228:THR:HG23	1.77	0.65
1:A:265:SER:HB3	1:A:278:PHE:CE2	2.31	0.65
1:A:382:ALA:HA	1:A:385:ARG:HD3	1.80	0.64
1:B:278:PHE:CZ	1:B:284:ILE:HG21	2.32	0.64
1:B:62:ASN:O	1:B:66:GLU:HB2	1.99	0.63
1:A:269:ARG:O	1:A:273:MET:HG3	1.98	0.62
1:B:283:ILE:HG13	1:B:400:THR:HG23	1.81	0.62
1:B:148:THR:OG1	1:B:182:THR:HG23	1.99	0.62
1:A:458:MET:HG3	1:A:463:HIS:HB3	1.82	0.62
1:B:225:LEU:HB3	1:B:228:THR:HG23	1.80	0.62
1:B:356:LEU:HD22	1:B:387:VAL:CG1	2.29	0.61
1:A:70:PRO:HG2	1:A:138:ARG:O	2.00	0.61
1:A:321:ARG:O	1:A:325:LEU:HG	2.01	0.60
1:A:160:VAL:HG21	1:A:194:TYR:CD2	2.36	0.60
1:A:371:LYS:N	1:A:372:PRO:CD	2.65	0.60
1:B:317:TYR:HB3	1:B:351:PRO:HG3	1.84	0.60
1:A:37:PRO:CG	1:A:225:LEU:HD22	2.33	0.59
1:B:203:ASN:CB	1:B:225:LEU:HD23	2.29	0.59
1:A:367:ILE:HD13	1:A:372:PRO:HD2	1.84	0.58
1:A:37:PRO:CD	1:A:225:LEU:CD2	2.80	0.58
1:A:156:ALA:O	1:A:158:SER:N	2.37	0.58
1:A:420:MET:HG2	1:A:492:GLY:CA	2.34	0.57
1:A:25:ILE:HD13	1:A:58:GLN:NE2	2.19	0.57
1:A:296:LEU:HD23	1:A:472:ILE:CD1	2.34	0.57
1:A:60:LEU:CD1	1:A:141:ARG:HB2	2.35	0.57
1:A:70:PRO:CG	1:A:138:ARG:O	2.52	0.57
1:A:420:MET:SD	1:A:449:MET:HE1	2.45	0.57
1:A:290:THR:HG22	1:B:456:PHE:HE2	1.70	0.56
1:A:370:PHE:C	1:A:372:PRO:HD3	2.30	0.56
1:B:313:ILE:HG13	1:B:372:PRO:HG3	1.86	0.56
1:B:225:LEU:HB3	1:B:228:THR:CG2	2.35	0.56
1:A:24:MET:HB2	1:A:62:ASN:HB3	1.86	0.56
1:A:454:ASN:HB2	1:A:467:ILE:HA	1.88	0.56
1:B:28:PHE:HB2	1:B:246:ILE:HD12	1.87	0.55
1:A:296:LEU:CD2	1:A:472:ILE:HD12	2.36	0.55
1:B:41:SER:CB	1:B:168:VAL:CG1	2.85	0.55
1:A:312:ALA:HA	1:A:374:ARG:O	2.06	0.55
1:B:63:GLY:HA3	1:B:141:ARG:NE	2.22	0.54
1:A:142:VAL:O	1:A:178:THR:HA	2.07	0.54
1:A:86:ASN:OD1	1:B:40:ARG:NH1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ARG:HA	1:B:482:SER:HA	1.89	0.54
1:A:283:ILE:HG13	1:A:400:THR:HG23	1.90	0.54
1:A:458:MET:HB2	1:A:463:HIS:CD2	2.43	0.54
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.43	0.54
1:B:27:GLY:HA2	1:B:248:PRO:HD3	1.89	0.54
1:B:170:ARG:O	1:B:174:ILE:CD1	2.54	0.54
1:A:321:ARG:HH11	1:A:321:ARG:HB3	1.73	0.54
1:B:261:VAL:HG13	1:B:280:LYS:CB	2.38	0.54
1:A:419:PHE:HZ	1:B:490:ILE:CD1	2.21	0.53
1:B:202:ASP:HA	1:B:226:ARG:NH2	2.23	0.53
1:A:397:ILE:HD13	1:A:433:ILE:HD13	1.90	0.53
1:B:271:ASP:HA	1:B:277:GLY:HA2	1.90	0.53
1:A:371:LYS:N	1:A:372:PRO:HD3	2.23	0.53
1:A:419:PHE:CZ	1:B:490:ILE:CD1	2.91	0.53
1:A:37:PRO:HD3	1:A:225:LEU:CD2	2.39	0.53
1:B:436:THR:OG1	1:B:458:MET:HE3	2.09	0.53
1:B:24:MET:HB2	1:B:62:ASN:HB3	1.91	0.53
1:A:298:VAL:HA	1:A:411:LEU:HD23	1.90	0.52
1:A:351:PRO:HB2	1:A:382:ALA:O	2.09	0.52
1:A:211:LEU:CD1	1:A:216:ARG:HD3	2.39	0.52
1:A:279:PHE:CE2	1:A:461:SER:HB2	2.44	0.52
1:B:300:ARG:NH2	1:B:475:LYS:O	2.38	0.52
1:B:267:VAL:HB	1:B:270:LEU:HB2	1.92	0.52
1:A:167:LEU:CD1	1:A:171:LEU:HD12	2.36	0.52
1:A:171:LEU:HD22	1:A:178:THR:CB	2.40	0.52
1:A:331:TRP:O	1:A:475:LYS:HA	2.10	0.52
1:B:21:MET:SD	1:B:141:ARG:NH2	2.83	0.52
1:B:279:PHE:CE2	1:B:461:SER:HB2	2.45	0.52
1:B:147:VAL:HG21	1:B:180:MET:HG2	1.92	0.52
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.46	0.51
1:A:21:MET:CB	1:A:141:ARG:HH12	2.24	0.51
1:A:335:PHE:O	1:A:339:GLU:HG3	2.09	0.51
1:A:157:SER:O	1:A:160:VAL:HG23	2.11	0.51
1:A:370:PHE:CD2	1:A:372:PRO:HG3	2.46	0.51
1:B:306:CYS:SG	1:B:338:MET:HG2	2.50	0.51
1:B:420:MET:HE3	1:B:492:GLY:C	2.35	0.51
1:A:25:ILE:CG2	1:A:244:ILE:CG2	2.84	0.51
1:B:24:MET:HG3	1:B:66:GLU:HG2	1.92	0.51
1:B:134:ILE:HA	1:B:139:ALA:HB3	1.90	0.51
1:B:174:ILE:HD12	1:B:174:ILE:N	2.26	0.51
1:B:363:ILE:O	1:B:367:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:MET:N	1:B:465:LYS:O	2.43	0.51
1:A:384:ALA:HB2	1:A:392:PHE:CZ	2.46	0.50
1:A:382:ALA:HA	1:A:385:ARG:CD	2.41	0.50
1:B:60:LEU:HD23	1:B:141:ARG:HB3	1.93	0.50
1:B:269:ARG:O	1:B:273:MET:HG3	2.12	0.50
1:A:312:ALA:HA	1:A:372:PRO:HB3	1.93	0.50
1:B:55:PHE:HE1	1:B:179:VAL:HG21	1.77	0.49
1:B:142:VAL:O	1:B:178:THR:HA	2.12	0.49
1:A:231:MET:HB3	1:A:235:TYR:OH	2.12	0.49
1:A:321:ARG:HB3	1:A:321:ARG:NH1	2.27	0.49
1:A:486:PHE:HA	1:A:495:THR:O	2.13	0.49
1:B:37:PRO:HB2	1:B:40:ARG:HB2	1.95	0.49
1:A:24:MET:HG3	1:A:66:GLU:HG3	1.95	0.49
1:B:440:LEU:HD23	1:B:453:ILE:HG13	1.94	0.49
1:B:331:TRP:O	1:B:475:LYS:HA	2.13	0.49
1:B:41:SER:CB	1:B:168:VAL:HG13	2.43	0.49
1:B:170:ARG:O	1:B:173:GLN:HB2	2.13	0.49
1:B:279:PHE:HE2	1:B:461:SER:HB2	1.76	0.48
1:A:301:PHE:CZ	1:A:374:ARG:HD3	2.47	0.48
1:B:174:ILE:HD12	1:B:174:ILE:H	1.77	0.48
1:A:129:ARG:HH21	1:A:129:ARG:HB2	1.78	0.48
1:B:52:LYS:HB3	1:B:181:THR:HG23	1.95	0.48
1:B:72:VAL:HB	1:B:142:VAL:HG22	1.95	0.48
1:B:296:LEU:CD2	1:B:472:ILE:HG12	2.43	0.48
1:A:287:THR:HG22	1:A:439:LEU:CB	2.44	0.48
1:B:278:PHE:HZ	1:B:438:ILE:HD12	1.79	0.48
1:B:367:ILE:HD13	1:B:375:ILE:HG21	1.96	0.48
1:B:313:ILE:HG13	1:B:372:PRO:CG	2.44	0.47
