



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:18 PM UTC

PDB ID : 1CKN / pdb_00001ckn
Title : STRUCTURE OF GUANYLYLATED MRNA CAPPING ENZYME COM-
PLEXED WITH GTP
Authors : Hakansson, K.; Doherty, A.J.; Wigley, D.B.
Deposited on : 1997-04-20
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

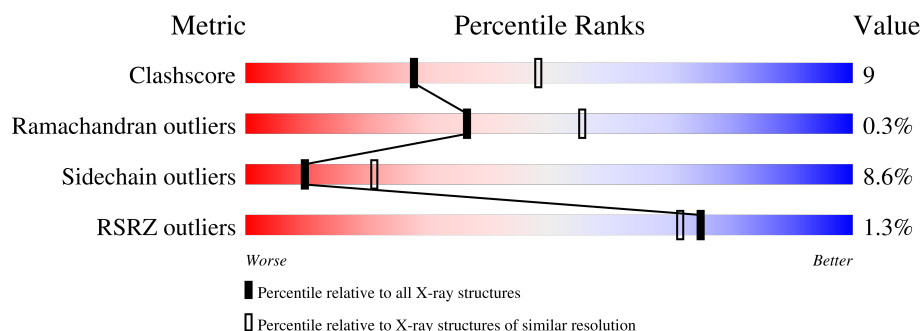
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	330	63%27%6%.
2	B	330	58%31%7%.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5525 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 MRNA CAPPING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2561	1657	429	463	12			

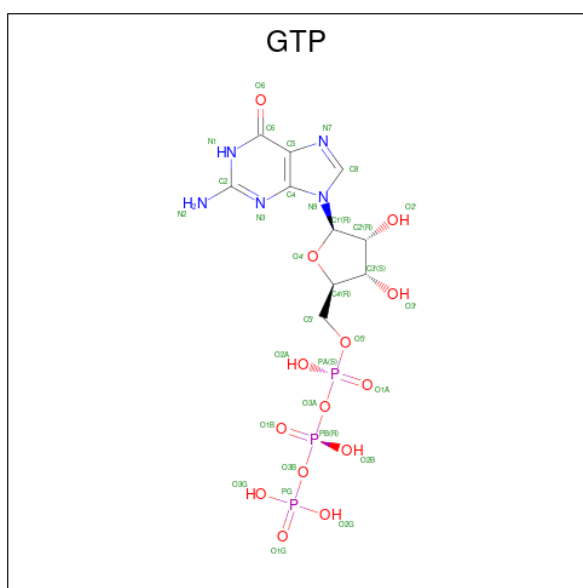
- Molecule 2 is a protein called MRNA CAPPING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	317	Total	C	N	O	P	S	0	0
			2584	1667	434	470	1	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	GPL	LYS	conflict	UNP Q84424

