Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 05:39 PM EST

PDB ID	:	4JYZ
Title	:	Crystal structure of E. coli glutaminyl-tRNA synthetase bound to ATP and native tRNA(Gln) containing the cmnm5s2U34 anticodon wobble base
Authors	:	Perona, J.J.; Rodriguez-Hernandez, A.
Deposited on	:	2013-04-01
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

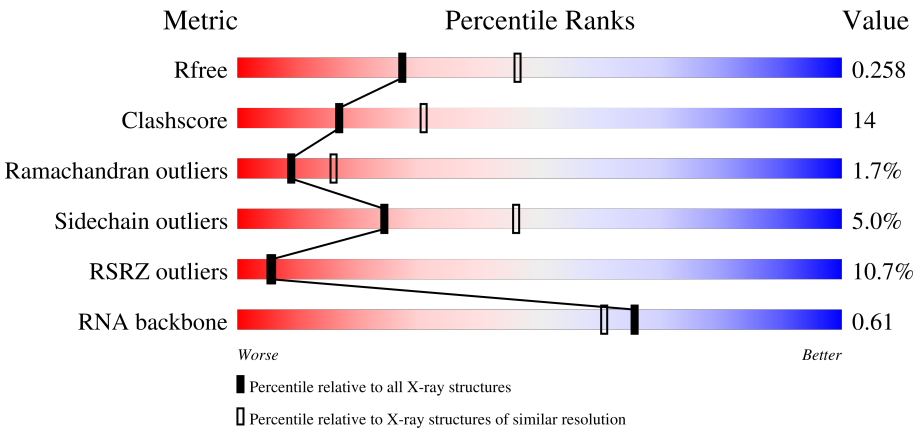
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	553	10% 69% 26% • •
2	B	75	9% 63% 17% 12% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	603	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6022 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

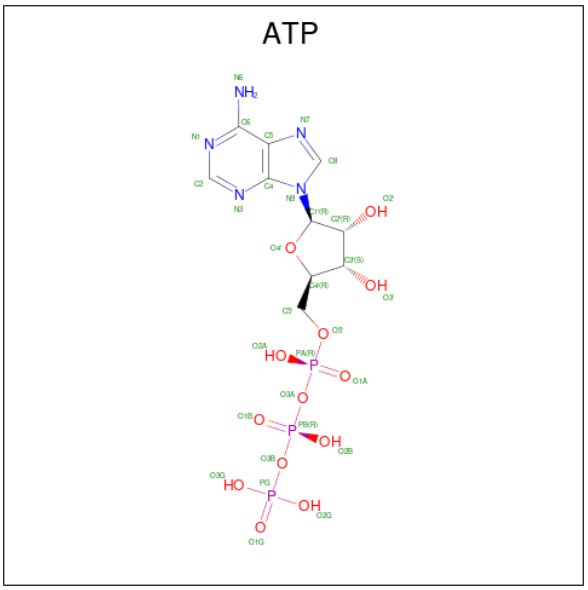
- Molecule 1 is a protein called Glutamine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	542	4328	2737	764	806	21	0	0	0

- Molecule 2 is a RNA chain called RNA (72-MER).

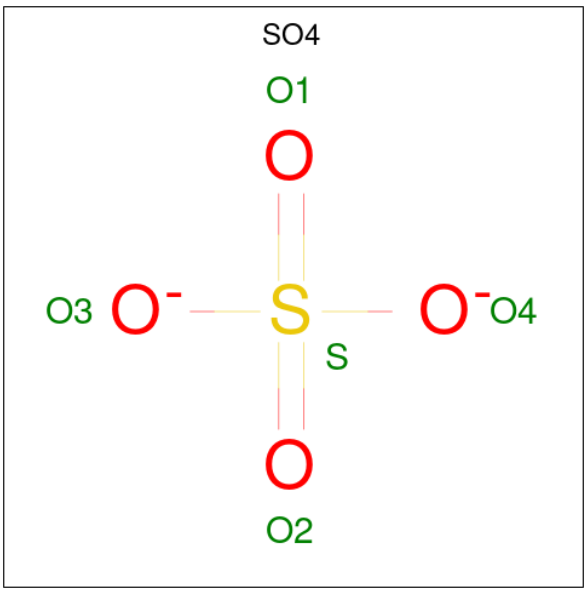
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	B	72	1543	691	275	503	72	2	0	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	5	13	3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

