Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:56 PM GMT

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)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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.
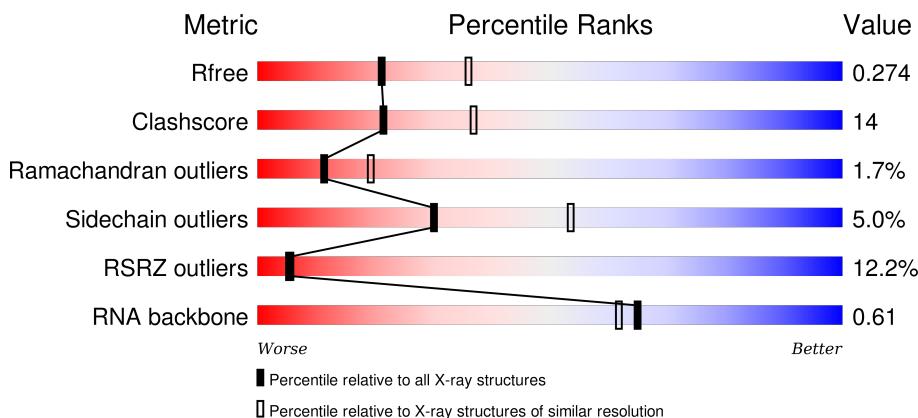
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	
2	B	75	

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
1	A	542	Total	C	N	O	S	0	0	0
			4328	2737	764	806	21			

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

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
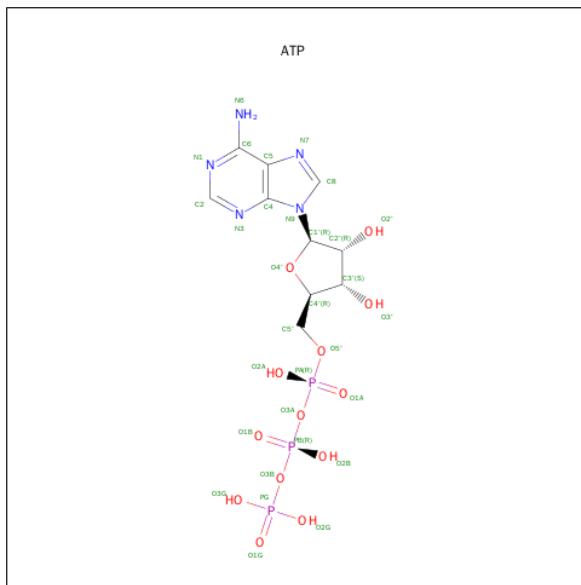
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
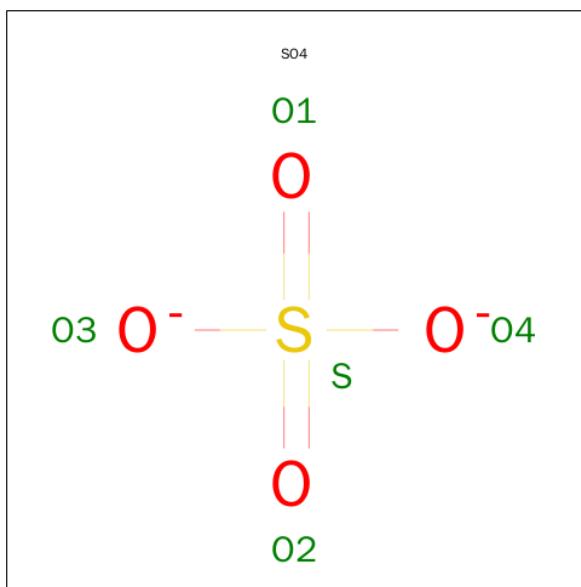
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total O S			0	0
			5	4	1		
4	A	1	Total O S			0	0
			5	4	1		