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

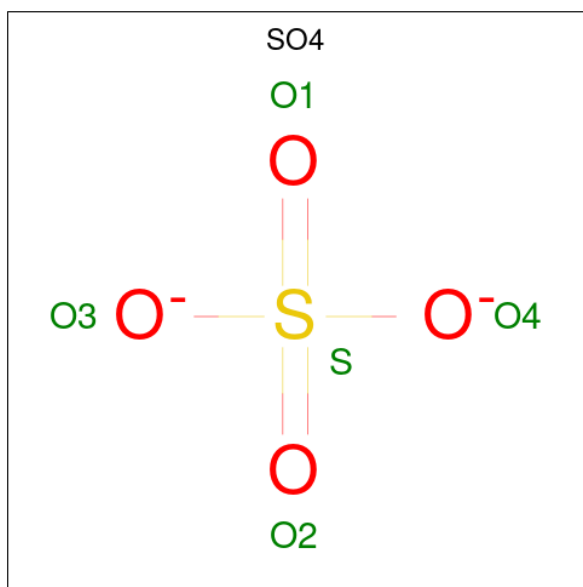


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

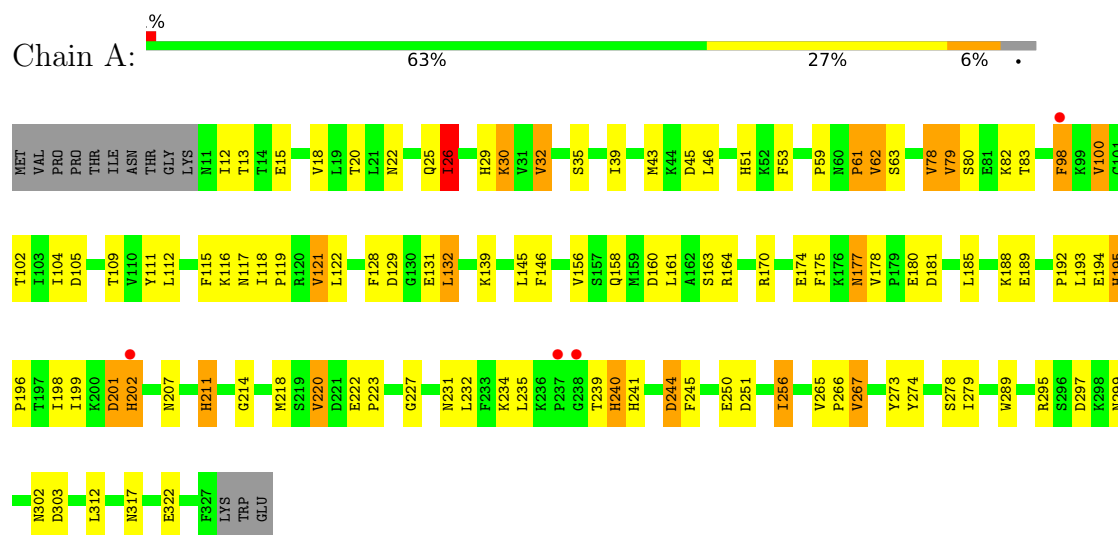
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	165	Total	O	0	0
			165	165		
6	B	177	Total	O	0	0
			177	177		

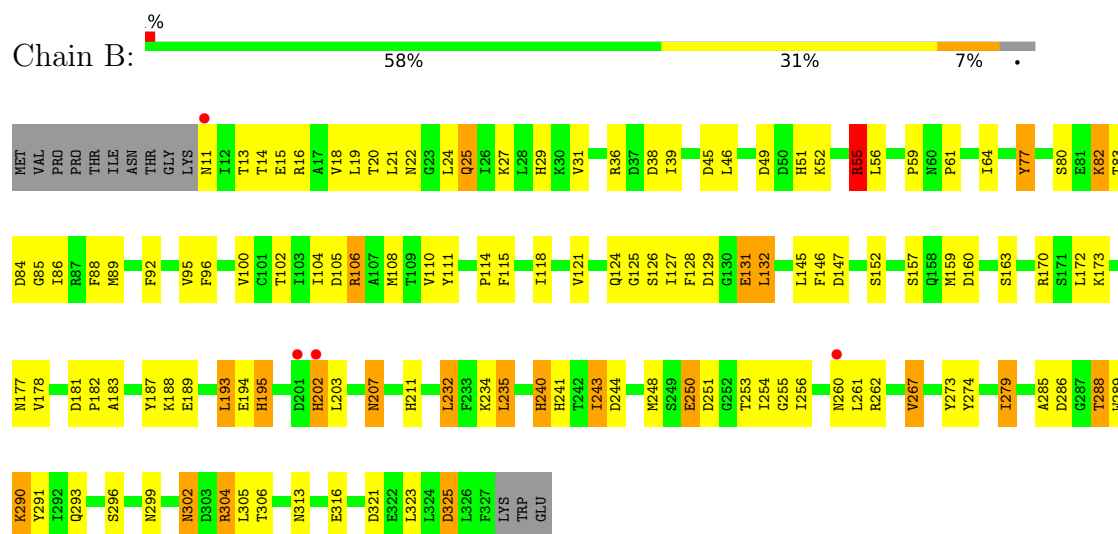
3 Residue-property plots [i](#)

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: MRNA CAPPING ENZYME



• Molecule 2: MRNA CAPPING ENZYME



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	94.91Å 212.95Å 105.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (10.00-2.50) 93.9 (10.00-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.51Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.224 , 0.299 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 73.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5525	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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, GPL, MN, 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	0.98	7/2616 (0.3%)	1.69	45/3530 (1.3%)
2	B	0.98	8/2606 (0.3%)	1.73	59/3516 (1.7%)
All	All	0.98	15/5222 (0.3%)	1.71	104/7046 (1.5%)

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	5
2	B	0	6
All	All	0	11

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	HIS	CD2-NE2	-8.05	1.28	1.37
2	B	240	HIS	CD2-NE2	-7.50	1.29	1.37
1	A	211	HIS	CD2-NE2	-7.31	1.29	1.37
2	B	241	HIS	CD2-NE2	-7.14	1.29	1.37
1	A	241	HIS	CD2-NE2	-6.93	1.30	1.37
2	B	29	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	195	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	29	HIS	CD2-NE2	-6.24	1.30	1.37
2	B	202	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	202	HIS	CD2-NE2	-6.15	1.31	1.37
2	B	51	HIS	CD2-NE2	-6.15	1.31	1.37
2	B	195	HIS	CD2-NE2	-6.09	1.31	1.37
2	B	211	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	240	HIS	CD2-NE2	-5.40	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	HIS	CG-ND1	-5.30	1.32	1.38

