



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:51 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 wwPDB X-ray Structure Validation Summary 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

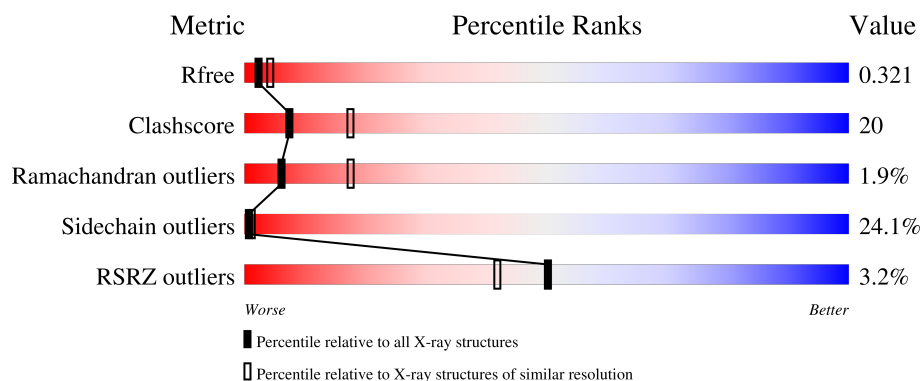
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

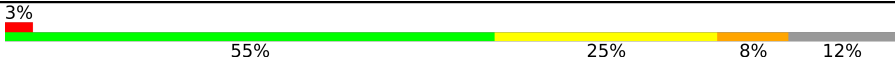
The reported resolution of this entry is 2.93 Å.

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.

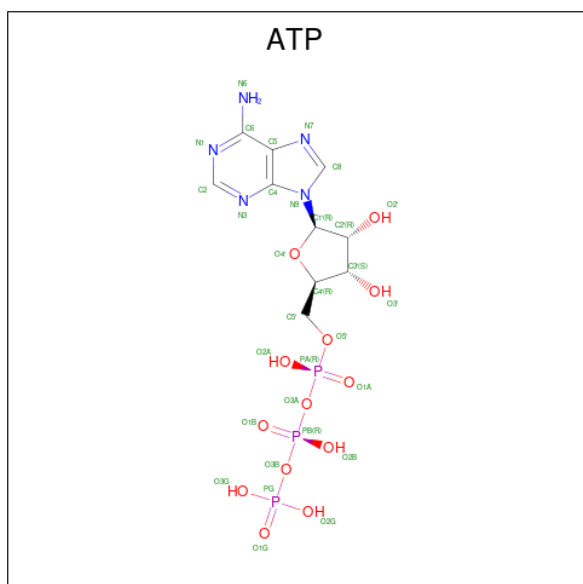
- Molecule 1 is a protein called Circadian clock oscillator protein KaiC.

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		

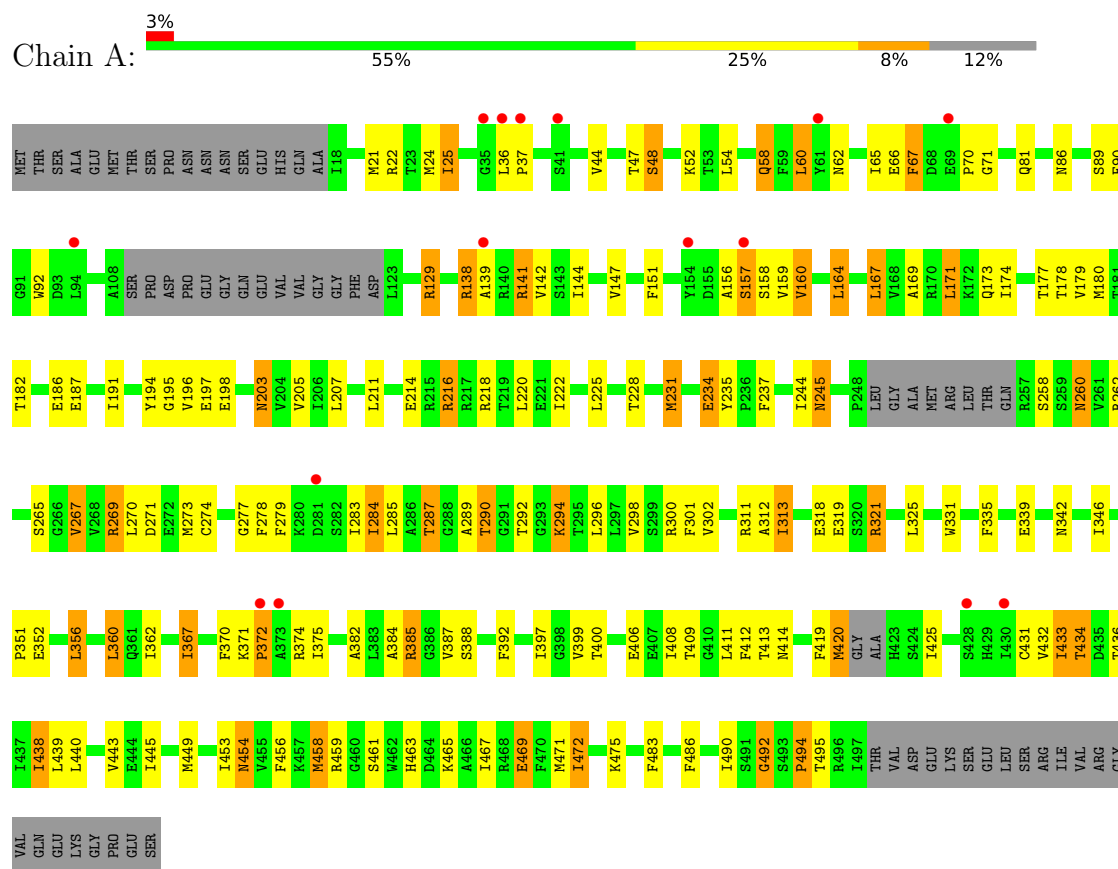
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	9	Total	O	0	0
			9	9		

