



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:12 PM UTC

PDB ID : 8X5T / pdb_00008x5t
Title : Crystal structure of Thermus thermophilus peptidyl-tRNA hydrolase in complex with adenosine 5'-monophosphate
Authors : Uehara, Y.; Matsumoto, A.; Nakazawa, T.; Fukuta, A.; Ando, K.; Oka, N.; Uchiumi, T.; Ito, K.
Deposited on : 2023-11-19
Resolution : 1.60 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

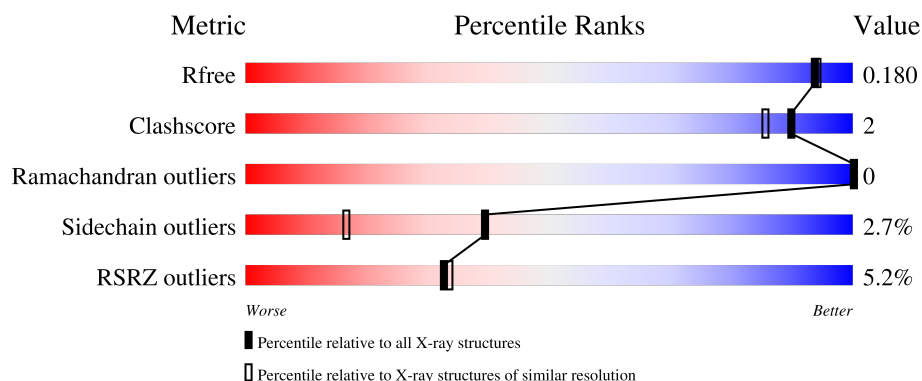
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	187	2% 76% 22% ..
1	B	187	66% 29% ..
1	C	187	14% 71% 25% ...

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5000 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 Peptidyl-tRNA hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1444	923	266	249	6			
1	B	185	Total	C	N	O	S	0	0	0
			1440	919	266	249	6			
1	C	184	Total	C	N	O	S	0	0	0
			1436	917	265	248	6			

There are 12 discrepancies between the modelled and reference sequences:

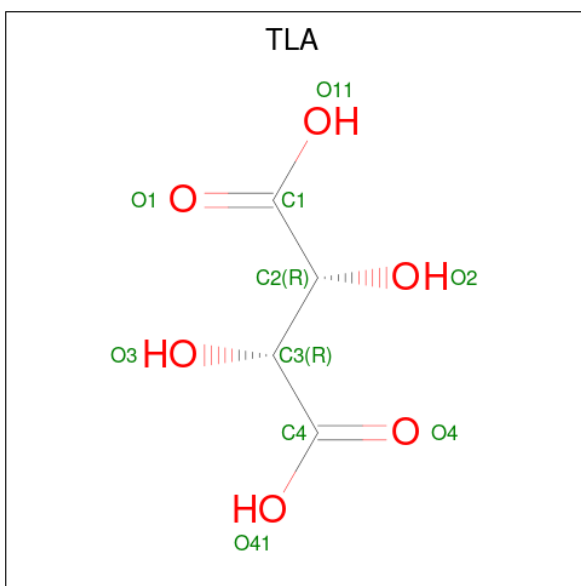
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q5SHZ2
A	-2	SER	-	expression tag	UNP Q5SHZ2
A	-1	HIS	-	expression tag	UNP Q5SHZ2
A	0	MET	-	expression tag	UNP Q5SHZ2
B	-3	GLY	-	expression tag	UNP Q5SHZ2
B	-2	SER	-	expression tag	UNP Q5SHZ2
B	-1	HIS	-	expression tag	UNP Q5SHZ2
B	0	MET	-	expression tag	UNP Q5SHZ2
C	-3	GLY	-	expression tag	UNP Q5SHZ2
C	-2	SER	-	expression tag	UNP Q5SHZ2
C	-1	HIS	-	expression tag	UNP Q5SHZ2
C	0	MET	-	expression tag	UNP Q5SHZ2

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

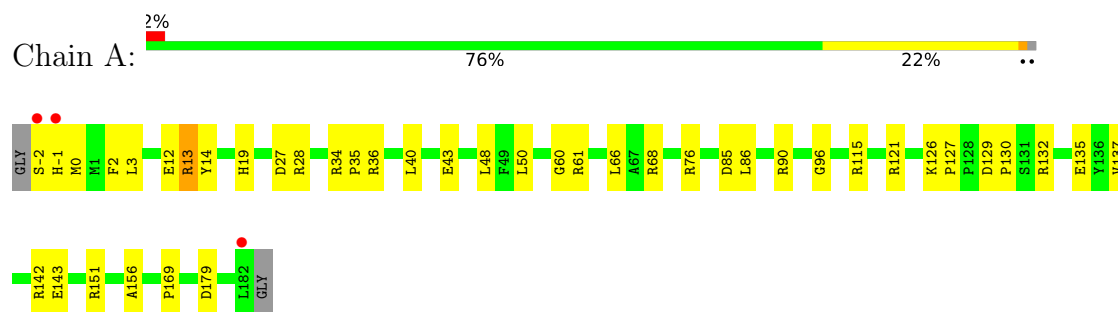
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	226	Total	O	0	0
			226	226		
5	B	222	Total	O	0	0
			222	222		
5	C	148	Total	O	0	0
			148	148		

