



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:33 PM UTC

PDB ID : 4JXX / pdb_00004jxx
Title : Crystal structure of E coli E. coli glutaminyl-tRNA synthetase bound to tRNA(Gln)(CUG) and ATP from novel cryostabilization conditions
Authors : Perona, J.J.; Rodriguez-Hernandez, A.
Deposited on : 2013-03-28
Resolution : 2.30 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

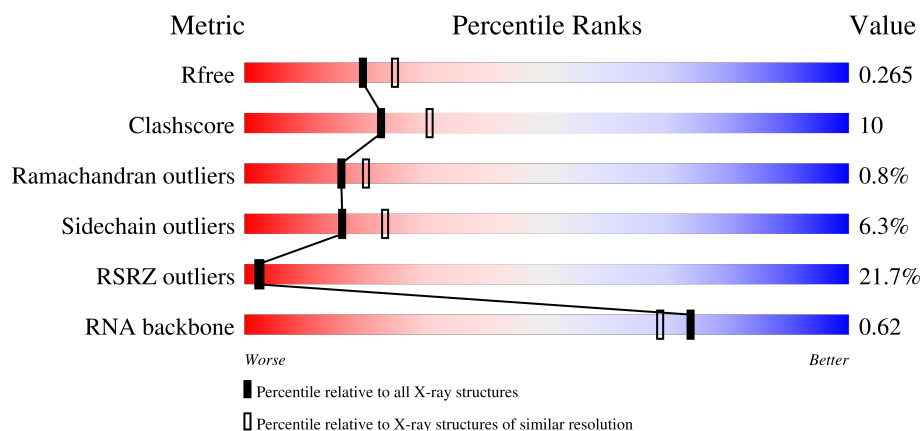
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)
RNA backbone	3983	1090 (2.60-2.00)

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	553	23% 71% 22% • •
2	B	75	9% 75% 16% • 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6050 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.

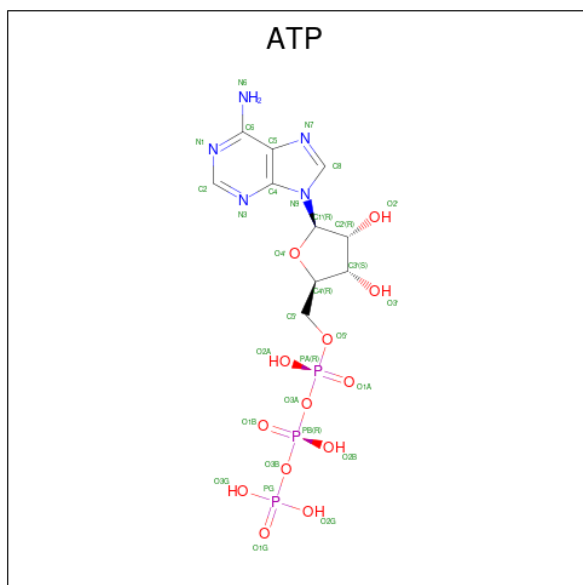
- Molecule 1 is a protein called Glutamine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4295	2715	755	804	21			

- Molecule 2 is a RNA chain called RNA (71-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	71	Total	C	N	O	P	0	0	0
			1511	674	270	496	71			

- 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 SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

