



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:23 PM UTC

PDB ID : 1GTS / pdb_00001gts
Title : STRUCTURAL BASIS FOR TRANSFER RNA AMINOACYLATION BY
ESCHERICHIA COLI GLUTAMINYL-TRNA SYNTHETASE
Authors : Perona, J.J.; Steitz, T.A.; Rould, M.A.
Deposited on : 1993-09-15
Resolution : 2.80 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

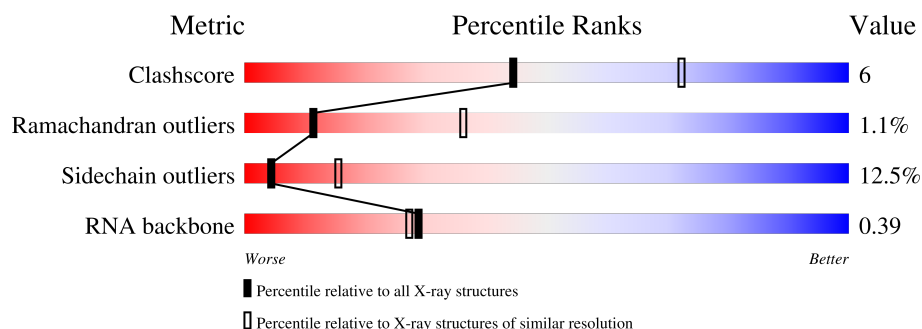
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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 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 6004 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.

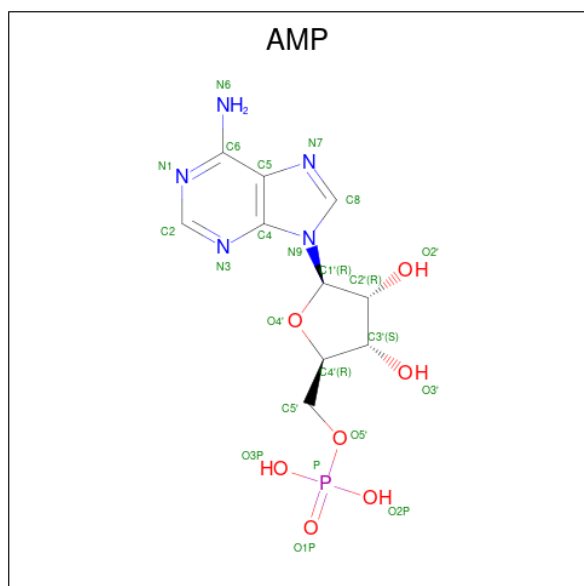
- Molecule 1 is a RNA chain called TRNAGLN.

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 PROTEIN (GLUTAMINYL-TRNA SYNTHETASE (E.C.6.1.1.18)).

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 MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

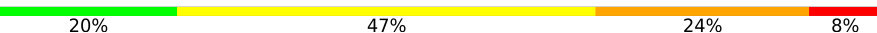
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	17	Total 17	O 17	0	0
4	A	112	Total 112	O 112	0	0

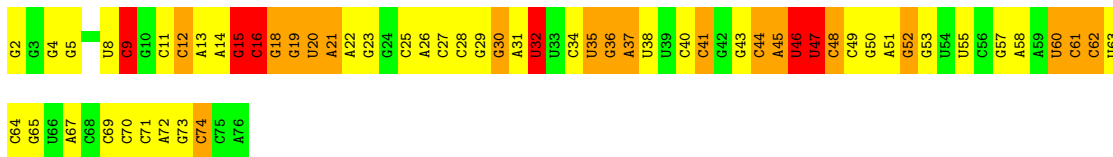
3 Residue-property plots

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.

