



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:59 PM GMT

PDB ID : 4JYZ
Title : Crystal structure of E. coli glutamyl-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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

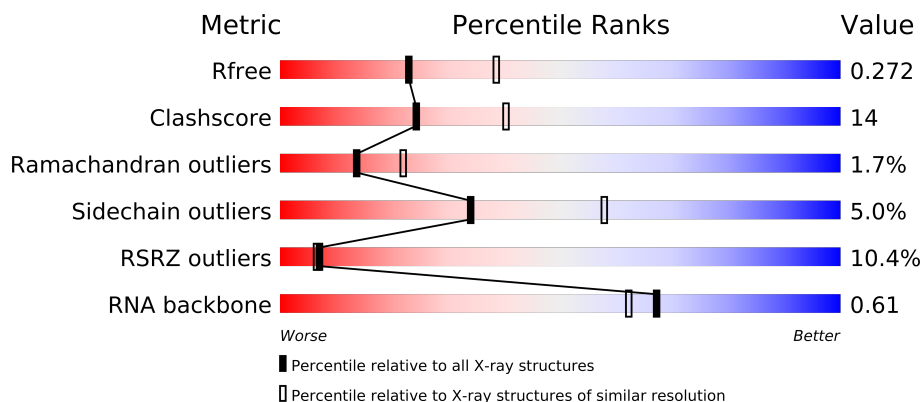
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)
RNA backbone	1838	1107 (3.10-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	553	
2	B	75	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	A	602	-	X
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 hydrogen and 0 are deuterium.

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.

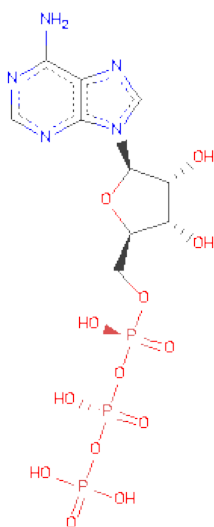
- Molecule 1 is a protein called Glutamine-tRNA ligase.

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: O₄S).



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		

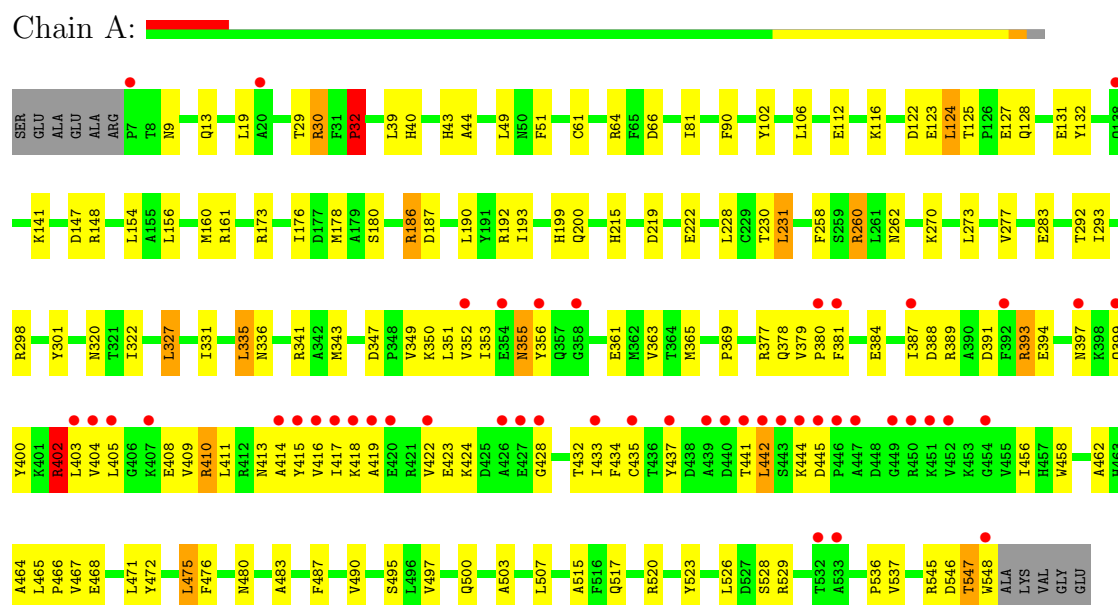
- Molecule 5 is water.