1:B:207:LEU:N	1:B:207:LEU:HD23	2.28	0.47
1:B:367:ILE:HG23	1:B:372:PRO:CG	2.44	0.47
1:A:191:ILE:HG21	1:A:198:GLU:HB3	1.95	0.47
1:A:318:GLU:CD	1:B:432:VAL:HG11	2.39	0.47
1:A:164:LEU:HD12	1:A:197:GLU:HG3	1.97	0.47
1:A:270:LEU:HD11	1:A:438:ILE:CD1	2.45	0.47
1:B:321:ARG:O	1:B:325:LEU:HG	2.15	0.47
1:A:167:LEU:CD1	1:A:171:LEU:CD1	2.93	0.47
1:A:419:PHE:CZ	1:B:490:ILE:HD12	2.50	0.46
1:A:265:SER:CB	1:A:278:PHE:CE2	2.97	0.46
1:A:311:ARG:HD2	1:A:370:PHE:CE1	2.51	0.46
1:B:296:LEU:HD23	1:B:472:ILE:HG12	1.97	0.46
1:B:397:ILE:CD1	1:B:433:ILE:HD13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:THR:O	1:A:52:LYS:NZ	2.48	0.46
1:A:271:ASP:HA	1:A:277:GLY:HA2	1.97	0.46
1:A:129:ARG:HH21	1:A:129:ARG:CB	2.29	0.46
1:A:311:ARG:CB	1:A:372:PRO:HA	2.46	0.46
1:A:360:LEU:HD23	1:A:360:LEU:HA	1.83	0.46
1:B:220:LEU:C	1:B:220:LEU:HD23	2.41	0.46
1:A:245:ASN:HD22	1:A:245:ASN:HA	1.56	0.46
1:B:54:LEU:C	1:B:54:LEU:HD12	2.41	0.46
1:B:367:ILE:HG23	1:B:372:PRO:HD2	1.98	0.46
1:A:289:ALA:O	1:A:294:LYS:NZ	2.48	0.46
1:B:43:LEU:HD11	1:B:182:THR:OG1	2.16	0.46
1:B:312:ALA:HA	1:B:374:ARG:O	2.15	0.46
1:A:313:ILE:HG13	1:A:372:PRO:CG	2.28	0.46
1:A:164:LEU:CD1	1:A:197:GLU:HG3	2.46	0.45
1:B:27:GLY:CA	1:B:248:PRO:HD3	2.46	0.45
1:B:73:PHE:O	1:B:105:ILE:HA	2.16	0.45
1:B:265:SER:HB3	1:B:278:PHE:CD2	2.50	0.45
1:A:197:GLU:OE2	1:A:197:GLU:N	2.49	0.45
1:A:287:THR:HA	1:A:414:ASN:O	2.16	0.45
1:A:294:LYS:HE2	2:A:602:ATP:O1B	2.16	0.45
1:B:28:PHE:CE2	1:B:36:LEU:HD21	2.52	0.45
1:B:367:ILE:CG2	1:B:372:PRO:HD2	2.47	0.45
1:B:414:ASN:ND2	1:B:414:ASN:C	2.75	0.45
1:A:167:LEU:HD12	1:A:167:LEU:C	2.42	0.45
1:B:419:PHE:C	1:B:419:PHE:CD2	2.95	0.45
1:B:145:ASP:HA	1:B:146:SER:HA	1.68	0.44
1:B:397:ILE:CD1	1:B:433:ILE:CD1	2.95	0.44
1:B:406:GLU:HB2	1:B:408:ILE:CD1	2.47	0.44
1:A:260:ASN:HD22	1:A:279:PHE:HE1	1.66	0.44
1:B:412:PHE:N	1:B:412:PHE:CD1	2.83	0.44
1:B:317:TYR:O	1:B:351:PRO:HD3	2.17	0.44
1:B:356:LEU:CD2	1:B:387:VAL:CG1	2.82	0.44
1:A:284:ILE:HG23	1:A:436:THR:HB	2.00	0.44
1:B:30:ASP:N	1:B:30:ASP:OD1	2.50	0.44
1:A:211:LEU:HD12	1:A:216:ARG:HD3	1.99	0.44
1:B:58:GLN:OE1	1:B:243:GLY:HA3	2.17	0.43
1:A:419:PHE:CZ	1:B:490:ILE:HD11	2.53	0.43
1:B:392:PHE:O	1:B:396:VAL:HG23	2.19	0.43
1:A:211:LEU:HD13	1:A:216:ARG:HD3	2.00	0.43
1:A:203:ASN:HB3	1:A:225:LEU:HD23	2.00	0.43
1:B:206:ILE:HD11	1:B:223:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:CD1	1:A:67:PHE:N	2.84	0.43
1:A:311:ARG:HB3	1:A:372:PRO:HA	2.01	0.43
1:A:439:LEU:C	1:A:439:LEU:HD12	2.44	0.43
1:B:148:THR:OG1	1:B:182:THR:CG2	2.65	0.43
1:A:220:LEU:HB2	1:A:237:PHE:CD2	2.54	0.43
1:A:267:VAL:HB	1:A:270:LEU:HB2	2.01	0.43
1:B:363:ILE:O	1:B:367:ILE:CG1	2.67	0.43
1:A:220:LEU:O	1:A:234:GLU:HA	2.19	0.42
1:B:356:LEU:HD12	1:B:356:LEU:HA	1.82	0.42
1:A:203:ASN:HB3	1:A:225:LEU:CD2	2.49	0.42
1:A:436:THR:OG1	1:A:458:MET:HE3	2.19	0.42
1:B:468:ARG:NH1	1:B:480:LYS:O	2.52	0.42
1:A:214:GLU:HB3	1:B:234:GLU:HG3	2.02	0.42
1:A:287:THR:O	1:A:439:LEU:HA	2.20	0.42
1:A:367:ILE:HD13	1:A:367:ILE:HA	1.84	0.42
1:A:412:PHE:N	1:A:412:PHE:CD1	2.87	0.42
1:A:370:PHE:CB	1:A:372:PRO:HD3	2.50	0.42
1:A:362:ILE:N	1:A:362:ILE:HD12	2.34	0.42
1:B:37:PRO:CG	1:B:225:LEU:HD22	2.50	0.42
1:B:397:ILE:HD13	1:B:397:ILE:HA	1.87	0.42
1:B:278:PHE:CZ	1:B:438:ILE:HD12	2.55	0.41
1:A:54:LEU:O	1:A:58:GLN:HB2	2.19	0.41
1:A:406:GLU:HB2	1:A:408:ILE:CD1	2.50	0.41
1:B:55:PHE:CD1	1:B:55:PHE:C	2.97	0.41
1:B:278:PHE:CD2	1:B:284:ILE:HD13	2.55	0.41
1:B:54:LEU:CD2	1:B:90:PHE:CZ	3.03	0.41
1:B:278:PHE:CE1	1:B:284:ILE:HG21	2.56	0.41
1:B:323:GLN:HG3	1:B:327:ASN:HD21	1.85	0.41
1:B:382:ALA:O	1:B:385:ARG:HG3	2.19	0.41
1:A:211:LEU:HD21	1:B:234:GLU:OE1	2.21	0.41
1:B:54:LEU:HD21	1:B:90:PHE:CZ	2.56	0.41
1:B:458:MET:HG3	1:B:463:HIS:HB3	2.01	0.41
1:A:262:ARG:NH1	1:A:274:CYS:O	2.44	0.41
1:A:70:PRO:HG3	1:A:138:ARG:O	2.21	0.41
1:B:305:ALA:CB	1:B:374:ARG:HD3	2.48	0.41
1:B:167:LEU:CD1	1:B:171:LEU:HD12	2.51	0.41
1:B:273:MET:SD	1:B:468:ARG:HD2	2.60	0.41
1:B:397:ILE:HD13	1:B:433:ILE:CD1	2.50	0.41
1:B:60:LEU:CD2	1:B:141:ARG:HB3	2.50	0.41
1:B:414:ASN:ND2	1:B:414:ASN:O	2.46	0.41
1:B:414:ASN:HD22	1:B:414:ASN:C	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.81	0.41
1:B:40:ARG:HH21	1:B:40:ARG:HG3	1.84	0.41
1:B:313:ILE:HG13	1:B:372:PRO:HB3	2.02	0.41
1:B:397:ILE:HD13	1:B:433:ILE:HD13	2.03	0.41
1:B:231:MET:HB3	1:B:235:TYR:OH	2.22	0.40
1:B:313:ILE:HD11	1:B:370:PHE:HB3	2.02	0.40
1:A:262:ARG:NH2	1:A:461:SER:OG	2.54	0.40
1:A:439:LEU:HD23	1:A:456:PHE:HB2	2.03	0.40
1:B:198:GLU:HB2	1:B:204:VAL:HG21	2.03	0.40
1:A:285:LEU:HD22	1:A:434:THR:HG21	2.03	0.40
1:A:44:VAL:HA	1:A:205:VAL:O	2.21	0.40
1:A:167:LEU:HD11	1:A:171:LEU:CD1	2.52	0.40
1:B:367:ILE:HG23	1:B:372:PRO:CD	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLY:O	1:B:193:ARG:NH2[2_655]	2.03	0.17