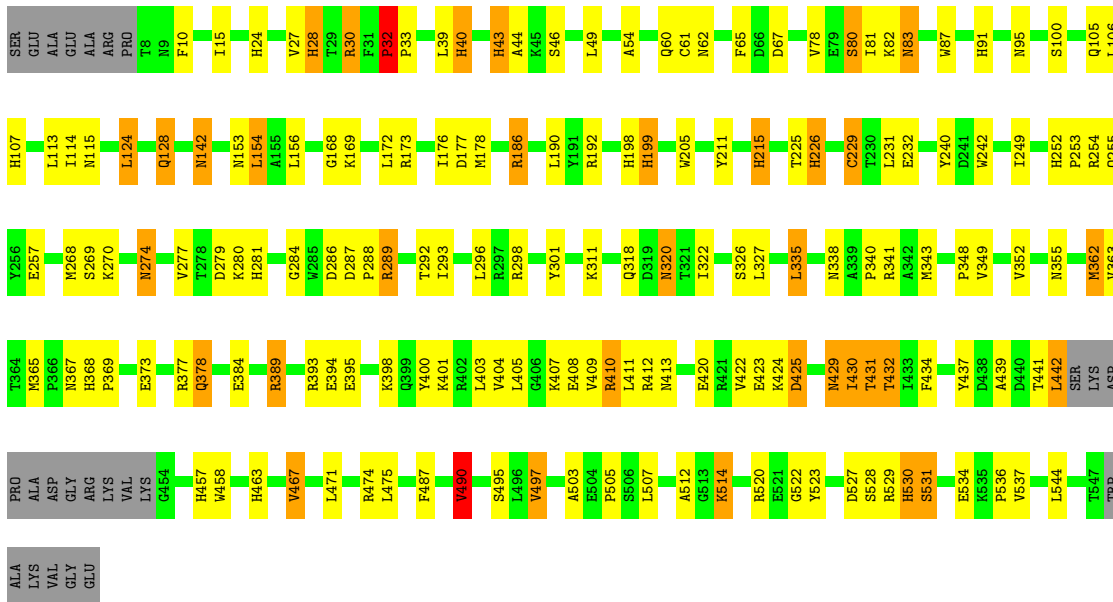
- Molecule 1: TRNAGLN

Chain B: 



- Molecule 2: PROTEIN (GLUTAMINYL-TRNA SYNTHETASE (E.C.6.1.1.18))

Chain A: 



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	242.84Å 93.59Å 115.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6004	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP

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	0.94	0/1756	2.72	134/2734 (4.9%)
2	A	0.98	20/4379 (0.5%)	1.55	37/5928 (0.6%)
All	All	0.97	20/6135 (0.3%)	1.99	171/8662 (2.0%)

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
2	A	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	252	HIS	CD2-NE2	-7.08	1.30	1.37
2	A	43	HIS	CD2-NE2	-7.03	1.30	1.37
2	A	226	HIS	CD2-NE2	-6.96	1.30	1.37
2	A	91	HIS	CD2-NE2	-6.96	1.30	1.37
2	A	457	HIS	CD2-NE2	-6.96	1.30	1.37
2	A	530	HIS	CD2-NE2	-6.90	1.30	1.37
2	A	215	HIS	CD2-NE2	-6.38	1.30	1.37
2	A	198	HIS	CD2-NE2	-6.32	1.30	1.37
2	A	463	HIS	CD2-NE2	-6.11	1.31	1.37
2	A	368	HIS	CD2-NE2	-6.00	1.31	1.37
2	A	281	HIS	CD2-NE2	-5.81	1.31	1.37
2	A	28	HIS	CD2-NE2	-5.80	1.31	1.37
2	A	24	HIS	CD2-NE2	-5.78	1.31	1.37
2	A	107	HIS	CD2-NE2	-5.68	1.31	1.37
2	A	40	HIS	CD2-NE2	-5.67	1.31	1.37
2	A	215	HIS	CG-ND1	-5.50	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	249	ILE	CA-CB	5.32	1.61	1.54
2	A	199	HIS	CD2-NE2	-5.28	1.32	1.37
2	A	252	HIS	CG-ND1	-5.13	1.32	1.38
2	A	107	HIS	CG-ND1	-5.11	1.32	1.38