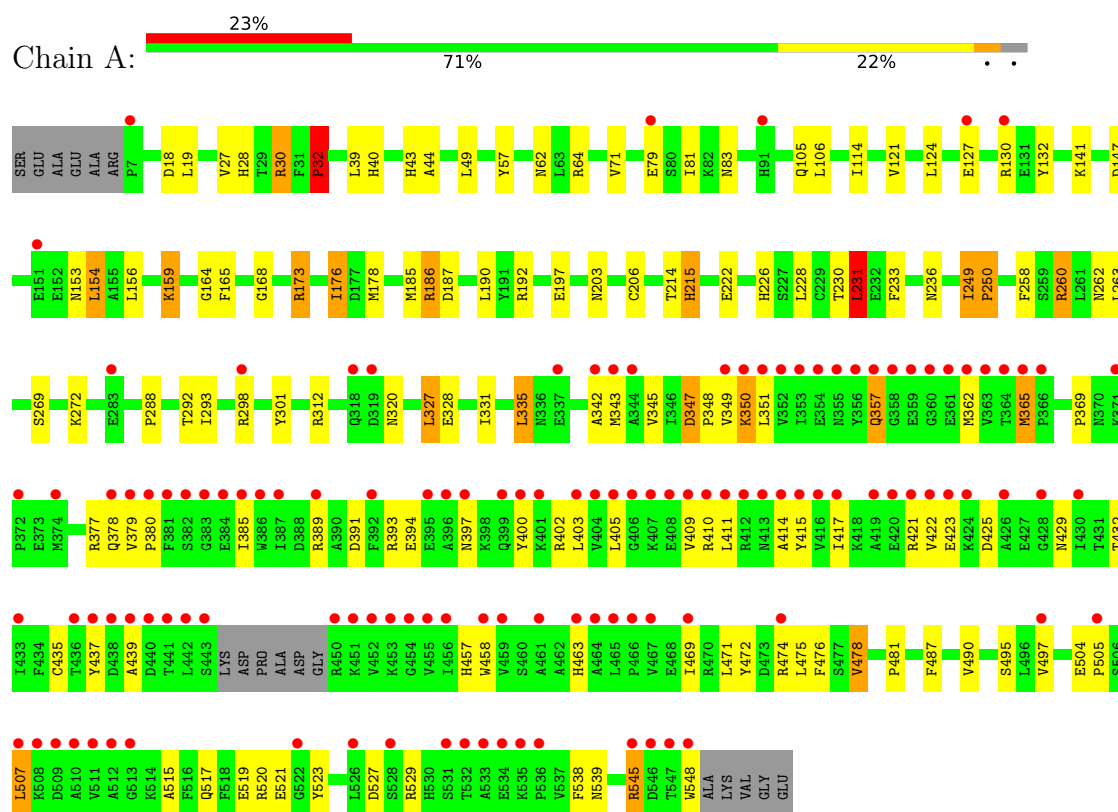
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	179	Total	O	0	0
			179	179		
5	B	29	Total	O	0	0
			29	29		

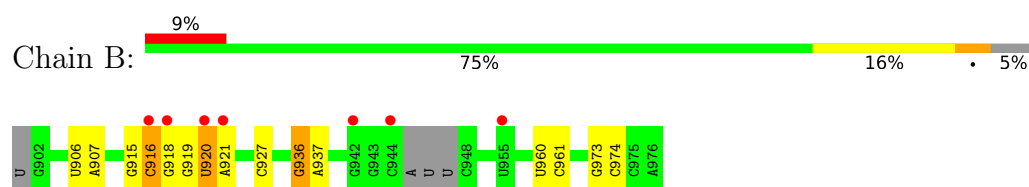
3 Residue-property plots [i](#)

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: Glutamine-tRNA ligase



• Molecule 2: RNA (71-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	93.66Å 234.28Å 113.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.10 – 2.30 41.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.10-2.30) 97.0 (41.10-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.258 0.234 , 0.265	Depositor DCC
R_{free} test set	10451 reflections (9.80%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6050	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, SO4

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	0.45	0/4398	0.90	15/5962 (0.3%)
2	B	0.30	0/1686	0.66	0/2623
All	All	0.42	0/6084	0.83	15/8585 (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
2	B	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	PRO	N-CA-C	7.00	122.60	113.86
1	A	347	ASP	CA-C-N	6.56	126.32	119.76
1	A	347	ASP	C-N-CA	6.56	126.32	119.76
1	A	214	THR	N-CA-C	6.15	117.78	111.14
1	A	147	ASP	N-CA-C	6.13	119.71	112.72
1	A	249	ILE	CA-C-N	5.95	125.57	119.56
1	A	249	ILE	C-N-CA	5.95	125.57	119.56
1	A	478	VAL	CA-C-N	5.88	125.36	119.24
1	A	478	VAL	C-N-CA	5.88	125.36	119.24
1	A	215	HIS	N-CA-C	5.69	117.17	110.97
1	A	231	LEU	N-CA-C	5.52	118.01	111.33
1	A	312	ARG	N-CA-C	5.40	117.25	111.36
1	A	348	PRO	N-CA-C	5.27	119.46	111.19
1	A	206	CYS	N-CA-C	-5.21	105.80	113.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	A	71	VAL	N-CA-C	5.08	116.41	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	915	G	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	4295	0	4133	106	0
2	B	1511	0	770	11	0
3	A	31	0	12	0	0
4	A	5	0	0	0	0
5	A	179	0	0	6	0
5	B	29	0	0	1	0
All	All	6050	0	4915	113	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 10.

