



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 05:14 pm BST

PDB ID : 1B76
Title : GLYCYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS
COMPLEXED WITH ATP
Authors : Arnez, J.G.; Moras, D.
Deposited on : 1999-01-27
Resolution : 3.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

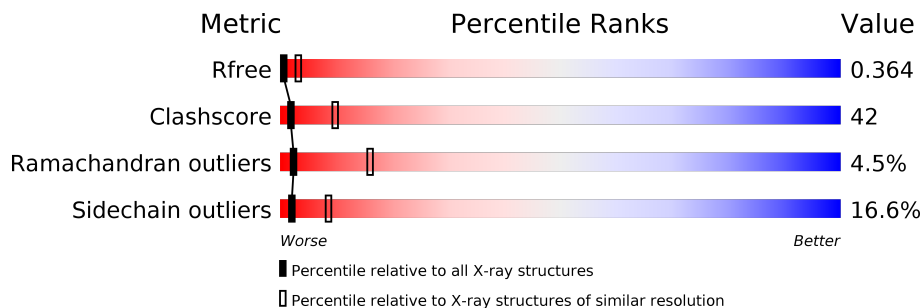
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	442	 39% 49% 11% •
1	B	442	 39% 47% 13% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8961 atoms, of which 1686 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 Glycine-tRNA ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	442	4451	2297	841	649	656	8	0	0	0
1	B	442	4440	2288	839	649	656	8	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

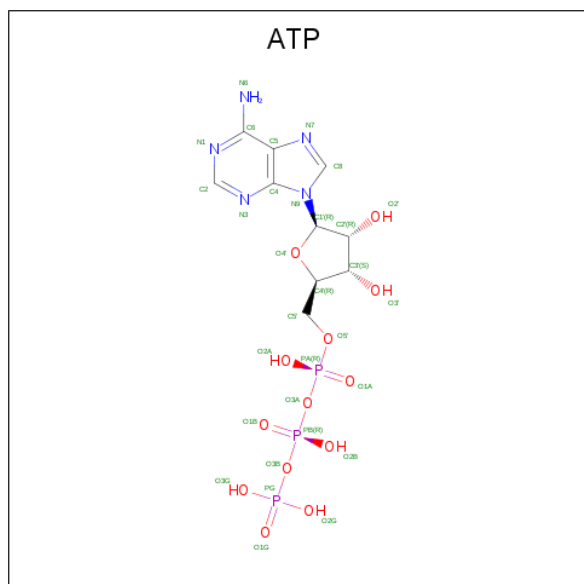
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	PRO	conflict	UNP P56206
A	91	ALA	ARG	conflict	UNP P56206
A	92	LYS	ILE	conflict	UNP P56206
A	93	ALA	THR	conflict	UNP P56206
A	94	ARG	LYS	conflict	UNP P56206
A	95	TYR	LYS	conflict	UNP P56206
A	170	GLN	LYS	conflict	UNP P56206
A	171	ASP	THR	conflict	UNP P56206
A	172	LEU	TYR	conflict	UNP P56206
A	173	ARG	VAL	conflict	UNP P56206
A	176	ARG	VAL	conflict	UNP P56206
A	177	GLY	GLU	conflict	UNP P56206
A	178	GLY	ASP	conflict	UNP P56206
A	179	ARG	GLU	conflict	UNP P56206
A	180	GLY	ALA	conflict	UNP P56206
A	181	LEU	SER	conflict	UNP P56206
A	209	GLY	PRO	conflict	UNP P56206
A	283	SER	GLU	conflict	UNP P56206
A	284	SER	LEU	conflict	UNP P56206
A	302	SER	LEU	conflict	UNP P56206
A	303	LEU	GLU	conflict	UNP P56206
A	310	GLN	ASN	conflict	UNP P56206
B	1	ALA	PRO	conflict	UNP P56206
B	91	ALA	ARG	conflict	UNP P56206
B	92	LYS	ILE	conflict	UNP P56206