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	G	O3'-P-O5'	43.10	168.65	104.00
1	B	46	U	O3'-P-O5'	23.82	139.72	104.00
1	B	47	U	O3'-P-O5'	-22.18	70.73	104.00
1	B	15	G	O3'-P-O5'	-21.48	71.78	104.00
1	B	31	A	OP2-P-O3'	19.49	166.48	108.00
1	B	40	C	O3'-P-O5'	-19.48	74.78	104.00
1	B	13	A	O3'-P-O5'	19.20	132.81	104.00
1	B	31	A	O3'-P-O5'	-18.55	76.18	104.00
1	B	14	A	O3'-P-O5'	17.52	130.28	104.00
1	B	32	U	OP1-P-O3'	-17.50	55.49	108.00
1	B	32	U	O3'-P-O5'	16.23	128.35	104.00
1	B	15	G	OP1-P-O3'	15.94	155.82	108.00
1	B	61	C	O3'-P-O5'	15.60	127.40	104.00
1	B	37	A	OP1-P-O3'	-14.81	63.56	108.00
1	B	46	U	OP2-P-O3'	-14.74	63.77	108.00
1	B	28	C	O3'-P-O5'	14.59	125.88	104.00
1	B	43	G	OP2-P-O3'	-14.26	65.23	108.00
1	B	31	A	OP1-P-O3'	-13.58	67.26	108.00
1	B	61	C	OP1-P-O3'	-13.47	67.60	108.00
1	B	71	C	O3'-P-O5'	13.41	124.11	104.00
1	B	37	A	OP2-P-O3'	13.02	147.05	108.00
1	B	27	C	O3'-P-O5'	12.47	122.71	104.00
1	B	44	C	O3'-P-O5'	-12.47	85.30	104.00
1	B	64	C	O3'-P-O5'	-12.27	85.59	104.00
1	B	20	U	OP1-P-O3'	-12.23	71.31	108.00
1	B	52	G	O3'-P-O5'	12.18	122.27	104.00
1	B	21	A	OP1-P-O3'	-11.99	72.03	108.00
1	B	51	A	OP1-P-O3'	-11.65	73.04	108.00
1	B	19	G	OP1-P-O3'	11.52	142.55	108.00
1	B	18	G	O3'-P-O5'	-11.44	86.84	104.00
1	B	20	U	O3'-P-O5'	11.43	121.15	104.00
1	B	51	A	OP2-P-O3'	11.33	141.99	108.00
1	B	40	C	OP2-P-O3'	11.29	141.88	108.00
1	B	19	G	OP2-P-O3'	-10.93	75.20	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	U	OP2-P-O3'	10.55	139.65	108.00
1	B	16	C	OP2-P-O3'	10.54	139.61	108.00
1	B	8	U	O3'-P-O5'	10.28	119.42	104.00
1	B	47	U	OP2-P-O3'	10.25	138.75	108.00
1	B	34	C	O3'-P-O5'	-10.20	88.70	104.00
1	B	50	G	OP1-P-O3'	-10.19	77.42	108.00
1	B	34	C	OP1-P-O3'	10.12	138.36	108.00
1	B	72	A	O3'-P-O5'	-9.78	89.32	104.00
1	B	16	C	OP1-P-O3'	-9.71	78.87	108.00
1	B	52	G	OP1-P-O3'	-9.50	79.51	108.00
1	B	53	G	O3'-P-O5'	9.43	118.15	104.00
1	B	11	C	O3'-P-O5'	9.36	118.04	104.00
1	B	4	G	OP2-P-O3'	9.35	136.06	108.00
1	B	70	C	O3'-P-O5'	-9.28	90.08	104.00
1	B	23	G	O3'-P-O5'	9.25	117.88	104.00
1	B	13	A	OP1-P-O3'	-9.21	80.36	108.00
2	A	215	HIS	CA-CB-CG	-9.12	104.68	113.80
1	B	26	A	OP1-P-O3'	-9.07	80.79	108.00
1	B	62	C	O3'-P-O5'	9.01	117.51	104.00
1	B	73	G	O3'-P-O5'	-8.85	90.73	104.00
1	B	15	G	OP2-P-O3'	-8.83	81.51	108.00
1	B	74	C	O3'-P-O5'	-8.79	90.81	104.00
1	B	65	G	O3'-P-O5'	-8.73	90.90	104.00
1	B	29	G	OP1-P-O3'	-8.69	81.94	108.00
1	B	63	U	OP1-P-O3'	-8.57	82.28	108.00
2	A	490	VAL	N-CA-CB	-8.55	101.02	112.22
1	B	49	C	OP1-P-O3'	-8.39	82.83	108.00
1	B	25	C	OP1-P-O3'	-8.17	83.49	108.00