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%)	393 (88%)	47 (10%)	8 (2%)	6	19
1	B	447/519 (86%)	391 (88%)	47 (10%)	9 (2%)	6	17
All	All	895/1038 (86%)	784 (88%)	94 (10%)	17 (2%)	6	17

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	SER
1	A	425	ILE
1	A	138	ARG
1	A	177	THR
1	B	429	HIS
1	B	426	THR
1	B	430	ILE
1	B	196	VAL
1	B	427	ASP
1	A	196	VAL
1	B	132	TYR
1	B	280	LYS
1	B	417	ASP
1	A	139	ALA
1	A	492	GLY
1	B	134	ILE
1	A	494	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/444 (67%)	225 (75%)	74 (25%)	1	1
1	B	295/444 (66%)	226 (77%)	69 (23%)	1	1
All	All	594/888 (67%)	451 (76%)	143 (24%)	1	1

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	36	LEU
1	A	48	SER
1	A	58	GLN
1	A	60	LEU
1	A	65	ILE
1	A	67	PHE

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Mol	Chain	Res	Type
1	A	81	GLN
1	A	129	ARG
1	A	141	ARG
1	A	144	ILE
1	A	147	VAL
1	A	151	PHE
1	A	159	VAL
1	A	160	VAL
1	A	164	LEU
1	A	167	LEU
1	A	171	LEU
1	A	174	ILE
1	A	179	VAL
1	A	180	MET
1	A	182	THR
1	A	186	GLU
1	A	187	GLU
1	A	203	ASN
1	A	207	LEU
1	A	216	ARG
1	A	218	ARG
1	A	222	ILE
1	A	231	MET
1	A	234	GLU
1	A	245	ASN
1	A	258	SER
1	A	260	ASN
1	A	267	VAL
1	A	269	ARG
1	A	284	ILE
1	A	287	THR
1	A	290	THR
1	A	292	THR
1	A	294	LYS
1	A	300	ARG
1	A	302	VAL
1	A	313	ILE
1	A	319	GLU
1	A	321	ARG
1	A	342	ASN
1	A	346	ILE
1	A	352	GLU

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Mol	Chain	Res	Type
1	A	356	LEU
1	A	360	LEU
1	A	367	ILE
1	A	372	PRO
1	A	375	ILE
1	A	385	ARG
1	A	388	SER
1	A	399	VAL
1	A	409	THR
1	A	413	THR
1	A	420	MET
1	A	431	CYS
1	A	433	ILE
1	A	434	THR
1	A	438	ILE
1	A	440	LEU
1	A	443	VAL
1	A	453	ILE
1	A	454	ASN
1	A	458	MET
1	A	465	LYS
1	A	469	GLU
1	A	471	MET
1	A	472	ILE
1	A	490	ILE
1	B	25	ILE
1	B	30	ASP
1	B	42	THR
1	B	43	LEU
1	B	48	SER
1	B	54	LEU
1	B	75	THR
1	B	83	ILE
1	B	144	ILE
1	B	147	VAL
1	B	168	VAL
1	B	171	LEU
1	B	179	VAL
1	B	180	MET
1	B	187	GLU
1	B	203	ASN
1	B	216	ARG

