



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:02 AM UTC

PDB ID : 4KR2 / pdb_00004kr2
Title : Glycyl-tRNA synthetase in complex with tRNA-Gly
Authors : Qin, X.; Hao, Z.; Tian, Q.; Zhang, Z.; Zhou, C.; Xie, W.
Deposited on : 2013-05-16
Resolution : 3.29 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

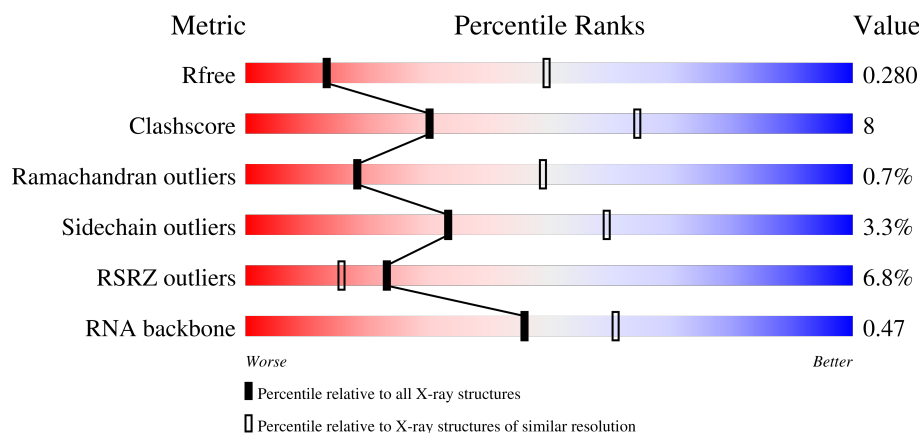
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	637	4% 55% 15% 28%
2	C	74	12% 47% 35% 9% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5044 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 Glycine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3540	2255	616	651	18			

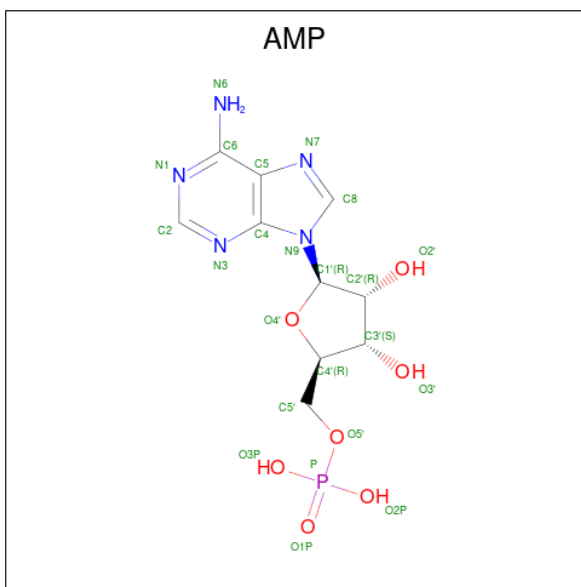
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	MET	-	expression tag	UNP P41250
A	58	ALA	-	expression tag	UNP P41250
A	59	SER	-	expression tag	UNP P41250
A	686	LEU	-	expression tag	UNP P41250
A	687	GLU	-	expression tag	UNP P41250
A	688	HIS	-	expression tag	UNP P41250
A	689	HIS	-	expression tag	UNP P41250
A	690	HIS	-	expression tag	UNP P41250
A	691	HIS	-	expression tag	UNP P41250
A	692	HIS	-	expression tag	UNP P41250
A	693	HIS	-	expression tag	UNP P41250

- Molecule 2 is a RNA chain called Gly-tRNA-CCC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	69	Total	C	N	O	P	0	0	0
			1476	653	254	498	71			

- 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	A	4	Total	O	0	0
			4	4		
4	C	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.96Å 88.50Å 80.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.25 – 3.29 32.25 – 3.29	Depositor EDS
% Data completeness (in resolution range)	89.3 (32.25-3.29) 88.7 (32.25-3.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.236 , 0.277 0.237 , 0.280	Depositor DCC
R_{free} test set	691 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	1.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5044	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: AMP, GTP

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	0.36	0/3622	0.88	8/4915 (0.2%)
2	C	0.13	0/1610	0.33	0/2507
All	All	0.31	0/5232	0.74	8/7422 (0.1%)

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	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	413	TYR	N-CA-C	12.70	125.60	108.07
1	A	414	ASP	N-CA-C	-6.47	105.52	113.41
1	A	369	SER	CA-C-N	5.41	124.87	119.24
1	A	369	SER	C-N-CA	5.41	124.87	119.24
1	A	626	THR	CA-C-N	-5.31	113.21	119.84
1	A	626	THR	C-N-CA	-5.31	113.21	119.84
1	A	412	CYS	CA-C-N	-5.27	114.44	122.23
1	A	412	CYS	C-N-CA	-5.27	114.44	122.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	412	CYS	Peptide

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	3540	0	3378	63	0
2	C	1476	0	743	18	0
3	A	23	0	12	0	0
4	A	4	0	0	1	0
4	C	1	0	0	0	0
All	All	5044	0	4133	77	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 8.