- Molecule 5 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

- Molecule 2: RNA (72-MER)
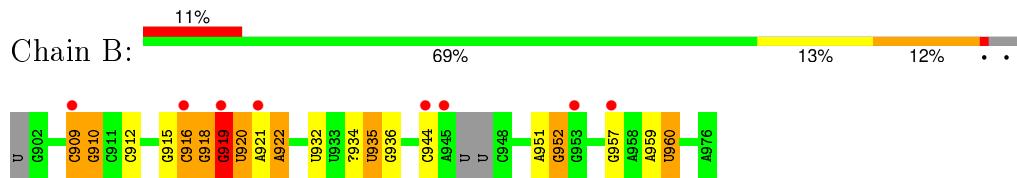
4 Data and refinement statistics (i)

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 0.241 , 0.274	Depositor DCC
R_{free} test set	4269 reflections (9.89%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 82840 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 5MU, OMG, ATP, H2U, 1RN, 2MA, SO4, OMU, 4SU, PSU

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
2:B:918:OMG:H2'	2:B:957:G:N2	2.12	0.65
1:A:351:LEU:HD23	1:A:351:LEU:O	1.96	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:HH11	1:A:260:ARG:HG2	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

Continued on next page...

Continued from previous page...

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:417:ILE:HG12	1:A:418:LYS:N	2.19	0.57
1:A:40:HIS:HA	1:A:292:THR:HA	1.86	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:415:TYR:HD1	1:A:442:LEU:H	1.54	0.55
1:A:161:ARG:HD3	5:A:751:HOH:O	2.06	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:422:VAL:HG12	1:A:423:GLU:N	2.26	0.50
1:A:379:VAL:HG12	1:A:380:PRO:HD2	1.93	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
2:B:934:1RN:O2'	2:B:934:1RN:C6	2.59	0.49
1:A:123:GLU:OE1	1:A:148:ARG:NH2	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:OD1	1:A:124:LEU:HB2	2.12	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
2:B:918:OMG:HM23	2:B:918:OMG:N3	2.28	0.48
1:A:180:SER:O	1:A:186:ARG:NH1	2.42	0.48
1:A:408:GLU:HB3	1:A:418:LYS:HG3	1.95	0.48
1:A:178:MET:O	1:A:186:ARG:HD2	2.14	0.48
1:A:381:PHE:CE2	1:A:414:ALA:HB1	2.46	0.47
1:A:377:ARG:HG2	1:A:377:ARG:HH11	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:HG23	1:A:547:THR:O	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:379:VAL:CG1	1:A:380:PRO:HD2	2.46	0.46
1:A:343:MET:HE1	1:A:458:TRP:H	1.81	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:352:VAL:HG23	1:A:352:VAL:O	2.18	0.44
1:A:347:ASP:O	1:A:388:ASP:HA	2.16	0.44
1:A:387:ILE:HG12	1:A:388:ASP:N	2.33	0.44
1:A:29:THR:O	1:A:61:CYS:HA	2.18	0.44
1:A:352:VAL:HG12	1:A:384:GLU:HG2	2.00	0.44
1:A:343:MET:HE3	1:A:458:TRP:O	2.17	0.44
1:A:43:HIS:CE1	1:A:270:LYS:HE3	2.52	0.44

Continued on next page...

Continued from previous page...

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:408:GLU:HB2	1:A:417:ILE:O	2.18	0.44
1:A:102:TYR:O	1:A:106:LEU:HD22	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:497:VAL:O	1:A:497:VAL:HG23	2.18	0.43
1:A:298:ARG:HH12	1:A:529:ARG:CZ	2.31	0.43
1:A:355:ASN:HD22	1:A:355:ASN:C	2.22	0.43
1:A:410:ARG:HE	2:B:934:1RN:C4	2.32	0.43
1:A:471:LEU:HB2	1:A:497:VAL:HG23	2.00	0.43
1:A:467:VAL:HG12	1:A:536:PRO:HG2	2.00	0.43
2:B:918:OMG:H5'	2:B:919:G:P	2.59	0.43
1:A:545:ARG:HH12	1:A:547:THR:HG21	1.83	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: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:934:1RN:H1	2:B:934:1RN:H9	2.01	0.42
2:B:915:G:H2'	2:B:959:A:H61	1.84	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
1:A:283:GLU:HB3	1:A:529:ARG:NH1	2.34	0.42
2:B:909:C:H5	2:B:912:C:N4	2.18	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
1:A:132:TYR:CG	1:A:141:LYS:HE3	2.55	0.42
2:B:932:OMU:H1'	2:B:932:OMU:HM23	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:402:ARG:HB3	1:A:403:LEU:H	1.67	0.41
1:A:30:ARG:HD2	1:A:219:ASP:OD1	2.20	0.41
1:A:381:PHE:C	1:A:381:PHE:CD1	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

Continued on next page...