All (113) 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:39:LEU:HD13	1:A:81:ILE:HG12	1.41	1.02
1:A:40:HIS:H	1:A:43:HIS:HD2	1.12	0.96
1:A:394:GLU:HA	1:A:405:LEU:HD23	1.58	0.85
1:A:40:HIS:H	1:A:43:HIS:CD2	2.02	0.74
1:A:343:MET:HG3	1:A:365:MET:HE1	1.69	0.74
1:A:435:CYS:HB3	5:A:842:HOH:O	1.85	0.74
1:A:159:LYS:HD3	1:A:164:GLY:HA3	1.69	0.74
1:A:380:PRO:HB2	1:A:463:HIS:CD2	2.24	0.72
1:A:83:ASN:HB2	5:A:808:HOH:O	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:GLN:HG3	1:A:523:TYR:CE1	2.26	0.71
1:A:39:LEU:CD1	1:A:81:ILE:HG12	2.21	0.68
1:A:471:LEU:HB2	1:A:497:VAL:HG13	1.76	0.67
1:A:40:HIS:HA	1:A:292:THR:HA	1.76	0.67
1:A:393:ARG:HD3	1:A:400:TYR:CZ	2.29	0.67
1:A:487:PHE:O	1:A:490:VAL:HG12	1.96	0.65
1:A:114:ILE:HG21	1:A:154:LEU:HD13	1.80	0.63
1:A:515:ALA:HB2	5:A:875:HOH:O	1.98	0.63
1:A:349:VAL:HB	1:A:389:ARG:HG2	1.80	0.62
1:A:357:GLN:H	1:A:357:GLN:CD	2.09	0.61
1:A:178:MET:O	1:A:186:ARG:HD2	2.02	0.59
1:A:40:HIS:N	1:A:43:HIS:HD2	1.92	0.59
1:A:30:ARG:NH2	1:A:228:LEU:O	2.37	0.57
1:A:394:GLU:HA	1:A:405:LEU:CD2	2.34	0.57
1:A:417:ILE:HB	5:A:842:HOH:O	2.04	0.57
1:A:114:ILE:CG2	1:A:154:LEU:HD13	2.35	0.56
1:A:365:MET:HE3	1:A:379:VAL:HG21	1.87	0.56
1:A:32:PRO:HA	1:A:64:ARG:O	2.05	0.56
1:A:173:ARG:HD2	1:A:187:ASP:O	2.05	0.55
1:A:520:ARG:NH1	2:B:936:G:OP1	2.38	0.55
1:A:421:ARG:HG2	1:A:422:VAL:H	1.70	0.55
1:A:437:TYR:CE2	1:A:439:ALA:HA	2.42	0.55
1:A:260:ARG:HG2	1:A:260:ARG:HH11	1.70	0.55
1:A:471:LEU:HB2	1:A:497:VAL:CG1	2.36	0.55
1:A:391:ASP:HA	1:A:402:ARG:HG2	1.90	0.54
1:A:159:LYS:HD2	1:A:165:PHE:CD2	2.43	0.53
1:A:377:ARG:HH11	1:A:377:ARG:HG2	1.74	0.53
1:A:351:LEU:HD23	1:A:351:LEU:O	2.09	0.52
1:A:298:ARG:NH1	1:A:529:ARG:NH1	2.57	0.52
1:A:545:ARG:HG2	1:A:545:ARG:NH1	2.25	0.52
1:A:520:ARG:HG2	1:A:520:ARG:HH11	1.75	0.52
1:A:545:ARG:HG2	1:A:545:ARG:HH11	1.73	0.52
1:A:132:TYR:CD2	1:A:141:LYS:HG3	2.45	0.51
1:A:422:VAL:HG12	1:A:423:GLU:N	2.25	0.51
1:A:403:LEU:HD13	1:A:409:VAL:HG22	1.93	0.51
2:B:936:G:H3'	2:B:937:A:H5'	1.93	0.51
1:A:365:MET:CE	1:A:379:VAL:HG11	2.41	0.51
1:A:504:GLU:HB2	1:A:505:PRO:HD2	1.93	0.50
1:A:393:ARG:HD3	1:A:400:TYR:CE1	2.46	0.50
1:A:298:ARG:HH12	1:A:529:ARG:NH1	2.10	0.50
2:B:920:U:H2'	2:B:920:U:O2	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HA	1:A:43:HIS:CD2	2.47	0.49
1:A:18:ASP:OD2	1:A:226:HIS:HE1	1.94	0.49
1:A:357:GLN:H	1:A:357:GLN:NE2	2.10	0.49
1:A:421:ARG:HG2	1:A:422:VAL:N	2.28	0.49
1:A:343:MET:HE3	1:A:458:TRP:O	2.13	0.49
1:A:365:MET:HE2	1:A:379:VAL:HG11	1.95	0.49
1:A:30:ARG:NH1	1:A:215:HIS:NE2	2.60	0.48
1:A:411:LEU:HB2	1:A:414:ALA:HB3	1.95	0.48
1:A:197:GLU:HG3	1:A:203:ASN:ND2	2.29	0.48