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

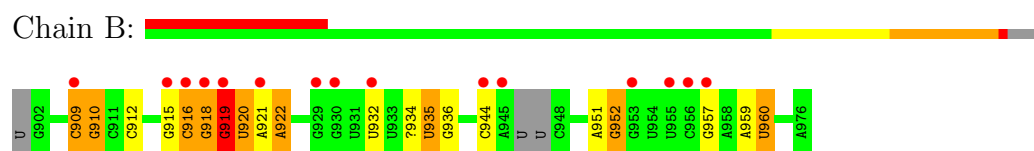
3 Residue-property plots

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

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
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.263 0.237 , 0.272	Depositor DCC
R_{free} test set	4269 reflections (10.97%)	DCC
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (151) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:122:ASP:OD1	1:A:124:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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	540/553 (98%)	497 (92%)	34 (6%)	9 (2%)	14 22

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 ⓘ

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%)	34 58

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

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Mol	Chain	Res	Type
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 ⓘ

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

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Mol	Chain	Res	Type
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 ⓘ

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	19,21,22	5.14	2 (10%)	23,30,33	25.94	1 (4%)
2	OMG	B	918	2	24,26,27	0.87	1 (4%)	32,38,41	6.02	6 (18%)
2	H2U	B	920	2	19,21,22	2.70	6 (31%)	27,30,33	6.94	12 (44%)
2	OMU	B	932	2	20,22,23	0.76	0	24,31,34	1.15	2 (8%)
2	1RN	B	934	2	25,27,28	4.80	7 (28%)	28,38,41	2.27	7 (25%)
2	2MA	B	937	2	23,25,26	1.88	3 (13%)	32,37,40	1.98	3 (9%)
2	PSU	B	938	2	19,21,22	1.12	1 (5%)	23,30,33	1.12	2 (8%)
2	5MU	B	954	2	20,22,23	0.97	3 (15%)	25,32,35	2.06	2 (8%)
2	PSU	B	955	2	19,21,22	1.24	2 (10%)	23,30,33	1.09	2 (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
2	4SU	B	908	2	-	0/6/25/26	0/2/2/2
2	OMG	B	918	2	-	1/10/27/28	0/1/3/3
2	H2U	B	920	2	-	0/8/38/39	0/2/2/2
2	OMU	B	932	2	-	0/8/27/28	0/2/2/2
2	1RN	B	934	2	-	0/12/31/32	0/2/2/2
2	2MA	B	937	2	-	0/8/25/26	0/1/3/3
2	PSU	B	938	2	-	0/8/25/26	0/2/2/2
2	5MU	B	954	2	-	0/6/25/26	0/2/2/2
2	PSU	B	955	2	-	0/8/25/26	0/2/2/2

All (25) 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	-18.90	1.23	1.70
2	B	934	1RN	C7-N2	-11.12	1.23	1.46
2	B	937	2MA	CM2-C2	-7.77	1.39	1.49
2	B	934	1RN	C7-C1	-6.29	1.31	1.51
2	B	920	H2U	O2-C2	6.03	1.35	1.23
2	B	920	H2U	C6-C5	5.50	1.61	1.52
2	B	920	H2U	O4-C4	5.41	1.35	1.23
2	B	934	1RN	C5-C3	-5.37	1.40	1.47
2	B	920	H2U	C6-N1	-4.70	1.40	1.47
2	B	955	PSU	C6-N1	3.74	1.35	1.32
2	B	938	PSU	C6-N1	3.63	1.35	1.32
2	B	908	4SU	C5-C4	3.20	1.43	1.38
2	B	920	H2U	C4-N3	-2.96	1.32	1.37
2	B	955	PSU	P-OP1	2.71	1.49	1.46
2	B	934	1RN	C3-N2	2.50	1.35	1.27
2	B	937	2MA	C2-N3	2.42	1.35	1.31
2	B	937	2MA	P-OP1	2.28	1.49	1.46
2	B	954	5MU	P-OP1	2.18	1.49	1.46
2	B	920	H2U	C2-N3	2.15	1.42	1.38
2	B	954	5MU	C6-N1	2.15	1.39	1.34
2	B	918	OMG	P-OP1	2.14	1.49	1.46
2	B	934	1RN	P-OP2	2.12	1.49	1.46
2	B	934	1RN	C6-C5	-2.08	1.34	1.39
2	B	954	5MU	C6-C5	-2.03	1.34	1.40