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Chain	Residue	Modelled	Actual	Comment	Reference
B	93	ALA	THR	conflict	UNP P56206
B	94	ARG	LYS	conflict	UNP P56206
B	95	TYR	LYS	conflict	UNP P56206
B	170	GLN	LYS	conflict	UNP P56206
B	171	ASP	THR	conflict	UNP P56206
B	172	LEU	TYR	conflict	UNP P56206
B	173	ARG	VAL	conflict	UNP P56206
B	176	ARG	VAL	conflict	UNP P56206
B	177	GLY	GLU	conflict	UNP P56206
B	178	GLY	ASP	conflict	UNP P56206
B	179	ARG	GLU	conflict	UNP P56206
B	180	GLY	ALA	conflict	UNP P56206
B	181	LEU	SER	conflict	UNP P56206
B	209	GLY	PRO	conflict	UNP P56206
B	283	SER	GLU	conflict	UNP P56206
B	284	SER	LEU	conflict	UNP P56206
B	302	SER	LEU	conflict	UNP P56206
B	303	LEU	GLU	conflict	UNP P56206
B	310	GLN	ASN	conflict	UNP P56206

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O	P		
2	A	1	34	10	3	5	13	3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	B	1	34	10	3	5	13	3	0	0

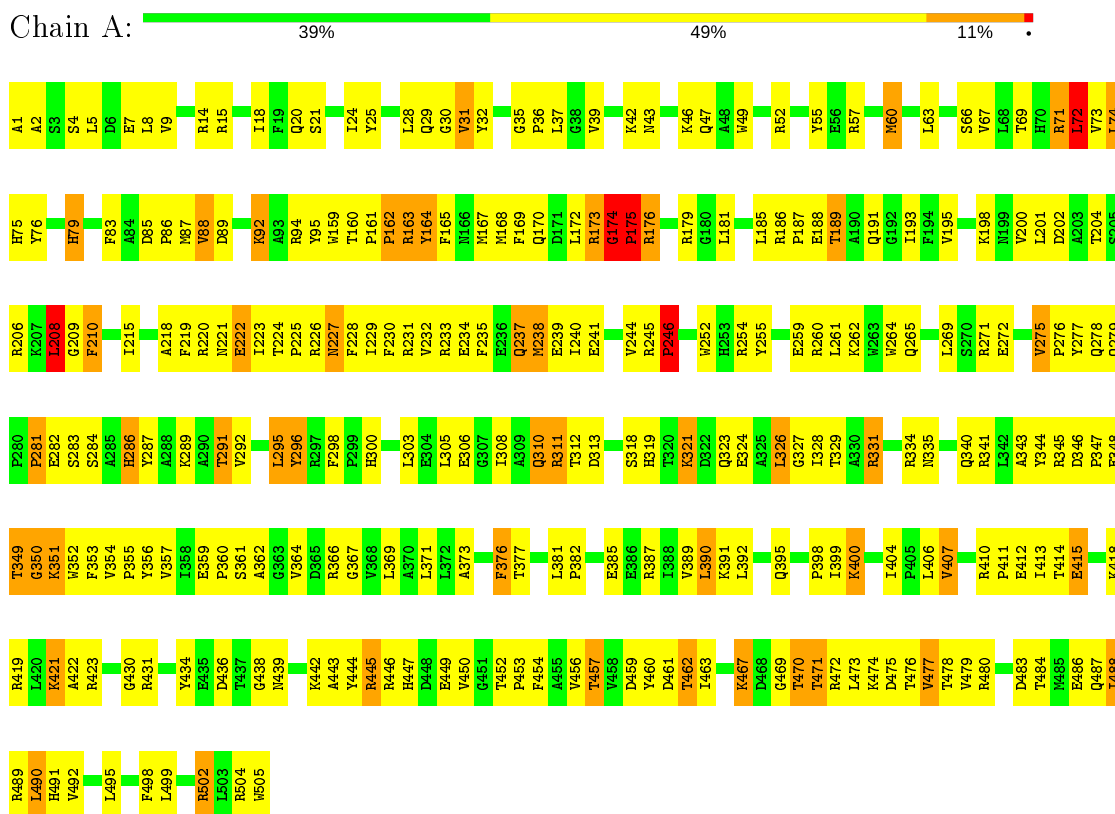
- Molecule 3 is water.