1:A:410:ARG:HD3	1:A:415:TYR:O	2.14	0.48
2:B:960:U:H5''	2:B:961:C:H5	1.77	0.48
1:A:121:VAL:H	1:A:153:ASN:ND2	2.12	0.47
1:A:342:ALA:HB1	1:A:507:LEU:HD21	1.96	0.47
1:A:457:HIS:HE1	5:A:809:HOH:O	1.98	0.47
1:A:402:ARG:HB3	1:A:403:LEU:H	1.58	0.47
1:A:345:VAL:HA	5:A:809:HOH:O	2.14	0.46
1:A:350:LYS:HG3	1:A:351:LEU:N	2.31	0.46
1:A:519:GLU:C	1:A:521:GLU:H	2.24	0.46
1:A:331:ILE:HG13	1:A:335:LEU:HD22	1.98	0.45
1:A:472:TYR:HA	1:A:495:SER:O	2.16	0.45
1:A:362:MET:CG	1:A:378:GLN:HG3	2.47	0.45
1:A:478:VAL:O	1:A:481:PRO:HD3	2.17	0.45
1:A:288:PRO:HD3	1:A:298:ARG:CZ	2.47	0.45
1:A:507:LEU:HD12	1:A:538:PHE:CZ	2.52	0.44
1:A:377:ARG:HG2	1:A:377:ARG:NH1	2.32	0.44
1:A:231:LEU:HD13	1:A:258:PHE:C	2.43	0.44
1:A:349:VAL:HG23	1:A:389:ARG:NH1	2.33	0.44
1:A:425:ASP:OD1	1:A:429:ASN:HB2	2.17	0.44
1:A:347:ASP:OD2	1:A:389:ARG:HD3	2.17	0.44
1:A:64:ARG:HD3	1:A:222:GLU:OE2	2.17	0.44
1:A:130:ARG:HG3	2:B:973:G:OP2	2.18	0.44
2:B:936:G:H3'	2:B:937:A:C5'	2.48	0.44
1:A:260:ARG:HH11	1:A:260:ARG:CG	2.31	0.43
1:A:176:ILE:HG21	1:A:185:MET:HE3	1.99	0.43
1:A:351:LEU:HD22	1:A:385:ILE:HD11	2.00	0.43
1:A:44:ALA:HB2	1:A:293:ILE:HD11	2.00	0.43
1:A:269:SER:OG	1:A:272:LYS:HG3	2.19	0.43
1:A:301:TYR:HE2	1:A:327:LEU:HD22	1.83	0.42
1:A:28:HIS:HE1	1:A:62:ASN:OD1	2.02	0.42
1:A:400:TYR:CE2	1:A:402:ARG:HB2	2.54	0.42
2:B:916:C:H5'	2:B:960:U:O2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG21	1:A:57:TYR:HB2	2.01	0.42
1:A:262:ASN:HB2	1:A:320:ASN:O	2.18	0.42
1:A:469:ILE:HD12	1:A:469:ILE:N	2.34	0.42
1:A:474:ARG:HD3	1:A:476:PHE:O	2.19	0.42
1:A:301:TYR:CE2	1:A:327:LEU:HD22	2.55	0.42
2:B:906:U:O2'	2:B:907:A:H5'	2.19	0.41
1:A:249:ILE:HG13	1:A:250:PRO:HD2	2.02	0.41
1:A:343:MET:HE2	1:A:365:MET:HE1	2.00	0.41
2:B:920:U:H3'	5:B:1021:HOH:O	2.19	0.41
1:A:400:TYR:CZ	1:A:402:ARG:HB2	2.55	0.41
1:A:168:GLY:HA2	2:B:974:C:N3	2.35	0.41
1:A:328:GLU:O	1:A:331:ILE:HG22	2.19	0.41
1:A:527:ASP:HB2	1:A:539:ASN:ND2	2.35	0.41
1:A:349:VAL:O	1:A:349:VAL:HG13	2.20	0.41
1:A:362:MET:HG2	1:A:378:GLN:HG3	2.03	0.40
1:A:545:ARG:NH2	2:B:927:C:OP2	2.49	0.40
1:A:154:LEU:HD12	1:A:154:LEU:HA	1.94	0.40
1:A:230:THR:HA	1:A:258:PHE:O	2.21	0.40
1:A:233:PHE:HA	1:A:236:ASN:HD22	1.87	0.40
1:A:349:VAL:HG23	1:A:389:ARG:HH12	1.86	0.40
1:A:394:GLU:CA	1:A:405:LEU:HD23	2.41	0.40
1:A:335:LEU:HD23	1:A:523:TYR:HB3	2.03	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
1	A	532/553 (96%)	501 (94%)	27 (5%)	4 (1%)	16 20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	PRO
1	A	397	ASN
1	A	369	PRO
1	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	
1	A	457/481 (95%)	428 (94%)	29 (6%)	16	23

