



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:51 PM UTC

PDB ID : 4QEI / pdb_00004qei
Title : Two distinct conformational states of GlyRS captured in crystal lattice
Authors : Xie, W.; Qin, X.; Deng, X.; Zhang, Q.; Li, Q.
Deposited on : 2014-05-16
Resolution : 2.88 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

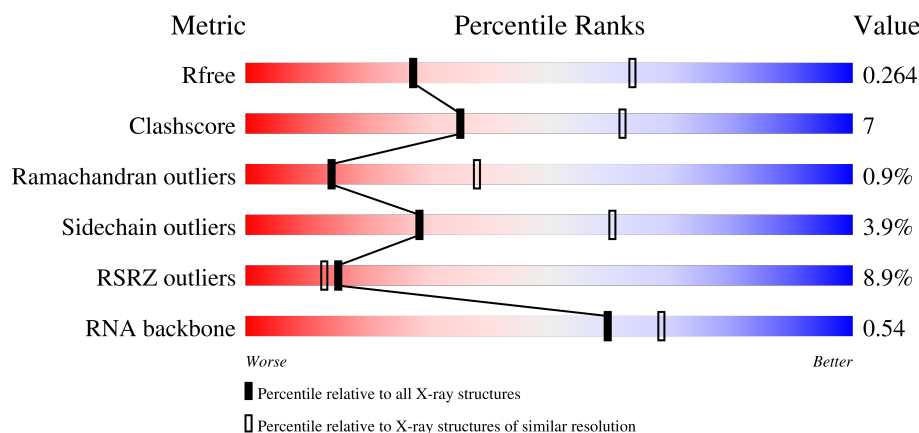
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)
RNA backbone	3983	1174 (3.10-2.66)

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	630	9% 67% 19% • 11%
2	C	69	% 61% 36% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5764 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
			Total	C	N	O	S			
1	A	562	4232	2691	738	781	22	0	0	0

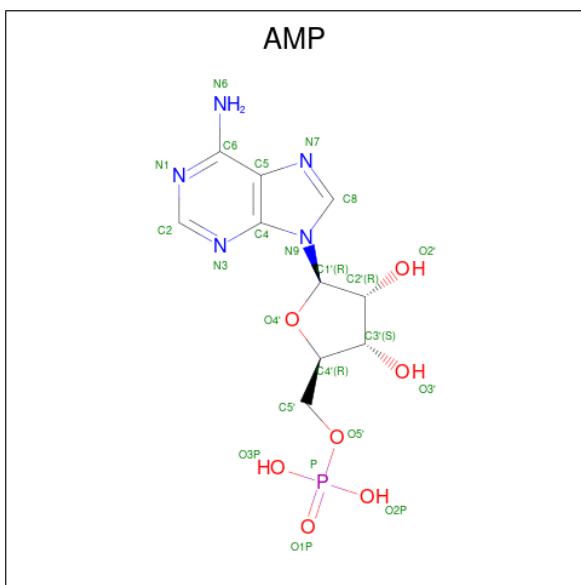
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	GLY	GLU	engineered mutation	UNP P41250
A	157	ARG	CYS	engineered mutation	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 tRNA-Gly-CCC-2-2.

