



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2025 – 12:05 PM EDT

PDB ID : 9Y02 / pdb\_00009y02  
Title : QatB-QatC complex in qatABCD anti-phage defense with ATP  
Authors : Gao, A.; Wassarman, D.R.; Kranzusch, P.J.  
Deposited on : 2025-08-28  
Resolution : 1.73 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](mailto: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>.

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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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

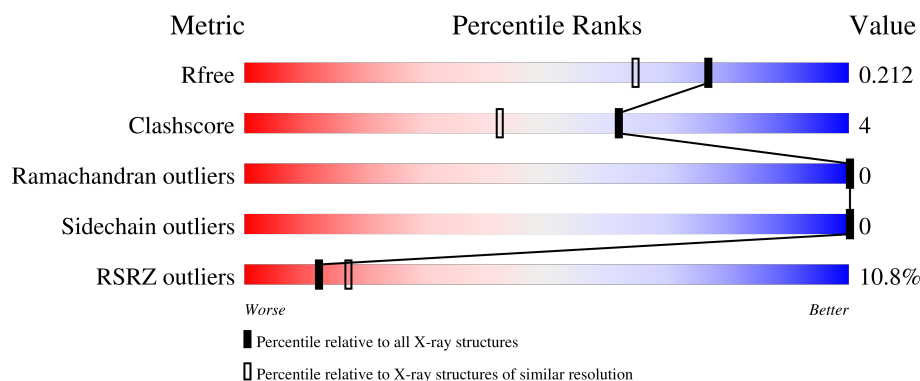
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 1.73 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	1043 (1.74-1.74)
Clashscore	180529	1119 (1.74-1.74)
Ramachandran outliers	177936	1112 (1.74-1.74)
Sidechain outliers	177891	1112 (1.74-1.74)
RSRZ outliers	164620	1043 (1.74-1.74)

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  $\geq 3$ , 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	287	
2	B	466	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5500 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 QatB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1564	961	285	312	6			

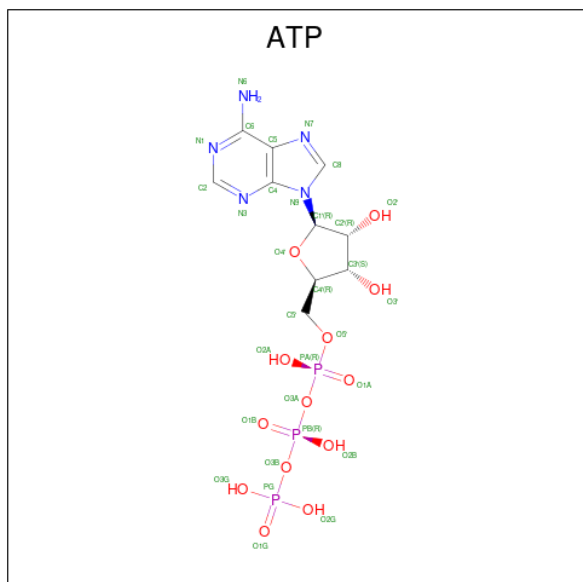
- Molecule 2 is a protein called QatC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3321	2085	595	624	17			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

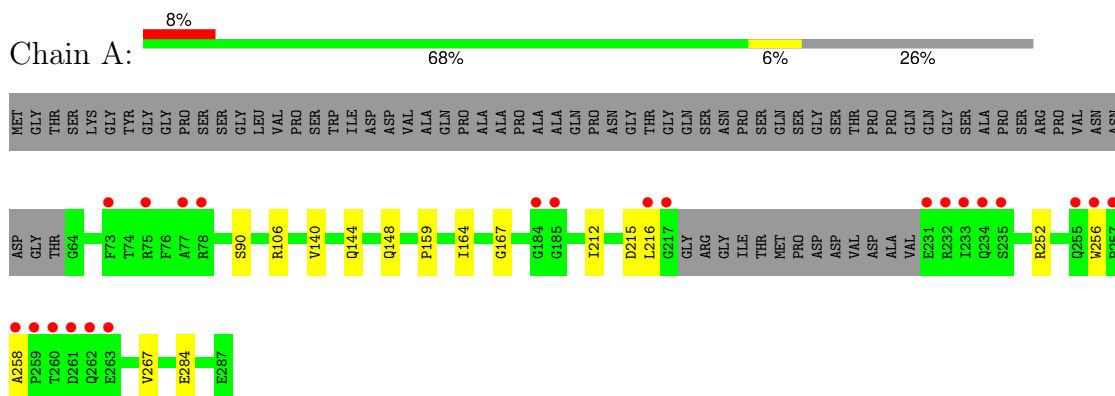
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	169	Total	O	0	0
			169	169		
6	B	413	Total	O	0	0
			413	413		

