



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:29 PM UTC

PDB ID : 8WIH / pdb_00008wih
Title : Crystal structure of E. coli ThrS catalytic domain mutant G463A in complex with ATP
Authors : Qiao, H.; Wang, Z.; Wang, J.; Fang, P.
Deposited on : 2023-09-24
Resolution : 2.44 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

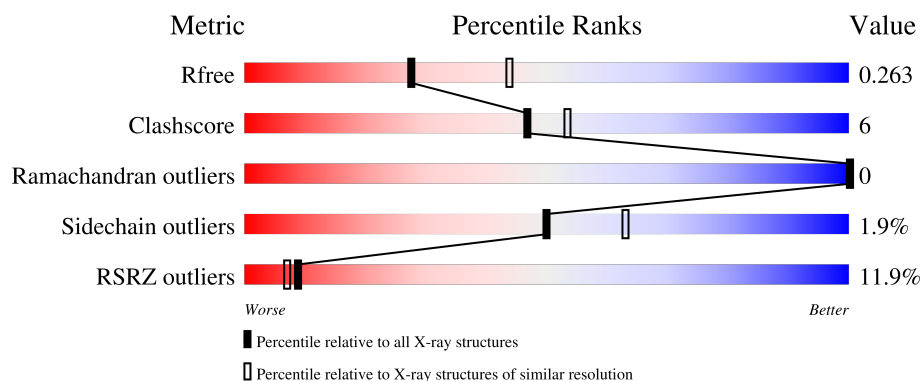
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	410	10% 81% 16% .
1	B	410	13% 84% 13% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6498 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.

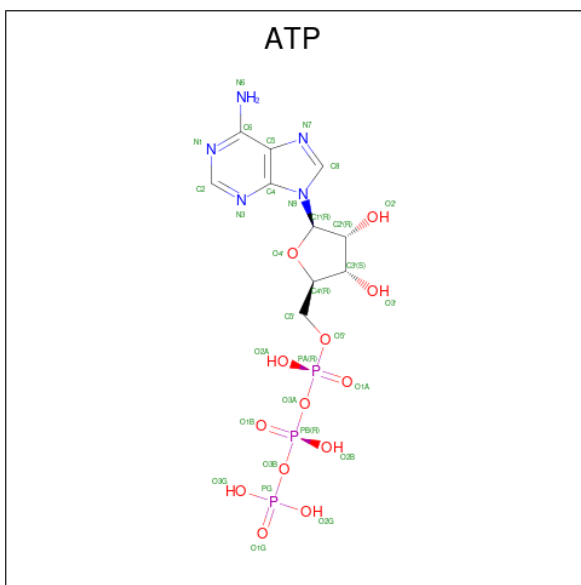
- Molecule 1 is a protein called Threonine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3204	2030	566	587	21			
1	B	399	Total	C	N	O	S	0	0	0
			3194	2025	567	579	23			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	initiating methionine	UNP A0A8S7FUD7
A	463	ALA	GLY	engineered mutation	UNP A0A8S7FUD7
A	643	LEU	-	expression tag	UNP A0A8S7FUD7
A	644	GLU	-	expression tag	UNP A0A8S7FUD7
A	645	HIS	-	expression tag	UNP A0A8S7FUD7
A	646	HIS	-	expression tag	UNP A0A8S7FUD7
A	647	HIS	-	expression tag	UNP A0A8S7FUD7
A	648	HIS	-	expression tag	UNP A0A8S7FUD7
A	649	HIS	-	expression tag	UNP A0A8S7FUD7
A	650	HIS	-	expression tag	UNP A0A8S7FUD7
B	241	MET	-	initiating methionine	UNP A0A8S7FUD7
B	463	ALA	GLY	engineered mutation	UNP A0A8S7FUD7
B	643	LEU	-	expression tag	UNP A0A8S7FUD7
B	644	GLU	-	expression tag	UNP A0A8S7FUD7
B	645	HIS	-	expression tag	UNP A0A8S7FUD7
B	646	HIS	-	expression tag	UNP A0A8S7FUD7
B	647	HIS	-	expression tag	UNP A0A8S7FUD7
B	648	HIS	-	expression tag	UNP A0A8S7FUD7
B	649	HIS	-	expression tag	UNP A0A8S7FUD7
B	650	HIS	-	expression tag	UNP A0A8S7FUD7