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	908	4SU	C4-N3-C2	124.35	126.92	121.60
2	B	918	OMG	C6-C5-N7	-26.82	130.53	134.14
2	B	920	H2U	C4-N3-C2	-21.09	107.59	125.83
2	B	918	OMG	O4'-C1'-N9	19.65	126.72	108.44
2	B	920	H2U	N3-C2-N1	-15.66	101.35	116.71
2	B	920	H2U	C6-N1-C1'	-12.72	94.02	119.30
2	B	920	H2U	O2-C2-N3	-11.88	97.63	121.42
2	B	920	H2U	C5-C4-N3	-10.24	107.13	116.76
2	B	954	5MU	C6-N1-C2	-8.68	119.94	122.41
2	B	934	1RN	C5-C4-N3	-7.68	114.78	119.13
2	B	920	H2U	O2-C2-N1	-7.12	113.84	123.25
2	B	920	H2U	O4-C4-C5	-6.91	105.74	122.25
2	B	937	2MA	C2-N3-C4	-6.80	111.39	117.69
2	B	937	2MA	N1-C2-N3	5.92	127.44	122.57
2	B	920	H2U	C6-N1-C2	-5.59	110.92	121.51
2	B	920	H2U	O4-C4-N3	-5.51	111.69	120.44
2	B	920	H2U	C1'-N1-C2	-4.76	111.48	118.16
2	B	934	1RN	O2'-C2'-C3'	4.64	126.94	111.83
2	B	934	1RN	C1-C7-N2	4.25	117.73	111.61
2	B	937	2MA	CM2-C2-N3	-4.09	116.29	119.96
2	B	954	5MU	C5-C6-N1	3.24	124.73	121.59
2	B	918	OMG	C6-N1-C2	3.21	125.13	119.51
2	B	920	H2U	C5-C6-N1	-3.15	107.17	110.71
2	B	934	1RN	C6-C5-C4	2.99	119.55	114.29
2	B	934	1RN	C5-C3-N2	-2.82	115.36	122.94
2	B	938	PSU	C4-N3-C2	-2.69	119.90	125.36
2	B	955	PSU	C4-N3-C2	-2.60	120.10	125.36
2	B	934	1RN	O2'-C2'-C1'	-2.51	103.64	111.23
2	B	918	OMG	O4'-C4'-C3'	-2.43	100.25	105.17
2	B	918	OMG	C2-N3-C4	-2.22	111.98	115.09
2	B	918	OMG	O4'-C1'-C2'	-2.21	104.89	106.95
2	B	955	PSU	C3'-C2'-C1'	-2.20	99.27	101.85
2	B	938	PSU	O4'-C1'-C5	-2.17	106.84	109.55
2	B	920	H2U	C6-C5-C4	-2.17	105.21	116.61
2	B	934	1RN	O3'-C3'-C2'	2.16	118.87	111.83
2	B	932	OMU	O4'-C1'-C2'	-2.16	104.93	106.95
2	B	932	OMU	O4'-C4'-C3'	-2.12	100.88	105.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	918	OMG	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	33,33,33	1.54	5 (15%)	52,52,52	2.47	11 (21%)
4	SO4	A	602	-	4,4,4	0.30	0	6,6,6	0.06	0
4	SO4	A	603	-	4,4,4	0.32	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	-	-	0/22/38/38	0/1/3/3
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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	ATP	C2-N3	4.05	1.40	1.32
3	A	601	ATP	C2-N1	3.26	1.40	1.33
3	A	601	ATP	C4-N9	-3.18	1.33	1.37
3	A	601	ATP	C5-C4	-2.96	1.33	1.40
3	A	601	ATP	C8-N9	-2.16	1.33	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ATP	N3-C2-N1	-13.01	117.83	128.71
3	A	601	ATP	O4'-C1'-N9	5.73	113.77	108.44