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	30	ARG
1	A	32	PRO
1	A	49	LEU
1	A	79	GLU
1	A	105	GLN
1	A	106	LEU
1	A	124	LEU
1	A	127	GLU
1	A	154	LEU
1	A	156	LEU
1	A	159	LYS
1	A	173	ARG
1	A	186	ARG
1	A	190	LEU
1	A	192	ARG
1	A	231	LEU
1	A	260	ARG
1	A	263	LEU
1	A	327	LEU
1	A	335	LEU
1	A	350	LYS
1	A	357	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	365	MET
1	A	432	THR
1	A	475	LEU
1	A	507	LEU
1	A	545	ARG
1	A	548	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	43	HIS
1	A	60	GLN
1	A	105	GLN
1	A	115	ASN
1	A	142	ASN
1	A	153	ASN
1	A	203	ASN
1	A	226	HIS
1	A	236	ASN
1	A	318	GLN
1	A	355	ASN
1	A	367	ASN
1	A	413	ASN
1	A	429	ASN
1	A	457	HIS
1	A	463	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	69/75 (92%)	6 (8%)	2 (2%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	916	C
2	B	918	G
2	B	919	G
2	B	920	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	921	A
2	B	936	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	916	C
2	B	920	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](#)

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	$\# Z > 2$
3	ATP	A	601	-	32,33,33	1.65	7 (21%)	48,52,52	1.90	10 (20%)
4	SO4	A	602	-	4,4,4	0.38	0	6,6,6	0.06	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
3	ATP	A	601	-	-	4/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ATP	C2-N1	3.65	1.40	1.33
3	A	601	ATP	C2-N3	3.60	1.40	1.33
3	A	601	ATP	C5-N7	-3.11	1.33	1.39
3	A	601	ATP	C5-C4	-2.99	1.33	1.39
3	A	601	ATP	C5-C6	-2.70	1.33	1.41
3	A	601	ATP	C8-N9	-2.30	1.33	1.37
3	A	601	ATP	C4-N9	-2.08	1.33	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ATP	N3-C2-N1	-7.10	117.84	128.58
3	A	601	ATP	C5-C4-N3	-4.34	120.74	126.72
3	A	601	ATP	N9-C8-N7	-4.29	107.85	113.94
3	A	601	ATP	C2-N3-C4	3.31	119.91	111.83
3	A	601	ATP	C5-N7-C8	3.00	108.16	103.45
3	A	601	ATP	C5-C6-N6	-2.79	116.38	123.29
3	A	601	ATP	C6-C5-C4	2.57	120.68	117.18
3	A	601	ATP	N3-C4-N9	2.46	131.34	127.17
3	A	601	ATP	C4-C5-N7	-2.32	107.93	110.58
3	A	601	ATP	C4-N9-C8	2.28	108.14	105.74

There are no chirality outliers.