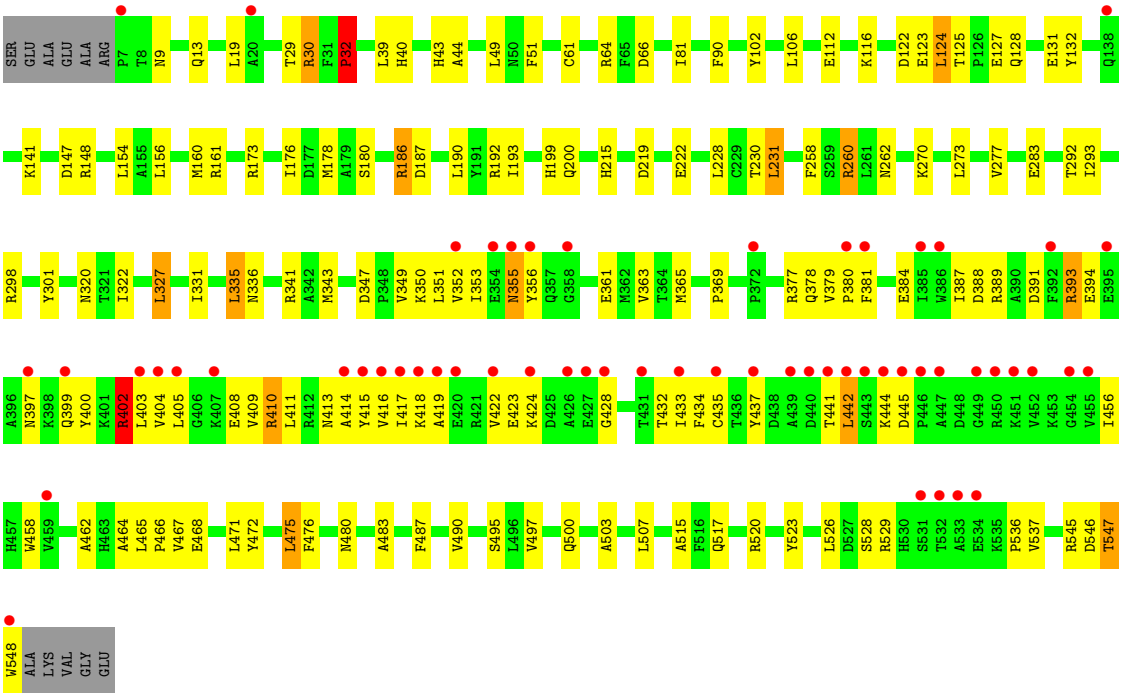
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	79	Total O 79 79	0	0
5	B	31	Total O 31 31	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

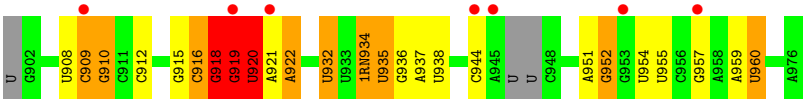
• Molecule 1: Glutamine–tRNA ligase

Chain A:



• Molecule 2: RNA (72-MER)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	93.40Å 234.62Å 113.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 2.50 47.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.60-2.50) 99.1 (47.55-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.263 0.227 , 0.258	Depositor DCC
R_{free} test set	8176 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6022	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, OMG, 4SU, SO4, H2U, 1RN, OMU, 5MU, 2MA, ATP

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	0.39	0/4432	0.59	0/6009
2	B	0.44	0/1505	0.97	1/2340 (0.0%)
All	All	0.40	0/5937	0.72	1/8349 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	960	U	C2'-C3'-O3'	6.83	124.63	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	919	G	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4328	0	4179	132	0
2	B	1543	0	791	24	0
3	A	31	0	12	2	0
4	A	10	0	0	0	0
5	A	79	0	0	4	0
5	B	31	0	0	1	0
All	All	6022	0	4982	151	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 14.

