



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:26 pm GMT

PDB ID : 1EUY  
Title : GLUTAMINYL-TRNA SYNTHETASE COMPLEXED WITH A TRNA MUTANT AND AN ACTIVE SITE INHIBITOR  
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Deposited on : 2000-04-19  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

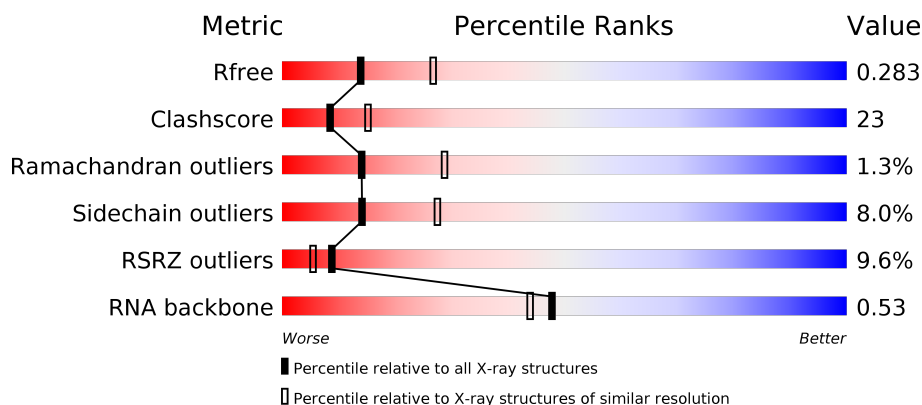
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)
RNA backbone	2435	1140 (3.00-2.20)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	74	
2	A	548	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5915 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.

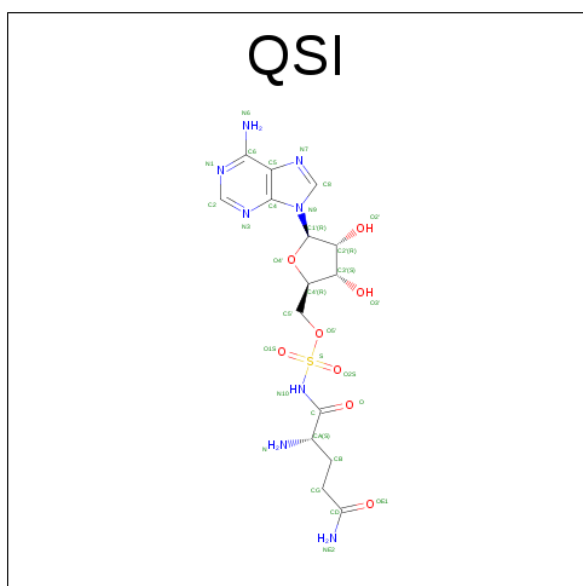
- Molecule 1 is a RNA chain called GLUTAMINYL TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	73	Total	C	N	O	P	0	0	0
			1555	695	282	506	72			

- Molecule 2 is a protein called GLUTAMINYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	529	Total	C	N	O	S	0	0	0
			4274	2701	751	801	21			

- Molecule 3 is 5'-O-[N-(L-GLUTAMINYL)-SULFAMOYL]ADENOSINE (three-letter code: QSI) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>8</sub>O<sub>8</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	15	8	8	1		

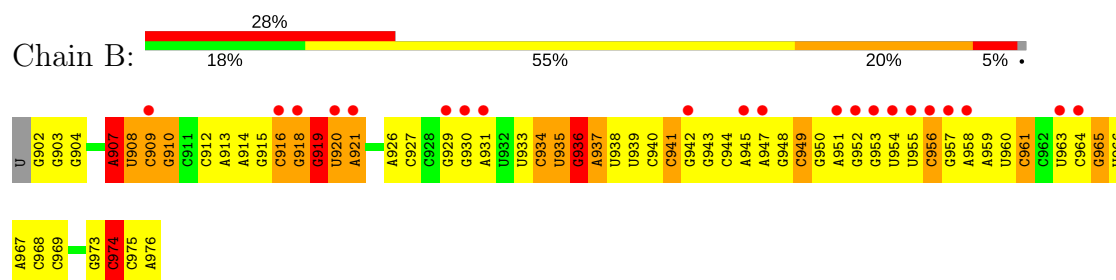
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total 36	O 36	0	0
4	B	18	Total 18	O 18	0	0

