



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:49 AM GMT

PDB ID : 1QRS  
Title : GLUTAMINYL-TRNA SYNTHETASE MUTANT D235N COMPLEXED  
WITH GLUTAMINE TRANSFER RNA  
Authors : Arnez, J.G.; Steitz, T.A.  
Deposited on : 1996-06-14  
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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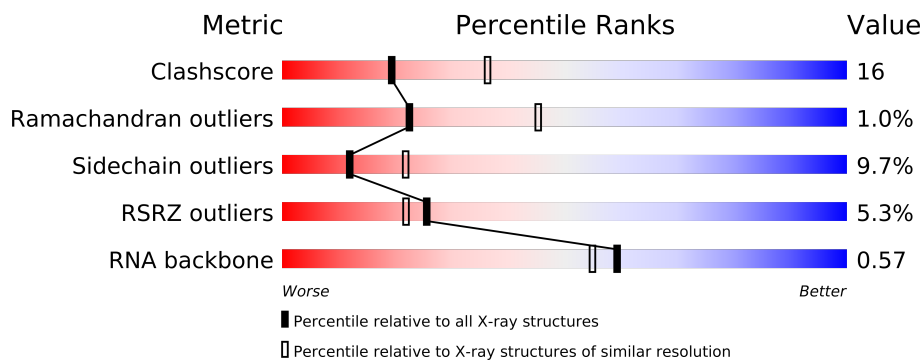
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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))
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)
RNA backbone	1838	1002 (3.12-2.08)

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  $\geq 3$ , 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	B	75	
2	A	553	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7205 atoms, of which 1209 are hydrogens 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 RNA chain called TRNAGLN2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
1	B	74	1802	702	229	279	518	74	0	0	0

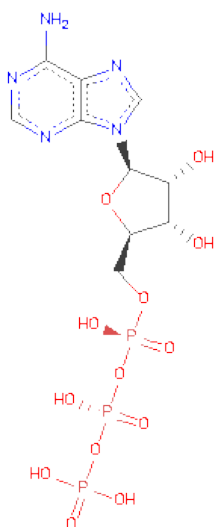
- Molecule 2 is a protein called PROTEIN (GLUTAMINYL-TRNA SYNTHETASE (E.C.6.1.1.18)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	A	529	5256	2704	977	753	801	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	ASN	ASP	ENGINEERED	UNP P00962

- 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	H	N	O	P	0	0
			34	10	3	5	13	3		

- Molecule 4 is water.

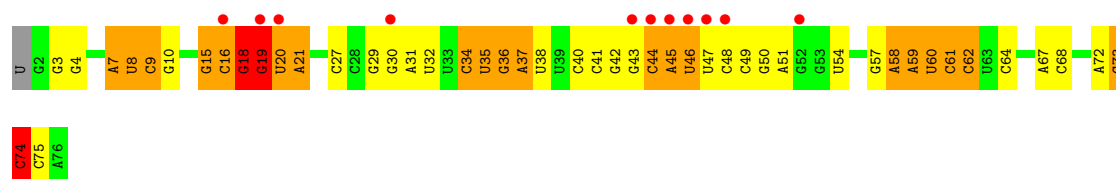
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total	O	0	0
			90	90		
4	B	23	Total	O	0	0
			23	23		