1	B	58	A	OP1-P-O3'	8.05	132.14	108.00
1	B	29	G	OP2-P-O3'	7.98	131.94	108.00
1	B	4	G	OP1-P-O3'	-7.97	84.10	108.00
1	B	28	C	OP1-P-O3'	-7.82	84.54	108.00
2	A	527	ASP	CA-CB-CG	7.74	120.34	112.60
1	B	21	A	OP2-P-O3'	7.72	131.17	108.00
1	B	45	A	OP1-P-O3'	7.71	131.12	108.00
1	B	43	G	OP1-P-O3'	-7.67	84.99	108.00
1	B	63	U	O3'-P-O5'	-7.63	92.56	104.00
2	A	40	HIS	CA-CB-CG	7.47	121.27	113.80
1	B	27	C	OP1-P-O3'	-7.42	85.73	108.00
1	B	38	U	O3'-P-O5'	7.27	114.91	104.00
1	B	2	G	OP1-P-O3'	-7.05	86.85	108.00
1	B	55	U	OP2-P-O3'	7.02	129.06	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9	C	OP2-P-O3'	6.99	128.96	108.00
1	B	67	A	OP1-P-O3'	6.98	128.94	108.00
1	B	25	C	O3'-P-O5'	6.84	114.26	104.00
2	A	355	ASN	CA-CB-CG	6.84	119.44	112.60
1	B	49	C	OP2-P-O3'	6.73	128.20	108.00
2	A	115	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	B	14	A	OP1-P-O3'	-6.69	87.93	108.00
1	B	11	C	OP1-P-O3'	-6.66	88.03	108.00
1	B	69	C	O3'-P-O5'	-6.63	94.05	104.00
1	B	60	U	OP2-P-O3'	6.63	127.89	108.00
1	B	19	G	O3'-P-O5'	-6.59	94.11	104.00
1	B	34	C	O4'-C1'-C2'	-6.57	99.23	105.80
1	B	67	A	O3'-P-O5'	-6.56	94.16	104.00
1	B	26	A	O3'-P-O5'	6.53	113.80	104.00
1	B	57	G	O3'-P-O5'	-6.53	94.20	104.00
1	B	30	G	C1'-O4'-C4'	-6.51	103.39	109.90
2	A	62	ASN	CA-CB-CG	6.49	119.09	112.60
1	B	5	G	O3'-P-O5'	-6.45	94.33	104.00
1	B	9	C	OP1-P-O3'	-6.39	88.84	108.00
1	B	55	U	OP1-P-O3'	-6.30	89.10	108.00
2	A	242	TRP	CG-CD2-CE3	6.24	140.14	133.90
1	B	58	A	O3'-P-O5'	-6.20	94.70	104.00
1	B	12	C	C4'-C3'-C2'	-6.19	96.41	102.60
1	B	46	U	C1'-O4'-C4'	-6.16	103.74	109.90
1	B	47	U	O4'-C1'-C2'	-6.15	99.65	105.80
1	B	32	U	P-O5'-C5'	6.13	130.09	120.90
1	B	45	A	OP2-P-O3'	-6.12	89.63	108.00
1	B	26	A	O4'-C4'-C3'	-6.11	97.89	104.00
2	A	10	PHE	CA-CB-CG	6.04	119.83	113.80
1	B	15	G	N9-C1'-C2'	-6.03	104.95	114.00
1	B	63	U	C5'-C4'-C3'	-6.02	106.97	116.00
2	A	173	ARG	CB-CG-CD	-6.01	97.48	111.30
1	B	41	C	P-O5'-C5'	6.00	129.91	120.90
1	B	34	C	OP2-P-O3'	-5.99	90.04	108.00
1	B	29	G	C5'-C4'-C3'	-5.96	107.06	116.00
1	B	22	A	C5'-C4'-C3'	-5.96	107.07	116.00
1	B	32	U	O4'-C1'-N1	5.95	117.42	108.50
1	B	32	U	N1-C1'-C2'	-5.93	103.10	112.00
2	A	83	ASN	CA-CB-CG	5.90	118.50	112.60
1	B	4	G	O3'-P-O5'	-5.86	95.20	104.00
1	B	50	G	O3'-P-O5'	5.83	112.75	104.00
1	B	71	C	OP1-P-O3'	-5.79	90.62	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	G	C5'-C4'-C3'	-5.76	107.37	116.00
2	A	128	GLN	OE1-CD-NE2	-5.75	116.84	122.60
1	B	40	C	OP1-P-O3'	-5.72	90.84	108.00
2	A	279	ASP	CA-CB-CG	5.72	118.32	112.60
2	A	274	ASN	OD1-CG-ND2	-5.71	116.89	122.60
2	A	255	GLN	OE1-CD-NE2	-5.70	116.90	122.60