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

- 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		

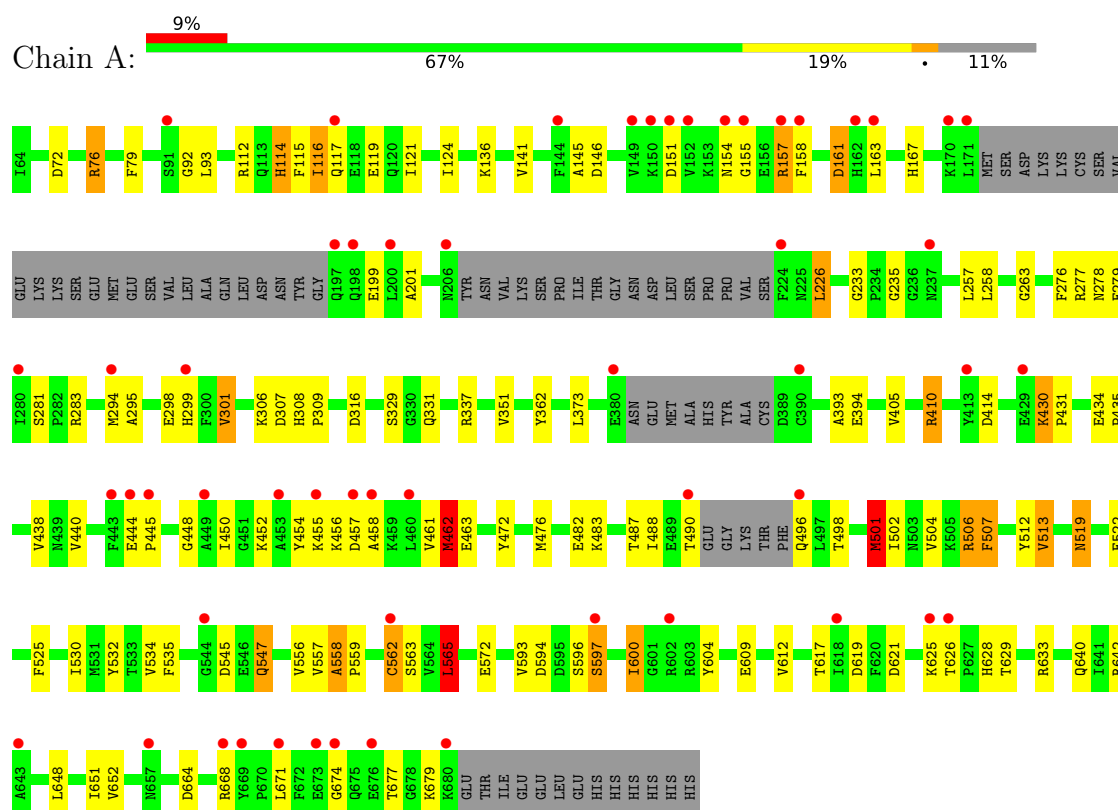
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	C	9	Total	O	0	0
			9	9		

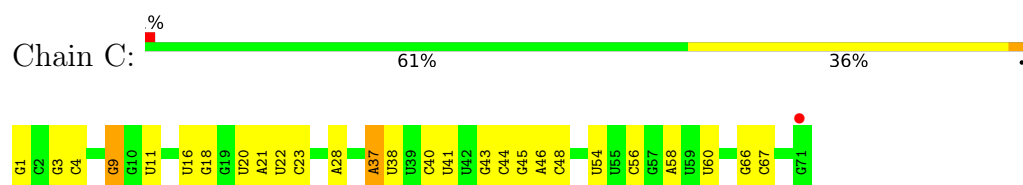
3 Residue-property plots

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 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: Glycine-tRNA ligase



• Molecule 2: tRNA-Gly-CCC-2-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.60Å 88.45Å 81.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.90 – 2.88 36.90 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.0 (36.90-2.88) 97.6 (36.90-2.88)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.213 , 0.265 0.217 , 0.264	Depositor DCC
R_{free} test set	1134 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	1.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.4	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	0.93	EDS
Total number of atoms	5764	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: GTP, 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	A	0.78	0/4322	1.36	47/5861 (0.8%)
2	C	0.36	0/1610	0.54	0/2507
All	All	0.69	0/5932	1.17	47/8368 (0.6%)