### 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.

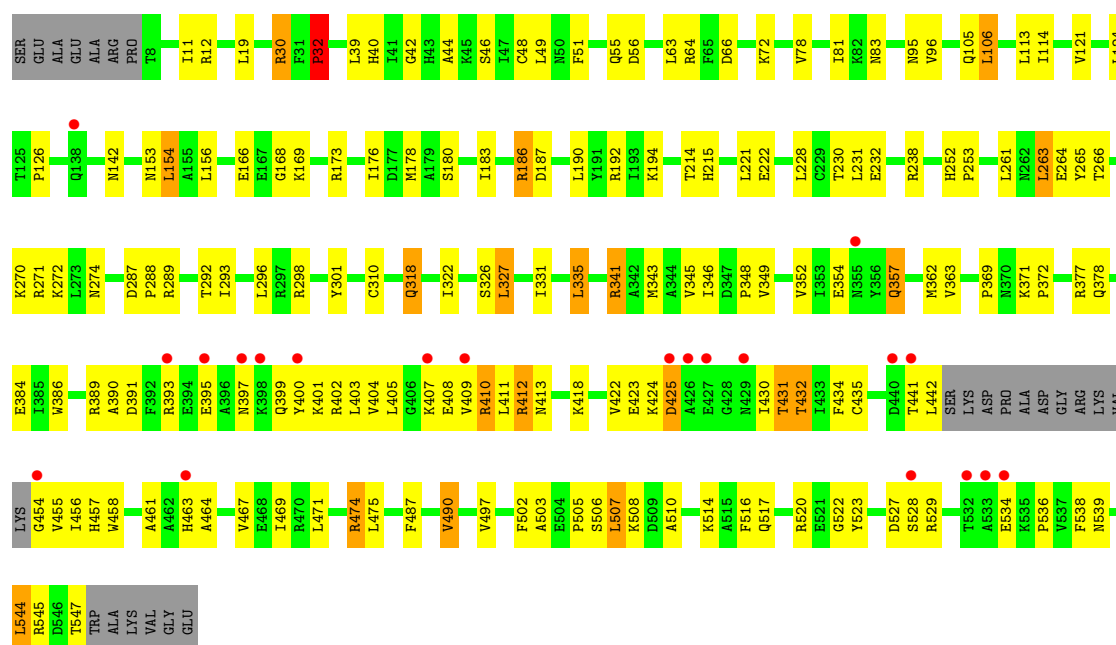
#### • Molecule 1: TRNAGLN2

Chain B: 



#### • Molecule 2: PROTEIN (GLUTAMINYL-TRNA SYNTHETASE (E.C.6.1.1.18))

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	243.70Å 93.70Å 115.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60 8.08 – 2.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.60) 89.9 (8.08-2.59)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.59Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.207 , (Not available) 0.199 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 36332 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: 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	B	0.53	0/1756	0.86	3/2734 (0.1%)
2	A	0.47	0/4379	0.69	0/5928
All	All	0.49	0/6135	0.75	3/8662 (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
1	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	19	G	N9-C1'-C2'	8.03	124.43	114.00
1	B	18	G	N9-C1'-C2'	5.27	120.85	114.00
1	B	74	C	N1-C1'-C2'	5.21	120.78	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	19	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	B	1573	229	571	77	0
2	A	4279	977	3199	114	0
3	A	31	3	9	2	0
4	A	90	0	0	4	0
4	B	23	0	0	2	0
All	All	5996	1209	3779	176	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 16.

