wwPDB X-ray Structure Validation Summary Report (i)

Sep 30, 2024 – 04:09 PM EDT

PDB ID	:	9BQ0
Title	:	Complex structure of protein crystal of Tri17 with ATP
Authors	:	Zhai, R.; Zhang, W.
Deposited on	:	2024-05-08
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

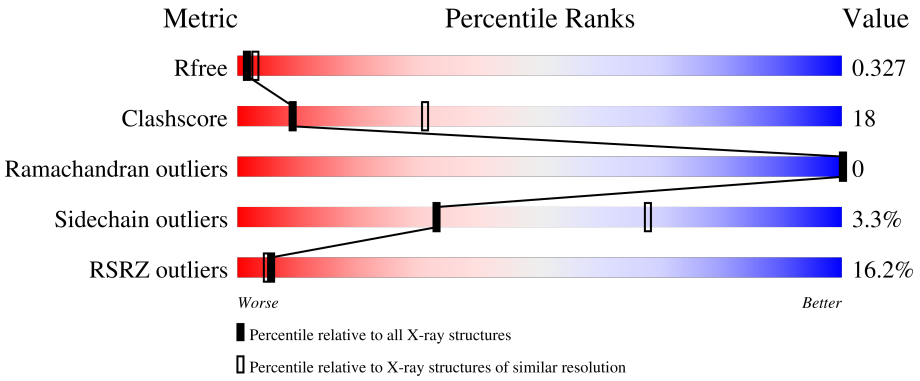
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	564	16% 56% 30% • 14%
1	B	564	8% 57% 27% • 15%
1	C	564	15% 52% 32% 15%
1	D	564	16% 57% 27% • 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	C	602	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29878 atoms, of which 14521 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 AMP-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	487	Total	C	H	N	O	S	0	0	0
			7410	2385	3653	662	697	13			
1	B	479	Total	C	H	N	O	S	0	0	0
			7300	2350	3599	652	686	13			
1	C	480	Total	C	H	N	O	S	0	0	0
			7335	2361	3622	652	687	13			
1	D	482	Total	C	H	N	O	S	0	0	0
			7333	2375	3599	657	689	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5H2UY12
A	557	LEU	-	expression tag	UNP A0A5H2UY12
A	558	GLU	-	expression tag	UNP A0A5H2UY12
A	559	HIS	-	expression tag	UNP A0A5H2UY12
A	560	HIS	-	expression tag	UNP A0A5H2UY12
A	561	HIS	-	expression tag	UNP A0A5H2UY12
A	562	HIS	-	expression tag	UNP A0A5H2UY12
A	563	HIS	-	expression tag	UNP A0A5H2UY12
A	564	HIS	-	expression tag	UNP A0A5H2UY12
B	1	MET	-	initiating methionine	UNP A0A5H2UY12
B	557	LEU	-	expression tag	UNP A0A5H2UY12
B	558	GLU	-	expression tag	UNP A0A5H2UY12
B	559	HIS	-	expression tag	UNP A0A5H2UY12
B	560	HIS	-	expression tag	UNP A0A5H2UY12
B	561	HIS	-	expression tag	UNP A0A5H2UY12
B	562	HIS	-	expression tag	UNP A0A5H2UY12
B	563	HIS	-	expression tag	UNP A0A5H2UY12
B	564	HIS	-	expression tag	UNP A0A5H2UY12
C	1	MET	-	initiating methionine	UNP A0A5H2UY12
C	557	LEU	-	expression tag	UNP A0A5H2UY12
C	558	GLU	-	expression tag	UNP A0A5H2UY12

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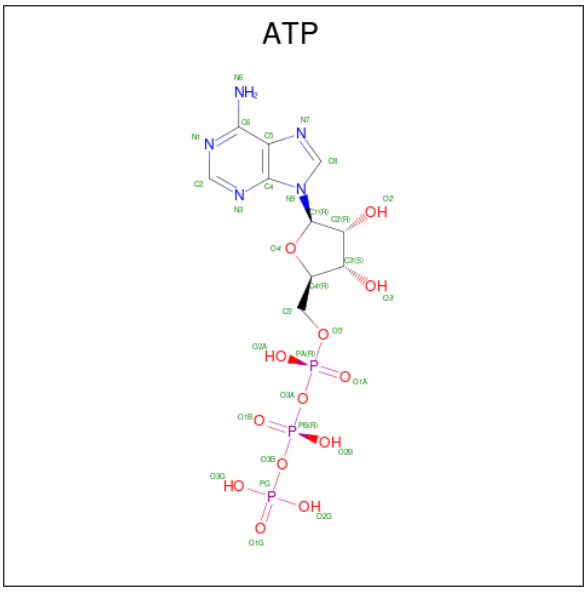
Chain	Residue	Modelled	Actual	Comment	Reference
C	559	HIS	-	expression tag	UNP A0A5H2UY12
C	560	HIS	-	expression tag	UNP A0A5H2UY12
C	561	HIS	-	expression tag	UNP A0A5H2UY12
C	562	HIS	-	expression tag	UNP A0A5H2UY12
C	563	HIS	-	expression tag	UNP A0A5H2UY12
C	564	HIS	-	expression tag	UNP A0A5H2UY12
D	1	MET	-	initiating methionine	UNP A0A5H2UY12
D	557	LEU	-	expression tag	UNP A0A5H2UY12
D	558	GLU	-	expression tag	UNP A0A5H2UY12
D	559	HIS	-	expression tag	UNP A0A5H2UY12
D	560	HIS	-	expression tag	UNP A0A5H2UY12
D	561	HIS	-	expression tag	UNP A0A5H2UY12
D	562	HIS	-	expression tag	UNP A0A5H2UY12
D	563	HIS	-	expression tag	UNP A0A5H2UY12
D	564	HIS	-	expression tag	UNP A0A5H2UY12

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	2	Total	Mg	0	0
			2	2		
3	C	1	Total	Mg	0	0
			1	1		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