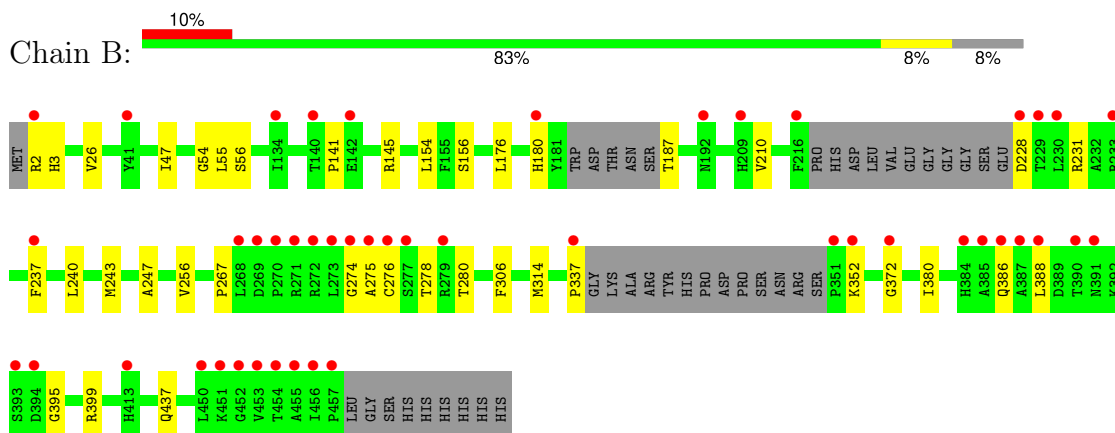
### 3 Residue-property plots [i](#)

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: QatB



#### • Molecule 2: QatC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.62Å 74.25Å 134.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.05 – 1.73 67.05 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.7 (67.05-1.73) 99.7 (67.05-1.73)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 1.73Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.184 , 0.212 0.184 , 0.212	Depositor DCC
$R_{free}$ test set	3665 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5500	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ZN

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	0.25	0/1582	0.44	0/2132
2	B	0.28	0/3388	0.48	0/4594
All	All	0.27	0/4970	0.47	0/6726

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	1564	0	1539	12	0
2	B	3321	0	3275	29	0
3	B	1	0	0	0	0
4	B	31	0	12	1	0
5	B	1	0	0	0	0
6	A	169	0	0	2	0
6	B	413	0	0	11	1
All	All	5500	0	4826	39	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 4.