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ASP	CA-CB-CG	11.99	124.59	112.60
1	A	240	HIS	CA-CB-CG	9.50	123.30	113.80
1	A	241	HIS	CB-CG-CD2	-9.04	119.45	131.20
2	B	105	ASP	CA-CB-CG	8.15	120.75	112.60
2	B	267	VAL	N-CA-CB	-8.01	98.01	111.23
2	B	160	ASP	CA-CB-CG	7.98	120.58	112.60
2	B	38	ASP	CA-CB-CG	7.77	120.37	112.60
2	B	302	ASN	OD1-CG-ND2	-7.72	114.88	122.60
1	A	195	HIS	CB-CG-CD2	-7.69	121.21	131.20
1	A	160	ASP	CA-CB-CG	7.58	120.18	112.60
1	A	98	PHE	CA-CB-CG	-7.42	106.38	113.80
2	B	251	ASP	N-CA-C	7.34	121.82	113.01
2	B	316	GLU	N-CA-C	-7.34	98.80	109.59
2	B	172	LEU	N-CA-C	-7.30	103.68	112.59
1	A	121	VAL	CB-CA-C	-7.16	102.48	112.14
2	B	84	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	241	HIS	CB-CG-ND1	6.91	133.07	122.70
2	B	55	ARG	CB-CA-C	-6.87	97.83	110.62
2	B	293	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	A	317	ASN	CA-CB-CG	6.79	119.39	112.60
2	B	11	ASN	OD1-CG-ND2	-6.62	115.98	122.60
2	B	11	ASN	CA-CB-CG	-6.53	106.07	112.60
1	A	45	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	207	ASN	OD1-CG-ND2	-6.47	116.13	122.60
2	B	211	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	A	211	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	A	26	ILE	CB-CA-C	-6.32	101.27	110.63
2	B	22	ASN	OD1-CG-ND2	-6.30	116.30	122.60
2	B	241	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	A	195	HIS	CB-CG-ND1	6.25	132.08	122.70
2	B	302	ASN	CB-CG-ND2	6.24	125.76	116.40
1	A	62	VAL	CB-CA-C	6.22	120.40	110.82
2	B	29	HIS	CB-CG-CD2	-6.21	123.12	131.20
1	A	100	VAL	N-CA-CB	-6.21	102.84	111.41
1	A	22	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	A	198	ILE	N-CA-C	-6.19	105.02	111.58
2	B	240	HIS	CB-CG-CD2	-6.15	123.21	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	289	TRP	CE2-CD2-CG	-6.10	99.88	107.20
2	B	286	ASP	CA-CB-CG	6.09	118.69	112.60
2	B	243	ILE	N-CA-C	-6.08	98.95	108.86
1	A	194	GLU	N-CA-C	-6.06	105.47	112.92
2	B	202	HIS	CB-CG-CD2	-6.04	123.34	131.20
2	B	260	ASN	OD1-CG-ND2	-6.04	116.56	122.60
2	B	11	ASN	CB-CG-ND2	6.02	125.43	116.40
1	A	189	GLU	CB-CG-CD	6.00	122.80	112.60
1	A	297	ASP	CA-CB-CG	5.97	118.58	112.60
2	B	299	ASN	N-CA-CB	-5.96	101.58	111.06
2	B	279	ILE	N-CA-CB	5.93	117.18	110.72
2	B	299	ASN	CA-CB-CG	5.91	118.51	112.60
2	B	106	ARG	N-CA-C	5.90	119.30	111.75
2	B	251	ASP	CA-C-N	-5.89	114.05	122.00
2	B	251	ASP	C-N-CA	-5.89	114.05	122.00
2	B	261	LEU	N-CA-C	-5.88	106.73	114.31
2	B	22	ASN	CB-CG-ND2	5.84	125.17	116.40
1	A	303	ASP	CA-CB-CG	5.79	118.39	112.60
2	B	55	ARG	CA-CB-CG	5.78	125.66	114.10
2	B	51	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	A	121	VAL	N-CA-CB	5.69	118.28	110.54
1	A	273	TYR	N-CA-C	-5.68	100.44	109.59
2	B	147	ASP	CA-CB-CG	5.68	118.28	112.60
2	B	181	ASP	CA-C-N	5.63	125.30	119.05
2	B	181	ASP	C-N-CA	5.63	125.30	119.05
2	B	177	ASN	CA-CB-CG	5.62	118.22	112.60
2	B	253	THR	N-CA-C	-5.62	101.73	110.10
1	A	177	ASN	CB-CA-C	-5.59	100.08	109.53
2	B	289	TRP	CG-CD2-CE3	5.55	139.45	133.90
1	A	244	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	146	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	29	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	A	61	PRO	N-CA-C	5.47	119.81	111.34
1	A	231	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	26	ILE	N-CA-CB	5.46	118.94	111.41
2	B	178	VAL	CA-C-N	5.46	125.13	119.56
2	B	178	VAL	C-N-CA	5.46	125.13	119.56
2	B	211	HIS	N-CA-C	-5.44	99.86	108.73
1	A	201	ASP	CA-CB-CG	-5.42	107.18	112.60
1	A	129	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	79	VAL	N-CA-C	5.38	116.48	108.46
2	B	129	ASP	CA-CB-CG	5.38	117.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	VAL	N-CA-CB	-5.33	103.36	111.57
1	A	32	VAL	N-CA-CB	-5.31	103.53	112.44
1	A	181	ASP	CA-CB-CG	5.29	117.89	112.60
2	B	157	SER	N-CA-C	5.29	118.83	112.38
2	B	304	ARG	CA-CB-CG	5.25	124.60	114.10
2	B	195	HIS	CB-CG-CD2	-5.24	124.38	131.20
1	A	62	VAL	N-CA-C	-5.23	100.80	108.85
1	A	251	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	289	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	A	202	HIS	CB-CG-CD2	-5.18	124.46	131.20
2	B	316	GLU	CA-C-N	-5.17	115.26	123.12
2	B	316	GLU	C-N-CA	-5.17	115.26	123.12
2	B	25	GLN	CG-CD-NE2	5.15	124.12	116.40
2	B	207	ASN	OD1-CG-ND2	-5.15	117.45	122.60
2	B	306	THR	N-CA-C	-5.15	105.58	111.14
1	A	256	ILE	N-CA-C	-5.14	100.48	108.86
2	B	289	TRP	CB-CG-CD1	-5.13	119.20	126.90
1	A	299	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	53	PHE	CA-C-N	5.12	124.88	119.76
1	A	53	PHE	C-N-CA	5.12	124.88	119.76
2	B	15	GLU	N-CA-C	-5.07	101.02	108.99
2	B	131	GLU	CB-CA-C	-5.06	100.45	109.71
2	B	267	VAL	CB-CA-C	5.05	119.57	111.29
2	B	290	LYS	CB-CG-CD	-5.02	99.75	111.30
2	B	288	THR	N-CA-CB	-5.01	103.54	111.05