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

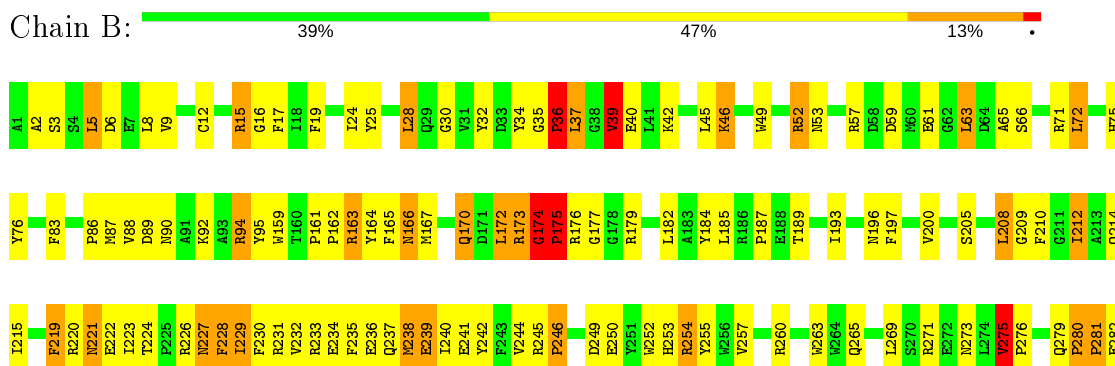
3 Residue-property plots

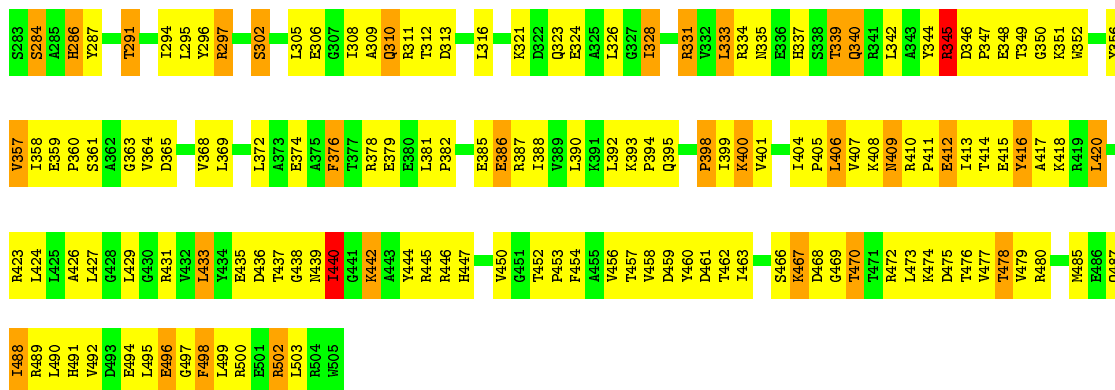
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: Glycine-tRNA ligase



- Molecule 1: Glycine-tRNA ligase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.80Å 250.90Å 105.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 3.40 12.16 – 3.30	Depositor EDS
% Data completeness (in resolution range)	83.0 (9.00-3.40) 80.4 (12.16-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	9.50	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.28Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.227 , 0.318 0.297 , 0.364	Depositor DCC
R_{free} test set	784 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å ²)	79.4	Xtrriage
Anisotropy	0.283	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 108.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	8961	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.71	0/3696	0.92	6/4999 (0.1%)
1	B	0.66	0/3686	0.91	9/4986 (0.2%)
All	All	0.69	0/7382	0.91	15/9985 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	174	GLY	C-N-CD	-9.31	100.11	120.60
1	A	174	GLY	C-N-CD	-8.00	102.99	120.60
1	B	39	VAL	CB-CA-C	-7.07	97.96	111.40
1	A	208	LEU	N-CA-C	6.75	129.23	111.00
1	B	208	LEU	N-CA-C	6.64	128.94	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	TYR	Sidechain

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	3610	841	3565	308	0
1	B	3601	839	3547	319	0
2	A	31	3	12	5	0
2	B	31	3	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	7275	1686	7136	599	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 42.