Continued from previous page...

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%)	11 19

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%)	30	53

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

Some 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	4SU	B	908	2	11,21,22	6.77	2 (18%)	13,30,33	2.71	1 (7%)
2	OMG	B	918	2	17,26,27	1.11	1 (5%)	21,38,41	3.32	5 (23%)
2	H2U	B	920	2	17,21,22	2.92	6 (35%)	23,30,33	7.25	11 (47%)
2	OMU	B	932	2	12,22,23	1.18	1 (8%)	19,31,34	3.28	3 (15%)
2	1RN	B	934	2	16,27,28	6.04	7 (43%)	17,38,41	3.20	5 (29%)
2	2MA	B	937	2	16,25,26	1.24	2 (12%)	18,37,40	1.97	1 (5%)
2	PSU	B	938	2	13,21,22	1.47	2 (15%)	18,30,33	3.48	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	5MU	B	954	2	12,22,23	1.50	3 (25%)	14,32,35	4.66	2 (14%)
2	PSU	B	955	2	13,21,22	2.40	2 (15%)	18,30,33	3.81	5 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4SU	B	908	2	-	0/3/25/26	0/2/2/2
2	OMG	B	918	2	-	0/5/27/28	0/3/3/3
2	H2U	B	920	2	-	0/7/38/39	0/2/2/2
2	OMU	B	932	2	-	0/5/27/28	0/2/2/2
2	1RN	B	934	2	-	0/7/31/32	0/2/2/2
2	2MA	B	937	2	-	0/3/25/26	0/3/3/3
2	PSU	B	938	2	-	0/7/25/26	0/2/2/2
2	5MU	B	954	2	-	0/3/25/26	0/2/2/2
2	PSU	B	955	2	-	0/7/25/26	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	908	4SU	C4-S4	-21.87	1.25	1.67
2	B	934	1RN	C2-S2	-21.03	1.23	1.66
2	B	934	1RN	C7-N2	-9.11	1.23	1.47
2	B	955	PSU	C5-C1'	-7.86	1.45	1.52
2	B	920	H2U	C6-N1	-5.13	1.40	1.47
2	B	934	1RN	C5-C3	-4.60	1.40	1.47
2	B	938	PSU	C5-C1'	-3.76	1.49	1.52
2	B	934	1RN	C6-C5	-3.26	1.34	1.39
2	B	937	2MA	CM2-C2	-3.21	1.39	1.49
2	B	920	H2U	C4-N3	-2.92	1.32	1.37
2	B	954	5MU	C6-C5	-2.04	1.34	1.40
2	B	920	H2U	C2-N3	2.23	1.42	1.38
2	B	934	1RN	C6-N1	2.39	1.38	1.35
2	B	934	1RN	C3-N2	2.53	1.35	1.27
2	B	937	2MA	C6-N6	2.64	1.33	1.29
2	B	932	OMU	C4-N3	2.66	1.38	1.33
2	B	954	5MU	C6-N1	3.02	1.39	1.35
2	B	954	5MU	C4-N3	3.11	1.38	1.33
2	B	955	PSU	C4-N3	3.14	1.38	1.33
2	B	938	PSU	C4-N3	3.23	1.39	1.33

