



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:57 AM UTC

PDB ID : 1GTR / pdb_00001gtr
Title : STRUCTURAL BASIS OF ANTICODON LOOP RECOGNITION BY
GLUTAMINYL-TRNA SYNTHETASE
Authors : Rould, M.A.; Perona, J.J.; Steitz, T.A.
Deposited on : 1993-09-15
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

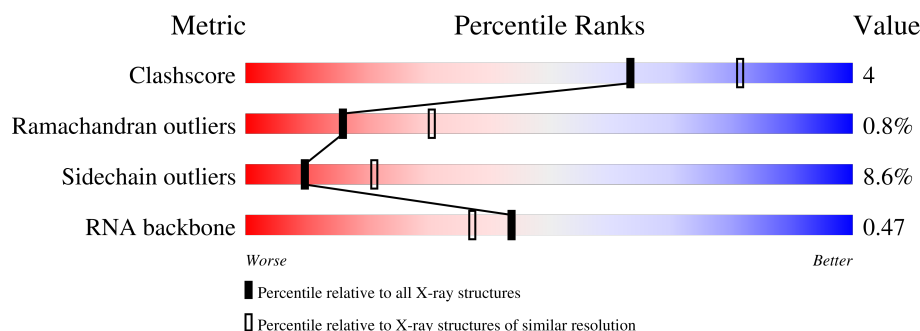
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	74	
2	A	553	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6114 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.

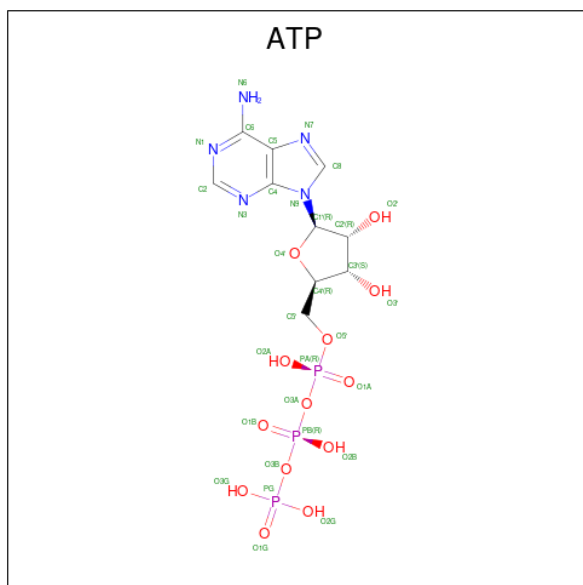
- Molecule 1 is a RNA chain called RNA (74-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			

- Molecule 2 is a protein called GLUTAMINYL-tRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	529	Total	C	N	O	S	0	0	0
			4279	2704	752	802	21			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is water.

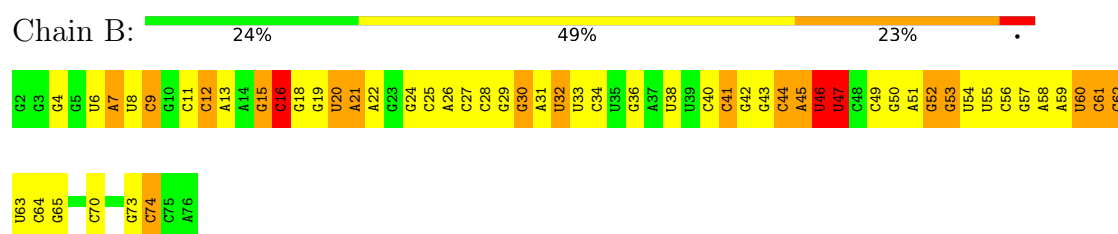
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	47	Total 47	O 47	0	0
4	A	184	Total 184	O 184	0	0