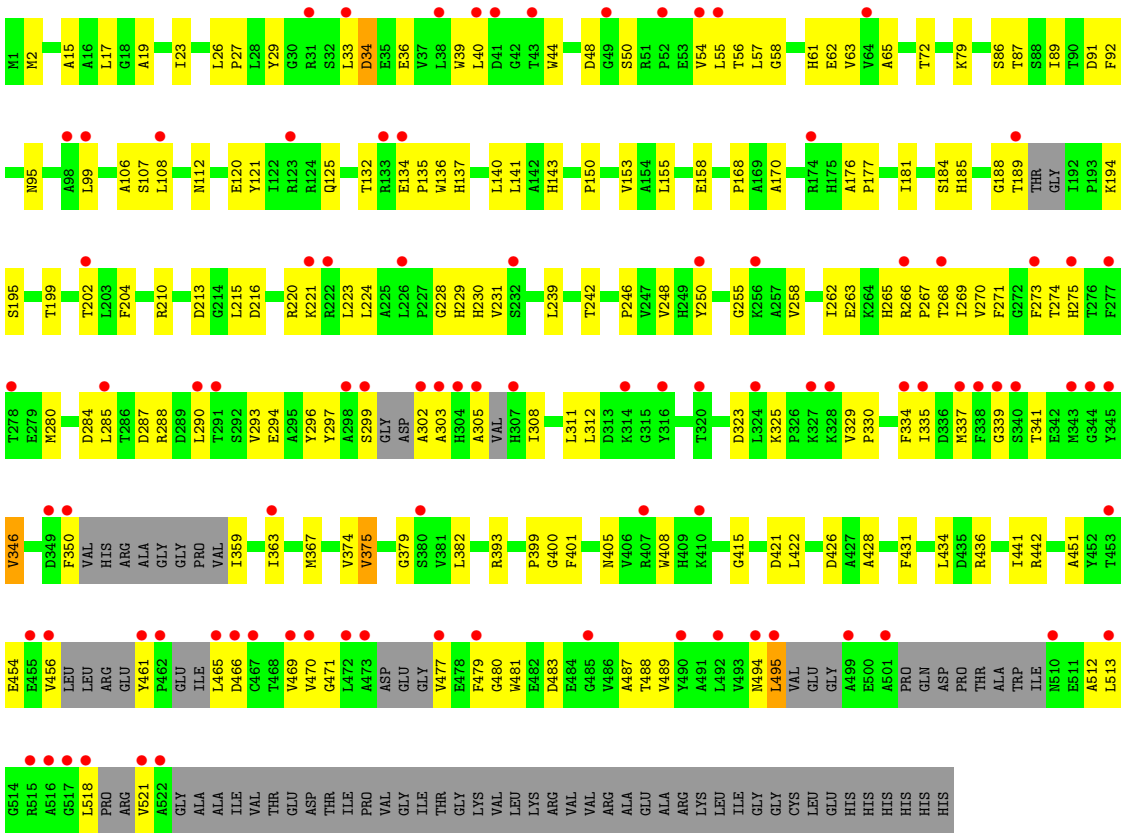
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total	O	0	0
			118	118		
4	B	74	Total	O	0	0
			74	74		
4	C	68	Total	O	0	0
			68	68		
4	D	62	Total	O	0	0
			62	62		

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.

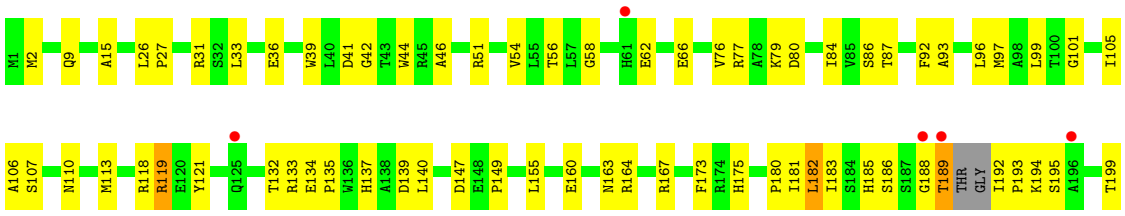
• Molecule 1: AMP-binding protein

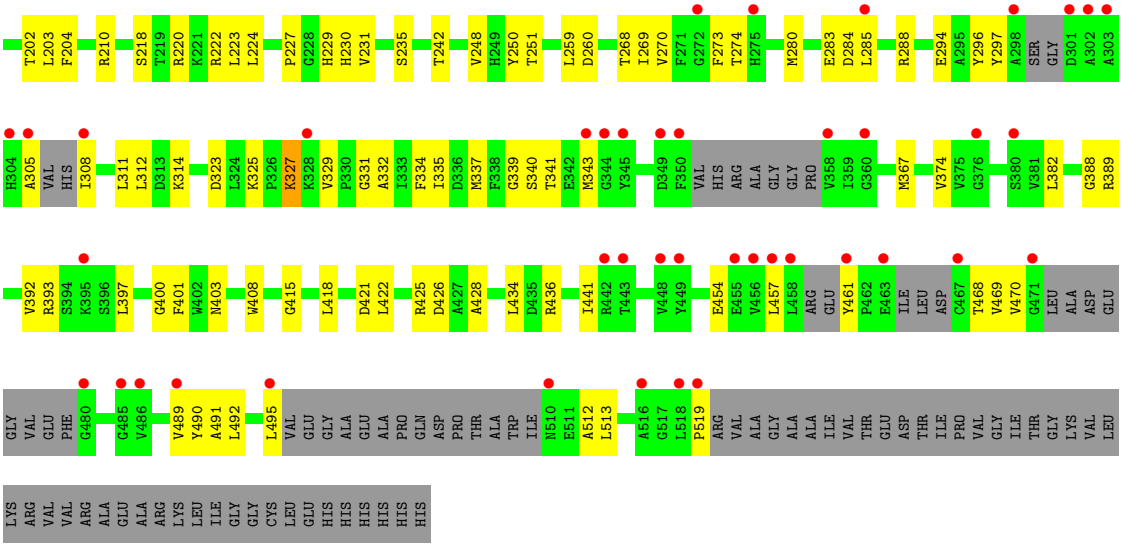
Chain A:



• Molecule 1: AMP-binding protein

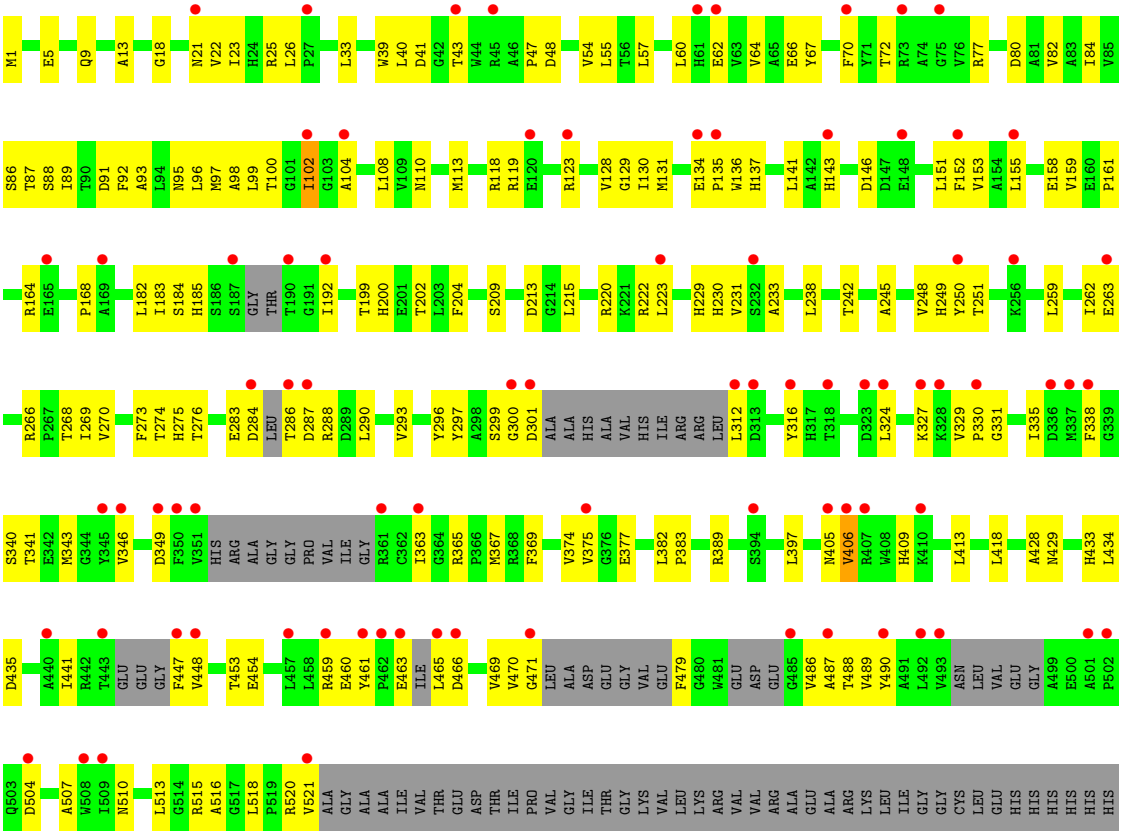
Chain B:





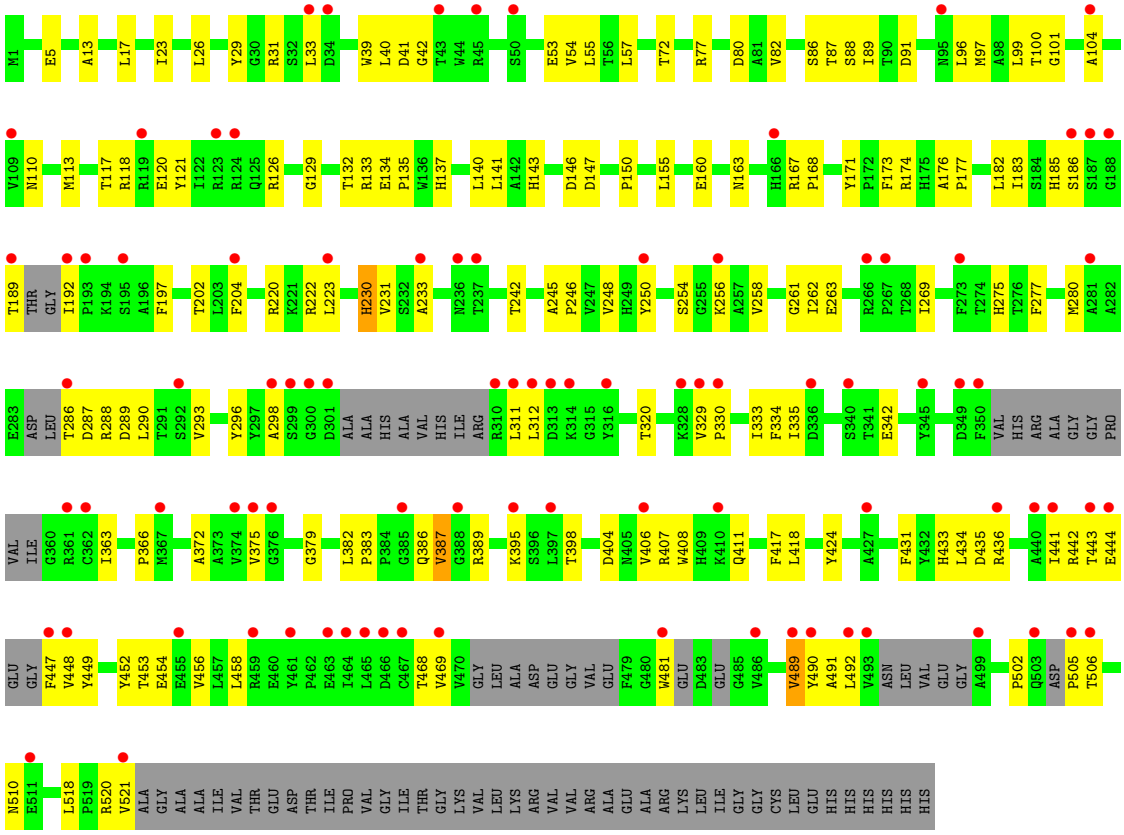
• Molecule 1: AMP-binding protein

Chain C:



• Molecule 1: AMP-binding protein

Chain D:


M1 E5 A13 L17 I23 L26 Y29 G30 R31 S32 L33 D34 W39 L40 D41 G42 T43 W44 R45 S50 E53 V54 L55 T56 L57 T72 R77 D80 A81 V82 S86 T87 S88 I89 T90 D91 N95 L96 M97 A98 L99 T100 G101 A104
V109 N110 M113 T117 R118 R119 E120 Y121 I122 R123 R124 Q125 R126 G129 T132 R133 E134 P135 W136 H137 L140 L141 A142 H143 D146 D147 P150 L155 E160 N163 H166 R167 P168 Y171 P172 F173 R174 H176 A176 P177 L182 I183 S184 H185 S186 S187 G188
T189 THR GLY I192 P193 K194 S195 A196 F197 T202 L203 F204 R220 K221 R222 L223 H230 V231 S232 A233 N236 T237 T242 A245 P246 V247 V248 H249 Y250 S254 G255 K256 A257 V258 G261 I262 E263 R266 P267 T268 I269 F273 T274 H275 T276 F277 M280 A281 A282
E283 ASP LEU T286 D287 R288 D289 L290 T291 S292 V293 Y296 Y297 A298 S299 G300 D301 ALA ALA HIS ALA VAL HIS ILE ARG R310 L311 L312 D313 K314 G315 Y316 T320 K328 V329 P330 I333 F334 I335 D336 S340 T341 E342 Y345 D349 F350 VAL HIS ARG ALA GLY GLY PRO
VAL ILE G360 R361 C362 I363 P366 M367 A372 A373 V374 V375 G376 G379 L382 P383 P384 G385 Q386 V387 G388 R389 K395 S396 L397 T398 D404 N405 V406 R407 W408 H409 K410 Q411 F417 L418 Y424 A427 F431 Y432 H433 L434 D435 R436 A440 I441 R442 T443 E444
GLU GLY F447 V448 Y449 Y452 T453 E454 E455 V456 L457 L458 R459 E460 Y461 P462 E463 I464 L465 D466 C467 T468 V469 V470 GLY LEU ALA ASP GLU GLY VAL GLU F479 G480 W481 GLU D483 GLU G485 V486 V489 Y490 A491 L492 V493 ASN LEU VAL GLU GLY A499 P502 Q503 ASP P505 T506
N510 E511 L518 P519 R520 V521 ALA GLY ALA ALA ILE VAL THR GLU ASP THR ILE PRO VAL GLY ILE THR GLY LYS VAL LEU LYS ARG VAL VAL ARG ALA GLU ALA ARG LYS LEU ILE GLY GLY CYS LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	87.09Å 152.33Å 229.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.44 – 2.90 46.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.44-2.90) 99.9 (46.44-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.278 , 0.330 0.278 , 0.327	Depositor DCC
R_{free} test set	3421 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	29878	wwPDB-VP
Average B, all atoms (Å^2)	61.0	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 60.77 % 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 1.4473e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.71	0/3841	0.88	0/5213
1	B	0.67	0/3786	0.83	0/5142
1	C	0.62	0/3801	0.84	0/5165
1	D	0.62	0/3821	0.83	0/5188
All	All	0.66	0/15249	0.85	0/20708

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	3757	3653	3673	148	0
1	B	3701	3599	3626	121	0
1	C	3713	3622	3630	147	0
1	D	3734	3599	3658	130	0
2	A	31	12	12	0	0
2	B	31	12	12	0	0
2	C	31	12	12	0	0
2	D	31	12	12	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	118	0	0	9	0
4	B	74	0	0	1	0
4	C	68	0	0	2	0
4	D	62	0	0	0	0
All	All	15357	14521	14635	535	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 18.

The worst 5 of 535 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:C:274:THR:HG21	1:C:301:ASP:HB2	1.54	0.89
1:C:39:TRP:HB2	1:C:248:VAL:HG22	1.54	0.87
1:C:343:MET:HA	1:C:397:LEU:HD23	1.58	0.86
1:C:39:TRP:CB	1:C:248:VAL:HG22	2.06	0.85
1:D:137:HIS:HD2	1:D:155:LEU:HG	1.40	0.84

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	465/564 (82%)	443 (95%)	22 (5%)	0	100	100
1	B	461/564 (82%)	447 (97%)	14 (3%)	0	100	100
1	C	460/564 (82%)	442 (96%)	18 (4%)	0	100	100
1	D	461/564 (82%)	436 (95%)	25 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1847/2256 (82%)	1768 (96%)	79 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	387/447 (87%)	376 (97%)	11 (3%)	38 73
1	B	383/447 (86%)	373 (97%)	10 (3%)	41 74
1	C	385/447 (86%)	367 (95%)	18 (5%)	22 55
1	D	387/447 (87%)	375 (97%)	12 (3%)	35 70
All	All	1542/1788 (86%)	1491 (97%)	51 (3%)	33 68

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	215	LEU
1	C	459	ARG
1	D	481	TRP
1	C	250	TYR
1	C	406	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	433	HIS
1	D	163	ASN
1	D	137	HIS
1	D	185	HIS
1	B	185	HIS