All (151) 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:B:919:G:H4'	2:B:920:H2U:OP1	1.53	1.04
1:A:503:ALA:HB1	1:A:507:LEU:HD12	1.57	0.84
1:A:39:LEU:HD13	1:A:81:ILE:HG12	1.61	0.81
1:A:403:LEU:HD13	1:A:409:VAL:HG12	1.63	0.80
1:A:397:ASN:ND2	1:A:399:GLN:HB2	2.00	0.77
1:A:416:VAL:HG23	1:A:441:THR:HG21	1.70	0.71
1:A:64:ARG:HD3	1:A:222:GLU:OE2	1.96	0.66
1:A:391:ASP:HA	1:A:402:ARG:HG2	1.78	0.65
1:A:351:LEU:HD23	1:A:351:LEU:O	1.96	0.65
2:B:918:OMG:H2'	2:B:957:G:N2	2.12	0.65
1:A:336:ASN:ND2	1:A:341:ARG:HH22	1.96	0.64
1:A:331:ILE:HG13	1:A:335:LEU:HD22	1.81	0.63
1:A:363:VAL:HG11	1:A:413:ASN:O	1.97	0.63
1:A:30:ARG:NH1	1:A:215:HIS:NE2	2.47	0.62
1:A:444:LYS:HA	2:B:934:1RN:H12	1.81	0.62
1:A:515:ALA:HB2	5:A:752:HOH:O	1.98	0.62
1:A:43:HIS:HD2	3:A:601:ATP:H5'2	1.64	0.62
1:A:487:PHE:O	1:A:490:VAL:HG22	2.00	0.62
1:A:336:ASN:HD22	1:A:341:ARG:HH22	1.48	0.61
2:B:909:C:H4'	2:B:910:G:OP1	1.99	0.61
1:A:381:PHE:HE2	1:A:414:ALA:HB1	1.63	0.61
1:A:391:ASP:O	1:A:402:ARG:HB3	2.00	0.61
1:A:410:ARG:HH11	1:A:410:ARG:HG3	1.65	0.61
1:A:260:ARG:HG2	1:A:260:ARG:HH11	1.66	0.61
1:A:173:ARG:HD2	1:A:187:ASP:O	2.00	0.60
1:A:32:PRO:HA	1:A:64:ARG:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ALA:HB2	1:A:293:ILE:HD11	1.85	0.58
1:A:352:VAL:HG22	1:A:432:THR:CG2	2.34	0.58
1:A:349:VAL:HB	1:A:389:ARG:HD3	1.86	0.57
1:A:40:HIS:HA	1:A:292:THR:HA	1.86	0.57
1:A:417:ILE:HG12	1:A:418:LYS:N	2.19	0.57
1:A:409:VAL:HG22	1:A:410:ARG:H	1.69	0.57
1:A:465:LEU:HD12	1:A:466:PRO:HD2	1.86	0.57
1:A:410:ARG:HG3	1:A:410:ARG:NH1	2.20	0.57
2:B:915:G:H2'	2:B:959:A:N1	2.21	0.56
1:A:402:ARG:N	1:A:402:ARG:HD3	2.21	0.56
1:A:409:VAL:HG22	1:A:410:ARG:N	2.21	0.55
1:A:471:LEU:HB2	1:A:497:VAL:CG2	2.36	0.55
1:A:416:VAL:HG23	1:A:441:THR:CG2	2.35	0.55
1:A:161:ARG:HD3	5:A:751:HOH:O	2.06	0.55
1:A:415:TYR:HD1	1:A:442:LEU:H	1.54	0.55
1:A:125:THR:OG1	1:A:128:GLN:HG3	2.07	0.55
1:A:43:HIS:CD2	3:A:601:ATP:H5'2	2.41	0.54
2:B:915:G:P	2:B:916:C:H41	2.30	0.54
1:A:301:TYR:HE2	1:A:327:LEU:HD22	1.72	0.54
1:A:517:GLN:HG3	1:A:523:TYR:CE1	2.43	0.54
1:A:393:ARG:O	1:A:404:VAL:HA	2.08	0.53
1:A:353:ILE:HD11	1:A:437:TYR:HD1	1.74	0.53
1:A:365:MET:HG2	1:A:413:ASN:HD22	1.73	0.53
1:A:301:TYR:CE2	1:A:327:LEU:HD22	2.43	0.53
1:A:528:SER:HB3	5:A:768:HOH:O	2.08	0.52
1:A:365:MET:HG2	1:A:413:ASN:ND2	2.25	0.52
1:A:480:ASN:ND2	1:A:483:ALA:HB2	2.24	0.52
1:A:365:MET:HG2	1:A:413:ASN:CB	2.40	0.51
1:A:231:LEU:HD13	1:A:258:PHE:C	2.31	0.51
1:A:410:ARG:NH2	1:A:441:THR:HG22	2.26	0.51
1:A:379:VAL:HG12	1:A:380:PRO:HD2	1.93	0.50
1:A:422:VAL:HG12	1:A:423:GLU:N	2.26	0.50
1:A:475:LEU:HD13	1:A:476:PHE:CE2	2.47	0.49
1:A:475:LEU:HD22	1:A:475:LEU:O	2.12	0.49
1:A:260:ARG:HH11	1:A:260:ARG:CG	2.26	0.49
1:A:415:TYR:HE1	1:A:442:LEU:HB2	1.78	0.49
2:B:951:A:H2'	2:B:952:G:O4'	2.11	0.49
1:A:132:TYR:CD2	1:A:141:LYS:HG3	2.47	0.49
1:A:199:HIS:ND1	1:A:200:GLN:HG2	2.27	0.49
1:A:122:ASP:OD1	1:A:124:LEU:HB2	2.12	0.49
1:A:123:GLU:OE1	1:A:148:ARG:NH2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:934:1RN:C6	2:B:934:1RN:O2'	2.59	0.49
1:A:273:LEU:O	1:A:277:VAL:HG23	2.13	0.49
2:B:918:OMG:H5'	2:B:919:G:OP1	2.13	0.48
1:A:545:ARG:NH1	1:A:547:THR:HG21	2.28	0.48
1:A:352:VAL:HG22	1:A:432:THR:HG21	1.95	0.48
1:A:424:LYS:HD3	1:A:428:GLY:O	2.14	0.48
1:A:180:SER:O	1:A:186:ARG:NH1	2.42	0.48
2:B:918:OMG:N3	2:B:918:OMG:HM23	2.28	0.48
1:A:178:MET:O	1:A:186:ARG:HD2	2.14	0.48
1:A:408:GLU:HB3	1:A:418:LYS:HG3	1.95	0.48