- 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
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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

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

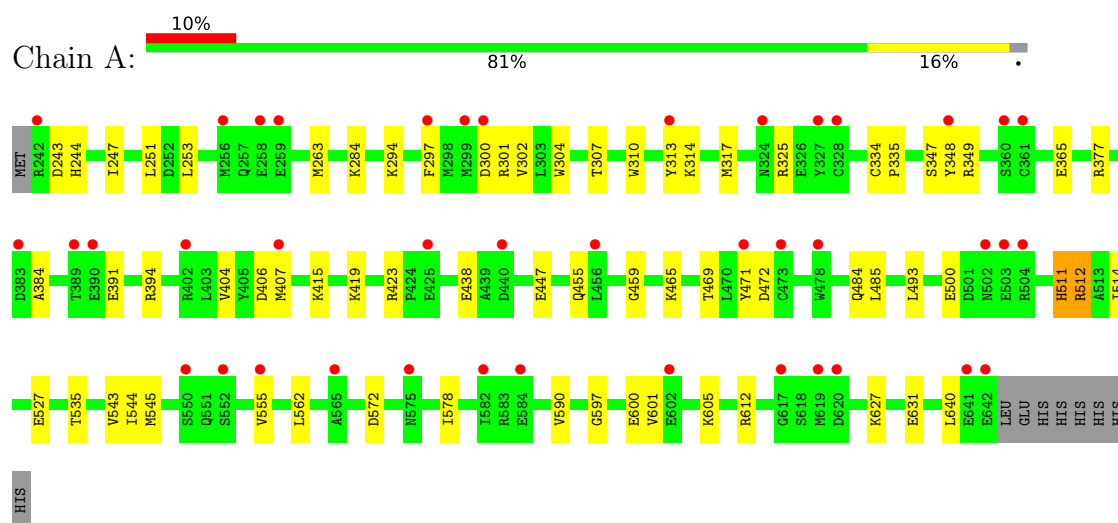
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	24	Total	O	0	0
			24	24		

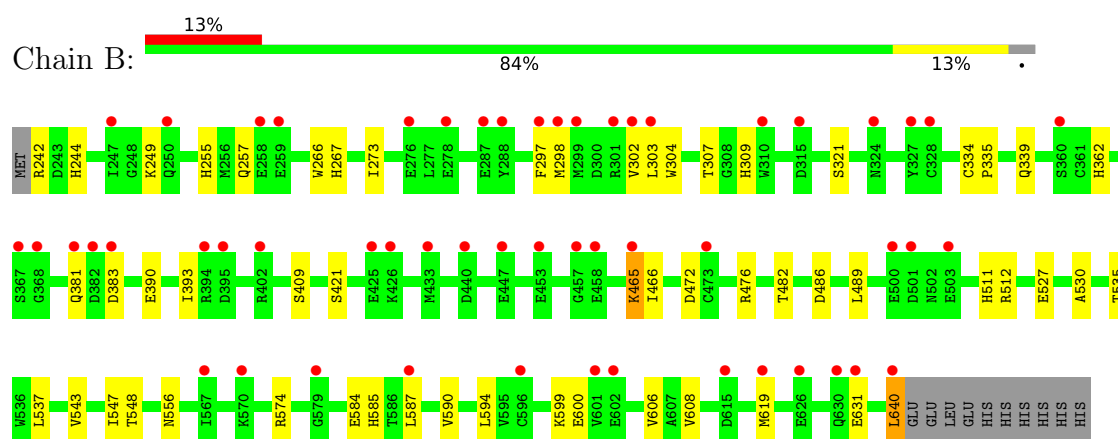
3 Residue-property plots [i](#)

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: Threonine-tRNA ligase



• Molecule 1: Threonine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.17Å 109.38Å 113.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.48 – 2.44 50.48 – 2.44	Depositor EDS
% Data completeness (in resolution range)	88.5 (50.48-2.44) 88.6 (50.48-2.44)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.240 , 0.264 0.240 , 0.263	Depositor DCC
R_{free} test set	1853 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6498	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	0.15	0/3275	0.32	0/4422
1	B	0.19	0/3265	0.35	1/4407 (0.0%)
All	All	0.17	0/6540	0.33	1/8829 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	465	LYS	N-CA-C	5.25	117.73	108.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3204	0	3091	41	0
1	B	3194	0	3099	33	0
2	A	27	0	12	0	0
2	B	23	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	24	0	0	2	0
4	B	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6498	0	6214	72	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 6.