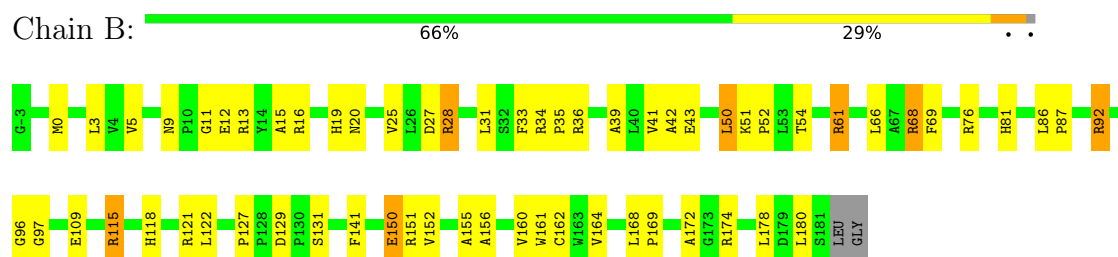
3 Residue-property plots [i](#)

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.

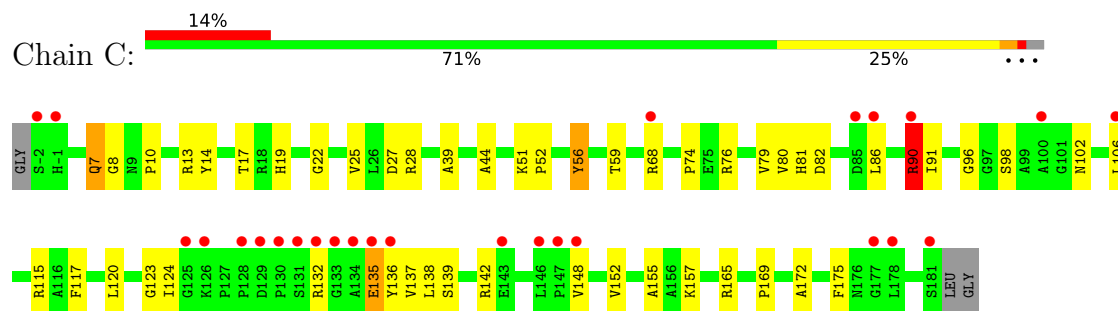
- Molecule 1: Peptidyl-tRNA hydrolase



- Molecule 1: Peptidyl-tRNA hydrolase



- Molecule 1: Peptidyl-tRNA hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.31Å 120.31Å 185.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	104.20 – 1.60 104.20 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (104.20-1.60) 99.9 (104.20-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	17.21 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.144 , 0.168 0.159 , 0.180	Depositor DCC
R_{free} test set	5230 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5000	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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, GOL, TLA

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	1.87	33/1479 (2.2%)	1.64	13/2000 (0.7%)
1	B	2.01	44/1475 (3.0%)	1.89	43/1994 (2.2%)
1	C	1.84	27/1471 (1.8%)	1.63	18/1989 (0.9%)
All	All	1.91	104/4425 (2.4%)	1.73	74/5983 (1.2%)