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Mol	Chain	Res	Type
1	B	222	ILE
1	B	224	LYS
1	B	231	MET
1	B	234	GLU
1	B	239	ILE
1	B	244	ILE
1	B	260	ASN
1	B	268	VAL
1	B	269	ARG
1	B	270	LEU
1	B	292	THR
1	B	294	LYS
1	B	302	VAL
1	B	319	GLU
1	B	321	ARG
1	B	323	GLN
1	B	338	MET
1	B	339	GLU
1	B	342	ASN
1	B	346	ILE
1	B	347	VAL
1	B	352	GLU
1	B	356	LEU
1	B	357	GLU
1	B	358	ASP
1	B	360	LEU
1	B	367	ILE
1	B	374	ARG
1	B	375	ILE
1	B	377	ILE
1	B	385	ARG
1	B	388	SER
1	B	397	ILE
1	B	399	VAL
1	B	412	PHE
1	B	413	THR
1	B	414	ASN
1	B	430	ILE
1	B	431	CYS
1	B	433	ILE
1	B	439	LEU
1	B	440	LEU

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Mol	Chain	Res	Type
1	B	449	MET
1	B	453	ILE
1	B	454	ASN
1	B	458	MET
1	B	459	ARG
1	B	465	LYS
1	B	468	ARG
1	B	469	GLU
1	B	471	MET
1	B	490	ILE

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	260	ASN
1	A	304	ASN
1	A	361	GLN
1	B	414	ASN
1	B	441	GLN
1	B	454	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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	B	602	3	32,33,33	0.51	0	48,52,52	0.59	0
2	ATP	B	601	3	32,33,33	0.63	0	48,52,52	0.87	2 (4%)
2	ATP	A	602	3	32,33,33	0.57	0	48,52,52	1.03	2 (4%)
2	ATP	A	601	3	32,33,33	0.53	0	48,52,52	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	602	3	-	0/22/38/38	0/3/3/3
2	ATP	B	601	3	-	7/22/38/38	0/3/3/3
2	ATP	A	602	3	-	9/22/38/38	0/3/3/3
2	ATP	A	601	3	-	6/22/38/38	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	602	ATP	O4'-C1'-N9	3.81	115.41	108.09
2	B	601	ATP	C1'-N9-C8	2.52	132.69	127.09
2	A	602	ATP	O4'-C4'-C5'	-2.42	101.57	109.33
2	B	601	ATP	C4-N9-C1'	-2.30	121.25	126.63

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O1A
2	A	601	ATP	C5'-O5'-PA-O3A
2	A	602	ATP	C5'-O5'-PA-O1A

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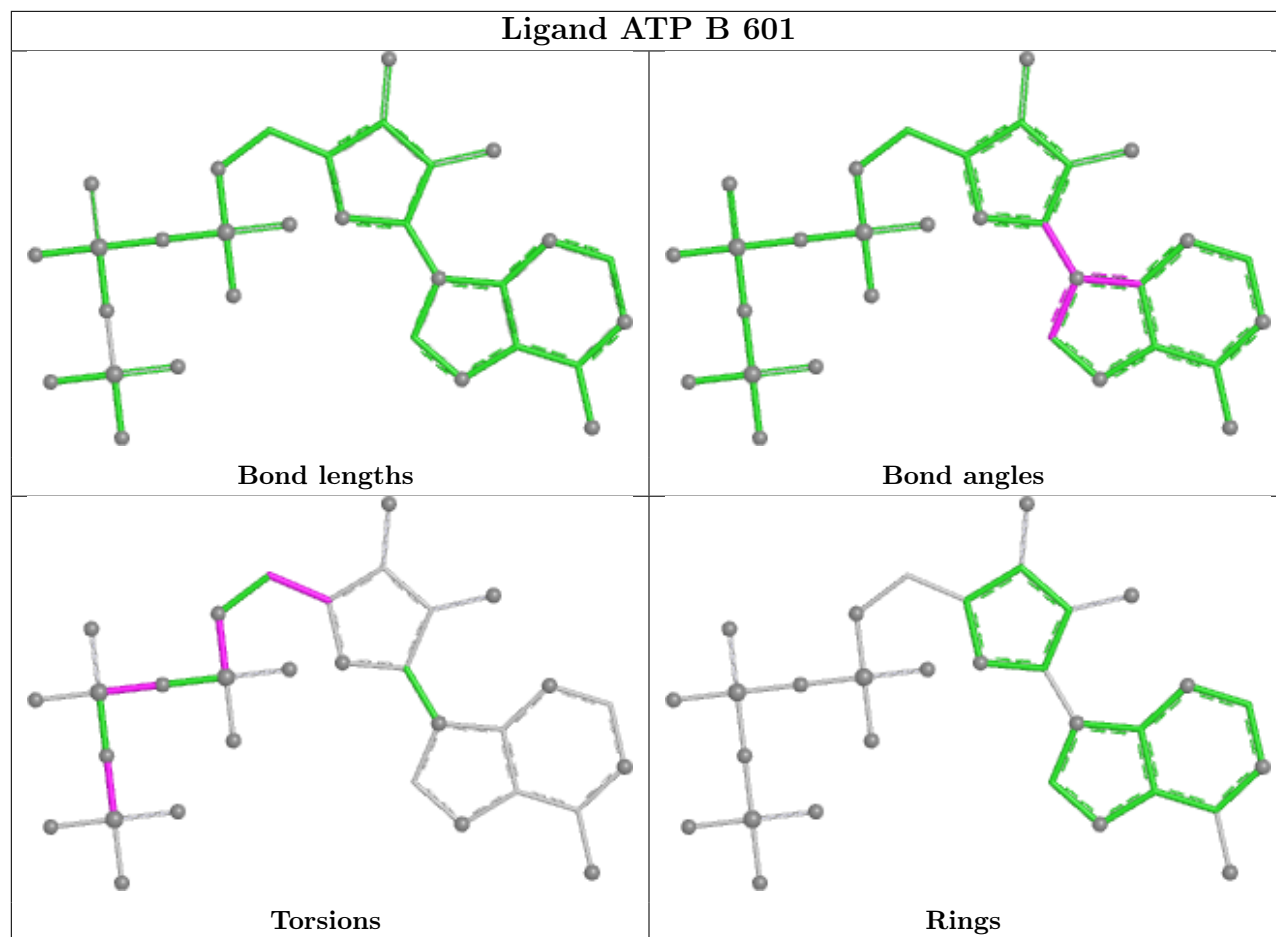
Mol	Chain	Res	Type	Atoms
2	A	602	ATP	C5'-O5'-PA-O3A
2	B	601	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	C5'-O5'-PA-O2A
2	B	601	ATP	C5'-O5'-PA-O3A
2	A	601	ATP	C3'-C4'-C5'-O5'
2	A	602	ATP	C3'-C4'-C5'-O5'
2	A	602	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	C3'-C4'-C5'-O5'
2	A	601	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	O4'-C4'-C5'-O5'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