2	A	530	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	B	2	G	O3'-P-O5'	5.68	112.52	104.00
1	B	53	G	OP1-P-O3'	-5.65	91.05	108.00
1	B	12	C	O3'-P-O5'	5.65	112.47	104.00
2	A	320	ASN	OD1-CG-ND2	-5.64	116.96	122.60
2	A	429	ASN	N-CA-C	5.64	120.43	113.50
1	B	38	U	C5'-C4'-C3'	-5.63	107.55	116.00
2	A	348	PRO	N-CA-C	5.63	124.08	112.47
2	A	142	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	B	48	C	P-O5'-C5'	5.59	129.28	120.90
1	B	60	U	O3'-P-O5'	-5.57	95.64	104.00
2	A	95	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	B	5	G	OP1-P-O3'	5.55	124.66	108.00
2	A	242	TRP	CB-CG-CD1	-5.52	118.63	126.90
2	A	65	PHE	CA-CB-CG	-5.51	108.29	113.80
1	B	32	U	O4'-C4'-C3'	-5.47	98.53	104.00
1	B	20	U	OP2-P-O3'	5.46	124.37	108.00
1	B	45	A	P-O3'-C3'	5.45	128.38	120.20
2	A	172	LEU	CA-C-O	-5.44	114.76	120.80
1	B	60	U	C5'-C4'-C3'	-5.43	107.06	115.20
2	A	43	HIS	CB-CG-CD2	-5.42	124.15	131.20
2	A	177	ASP	CA-CB-CG	5.41	118.01	112.60
2	A	280	LYS	CA-CB-CG	5.38	124.86	114.10
2	A	153	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	B	15	G	O4'-C4'-C3'	-5.37	100.73	106.10
1	B	72	A	OP2-P-O3'	5.33	123.98	108.00
2	A	67	ASP	N-CA-C	5.26	118.00	110.68
2	A	87	TRP	CG-CD2-CE3	5.24	139.14	133.90
1	B	69	C	OP1-P-O3'	5.24	123.71	108.00
2	A	467	VAL	N-CA-CB	-5.24	103.88	111.52
1	B	30	G	O4'-C4'-C3'	-5.19	98.81	104.00
2	A	82	LYS	CA-C-N	5.18	127.17	120.44
2	A	82	LYS	C-N-CA	5.18	127.17	120.44
1	B	55	U	O3'-P-O5'	-5.15	96.28	104.00
1	B	50	G	OP2-P-O3'	5.12	123.36	108.00
1	B	35	U	OP1-P-O3'	-5.12	92.64	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	G	C4'-C3'-C2'	-5.11	97.49	102.60
2	A	338	ASN	OD1-CG-ND2	-5.08	117.52	122.60
2	A	205	TRP	CE2-CD2-CG	-5.07	101.11	107.20
1	B	4	G	P-O5'-C5'	5.06	128.49	120.90
1	B	64	C	C5'-C4'-C3'	-5.05	108.42	116.00
1	B	46	U	C5'-C4'-O4'	5.05	117.37	109.80
1	B	30	G	O3'-P-O5'	5.04	111.56	104.00
1	B	15	G	O4'-C1'-N9	5.03	115.75	108.20
2	A	32	PRO	N-CA-C	5.02	116.83	110.70
2	A	153	ASN	CB-CG-ND2	5.02	123.93	116.40
1	B	30	G	O4'-C1'-N9	5.00	116.00	108.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	211	TYR	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	B	1573	0	800	11	0
2	A	4279	0	4172	57	0
3	A	23	0	12	0	0
4	A	112	0	0	0	0
4	B	17	0	0	0	0
All	All	6004	0	4984	64	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 (64) 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:39:LEU:HD13	2:A:81:ILE:HG12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:424:LYS:HA	2:A:430:ILE:HA	1.63	0.79
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.71	0.73