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 (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	ALA	CA-C-N	12.53	135.51	119.84
1	A	558	ALA	C-N-CA	12.53	135.51	119.84
1	A	456	LYS	N-CA-C	-11.58	99.85	114.56
1	A	462	MET	N-CA-C	-10.83	99.06	114.12
1	A	482	GLU	N-CA-C	-10.12	87.94	107.57
1	A	430	LYS	CA-C-N	9.15	129.09	119.85
1	A	430	LYS	C-N-CA	9.15	129.09	119.85
1	A	547	GLN	N-CA-C	-8.84	101.09	112.23
1	A	501	MET	N-CA-C	-8.69	99.46	113.19
1	A	444	GLU	CA-C-N	8.40	130.57	120.23
1	A	444	GLU	C-N-CA	8.40	130.57	120.23
1	A	235	GLY	N-CA-C	-8.12	104.29	113.79
1	A	199	GLU	N-CA-C	-8.11	101.71	111.69
1	A	463	GLU	N-CA-C	-8.03	102.51	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	VAL	N-CA-C	-7.96	97.18	108.80
1	A	600	ILE	N-CA-C	-7.70	103.03	110.42
1	A	513	VAL	N-CA-C	7.51	118.26	108.35
1	A	488	ILE	N-CA-C	7.50	119.52	108.65
1	A	626	THR	CA-C-N	-7.28	110.74	119.84
1	A	626	THR	C-N-CA	-7.28	110.74	119.84
1	A	593	VAL	CA-C-N	-7.06	112.76	123.07
1	A	593	VAL	C-N-CA	-7.06	112.76	123.07
1	A	597	SER	CA-C-N	-6.95	115.46	122.69
1	A	597	SER	C-N-CA	-6.95	115.46	122.69
1	A	233	GLY	CA-C-N	-6.85	111.27	119.84
1	A	233	GLY	C-N-CA	-6.85	111.27	119.84
1	A	445	PRO	N-CA-C	6.85	121.26	110.50
1	A	226	LEU	N-CA-C	-6.83	104.95	113.28
1	A	455	LYS	N-CA-C	6.62	121.90	113.55
1	A	279	GLU	N-CA-C	6.55	119.73	110.23
1	A	163	LEU	N-CA-C	-6.53	104.09	111.14
1	A	519	ASN	CA-C-N	-5.80	114.92	122.99
1	A	519	ASN	C-N-CA	-5.80	114.92	122.99
1	A	414	ASP	N-CA-C	5.80	117.27	111.07
1	A	438	VAL	N-CA-C	5.76	116.42	108.12
1	A	351	VAL	N-CA-C	-5.72	105.28	110.82
1	A	116	ILE	CB-CA-C	-5.67	104.48	112.14
1	A	562	CYS	N-CA-C	5.58	118.19	108.76
1	A	594	ASP	N-CA-C	-5.44	98.50	108.02
1	A	628	HIS	N-CA-C	5.41	117.05	108.67
1	A	201	ALA	N-CA-C	-5.39	105.31	111.14
1	A	674	GLY	N-CA-C	5.25	116.94	111.95
1	A	565	LEU	CA-C-N	5.23	127.10	120.51
1	A	565	LEU	C-N-CA	5.23	127.10	120.51
1	A	79	PHE	N-CA-C	-5.20	105.51	111.07
1	A	507	PHE	N-CA-C	5.18	116.30	108.07
1	A	115	PHE	N-CA-C	5.08	116.67	111.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	ARG	Mainchain

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	4232	0	3955	65	0
2	C	1476	0	743	14	0
3	A	23	0	12	0	0
4	A	24	0	0	1	0
4	C	9	0	0	1	0
All	All	5764	0	4710	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 7.