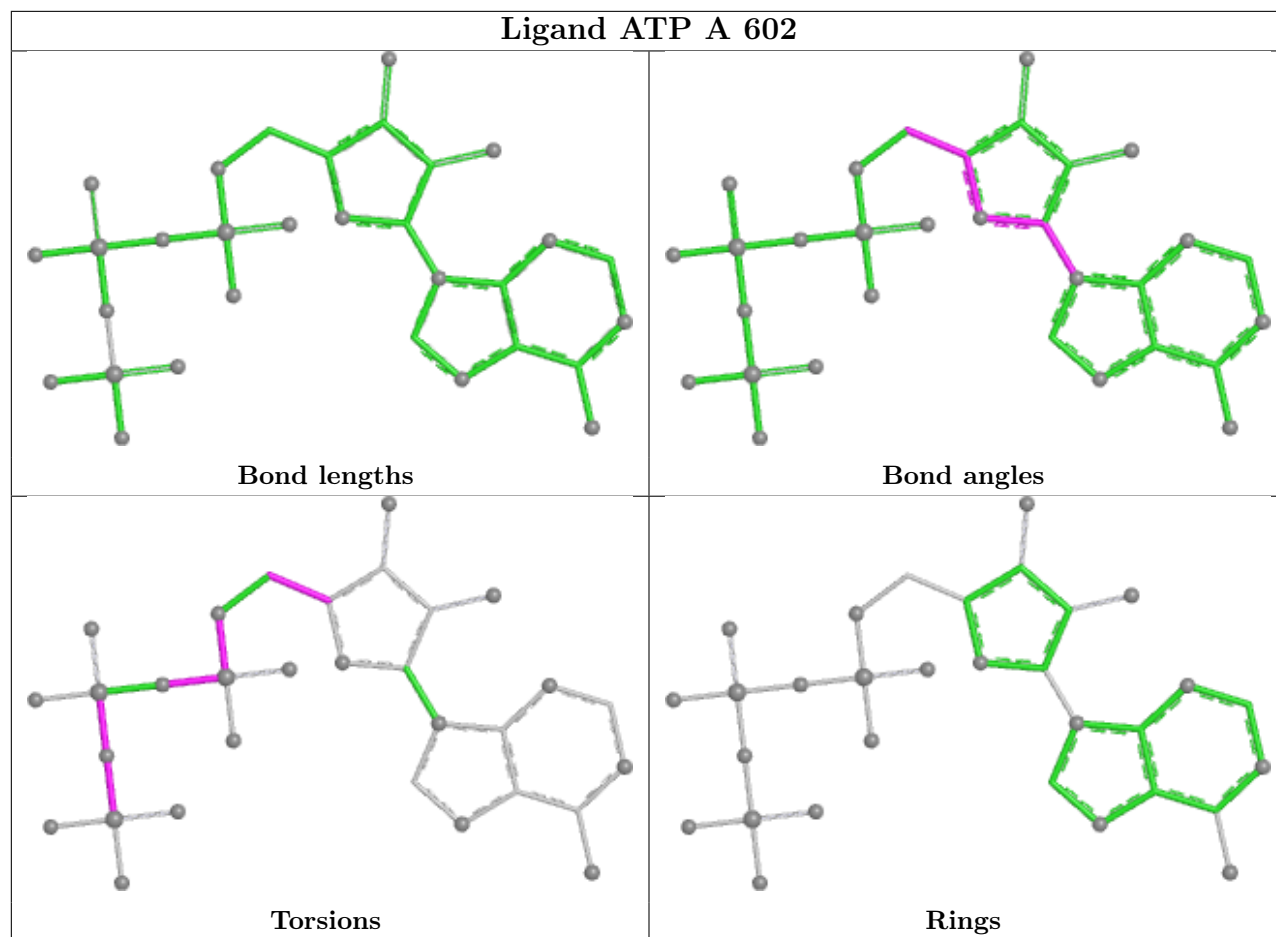
There are no ring outliers.

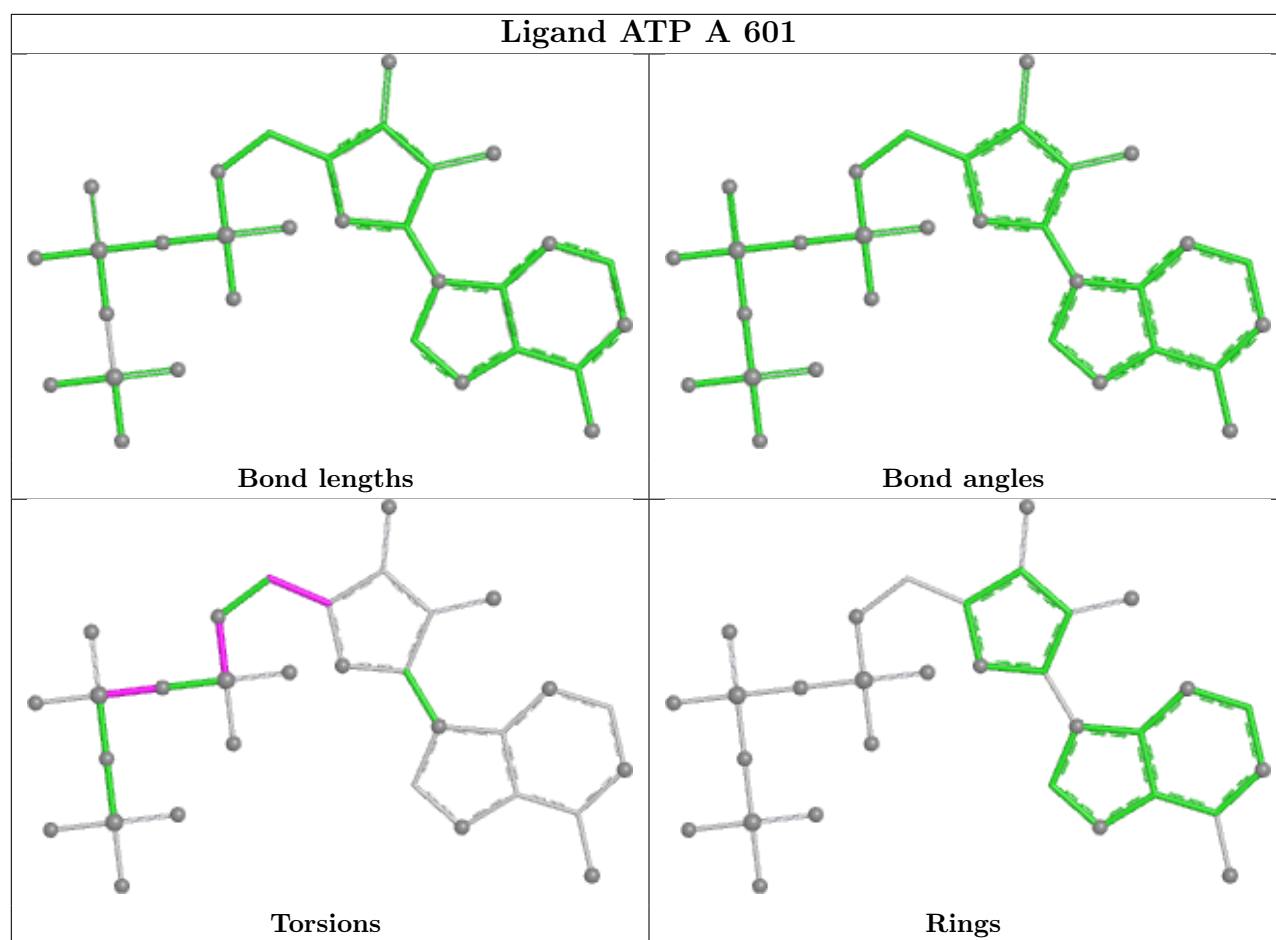
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	ATP	1	0
2	A	601	ATP	2	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	456/519 (87%)	0.49	15 (3%)	49	41	55, 80, 118, 143	0
1	B	455/519 (87%)	0.47	14 (3%)	51	43	53, 80, 124, 148	0
All	All	911/1038 (87%)	0.48	29 (3%)	50	42	53, 80, 122, 148	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	PRO	4.0
1	A	41	SER	3.2
1	B	57	ILE	3.0
1	B	137	TYR	2.9
1	B	353	SER	2.8
1	A	139	ALA	2.8
1	B	34	GLY	2.6
1	A	430	ILE	2.5
1	A	61	TYR	2.5
1	B	69	GLU	2.5
1	B	35	GLY	2.4
1	A	157	SER	2.4
1	A	428	SER	2.4
1	A	35	GLY	2.4
1	B	36	LEU	2.3
1	B	139	ALA	2.3
1	A	373	ALA	2.3
1	A	37	PRO	2.3
1	A	36	LEU	2.2
1	A	154	TYR	2.2
1	B	489	ILE	2.1
1	A	94	LEU	2.1
1	B	430	ILE	2.1
1	B	470	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	281	ASP	2.1
1	B	156	ALA	2.1
1	B	244	ILE	2.1
1	A	69	GLU	2.1
1	B	41	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