2:A:44:ALA:HB2	2:A:293:ILE:HD11	1.72	0.71
2:A:352:VAL:HG12	2:A:384:GLU:HG2	1.71	0.71
2:A:363:VAL:HG11	2:A:413:ASN:O	1.92	0.69
2:A:40:HIS:HA	2:A:292:THR:HA	1.81	0.63
1:B:46:U:H4'	1:B:47:U:C5	2.34	0.62
2:A:114:ILE:HG21	2:A:154:LEU:HD13	1.83	0.58
1:B:12:C:H5''	2:A:320:ASN:HB2	1.86	0.58
2:A:393:ARG:O	2:A:404:VAL:HA	2.04	0.57
2:A:287:ASP:OD1	2:A:289:ARG:HD3	2.05	0.57
1:B:60:U:H5''	1:B:61:C:H5	1.69	0.56
2:A:277:VAL:HG13	2:A:284:GLY:HA2	1.91	0.53
2:A:43:HIS:HE1	2:A:270:LYS:HE2	1.73	0.52
2:A:425:ASP:HB2	2:A:431:THR:HG23	1.90	0.52
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.91	0.51
1:B:32:U:H3'	1:B:32:U:OP2	2.11	0.51
2:A:114:ILE:CG2	2:A:154:LEU:HD13	2.40	0.51
2:A:30:ARG:NH1	2:A:215:HIS:CE1	2.79	0.50
2:A:288:PRO:HG3	2:A:298:ARG:HG2	1.93	0.50
2:A:487:PHE:O	2:A:490:VAL:HG12	2.12	0.50
1:B:74:C:N3	2:A:168:GLY:HA2	2.26	0.50
2:A:240:TYR:OH	2:A:253:PRO:HB2	2.12	0.49
2:A:225:THR:OG1	2:A:226:HIS:HD2	1.94	0.49
2:A:335:LEU:HB3	2:A:523:TYR:CD2	2.48	0.48
2:A:424:LYS:HG2	2:A:430:ILE:HG13	1.94	0.48
2:A:229:CYS:O	2:A:257:GLU:HA	2.13	0.48
2:A:340:PRO:HG3	2:A:514:LYS:HE2	1.96	0.47
2:A:437:TYR:CE2	2:A:439:ALA:HA	2.49	0.47
1:B:9:C:H5	1:B:12:C:N4	2.12	0.46
2:A:286:ASP:O	2:A:298:ARG:HD3	2.16	0.46
2:A:80:SER:O	2:A:83:ASN:HB3	2.16	0.46
2:A:296:LEU:O	2:A:301:TYR:HB2	2.17	0.45
2:A:411:LEU:HB3	2:A:458:TRP:CD1	2.52	0.45
2:A:349:VAL:HB	2:A:389:ARG:HD3	1.99	0.44
2:A:367:ASN:OD1	2:A:377:ARG:HD3	2.17	0.44
1:B:35:U:H1'	2:A:520:ARG:HG2	2.00	0.44
2:A:124:LEU:HG	2:A:128:GLN:HB3	2.00	0.44
2:A:512:ALA:HB2	2:A:528:SER:OG	2.18	0.43
1:B:36:G:C6	2:A:401:LYS:HG2	2.53	0.43
2:A:394:GLU:HG2	2:A:405:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:425:ASP:HB3	2:A:429:ASN:HB2	1.99	0.43
2:A:423:GLU:HB2	2:A:434:PHE:HE1	1.82	0.43
2:A:178:MET:O	2:A:186:ARG:HD2	2.19	0.43
2:A:28:HIS:CD2	2:A:60:GLN:HB2	2.54	0.43
2:A:530:HIS:HB3	2:A:537:VAL:HG21	1.99	0.43
2:A:142:ASN:HD22	2:A:178:MET:HG3	1.84	0.43
2:A:531:SER:HB3	2:A:537:VAL:H	1.83	0.42
1:B:15:G:O2'	1:B:16:C:P	2.77	0.42
1:B:46:U:OP1	1:B:47:U:H5'	2.19	0.42
2:A:362:MET:HG2	2:A:378:GLN:HG3	2.01	0.42
1:B:46:U:H6	1:B:46:U:H2'	1.68	0.41
2:A:423:GLU:HB3	2:A:432:THR:HG23	2.01	0.41
2:A:503:ALA:HB1	2:A:507:LEU:CD2	2.50	0.41
2:A:343:MET:HE3	2:A:458:TRP:H	1.85	0.41
2:A:407:LYS:HG2	2:A:408:GLU:H	1.85	0.41
2:A:410:ARG:HH21	2:A:442:LEU:HA	1.85	0.41
2:A:522:GLY:HA2	2:A:544:LEU:HD13	2.02	0.41
2:A:393:ARG:HB2	2:A:400:TYR:CZ	2.55	0.41
2:A:534:GLU:C	2:A:536:PRO:HD3	2.46	0.41
2:A:254:ARG:HA	2:A:254:ARG:HD3	1.86	0.40
2:A:54:ALA:HB2	2:A:61:CYS:HB2	2.02	0.40
2:A:15:ILE:HG12	2:A:226:HIS:CE1	2.57	0.40