3	A	601	ATP	PB-O3B-PG	-4.32	119.02	131.68
3	A	601	ATP	PA-O3A-PB	-3.86	120.37	131.68
3	A	601	ATP	C4'-O4'-C1'	-3.14	106.34	109.75
3	A	601	ATP	N3-C4-N9	3.09	131.01	125.43
3	A	601	ATP	N7-C8-N9	-2.45	107.43	114.36
3	A	601	ATP	C4-C5-N7	-2.36	107.50	109.52
3	A	601	ATP	C5-C4-N3	-2.15	121.01	125.70
3	A	601	ATP	C8-N9-C4	2.14	108.53	106.90
3	A	601	ATP	C2-N3-C4	2.02	119.76	114.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	542/553 (98%)	0.74	48 (8%)	10 9	27, 48, 90, 115	0
2	B	71/75 (94%)	1.17	15 (21%)	1 1	37, 74, 98, 112	0
All	All	613/628 (97%)	0.79	63 (10%)	7 6	27, 50, 93, 115	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	452	VAL	7.7
1	A	426	ALA	6.4
2	B	918	OMG	5.5
2	B	932	OMU	4.9
1	A	404	VAL	4.6
1	A	450	ARG	4.5
1	A	441	THR	4.5
1	A	419	ALA	4.3
1	A	443	SER	4.2
1	A	405	LEU	4.2
2	B	945	A	4.1
1	A	381	PHE	4.0
1	A	446	PRO	3.9
1	A	444	LYS	3.8
2	B	944	C	3.8
1	A	440	ASP	3.7
1	A	447	ALA	3.6
1	A	445	ASP	3.6
2	B	919	G	3.6
1	A	427	GLU	3.6
1	A	435	CYS	3.5
1	A	418	LYS	3.4
1	A	454	GLY	3.3
1	A	451	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	415	TYR	3.2
1	A	356	TYR	3.2
1	A	414	ALA	3.2
1	A	437	TYR	3.1
1	A	442	LEU	3.0
1	A	380	PRO	3.0
1	A	532	THR	2.9
1	A	428	GLY	2.8
1	A	433	ILE	2.8
1	A	403	LEU	2.7
2	B	957	G	2.7
2	B	916	C	2.6
1	A	392	PHE	2.6
1	A	387	ILE	2.6
1	A	399	GLN	2.6
2	B	921	A	2.5
1	A	138	GLN	2.5
2	B	929	G	2.5
1	A	407	LYS	2.4
2	B	955	PSU	2.4
1	A	533	ALA	2.4
1	A	358	GLY	2.4
2	B	909	C	2.4
1	A	354	GLU	2.4
1	A	422	VAL	2.4
1	A	548	TRP	2.4
1	A	449	GLY	2.3
2	B	915	G	2.3
2	B	930	G	2.3
1	A	416	VAL	2.3
1	A	7	PRO	2.2
1	A	397	ASN	2.2
2	B	953	G	2.2
1	A	420	GLU	2.2
1	A	417	ILE	2.1
1	A	20	ALA	2.1
1	A	352	VAL	2.1
2	B	956	C	2.1
1	A	439	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PSU	B	955	20/21	0.28	1.73	84,98,105,105	0
2	OMU	B	932	21/22	0.21	1.72	89,93,95,97	0
2	5MU	B	954	21/22	0.23	1.21	87,97,100,104	0
2	OMG	B	918	24/25	0.26	0.34	81,90,96,97	0
2	4SU	B	908	20/21	0.23	0.14	64,78,104,123	0
2	1RN	B	934	26/27	0.26	-0.55	86,97,114,115	0
2	2MA	B	937	23/24	0.16	-1.11	64,70,71,72	0
2	PSU	B	938	20/21	0.16	-1.25	66,71,84,85	0
2	H2U	B	920	20/21	0.26	-1.74	89,91,93,93	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	A	603	5/5	0.54	13.21	142,142,143,143	0
4	SO4	A	602	5/5	0.27	2.12	128,129,129,129	0
3	ATP	A	601	31/31	0.19	-0.45	36,41,68,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.