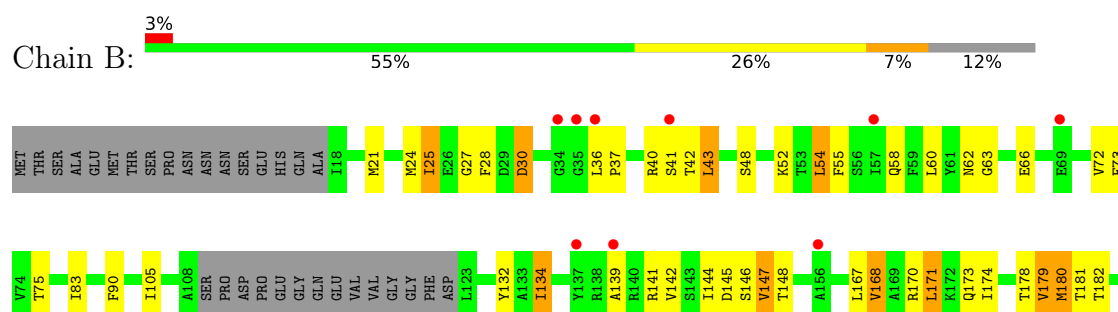
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Circadian clock oscillator protein KaiC



• Molecule 1: Circadian clock oscillator protein KaiC



GLU	E187	L270	E357	I437	GLU
SER	I191	D271	D358	I438	
	A192	E272	H559	L439	
	R193	M273	L360	L440	
			Q441		
	V196	G277	I363	M449	
	E197	F278	I367	I453	
	E198	F279	F370	N454	
		K280	K371	V455	
	D202	I283	P372	F456	
	N203	I284	A373	K457	
	V204	T287	R374	M458	
	V205		I375	R459	
	I206	T292	A376	G460	
	L207	G293	I377	S461	
		K294		V462	
	R216	T295	A382	H463	
		L296		D464	
	L220		R385	K465	
	E221	R300	G386		
	I222	F301	V387	R468	
	L223	V302	S388	E469	
	K224			F470	
	L225	A305	F392	M471	
	R226	C306		I472	
	G227		V396	K475	
	T228	A312	I397		
	M231	I313	G398	K480	
			V399	D481	
	E234	Y317	T400	S482	
	Y235	E318			
	I239	E319	E406	I489	
		S320	E407	I490	
		R321	A322	S491	
	G243	Q323	I403	G492	
	I244	L324	F412		
	R245	L325	T413		
	I246	R326	M414		
	F247	N327			
	P248		D417		
	L249		Q418		
	GLY	W331	F419		
	ALA		M420		
	MET	R338	GLY		
	ARG	E339	ALA		
	LEU		HIS		
	THR	N342	SER		
	GLN	L343	I425		
	R257	L344	T426		
		I345	D427		
	N260	V347	S428		
	V261		H429		
			I430		
	S265	P351	C431		
	G266	E352	V432		
	V267	S353	I433		
	V268				
	R269	L356			

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.

The worst 5 of 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

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

5 of 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

5.3.2 Protein sidechains [i](#)

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

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	358	ASP
1	B	375	ILE
1	B	433	ILE
1	A	352	GLU
1	A	346	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	GLN
1	B	414	ASN
1	B	454	ASN
1	B	441	GLN
1	A	304	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.

5 of 22 torsion outliers are listed below:

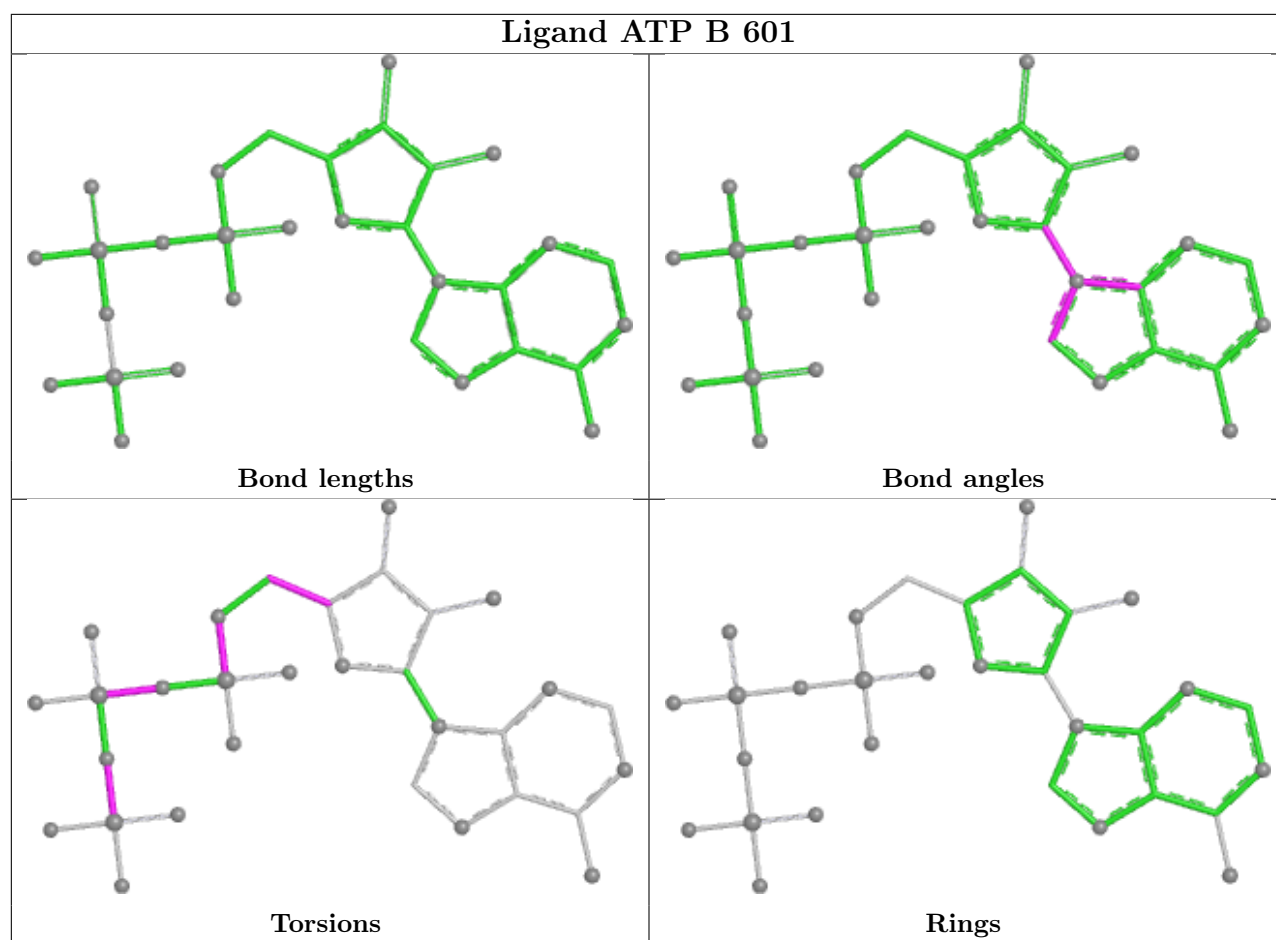
Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O1A
2	A	601	ATP	C5'-O5'-PA-O3A
2	A	602	ATP	C5'-O5'-PA-O1A
2	A	602	ATP	C5'-O5'-PA-O3A
2	B	601	ATP	C5'-O5'-PA-O1A