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
2	A	525/553 (95%)	490 (93%)	29 (6%)	6 (1%)	11 36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	32	PRO
2	A	199	HIS
2	A	398	LYS
2	A	430	ILE
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%)	405 (88%)	58 (12%)	4 15

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	27	VAL
2	A	30	ARG
2	A	32	PRO
2	A	33	PRO
2	A	46	SER
2	A	49	LEU
2	A	78	VAL
2	A	80	SER
2	A	100	SER
2	A	105	GLN
2	A	106	LEU
2	A	113	LEU
2	A	124	LEU
2	A	154	LEU
2	A	156	LEU
2	A	169	LYS
2	A	186	ARG
2	A	190	LEU
2	A	192	ARG
2	A	229	CYS
2	A	231	LEU

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Mol	Chain	Res	Type
2	A	232	GLU
2	A	268	MET
2	A	269	SER
2	A	274	ASN
2	A	289	ARG
2	A	311	LYS
2	A	318	GLN
2	A	322	ILE
2	A	326	SER
2	A	327	LEU
2	A	335	LEU
2	A	341	ARG
2	A	362	MET
2	A	365	MET
2	A	369	PRO
2	A	373	GLU
2	A	378	GLN
2	A	389	ARG
2	A	395	GLU
2	A	410	ARG
2	A	412	ARG
2	A	420	GLU
2	A	422	VAL
2	A	425	ASP
2	A	431	THR
2	A	432	THR
2	A	441	THR
2	A	442	LEU
2	A	467	VAL
2	A	474	ARG
2	A	475	LEU
2	A	490	VAL
2	A	495	SER
2	A	497	VAL
2	A	505	PRO
2	A	514	LYS
2	A	531	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	55	GLN