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)
2:C:54:U:H3	2:C:58:A:H2	1.21	0.86
1:A:498:THR:HA	1:A:501:MET:HE2	1.62	0.81
1:A:112:ARG:HD2	4:A:807:HOH:O	1.84	0.75
1:A:155:GLY:O	1:A:157:ARG:NH1	2.24	0.70
1:A:664:ASP:HB3	1:A:668:ARG:NH2	2.10	0.67
1:A:431:PRO:HA	1:A:513:VAL:HG12	1.78	0.66
1:A:498:THR:HG21	1:A:502:ILE:HG13	1.76	0.66
1:A:393:ALA:HB3	1:A:405:VAL:HB	1.79	0.65
1:A:298:GLU:OE2	1:A:522:GLU:HG3	1.96	0.64
1:A:410:ARG:NH1	1:A:522:GLU:OE1	2.31	0.64
1:A:76:ARG:NH2	1:A:609:GLU:OE2	2.28	0.59
1:A:600:ILE:HG13	1:A:604:TYR:CE1	2.38	0.59
1:A:621:ASP:OD2	1:A:677:THR:OG1	2.16	0.59
1:A:664:ASP:O	1:A:668:ARG:HG3	2.02	0.59
1:A:619:ASP:OD2	1:A:642:ARG:NH2	2.37	0.58
1:A:295:ALA:HB3	1:A:525:PHE:HB2	1.86	0.57
1:A:454:TYR:HB2	1:A:458:ALA:HB2	1.89	0.55
1:A:487:THR:HG23	1:A:496:GLN:C	2.32	0.55
1:A:450:ILE:HG22	1:A:458:ALA:HB1	1.90	0.54
1:A:556:VAL:HG23	1:A:557:VAL:HG13	1.88	0.54
1:A:458:ALA:HA	1:A:461:VAL:HB	1.90	0.53
1:A:72:ASP:O	1:A:76:ARG:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:O	1:A:278:ASN:N	2.41	0.52
1:A:151:ASP:HB3	1:A:154:ASN:O	2.08	0.52
1:A:648:LEU:HD23	1:A:651:ILE:HD12	1.92	0.52
2:C:9:G:H5''	4:C:201:HOH:O	2.10	0.50
1:A:316:ASP:OD1	1:A:337:ARG:NH1	2.43	0.49
1:A:114:HIS:CD2	1:A:362:TYR:HB2	2.48	0.49
1:A:596:SER:OG	1:A:597:SER:N	2.46	0.49
1:A:299:HIS:CD2	1:A:301:VAL:HG22	2.48	0.48
1:A:276:PHE:C	1:A:277:ARG:HG2	2.38	0.48
1:A:329:SER:OG	1:A:331:GLN:NE2	2.37	0.48
1:A:532:TYR:O	1:A:535:PHE:HB2	2.14	0.47
1:A:158:PHE:CB	1:A:161:ASP:HB2	2.44	0.47
1:A:116:ILE:HA	1:A:121:ILE:HB	1.96	0.47
1:A:440:VAL:O	1:A:506:ARG:HA	2.15	0.47
1:A:141:VAL:O	1:A:145:ALA:HB3	2.15	0.46
1:A:448:GLY:O	1:A:452:LYS:HG3	2.16	0.46
1:A:565:LEU:O	1:A:617:THR:HA	2.15	0.46
1:A:558:ALA:HA	1:A:559:PRO:HD3	1.73	0.46
1:A:124:ILE:HG21	1:A:257:LEU:HD21	1.98	0.46
1:A:562:CYS:HB2	1:A:652:VAL:HG11	1.97	0.46
1:A:619:ASP:CG	1:A:642:ARG:HH22	2.23	0.45
1:A:633:ARG:HB2	1:A:640:GLN:HE21	1.81	0.45
1:A:462:MET:HE3	1:A:462:MET:HB3	1.75	0.45
1:A:472:TYR:O	1:A:476:MET:HG2	2.16	0.45
1:A:294:MET:HB3	1:A:294:MET:HE3	1.60	0.45
1:A:454:TYR:HB3	1:A:457:ASP:CB	2.47	0.45
2:C:44:C:O2'	2:C:45:G:H5'	2.17	0.45
1:A:430:LYS:HA	1:A:431:PRO:HD3	1.62	0.45
1:A:547:GLN:HB3	2:C:37:A:N7	2.32	0.44
2:C:58:A:H8	2:C:60:U:C6	2.36	0.44
1:A:633:ARG:HB2	1:A:640:GLN:HG2	1.99	0.44
1:A:530:ILE:O	1:A:534:VAL:HG23	2.18	0.44
1:A:119:GLU:HB2	1:A:121:ILE:HG13	1.99	0.43
1:A:629:THR:O	1:A:642:ARG:NH1	2.51	0.43
2:C:22:U:H2'	2:C:23:C:C6	2.54	0.43
1:A:92:GLY:O	1:A:93:LEU:HD23	2.19	0.43
2:C:58:A:H8	2:C:60:U:C5	2.37	0.43
1:A:498:THR:HG21	1:A:502:ILE:CG1	2.46	0.43
2:C:40:C:H2'	2:C:41:U:C6	2.54	0.43
1:A:512:TYR:CD2	1:A:512:TYR:N	2.87	0.42
2:C:21:A:H61	2:C:46:A:H2'	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LYS:HE3	1:A:519:ASN:HD22	1.84	0.41
1:A:373:LEU:HD12	1:A:394:GLU:O	2.20	0.41
1:A:563:SER:HB3	1:A:612:VAL:HG11	2.03	0.41
1:A:671:LEU:N	1:A:671:LEU:HD12	2.35	0.41
2:C:16:U:H2'	2:C:60:U:O2	2.21	0.41
1:A:308:HIS:HA	1:A:309:PRO:HD2	1.88	0.41
1:A:506:ARG:O	1:A:507:PHE:HB3	2.21	0.41
2:C:66:G:C6	2:C:67:C:C4	3.09	0.41
1:A:434:GLU:HA	1:A:435:PRO:HD2	1.84	0.41
2:C:3:G:H2'	2:C:4:C:C6	2.56	0.41
2:C:28:A:C2	2:C:43:G:C4	3.09	0.41
1:A:72:ASP:OD1	2:C:11:U:O2'	2.36	0.40
1:A:136:LYS:HE2	1:A:136:LYS:HB2	1.89	0.40
1:A:258:LEU:HG	1:A:263:GLY:HA2	2.02	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	552/630 (88%)	515 (93%)	32 (6%)	5 (1%)	14 38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
1	A	114	HIS
1	A	146	ASP
1	A	545	ASP
1	A	483	LYS

