



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:27 pm BST

PDB ID : 4AT1
Title : STRUCTURAL CONSEQUENCES OF EFFECTOR BINDING TO THE
T STATE OF ASPARTATE CARBAMOYLTRANSFERASE. CRYSTAL
STRUCTURES OF THE UNLIGATED AND ATP-, AND CTP-
COMPLEXED ENZYMES AT 2.6-ANGSTROMS RESOLUTION
Authors : Stevens, R.C.; Gouaux, J.E.; Lipscomb, W.N.
Deposited on : 1990-04-26
Resolution : 2.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

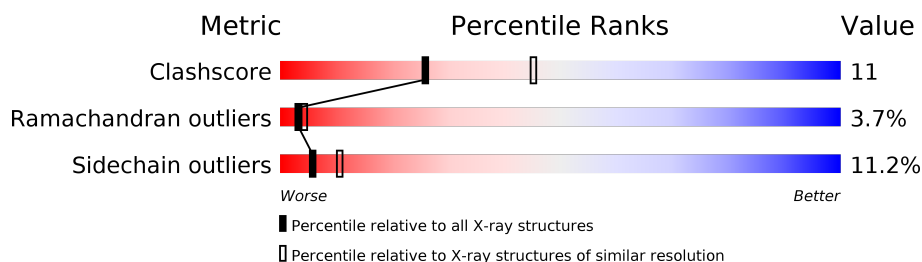
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	
1	C	310	
2	B	153	
2	D	153	

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
4	ATP	B	155	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7170 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 ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	CONFLICT	UNP P0A786
A	147	GLN	GLU	CONFLICT	UNP P0A786
A	149	GLU	GLN	CONFLICT	UNP P0A786
A	196	GLU	GLN	CONFLICT	UNP P0A786
C	60	GLN	GLU	CONFLICT	UNP P0A786
C	147	GLN	GLU	CONFLICT	UNP P0A786
C	149	GLU	GLN	CONFLICT	UNP P0A786
C	196	GLU	GLN	CONFLICT	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

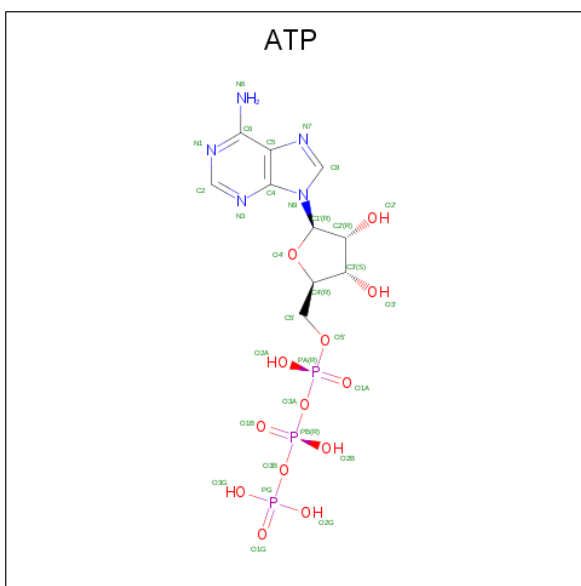
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	CONFLICT	UNP P0A7F3
D	8	GLY	GLN	CONFLICT	UNP P0A7F3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