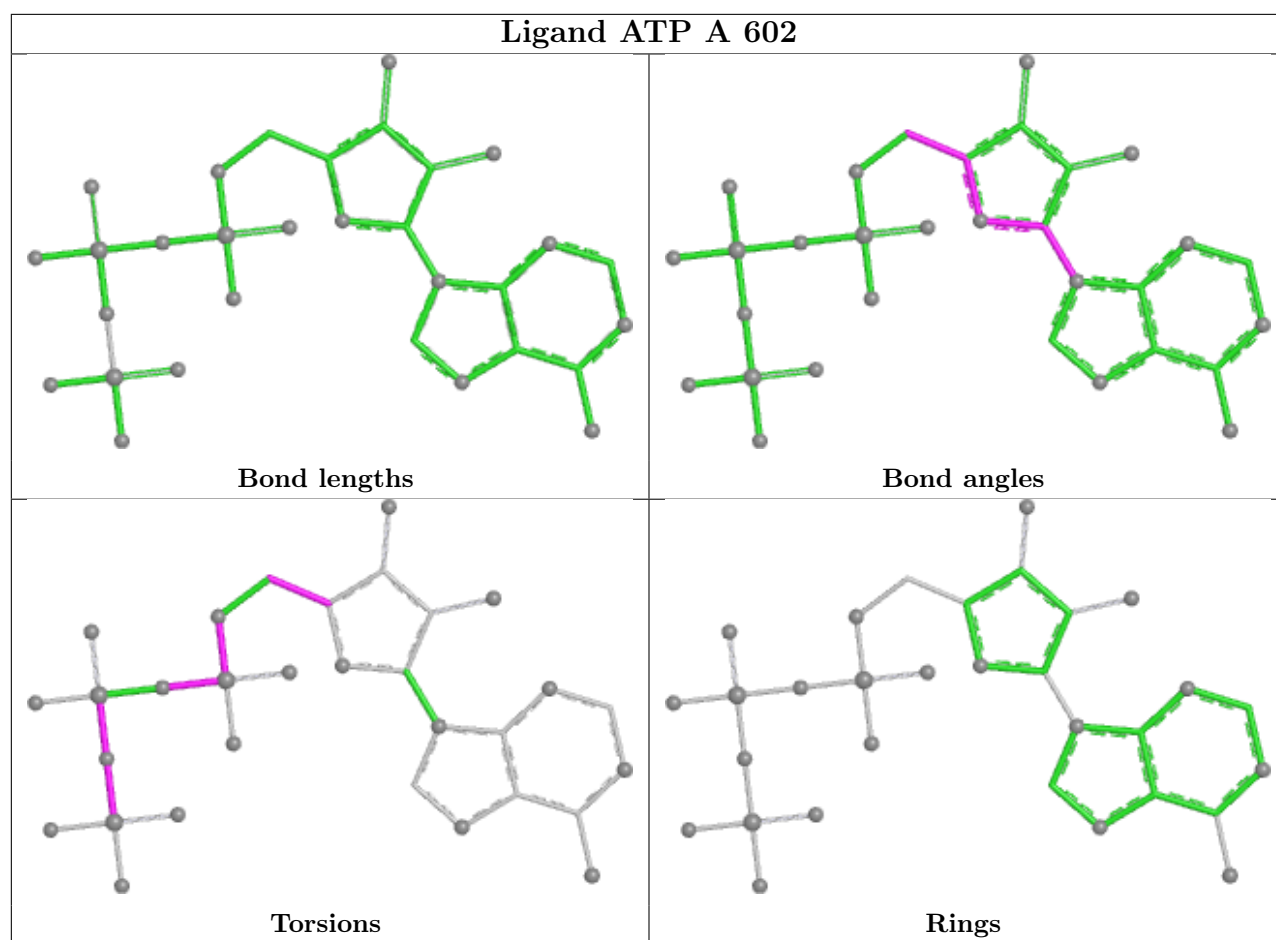
There are no ring outliers.

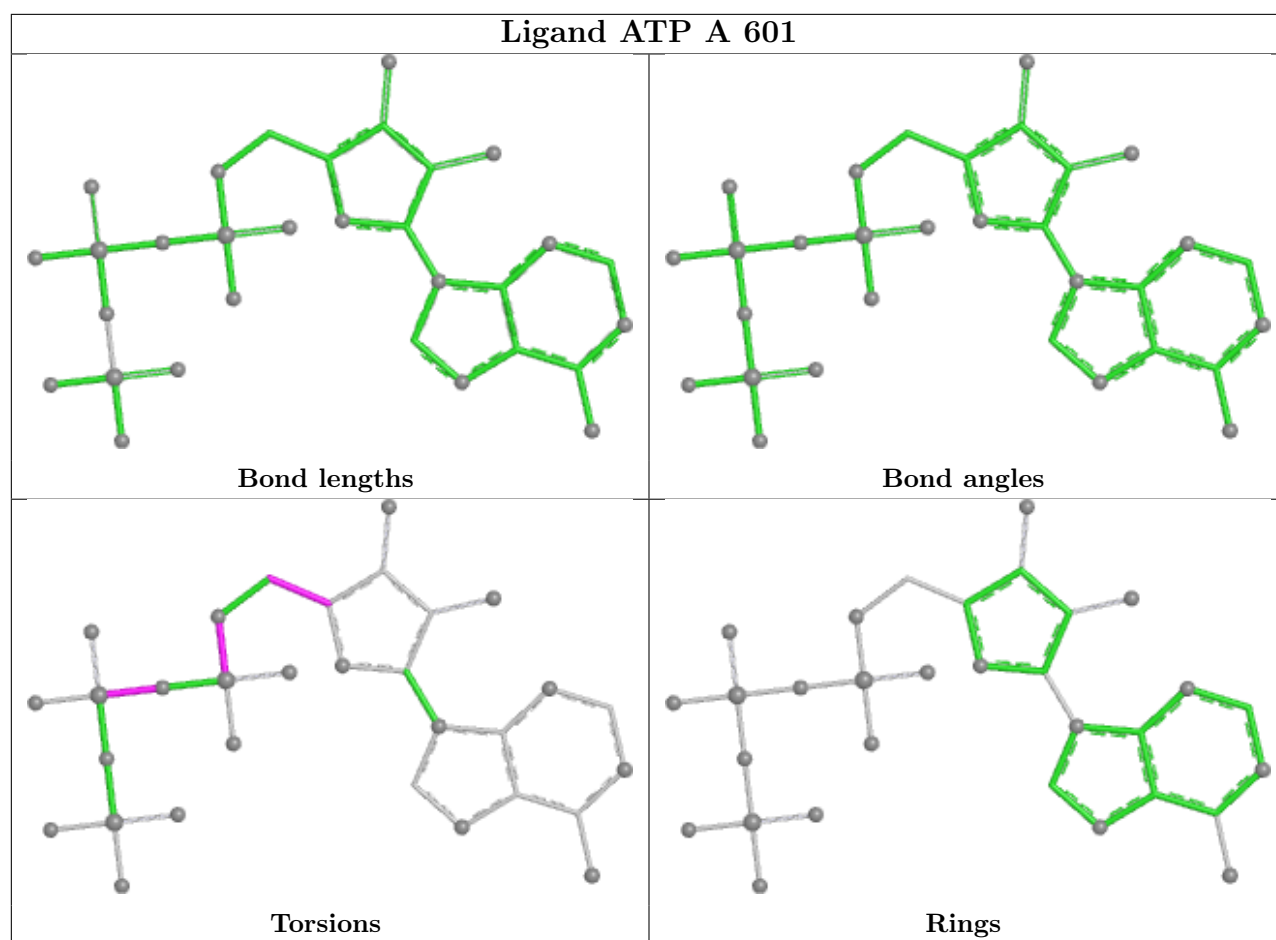
2 monomers are involved in 3 short contacts:

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

The worst 5 of 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

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](#)

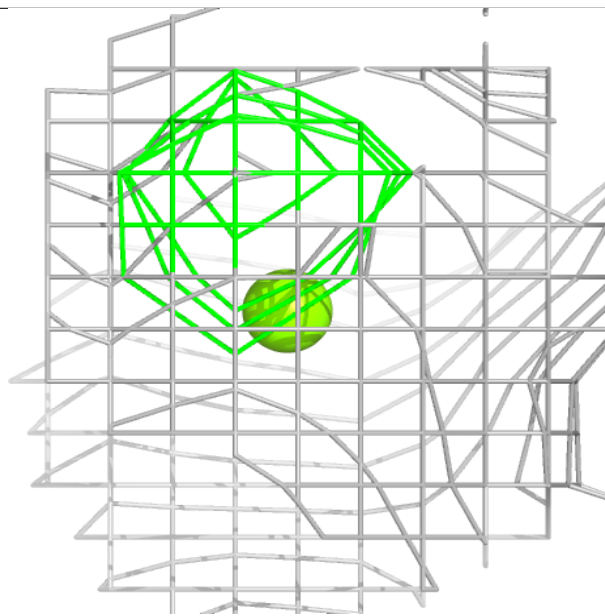
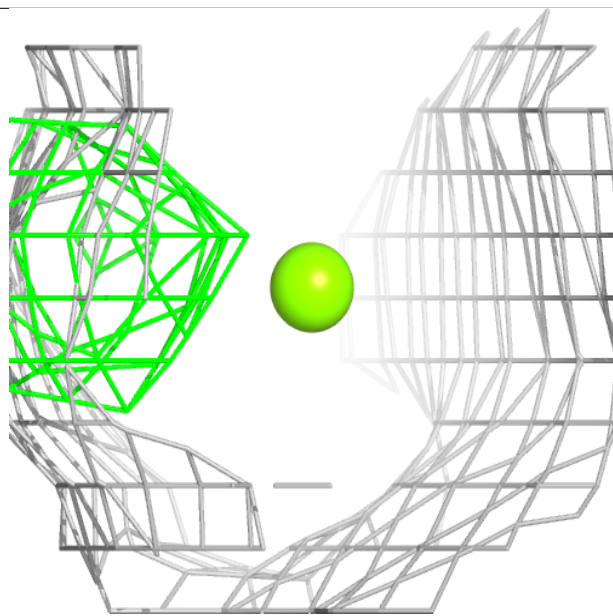
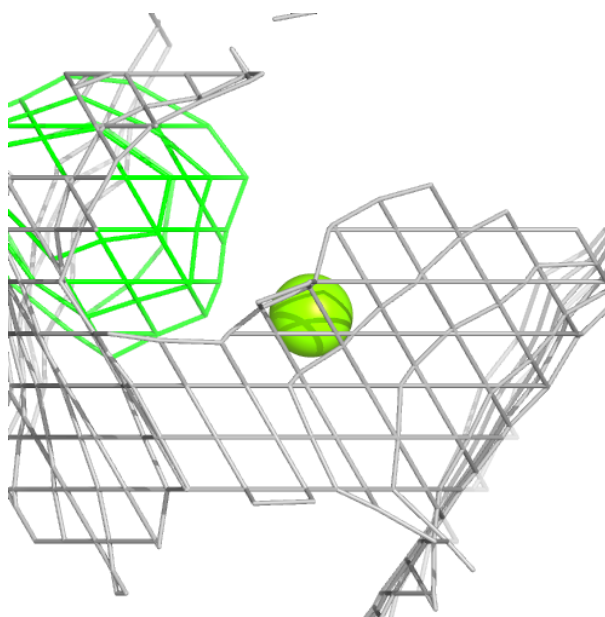
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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.