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	415/549 (76%)	399 (96%)	16 (4%)	28 60

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	117	GLN
1	A	157	ARG
1	A	161	ASP
1	A	281	SER
1	A	301	VAL
1	A	307	ASP
1	A	410	ARG
1	A	462	MET
1	A	490	THR
1	A	501	MET
1	A	506	ARG
1	A	565	LEU
1	A	572	GLU
1	A	625	LYS
1	A	679	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	299	HIS
1	A	481	ASN
1	A	508	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	67/69 (97%)	7 (10%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	9	G
2	C	18	G
2	C	20	U
2	C	37	A
2	C	38	U
2	C	48	C
2	C	56	C

There are no RNA pucker outliers to report.

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	2.74	14 (42%)	50,54,54	2.11	11 (22%)

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	-	6/22/38/38	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	9.63	1.41	1.23
2	C	1	GTP	C2'-C3'	-4.85	1.40	1.53
2	C	1	GTP	C2-N2	4.53	1.44	1.34
2	C	1	GTP	C5-N7	-4.07	1.30	1.39
2	C	1	GTP	C8-N9	-3.43	1.29	1.37
2	C	1	GTP	PB-O3A	-3.41	1.55	1.59
2	C	1	GTP	C5-C4	3.31	1.47	1.38
2	C	1	GTP	O4'-C4'	-2.93	1.38	1.45
2	C	1	GTP	C8-N7	-2.88	1.24	1.32
2	C	1	GTP	C4-N9	2.36	1.44	1.38
2	C	1	GTP	PA-O3A	-2.28	1.57	1.59
2	C	1	GTP	C3'-C4'	-2.19	1.47	1.53
2	C	1	GTP	O3'-C3'	-2.15	1.37	1.43
2	C	1	GTP	PB-O2B	-2.01	1.46	1.55

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GTP	N9-C4-N3	6.04	138.02	125.95
2	C	1	GTP	C5-C4-N3	-5.83	119.11	128.39
2	C	1	GTP	C8-N7-C5	5.45	113.97	104.26
2	C	1	GTP	C2-N3-C4	4.63	120.27	112.30
2	C	1	GTP	C4-C5-N7	-4.22	103.98	110.67
2	C	1	GTP	C6-C5-N7	4.07	137.69	130.29
2	C	1	GTP	O5'-C5'-C4'	3.17	119.78	108.99
2	C	1	GTP	O2A-PA-O3A	2.62	114.35	107.27
2	C	1	GTP	C2-N1-C6	-2.33	120.89	125.11
2	C	1	GTP	C5-C6-N1	2.30	119.12	113.25
2	C	1	GTP	O6-C6-C5	-2.04	121.16	126.53

There are no chirality outliers.

All (6) 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'
2	C	1	GTP	C3'-C4'-C5'-O5'
2	C	1	GTP	PB-O3B-PG-O2G

There are no ring outliers.

No monomer is involved in short contacts.

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	1.39	4 (16%)	37,38,38	1.74	8 (21%)

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	-	-	1/10/26/26	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	4.84	1.47	1.39
3	A	701	AMP	C8-N7	2.57	1.36	1.31
3	A	701	AMP	C5-C6	2.38	1.47	1.41
3	A	701	AMP	C4-N9	-2.09	1.33	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	AMP	C5-C4-N3	-4.97	119.88	126.72
3	A	701	AMP	N3-C4-N9	4.49	134.80	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	AMP	C4-N9-C8	3.40	109.31	105.74
3	A	701	AMP	C2-N3-C4	3.14	119.50	111.83
3	A	701	AMP	N3-C2-N1	-2.78	124.38	128.58
3	A	701	AMP	C4-C5-N7	-2.21	108.05	110.58
3	A	701	AMP	N6-C6-N1	2.10	123.06	118.38
3	A	701	AMP	N9-C8-N7	-2.04	111.05	113.94

There are no chirality outliers.