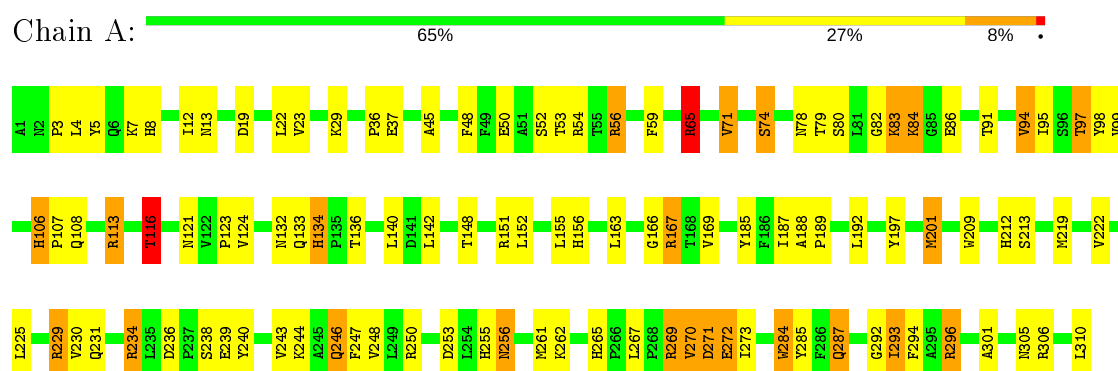
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

3 Residue-property plots

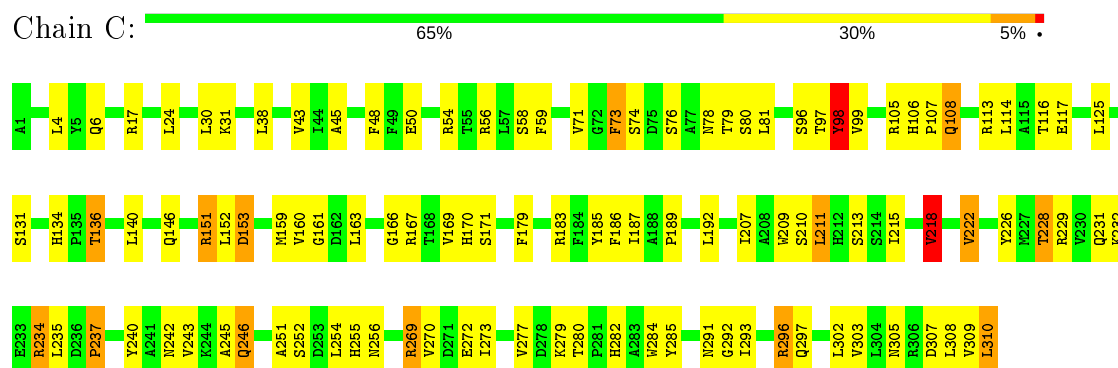
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

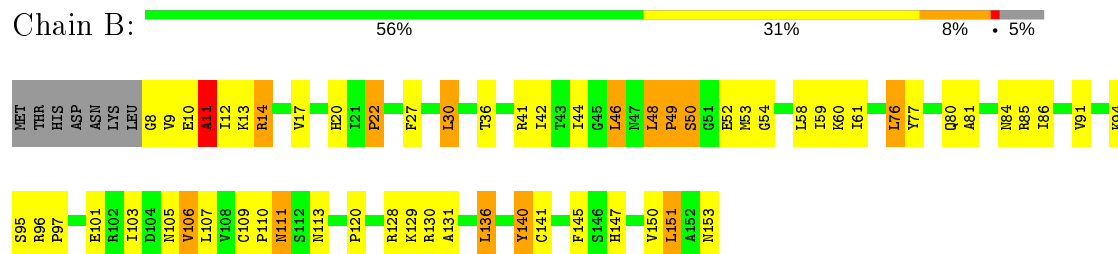
• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN



• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN



• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



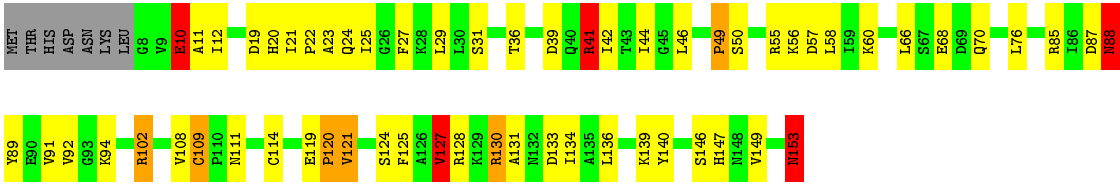
• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN

Chain D:

56%

32%

• • 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.00 Å 122.00 Å 142.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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: ZN, 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	0.86	0/2461	1.64	40/3339 (1.2%)
1	C	0.89	0/2461	1.66	40/3339 (1.2%)
2	B	0.82	0/1155	1.58	12/1561 (0.8%)
2	D	0.78	0/1155	1.55	13/1561 (0.8%)
All	All	0.85	0/7232	1.62	105/9800 (1.1%)

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	5
1	C	0	4
2	B	0	3
All	All	0	12

There are no bond length outliers.

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH1	-13.45	113.57	120.30
1	C	269	ARG	NE-CZ-NH2	13.14	126.87	120.30
1	A	54	ARG	NE-CZ-NH1	-12.90	113.85	120.30
1	C	56	ARG	NE-CZ-NH1	-12.77	113.92	120.30
1	C	269	ARG	NE-CZ-NH1	-12.73	113.94	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	HIS	Sidechain
1	A	156	HIS	Sidechain
1	A	294	PHE	Sidechain
1	A	5	TYR	Sidechain
1	A	59	PHE	Sidechain

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	2415	0	2422	51	0
1	C	2415	0	2422	36	0
2	B	1138	0	1154	36	0
2	D	1138	0	1154	34	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	31	0	10	10	0
4	D	31	0	12	8	0
All	All	7170	0	7174	151	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 11.

The worst 5 of 151 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:11:ALA:HA	4:B:155:ATP:N1	1.48	1.26
2:B:8:GLY:N	2:B:50:SER:HG	1.68	0.89
1:A:8:HIS:HD2	1:A:124:VAL:H	1.19	0.84
2:D:60:LYS:NZ	4:D:155:ATP:N3	2.25	0.84
2:D:11:ALA:HA	4:D:155:ATP:N1	1.94	0.82

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	308/310 (99%)	283 (92%)	17 (6%)	8 (3%)	5	9
1	C	308/310 (99%)	283 (92%)	18 (6%)	7 (2%)	6	11
2	B	144/153 (94%)	121 (84%)	15 (10%)	8 (6%)	2	2
2	D	144/153 (94%)	124 (86%)	10 (7%)	10 (7%)	1	1
All	All	904/926 (98%)	811 (90%)	60 (7%)	33 (4%)	3	4

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	SER
2	B	22	PRO
2	B	50	SER
2	B	53	MET
1	C	78	ASN

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	261/261 (100%)	238 (91%)	23 (9%)	10	19
1	C	261/261 (100%)	228 (87%)	33 (13%)	4	8
2	B	129/136 (95%)	113 (88%)	16 (12%)	4	8
2	D	129/136 (95%)	114 (88%)	15 (12%)	5	10
All	All	780/794 (98%)	693 (89%)	87 (11%)	6	10

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	6	GLN
1	C	114	LEU
2	D	87	ASP
1	C	17	ARG
1	C	74	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	A	291	ASN
1	C	282	HIS
1	A	282	HIS
1	C	170	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
4	ATP	D	155	-	26,33,33	3.07	12 (46%)	31,52,52	2.88	12 (38%)
4	ATP	B	155	-	26,33,33	2.67	11 (42%)	31,52,52	3.72	12 (38%)

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	D	155	-	-	5/18/38/38	0/3/3/3
4	ATP	B	155	-	-	6/18/38/38	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	155	ATP	C4-N3	-8.12	1.24	1.35
4	B	155	ATP	C3'-C4'	-5.54	1.38	1.53
4	D	155	ATP	C3'-C4'	-5.53	1.38	1.53
4	D	155	ATP	O4'-C4'	4.64	1.55	1.45
4	B	155	ATP	O4'-C4'	4.61	1.55	1.45