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
1	B	0	1

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	GLU	CA-CB	9.08	1.67	1.53
1	A	151	ARG	CD-NE	-8.87	1.33	1.46
1	A	50	LEU	CB-CG	-8.84	1.35	1.53
1	A	127	PRO	C-O	-8.46	1.15	1.24
1	A	3	LEU	CB-CG	-7.92	1.37	1.53
1	A	76	ARG	CD-NE	-7.88	1.35	1.46
1	C	52	PRO	CA-C	-7.34	1.43	1.52
1	B	76	ARG	NE-CZ	7.30	1.41	1.33
1	C	8	GLY	N-CA	-7.29	1.37	1.45
1	C	82	ASP	N-CA	7.24	1.55	1.46
1	C	25	VAL	CA-CB	-7.21	1.46	1.54
1	B	152	VAL	CA-C	-7.16	1.43	1.52
1	A	121	ARG	CD-NE	-7.13	1.36	1.46
1	A	132	ARG	CA-CB	-7.07	1.43	1.53
1	A	127	PRO	CA-C	-7.01	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	172	ALA	CA-C	6.95	1.61	1.52
1	B	86	LEU	CA-C	-6.88	1.45	1.52
1	A	142	ARG	CD-NE	-6.85	1.36	1.46
1	C	56	TYR	C-O	-6.80	1.16	1.24
1	B	41	VAL	N-CA	6.79	1.54	1.46
1	C	120	LEU	CA-C	-6.75	1.44	1.53
1	C	123	GLY	CA-C	-6.73	1.44	1.52
1	B	121	ARG	CD-NE	-6.72	1.36	1.46
1	A	34	ARG	N-CA	6.69	1.51	1.45
1	B	11	GLY	N-CA	6.66	1.51	1.45
1	B	3	LEU	CA-C	-6.59	1.44	1.52
1	A	35	PRO	CA-C	-6.56	1.45	1.52
1	A	129	ASP	N-CA	-6.54	1.35	1.45
1	A	126	LYS	CA-C	-6.46	1.45	1.52
1	B	35	PRO	N-CA	-6.43	1.39	1.47
1	C	22	GLY	C-O	6.42	1.31	1.23
1	B	16	ARG	N-CA	-6.36	1.38	1.46
1	B	109	GLU	N-CA	6.27	1.53	1.46
1	C	175	PHE	CA-CB	6.22	1.62	1.53
1	B	33	PHE	C-N	-6.17	1.25	1.33
1	B	172	ALA	C-O	-6.15	1.17	1.24
1	B	155	ALA	CA-CB	-6.10	1.43	1.53
1	A	90	ARG	NE-CZ	6.07	1.39	1.33
1	C	124	ILE	CA-C	6.05	1.58	1.52
1	B	68	ARG	CZ-NH1	6.03	1.41	1.32
1	B	15	ALA	C-O	6.00	1.31	1.24
1	A	135	GLU	CD-OE2	5.97	1.36	1.25
1	C	86	LEU	CA-C	-5.95	1.47	1.52
1	B	50	LEU	CB-CG	-5.92	1.41	1.53
1	C	14	TYR	N-CA	-5.91	1.38	1.46
1	B	12	GLU	CA-CB	5.89	1.62	1.53
1	C	39	ALA	CA-CB	-5.89	1.44	1.53
1	B	25	VAL	C-O	5.86	1.30	1.24
1	A	12	GLU	CA-C	-5.83	1.44	1.52
1	B	151	ARG	CA-CB	-5.79	1.44	1.53
1	B	27	ASP	CB-CG	-5.76	1.37	1.52
1	C	137	VAL	N-CA	5.75	1.53	1.46
1	A	90	ARG	CD-NE	5.72	1.54	1.46
1	C	80	VAL	C-N	5.69	1.40	1.33
1	B	160	VAL	N-CA	-5.66	1.40	1.46
1	A	36	ARG	N-CA	-5.65	1.39	1.46
1	B	50	LEU	CA-CB	-5.65	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	ASP	N-CA	5.62	1.53	1.46
1	B	87	PRO	CA-C	-5.62	1.45	1.52
1	B	31	LEU	N-CA	-5.61	1.39	1.45
1	A	90	ARG	CZ-NH1	5.53	1.40	1.32
1	B	61	ARG	CA-CB	5.51	1.62	1.53
1	A	14	TYR	CE1-CZ	-5.44	1.25	1.38
1	B	81	HIS	CA-C	-5.43	1.45	1.52
1	B	27	ASP	CA-C	-5.43	1.45	1.52
1	A	130	PRO	N-CA	-5.41	1.40	1.47
1	B	69	PHE	C-O	5.41	1.30	1.24
1	B	0	MET	CG-SD	-5.39	1.67	1.80
1	A	68	ARG	CZ-NH1	5.37	1.40	1.32
1	C	59	THR	C-O	5.35	1.30	1.24
1	C	10	PRO	CA-C	-5.34	1.46	1.52
1	B	66	LEU	C-O	5.33	1.30	1.24
1	B	76	ARG	CZ-NH1	5.32	1.40	1.32
1	B	118	HIS	C-O	5.32	1.30	1.23
1	C	102	ASN	CA-C	5.31	1.59	1.52
1	C	44	ALA	CA-CB	-5.29	1.45	1.53
1	B	178	LEU	CA-CB	-5.29	1.44	1.53
1	C	148	VAL	N-CA	-5.27	1.40	1.46
1	B	160	VAL	CA-CB	5.26	1.60	1.54
1	B	76	ARG	CD-NE	-5.26	1.38	1.46
1	A	60	GLY	CA-C	-5.25	1.45	1.52
1	B	41	VAL	C-O	5.24	1.29	1.24
1	C	51	LYS	CA-C	5.23	1.59	1.52
1	B	15	ALA	CA-C	-5.23	1.45	1.52
1	C	79	VAL	C-O	5.22	1.29	1.24
1	B	115	ARG	CZ-NH1	5.21	1.40	1.32
1	C	17	THR	CA-C	-5.21	1.46	1.53
1	A	86	LEU	N-CA	-5.21	1.39	1.45
1	A	34	ARG	CA-CB	-5.20	1.47	1.53
1	A	137	VAL	CA-C	-5.19	1.45	1.52
1	A	156	ALA	N-CA	-5.18	1.40	1.46
1	B	161	TRP	NE1-CE2	-5.16	1.31	1.37
1	C	155	ALA	N-CA	-5.16	1.40	1.46
1	B	122	LEU	C-O	5.15	1.30	1.24
1	B	43	GLU	C-O	5.14	1.30	1.24
1	A	14	TYR	CA-C	-5.13	1.45	1.52
1	C	52	PRO	N-CA	5.11	1.53	1.47
1	B	42	ALA	CA-CB	-5.11	1.42	1.53
1	A	179	ASP	CA-C	-5.08	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	ARG	C-O	5.05	1.29	1.23
1	C	7	GLN	CA-C	-5.04	1.46	1.52
1	A	40	LEU	CA-CB	-5.04	1.46	1.53
1	A	142	ARG	CZ-NH1	5.03	1.39	1.32
1	B	127	PRO	C-N	5.01	1.40	1.34