The worst 5 of 599 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:B:88:VAL:HG22	1:B:162:PRO:HB3	1.26	1.09
1:B:413:ILE:HG12	1:B:463:ILE:HD11	1.35	1.04
1:A:366:ARG:NH1	2:A:1552:ATP:H2'	1.72	1.02
1:A:400:LYS:HD3	1:A:430:GLY:HA3	1.43	1.00
1:B:442:LYS:HA	1:B:445:ARG:HD3	1.46	0.96

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	438/442 (99%)	355 (81%)	65 (15%)	18 (4%)	3 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	438/442 (99%)	354 (81%)	63 (14%)	21 (5%)	2	15
All	All	876/884 (99%)	709 (81%)	128 (15%)	39 (4%)	2	16

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	PRO
1	A	281	PRO
1	A	286	HIS
1	A	438	GLY
1	B	92	LYS

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	375/376 (100%)	315 (84%)	60 (16%)	2	10
1	B	374/376 (100%)	310 (83%)	64 (17%)	2	8
All	All	749/752 (100%)	625 (83%)	124 (17%)	2	8

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	478	THR
1	B	52	ARG
1	B	442	LYS
1	A	488	ILE
1	B	6	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	487	GLN
1	B	44	ASN

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Mol	Chain	Res	Type
1	B	237	GLN
1	A	340	GLN
1	B	253	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	1552	-	26,33,33	0.67	0	31,52,52	0.76	0
2	ATP	B	2552	-	26,33,33	0.68	0	31,52,52	0.76	1 (3%)

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	1552	-	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	2552	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	2552	ATP	C5-C6-N6	2.33	123.90	120.35

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

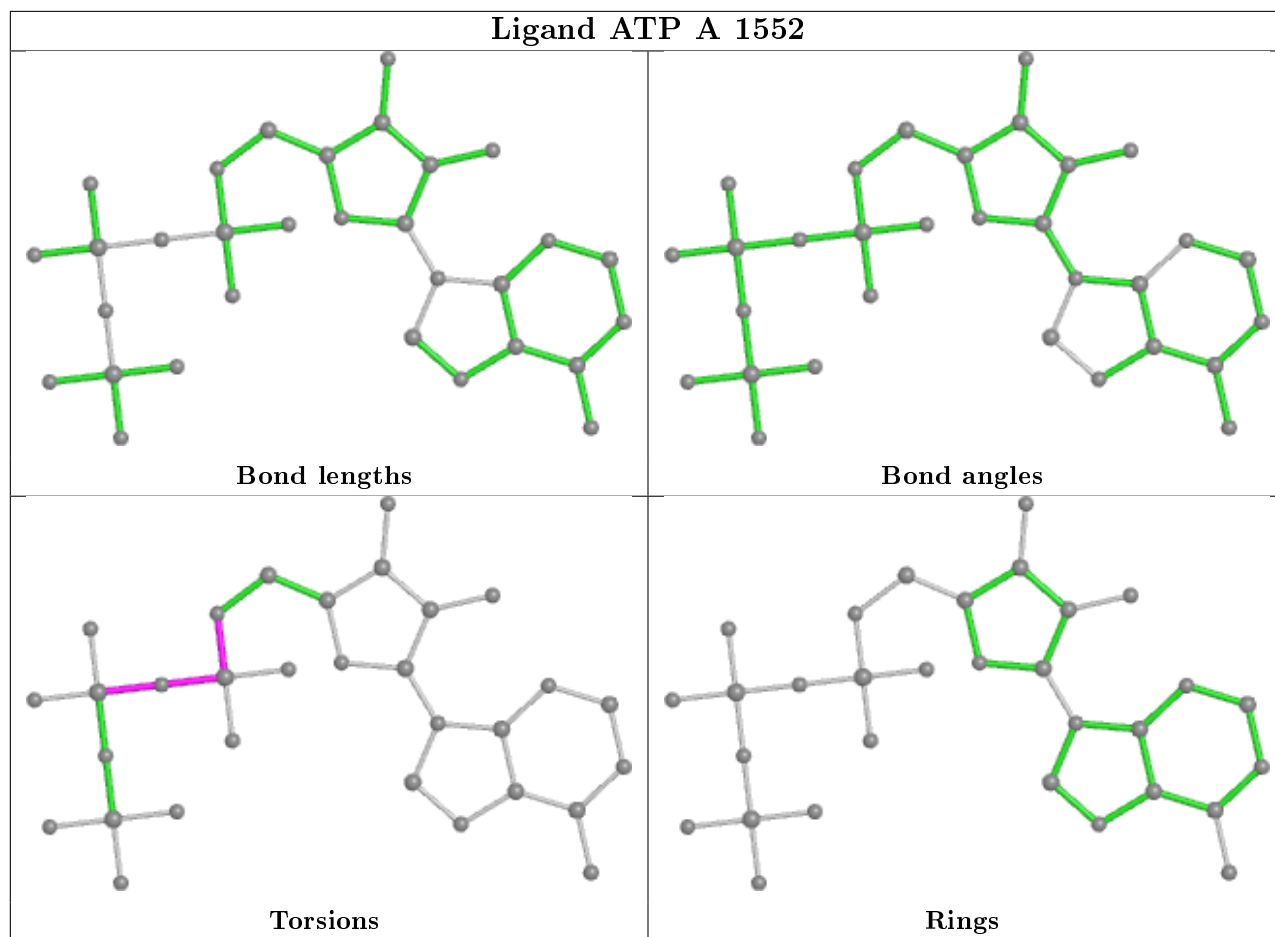
Mol	Chain	Res	Type	Atoms
2	A	1552	ATP	PB-O3A-PA-O5'
2	A	1552	ATP	C5'-O5'-PA-O2A
2	A	1552	ATP	C5'-O5'-PA-O3A
2	B	2552	ATP	PB-O3A-PA-O5'
2	B	2552	ATP	PB-O3B-PG-O1G