3 Residue-property plots [i](#)

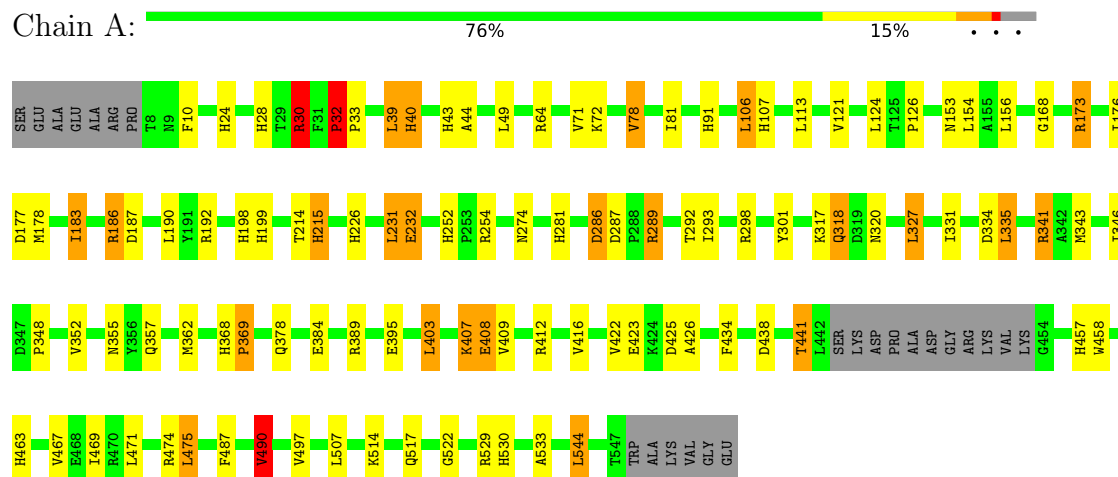
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: RNA (74-MER)



• Molecule 2: GLUTAMINYL-tRNA SYNTHETASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	242.80 Å 94.30 Å 115.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6114	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: 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	B	0.85	0/1756	2.45	111/2734 (4.1%)
2	A	0.83	26/4379 (0.6%)	1.28	16/5928 (0.3%)
All	All	0.84	26/6135 (0.4%)	1.74	127/8662 (1.5%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	252	HIS	CD2-NE2	-7.16	1.29	1.37
2	A	198	HIS	CD2-NE2	-6.96	1.30	1.37
2	A	457	HIS	CD2-NE2	-6.63	1.30	1.37
2	A	368	HIS	CD2-NE2	-6.62	1.30	1.37
2	A	28	HIS	CD2-NE2	-6.57	1.30	1.37
2	A	226	HIS	CD2-NE2	-6.56	1.30	1.37
2	A	215	HIS	CD2-NE2	-6.54	1.30	1.37
2	A	24	HIS	CD2-NE2	-6.51	1.30	1.37
2	A	281	HIS	CD2-NE2	-6.51	1.30	1.37
2	A	40	HIS	CD2-NE2	-6.47	1.30	1.37
2	A	530	HIS	CD2-NE2	-6.42	1.30	1.37
2	A	43	HIS	CD2-NE2	-6.40	1.30	1.37
2	A	107	HIS	CD2-NE2	-6.26	1.30	1.37
2	A	463	HIS	CD2-NE2	-6.17	1.31	1.37
2	A	91	HIS	CD2-NE2	-6.05	1.31	1.37
2	A	78	VAL	CA-CB	6.01	1.62	1.54
2	A	199	HIS	CD2-NE2	-5.99	1.31	1.37
2	A	40	HIS	CG-ND1	-5.55	1.32	1.38
2	A	215	HIS	CG-ND1	-5.36	1.32	1.38
2	A	28	HIS	CG-ND1	-5.30	1.32	1.38
2	A	43	HIS	CG-ND1	-5.28	1.32	1.38
2	A	252	HIS	CG-ND1	-5.24	1.32	1.38
2	A	198	HIS	CG-ND1	-5.20	1.32	1.38
2	A	368	HIS	CG-ND1	-5.19	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	24	HIS	CG-ND1	-5.18	1.32	1.38
2	A	226	HIS	CG-ND1	-5.15	1.32	1.38