All (176) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:46:U:H4'	1:B:47:U:C5	1.90	1.05
1:B:46:U:H4'	1:B:47:U:C6	1.92	1.03
1:B:58:A:H4'	1:B:59:A:OP1	1.56	1.03
1:B:21:A:H61	1:B:47:U:H1'	1.26	0.97
1:B:40:C:O2'	1:B:41:C:H5'	1.71	0.91
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.50	0.90
1:B:7:A:H5'	2:A:318:GLN:HE21	1.37	0.90
1:B:34:C:H4'	1:B:35:U:OP1	1.74	0.87
1:B:36:G:H4'	1:B:37:A:OP2	1.72	0.87
2:A:522:GLY:HA2	2:A:544:LEU:HD13	1.58	0.85
2:A:30:ARG:NH1	2:A:215:HIS:HE1	1.77	0.82
2:A:352:VAL:HG12	2:A:384:GLU:HG2	1.62	0.82
1:B:47:U:H2'	1:B:47:U:O2	1.79	0.81
1:B:46:U:C4'	1:B:47:U:C5	2.65	0.79
2:A:363:VAL:HG11	2:A:413:ASN:O	1.83	0.78
2:A:467:VAL:HG23	2:A:536:PRO:HB2	1.65	0.78
1:B:44:C:H5''	1:B:44:C:H6	1.49	0.77
2:A:407:LYS:HG2	2:A:408:GLU:H	1.49	0.77
1:B:16:C:OP2	1:B:16:C:H3'	1.85	0.75
1:B:7:A:H5'	2:A:318:GLN:NE2	2.03	0.73
2:A:30:ARG:NH1	2:A:215:HIS:CE1	2.57	0.72
1:B:18:G:O2'	1:B:57:G:N2	2.21	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:30:ARG:HH11	2:A:215:HIS:CE1	2.08	0.71
2:A:534:GLU:O	2:A:536:PRO:HD3	1.90	0.71
2:A:30:ARG:HH11	2:A:215:HIS:HE1	1.38	0.71
1:B:61:C:O2'	1:B:62:C:H5'	1.91	0.71
1:B:58:A:C4'	1:B:59:A:OP1	2.39	0.68
1:B:60:U:OP2	1:B:60:U:H6	1.78	0.67
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.77	0.67
2:A:362:MET:CG	2:A:378:GLN:HG3	2.24	0.67
2:A:349:VAL:HB	2:A:389:ARG:HD3	1.79	0.65
1:B:34:C:C4'	1:B:35:U:OP1	2.46	0.64
2:A:341:ARG:HD3	2:A:369:PRO:HD2	1.79	0.64
1:B:21:A:N6	1:B:47:U:H1'	2.06	0.62
2:A:441:THR:O	2:A:442:LEU:HB3	1.99	0.62
1:B:44:C:C5'	1:B:44:C:H6	2.11	0.62
2:A:393:ARG:O	2:A:404:VAL:HA	2.00	0.61
1:B:40:C:H2'	1:B:41:C:C6	2.36	0.61
2:A:397:ASN:HD21	2:A:399:GLN:CG	2.13	0.61
2:A:142:ASN:HD22	2:A:178:MET:HG3	1.65	0.61
2:A:40:HIS:HA	2:A:292:THR:HA	1.83	0.60
2:A:346:ILE:HG12	2:A:469:ILE:HD13	1.82	0.60
1:B:19:G:HO2'	1:B:20:U:H5	1.50	0.60
1:B:44:C:OP1	1:B:44:C:H4'	2.01	0.60
1:B:40:C:H2'	1:B:41:C:H6	1.67	0.59
2:A:46:SER:OG	3:A:999:ATP:H1'	2.02	0.59
2:A:48:CYS:HG	2:A:310:CYS:HG	1.45	0.59
2:A:362:MET:HG3	2:A:378:GLN:HG3	1.84	0.59
1:B:35:U:H1'	2:A:520:ARG:HG2	1.85	0.58
2:A:51:PHE:O	2:A:55:GLN:HG2	2.03	0.58
1:B:36:G:C4'	1:B:37:A:OP2	2.48	0.58
2:A:264:GLU:HG2	2:A:265:TYR:CD2	2.38	0.58
1:B:9:C:H6	4:B:801:HOH:O	1.87	0.58
1:B:34:C:O2'	2:A:412:ARG:NH2	2.38	0.57
1:B:15:G:HO2'	1:B:16:C:P	2.28	0.56
1:B:50:G:H2'	1:B:51:A:C8	2.40	0.56
2:A:487:PHE:O	2:A:490:VAL:HG12	2.05	0.56
2:A:474:ARG:HD3	4:A:704:HOH:O	2.05	0.56
1:B:42:G:O2'	1:B:43:G:H5'	2.05	0.56
2:A:362:MET:HG2	2:A:378:GLN:HG3	1.87	0.56