1:A:381:PHE:CE2	1:A:414:ALA:HB1	2.46	0.47
1:A:377:ARG:HH11	1:A:377:ARG:HG2	1.80	0.47
1:A:391:ASP:OD2	1:A:456:ILE:HB	2.15	0.47
1:A:411:LEU:HB2	1:A:414:ALA:HB3	1.97	0.47
1:A:547:THR:O	1:A:547:THR:HG23	2.15	0.47
1:A:468:GLU:HG3	1:A:500:GLN:HE22	1.79	0.46
1:A:351:LEU:HD21	1:A:417:ILE:CD1	2.44	0.46
1:A:356:TYR:HD1	1:A:437:TYR:CE1	2.33	0.46
1:A:352:VAL:O	1:A:434:PHE:HA	2.15	0.46
1:A:343:MET:HE1	1:A:458:TRP:H	1.81	0.46
1:A:379:VAL:CG1	1:A:380:PRO:HD2	2.46	0.46
1:A:353:ILE:HD11	1:A:437:TYR:CD1	2.51	0.46
1:A:520:ARG:HG2	2:B:935:U:O2'	2.16	0.46
2:B:944:C:H1'	5:B:1016:HOH:O	2.17	0.45
1:A:322:ILE:HD12	1:A:322:ILE:N	2.31	0.45
1:A:127:GLU:O	1:A:131:GLU:HG3	2.16	0.45
1:A:160:MET:HG2	1:A:193:ILE:HD11	1.97	0.45
1:A:365:MET:HG2	1:A:413:ASN:HB2	1.99	0.45
1:A:356:TYR:OH	1:A:361:GLU:HG2	2.17	0.45
1:A:394:GLU:HA	1:A:405:LEU:CB	2.47	0.45
1:A:417:ILE:HD11	1:A:435:CYS:SG	2.57	0.44
2:B:915:G:HO2'	2:B:916:C:P	2.39	0.44
1:A:30:ARG:NH2	1:A:228:LEU:O	2.50	0.44
1:A:472:TYR:HA	1:A:495:SER:O	2.17	0.44
1:A:29:THR:O	1:A:61:CYS:HA	2.18	0.44
1:A:347:ASP:O	1:A:388:ASP:HA	2.16	0.44
1:A:352:VAL:O	1:A:352:VAL:HG23	2.18	0.44
1:A:387:ILE:HG12	1:A:388:ASP:N	2.33	0.44
1:A:343:MET:HE3	1:A:458:TRP:O	2.17	0.44
1:A:352:VAL:HG12	1:A:384:GLU:HG2	2.00	0.44
1:A:43:HIS:CE1	1:A:270:LYS:HE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASN:HB2	1:A:320:ASN:O	2.17	0.44
2:B:921:A:H2'	2:B:922:A:OP2	2.18	0.44
1:A:102:TYR:O	1:A:106:LEU:HD22	2.18	0.44
1:A:408:GLU:HB2	1:A:417:ILE:O	2.18	0.44
1:A:400:TYR:CE2	1:A:402:ARG:HB2	2.53	0.43
1:A:433:ILE:HG22	1:A:435:CYS:SG	2.59	0.43
1:A:353:ILE:O	1:A:353:ILE:HG12	2.17	0.43
1:A:13:GLN:HE22	2:B:916:C:N4	2.17	0.43
1:A:298:ARG:HH12	1:A:529:ARG:CZ	2.31	0.43
1:A:497:VAL:O	1:A:497:VAL:HG23	2.18	0.43
1:A:355:ASN:C	1:A:355:ASN:HD22	2.22	0.43
1:A:410:ARG:HE	2:B:934:1RN:C4	2.32	0.43
1:A:467:VAL:HG12	1:A:536:PRO:HG2	2.00	0.43
1:A:471:LEU:HB2	1:A:497:VAL:HG23	2.00	0.43
1:A:51:PHE:HB3	1:A:90:PHE:CD1	2.54	0.43
1:A:112:GLU:O	1:A:116:LYS:HG3	2.17	0.43
1:A:545:ARG:HH12	1:A:547:THR:HG21	1.83	0.43
2:B:918:OMG:H5'	2:B:919:G:P	2.59	0.43
1:A:9:ASN:O	1:A:13:GLN:HG3	2.18	0.43
2:B:909:C:H5	2:B:912:C:H41	1.67	0.42
1:A:416:VAL:H	1:A:441:THR:HG21	1.85	0.42
2:B:915:G:H2'	2:B:959:A:H61	1.84	0.42
2:B:934:1RN:H1	2:B:934:1RN:H9	2.01	0.42
1:A:283:GLU:HB3	1:A:529:ARG:NH1	2.34	0.42
1:A:397:ASN:HD21	1:A:399:GLN:HB2	1.79	0.42
1:A:397:ASN:HD22	1:A:399:GLN:HB2	1.79	0.42
2:B:909:C:H5	2:B:912:C:N4	2.18	0.42
1:A:132:TYR:CG	1:A:141:LYS:HE3	2.55	0.42
1:A:351:LEU:HD21	1:A:417:ILE:HD11	2.01	0.42
1:A:361:GLU:HG3	1:A:381:PHE:HB3	2.01	0.42
2:B:932:OMU:HM23	2:B:932:OMU:H1'	1.82	0.42
1:A:419:ALA:HA	1:A:435:CYS:SG	2.60	0.42
1:A:161:ARG:HG2	5:A:754:HOH:O	2.19	0.41
1:A:410:ARG:HH21	2:B:934:1RN:C4	2.32	0.41
1:A:30:ARG:HD2	1:A:219:ASP:OD1	2.20	0.41
1:A:402:ARG:HB3	1:A:403:LEU:H	1.67	0.41
1:A:381:PHE:CD1	1:A:381:PHE:C	2.94	0.41
1:A:230:THR:HA	1:A:258:PHE:O	2.21	0.41
1:A:391:ASP:HB3	1:A:456:ILE:HG21	2.03	0.41
1:A:526:LEU:HD12	1:A:537:VAL:O	2.20	0.41
1:A:350:LYS:O	1:A:432:THR:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ASP:O	1:A:547:THR:HB	2.21	0.40
2:B:921:A:C2'	2:B:922:A:OP2	2.69	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	540/553 (98%)	497 (92%)	34 (6%)	9 (2%)	9 16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	ALA
1	A	32	PRO
1	A	402	ARG
1	A	442	LEU
1	A	547	THR
1	A	445	ASP
1	A	462	ALA
1	A	176	ILE
1	A	369	PRO