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	TYR	Sidechain
1	A	170	ARG	Sidechain
1	A	274	TYR	Sidechain
1	A	295	ARG	Sidechain
1	A	98	PHE	Sidechain
2	B	106	ARG	Sidechain
2	B	111	TYR	Sidechain
2	B	187	TYR	Sidechain
2	B	273	TYR	Sidechain
2	B	274	TYR	Sidechain
2	B	77	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	A	2561	0	2607	42	0
2	B	2584	0	2617	54	0
3	A	32	0	12	5	0
4	B	1	0	0	0	0
5	B	5	0	0	0	0
6	A	165	0	0	7	0
6	B	177	0	0	4	0
All	All	5525	0	5236	94	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 9.

All (94) 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:26:ILE:HD11	1:A:132:LEU:HD11	1.61	0.81
2:B:89:MET:HE2	2:B:127:ILE:HG22	1.70	0.74
1:A:156:VAL:HG12	1:A:164:ARG:HG2	1.71	0.73
2:B:83:THR:HB	2:B:131:GLU:HG3	1.74	0.69
2:B:159:MET:CE	2:B:163:SER:HB3	2.26	0.66
2:B:159:MET:HE2	2:B:163:SER:HB3	1.80	0.64
1:A:158:GLN:HA	1:A:223:PRO:HB3	1.81	0.63
2:B:285:ALA:HB2	2:B:290:LYS:HD2	1.80	0.62
2:B:21:LEU:HD21	2:B:86:ILE:HG13	1.82	0.61
1:A:39:ILE:HD13	1:A:102:THR:HG21	1.82	0.61
2:B:104:ILE:HG12	2:B:110:VAL:HG22	1.82	0.61
2:B:202:HIS:HB2	6:B:1105:HOH:O	2.00	0.61
1:A:20:THR:HG23	1:A:25:GLN:HG2	1.84	0.60
1:A:61:PRO:HG2	3:A:899:GTP:H5'	1.82	0.60
2:B:131:GLU:HG2	2:B:146:PHE:HZ	1.68	0.58
2:B:248:MET:SD	2:B:255:GLY:HA3	2.43	0.58
2:B:77:TYR:HB2	2:B:193:LEU:HD12	1.85	0.58
2:B:100:VAL:HG12	2:B:102:THR:HG23	1.87	0.57
1:A:79:VAL:HG11	1:A:199:ILE:HD13	1.87	0.56
1:A:156:VAL:HG11	1:A:164:ARG:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LEU:O	2:B:188:LYS:HB2	2.06	0.55
1:A:214:GLY:HA3	1:A:235:LEU:O	2.07	0.55
2:B:321:ASP:O	2:B:325:ASP:HB2	2.06	0.55
1:A:18:VAL:HA	1:A:26:ILE:O	2.07	0.55
1:A:12:ILE:HG23	1:A:35:SER:HB3	1.89	0.54
1:A:163:SER:HA	6:A:1026:HOH:O	2.08	0.54
2:B:82:GPL:HE2	2:B:234:LYS:HD2	1.89	0.54
2:B:61:PRO:HG3	2:B:232:LEU:HD13	1.88	0.54
2:B:95:VAL:HG12	2:B:96:PHE:CD2	2.43	0.54
1:A:82:LYS:HE3	3:A:899:GTP:H5''	1.90	0.53
2:B:121:VAL:HG22	2:B:152:SER:HB3	1.91	0.53
1:A:177:ASN:HD21	1:A:185:LEU:H	1.55	0.53
2:B:240:HIS:NE2	2:B:290:LYS:HE2	2.24	0.53
1:A:59:PRO:HA	1:A:227:GLY:O	2.09	0.52
2:B:115:PHE:HB2	2:B:118:ILE:CD1	2.40	0.52
2:B:121:VAL:HG23	2:B:124:GLN:OE1	2.09	0.52
1:A:119:PRO:HB2	1:A:122:LEU:HD23	1.92	0.51
2:B:64:ILE:HG21	2:B:235:LEU:HG	1.91	0.51
1:A:202:HIS:HB2	6:A:1012:HOH:O	2.11	0.50
1:A:15:GLU:O	1:A:30:LYS:N	2.44	0.50
2:B:244:ASP:H	2:B:302:ASN:ND2	2.09	0.50
1:A:188:LYS:NZ	3:A:899:GTP:O6	2.44	0.50
2:B:313:ASN:HA	6:B:1023:HOH:O	2.12	0.50