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	GLY	CA-C-O	9.60	128.86	122.23
1	B	34	ARG	O-C-N	-8.90	115.56	121.88
1	A	28	ARG	NE-CZ-NH1	-8.76	112.74	121.50
1	A	28	ARG	NH1-CZ-NH2	8.34	130.14	119.30
1	B	141	PHE	CA-C-O	-8.19	112.63	121.56
1	B	156	ALA	N-CA-C	8.00	120.00	111.28
1	C	138	LEU	N-CA-C	7.64	122.18	113.02
1	B	9	ASN	O-C-N	7.56	130.31	121.39
1	B	96	GLY	O-C-N	7.52	130.65	122.60
1	B	150	GLU	CA-C-O	-7.28	112.83	120.55
1	A	12	GLU	CB-CG-CD	6.99	124.48	112.60
1	C	56	TYR	CA-C-O	6.98	128.17	120.63
1	B	169	PRO	N-CA-C	6.81	119.01	110.70
1	A	13	ARG	CG-CD-NE	-6.75	97.15	112.00
1	C	56	TYR	N-CA-C	6.66	119.39	111.33
1	C	124	ILE	O-C-N	6.54	128.52	121.78
1	C	28	ARG	CG-CD-NE	-6.51	97.68	112.00
1	A	61	ARG	CG-CD-NE	6.48	126.25	112.00
1	C	169	PRO	N-CA-C	6.46	118.58	110.70
1	B	52	PRO	O-C-N	6.43	130.98	123.01
1	B	11	GLY	O-C-N	-6.41	115.21	122.64
1	B	31	LEU	CA-C-O	-6.40	114.41	121.89
1	B	150	GLU	O-C-N	6.37	128.87	122.12
1	B	162	CYS	CA-C-O	6.24	127.37	120.82
1	B	39	ALA	N-CA-C	6.24	118.26	108.96
1	A	68	ARG	NE-CZ-NH2	-6.22	113.60	119.20
1	B	131	SER	CA-CB-OG	-6.20	98.70	111.10
1	B	5	VAL	O-C-N	-6.13	116.70	123.20
1	B	15	ALA	O-C-N	-6.07	115.12	122.22
1	A	90	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	B	25	VAL	O-C-N	-6.06	115.59	121.90
1	C	139	SER	O-C-N	5.99	126.59	121.20
1	B	39	ALA	CA-C-O	-5.89	115.15	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	VAL	O-C-N	-5.89	115.77	121.83
1	C	152	VAL	CA-C-O	-5.89	114.61	120.85
1	C	157	LYS	CA-C-O	5.88	126.99	120.82
1	A	169	PRO	CB-CA-C	5.84	118.05	110.92
1	B	141	PHE	O-C-N	5.84	129.75	122.86
1	B	61	ARG	CB-CA-C	-5.83	99.83	110.63
1	B	51	LYS	O-C-N	-5.83	114.64	120.83
1	A	12	GLU	N-CA-C	5.81	118.39	111.71
1	B	13	ARG	CA-C-O	5.77	126.86	120.63
1	B	20	ASN	CA-C-O	-5.75	112.83	119.56
1	B	25	VAL	CA-C-N	5.75	127.99	120.28
1	B	25	VAL	C-N-CA	5.75	127.99	120.28
1	B	92	ARG	O-C-N	-5.74	116.38	123.44
1	C	90	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	C	81	HIS	O-C-N	5.66	129.72	123.33
1	B	156	ALA	CA-C-O	5.62	126.51	120.55
1	B	164	VAL	O-C-N	5.59	127.37	121.89
1	A	76	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	B	31	LEU	N-CA-C	5.50	118.57	110.59
1	B	174	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	C	148	VAL	O-C-N	5.38	127.37	121.83
1	B	92	ARG	CA-C-O	5.34	127.42	120.21
1	C	136	TYR	O-C-N	5.33	127.56	122.07
1	A	66	LEU	N-CA-CB	5.31	117.77	110.07
1	C	136	TYR	N-CA-C	-5.29	105.41	111.07
1	C	27	ASP	O-C-N	5.24	129.69	122.46
1	B	129	ASP	CA-C-N	5.17	124.97	119.28
1	B	129	ASP	C-N-CA	5.17	124.97	119.28
1	C	165	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	B	28	ARG	NE-CZ-NH2	-5.14	114.58	119.20
1	B	34	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	A	85	ASP	CB-CG-OD2	-5.12	106.62	118.40
1	B	5	VAL	CA-C-O	5.12	125.71	120.39
1	B	127	PRO	CB-CA-C	5.10	117.14	110.92
1	B	54	THR	CA-C-N	5.09	131.26	121.54
1	B	54	THR	C-N-CA	5.09	131.26	121.54
1	C	76	ARG	N-CA-C	-5.07	105.56	112.26
1	A	2	PHE	CA-C-O	-5.07	116.01	121.38
1	B	168	LEU	CA-C-N	-5.04	115.19	120.38
1	B	168	LEU	C-N-CA	-5.04	115.19	120.38
1	C	13	ARG	N-CA-C	5.01	118.17	111.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	61	ARG	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	1444	0	1464	4	0
1	B	1440	0	1456	5	0
1	C	1436	0	1453	7	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
3	A	20	0	8	0	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
5	A	226	0	0	0	0
5	B	222	0	0	2	0
5	C	148	0	0	2	0
All	All	5000	0	4429	16	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 2.