All (4) torsion outliers are listed below:

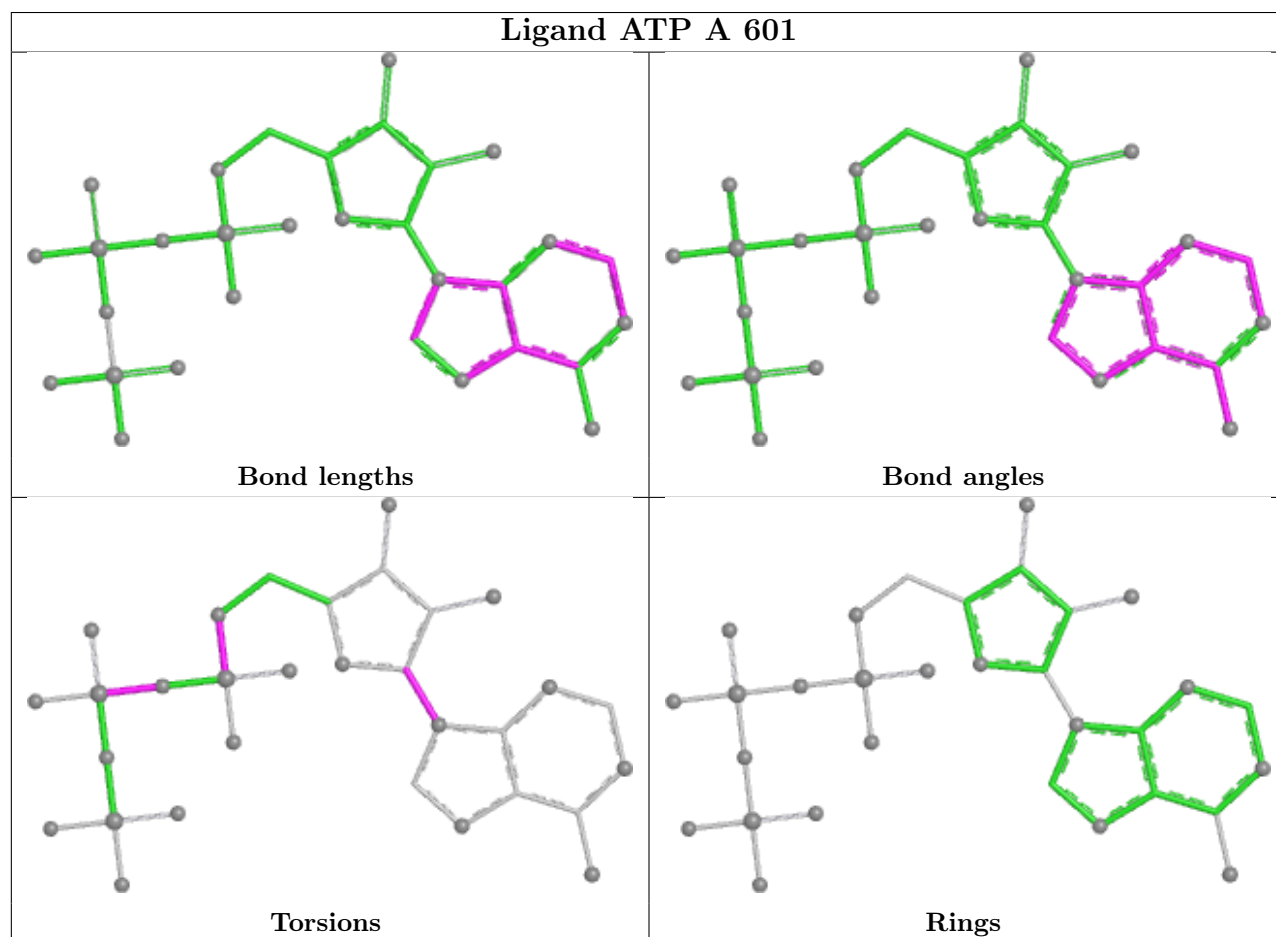
Mol	Chain	Res	Type	Atoms
3	A	601	ATP	C5'-O5'-PA-O3A
3	A	601	ATP	C5'-O5'-PA-O1A
3	A	601	ATP	C2'-C1'-N9-C8
3	A	601	ATP	PA-O3A-PB-O1B