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	G	O3'-P-O5'	30.50	149.76	104.00
1	B	43	G	O3'-P-O5'	28.15	146.22	104.00
1	B	31	A	O3'-P-O5'	-24.40	67.40	104.00
1	B	40	C	O3'-P-O5'	-22.45	70.33	104.00
1	B	46	U	O3'-P-O5'	20.87	135.31	104.00
1	B	61	C	O3'-P-O5'	17.74	130.60	104.00
1	B	15	G	O3'-P-O5'	-17.27	78.10	104.00
1	B	43	G	OP1-P-O3'	-16.29	59.12	108.00
1	B	31	A	OP2-P-O3'	15.91	155.72	108.00
1	B	63	U	OP1-P-O3'	-15.85	60.44	108.00
1	B	52	G	OP1-P-O3'	-15.10	62.69	108.00
1	B	51	A	O3'-P-O5'	-14.72	81.92	104.00
1	B	40	C	OP2-P-O3'	14.70	152.11	108.00
1	B	21	A	O3'-P-O5'	14.47	125.71	104.00
1	B	20	U	O3'-P-O5'	-14.21	82.68	104.00
1	B	63	U	OP2-P-O3'	14.20	150.61	108.00
1	B	20	U	OP2-P-O3'	13.24	147.72	108.00
1	B	47	U	O3'-P-O5'	-13.02	84.46	104.00
1	B	61	C	OP1-P-O3'	-12.80	69.60	108.00
1	B	13	A	O3'-P-O5'	12.59	122.89	104.00
1	B	29	G	O3'-P-O5'	12.11	122.17	104.00
1	B	15	G	OP1-P-O3'	12.04	144.12	108.00
1	B	64	C	O3'-P-O5'	-11.70	86.45	104.00
1	B	45	A	O3'-P-O5'	-11.37	86.94	104.00
1	B	33	U	O3'-P-O5'	11.08	120.62	104.00
1	B	32	U	O3'-P-O5'	11.08	120.62	104.00
1	B	21	A	OP1-P-O3'	-10.99	75.04	108.00
1	B	29	G	OP1-P-O3'	-10.97	75.10	108.00
1	B	32	U	OP1-P-O3'	-10.69	75.93	108.00
1	B	49	C	OP1-P-O3'	-10.56	76.30	108.00
1	B	7	A	OP2-P-O3'	10.27	138.81	108.00
1	B	49	C	OP2-P-O3'	10.08	138.24	108.00
1	B	16	C	OP1-P-O3'	-9.92	78.23	108.00
1	B	44	C	OP2-P-O3'	9.81	137.43	108.00
1	B	7	A	OP1-P-O3'	-9.48	79.56	108.00
1	B	46	U	OP2-P-O3'	-8.93	81.22	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	C	OP2-P-O3'	8.87	134.62	108.00
1	B	33	U	OP1-P-O3'	-8.84	81.48	108.00
1	B	62	C	OP2-P-O3'	8.82	134.47	108.00
1	B	12	C	O3'-P-O5'	8.82	117.23	104.00
1	B	31	A	OP1-P-O3'	-8.81	81.55	108.00
1	B	53	G	O3'-P-O5'	-8.63	91.06	104.00
1	B	73	G	O3'-P-O5'	-8.51	91.23	104.00
1	B	44	C	O3'-P-O5'	-8.46	91.31	104.00
1	B	36	G	OP1-P-O3'	-8.41	82.78	108.00
1	B	20	U	OP1-P-O3'	-8.25	83.25	108.00
1	B	51	A	OP2-P-O3'	8.25	132.75	108.00
1	B	58	A	OP1-P-O3'	8.21	132.62	108.00
1	B	50	G	OP1-P-O3'	-8.16	83.53	108.00
1	B	40	C	OP1-P-O3'	-8.08	83.75	108.00
1	B	62	C	OP1-P-O3'	-8.06	83.81	108.00
1	B	42	G	O3'-P-O5'	7.96	115.94	104.00
1	B	20	U	P-O3'-C3'	7.76	131.84	120.20
1	B	42	G	OP1-P-O3'	-7.76	84.73	108.00
1	B	63	U	C5'-C4'-C3'	-7.70	104.45	116.00
1	B	11	C	OP1-P-O3'	-7.63	85.11	108.00
1	B	28	C	O3'-P-O5'	7.54	115.31	104.00
1	B	24	G	O3'-P-O5'	7.45	115.17	104.00
1	B	27	C	OP1-P-O3'	-7.42	85.73	108.00
1	B	59	A	O3'-P-O5'	-7.26	93.10	104.00
1	B	36	G	C5'-C4'-C3'	-7.24	104.34	115.20
2	A	490	VAL	N-CA-CB	-7.21	102.69	112.28
1	B	58	A	O3'-P-O5'	-7.20	93.19	104.00
1	B	12	C	C4'-C3'-C2'	-7.20	95.40	102.60