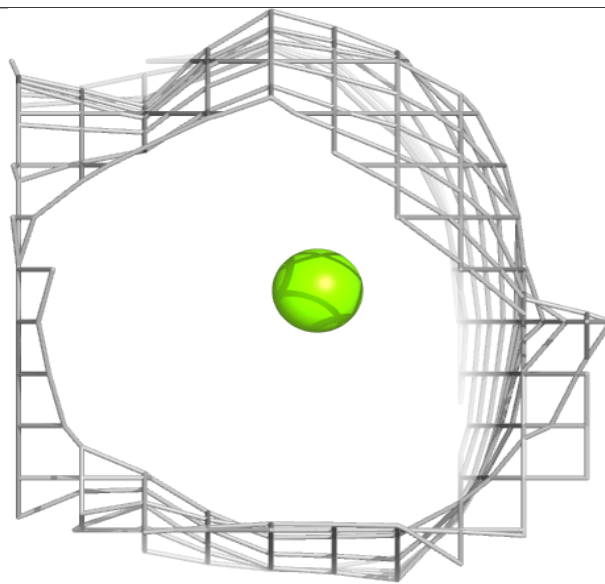
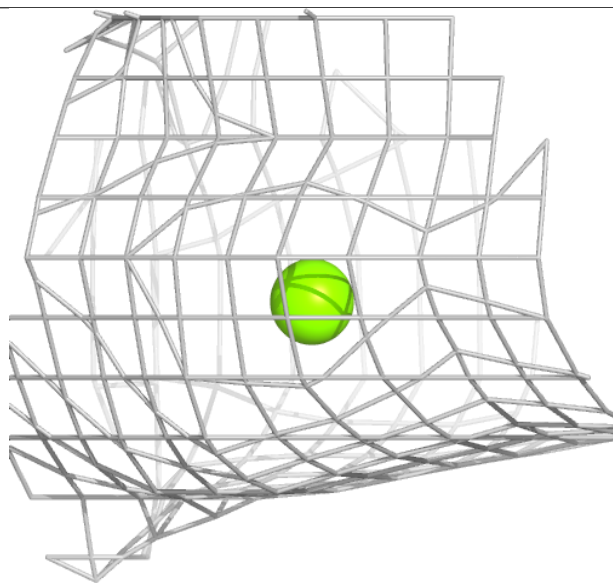
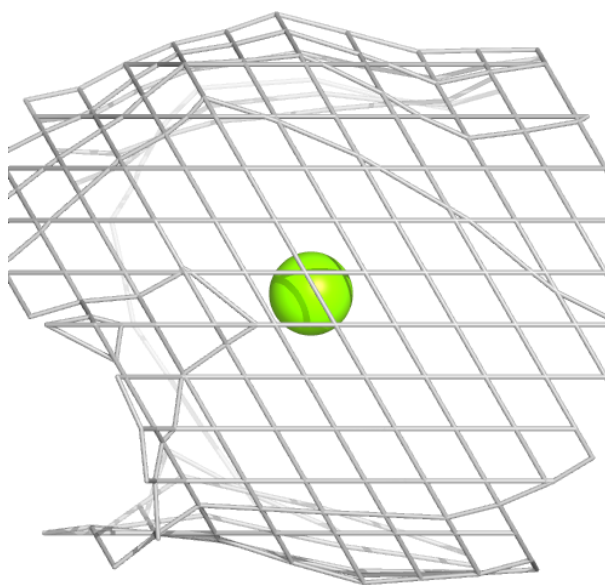
Electron density around MG A 603:

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



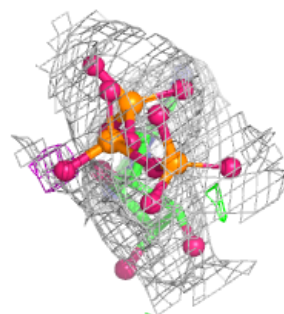
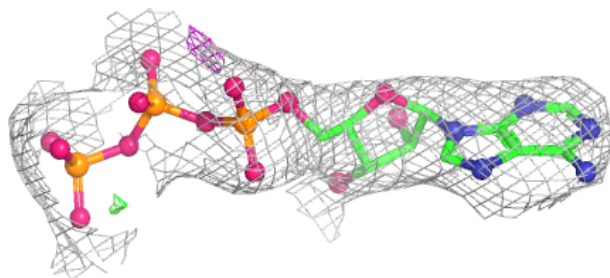
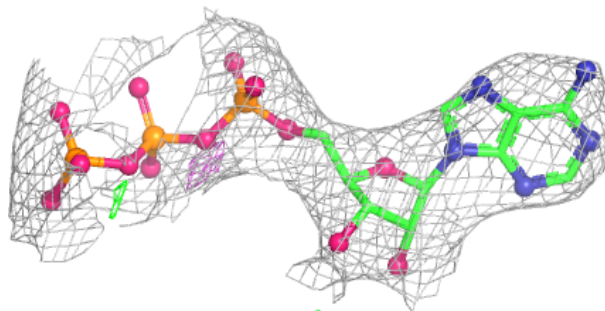
Electron density around MG B 603:

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

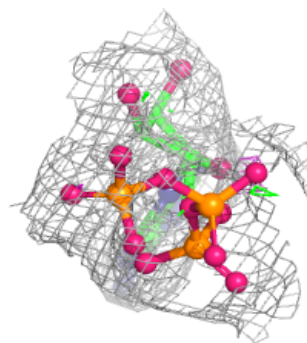
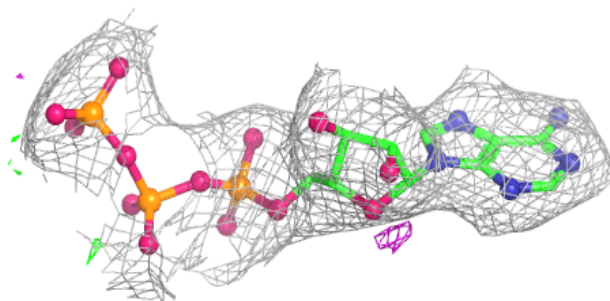
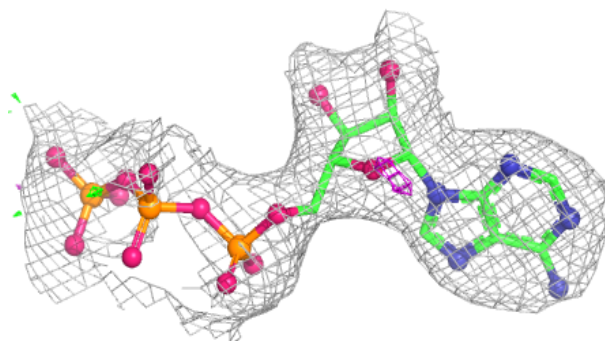


Electron density around ATP B 601:

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

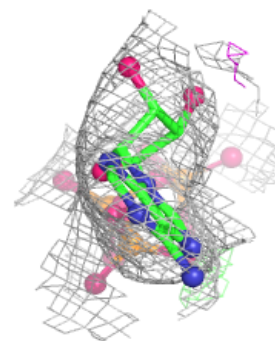
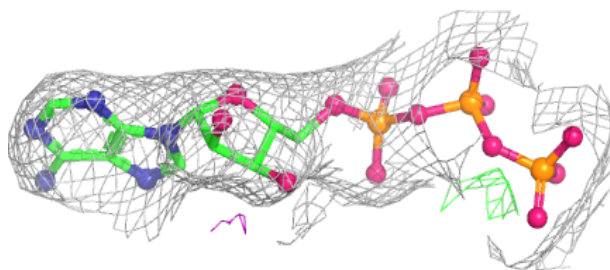
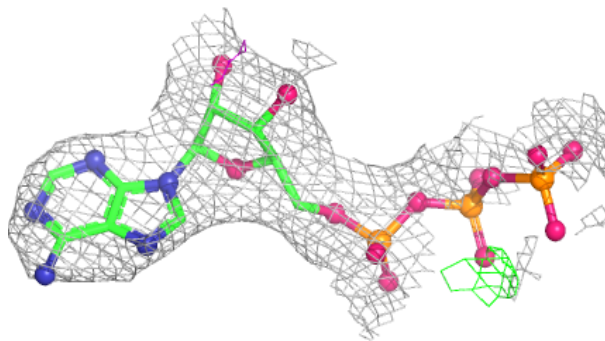
**Electron density around ATP A 602:**

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



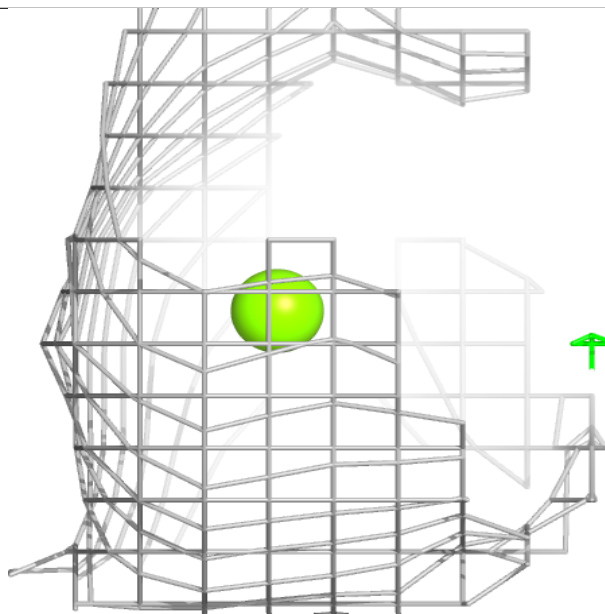
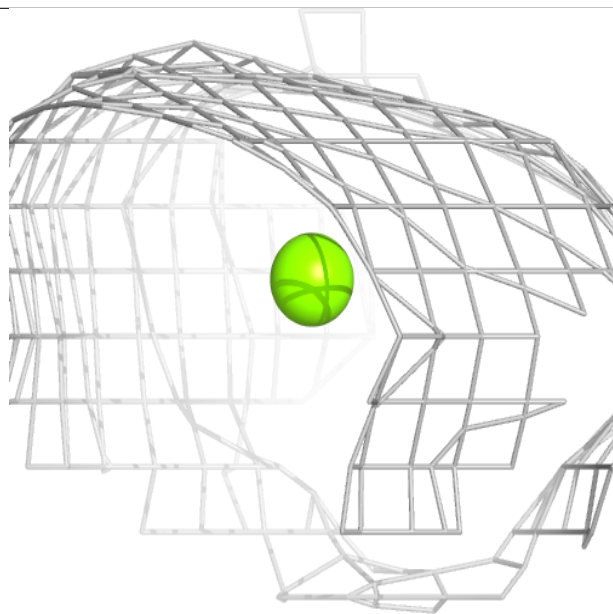
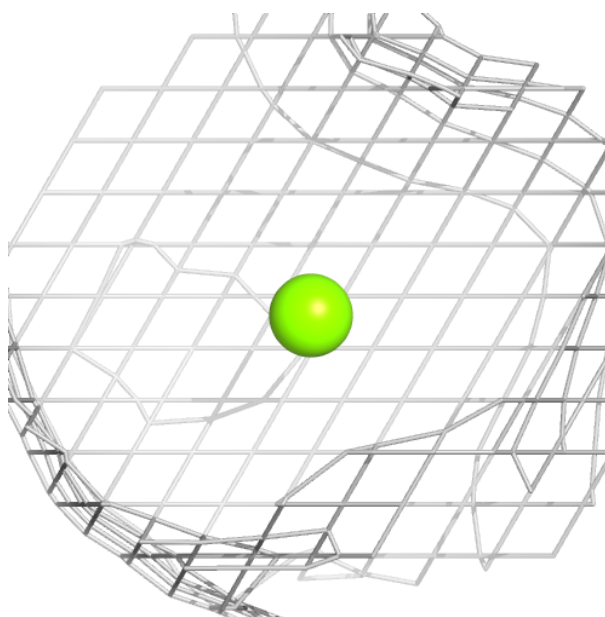
Electron density around ATP A 601:

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



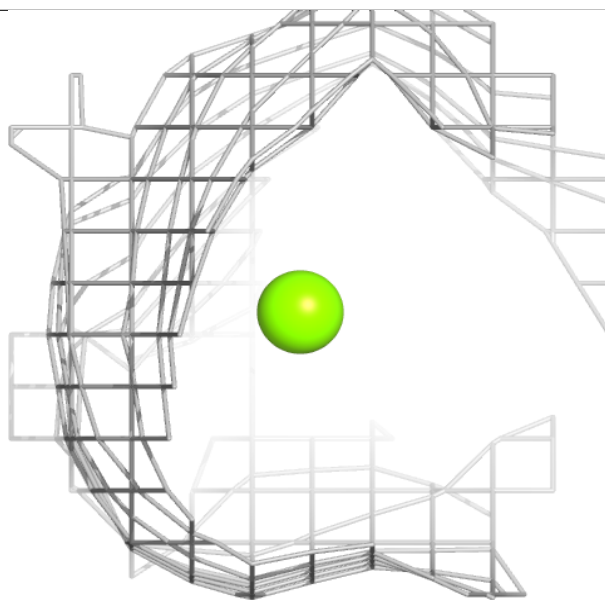
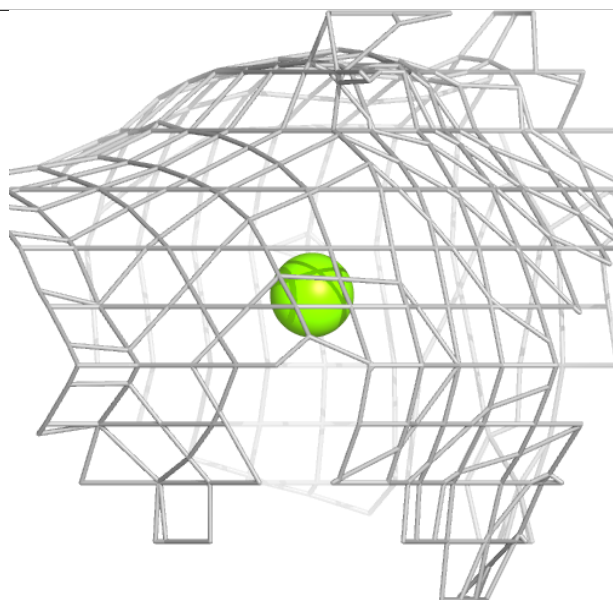
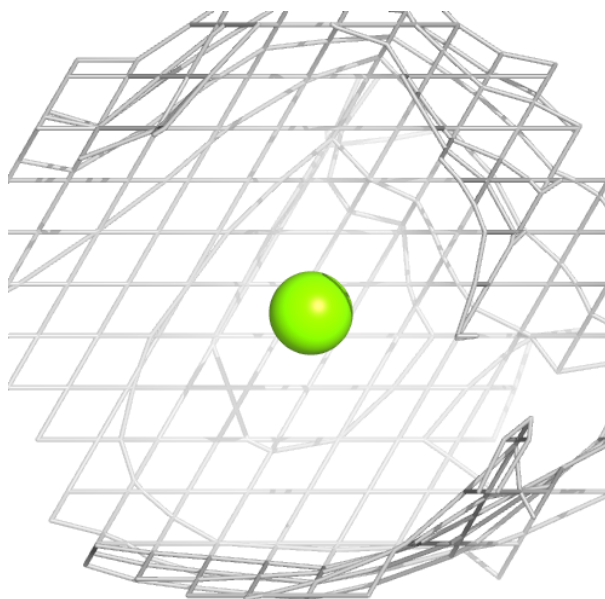
Electron density around MG A 604:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.