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 10 ligands modelled in this entry, 6 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	28,33,33	0.81	1 (3%)	34,52,52	0.81	1 (2%)
2	ATP	C	601	3	28,33,33	0.85	1 (3%)	34,52,52	0.82	1 (2%)
2	ATP	A	601	3	28,33,33	0.80	0	34,52,52	0.85	1 (2%)
2	ATP	D	601	3	28,33,33	0.77	0	34,52,52	0.80	1 (2%)

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	-	8/18/38/38	0/3/3/3
2	ATP	C	601	3	-	8/18/38/38	0/3/3/3
2	ATP	A	601	3	-	7/18/38/38	0/3/3/3
2	ATP	D	601	3	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	ATP	C1'-N9	-2.14	1.44	1.49
2	B	601	ATP	C1'-N9	-2.06	1.44	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	ATP	C5-C6-N6	2.52	124.15	120.31
2	D	601	ATP	C5-C6-N6	2.34	123.88	120.31
2	B	601	ATP	C5-C6-N6	2.31	123.83	120.31
2	C	601	ATP	C5-C6-N6	2.05	123.44	120.31

There are no chirality outliers.

5 of 29 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-O2A
2	A	601	ATP	C5'-O5'-PA-O3A
2	B	601	ATP	C5'-O5'-PA-O1A
2	B	601	ATP	C5'-O5'-PA-O2A

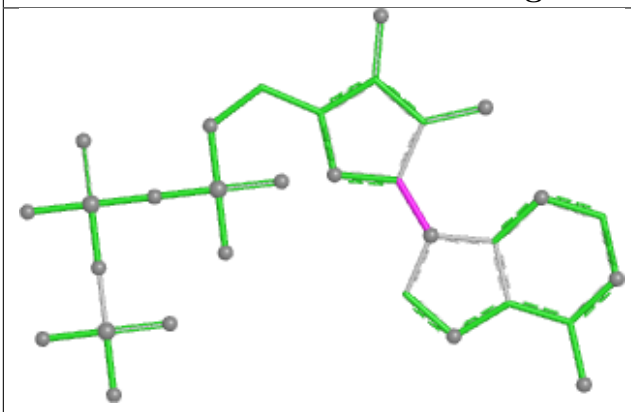
There are no ring outliers.

1 monomer is involved in 1 short contact:

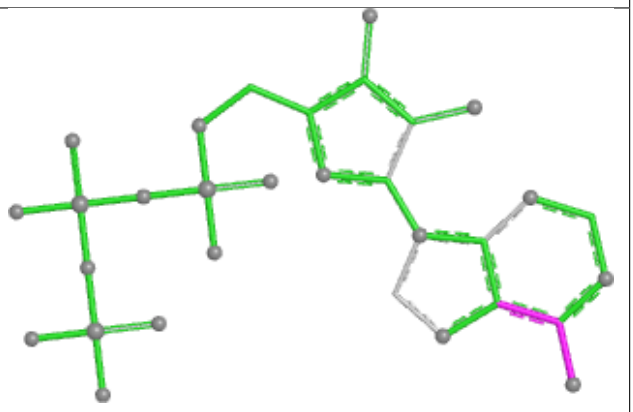
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