1:A:240:HIS:ND1	2:B:291:TYR:HB3	2.27	0.49
1:A:115:PHE:HB2	1:A:118:ILE:HG12	1.95	0.49
1:A:83:THR:HB	1:A:131:GLU:HG2	1.96	0.48
1:A:78:VAL:HG13	1:A:220:VAL:HG23	1.95	0.47
2:B:115:PHE:HE2	2:B:183:ALA:O	1.97	0.47
2:B:20:THR:HA	2:B:24:LEU:O	2.14	0.47
2:B:46:LEU:HD23	2:B:127:ILE:HG13	1.96	0.47
2:B:80:SER:OG	2:B:188:LYS:HE3	2.15	0.47
1:A:25:GLN:HG3	2:B:18:VAL:HG21	1.97	0.47
1:A:116:LYS:HD3	1:A:178:VAL:HG11	1.97	0.47
2:B:19:LEU:O	2:B:25:GLN:HA	2.15	0.46
2:B:159:MET:HE3	2:B:163:SER:HB3	1.96	0.46
1:A:61:PRO:CG	3:A:899:GTP:H5'	2.45	0.46
1:A:240:HIS:ND1	6:A:900:HOH:O	2.35	0.46
1:A:117:ASN:O	1:A:175:PHE:HD1	1.98	0.46
2:B:59:PRO:HB2	2:B:232:LEU:HD12	1.97	0.46
2:B:243:ILE:HA	2:B:302:ASN:HD22	1.79	0.46
1:A:30:LYS:HD2	1:A:109:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PRO:HB3	6:A:931:HOH:O	2.15	0.46
2:B:170:ARG:O	2:B:173:LYS:HG2	2.17	0.45
2:B:89:MET:HE3	2:B:128:PHE:C	2.41	0.45
1:A:244:ASP:H	1:A:302:ASN:ND2	2.14	0.45
1:A:234:LYS:HD2	3:A:899:GTP:O2A	2.17	0.44
2:B:195:HIS:CE1	6:B:1107:HOH:O	2.70	0.44
2:B:92:PHE:HE2	2:B:118:ILE:HD13	1.83	0.44
2:B:14:THR:HG22	2:B:31:VAL:HA	1.99	0.44
1:A:211:HIS:HD2	6:A:1018:HOH:O	2.01	0.44
2:B:56:LEU:HD22	2:B:89:MET:HB2	2.01	0.43
2:B:115:PHE:CD1	2:B:118:ILE:HD11	2.53	0.43
2:B:85:GLY:HA3	2:B:132:LEU:O	2.19	0.43
2:B:88:PHE:CD2	2:B:132:LEU:HB2	2.54	0.43
1:A:128:PHE:HB3	1:A:145:LEU:HD22	2.01	0.42
1:A:195:HIS:CE1	6:A:1063:HOH:O	2.72	0.42
2:B:114:PRO:HD2	2:B:182:PRO:HG3	2.02	0.42
2:B:92:PHE:CE2	2:B:118:ILE:HD13	2.53	0.42
2:B:290:LYS:NZ	6:B:1174:HOH:O	2.53	0.42
2:B:279:ILE:HD12	2:B:279:ILE:N	2.35	0.41
2:B:49:ASP:OD2	2:B:55:ARG:HD2	2.19	0.41
1:A:161:LEU:HD22	1:A:218:MET:HE3	2.02	0.41
2:B:285:ALA:CB	2:B:290:LYS:HD2	2.49	0.41
1:A:164:ARG:NH2	1:A:222:GLU:O	2.53	0.41
2:B:92:PHE:HD1	2:B:126:SER:HB2	1.86	0.41
1:A:43:MET:SD	1:A:104:ILE:HD12	2.60	0.41
1:A:196:PRO:HA	1:A:199:ILE:HD12	2.02	0.41
2:B:131:GLU:HG2	2:B:146:PHE:CZ	2.53	0.41
1:A:278:SER:HB3	6:A:930:HOH:O	2.21	0.40
2:B:31:VAL:HG11	2:B:39:ILE:HD12	2.01	0.40
2:B:36:ARG:NH1	2:B:108:MET:O	2.54	0.40
1:A:245:PHE:O	1:A:279:ILE:HA	2.22	0.40
2:B:203:LEU:O	2:B:207:ASN:ND2	2.50	0.40
1:A:265:VAL:HA	1:A:266:PRO:HD3	1.95	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	315/330 (96%)	298 (95%)	17 (5%)	0	100	100
2	B	314/330 (95%)	297 (95%)	15 (5%)	2 (1%)	21	38
All	All	629/660 (95%)	595 (95%)	32 (5%)	2 (0%)	36	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	250	GLU
2	B	125	GLY