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	155	ATP	O2'-C2'-C3'	-13.69	67.54	111.82
4	D	155	ATP	C2'-C3'-C4'	7.26	116.75	102.64
4	B	155	ATP	C2'-C3'-C4'	7.25	116.73	102.64
4	B	155	ATP	O3G-PG-O3B	6.67	127.02	104.64
4	D	155	ATP	O3G-PG-O3B	6.67	127.01	104.64

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

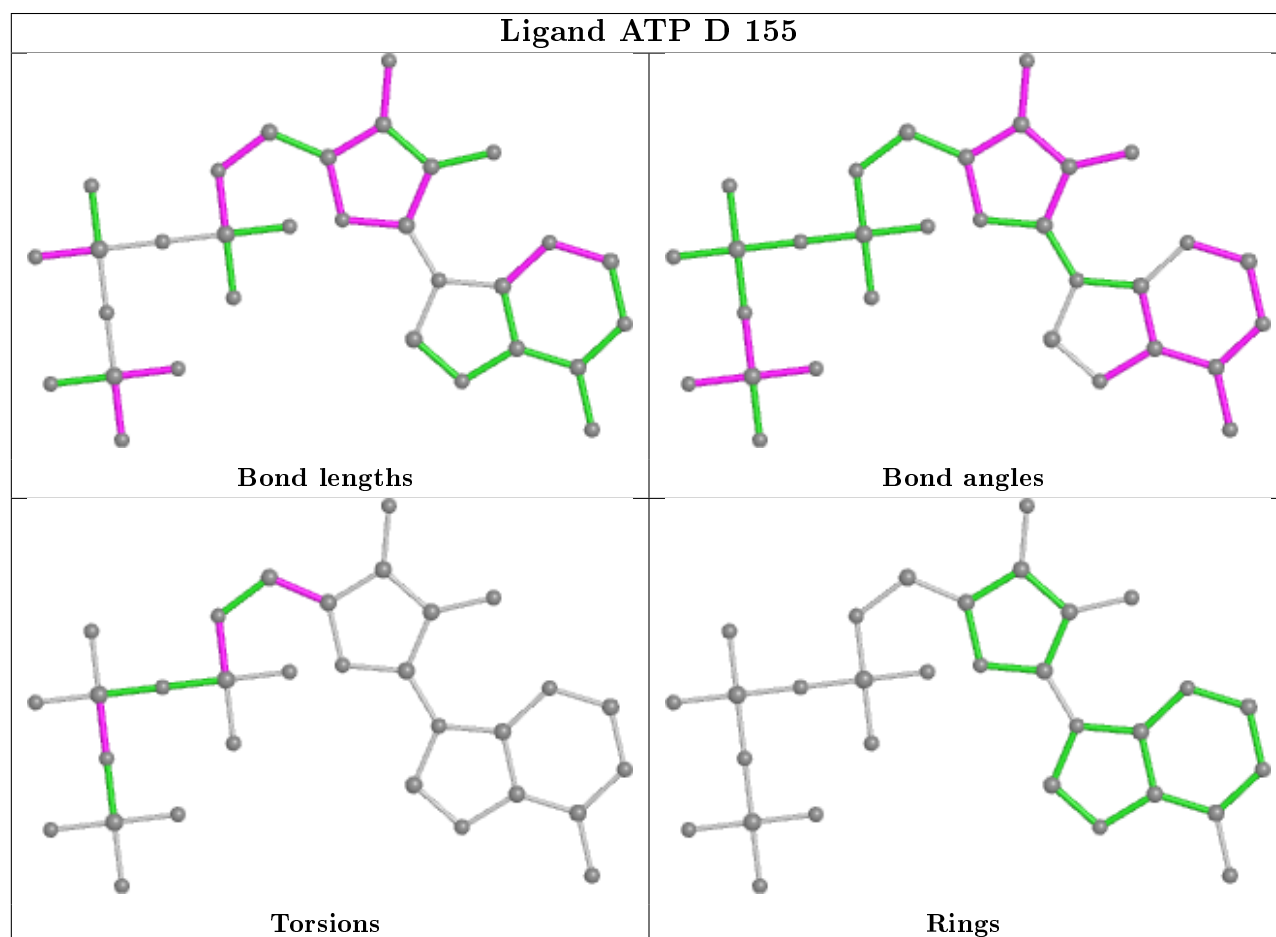
Mol	Chain	Res	Type	Atoms
4	D	155	ATP	C5'-O5'-PA-O3A
4	D	155	ATP	C3'-C4'-C5'-O5'
4	B	155	ATP	C5'-O5'-PA-O3A
4	B	155	ATP	C3'-C4'-C5'-O5'
4	D	155	ATP	O4'-C4'-C5'-O5'