1:B:50:G:H2'	1:B:51:A:H8	1.71	0.56
1:B:19:G:O2'	1:B:20:U:H5	1.88	0.56
2:A:263:LEU:HB3	2:A:266:THR:CG2	2.36	0.56
2:A:166:GLU:O	2:A:169:LYS:HB2	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:173:ARG:HD2	2:A:187:ASP:O	2.06	0.55
1:B:37:A:C2	1:B:38:U:H1'	2.42	0.54
2:A:296:LEU:O	2:A:301:TYR:HB2	2.07	0.54
1:B:45:A:HO2'	1:B:47:U:H6	1.55	0.54
2:A:418:LYS:O	2:A:435:CYS:HB3	2.07	0.54
1:B:16:C:H4'	1:B:18:G:OP2	2.08	0.53
2:A:331:ILE:HG13	2:A:335:LEU:HD22	1.90	0.53
1:B:19:G:C4	1:B:57:G:N2	2.76	0.53
2:A:335:LEU:HB3	2:A:523:TYR:CD1	2.43	0.53
2:A:343:MET:HE1	2:A:457:HIS:HA	1.90	0.53
2:A:106:LEU:HD21	2:A:214:THR:HG23	1.91	0.53
1:B:44:C:OP1	1:B:44:C:C4'	2.56	0.52
1:B:15:G:O2'	1:B:16:C:P	2.66	0.52
1:B:35:U:O2'	2:A:520:ARG:HG2	2.09	0.52
1:B:36:G:O6	2:A:402:ARG:NH2	2.42	0.52
2:A:408:GLU:HG2	2:A:418:LYS:HB2	1.90	0.52
2:A:44:ALA:HB2	2:A:293:ILE:HD11	1.91	0.52
2:A:527:ASP:HB2	2:A:539:ASN:ND2	2.25	0.52
1:B:36:G:C6	2:A:401:LYS:HG2	2.46	0.51
2:A:464:ALA:HB1	2:A:502:PHE:HB3	1.92	0.51
1:B:36:G:N3	2:A:401:LYS:HD3	2.25	0.51
2:A:407:LYS:CG	2:A:408:GLU:H	2.18	0.51
1:B:74:C:N3	2:A:168:GLY:HA2	2.25	0.51
2:A:288:PRO:HG3	2:A:298:ARG:HG2	1.93	0.51
2:A:39:LEU:CD1	2:A:81:ILE:HG12	2.34	0.51
2:A:401:LYS:O	2:A:454:GLY:HA2	2.12	0.50
2:A:30:ARG:NH1	2:A:32:PRO:HG3	2.26	0.50
2:A:517:GLN:HG3	2:A:523:TYR:CE1	2.46	0.50
1:B:36:G:C4	2:A:401:LYS:HD3	2.46	0.50
1:B:37:A:H2'	1:B:38:U:O4'	2.11	0.50
2:A:42:GLY:HA2	2:A:261:LEU:HD23	1.93	0.50
1:B:43:G:H2'	1:B:44:C:O4'	2.11	0.49
1:B:18:G:HO2'	1:B:57:G:H22	1.53	0.49
1:B:41:C:H2'	1:B:42:G:C8	2.46	0.49
2:A:425:ASP:HB3	2:A:431:THR:HG23	1.93	0.49
1:B:72:A:H5'	2:A:183:ILE:HG21	1.94	0.49
2:A:377:ARG:HG2	2:A:377:ARG:HH11	1.78	0.49
2:A:32:PRO:HA	2:A:64:ARG:O	2.13	0.48
2:A:12:ARG:HH22	2:A:56:ASP:CG	2.17	0.48
1:B:9:C:C4	1:B:45:A:C6	3.02	0.48
2:A:301:TYR:HE2	2:A:327:LEU:HD22	1.78	0.48
2:A:393:ARG:HB2	2:A:400:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:503:ALA:HB1	2:A:507:LEU:HD23	1.95	0.48
2:A:463:HIS:O	2:A:505:PRO:HD3	2.14	0.47
2:A:121:VAL:H	2:A:153:ASN:ND2	2.12	0.47
1:B:31:A:C2	1:B:32:U:C2	3.02	0.47
1:B:3:G:O2'	1:B:4:G:H5'	2.14	0.47
1:B:73:G:H2'	4:B:749:HOH:O	2.15	0.47
1:B:15:G:O2'	1:B:16:C:OP1	2.31	0.47
2:A:397:ASN:ND2	2:A:399:GLN:HG2	2.30	0.47
2:A:64:ARG:HD3	2:A:222:GLU:OE2	2.14	0.47
2:A:346:ILE:HG12	2:A:469:ILE:CD1	2.45	0.47
2:A:105:GLN:HG2	2:A:221:LEU:HD11	1.97	0.46
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.97	0.46
2:A:354:GLU:HG2	4:A:723:HOH:O	2.15	0.46
1:B:47:U:C2'	1:B:47:U:O2	2.50	0.46