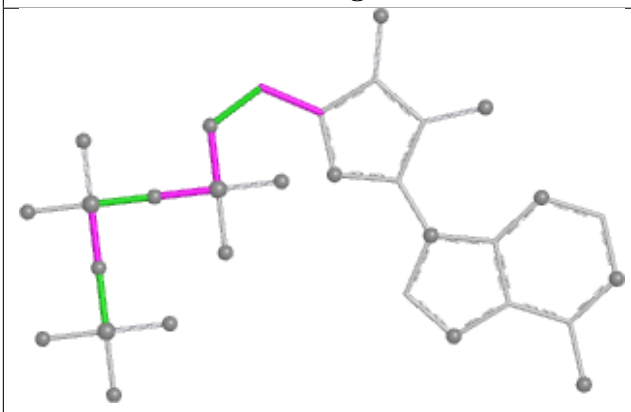
Ligand ATP B 601



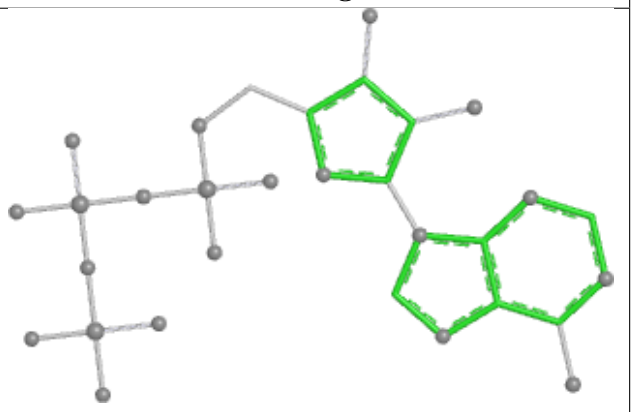
Bond lengths



Bond angles

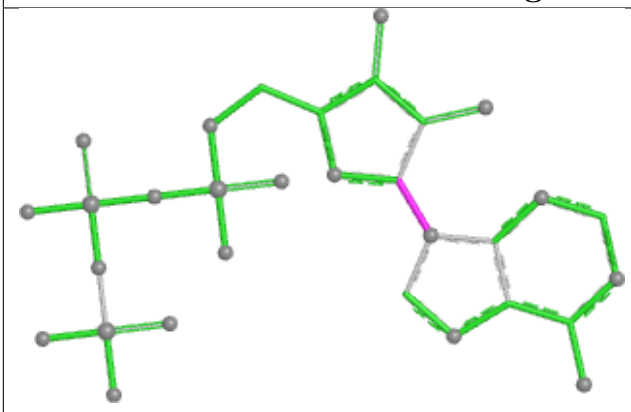


Torsions

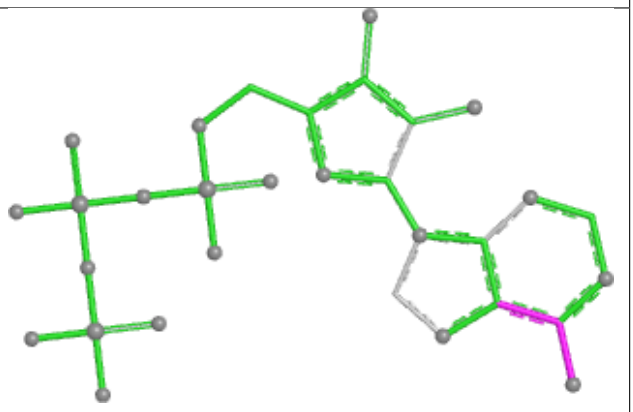


Rings

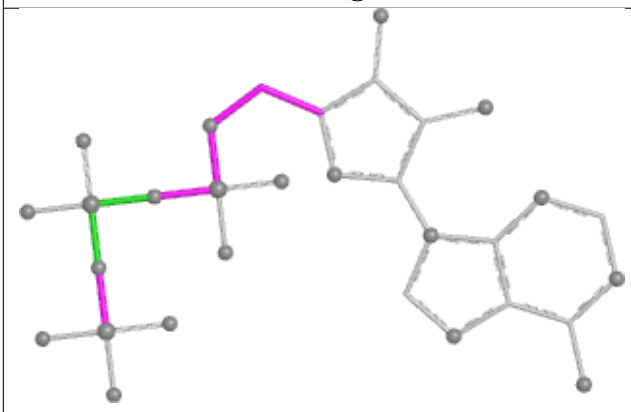
Ligand ATP C 601



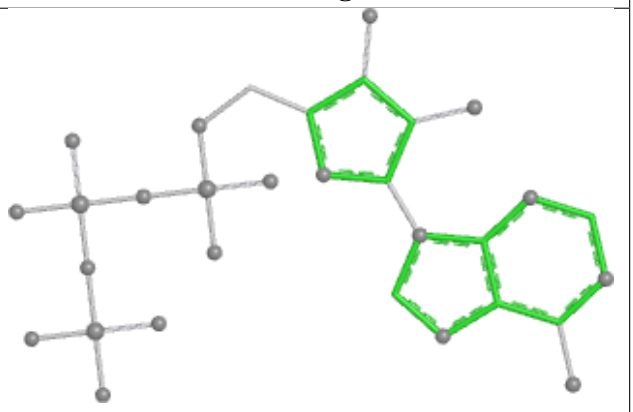
Bond lengths



Bond angles

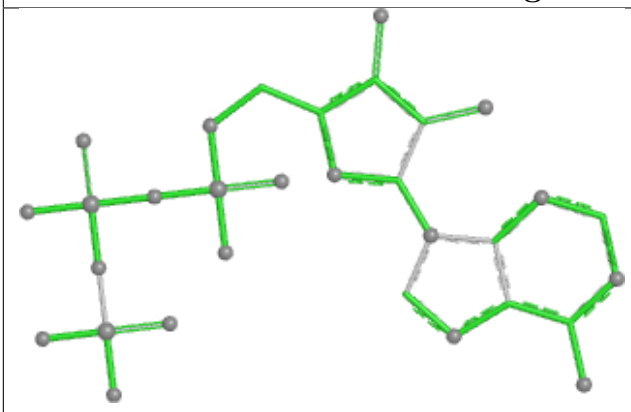


Torsions

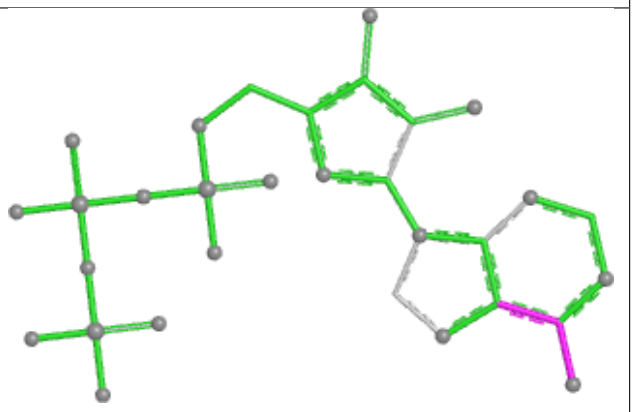


Rings

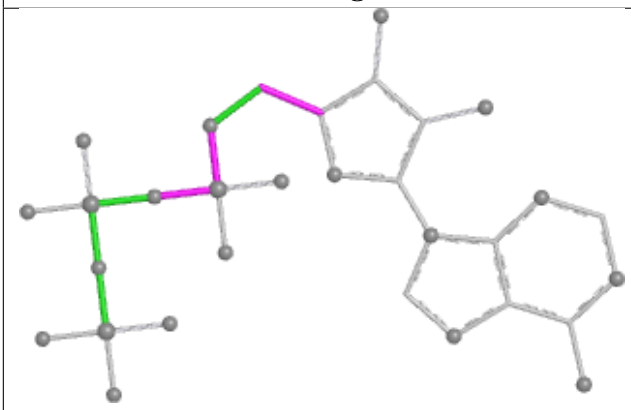
Ligand ATP A 601



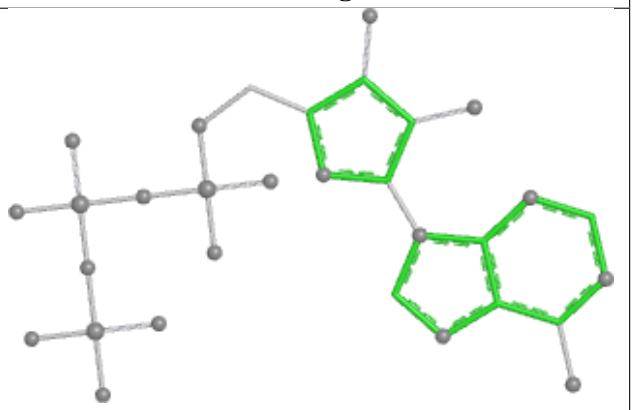
Bond lengths



Bond angles

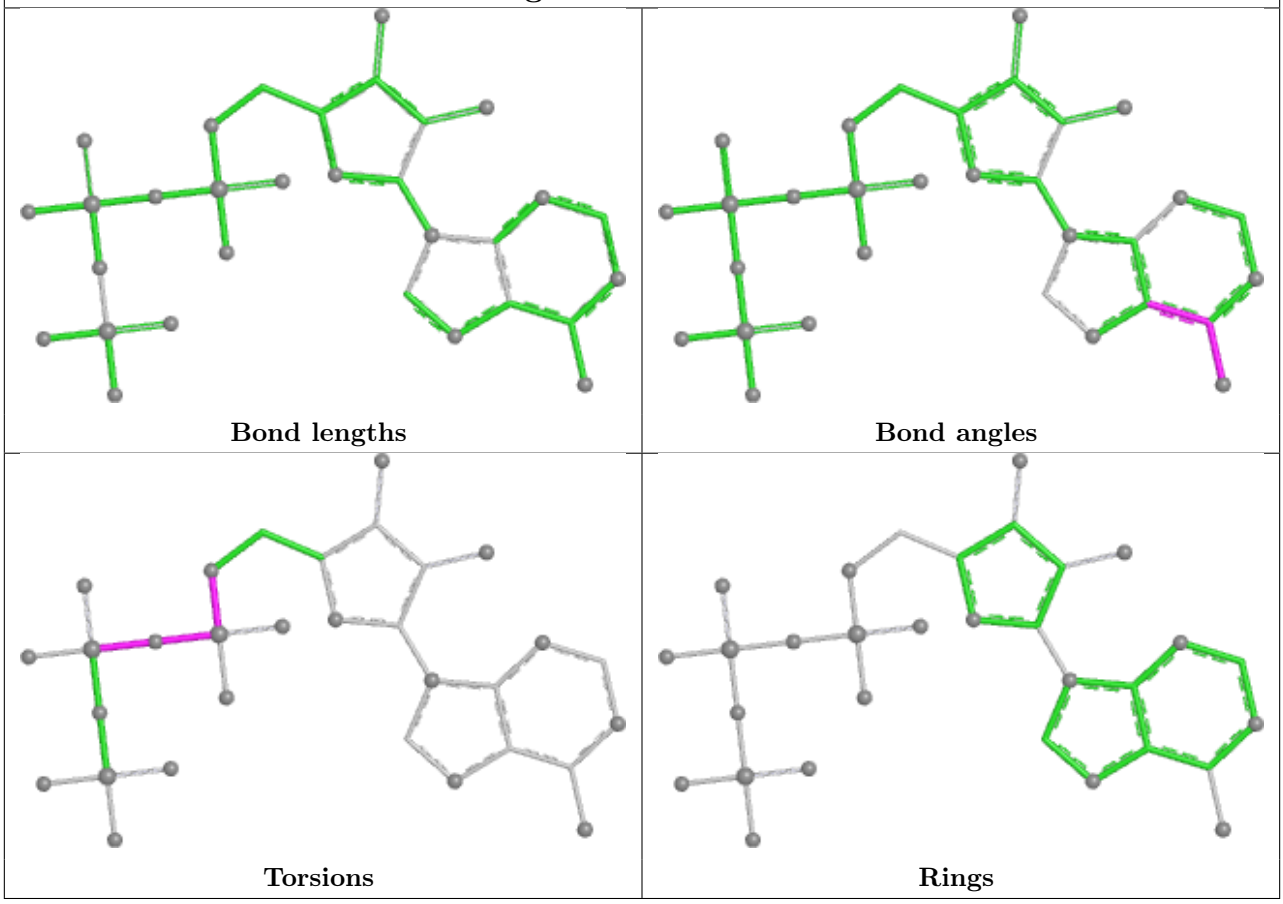


Torsions



Rings

Ligand ATP D 601