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	285/297 (96%)	259 (91%)	26 (9%)	9	19
2	B	284/296 (96%)	261 (92%)	23 (8%)	11	23
All	All	569/593 (96%)	520 (91%)	49 (9%)	10	21

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	26	ILE
1	A	30	LYS
1	A	32	VAL

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Mol	Chain	Res	Type
1	A	46	LEU
1	A	62	VAL
1	A	63	SER
1	A	78	VAL
1	A	80	SER
1	A	100	VAL
1	A	112	LEU
1	A	121	VAL
1	A	132	LEU
1	A	139	LYS
1	A	174	GLU
1	A	180	GLU
1	A	193	LEU
1	A	201	ASP
1	A	220	VAL
1	A	232	LEU
1	A	239	THR
1	A	250	GLU
1	A	256	ILE
1	A	267	VAL
1	A	312	LEU
1	A	322	GLU
2	B	13	THR
2	B	16	ARG
2	B	27	LYS
2	B	45	ASP
2	B	52	LYS
2	B	55	ARG
2	B	132	LEU
2	B	189	GLU
2	B	193	LEU
2	B	194	GLU
2	B	232	LEU
2	B	235	LEU
2	B	250	GLU
2	B	254	ILE
2	B	256	ILE
2	B	262	ARG
2	B	267	VAL
2	B	288	THR
2	B	296	SER
2	B	304	ARG

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Mol	Chain	Res	Type
2	B	305	LEU
2	B	323	LEU
2	B	325	ASP

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

Mol	Chain	Res	Type
1	A	11	ASN
1	A	60	ASN
1	A	158	GLN
1	A	177	ASN
1	A	211	HIS
1	A	231	ASN
1	A	302	ASN
1	A	313	ASN
2	B	29	HIS
2	B	51	HIS
2	B	264	ASN
2	B	293	GLN
2	B	302	ASN
2	B	317	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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	GPL	B	82	2,4	33,34,35	1.25	3 (9%)	43,49,51	1.92	5 (11%)