1	B	36	G	OP2-P-O3'	7.19	129.57	108.00
1	B	45	A	OP1-P-O3'	7.10	129.30	108.00
1	B	46	U	C1'-O4'-C4'	-6.99	102.91	109.90
1	B	15	G	P-O3'-C3'	6.97	130.65	120.20
1	B	28	C	OP1-P-O3'	-6.96	87.11	108.00
1	B	47	U	OP2-P-O3'	6.85	128.55	108.00
2	A	334	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	44	C	OP1-P-O3'	-6.68	87.95	108.00
1	B	60	U	C5'-C4'-C3'	-6.62	105.26	115.20
1	B	8	U	OP1-P-O3'	-6.59	88.21	108.00
1	B	45	A	P-O3'-C3'	6.54	130.02	120.20
1	B	15	G	OP2-P-O3'	-6.50	88.49	108.00
2	A	407	LYS	N-CA-C	6.50	120.14	109.94
1	B	47	U	O4'-C1'-C2'	-6.45	99.36	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	286	ASP	CA-CB-CG	6.44	119.04	112.60
1	B	54	U	O3'-P-O5'	-6.43	94.36	104.00
1	B	25	C	O3'-P-O5'	6.35	113.52	104.00
1	B	19	G	O3'-P-O5'	-6.27	94.60	104.00
1	B	29	G	C5'-C4'-C3'	-6.25	106.62	116.00
1	B	55	U	OP1-P-O3'	-6.22	89.35	108.00
1	B	13	A	OP1-P-O3'	-6.12	89.63	108.00
1	B	44	C	C5'-C4'-C3'	-6.01	106.99	116.00
1	B	74	C	O3'-P-O5'	-5.98	95.03	104.00
1	B	57	G	O3'-P-O5'	-5.95	95.08	104.00
1	B	52	G	C5'-C4'-C3'	-5.91	107.14	116.00
1	B	6	U	O3'-P-O5'	-5.88	95.19	104.00
1	B	24	G	OP1-P-O3'	-5.83	90.52	108.00
1	B	41	C	P-O5'-C5'	5.79	129.59	120.90
2	A	10	PHE	CA-CB-CG	5.76	119.56	113.80
1	B	56	C	O3'-P-O5'	-5.76	95.36	104.00
2	A	177	ASP	CA-CB-CG	5.75	118.35	112.60
2	A	389	ARG	CG-CD-NE	-5.74	99.36	112.00
1	B	4	G	OP1-P-O3'	-5.70	90.89	108.00
1	B	8	U	O3'-P-O5'	5.64	112.46	104.00
1	B	26	A	O3'-P-O5'	5.63	112.45	104.00
1	B	74	C	OP1-P-O3'	5.59	124.78	108.00
1	B	4	G	OP2-P-O3'	5.59	124.76	108.00
2	A	348	PRO	N-CA-C	5.58	121.00	111.68
1	B	70	C	OP1-P-O3'	-5.58	91.26	108.00
2	A	438	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	45	A	C1'-O4'-C4'	-5.56	104.14	109.70
1	B	22	A	C5'-C4'-C3'	-5.50	107.75	116.00
1	B	30	G	C1'-O4'-C4'	-5.49	104.41	109.90
2	A	355	ASN	CA-CB-CG	5.45	118.05	112.60
1	B	58	A	OP2-P-O3'	-5.45	91.65	108.00
1	B	73	G	OP2-P-O3'	5.44	124.31	108.00
1	B	32	U	O4'-C1'-N1	5.42	116.63	108.50
2	A	30	ARG	CA-CB-CG	5.41	124.92	114.10
1	B	65	G	C5'-C4'-C3'	-5.36	107.96	116.00
2	A	317	LYS	CB-CG-CD	-5.34	99.01	111.30
1	B	57	G	OP2-P-O3'	5.32	123.97	108.00
2	A	231	LEU	N-CA-C	5.28	118.83	112.38
2	A	403	LEU	N-CA-C	5.26	117.32	109.59
1	B	70	C	OP2-P-O3'	5.25	123.74	108.00
1	B	34	C	O3'-P-O5'	-5.20	96.21	104.00
1	B	16	C	P-O3'-C3'	5.16	127.94	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	G	OP2-P-O3'	5.12	123.36	108.00
1	B	9	C	O3'-P-O5'	-5.09	96.36	104.00
2	A	533	ALA	N-CA-C	-5.08	107.21	113.41
2	A	215	HIS	CA-CB-CG	-5.06	108.74	113.80
1	B	55	U	OP2-P-O3'	5.05	123.15	108.00
1	B	21	A	C4'-C3'-O3'	-5.01	105.49	113.00
1	B	41	C	O3'-P-O5'	-5.00	96.50	104.00