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	458/481 (95%)	435 (95%)	23 (5%)	24 46

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	30	ARG
1	A	32	PRO
1	A	49	LEU
1	A	66	ASP
1	A	124	LEU
1	A	147	ASP
1	A	154	LEU
1	A	156	LEU
1	A	186	ARG
1	A	190	LEU
1	A	192	ARG
1	A	231	LEU
1	A	260	ARG
1	A	327	LEU
1	A	335	LEU
1	A	355	ASN
1	A	378	GLN
1	A	393	ARG
1	A	402	ARG
1	A	410	ARG
1	A	475	LEU
1	A	548	TRP

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	336	ASN
1	A	338	ASN
1	A	413	ASN
1	A	500	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	68/75 (90%)	10 (14%)	4 (5%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	909	C
2	B	910	G
2	B	916	C
2	B	918	OMG
2	B	919	G
2	B	920	H2U
2	B	922	A
2	B	935	U
2	B	936	G
2	B	952	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	909	C
2	B	919	G
2	B	935	U
2	B	960	U

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

9 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	2MA	B	937	2	17,25,26	1.37	2 (11%)	17,37,40	1.28	3 (17%)
2	PSU	B	955	2	18,21,22	1.15	2 (11%)	22,30,33	1.66	4 (18%)
2	H2U	B	920	2	18,21,22	2.60	6 (33%)	21,30,33	7.16	7 (33%)
2	OMG	B	918	2	18,26,27	1.06	2 (11%)	19,38,41	1.18	2 (10%)
2	5MU	B	954	2	19,22,23	0.42	0	28,32,35	0.96	1 (3%)
2	OMU	B	932	2	19,22,23	0.39	0	26,31,34	0.90	1 (3%)
2	1RN	B	934	2	22,27,28	6.77	4 (18%)	24,38,41	1.47	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	4SU	B	908	2	18,21,22	5.43	1 (5%)	26,30,33	0.66	0
2	PSU	B	938	2	18,21,22	1.11	1 (5%)	22,30,33	1.81	4 (18%)