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Mol	Chain	Res	Type
2	A	60	GLN
2	A	83	ASN
2	A	107	HIS
2	A	142	ASN
2	A	153	ASN
2	A	203	ASN
2	A	226	HIS
2	A	246	ASN
2	A	336	ASN
2	A	355	ASN
2	A	378	GLN
2	A	413	ASN
2	A	429	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	73/74 (98%)	18 (24%)	6 (8%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	9	C
1	B	16	C
1	B	18	G
1	B	19	G
1	B	20	U
1	B	21	A
1	B	30	G
1	B	32	U
1	B	36	G
1	B	37	A
1	B	41	C
1	B	44	C
1	B	45	A
1	B	46	U
1	B	47	U
1	B	48	C
1	B	52	G
1	B	62	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	15	G
1	B	16	C
1	B	20	U
1	B	36	G
1	B	44	C
1	B	45	A

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	AMP	A	999	-	25,25,25	0.78	1 (4%)	37,38,38	0.93	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
3	AMP	A	999	-	-	0/10/26/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	AMP	P-O2P	-2.02	1.47	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	AMP	O4'-C1'-C2'	-2.08	102.16	106.62
3	A	999	AMP	O5'-P-O1P	2.05	111.99	106.44

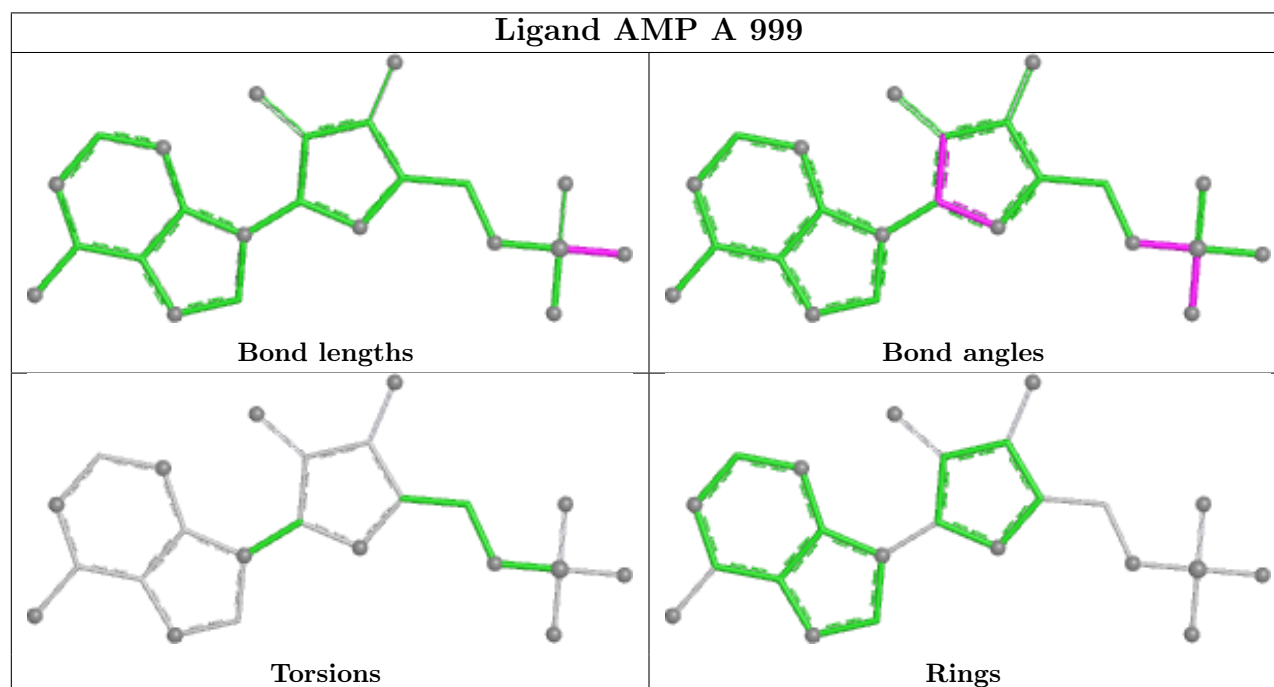
There are no chirality outliers.

There are no torsion outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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.