All (72) 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:612:ARG:HA	4:A:813:HOH:O	1.52	1.09
1:A:419:LYS:HD3	1:A:455:GLN:HB2	1.75	0.68
1:B:547:ILE:HG22	1:B:548:THR:HG23	1.75	0.67
1:A:578:ILE:HD12	1:A:578:ILE:H	1.61	0.66
1:A:544:ILE:HG22	1:A:555:VAL:HG13	1.79	0.65
1:A:484:GLN:HB2	1:A:511:HIS:HB2	1.78	0.65
1:A:545:MET:HB3	1:A:572:ASP:HB3	1.80	0.63
1:B:297:PHE:HZ	1:B:362:HIS:CE1	2.18	0.61
1:B:608:VAL:HG21	1:B:619:MET:HE2	1.83	0.61
1:A:627:LYS:HB3	1:A:640:LEU:HD21	1.83	0.60
1:A:244:HIS:HB3	1:A:527:GLU:HG3	1.85	0.58
1:B:381:GLN:NE2	1:B:383:ASP:OD2	2.37	0.57
1:B:599:LYS:NZ	1:B:600:GLU:OE2	2.35	0.55
1:B:255:HIS:ND1	1:B:267:HIS:HE1	2.05	0.54
1:B:242:ARG:HD3	1:B:530:ALA:HB2	1.90	0.54
1:B:486:ASP:OD2	1:B:489:LEU:HB2	2.07	0.54
1:B:303:LEU:HD21	1:B:339:GLN:HE21	1.73	0.54
1:A:459:GLY:HA2	1:A:465:LYS:HD3	1.91	0.53
1:A:391:GLU:H	1:A:391:GLU:CD	2.17	0.52
1:A:415:LYS:HD3	1:A:471:TYR:CD1	2.46	0.51
1:A:300:ASP:OD1	1:A:301:ARG:N	2.45	0.50
1:A:404:VAL:HG22	1:A:514:ILE:HG23	1.94	0.49
1:A:535:THR:OG1	1:A:631:GLU:OE2	2.21	0.49
1:A:423:ARG:HH21	1:A:438:GLU:CD	2.20	0.49
1:B:535:THR:OG1	1:B:631:GLU:OE2	2.20	0.48
1:B:543:VAL:HG11	1:B:585:HIS:CD2	2.47	0.48
1:B:594:LEU:HD22	1:B:608:VAL:HG22	1.95	0.48
1:B:466:ILE:O	1:B:482:THR:HA	2.13	0.48
1:A:472:ASP:HB2	1:A:527:GLU:OE1	2.13	0.48
1:A:263:MET:HE1	1:B:298:MET:HE3	1.95	0.48
1:A:600:GLU:HB3	1:A:605:LYS:O	2.12	0.48
1:A:612:ARG:HD3	4:A:810:HOH:O	2.12	0.48
1:A:544:ILE:HD11	1:A:562:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ILE:HG23	1:B:537:LEU:HD22	1.97	0.47
1:A:300:ASP:OD1	1:A:302:VAL:HG13	2.15	0.46
1:A:365:GLU:O	1:A:377:ARG:NH2	2.49	0.46
1:A:543:VAL:HG23	1:A:590:VAL:HG11	1.98	0.46
1:A:294:LYS:HB3	1:B:266:TRP:HB2	1.98	0.45
1:A:394:ARG:NH1	1:A:447:GLU:OE2	2.50	0.45
1:B:594:LEU:HB3	1:B:606:VAL:HG21	1.98	0.45
1:A:304:TRP:CZ3	1:A:335:PRO:HG2	2.51	0.45
1:B:304:TRP:CZ3	1:B:335:PRO:HG2	2.51	0.44
1:B:390:GLU:HA	1:B:393:ILE:HD12	1.97	0.44
1:B:249:LYS:HB3	1:B:249:LYS:HE3	1.73	0.44
1:A:348:TYR:CZ	1:A:500:GLU:HG2	2.52	0.44
1:A:391:GLU:OE1	1:A:391:GLU:N	2.44	0.44
1:B:556:ASN:HD22	1:B:556:ASN:HA	1.66	0.43
1:B:303:LEU:HD11	1:B:335:PRO:HB3	2.00	0.43
1:A:284:LYS:NZ	1:A:406:ASP:OD2	2.51	0.43
1:A:243:ASP:O	1:A:247:ILE:HG13	2.19	0.43
1:B:244:HIS:HB3	1:B:527:GLU:HG2	2.00	0.43
1:B:421:SER:HB2	1:B:465:LYS:HG3	1.99	0.43
1:A:511:HIS:CD2	1:A:511:HIS:N	2.87	0.42
1:A:251:LEU:HB2	1:A:253:LEU:HG	2.02	0.42
1:B:472:ASP:OD2	1:B:476:ARG:HB2	2.18	0.42
1:B:255:HIS:NE2	1:B:257:GLN:HG3	2.35	0.42
1:A:310:TRP:O	1:A:314:LYS:HD3	2.20	0.42
1:A:348:TYR:CE2	1:A:349:ARG:HD2	2.55	0.42
1:B:307:THR:OG1	1:B:309:HIS:ND1	2.50	0.42
1:B:472:ASP:HB2	1:B:527:GLU:OE1	2.19	0.42
1:B:574:ARG:NH2	1:B:584:GLU:OE2	2.53	0.41
1:A:597:GLY:O	1:A:601:VAL:HG23	2.20	0.41
1:A:284:LYS:HG3	1:A:407:MET:SD	2.61	0.41
1:A:307:THR:HG22	1:A:493:LEU:HD21	2.01	0.41
1:A:347:SER:OG	1:A:349:ARG:HD3	2.21	0.41
1:A:384:ALA:HB3	1:A:512:ARG:HD3	2.02	0.41
1:B:543:VAL:HG23	1:B:590:VAL:HG11	2.02	0.41
1:B:255:HIS:HE2	1:B:257:GLN:HG3	1.84	0.41
1:B:587:LEU:HD23	1:B:587:LEU:HA	1.91	0.41
1:B:640:LEU:HD22	1:B:640:LEU:HA	1.83	0.41
1:A:313:TYR:HB3	1:A:317:MET:HE2	2.03	0.41
1:A:485:LEU:HD12	1:A:485:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	399/410 (97%)	396 (99%)	3 (1%)	0	100	100
1	B	397/410 (97%)	391 (98%)	6 (2%)	0	100	100
All	All	796/820 (97%)	787 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	336/365 (92%)	330 (98%)	6 (2%)	51	64
1	B	336/365 (92%)	329 (98%)	7 (2%)	47	60
All	All	672/730 (92%)	659 (98%)	13 (2%)	50	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	PHE
1	A	325	ARG
1	A	334	CYS
1	A	469	THR
1	A	511	HIS
1	A	512	ARG
1	B	302	VAL
1	B	321	SER