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	B	1573	0	800	8	0
2	A	4279	0	4172	38	0
3	A	31	0	12	0	0
4	A	184	0	0	1	0
4	B	47	0	0	1	0
All	All	6114	0	4984	43	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 4.

All (43) 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:A:403:LEU:HD13	2:A:409:VAL:HG22	1.72	0.71
1:B:38:U:H5	4:B:891:HOH:O	1.74	0.70
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.75	0.69
2:A:346:ILE:HG12	2:A:469:ILE:HD13	1.82	0.62
2:A:407:LYS:HE2	2:A:408:GLU:HG3	1.83	0.61
2:A:30:ARG:NH1	2:A:215:HIS:HE1	1.99	0.60
2:A:30:ARG:HH11	2:A:215:HIS:HE1	1.48	0.60
1:B:12:C:H5''	2:A:320:ASN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:362:MET:HG3	2:A:378:GLN:HG3	1.86	0.55
2:A:416:VAL:HB	2:A:441:THR:HG21	1.87	0.55
2:A:40:HIS:HA	2:A:292:THR:HA	1.89	0.54
2:A:44:ALA:HB2	2:A:293:ILE:HD11	1.91	0.53
2:A:30:ARG:HH11	2:A:215:HIS:CE1	2.29	0.51
2:A:341:ARG:HG3	2:A:517:GLN:HB3	1.93	0.50
1:B:60:U:H5''	1:B:61:C:H5	1.78	0.49
2:A:287:ASP:OD1	2:A:289:ARG:HD3	2.13	0.49
2:A:423:GLU:HB2	2:A:434:PHE:HE1	1.78	0.48
1:B:46:U:H4'	1:B:47:U:C5	2.49	0.46
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.96	0.46
2:A:30:ARG:NH1	2:A:215:HIS:CE1	2.81	0.46
2:A:352:VAL:HG12	2:A:384:GLU:HG2	1.97	0.45
2:A:487:PHE:O	2:A:490:VAL:HG12	2.16	0.45
1:B:16:C:H5'	1:B:60:U:O2	2.16	0.45
1:B:46:U:OP1	1:B:47:U:H5'	2.17	0.45
2:A:173:ARG:HD2	2:A:187:ASP:O	2.17	0.45
2:A:407:LYS:HG2	2:A:408:GLU:H	1.82	0.45
2:A:232:GLU:HG3	4:A:818:HOH:O	2.16	0.44
2:A:32:PRO:HA	2:A:64:ARG:O	2.18	0.43
1:B:74:C:N3	2:A:168:GLY:HA2	2.33	0.43
2:A:289:ARG:HB3	2:A:475:LEU:HG	2.00	0.43
2:A:286:ASP:O	2:A:298:ARG:HD3	2.18	0.43
2:A:343:MET:HE3	2:A:458:TRP:H	1.82	0.43
2:A:331:ILE:HG13	2:A:335:LEU:HD22	1.99	0.42
2:A:183:ILE:HA	2:A:186:ARG:HG3	2.01	0.42
2:A:121:VAL:H	2:A:153:ASN:ND2	2.17	0.42
2:A:71:VAL:HG23	2:A:72:LYS:HG2	2.02	0.42
2:A:178:MET:O	2:A:186:ARG:HD2	2.19	0.41
2:A:106:LEU:HD21	2:A:214:THR:HG23	2.03	0.41
2:A:341:ARG:HD2	2:A:369:PRO:HD2	2.02	0.41
2:A:522:GLY:HA2	2:A:544:LEU:HD13	2.02	0.41
2:A:301:TYR:CE2	2:A:327:LEU:HD22	2.56	0.41
1:B:7:A:H4'	2:A:318:GLN:NE2	2.37	0.40
2:A:254:ARG:HD3	2:A:254:ARG:HA	1.87	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	
2	A	525/553 (95%)	502 (96%)	19 (4%)	4 (1%)	16	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	32	PRO
2	A	426	ALA
2	A	529	ARG
2	A	176	ILE