All (77) 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:410:ARG:NH1	1:A:522:GLU:OE1	2.11	0.84
1:A:410:ARG:HH22	1:A:522:GLU:HB3	1.45	0.81
1:A:563:SER:HB3	1:A:612:VAL:HG11	1.73	0.71
1:A:585:THR:HG23	1:A:591:HIS:HE1	1.56	0.70
1:A:349:ASN:HD21	1:A:352:LEU:HD13	1.57	0.68
2:C:1:GTP:H2'	2:C:2:C:C6	2.28	0.67
2:C:5:C:H42	2:C:68:G:H1	1.42	0.66
1:A:538:THR:HB	1:A:552:SER:H	1.61	0.65
2:C:58:A:O2'	2:C:60:U:OP2	2.13	0.65
1:A:297:ILE:HB	1:A:523:PRO:HG2	1.80	0.64
1:A:372:LYS:NZ	4:A:801:HOH:O	2.29	0.62
1:A:597:SER:OG	2:C:29:A:OP2	2.17	0.62
2:C:54:U:H3	2:C:58:A:H2	1.50	0.59
1:A:404:ILE:HG22	1:A:529:ARG:HB3	1.85	0.59
1:A:283:ARG:NH2	2:C:71:G:O6	2.36	0.59
1:A:641:ILE:HA	1:A:671:LEU:HA	1.86	0.58
1:A:317:LEU:HD11	1:A:360:TYR:CE2	2.41	0.56
1:A:308:HIS:HE1	1:A:310:LYS:HD3	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:SER:O	1:A:420:ARG:HG2	2.05	0.55
1:A:79:PHE:HA	1:A:99:VAL:HG23	1.88	0.55
1:A:243:ARG:NH1	1:A:271:GLN:OE1	2.40	0.55
2:C:18:G:O2'	2:C:57:G:N2	2.37	0.54
1:A:319:LEU:O	1:A:335:LYS:HA	2.08	0.53
2:C:20:U:H5''	2:C:21:A:OP1	2.08	0.53
1:A:655:LEU:HD11	1:A:665:VAL:HG21	1.90	0.53
1:A:104:LYS:HA	1:A:531:MET:HE1	1.91	0.52
1:A:317:LEU:HG	1:A:319:LEU:HD11	1.91	0.52
2:C:4:C:O2'	2:C:5:C:OP1	2.27	0.51
1:A:564:VAL:CG1	1:A:580:LEU:HD11	2.41	0.51
1:A:284:SER:HB2	1:A:287:ILE:HB	1.93	0.51
2:C:21:A:H61	2:C:46:A:H2'	1.76	0.50
1:A:322:TYR:HB3	1:A:376:ARG:HA	1.94	0.49
1:A:314:VAL:HG21	1:A:354:TYR:HA	1.95	0.49
2:C:15:G:H2'	2:C:16:U:C6	2.48	0.49
1:A:644:GLU:HB2	1:A:647:GLU:OE1	2.13	0.48
1:A:521:ILE:HG22	1:A:523:PRO:HD3	1.96	0.48
2:C:8:U:H5'	2:C:49:C:OP2	2.13	0.47
1:A:629:THR:HA	1:A:644:GLU:HA	1.96	0.47
1:A:124:ILE:HD11	1:A:250:ILE:HG12	1.97	0.47
1:A:312:GLN:HA	1:A:315:ALA:HB2	1.96	0.47
1:A:308:HIS:CE1	1:A:310:LYS:HB2	2.50	0.46
1:A:427:VAL:HG12	1:A:428:ALA:O	2.15	0.46
1:A:556:VAL:HG23	1:A:557:VAL:HG13	1.96	0.46
2:C:58:A:H8	2:C:60:U:C5	2.33	0.46
2:C:39:U:H2'	2:C:40:C:C6	2.50	0.46
1:A:393:ALA:HB3	1:A:405:VAL:HB	1.97	0.46
1:A:319:LEU:HD23	1:A:375:PHE:CE2	2.50	0.46
1:A:562:CYS:HB2	1:A:652:VAL:HG11	1.98	0.45
1:A:348:ASN:CG	1:A:349:ASN:HD22	2.25	0.45
1:A:580:LEU:HA	1:A:583:ALA:HB3	1.97	0.45
1:A:242:LEU:HB3	1:A:276:PHE:CD2	2.52	0.45
1:A:227:MET:HE3	1:A:244:PRO:HG3	1.98	0.45
1:A:531:MET:HE2	1:A:531:MET:HB2	1.85	0.45
1:A:341:ALA:O	1:A:346:VAL:HG12	2.17	0.45
1:A:580:LEU:HD21	1:A:618:ILE:HD11	1.99	0.45
1:A:661:THR:OG1	1:A:662:TRP:N	2.50	0.44
1:A:565:LEU:HA	1:A:566:PRO:HD3	1.88	0.44
1:A:651:ILE:O	1:A:655:LEU:HD12	2.17	0.44
1:A:605:ALA:O	1:A:609:GLU:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:GLN:HE21	2:C:36:C:H41	1.66	0.44
1:A:580:LEU:HD12	1:A:580:LEU:C	2.44	0.43
1:A:585:THR:HG23	1:A:591:HIS:CE1	2.46	0.43
1:A:634:ASP:HB2	1:A:662:TRP:CE2	2.54	0.43
1:A:641:ILE:HG22	1:A:671:LEU:HA	2.02	0.42
1:A:411:SER:HA	1:A:519:ASN:HA	2.01	0.42
1:A:631:THR:HG23	1:A:642:ARG:HH11	1.86	0.41
1:A:83:ALA:O	1:A:89:GLY:HA2	2.20	0.41
2:C:3:G:H2'	2:C:4:C:C6	2.55	0.41
2:C:9:G:O2'	2:C:10:G:N7	2.47	0.41
1:A:317:LEU:HG	1:A:319:LEU:CD1	2.51	0.41
1:A:565:LEU:O	1:A:617:THR:HA	2.21	0.41
1:A:640:GLN:NE2	2:C:36:C:H41	2.19	0.41
1:A:633:ARG:HB2	1:A:640:GLN:HG2	2.03	0.40
1:A:530:ILE:O	1:A:534:VAL:HG23	2.21	0.40
1:A:299:HIS:HB3	1:A:521:ILE:HB	2.02	0.40
1:A:348:ASN:OD1	1:A:348:ASN:C	2.63	0.40
1:A:603:ARG:HA	1:A:606:ARG:HD2	2.02	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
1	A	450/637 (71%)	427 (95%)	20 (4%)	3 (1%)	18 49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	PRO
1	A	411	SER
1	A	575	PRO