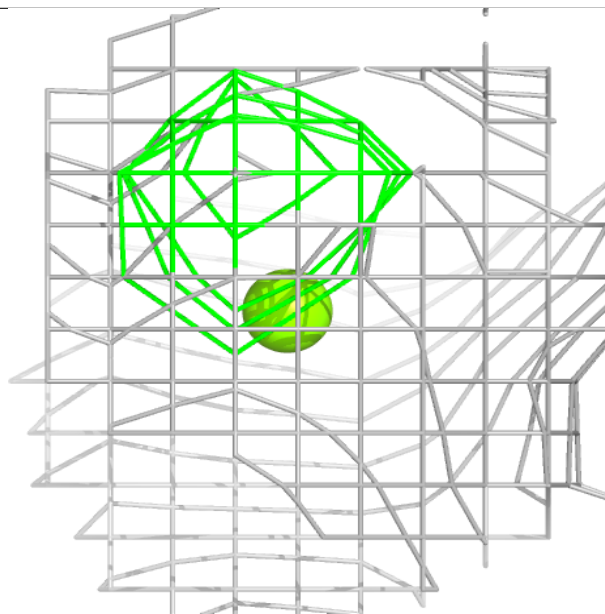
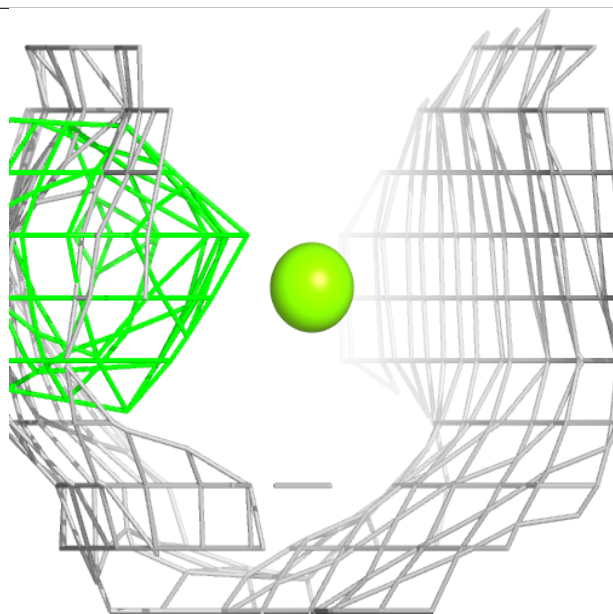
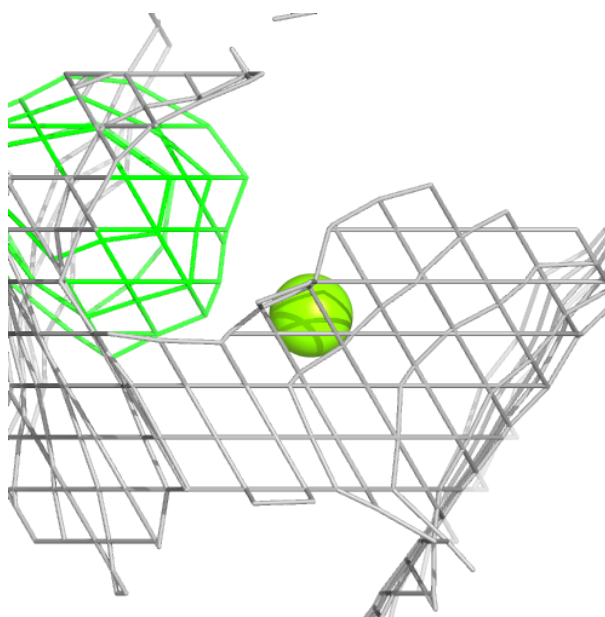
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	603	1/1	0.85	0.12	55,55,55,55	0
3	MG	B	603	1/1	0.88	0.08	52,52,52,52	0
2	ATP	B	601	31/31	0.89	0.09	78,85,89,90	0
2	ATP	A	602	31/31	0.91	0.09	49,52,67,69	0
2	ATP	A	601	31/31	0.92	0.08	80,86,88,89	0
2	ATP	B	602	31/31	0.92	0.08	55,58,68,69	0
3	MG	A	604	1/1	1.00	0.04	54,54,54,54	0
3	MG	B	604	1/1	1.00	0.04	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.