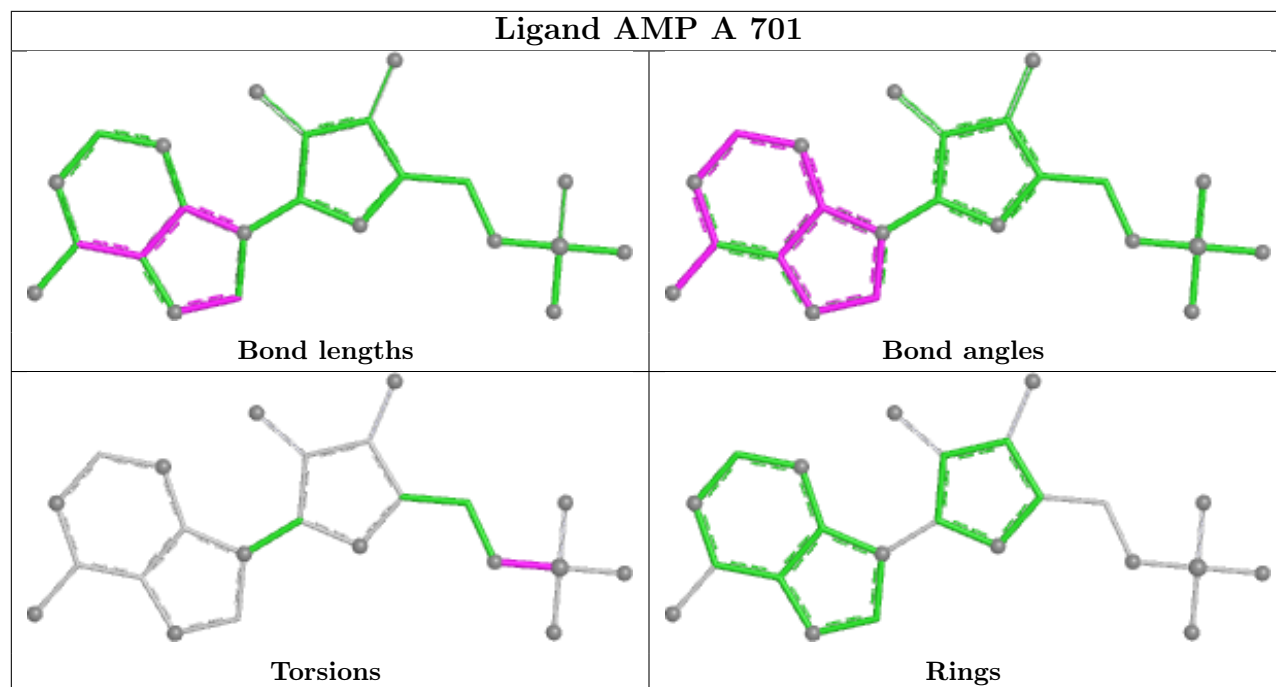
All (1) torsion outliers are listed below:

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

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	562/630 (89%)	0.72	55 (9%) 13 11	32, 53, 112, 128	0
2	C	68/69 (98%)	0.84	1 (1%) 72 64	44, 68, 122, 134	0
All	All	630/699 (90%)	0.74	56 (8%) 15 13	32, 55, 113, 134	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	5.7
1	A	206	ASN	4.2
1	A	668	ARG	3.6
1	A	602	ARG	3.6
1	A	673	GLU	3.6
1	A	294	MET	3.5
1	A	458	ALA	3.4
1	A	443	PHE	3.3
1	A	544	GLY	3.3
1	A	444	GLU	3.2
1	A	597	SER	3.2
1	A	151	ASP	3.0
1	A	155	GLY	3.0
1	A	224	PHE	2.8
1	A	496	GLN	2.7
1	A	162	HIS	2.7
1	A	626	THR	2.7
1	A	676	GLU	2.7
1	A	671	LEU	2.7
1	A	158	PHE	2.6
1	A	680	LYS	2.6
1	A	674	GLY	2.6
1	A	280	ILE	2.5
1	A	643	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	562	CYS	2.5
1	A	657	ASN	2.5
1	A	490	THR	2.5
1	A	150	LYS	2.5
1	A	457	ASP	2.4
1	A	380	GLU	2.4
1	A	237	ASN	2.4
1	A	429	GLU	2.4
1	A	449	ALA	2.4
1	A	91	SER	2.4
1	A	669	TYR	2.3
1	A	149	VAL	2.3
1	A	445	PRO	2.2
1	A	413	TYR	2.2
1	A	144	PHE	2.2
1	A	154	ASN	2.2
1	A	625	LYS	2.2
1	A	618	ILE	2.2
1	A	453	ALA	2.2
2	C	71	G	2.2
1	A	197	GLN	2.1
1	A	198	GLN	2.1
1	A	455	LYS	2.1
1	A	117	GLN	2.1
1	A	299	HIS	2.1
1	A	200	LEU	2.1
1	A	163	LEU	2.1
1	A	390	CYS	2.0
1	A	460	LEU	2.0
1	A	170	LYS	2.0
1	A	152	VAL	2.0
1	A	157	ARG	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	0.71	0.18	86,113,121,124	0