1:B:58:A:H4'	1:B:60:U:H5	1.81	0.46
2:A:12:ARG:HD2	4:A:776:HOH:O	2.15	0.46
2:A:114:ILE:HG21	2:A:154:LEU:HD13	1.96	0.46
2:A:345:VAL:HA	4:A:717:HOH:O	2.16	0.45
2:A:386:TRP:CD1	2:A:461:ALA:HA	2.51	0.45
1:B:46:U:H4'	1:B:47:U:H5	1.66	0.45
1:B:46:U:C4'	1:B:47:U:C6	2.83	0.45
1:B:37:A:C6	1:B:38:U:C2	3.03	0.45
2:A:322:ILE:N	2:A:322:ILE:HD12	2.32	0.45
2:A:510:ALA:HB1	2:A:516:PHE:HE2	1.81	0.45
2:A:252:HIS:HD2	2:A:253:PRO:O	2.00	0.45
2:A:180:SER:O	2:A:186:ARG:NH1	2.50	0.45
2:A:423:GLU:HB3	2:A:432:THR:HG23	1.99	0.45
2:A:397:ASN:HD21	2:A:399:GLN:HG3	1.82	0.44
2:A:467:VAL:HG21	2:A:538:PHE:CE1	2.53	0.44
1:B:54:U:O5'	1:B:54:U:H6	2.01	0.44
2:A:474:ARG:HE	2:A:474:ARG:HB3	1.59	0.43
1:B:43:G:C2'	1:B:44:C:OP1	2.67	0.43
1:B:8:U:OP2	2:A:318:GLN:NE2	2.51	0.43
1:B:27:C:OP2	2:A:545:ARG:NH2	2.47	0.43
1:B:41:C:H2'	1:B:42:G:O4'	2.19	0.43
1:B:61:C:C2'	1:B:62:C:H5'	2.49	0.43
2:A:424:LYS:HA	2:A:430:ILE:HA	2.00	0.43
1:B:67:A:H2'	1:B:68:C:O4'	2.19	0.43
2:A:545:ARG:HG3	2:A:545:ARG:HH11	1.84	0.43
1:B:50:G:O2'	1:B:51:A:H5'	2.19	0.43
2:A:397:ASN:HD21	2:A:399:GLN:HG2	1.84	0.42
1:B:59:A:H3'	1:B:60:U:C6	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:287:ASP:OD1	2:A:289:ARG:HD3	2.20	0.42
2:A:397:ASN:ND2	2:A:399:GLN:CG	2.82	0.42
2:A:357:GLN:CD	2:A:357:GLN:N	2.72	0.42
1:B:46:U:H1'	1:B:47:U:C4	2.54	0.42
1:B:19:G:O2'	1:B:20:U:C5	2.64	0.42
2:A:270:LYS:HE3	3:A:999:ATP:O1B	2.20	0.42
2:A:410:ARG:O	2:A:455:VAL:HA	2.20	0.42
1:B:59:A:H2'	1:B:60:U:O4'	2.20	0.42
1:B:7:A:C5'	2:A:318:GLN:NE2	2.79	0.42
1:B:37:A:C2'	1:B:38:U:H5'	2.50	0.41
2:A:271:ARG:HH12	2:A:272:LYS:NZ	2.18	0.41
1:B:46:U:H4'	1:B:47:U:H6	1.68	0.41
2:A:261:LEU:CD1	2:A:322:ILE:HD13	2.50	0.41
2:A:506:SER:C	2:A:508:LYS:H	2.22	0.41
2:A:402:ARG:HG2	2:A:456:ILE:HG22	2.02	0.41
2:A:371:LYS:HA	2:A:372:PRO:HD2	1.88	0.41
2:A:63:LEU:HD23	2:A:96:VAL:HG22	2.01	0.41
1:B:34:C:O2'	2:A:412:ARG:CZ	2.67	0.41
2:A:178:MET:O	2:A:186:ARG:HD2	2.21	0.41
2:A:411:LEU:HB3	2:A:458:TRP:CD1	2.55	0.41
2:A:467:VAL:CG2	2:A:536:PRO:HB2	2.42	0.41
1:B:8:U:C2	1:B:15:G:O6	2.74	0.41
2:A:11:ILE:HD13	2:A:228:LEU:HD22	2.03	0.40
2:A:545:ARG:HG2	2:A:547:THR:HG23	2.03	0.40
2:A:403:LEU:HA	2:A:409:VAL:HG11	2.03	0.40
2:A:423:GLU:HB2	2:A:434:PHE:HE1	1.87	0.40
2:A:422:VAL:HG11	2:A:430:ILE:HG12	2.03	0.40
2:A:389:ARG:C	2:A:391:ASP:H	2.25	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	
2	A	525/553 (95%)	492 (94%)	28 (5%)	5 (1%)	22	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	32	PRO
2	A	390	ALA
2	A	405	LEU
2	A	348	PRO
2	A	176	ILE