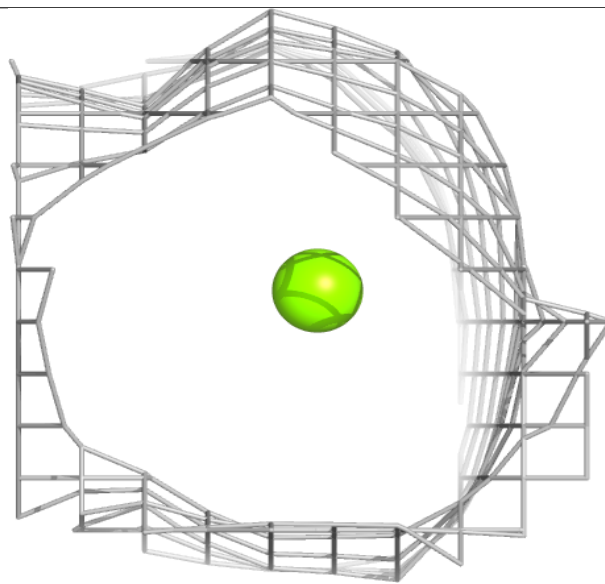
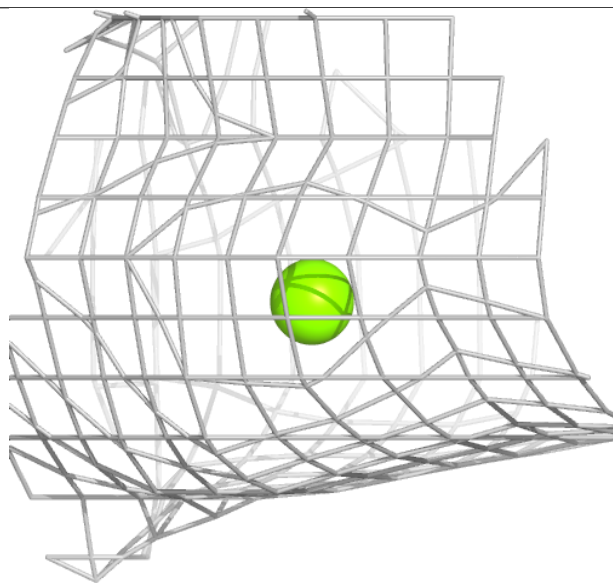
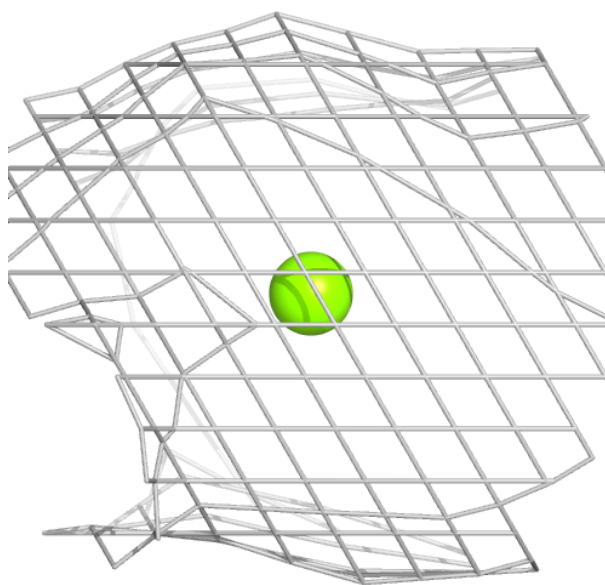
Electron density around MG A 603:

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



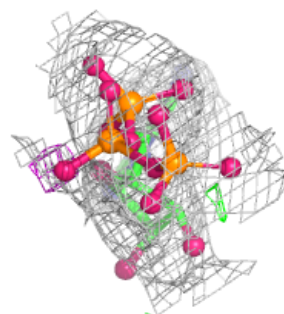
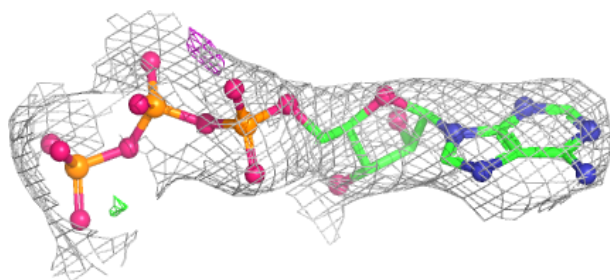
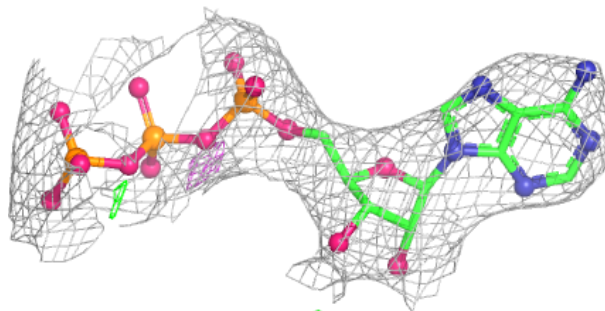
Electron density around MG B 603:

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

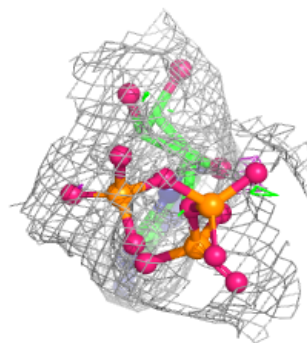
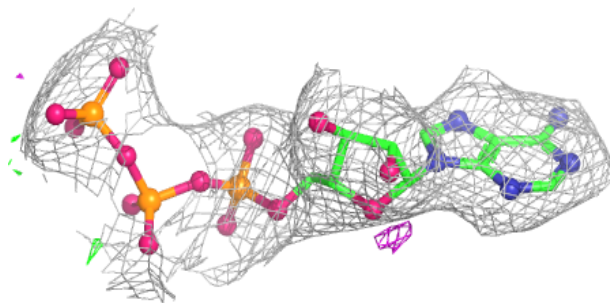
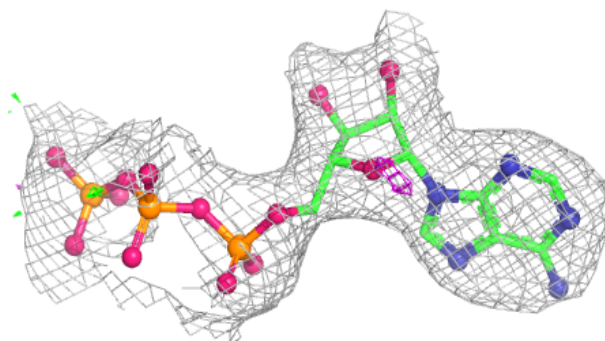


Electron density around ATP B 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

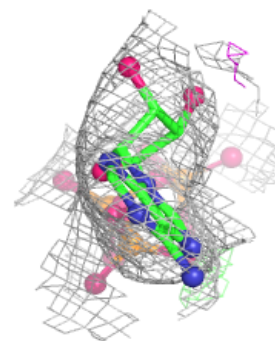
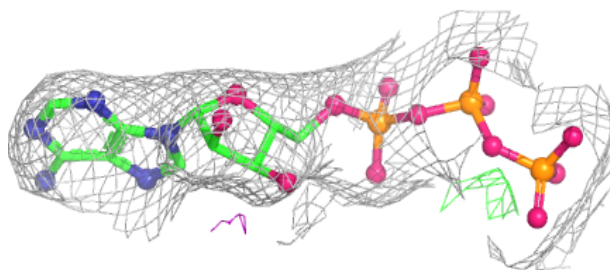
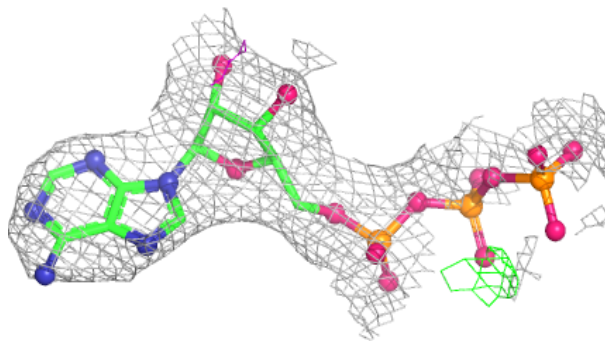
**Electron density around ATP A 602:**