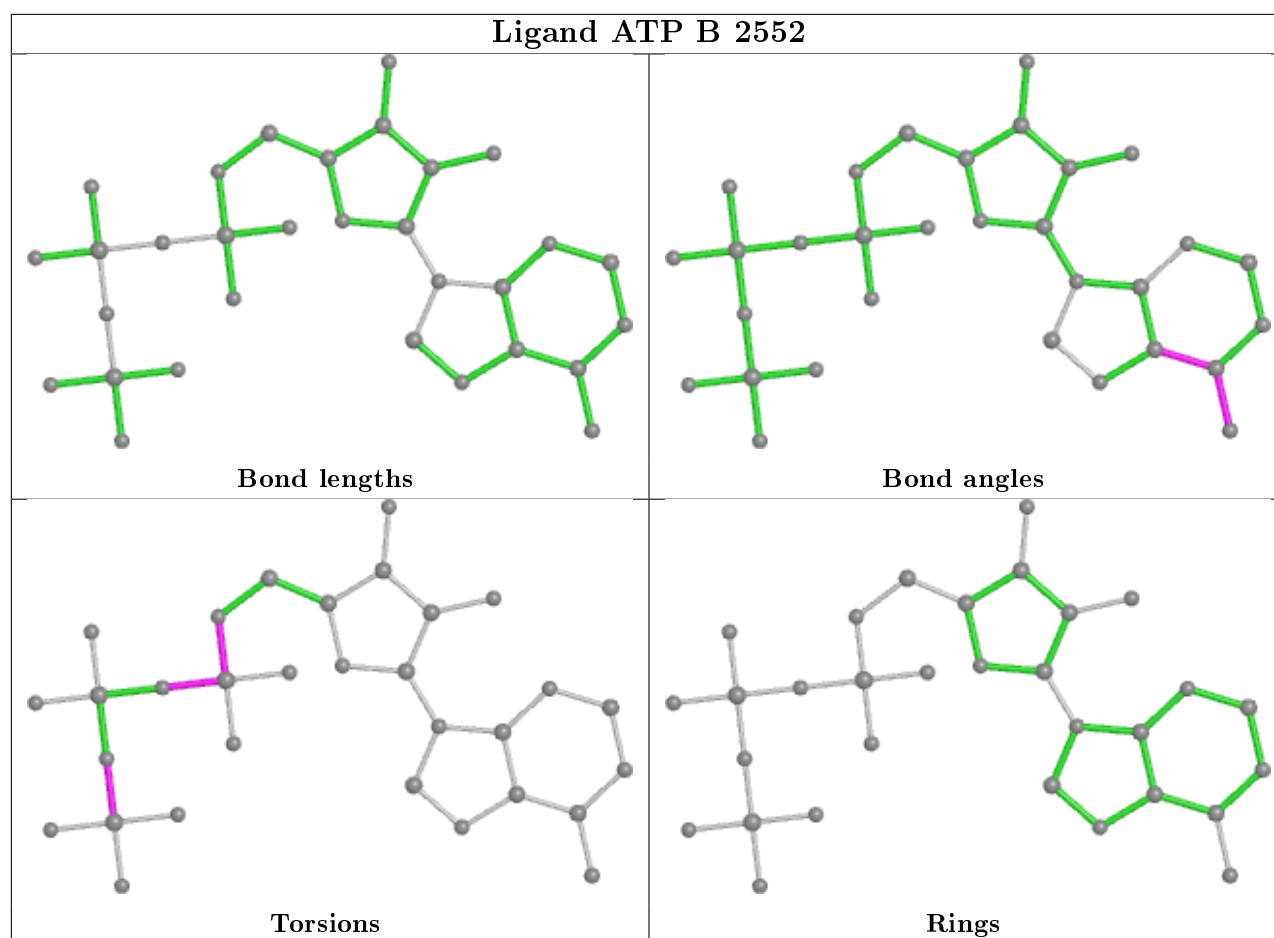
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1552	ATP	5	0
2	B	2552	ATP	3	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 [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	95:TYR	C	159:TRP	N	11.48
1	B	95:TYR	C	159:TRP	N	11.20