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	366/556 (66%)	354 (97%)	12 (3%)	33 59

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	THR
1	A	127	THR
1	A	280	ILE
1	A	338	LEU
1	A	352	LEU
1	A	378	HIS
1	A	517	VAL
1	A	597	SER
1	A	618	ILE
1	A	638	MET
1	A	641	ILE
1	A	655	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	A	378	HIS
1	A	640	GLN
1	A	653	GLN
1	A	657	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	68/74 (91%)	14 (20%)	4 (5%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	4	C
2	C	5	C
2	C	9	G
2	C	18	G
2	C	19	G
2	C	21	A
2	C	28	A
2	C	35	C
2	C	36	C
2	C	37	A
2	C	38	U
2	C	48	C
2	C	59	U
2	C	65	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	1	GTP
2	C	3	G
2	C	4	C
2	C	34	C

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
2	GTP	C	1	2	33,34,34	2.89	14 (42%)	50,54,54	1.99	10 (20%)

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	GTP	C	1	2	-	7/22/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	GTP	O6-C6	9.62	1.41	1.23
2	C	1	GTP	PB-O3A	-5.05	1.54	1.59
2	C	1	GTP	C2'-C3'	-5.03	1.39	1.53
2	C	1	GTP	C2-N2	4.68	1.45	1.34
2	C	1	GTP	C5-N7	-4.15	1.30	1.39
2	C	1	GTP	PA-O3A	-3.97	1.55	1.59
2	C	1	GTP	C8-N9	-3.47	1.29	1.37
2	C	1	GTP	O4'-C4'	-2.98	1.38	1.45
2	C	1	GTP	C5-C4	2.98	1.46	1.38
2	C	1	GTP	C8-N7	-2.94	1.24	1.32
2	C	1	GTP	C3'-C4'	-2.18	1.47	1.53
2	C	1	GTP	PB-O2B	-2.10	1.45	1.55
2	C	1	GTP	O3'-C3'	-2.03	1.37	1.43
2	C	1	GTP	C4-N9	2.02	1.43	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GTP	N9-C4-N3	5.71	137.37	125.95
2	C	1	GTP	C8-N7-C5	5.36	113.81	104.26
2	C	1	GTP	C5-C4-N3	-5.11	120.26	128.39