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, 95^{th} 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	487/564 (86%)	1.07	92 (18%) 4 3	28, 53, 101, 124	0
1	B	479/564 (84%)	0.63	47 (9%) 14 12	27, 50, 95, 116	0
1	C	480/564 (85%)	1.06	82 (17%) 5 4	28, 64, 94, 113	0
1	D	482/564 (85%)	1.14	91 (18%) 4 3	27, 64, 96, 118	0
All	All	1928/2256 (85%)	0.97	312 (16%) 5 5	27, 57, 96, 124	0

The worst 5 of 312 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	PHE	9.9
1	A	455	GLU	9.2
1	A	299	SER	7.2
1	A	41	ASP	7.1
1	A	302	ALA	7.0

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

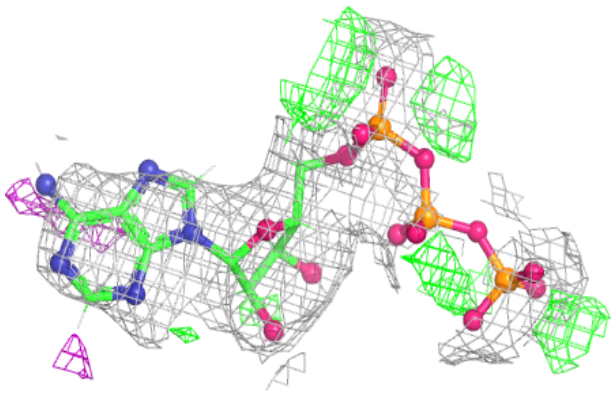
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