All (39) 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)
2:B:187:THR:N	6:B:601:HOH:O	2.21	0.74
2:B:372:GLY:N	6:B:602:HOH:O	2.25	0.68
1:A:167:GLY:HA2	2:B:275:ALA:HB3	1.78	0.66
2:B:55:LEU:HB3	2:B:247:ALA:HB1	1.84	0.59
1:A:252:ARG:HD3	6:A:304:HOH:O	2.05	0.57
2:B:437:GLN:CD	6:B:676:HOH:O	2.47	0.56
1:A:144:GLN:NE2	1:A:148:GLN:HG2	2.20	0.56
2:B:3:HIS:HB2	6:B:906:HOH:O	2.05	0.55
2:B:47:ILE:HG13	2:B:243:MET:HE1	1.91	0.53
2:B:228:ASP:N	6:B:607:HOH:O	2.44	0.50
2:B:56:SER:HB3	2:B:141:PRO:HD3	1.94	0.49
2:B:337:PRO:HA	2:B:352:LYS:O	2.13	0.49
2:B:154:LEU:HD12	2:B:256:VAL:HG22	1.95	0.49
2:B:231:ARG:NE	2:B:278:THR:HG22	2.28	0.49
2:B:176:LEU:HD21	2:B:210:VAL:HG23	1.97	0.47
2:B:54:GLY:HA3	2:B:145:ARG:HA	1.97	0.47
1:A:164:ILE:HA	2:B:276:CYS:SG	2.56	0.46
2:B:2:ARG:HA	6:B:892:HOH:O	2.15	0.46
1:A:256:TRP:CE2	1:A:267:VAL:HG22	2.51	0.46
2:B:306:PHE:CD2	2:B:314:MET:HE3	2.51	0.45
2:B:280:THR:HB	6:B:627:HOH:O	2.16	0.45
2:B:388:LEU:HB3	2:B:395:GLY:CA	2.47	0.44
2:B:2:ARG:HH21	2:B:26:VAL:HG21	1.82	0.43
2:B:380:ILE:HG23	2:B:386:GLN:HE22	1.83	0.43
1:A:140:VAL:HG23	1:A:144:GLN:CD	2.44	0.43
2:B:180:HIS:CD2	2:B:240:LEU:HD13	2.54	0.43
2:B:267:PRO:CG	2:B:274:GLY:HA2	2.49	0.43
2:B:180:HIS:CE1	2:B:237:PHE:HA	2.54	0.42
2:B:372:GLY:CA	6:B:602:HOH:O	2.67	0.42
2:B:3:HIS:HB3	6:B:632:HOH:O	2.19	0.42
2:B:399:ARG:CZ	6:B:615:HOH:O	2.67	0.41
2:B:156:SER:HB3	4:B:502:ATP:C4	2.55	0.41
1:A:90:SER:HB2	1:A:284:GLU:HG3	2.02	0.41
1:A:212:ILE:HG23	1:A:216:LEU:HD12	2.03	0.41
1:A:256:TRP:HD1	1:A:258:ALA:O	2.03	0.41
2:B:399:ARG:NH2	6:B:615:HOH:O	2.52	0.41
1:A:144:GLN:HE21	1:A:144:GLN:HB3	1.77	0.41
1:A:159:PRO:HD3	6:A:327:HOH:O	2.20	0.40
1:A:106:ARG:HH22	1:A:215:ASP:CG	2.30	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)
6:B:864:HOH:O	6:B:891:HOH:O[4_455]	1.93	0.27

## 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	207/287 (72%)	203 (98%)	4 (2%)	0	100	100
2	B	419/466 (90%)	411 (98%)	8 (2%)	0	100	100
All	All	626/753 (83%)	614 (98%)	12 (2%)	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	160/217 (74%)	160 (100%)	0	100	100
2	B	359/392 (92%)	359 (100%)	0	100	100
All	All	519/609 (85%)	519 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
2	B	317	GLN
2	B	386	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z  > 2$
4	ATP	B	502	5	28,33,33	0.88	2 (7%)	34,52,52	0.88	2 (5%)

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
4	ATP	B	502	5	-	4/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	ATP	PG-O3G	-2.37	1.46	1.54
4	B	502	ATP	PB-O3B	-2.30	1.57	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	ATP	O2B-PB-O3B	2.49	114.00	107.27
4	B	502	ATP	C5-C6-N6	2.18	123.64	120.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