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	GPL	B	82	2,4	-	2/19/37/39	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	82	GPL	P-O2P	-3.31	1.48	1.56
2	B	82	GPL	P-O1P	3.25	1.51	1.46
2	B	82	GPL	C3'-C4'	-2.06	1.47	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	82	GPL	P-NZ-CE	-9.47	111.40	124.61
2	B	82	GPL	O4'-C4'-C5'	3.14	119.39	109.33
2	B	82	GPL	O4'-C1'-N9	3.10	115.39	108.36
2	B	82	GPL	O2P-P-O1P	2.87	116.02	109.87
2	B	82	GPL	O5'-C5'-C4'	2.79	118.49	108.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	82	GPL	C4'-C5'-O5'-P
2	B	82	GPL	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	82	GPL	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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
5	SO4	B	1000	-	4,4,4	0.38	0	6,6,6	0.56	0
3	GTP	A	899	-	33,34,34	1.78	5 (15%)	50,54,54	0.85	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	A	899	-	-	4/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	899	GTP	PB-O3A	5.27	1.65	1.59
3	A	899	GTP	PB-O3B	4.99	1.64	1.59
3	A	899	GTP	PA-O3A	3.83	1.63	1.59
3	A	899	GTP	PA-O2A	-2.68	1.42	1.55
3	A	899	GTP	PG-O3G	-2.13	1.46	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	899	GTP	O5'-C5'-C4'	2.41	117.21	108.99
3	A	899	GTP	O3G-PG-O2G	2.04	115.47	107.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

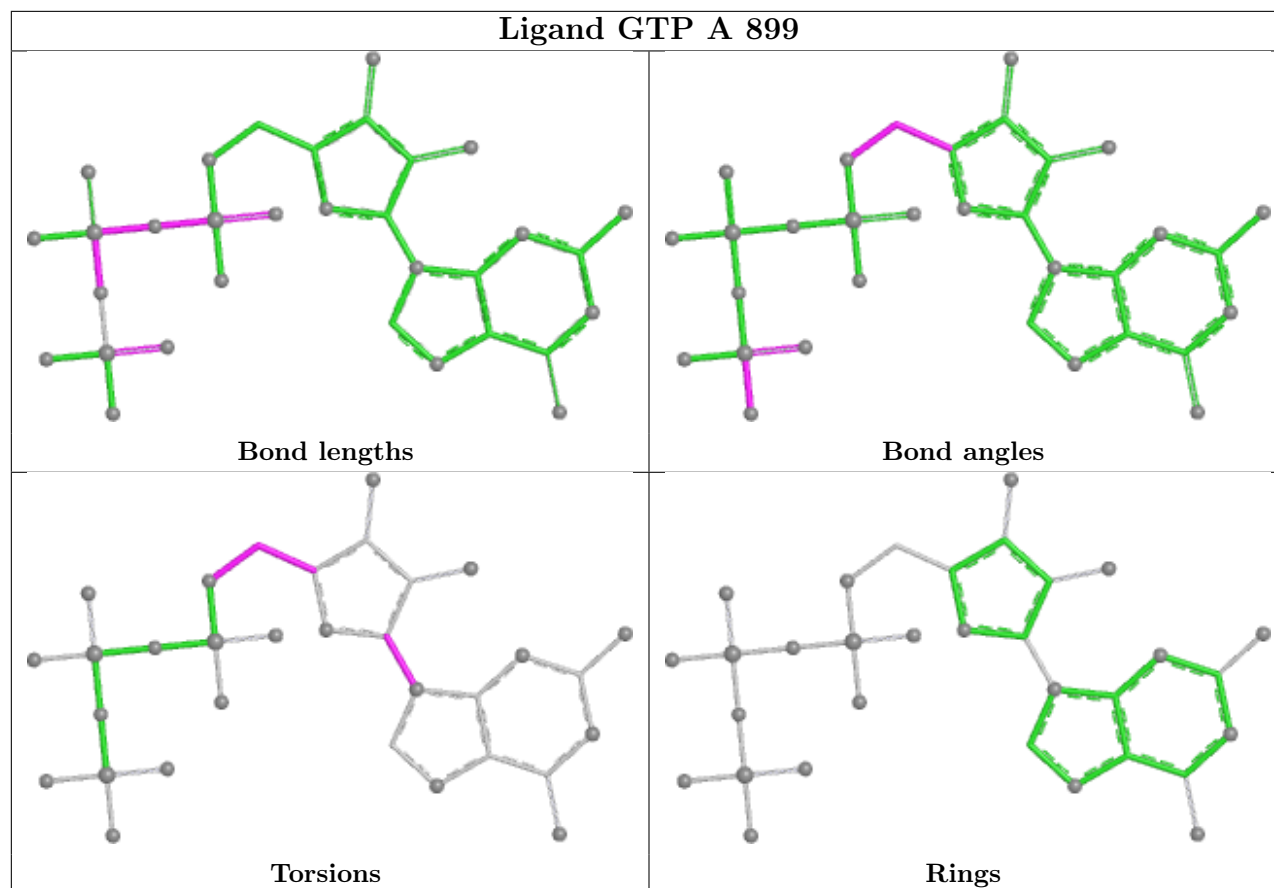
Mol	Chain	Res	Type	Atoms
3	A	899	GTP	O4'-C4'-C5'-O5'
3	A	899	GTP	C3'-C4'-C5'-O5'
3	A	899	GTP	C4'-C5'-O5'-PA
3	A	899	GTP	C2'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	899	GTP	5	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	317/330 (96%)	-0.49	4 (1%) 75 71	8, 25, 55, 89	0
2	B	316/330 (95%)	-0.48	4 (1%) 75 71	7, 25, 56, 93	0
All	All	633/660 (95%)	-0.49	8 (1%) 75 71	7, 25, 55, 93	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	11	ASN	2.9
1	A	98	PHE	2.5
2	B	260	ASN	2.4
1	A	238	GLY	2.2
1	A	237	PRO	2.2
2	B	201	ASP	2.1
1	A	202	HIS	2.1
2	B	202	HIS	2.1