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	
2	A	463/481 (96%)	423 (91%)	40 (9%)	10	21

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	30	ARG
2	A	32	PRO
2	A	33	PRO
2	A	39	LEU
2	A	49	LEU
2	A	78	VAL
2	A	106	LEU

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Mol	Chain	Res	Type
2	A	113	LEU
2	A	124	LEU
2	A	126	PRO
2	A	154	LEU
2	A	156	LEU
2	A	173	ARG
2	A	183	ILE
2	A	186	ARG
2	A	190	LEU
2	A	192	ARG
2	A	231	LEU
2	A	232	GLU
2	A	274	ASN
2	A	289	ARG
2	A	318	GLN
2	A	327	LEU
2	A	335	LEU
2	A	341	ARG
2	A	357	GLN
2	A	369	PRO
2	A	395	GLU
2	A	408	GLU
2	A	412	ARG
2	A	422	VAL
2	A	425	ASP
2	A	441	THR
2	A	467	VAL
2	A	474	ARG
2	A	475	LEU
2	A	490	VAL
2	A	507	LEU
2	A	514	LYS
2	A	544	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	9	ASN
2	A	60	GLN
2	A	83	ASN
2	A	128	GLN
2	A	153	ASN

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Mol	Chain	Res	Type
2	A	200	GLN
2	A	215	HIS
2	A	226	HIS
2	A	318	GLN
2	A	336	ASN
2	A	355	ASN
2	A	413	ASN
2	A	480	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	73/74 (98%)	14 (19%)	5 (6%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	9	C
1	B	16	C
1	B	18	G
1	B	21	A
1	B	30	G
1	B	32	U
1	B	41	C
1	B	44	C
1	B	45	A
1	B	46	U
1	B	47	U
1	B	52	G
1	B	53	G
1	B	62	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	15	G
1	B	16	C
1	B	20	U
1	B	45	A
1	B	47	U

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](#)

1 ligand is 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$
3	ATP	A	999	-	32,33,33	1.12	3 (9%)	48,52,52	0.92	2 (4%)

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
3	ATP	A	999	-	-	5/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	ATP	PB-O3B	3.35	1.63	1.59
3	A	999	ATP	PA-O3A	2.80	1.62	1.59
3	A	999	ATP	PB-O3A	2.00	1.61	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	ATP	O3G-PG-O2G	2.15	115.87	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	ATP	O5'-C5'-C4'	2.07	116.03	108.99

There are no chirality outliers.