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

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	536/553 (96%)	0.94	125 (23%) 2 2	30, 49, 93, 105	0
2	B	71/75 (94%)	0.81	7 (9%) 13 14	41, 77, 105, 118	0
All	All	607/628 (96%)	0.93	132 (21%) 2 2	30, 50, 96, 118	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	TRP	6.7
1	A	358	GLY	6.0
1	A	7	PRO	5.7
1	A	443	SER	5.6
1	A	406	GLY	5.3
1	A	360	GLY	5.1
1	A	381	PHE	5.0
1	A	452	VAL	5.0
1	A	439	ALA	4.6
1	A	356	TYR	4.6
1	A	355	ASN	4.5
1	A	414	ALA	4.5
1	A	419	ALA	4.4
1	A	507	LEU	4.4
1	A	440	ASP	4.4
1	A	465	LEU	4.3
1	A	397	ASN	4.3
1	A	442	LEU	4.3
1	A	411	LEU	4.2
1	A	352	VAL	4.2
1	A	409	VAL	4.2
1	A	533	ALA	4.2
1	A	547	THR	4.2
1	A	353	ILE	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	944	C	4.2
1	A	363	VAL	4.1
1	A	407	LYS	4.0
1	A	404	VAL	4.0
1	A	379	VAL	3.8
1	A	463	HIS	3.8
1	A	405	LEU	3.8
1	A	357	GLN	3.7
1	A	466	PRO	3.7
1	A	467	VAL	3.7
1	A	508	LYS	3.6
1	A	415	TYR	3.6
1	A	437	TYR	3.6
1	A	505	PRO	3.5
1	A	383	GLY	3.5
1	A	532	THR	3.5
1	A	453	LYS	3.4
1	A	380	PRO	3.4
1	A	359	GLU	3.4
2	B	921	A	3.4
1	A	455	VAL	3.4
1	A	382	SER	3.4
1	A	545	ARG	3.3
1	A	430	ILE	3.3
1	A	342	ALA	3.3
1	A	441	THR	3.3
1	A	416	VAL	3.3
1	A	464	ALA	3.2
1	A	426	ALA	3.2
2	B	920	U	3.1
1	A	401	LYS	3.0
1	A	384	GLU	3.0
1	A	458	TRP	3.0
1	A	422	VAL	2.9
1	A	366	PRO	2.9
1	A	354	GLU	2.9
1	A	459	VAL	2.9
1	A	343	MET	2.9
1	A	392	PHE	2.8
1	A	510	ALA	2.8
1	A	408	GLU	2.8
1	A	386	TRP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	372	PRO	2.8
1	A	526	LEU	2.8
1	A	385	ILE	2.7
1	A	371	LYS	2.7
1	A	433	ILE	2.7
1	A	450	ARG	2.7
1	A	469	ILE	2.7
1	A	399	GLN	2.7
1	A	522	GLY	2.6
1	A	454	GLY	2.6
1	A	417	ILE	2.6
1	A	350	LYS	2.6
1	A	319	ASP	2.5
1	A	362	MET	2.5
1	A	364	THR	2.5
1	A	412	ARG	2.5
1	A	421	ARG	2.5
1	A	374	MET	2.5
1	A	461	ALA	2.5
1	A	511	VAL	2.5
1	A	403	LEU	2.5
1	A	365	MET	2.5
1	A	509	ASP	2.5
2	B	918	G	2.5
1	A	151	GLU	2.5
1	A	337	GLU	2.4
1	A	420	GLU	2.4
1	A	424	LYS	2.4
1	A	451	LYS	2.4
1	A	546	ASP	2.4
1	A	531	SER	2.4
1	A	351	LEU	2.4
1	A	438	ASP	2.4
1	A	423	GLU	2.4
1	A	318	GLN	2.4
1	A	389	ARG	2.4
1	A	400	TYR	2.4
1	A	79	GLU	2.4
1	A	513	GLY	2.4
2	B	955	U	2.3
1	A	91	HIS	2.3
1	A	298	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	ARG	2.3
1	A	349	VAL	2.3
1	A	410	ARG	2.3
1	A	474	ARG	2.3
1	A	534	GLU	2.2
1	A	127	GLU	2.2
1	A	428	GLY	2.2
1	A	378	GLN	2.2
1	A	344	ALA	2.2
1	A	456	ILE	2.2
1	A	497	VAL	2.2
2	B	916	C	2.2
1	A	512	ALA	2.2
1	A	387	ILE	2.1
1	A	536	PRO	2.1
1	A	396	ALA	2.1
1	A	361	GLU	2.1
1	A	535	LYS	2.0
1	A	528	SER	2.0
1	A	283	GLU	2.0
1	A	395	GLU	2.0
2	B	942	G	2.0
1	A	413	ASN	2.0
1	A	436	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