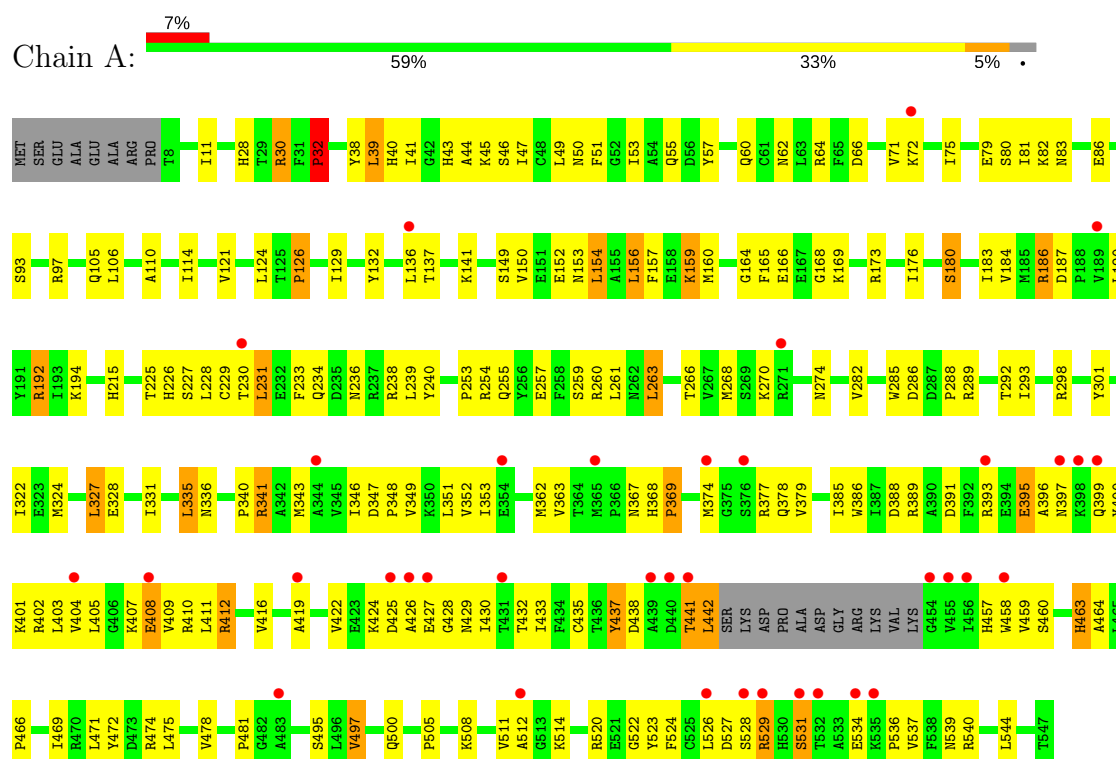
### 3 Residue-property plots

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



#### • Molecule 2: GLUTAMINYL-TRNA SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.20Å 94.20Å 113.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.48 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.5 (30.00-2.60) 98.7 (29.48-2.45)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.45Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.234 , 0.277 0.286 , 0.283	Depositor DCC
$R_{free}$ test set	3891 reflections (10.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.0	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 59.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QSI

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	0.51	0/1738	0.82	4/2708 (0.1%)
2	A	0.50	0/4374	0.72	0/5921
All	All	0.50	0/6112	0.76	4/8629 (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	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	974	C	N1-C1'-C2'	6.77	122.80	114.00
1	B	936	G	N9-C1'-C2'	6.66	122.66	114.00
1	B	934	C	N1-C1'-C2'	6.62	122.60	114.00
1	B	919	G	N9-C1'-C2'	6.10	121.93	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	907	A	Sidechain
1	B	919	G	Sidechain
1	B	936	G	Sidechain
1	B	974	C	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1555	0	792	95	0
2	A	4274	0	4165	162	0
3	A	32	0	22	2	0
4	A	36	0	0	0	0
4	B	18	0	0	2	0
All	All	5915	0	4979	246	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 23.