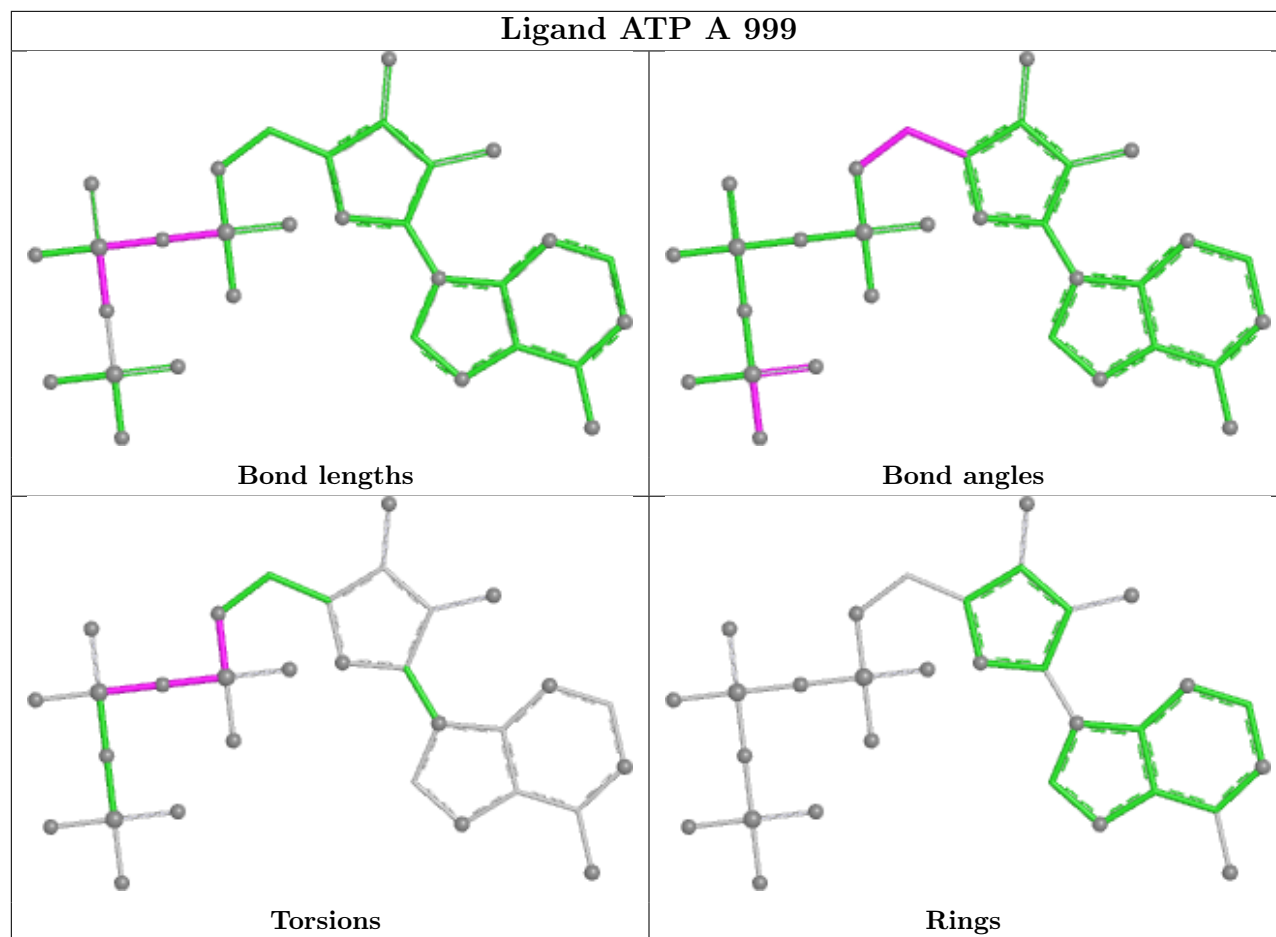
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	ATP	C5'-O5'-PA-O1A
3	A	999	ATP	PB-O3A-PA-O5'
3	A	999	ATP	PA-O3A-PB-O2B
3	A	999	ATP	C5'-O5'-PA-O3A
3	A	999	ATP	PA-O3A-PB-O1B

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

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.