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

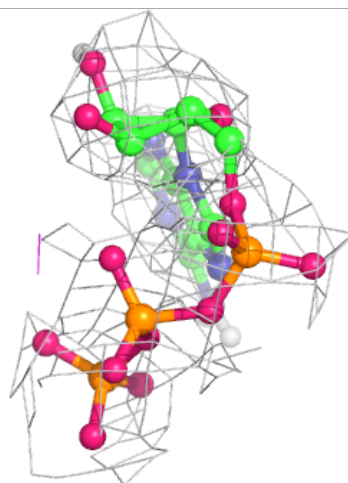
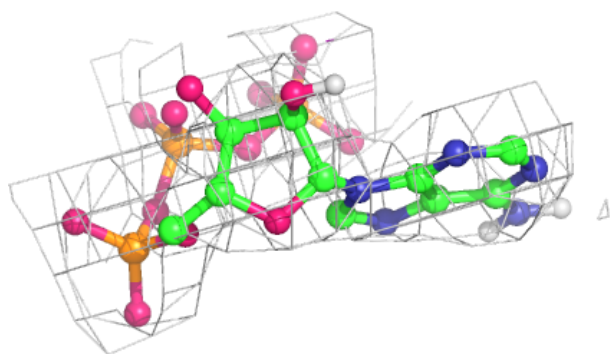
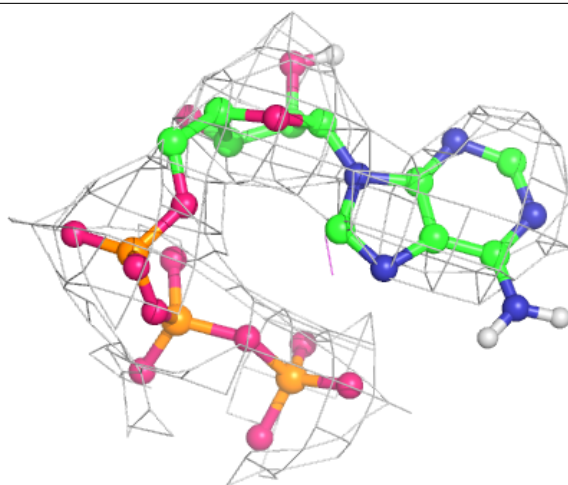
6.4 Ligands