2	C	1	GTP	C2-N3-C4	4.29	119.68	112.30
2	C	1	GTP	C6-C5-N7	3.98	137.53	130.29
2	C	1	GTP	C4-C5-N7	-3.87	104.53	110.67
2	C	1	GTP	O5'-C5'-C4'	2.51	117.53	108.99
2	C	1	GTP	C5-C6-N1	2.18	118.80	113.25
2	C	1	GTP	O6-C6-C5	-2.17	120.82	126.53
2	C	1	GTP	C3'-C2'-C1'	2.16	105.55	101.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	GTP	C5'-O5'-PA-O3A
2	C	1	GTP	C5'-O5'-PA-O1A
2	C	1	GTP	C5'-O5'-PA-O2A
2	C	1	GTP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1	GTP	C3'-C4'-C5'-O5'
2	C	1	GTP	PB-O3A-PA-O1A
2	C	1	GTP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GTP	1	0

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	701	-	25,25,25	1.47	4 (16%)	37,38,38	2.00	10 (27%)

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	701	-	-	4/10/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	AMP	C5-C4	4.96	1.47	1.39
3	A	701	AMP	C5-C6	2.85	1.48	1.41
3	A	701	AMP	C8-N7	2.58	1.36	1.31
3	A	701	AMP	C5-N7	-2.14	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	AMP	C5-C4-N3	-5.65	118.93	126.72
3	A	701	AMP	N3-C4-N9	4.41	134.67	127.17
3	A	701	AMP	C4-C5-N7	-4.07	105.93	110.58
3	A	701	AMP	C2-N3-C4	3.47	120.29	111.83
3	A	701	AMP	C4-N9-C8	3.22	109.12	105.74
3	A	701	AMP	C5-N7-C8	3.09	108.31	103.45
3	A	701	AMP	N3-C2-N1	-3.07	123.93	128.58
3	A	701	AMP	N9-C8-N7	-2.61	110.23	113.94
3	A	701	AMP	C6-C5-N7	2.29	136.51	132.09
3	A	701	AMP	C2-N1-C6	2.04	122.08	118.73

There are no chirality outliers.

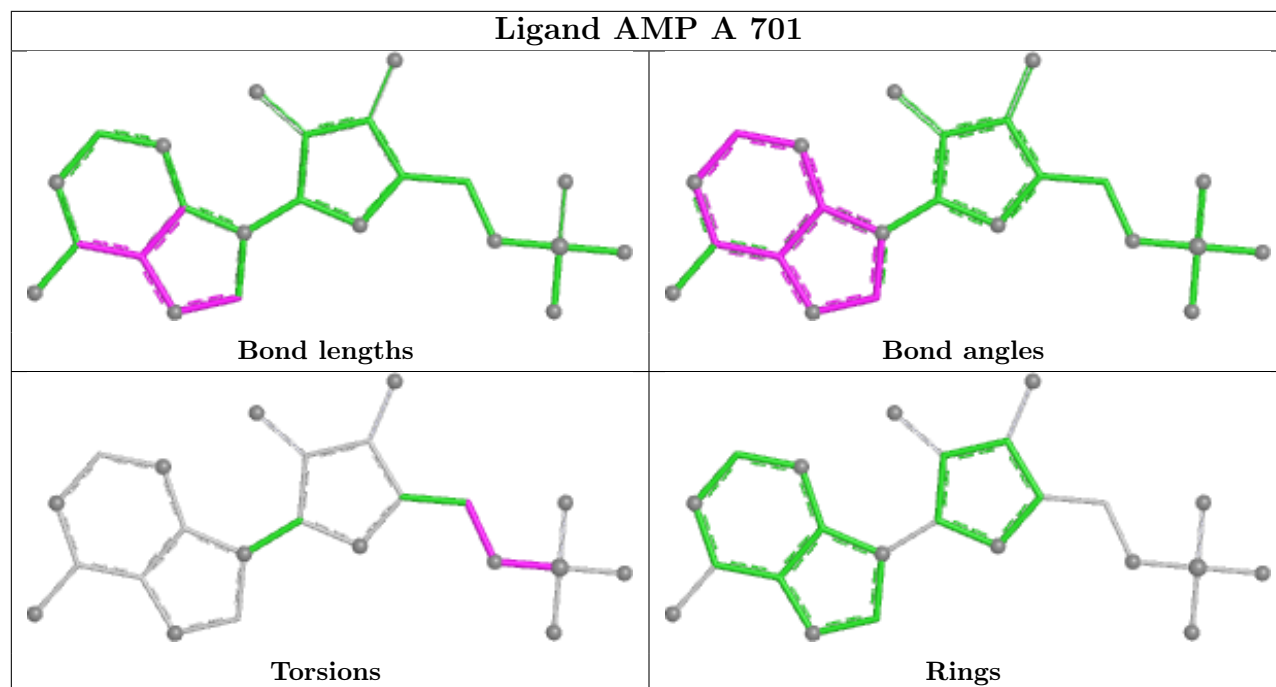
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	AMP	C5'-O5'-P-O1P
3	A	701	AMP	C5'-O5'-P-O2P
3	A	701	AMP	C5'-O5'-P-O3P
3	A	701	AMP	C4'-C5'-O5'-P