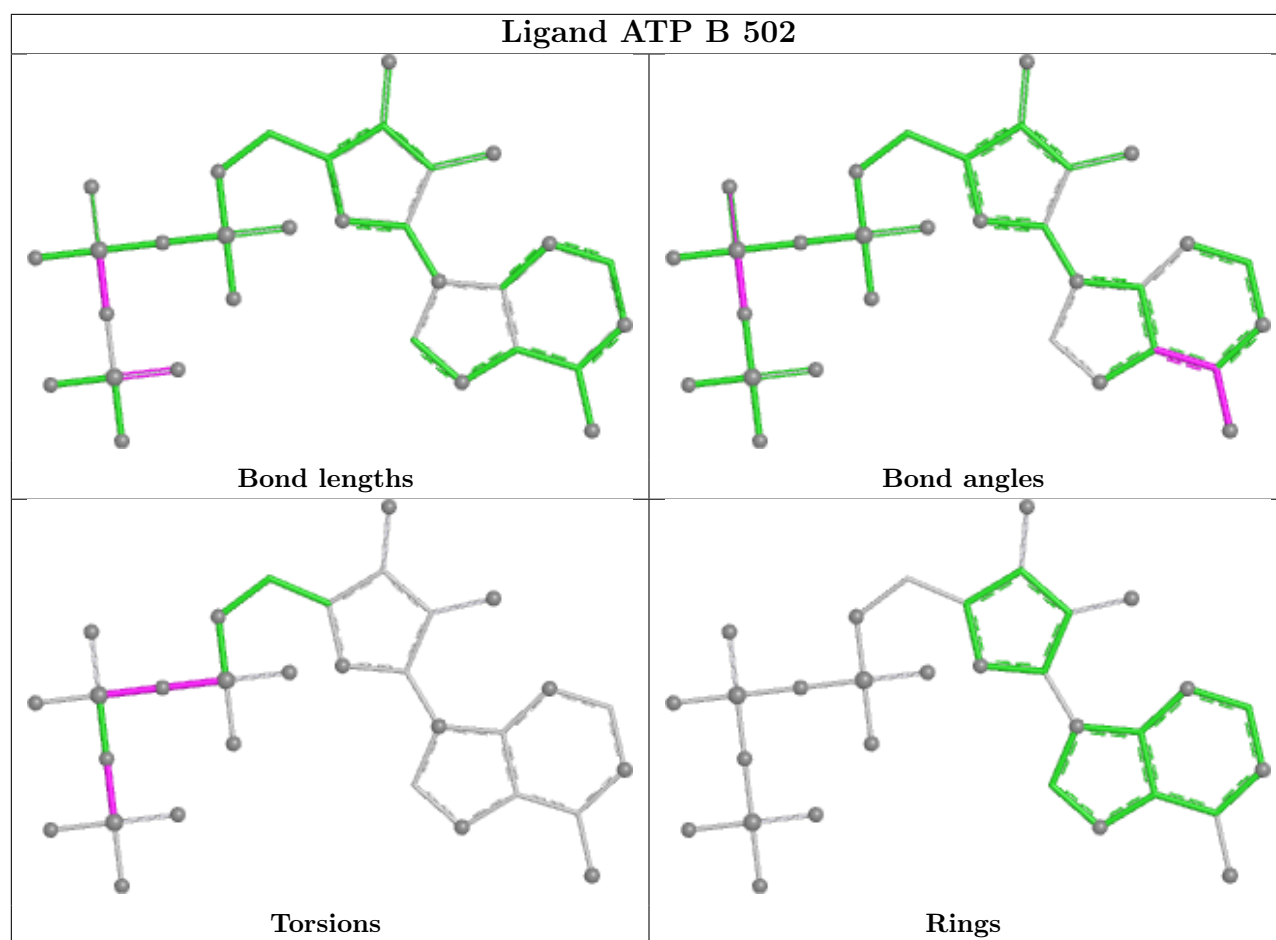
Mol	Chain	Res	Type	Atoms
4	B	502	ATP	PB-O3B-PG-O3G
4	B	502	ATP	PB-O3B-PG-O2G
4	B	502	ATP	PA-O3A-PB-O2B
4	B	502	ATP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	211/287 (73%)	0.41	22 (10%)	13 19	14, 28, 70, 100	0
2	B	427/466 (91%)	0.24	47 (11%)	12 17	15, 25, 55, 79	0
All	All	638/753 (84%)	0.30	69 (10%)	12 17	14, 26, 58, 100	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	PRO	8.0
2	B	274	GLY	6.4
1	A	259	PRO	6.1
1	A	256	TRP	6.0
2	B	180	HIS	5.7
2	B	275	ALA	5.3
2	B	277	SER	4.9
1	A	233	ILE	4.8
1	A	185	GLY	4.8
2	B	270	PRO	4.5
1	A	232	ARG	4.3
2	B	413	HIS	4.2
2	B	269	ASP	4.2
2	B	351	PRO	4.2
1	A	231	GLU	4.1
1	A	258	ALA	4.1
1	A	260	THR	4.0
1	A	216	LEU	4.0
2	B	230	LEU	4.0
2	B	273	LEU	4.0
2	B	276	CYS	3.9
2	B	272	ARG	3.9
1	A	261	ASP	3.9
2	B	268	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	388	LEU	3.9
2	B	216	PHE	3.7
2	B	456	ILE	3.6
2	B	452	GLY	3.6
2	B	453	VAL	3.5
2	B	450	LEU	3.5
2	B	372	GLY	3.4
2	B	337	PRO	3.4
1	A	184	GLY	3.4
2	B	229	THR	3.3
1	A	234	GLN	3.3
1	A	262	GLN	3.2
2	B	457	PRO	3.2
2	B	271	ARG	3.1
2	B	454	THR	3.1
2	B	390	THR	3.0
1	A	217	GLY	2.9
2	B	233	ARG	2.9
2	B	385	ALA	2.9
2	B	209	HIS	2.9
2	B	237	PHE	2.9
2	B	279	ARG	2.8
1	A	73	PHE	2.8
2	B	455	ALA	2.7
2	B	387	ALA	2.6
2	B	451	LYS	2.5
1	A	78	ARG	2.5
2	B	393	SER	2.5
2	B	386	GLN	2.5
2	B	142	GLU	2.5
1	A	263	GLU	2.4
2	B	228	ASP	2.4
1	A	255	GLN	2.3
2	B	2	ARG	2.3
2	B	41	TYR	2.3
1	A	235	SER	2.3
1	A	75	ARG	2.2
1	A	77	ALA	2.2
2	B	140	THR	2.2
2	B	394	ASP	2.2
2	B	192	ASN	2.2
2	B	384	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	134	ILE	2.1
2	B	352	LYS	2.1
2	B	391	ASN	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](#)