All (16) 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:B:68:ARG:HG3	5:B:347:HOH:O	1.69	0.90
1:A:-2:SER:HB2	1:A:0:MET:HE2	1.77	0.66
1:B:28:ARG:HH22	1:B:150:GLU:CD	2.04	0.66
1:B:28:ARG:NH2	1:B:150:GLU:OE1	2.28	0.64
1:C:68:ARG:NH2	5:C:201:HOH:O	2.35	0.59
1:B:92:ARG:CG	5:B:367:HOH:O	2.59	0.50
1:C:142:ARG:NH1	5:C:202:HOH:O	2.40	0.50
1:B:97:GLY:HA2	1:B:115:ARG:CZ	2.41	0.50
1:A:43:GLU:HG2	1:A:48:LEU:HD23	1.94	0.49
1:A:96:GLY:HA2	1:A:115:ARG:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:NH2	1:C:135:GLU:HG3	2.34	0.42
1:C:74:PRO:O	1:C:117:PHE:HA	2.19	0.42
1:C:7:GLN:HB3	1:C:56:TYR:CE2	2.55	0.42
1:A:-2:SER:CB	1:A:0:MET:HE2	2.48	0.42
1:C:96:GLY:HA2	1:C:115:ARG:O	2.20	0.42
1:C:90:ARG:HH21	1:C:90:ARG:HG3	1.85	0.41

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	183/187 (98%)	180 (98%)	3 (2%)	0	100	100
1	B	183/187 (98%)	179 (98%)	4 (2%)	0	100	100
1	C	182/187 (97%)	177 (97%)	5 (3%)	0	100	100
All	All	548/561 (98%)	536 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	147/147 (100%)	144 (98%)	3 (2%)	48	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	146/147 (99%)	143 (98%)	3 (2%)	47	23
1	C	146/147 (99%)	140 (96%)	6 (4%)	27	8
All	All	439/441 (100%)	427 (97%)	12 (3%)	39	16

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

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	13	ARG
1	A	19	HIS
1	B	19	HIS
1	B	50	LEU
1	B	180	LEU
1	C	19	HIS
1	C	90	ARG
1	C	91	ILE
1	C	98	SER
1	C	106	LEU
1	C	135	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	-1	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

7 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$
4	GOL	B	203	-	5,5,5	0.64	0	5,5,5	1.12	1 (20%)
3	TLA	A	202	-	9,9,9	1.56	2 (22%)	12,12,12	2.01	4 (33%)
4	GOL	B	202	-	5,5,5	0.74	0	5,5,5	1.31	1 (20%)
2	AMP	A	201	-	25,25,25	1.12	2 (8%)	37,38,38	2.65	10 (27%)
4	GOL	A	204	-	5,5,5	1.17	1 (20%)	5,5,5	0.59	0
2	AMP	B	201	-	25,25,25	1.07	4 (16%)	37,38,38	1.31	3 (8%)
3	TLA	A	203	-	9,9,9	1.45	2 (22%)	12,12,12	1.39	1 (8%)