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	934	1RN	C4-N3	3.24	1.39	1.33
2	B	918	OMG	C6-N1	3.52	1.39	1.33
2	B	908	4SU	C5-C4	4.02	1.43	1.38
2	B	920	H2U	C6-C5	5.46	1.61	1.52
2	B	920	H2U	O4-C4	5.67	1.35	1.23
2	B	920	H2U	O2-C2	6.26	1.35	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	920	H2U	C4-N3-C2	-22.06	107.59	125.79
2	B	920	H2U	N3-C2-N1	-15.27	101.35	116.60
2	B	955	PSU	N1-C2-N3	-14.15	119.30	128.33
2	B	938	PSU	N1-C2-N3	-12.68	120.24	128.33
2	B	920	H2U	O2-C2-N3	-12.20	97.63	121.48
2	B	920	H2U	C5-C4-N3	-10.16	107.13	116.71
2	B	908	4SU	C5-C4-N3	-9.35	114.47	123.63
2	B	954	5MU	C5-C4-N3	-8.88	115.25	125.14
2	B	918	OMG	C5-C6-N1	-8.80	111.55	123.59
2	B	920	H2U	C6-N1-C2	-7.48	110.92	122.23
2	B	920	H2U	O4-C4-C5	-7.40	105.74	122.34
2	B	937	2MA	C2-N3-C4	-7.27	111.39	115.34
2	B	920	H2U	O2-C2-N1	-7.23	113.84	123.30
2	B	920	H2U	O4-C4-N3	-5.62	111.69	120.45
2	B	934	1RN	C5-C4-N3	-5.12	114.78	124.04
2	B	920	H2U	C1'-N1-C2	-4.91	111.48	118.27
2	B	932	OMU	C5-C4-N3	-3.35	114.53	123.12
2	B	920	H2U	C5-C6-N1	-3.25	107.17	110.70
2	B	934	1RN	C5-C3-N2	-2.99	115.36	122.91
2	B	938	PSU	C5-C6-N1	-2.44	120.95	124.39
2	B	918	OMG	O4'-C4'-C3'	-2.43	100.25	105.15
2	B	918	OMG	N3-C2-N1	-2.32	123.92	127.44
2	B	955	PSU	C3'-C2'-C1'	-2.17	99.27	101.79
2	B	932	OMU	O4'-C4'-C3'	-2.12	100.88	105.15
2	B	920	H2U	C6-C5-C4	-2.08	105.21	116.24
2	B	955	PSU	C5-C6-N1	-2.05	121.50	124.39
2	B	934	1RN	O3'-C3'-C2'	2.16	118.87	111.83
2	B	938	PSU	C6-N1-C2	2.88	120.10	115.47
2	B	955	PSU	C6-N1-C2	3.27	120.73	115.47
2	B	934	1RN	O2'-C2'-C3'	4.65	126.94	111.83
2	B	938	PSU	C4-N3-C2	5.38	119.90	115.25
2	B	955	PSU	C4-N3-C2	5.61	120.10	115.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	918	OMG	C6-N1-C2	6.62	125.13	115.94
2	B	918	OMG	O4'-C1'-N9	8.90	126.72	108.10
2	B	934	1RN	C2-N3-C4	10.22	127.16	115.95
2	B	932	OMU	C4-N3-C2	13.12	127.14	114.14
2	B	954	5MU	C4-N3-C2	14.64	127.90	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	#$|Z| > 2$
3	ATP	A	601	-	24,33,33	1.64	4 (16%)	31,52,52	3.06	7 (22%)
4	SO4	A	602	-	4,4,4	0.25	0	6,6,6	0.06	0
4	SO4	A	603	-	4,4,4	0.27	0	6,6,6	0.07	0

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	-	-	0/18/38/38	0/3/3/3
4	SO4	A	602	-	-	0/0/0/0	0/0/0/0
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ATP	C5-C4	-2.96	1.33	1.40
3	A	601	ATP	O4'-C1'	2.42	1.44	1.41
3	A	601	ATP	C2-N1	3.38	1.40	1.33
3	A	601	ATP	C2-N3	4.51	1.40	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ATP	N3-C2-N1	-14.45	117.83	128.89
3	A	601	ATP	PA-O3A-PB	-4.40	120.37	132.73
3	A	601	ATP	PB-O3B-PG	-4.07	119.02	132.67
3	A	601	ATP	C4'-O4'-C1'	-3.08	106.34	109.72
3	A	601	ATP	C4-C5-N7	-2.15	107.50	109.48
3	A	601	ATP	C1'-N9-C4	-2.02	123.90	126.94
3	A	601	ATP	O4'-C1'-N9	2.71	113.77	108.10