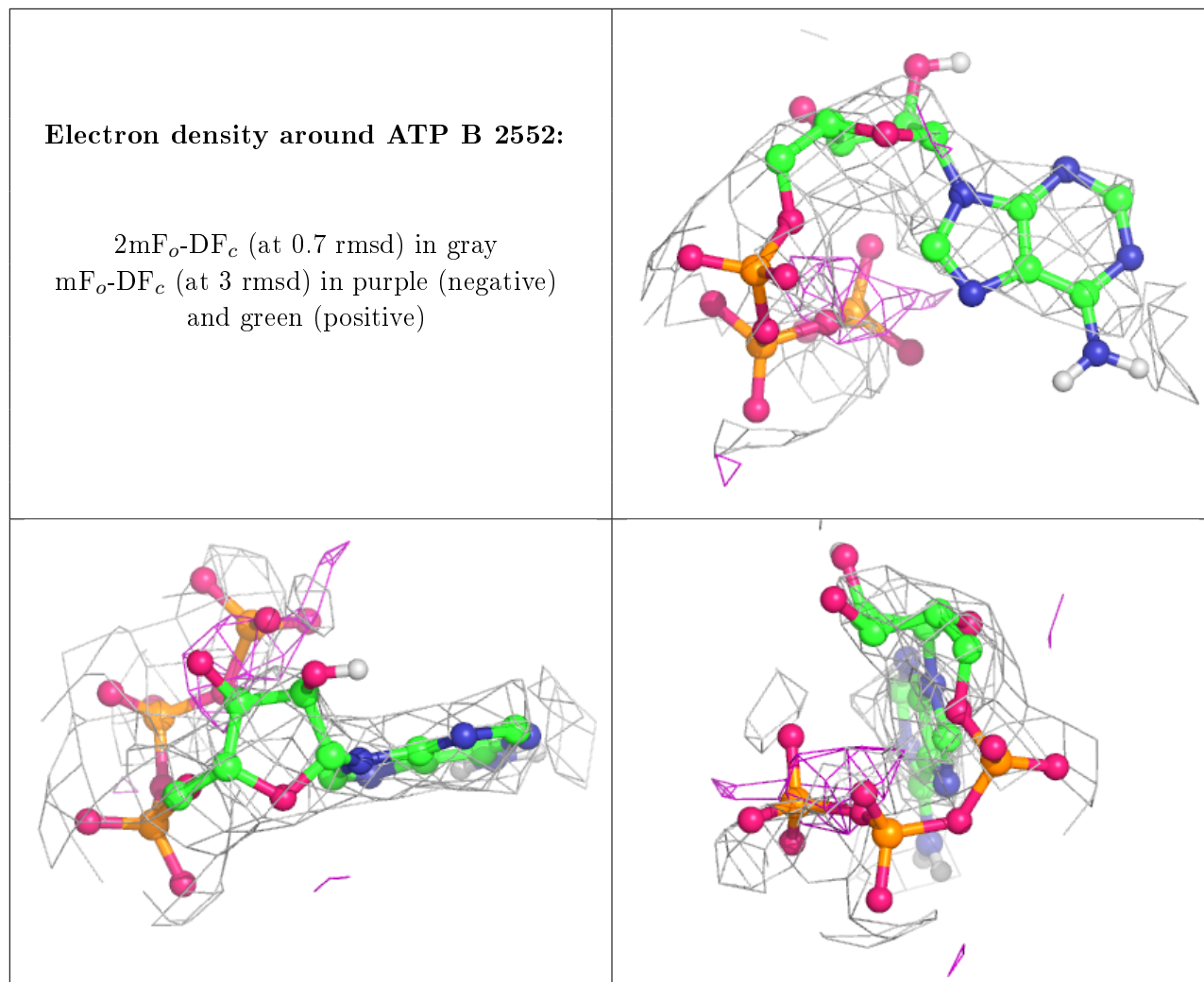
Unable to reproduce the depositors R factor - this section is therefore empty.

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 1552:

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





6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.