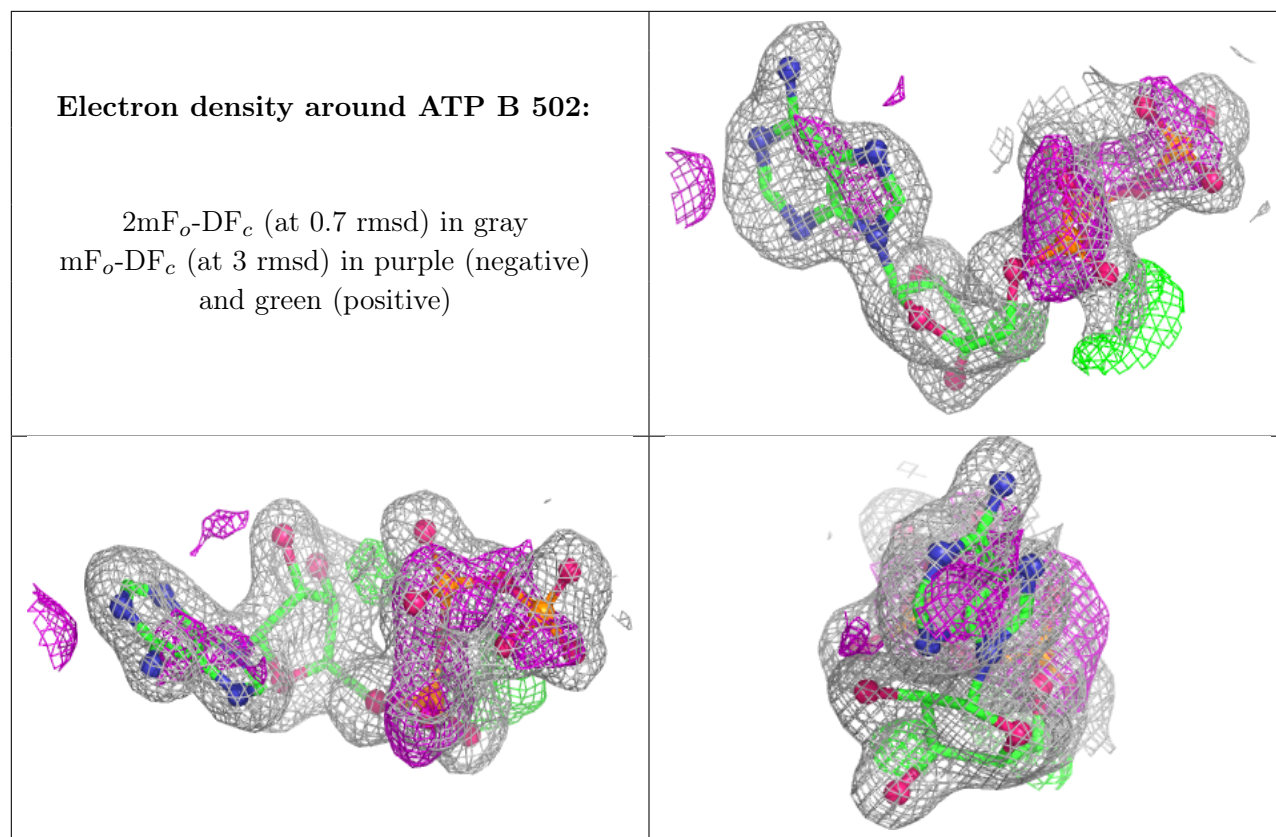
There are no oligosaccharides in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	ATP	B	502	31/31	0.92	0.09	19,26,31,34	0
3	ZN	B	501	1/1	0.97	0.05	25,25,25,25	0
5	MG	B	503	1/1	0.99	0.10	31,31,31,31	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.