6.3 Carbohydrates [i](#)

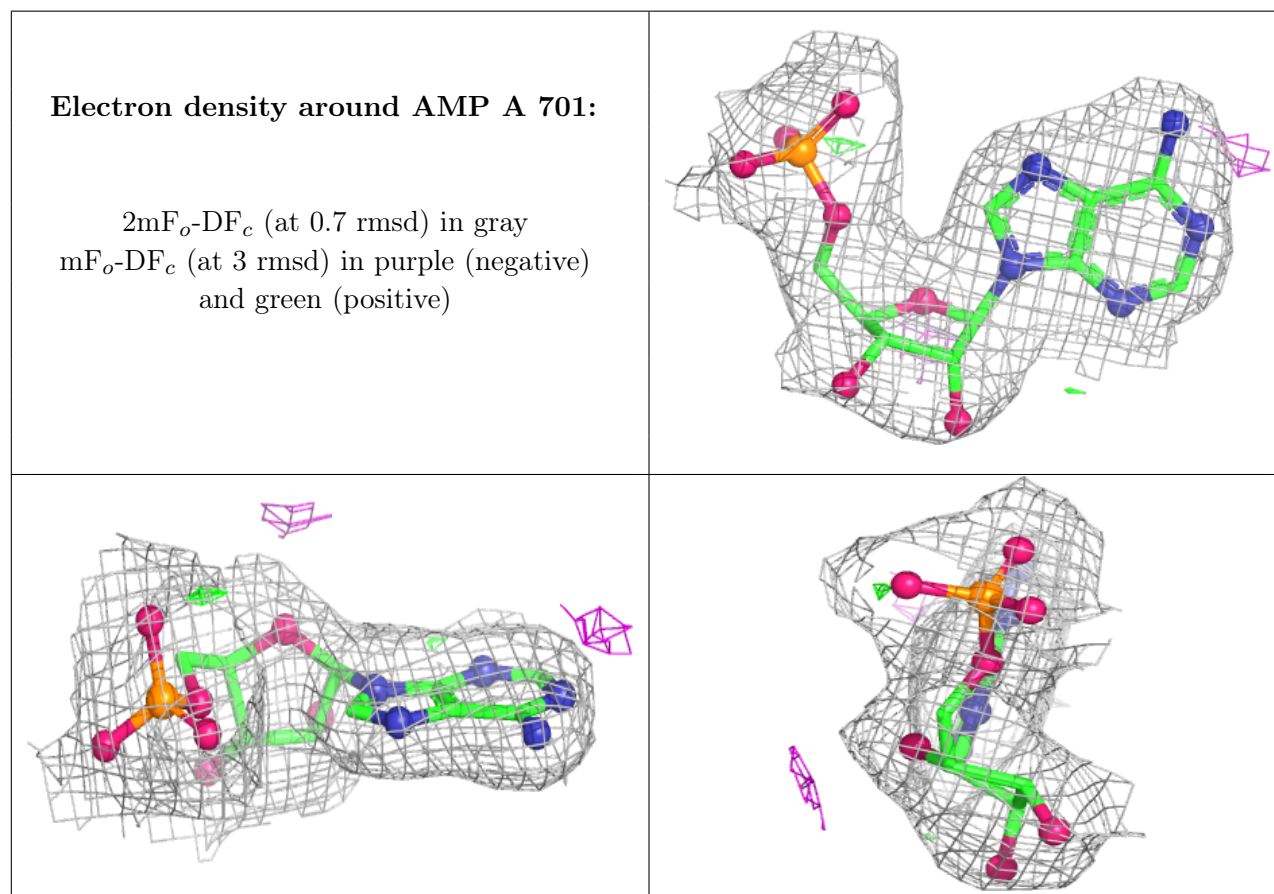
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	AMP	A	701	23/23	0.90	0.09	36,44,52,64	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 [i](#)

There are no such residues in this entry.