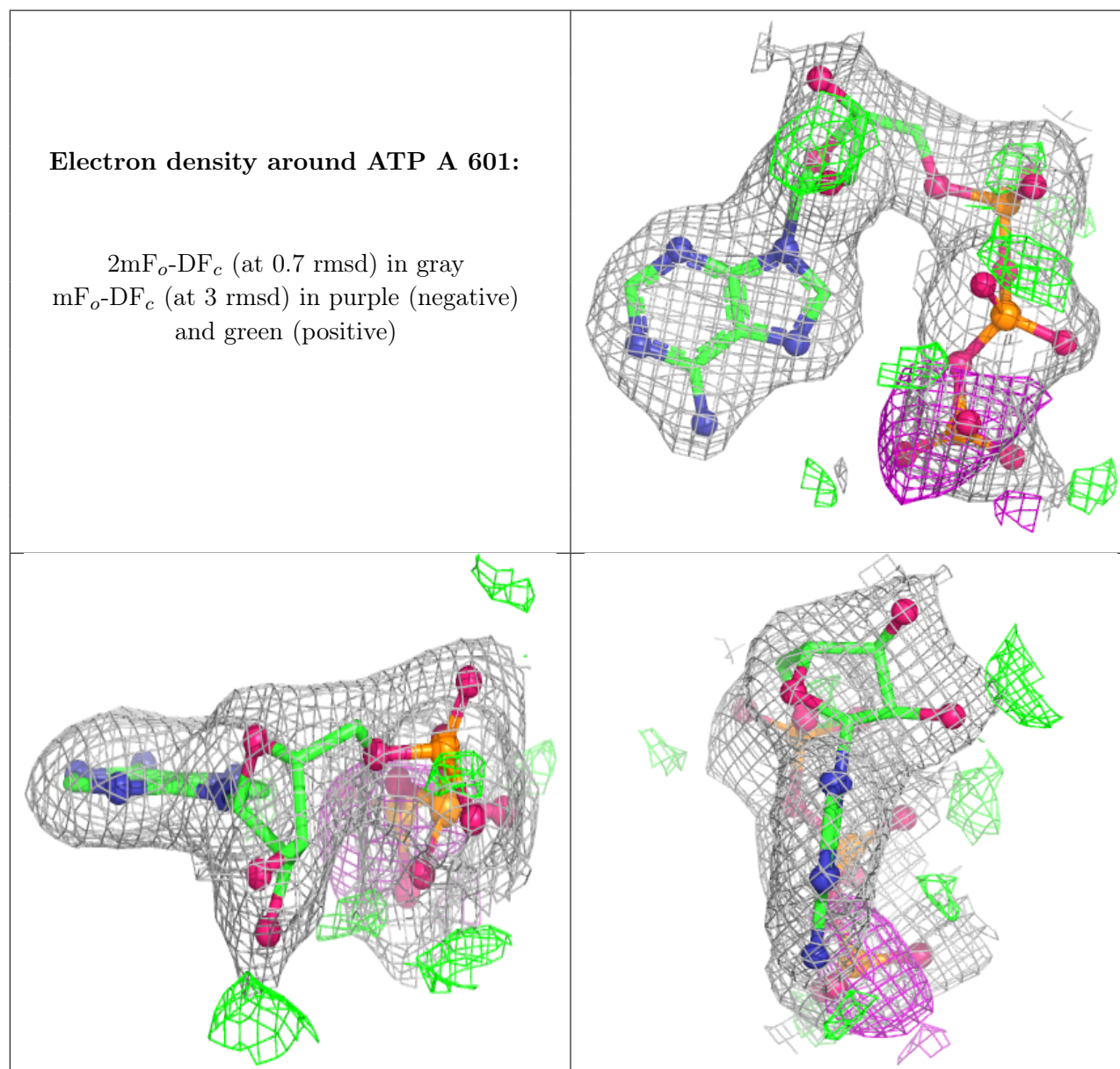
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
4	SO4	A	602	5/5	0.81	0.25	150,150,150,151	0
3	ATP	A	601	31/31	0.94	0.11	37,42,71,73	0

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.



6.5 Other polymers ⓘ

There are no such residues in this entry.