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers ⓘ

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%)	0.92	66 (12%)	5	5	27, 48, 90, 115	0
2	B	63/75 (84%)	0.85	8 (12%)	5	5	37, 71, 98, 112	0
All	All	605/628 (96%)	0.91	74 (12%)	5	5	27, 50, 92, 115	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	426	ALA	7.6
1	A	452	VAL	7.2
1	A	419	ALA	5.5
1	A	441	THR	5.5
1	A	450	ARG	5.5
1	A	404	VAL	5.4
1	A	440	ASP	4.9
1	A	405	LEU	4.4
1	A	443	SER	4.3
1	A	446	PRO	4.2
1	A	428	GLY	4.1
1	A	447	ALA	4.1
1	A	418	LYS	4.0
1	A	356	TYR	3.9
1	A	454	GLY	3.9
1	A	427	GLU	3.8
1	A	435	CYS	3.8
1	A	414	ALA	3.8
1	A	381	PHE	3.8
1	A	444	LYS	3.7
1	A	445	ASP	3.7
1	A	399	GLN	3.6
1	A	415	TYR	3.6
1	A	533	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	416	VAL	3.5
2	B	945	A	3.4
1	A	437	TYR	3.4
1	A	420	GLU	3.4
1	A	442	LEU	3.3
1	A	138	GLN	3.3
1	A	548	TRP	3.2
1	A	352	VAL	3.2
1	A	532	THR	3.1
1	A	392	PHE	3.1
2	B	919	G	3.0
1	A	358	GLY	3.0
2	B	944	C	3.0
1	A	403	LEU	3.0
1	A	380	PRO	3.0
1	A	422	VAL	2.8
1	A	449	GLY	2.8
1	A	433	ILE	2.8
1	A	451	LYS	2.8
1	A	20	ALA	2.7
2	B	957	G	2.7
1	A	354	GLU	2.6
1	A	7	PRO	2.5
1	A	417	ILE	2.5
1	A	355	ASN	2.5
1	A	455	VAL	2.5
1	A	397	ASN	2.5
1	A	395	GLU	2.4
1	A	534	GLU	2.4
2	B	921	A	2.4
1	A	531	SER	2.4
2	B	909	C	2.4
1	A	385	ILE	2.4
1	A	431	THR	2.4
1	A	424	LYS	2.3
2	B	953	G	2.2
1	A	386	TRP	2.2
1	A	407	LYS	2.2
1	A	459	VAL	2.2
1	A	464	ALA	2.2
1	A	372	PRO	2.2
1	A	546	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	438	ASP	2.1
1	A	439	ALA	2.1
2	B	916	C	2.1
1	A	547	THR	2.1
1	A	409	VAL	2.1
1	A	137	THR	2.1
1	A	483	ALA	2.0
1	A	410	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	2MA	B	937	23/24	0.95	0.16	-	64,70,71,72	0
2	OMU	B	932	21/22	0.87	0.22	-	89,93,95,97	0
2	PSU	B	955	20/21	0.81	0.28	-	84,98,105,105	0
2	PSU	B	938	20/21	0.95	0.17	-	66,71,84,85	0
2	1RN	B	934	26/27	0.86	0.27	-	86,97,114,115	0
2	H2U	B	920	20/21	0.92	0.28	-	89,91,93,93	0
2	5MU	B	954	21/22	0.81	0.25	-	87,97,100,104	0
2	OMG	B	918	24/25	0.85	0.26	-	81,90,96,97	0
2	4SU	B	908	20/21	0.82	0.24	-	64,78,104,123	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
4	SO4	A	603	5/5	0.58	0.53	10.59	142,142,143,143	0
4	SO4	A	602	5/5	0.84	0.28	1.63	128,129,129,129	0
3	ATP	A	601	31/31	0.96	0.20	-0.49	36,41,68,69	0

6.5 Other polymers (i)

There are no such residues in this entry.