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
4	GOL	B	203	-	-	1/4/4/4	-
3	TLA	A	202	-	-	0/12/12/12	-
4	GOL	B	202	-	-	0/4/4/4	-
2	AMP	A	201	-	-	1/10/26/26	0/3/3/3
4	GOL	A	204	-	-	0/4/4/4	-
2	AMP	B	201	-	-	3/10/26/26	0/3/3/3
3	TLA	A	203	-	-	0/12/12/12	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	TLA	O11-C1	-3.22	1.20	1.30
2	B	201	AMP	P-O2P	-2.24	1.46	1.54
3	A	203	TLA	C3-C4	-2.18	1.49	1.52
2	B	201	AMP	C2-N1	2.12	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	AMP	O3'-C3'	2.09	1.48	1.43
3	A	203	TLA	O2-C2	2.06	1.46	1.42
3	A	202	TLA	O41-C4	-2.04	1.24	1.30
2	A	201	AMP	C2-N1	2.04	1.37	1.33
2	B	201	AMP	C5-C4	2.04	1.42	1.39
4	A	204	GOL	O2-C2	2.02	1.49	1.43
2	A	201	AMP	P-O2P	-2.02	1.47	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	AMP	O3P-P-O2P	10.36	146.65	107.80
2	A	201	AMP	O2P-P-O1P	-6.53	85.37	110.83
3	A	202	TLA	O11-C1-O1	4.20	133.62	124.08
2	A	201	AMP	O2P-P-O5'	-3.99	96.27	106.67
2	A	201	AMP	O4'-C1'-C2'	-3.93	98.21	106.62
2	A	201	AMP	C4-N9-C8	-3.53	102.03	105.74
2	B	201	AMP	N3-C2-N1	-3.35	123.50	128.58
3	A	202	TLA	O1-C1-C2	-3.27	112.91	121.62
3	A	203	TLA	O4-C4-C3	-2.89	113.93	121.62
2	A	201	AMP	O3P-P-O5'	-2.70	99.62	106.67
2	B	201	AMP	C2-N1-C6	2.61	123.02	118.73
2	A	201	AMP	C6-C5-C4	2.47	120.56	117.18
3	A	202	TLA	O3-C3-C2	-2.42	105.25	110.17
2	B	201	AMP	C4-N9-C8	2.40	108.26	105.74
2	A	201	AMP	N9-C8-N7	2.33	117.25	113.94
2	A	201	AMP	C5-C6-N1	-2.27	111.76	117.51
4	B	202	GOL	O2-C2-C3	2.12	117.97	109.18
2	A	201	AMP	C6-C5-N7	-2.09	128.06	132.09
3	A	202	TLA	O3-C3-C4	-2.06	106.29	110.69
4	B	203	GOL	O2-C2-C3	-2.05	100.68	109.18

There are no chirality outliers.

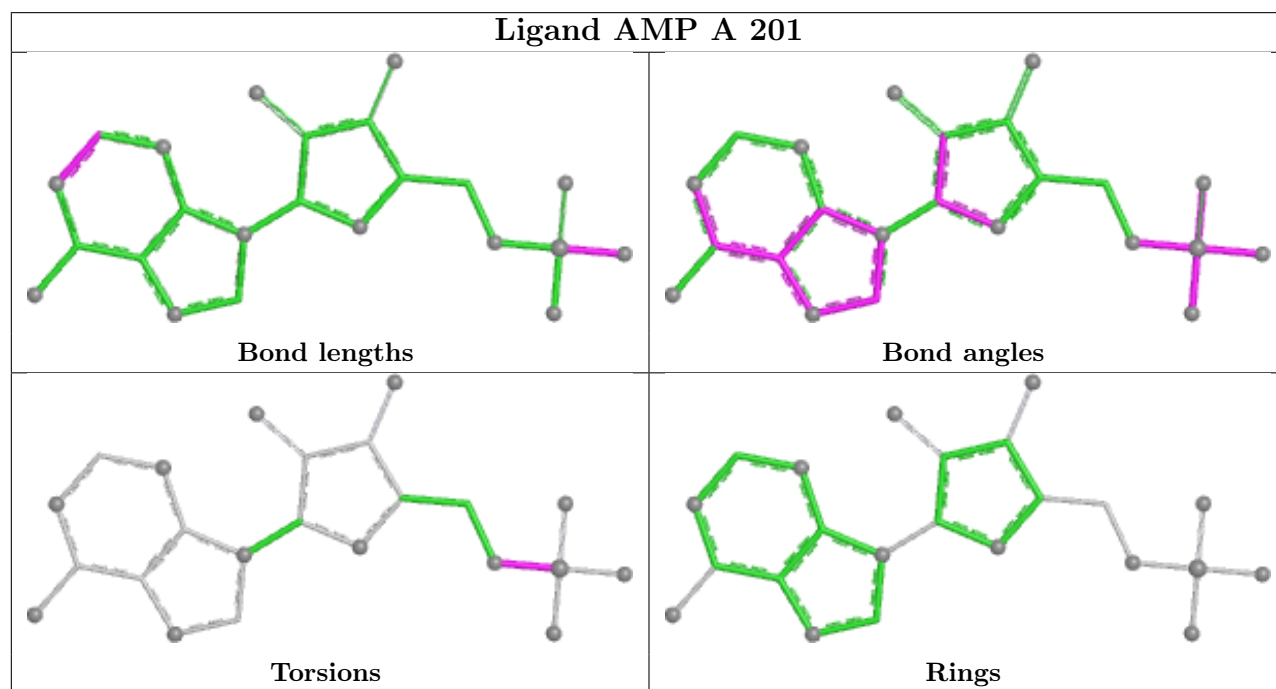
All (5) torsion outliers are listed below:

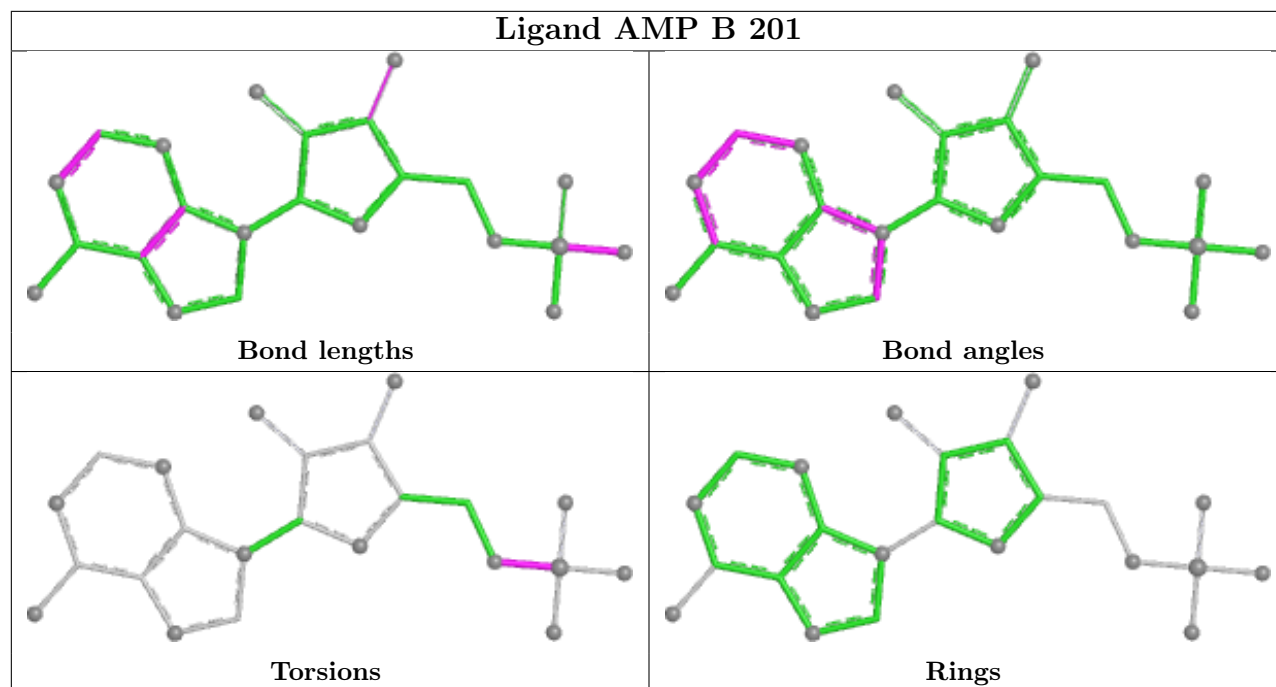
Mol	Chain	Res	Type	Atoms
2	A	201	AMP	C5'-O5'-P-O2P
2	B	201	AMP	C5'-O5'-P-O1P
4	B	203	GOL	O1-C1-C2-O2
2	B	201	AMP	C5'-O5'-P-O2P
2	B	201	AMP	C5'-O5'-P-O3P

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	185/187 (98%)	-0.43	3 (1%) 70 74	8, 12, 24, 63	0
1	B	185/187 (98%)	-0.20	0 100 100	9, 15, 29, 38	0
1	C	184/187 (98%)	0.57	26 (14%) 6 6	11, 23, 47, 67	0
All	All	554/561 (98%)	-0.02	29 (5%) 33 33	8, 15, 38, 67	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	HIS	5.2
1	C	128	PRO	5.0
1	C	129	ASP	4.0
1	A	-2	SER	4.0
1	C	-1	HIS	3.8
1	C	130	PRO	3.8
1	C	-2	SER	3.5
1	C	131	SER	3.4
1	A	182	LEU	3.3
1	C	177	GLY	3.2
1	C	132	ARG	3.0
1	C	85	ASP	2.8
1	C	136	TYR	2.6
1	C	125	GLY	2.6
1	C	100	ALA	2.6
1	C	68	ARG	2.5
1	C	90	ARG	2.4
1	C	86	LEU	2.3
1	C	135	GLU	2.3
1	C	143	GLU	2.3
1	C	106	LEU	2.3
1	C	148	VAL	2.3
1	C	134	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	181	SER	2.1
1	C	147	PRO	2.1
1	C	133	GLY	2.1
1	C	146	LEU	2.0
1	C	178	LEU	2.0
1	C	126	LYS	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](#)