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Mol	Chain	Res	Type
1	B	334	CYS
1	B	409	SER
1	B	511	HIS
1	B	512	ARG
1	B	640	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	455	GLN
1	A	564	ASN
1	B	257	GLN
1	B	267	HIS
1	B	362	HIS
1	B	371	HIS
1	B	381	GLN
1	B	455	GLN
1	B	556	ASN
1	B	564	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	A	701	-	28,29,33	0.75	1 (3%)	43,45,52	0.69	2 (4%)
2	ATP	B	701	-	25,25,33	0.51	0	37,38,52	0.55	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	A	701	-	-	4/16/32/38	0/3/3/3
2	ATP	B	701	-	-	5/10/26/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ATP	PB-O1B	3.01	1.59	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ATP	O3B-PB-O3A	2.24	112.15	104.64
2	A	701	ATP	O3B-PB-O2B	2.07	115.57	107.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ATP	C5'-O5'-PA-O1A
2	B	701	ATP	C5'-O5'-PA-O1A
2	B	701	ATP	C5'-O5'-PA-O2A
2	B	701	ATP	C5'-O5'-PA-O3A
2	B	701	ATP	O4'-C4'-C5'-O5'
2	A	701	ATP	O4'-C4'-C5'-O5'
2	A	701	ATP	C5'-O5'-PA-O2A
2	A	701	ATP	C5'-O5'-PA-O3A