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	2MA	B	937	2	-	0/3/25/26	0/3/3/3
2	PSU	B	955	2	-	0/7/25/26	0/2/2/2
2	H2U	B	920	2	-	2/7/38/39	0/2/2/2
2	OMG	B	918	2	-	2/5/27/28	0/3/3/3
2	5MU	B	954	2	-	0/7/25/26	0/2/2/2
2	OMU	B	932	2	-	0/9/27/28	0/2/2/2
2	1RN	B	934	2	-	2/13/31/32	0/2/2/2
2	4SU	B	908	2	-	0/7/25/26	0/2/2/2
2	PSU	B	938	2	-	0/7/25/26	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	934	1RN	C2-S2	-27.68	1.23	1.67
2	B	908	4SU	C4-S4	-22.92	1.25	1.68
2	B	934	1RN	C7-N2	-14.13	1.23	1.46
2	B	920	H2U	O2-C2	6.59	1.35	1.23
2	B	920	H2U	O4-C4	5.86	1.35	1.23
2	B	934	1RN	C3-N2	4.73	1.35	1.27
2	B	938	PSU	C6-C5	3.78	1.39	1.35
2	B	955	PSU	C6-C5	3.67	1.39	1.35
2	B	920	H2U	C6-N1	-3.67	1.40	1.47
2	B	920	H2U	C6-C5	3.64	1.61	1.52
2	B	937	2MA	CM2-C2	-3.59	1.39	1.49
2	B	920	H2U	C4-N3	-2.80	1.32	1.37
2	B	934	1RN	C3-C5	-2.68	1.40	1.45
2	B	918	OMG	C5-C6	-2.44	1.42	1.47
2	B	918	OMG	C8-N7	-2.30	1.31	1.35
2	B	920	H2U	C2-N3	2.26	1.42	1.38
2	B	955	PSU	C1'-C5	-2.10	1.45	1.50
2	B	937	2MA	C8-N7	-2.04	1.31	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	920	H2U	C4-N3-C2	-21.94	107.59	125.79
2	B	920	H2U	N3-C2-N1	-14.48	101.35	116.65
2	B	920	H2U	O2-C2-N3	-12.82	97.63	121.50
2	B	920	H2U	C5-C4-N3	-8.47	107.13	116.65
2	B	920	H2U	O4-C4-C5	-7.69	105.74	122.17
2	B	920	H2U	O2-C2-N1	-7.38	113.84	123.11
2	B	920	H2U	O4-C4-N3	-5.42	111.69	120.28
2	B	934	1RN	O2'-C2'-C3'	4.67	126.94	111.82
2	B	938	PSU	N1-C2-N3	4.51	120.24	115.13
2	B	938	PSU	C4-N3-C2	-4.47	119.90	126.34
2	B	955	PSU	C4-N3-C2	-4.33	120.10	126.34
2	B	955	PSU	N1-C2-N3	3.68	119.30	115.13
2	B	938	PSU	O2-C2-N1	-2.99	119.50	122.79
2	B	937	2MA	N1-C2-N3	2.65	127.44	123.06
2	B	938	PSU	C6-N1-C2	-2.53	120.10	122.68
2	B	955	PSU	O2-C2-N1	-2.51	120.02	122.79
2	B	918	OMG	O4'-C4'-C3'	-2.46	100.25	105.11
2	B	954	5MU	O4-C4-C5	-2.44	122.07	124.90
2	B	934	1RN	O2-C1-C7	-2.35	116.95	123.07
2	B	937	2MA	C5-C6-N1	2.20	117.81	114.02
2	B	934	1RN	O3'-C3'-C2'	2.18	118.87	111.82
2	B	932	OMU	O4'-C4'-C3'	-2.14	100.88	105.11
2	B	918	OMG	O6-C6-C5	2.11	128.49	124.37
2	B	955	PSU	C3'-C2'-C1'	-2.03	99.27	101.64
2	B	934	1RN	O1-C1-C7	2.03	117.11	111.57
2	B	937	2MA	C2'-C3'-C4'	-2.02	98.72	102.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	920	H2U	C2'-C1'-N1-C2
2	B	934	1RN	O2-C1-C7-N2
2	B	920	H2U	O4'-C1'-N1-C2
2	B	918	OMG	C3'-C2'-O2'-CM2
2	B	934	1RN	O4'-C4'-C5'-O5'
2	B	918	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	920	H2U	1	0
2	B	918	OMG	4	0
2	B	932	OMU	1	0
2	B	934	1RN	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	SO4	A	602	-	4,4,4	0.29	0	6,6,6	0.06	0
4	SO4	A	603	-	4,4,4	0.30	0	6,6,6	0.04	0
3	ATP	A	601	-	26,33,33	1.69	5 (19%)	31,52,52	1.90	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	601	-	-	3/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ATP	C2-N3	5.01	1.40	1.32
3	A	601	ATP	C2-N1	3.45	1.40	1.33
3	A	601	ATP	C5-C4	-2.69	1.33	1.40
3	A	601	ATP	C6-C5	-2.67	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ATP	O4'-C1'	2.28	1.44	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	ATP	N3-C2-N1	-6.94	117.83	128.68
3	A	601	ATP	PB-O3B-PG	-4.02	119.02	132.83
3	A	601	ATP	PA-O3A-PB	-3.63	120.37	132.83
3	A	601	ATP	C5-C6-N6	-2.19	117.03	120.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ATP	C5'-O5'-PA-O3A
3	A	601	ATP	O4'-C4'-C5'-O5'
3	A	601	ATP	PA-O3A-PB-O1B