### 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	
2	A	463/481 (96%)	418 (90%)	45 (10%)	12	22

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	19	LEU
2	A	30	ARG
2	A	32	PRO
2	A	49	LEU
2	A	66	ASP
2	A	72	LYS
2	A	78	VAL
2	A	83	ASN
2	A	95	ASN
2	A	106	LEU
2	A	113	LEU
2	A	124	LEU
2	A	126	PRO
2	A	154	LEU
2	A	156	LEU
2	A	186	ARG
2	A	190	LEU
2	A	192	ARG
2	A	194	LYS
2	A	230	THR
2	A	231	LEU
2	A	232	GLU

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Mol	Chain	Res	Type
2	A	238	ARG
2	A	263	LEU
2	A	274	ASN
2	A	318	GLN
2	A	326	SER
2	A	327	LEU
2	A	335	LEU
2	A	341	ARG
2	A	357	GLN
2	A	395	GLU
2	A	410	ARG
2	A	412	ARG
2	A	425	ASP
2	A	431	THR
2	A	432	THR
2	A	474	ARG
2	A	475	LEU
2	A	490	VAL
2	A	507	LEU
2	A	514	LYS
2	A	528	SER
2	A	529	ARG
2	A	544	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	55	GLN
2	A	95	ASN
2	A	142	ASN
2	A	153	ASN
2	A	215	HIS
2	A	234	GLN
2	A	274	ASN
2	A	318	GLN
2	A	336	ASN
2	A	397	ASN
2	A	413	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	73/75 (97%)	26 (35%)	16 (21%)

All (26) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	7	A
1	B	8	U
1	B	9	C
1	B	10	G
1	B	16	C
1	B	18	G
1	B	19	G
1	B	21	A
1	B	29	G
1	B	30	G
1	B	35	U
1	B	36	G
1	B	37	A
1	B	44	C
1	B	45	A
1	B	46	U
1	B	48	C
1	B	49	C
1	B	59	A
1	B	60	U
1	B	61	C
1	B	62	C
1	B	64	C
1	B	73	G
1	B	74	C
1	B	75	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	7	A
1	B	9	C
1	B	15	G
1	B	16	C
1	B	18	G
1	B	19	G
1	B	20	U
1	B	34	C

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Mol	Chain	Res	Type
1	B	35	U
1	B	36	G
1	B	45	A
1	B	48	C
1	B	58	A
1	B	60	U
1	B	73	G
1	B	74	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ATP	A	999	-	33,33,33	0.76	0	52,52,52	0.91	1 (1%)

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	999	-	-	0/22/38/38	0/1/3/3



There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	999	ATP	O3'-C3'-C4'	-2.92	102.48	111.08

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	74/75 (98%)	0.85	11 (14%) 3 2	8, 46, 79, 94	0
2	A	529/553 (95%)	-0.37	21 (3%) 36 32	3, 19, 67, 78	0
All	All	603/628 (96%)	-0.22	32 (5%) 25 22	3, 21, 69, 94	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	440	ASP	5.6
1	B	46	U	5.4
1	B	47	U	5.2
2	A	426	ALA	5.1
2	A	534	GLU	3.7
1	B	44	C	3.7
2	A	429	ASN	3.6
2	A	533	ALA	3.5
1	B	30	G	3.4
1	B	45	A	3.4
2	A	441	THR	3.2
2	A	454	GLY	3.1
1	B	20	U	3.1
1	B	43	G	3.0
2	A	425	ASP	3.0
2	A	400	TYR	2.9
1	B	48	C	2.9
2	A	532	THR	2.8
2	A	409	VAL	2.7
2	A	397	ASN	2.6
2	A	395	GLU	2.6
2	A	398	LYS	2.6
2	A	138	GLN	2.5
2	A	393	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	355	ASN	2.4
2	A	427	GLU	2.4
1	B	19	G	2.4
1	B	52	G	2.3
2	A	528	SER	2.3
2	A	407	LYS	2.3
1	B	16	C	2.2
2	A	463	HIS	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ATP	A	999	31/31	0.16	0.99	0,28,58,60	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.