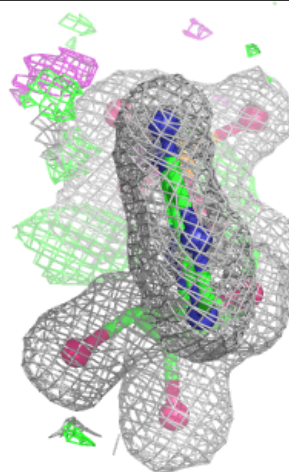
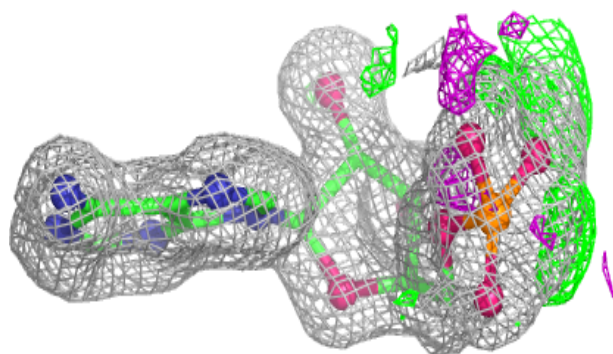
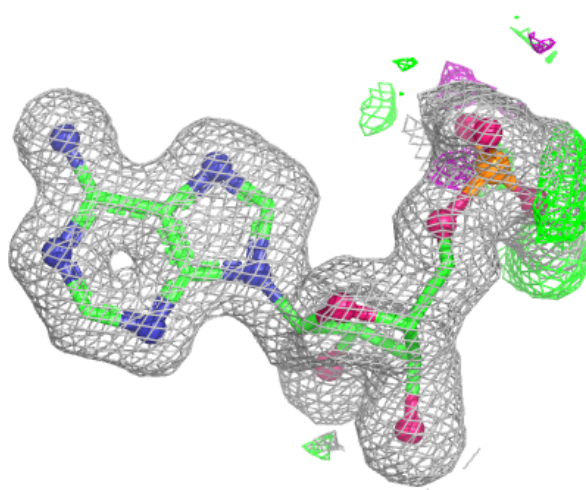
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	203	6/6	0.89	0.12	33,36,36,37	0
4	GOL	A	204	6/6	0.91	0.09	21,23,29,29	0
3	TLA	A	203	10/10	0.93	0.08	26,27,32,33	0
4	GOL	B	202	6/6	0.95	0.08	22,26,26,31	0
2	AMP	A	201	23/23	0.97	0.06	9,11,29,35	0
3	TLA	A	202	10/10	0.97	0.05	14,15,20,20	0
2	AMP	B	201	23/23	0.98	0.05	12,13,22,22	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.

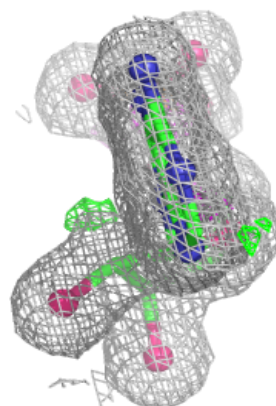
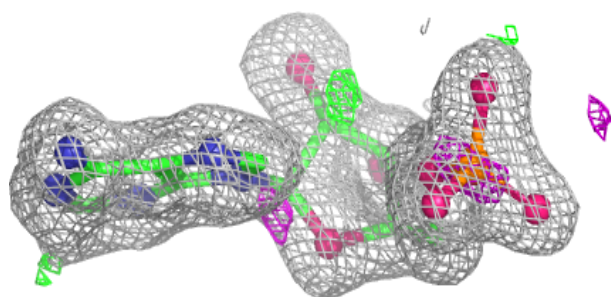
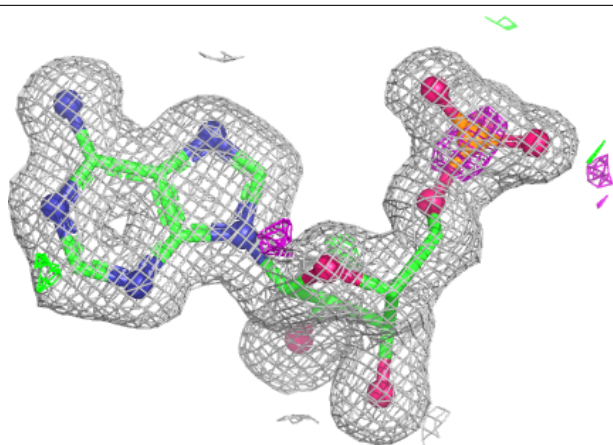
Electron density around AMP A 201:

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



Electron density around AMP B 201:

$2mF_o-DF_c$ (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.