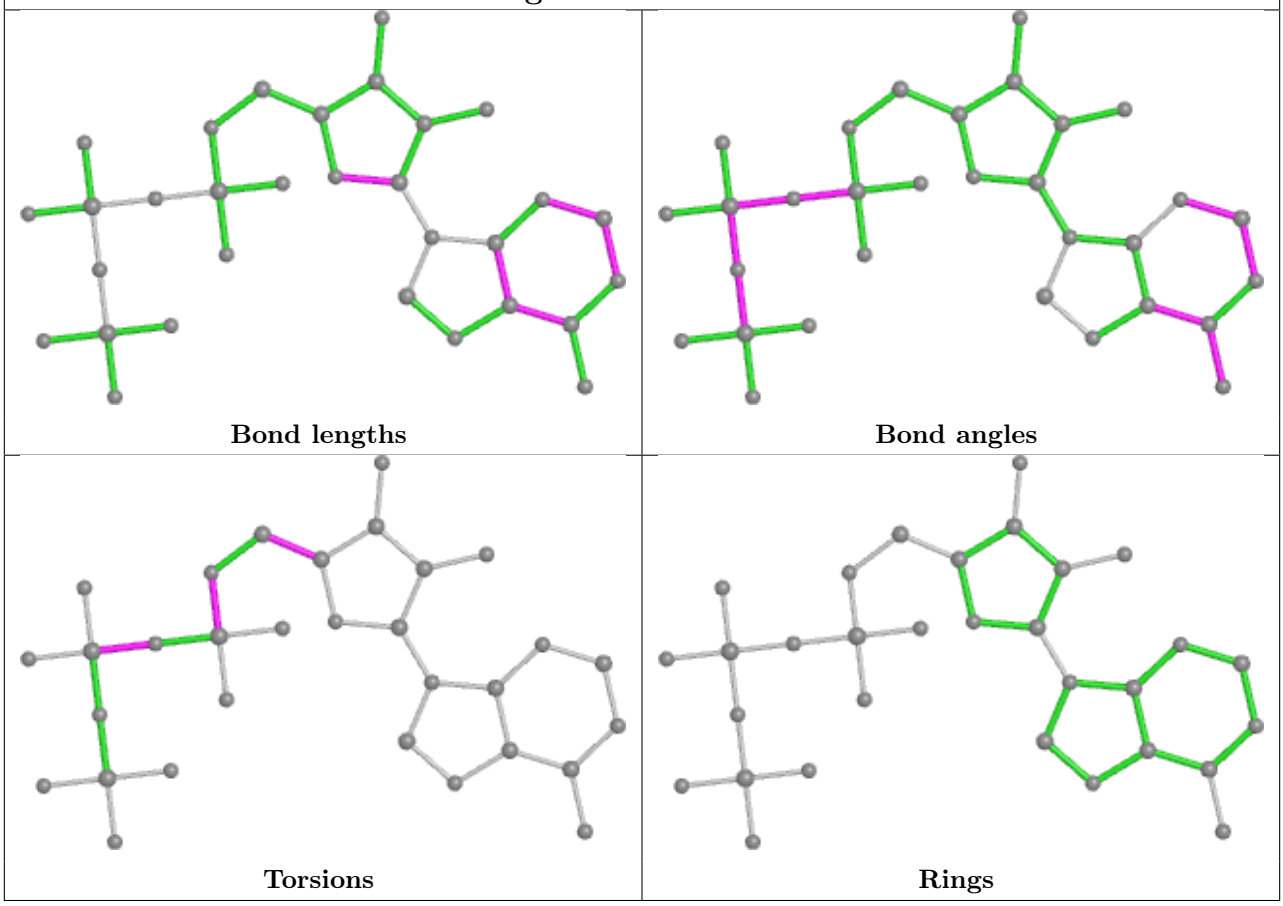
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ATP	2	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 then 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.