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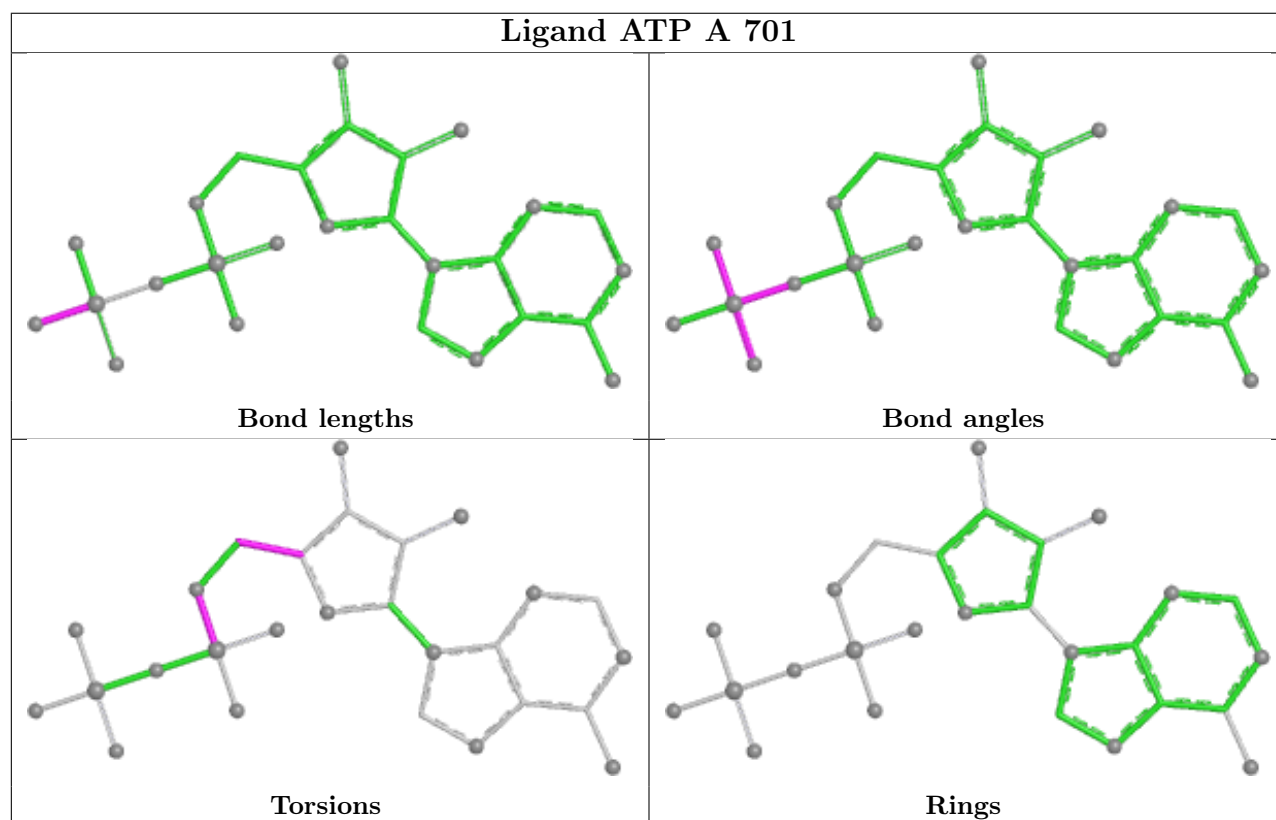
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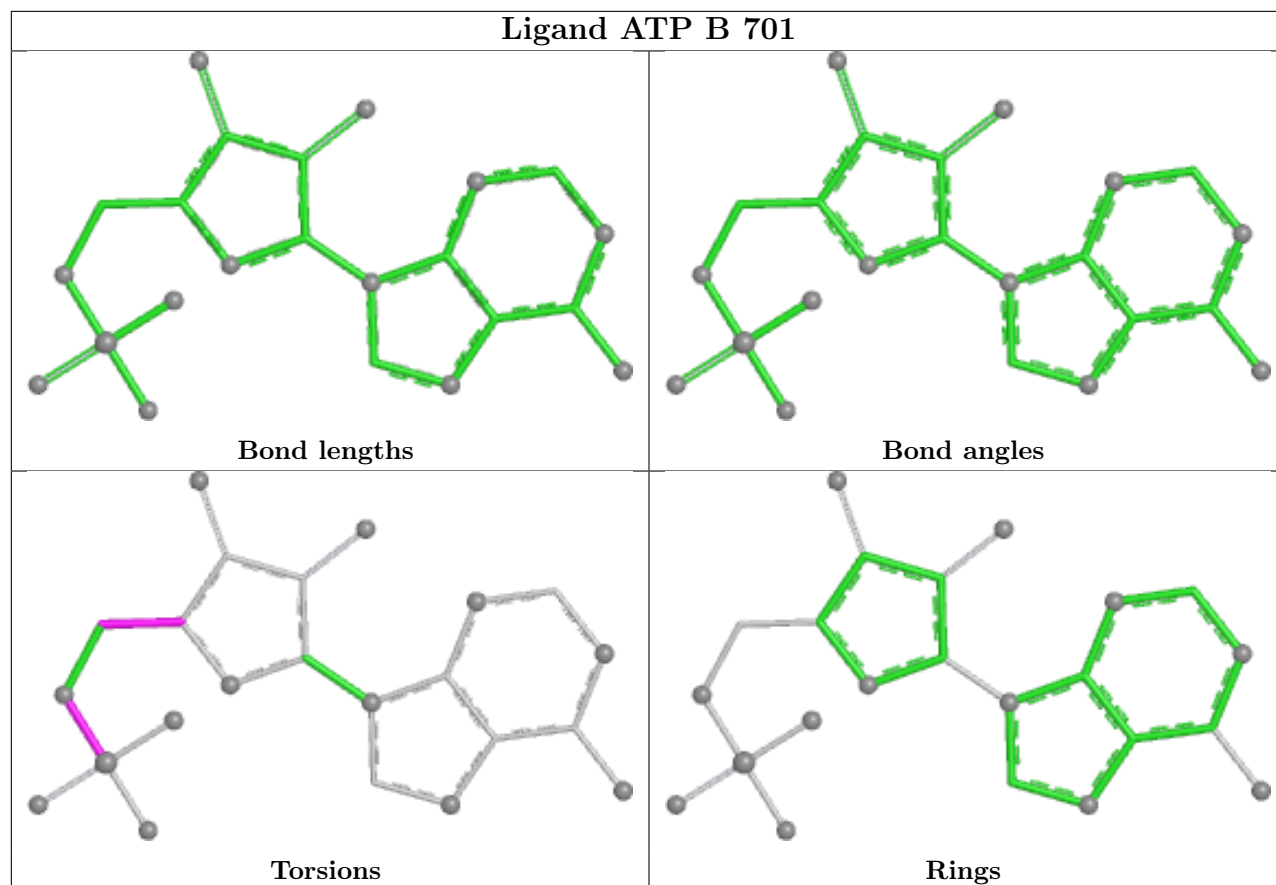
Mol	Chain	Res	Type	Atoms
2	B	701	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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	401/410 (97%)	0.81	41 (10%) 12 9	27, 40, 58, 87	220 (54%)
1	B	399/410 (97%)	0.94	54 (13%) 7 5	22, 38, 53, 75	238 (59%)
All	All	800/820 (97%)	0.87	95 (11%) 9 7	22, 39, 56, 87	458 (57%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	PHE	6.2
1	B	259	GLU	6.2
1	B	425	GLU	4.5
1	A	242	ARG	4.1
1	A	297	PHE	3.9
1	B	288	TYR	3.7
1	B	301	ARG	3.7
1	B	602	GLU	3.6
1	A	313	TYR	3.5
1	B	426	LYS	3.4
1	B	383	ASP	3.3
1	B	250	GLN	3.3
1	A	504	ARG	3.2
1	B	299	MET	3.2
1	B	247	ILE	3.2
1	A	550	SER	3.1
1	A	503	GLU	3.1
1	A	383	ASP	3.1
1	B	601	VAL	3.0
1	A	324	ASN	3.0
1	A	407	MET	3.0
1	B	447	GLU	3.0
1	B	402	ARG	2.9
1	A	328	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	473	CYS	2.9
1	A	300	ASP	2.9
1	A	327	TYR	2.9
1	A	299	MET	2.8
1	B	433	MET	2.8
1	B	631	GLU	2.8
1	A	555	VAL	2.8
1	A	471	TYR	2.8