All (246) 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:A:531:SER:HB3	2:A:537:VAL:H	1.28	0.98
1:B:933:U:H2'	1:B:935:U:OP1	1.66	0.94
2:A:529:ARG:HA	2:A:529:ARG:HE	1.36	0.88
1:B:954:U:O2'	1:B:955:U:H5'	1.78	0.83
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.62	0.81
2:A:341:ARG:HD3	2:A:369:PRO:HD2	1.63	0.81
1:B:954:U:H2'	1:B:955:U:H6	1.45	0.79
1:B:963:U:H2'	1:B:964:C:C6	2.18	0.79
1:B:921:A:H61	1:B:947:A:H2'	1.49	0.78
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.67	0.76
1:B:908:U:H5'	1:B:949:C:OP2	1.86	0.75
2:A:412:ARG:HH11	2:A:412:ARG:HG2	1.51	0.75
2:A:362:MET:HG2	2:A:378:GLN:HG3	1.68	0.75
1:B:943:G:O2'	1:B:944:C:H5'	1.86	0.75
1:B:918:G:H4'	1:B:919:G:OP1	1.87	0.74
1:B:919:G:O2'	1:B:920:U:C6	2.40	0.74
1:B:954:U:H2'	1:B:955:U:C6	2.23	0.73
1:B:950:G:O2'	1:B:951:A:H5'	1.91	0.71
2:A:463:HIS:O	2:A:505:PRO:HD3	1.91	0.71
1:B:907:A:H5'	1:B:908:U:OP2	1.92	0.70
1:B:958:A:HO2'	1:B:960:U:H5	1.40	0.70
2:A:362:MET:CG	2:A:378:GLN:HG3	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:939:U:H2'	1:B:940:C:O4'	1.93	0.68
2:A:289:ARG:HD3	2:A:495:SER:HB2	1.76	0.68
2:A:343:MET:HE1	2:A:457:HIS:HA	1.76	0.68
2:A:438:ASP:HB3	2:A:441:THR:OG1	1.94	0.68
1:B:958:A:O2'	1:B:960:U:H5	1.78	0.66
1:B:955:U:H2'	1:B:957:G:OP2	1.94	0.66
2:A:393:ARG:O	2:A:404:VAL:HA	1.96	0.65
2:A:412:ARG:HG2	2:A:412:ARG:NH1	2.09	0.64
1:B:918:G:H5''	1:B:919:G:OP1	1.97	0.64
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.79	0.64
2:A:410:ARG:HH21	2:A:442:LEU:HA	1.62	0.64
1:B:930:G:O2'	1:B:931:A:H5'	1.98	0.64
1:B:952:G:H2'	1:B:953:G:O4'	1.97	0.64
1:B:909:C:O2	1:B:945:A:N7	2.30	0.64
1:B:934:C:O2'	2:A:412:ARG:NH1	2.31	0.63
1:B:935:U:O4	2:A:341:ARG:NH1	2.31	0.63
2:A:346:ILE:HG13	2:A:469:ILE:HD12	1.81	0.63
1:B:956:C:H2'	1:B:957:G:O4'	1.99	0.63
1:B:909:C:C5'	1:B:910:G:OP2	2.47	0.62
1:B:903:G:O2'	1:B:904:G:H5'	1.99	0.62
1:B:909:C:C4	1:B:947:A:C2	2.87	0.62
2:A:28:HIS:HE1	2:A:62:ASN:OD1	1.83	0.62
1:B:939:U:C2	1:B:940:C:C6	2.87	0.62
1:B:918:G:O2'	1:B:957:G:N2	2.29	0.62
2:A:270:LYS:O	2:A:274:ASN:HB2	2.01	0.61
2:A:159:LYS:HD3	2:A:164:GLY:HA3	1.82	0.61
2:A:396:ALA:HB1	2:A:400:TYR:HB3	1.82	0.60
1:B:958:A:O2'	1:B:960:U:C5	2.51	0.60
2:A:159:LYS:HD2	2:A:165:PHE:CD2	2.36	0.60
2:A:349:VAL:HB	2:A:389:ARG:HG2	1.83	0.60
1:B:957:G:H2'	1:B:958:A:H5'	1.84	0.59