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	458/637 (71%)	0.67	27 (5%) 28 19	64, 96, 136, 185	0
2	C	68/74 (91%)	0.91	9 (13%) 7 6	86, 125, 170, 193	0
All	All	526/711 (73%)	0.70	36 (6%) 23 16	64, 99, 144, 193	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	562	CYS	6.2
2	C	59	U	4.0
1	A	582	GLU	3.5
1	A	74	LEU	3.5
1	A	662	TRP	3.4
1	A	664	ASP	3.1
1	A	100	GLY	2.9
1	A	641	ILE	2.9
2	C	48	C	2.8
1	A	552	SER	2.7
1	A	521	ILE	2.5
1	A	648	LEU	2.5
1	A	294	MET	2.5
2	C	12	G	2.5
1	A	230	THR	2.5
1	A	114	HIS	2.4
2	C	61	C	2.4
1	A	234	PRO	2.4
1	A	393	ALA	2.3
1	A	409	ASP	2.3
2	C	49	C	2.3
1	A	661	THR	2.3
2	C	34	C	2.2
1	A	438	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	342	VAL	2.2
1	A	85	ALA	2.1
1	A	408	ALA	2.1
1	A	413	TYR	2.1
1	A	79	PHE	2.1
1	A	538	THR	2.1
1	A	673	GLU	2.1
2	C	35	C	2.1
2	C	71	G	2.1
2	C	26	G	2.0
1	A	86	ILE	2.0
1	A	380	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	GTP	C	1	32/32	0.73	0.12	143,181,194,213	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

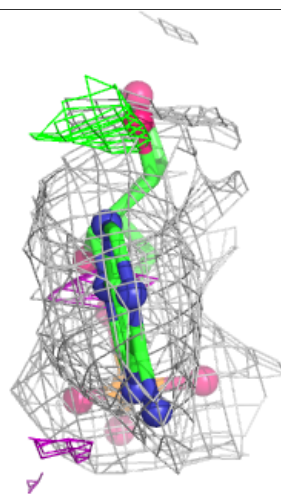
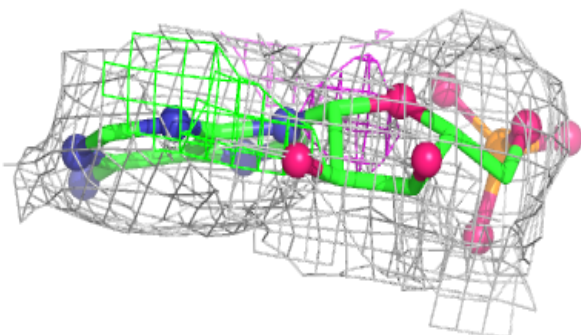
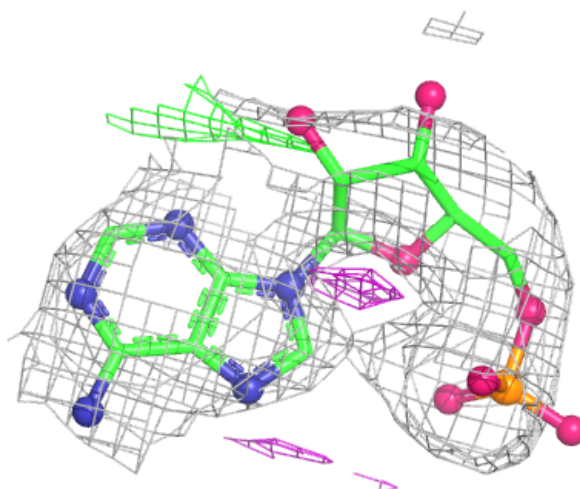
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AMP	A	701	23/23	0.69	0.16	74,130,188,198	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.

Electron density around AMP A 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.