1	A	642	GLU	2.8
1	A	259	GLU	2.8
1	B	298	MET	2.7
1	B	500	GLU	2.7
1	B	630	GLN	2.7
1	B	596	CYS	2.7
1	B	287	GLU	2.7
1	A	575	ASN	2.7
1	B	360	SER	2.7
1	A	258	GLU	2.7
1	A	390	GLU	2.6
1	B	382	ASP	2.6
1	A	402	ARG	2.6
1	B	619	MET	2.6
1	A	425	GLU	2.6
1	A	619	MET	2.6
1	A	641	GLU	2.6
1	A	440	ASP	2.6
1	B	579	GLY	2.6
1	B	328	CYS	2.6
1	B	258	GLU	2.5
1	B	303	LEU	2.5
1	B	302	VAL	2.5
1	A	602	GLU	2.5
1	B	458	GLU	2.5
1	B	465	LYS	2.5
1	B	453	GLU	2.5
1	B	368	GLY	2.5
1	B	567	ILE	2.5
1	A	256	MET	2.5
1	B	367	SER	2.4
1	A	360	SER	2.4
1	B	278	GLU	2.4
1	A	389	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	552	SER	2.4
1	B	310	TRP	2.4
1	B	440	ASP	2.3
1	B	501	ASP	2.3
1	B	324	ASN	2.3
1	A	582	ILE	2.3
1	A	473	CYS	2.3
1	A	361	CYS	2.3
1	B	315	ASP	2.2
1	B	276	GLU	2.2
1	B	615	ASP	2.2
1	B	381	GLN	2.2
1	B	626	GLU	2.2
1	B	570	LYS	2.2
1	A	502	ASN	2.1
1	A	456	LEU	2.1
1	B	457	GLY	2.1
1	B	640	LEU	2.1
1	B	327	TYR	2.1
1	A	478	TRP	2.1
1	A	565	ALA	2.1
1	A	620	ASP	2.1
1	A	617	GLY	2.1
1	B	587	LEU	2.1
1	B	394	ARG	2.1
1	B	395	ASP	2.1
1	A	584	GLU	2.0
1	B	503	GLU	2.0
1	A	348	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