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	GPL	B	82	32/33	0.97	0.06	4,16,25,31	0

6.3 Carbohydrates [i](#)

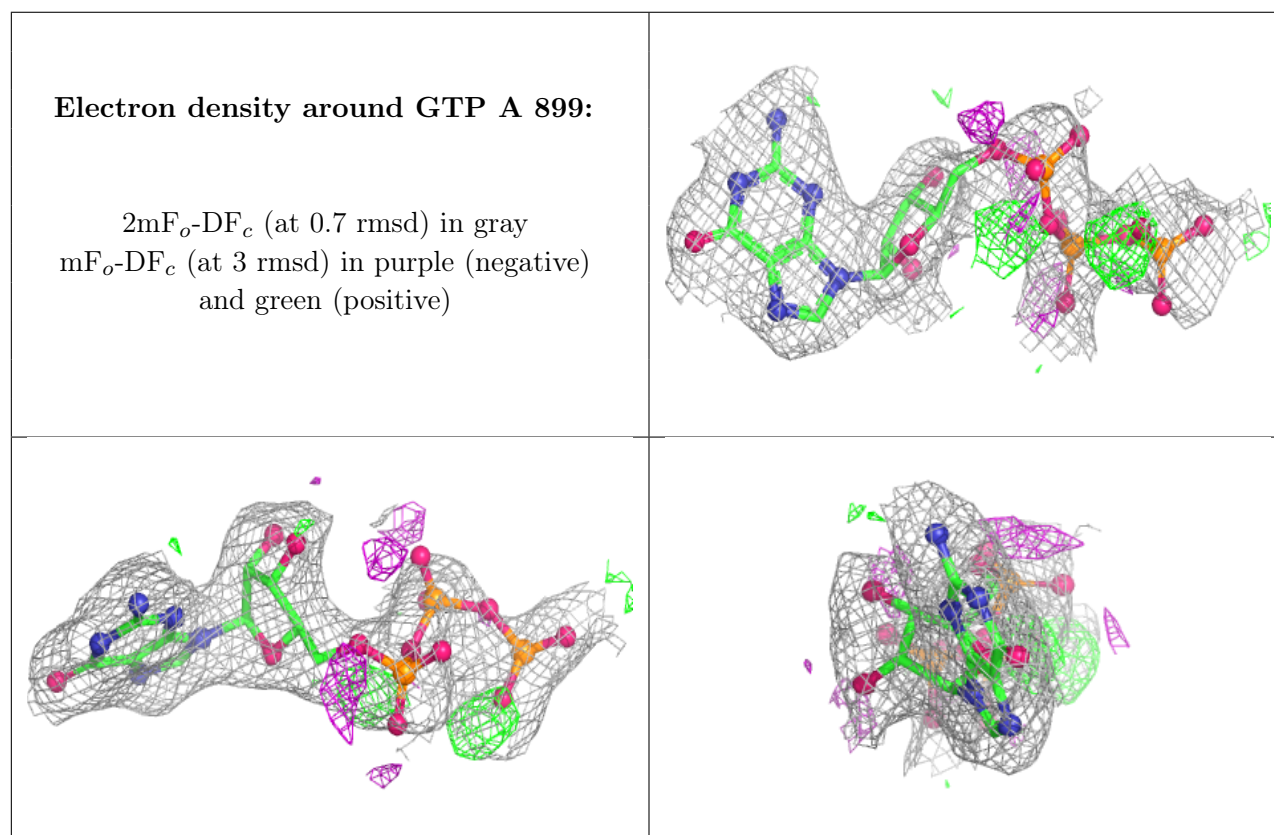
There are no oligosaccharides in this entry.

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
4	MN	B	1001	1/1	0.84	0.08	28,28,28,28	0
3	GTP	A	899	32/32	0.90	0.10	15,36,130,135	0
5	SO4	B	1000	5/5	0.92	0.11	35,48,57,65	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.