Ligand ATP A 601



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	542/553 (98%)	0.84	58 (10%)	6	5	27, 48, 90, 115	0
2	B	63/75 (84%)	0.68	7 (11%)	5	5	37, 71, 98, 112	0
All	All	605/628 (96%)	0.82	65 (10%)	6	5	27, 50, 92, 115	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	426	ALA	7.3
1	A	452	VAL	6.9
1	A	450	ARG	5.3
1	A	419	ALA	5.3
1	A	441	THR	5.2
1	A	404	VAL	5.1
1	A	440	ASP	4.7
1	A	405	LEU	4.3
1	A	443	SER	4.2
1	A	428	GLY	3.9
1	A	418	LYS	3.9
1	A	446	PRO	3.9
1	A	447	ALA	3.8
1	A	356	TYR	3.7
1	A	454	GLY	3.7
1	A	427	GLU	3.7
1	A	414	ALA	3.6
1	A	444	LYS	3.6
1	A	381	PHE	3.6
1	A	435	CYS	3.6
1	A	415	TYR	3.6
1	A	399	GLN	3.5
1	A	533	ALA	3.5
1	A	445	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	416	VAL	3.3
2	B	945	A	3.3
1	A	437	TYR	3.3
1	A	420	GLU	3.2
1	A	442	LEU	3.2
1	A	138	GLN	3.1
1	A	548	TRP	3.1
1	A	352	VAL	3.1
1	A	532	THR	3.0
1	A	392	PHE	3.0
2	B	919	G	2.9
1	A	403	LEU	2.9
2	B	944	C	2.8
1	A	358	GLY	2.8
1	A	380	PRO	2.8
1	A	451	LYS	2.7
1	A	433	ILE	2.7
1	A	449	GLY	2.7
1	A	422	VAL	2.7
1	A	20	ALA	2.6
2	B	957	G	2.5
1	A	354	GLU	2.5
1	A	7	PRO	2.4
1	A	397	ASN	2.4
1	A	395	GLU	2.4
1	A	531	SER	2.3
1	A	355	ASN	2.3
1	A	417	ILE	2.3
1	A	534	GLU	2.3
1	A	455	VAL	2.3
2	B	921	A	2.3
1	A	385	ILE	2.2
2	B	909	C	2.2
1	A	431	THR	2.2
1	A	424	LYS	2.2
1	A	386	TRP	2.1
1	A	407	LYS	2.1
2	B	953	G	2.1
1	A	372	PRO	2.0
1	A	459	VAL	2.0
1	A	439	ALA	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	5MU	B	954	21/22	0.81	0.25	87,97,100,104	0
2	PSU	B	955	20/21	0.81	0.28	84,98,105,105	0
2	4SU	B	908	20/21	0.82	0.24	64,78,104,123	0
2	OMG	B	918	24/25	0.85	0.26	81,90,96,97	0
2	1RN	B	934	26/27	0.85	0.27	86,97,114,115	0
2	OMU	B	932	21/22	0.87	0.22	89,93,95,97	0
2	H2U	B	920	20/21	0.92	0.28	89,91,93,93	0
2	2MA	B	937	23/24	0.95	0.16	64,70,71,72	0
2	PSU	B	938	20/21	0.95	0.17	66,71,84,85	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

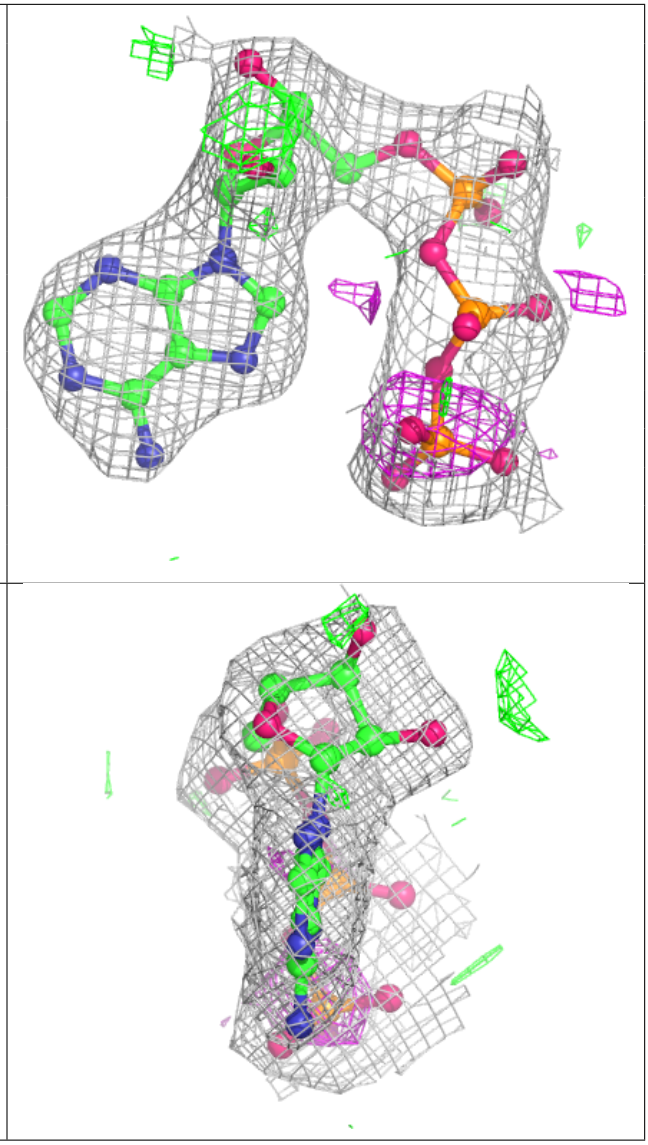
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	A	603	5/5	0.57	0.53	142,142,143,143	0
4	SO4	A	602	5/5	0.84	0.28	128,129,129,129	0
3	ATP	A	601	31/31	0.96	0.20	36,41,68,69	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 ATP A 601:

$2mF_o$-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.