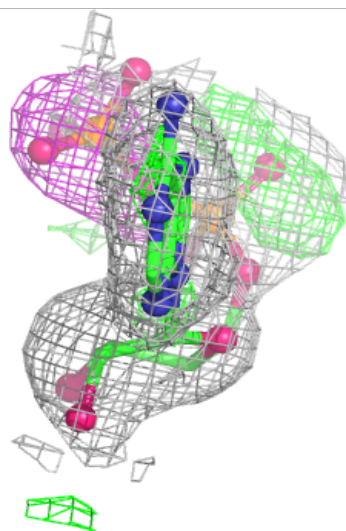
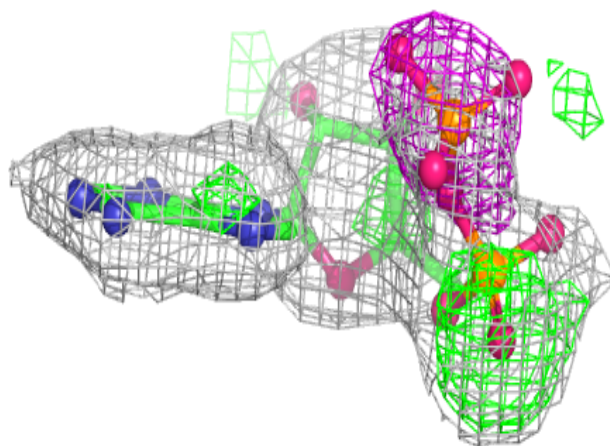
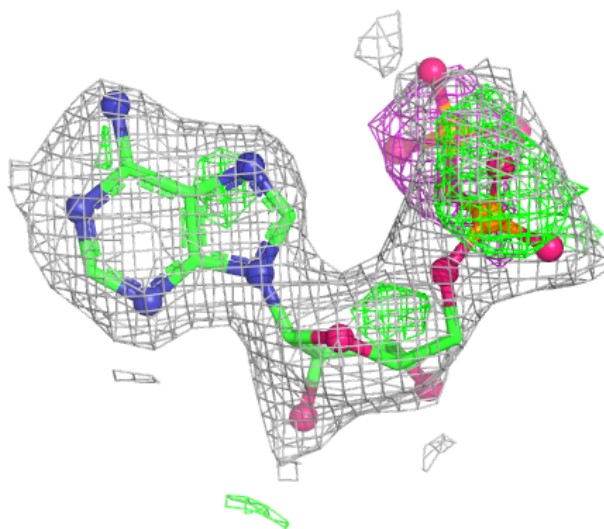
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ATP	A	701	27/31	0.74	0.24	39,40,44,44	27
2	ATP	B	701	23/31	0.89	0.14	38,38,39,40	23
3	ZN	B	702	1/1	0.97	0.04	38,38,38,38	0
3	ZN	A	702	1/1	0.98	0.04	38,38,38,38	1