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



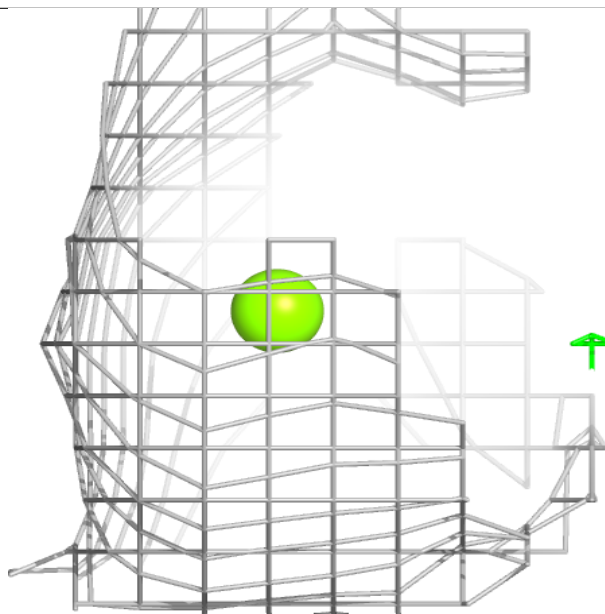
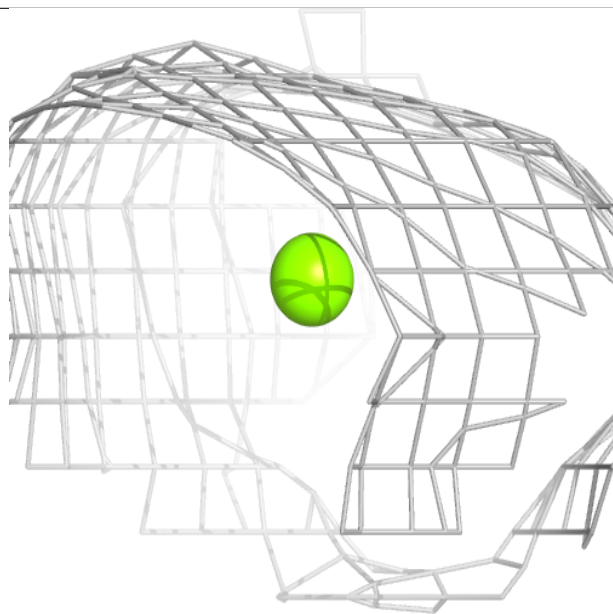
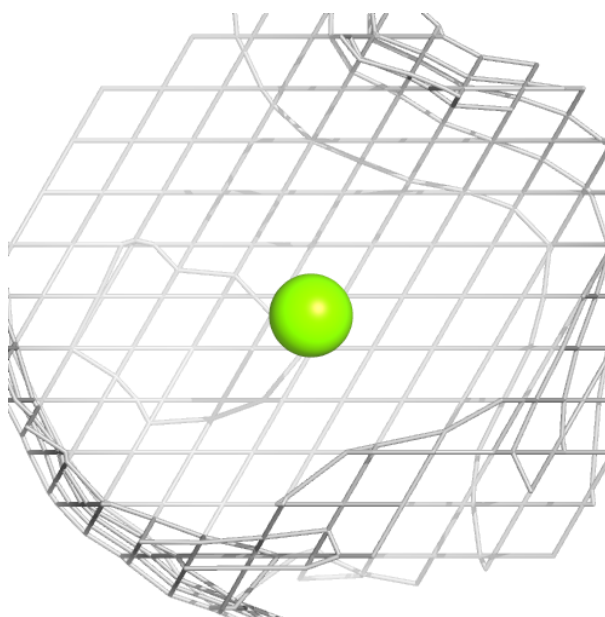
Electron density around ATP A 601:

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



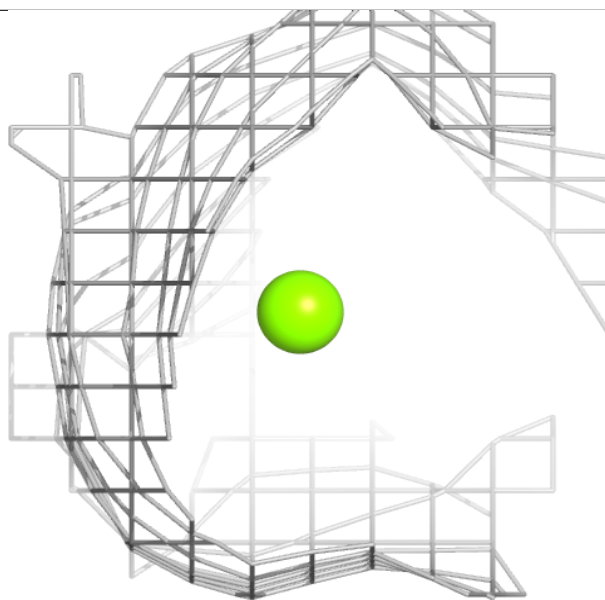
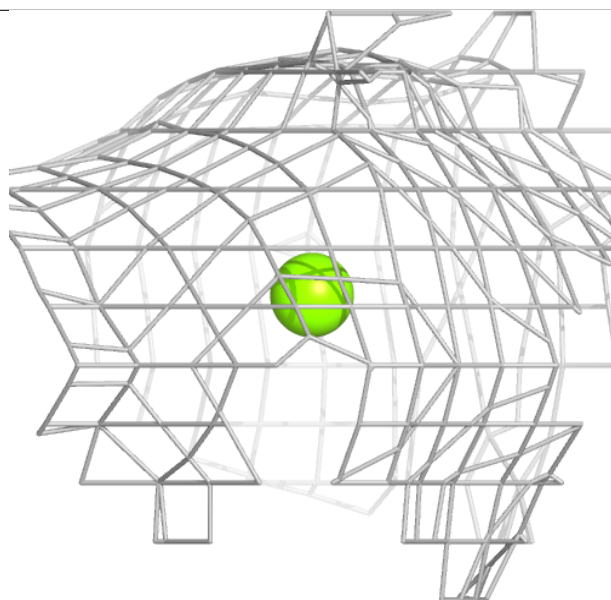
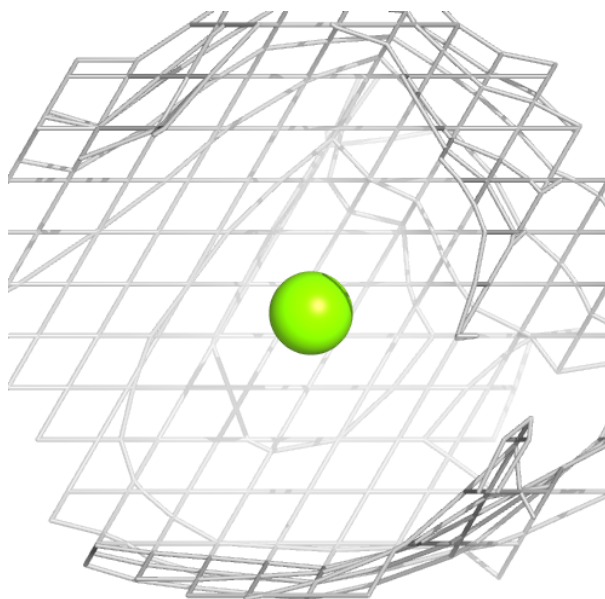
Electron density around MG A 604:

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



Electron density around MG B 604:

$2mF_o-DF_c$ (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.