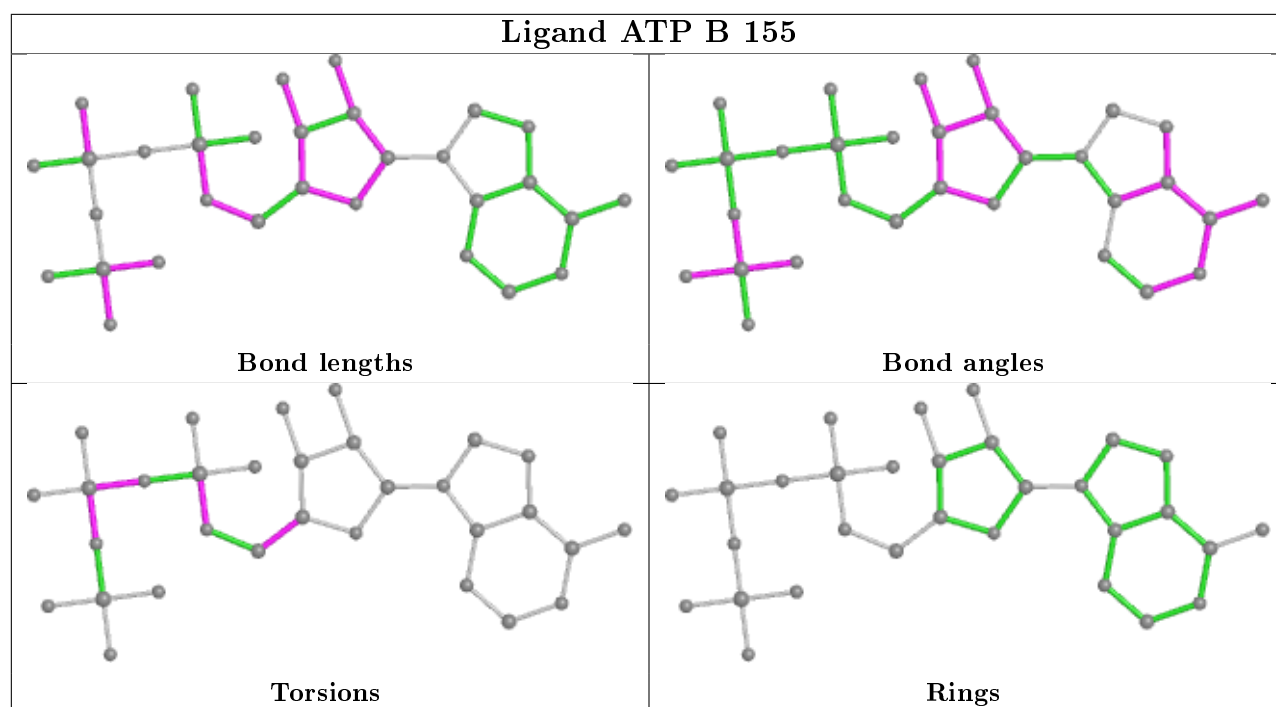
There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	155	ATP	8	0
4	B	155	ATP	10	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.