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

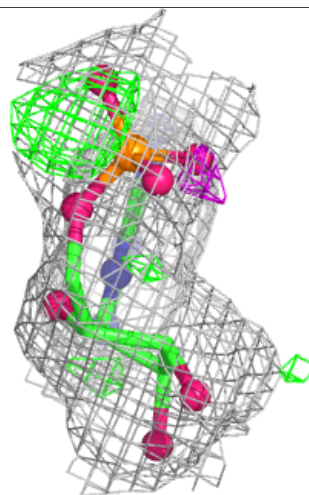
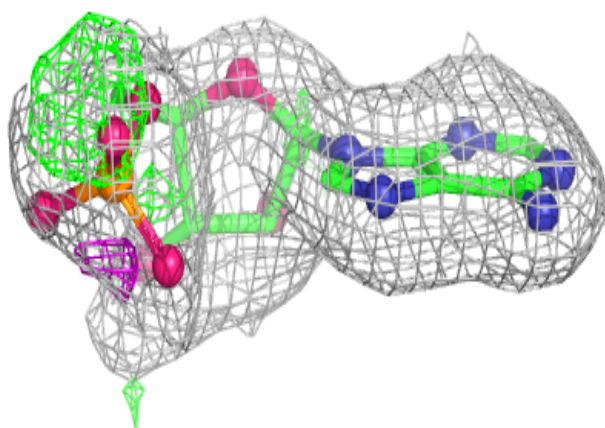
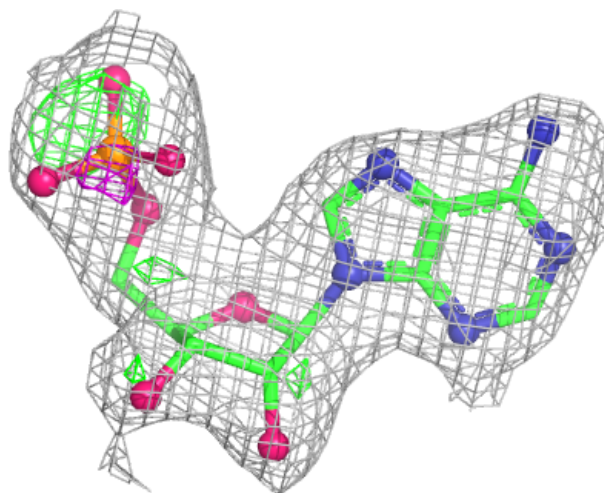
Electron density around ATP A 701:

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



Electron density around ATP B 701:

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.