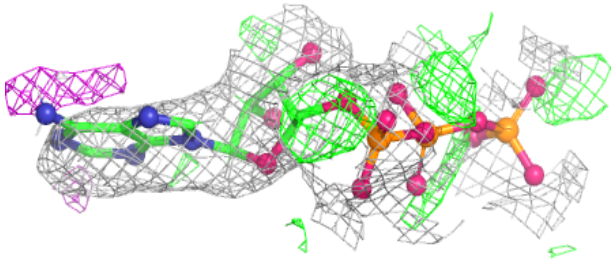
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	603	1/1	0.42	0.17	30,30,30,30	0
3	MG	C	602	1/1	0.49	0.46	85,85,85,85	0
2	ATP	C	601	31/31	0.71	0.21	53,86,103,124	0
2	ATP	D	601	31/31	0.79	0.17	57,74,102,114	0
3	MG	B	602	1/1	0.87	0.37	50,50,50,50	0
2	ATP	A	601	31/31	0.87	0.14	45,70,90,109	0
2	ATP	B	601	31/31	0.87	0.14	45,64,81,83	0
3	MG	A	602	1/1	0.88	0.28	48,48,48,48	0
3	MG	B	603	1/1	0.89	0.12	30,30,30,30	0
3	MG	D	602	1/1	0.90	0.40	50,50,50,50	0

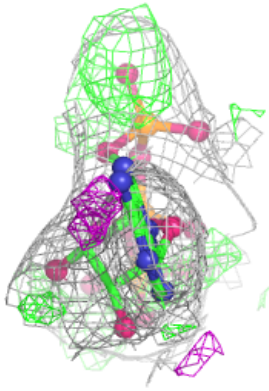
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 601:

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

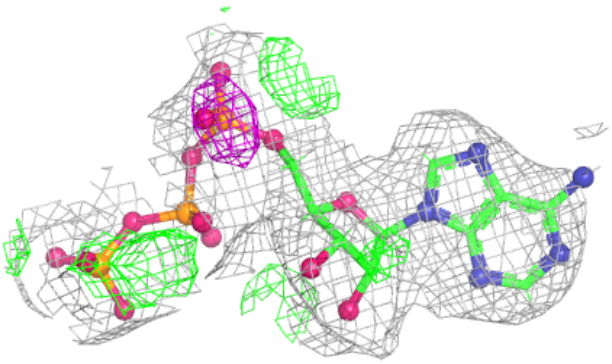


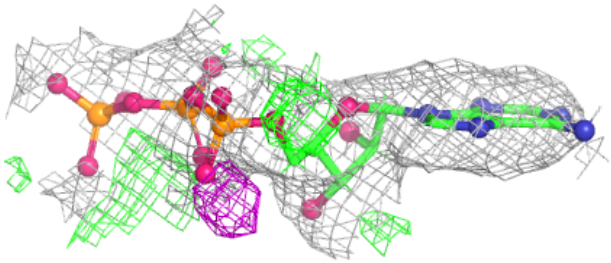


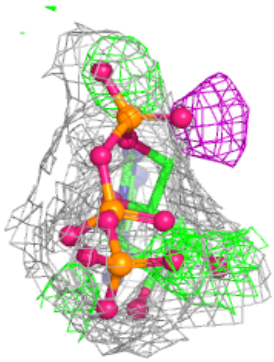


Electron density around ATP D 601:

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

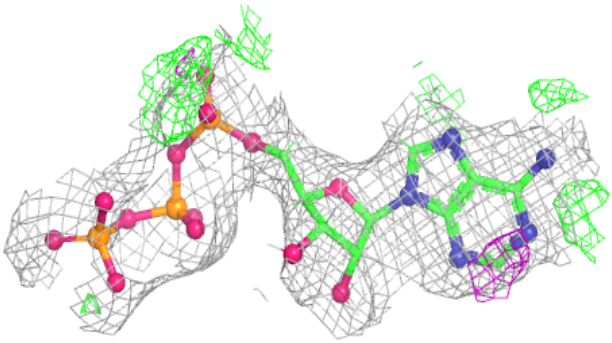


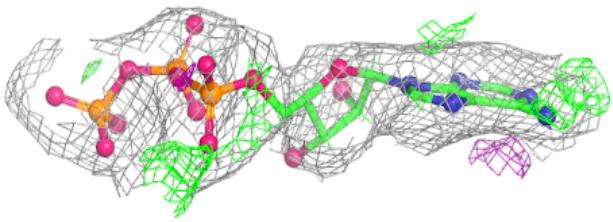


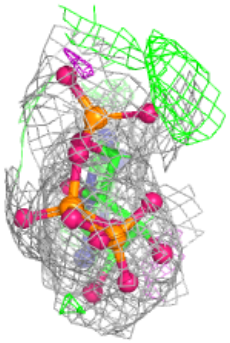


Electron density around ATP A 601:

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

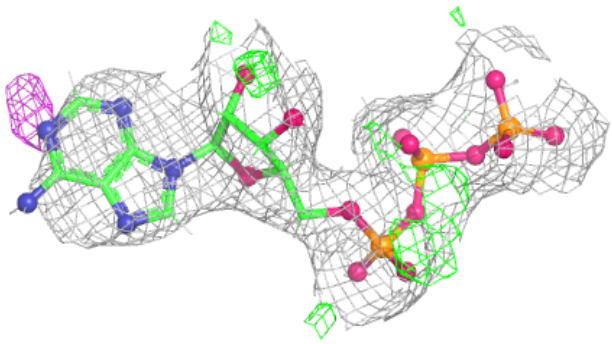


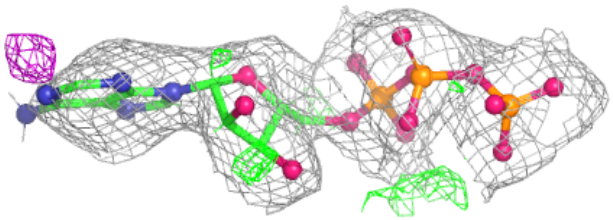


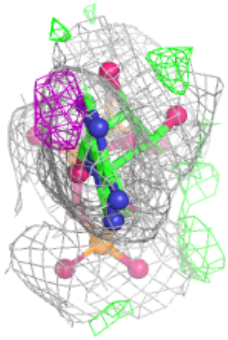


Electron density around ATP B 601:

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







6.5 Other polymers

There are no such residues in this entry.