1:B:963:U:H2'	1:B:964:C:H6	1.64	0.59
1:B:918:G:C4'	1:B:919:G:OP1	2.50	0.59
2:A:529:ARG:CA	2:A:529:ARG:HE	2.14	0.59
1:B:908:U:H4'	1:B:948:G:H4'	1.85	0.59
1:B:909:C:H41	1:B:913:A:H2	1.45	0.58
2:A:433:ILE:HG22	2:A:435:CYS:SG	2.42	0.58
2:A:114:ILE:HG21	2:A:154:LEU:HD13	1.83	0.58
2:A:40:HIS:HA	2:A:292:THR:HA	1.85	0.58
2:A:416:VAL:HB	2:A:441:THR:HG21	1.86	0.58
2:A:478:VAL:O	2:A:481:PRO:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:916:C:H5'	1:B:960:U:O2	2.03	0.58
1:B:916:C:H3'	1:B:916:C:OP2	2.03	0.58
2:A:32:PRO:HA	2:A:64:ARG:O	2.04	0.57
1:B:948:G:O2'	1:B:949:C:P	2.62	0.57
1:B:941:C:C2	1:B:942:G:C8	2.92	0.57
2:A:531:SER:HB3	2:A:537:VAL:N	2.10	0.57
2:A:424:LYS:HD3	2:A:428:GLY:O	2.05	0.57
1:B:921:A:H61	1:B:947:A:C2'	2.14	0.57
2:A:126:PRO:O	2:A:129:ILE:HG22	2.05	0.57
2:A:528:SER:O	2:A:529:ARG:NE	2.37	0.57
2:A:410:ARG:NH2	2:A:442:LEU:HA	2.20	0.57
2:A:343:MET:CE	2:A:412:ARG:HB3	2.36	0.56
2:A:419:ALA:HA	2:A:435:CYS:SG	2.46	0.56
2:A:512:ALA:HB1	2:A:528:SER:HB2	1.86	0.56
1:B:914:A:C6	1:B:915:G:C2	2.94	0.56
2:A:30:ARG:NH1	2:A:215:HIS:NE2	2.53	0.55
2:A:166:GLU:O	2:A:169:LYS:HB2	2.06	0.55
1:B:975:C:H2'	1:B:976:A:O4'	2.07	0.54
2:A:240:TYR:OH	2:A:253:PRO:HB2	2.08	0.54
2:A:363:VAL:HG22	2:A:379:VAL:O	2.07	0.54
1:B:960:U:H5'	1:B:961:C:OP2	2.08	0.53
2:A:331:ILE:HG13	2:A:335:LEU:HD22	1.89	0.53
2:A:149:SER:OG	2:A:152:GLU:HG3	2.08	0.53
1:B:902:G:C8	2:A:137:THR:HG22	2.43	0.53
2:A:263:LEU:HD22	2:A:324:MET:HE2	1.91	0.53
2:A:30:ARG:NH2	2:A:228:LEU:O	2.42	0.53
2:A:410:ARG:HD3	2:A:416:VAL:HG22	1.91	0.53
1:B:955:U:C2'	1:B:957:G:OP2	2.57	0.52
2:A:152:GLU:O	2:A:156:LEU:HD22	2.09	0.52
2:A:529:ARG:NE	2:A:529:ARG:HA	2.17	0.52
1:B:947:A:O2'	1:B:948:G:H5'	2.10	0.52
2:A:282:VAL:HG12	2:A:289:ARG:NH1	2.26	0.51
2:A:136:LEU:HD23	2:A:183:ILE:HD11	1.92	0.51
2:A:322:ILE:HD12	2:A:322:ILE:N	2.26	0.51
2:A:512:ALA:HB1	2:A:528:SER:CB	2.40	0.51
2:A:324:MET:O	2:A:328:GLU:HG3	2.11	0.51
2:A:132:TYR:CD2	2:A:141:LYS:HG3	2.45	0.51
1:B:944:C:H2'	1:B:945:A:C4	2.46	0.51
2:A:180:SER:O	2:A:186:ARG:NH1	2.43	0.51
2:A:397:ASN:HD21	2:A:399:GLN:HB2	1.76	0.51
1:B:921:A:N1	1:B:947:A:C4	2.78	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:G:C5'	1:B:919:G:OP1	2.60	0.50
1:B:939:U:C4	1:B:940:C:C5	2.99	0.50
2:A:301:TYR:CE2	2:A:327:LEU:HD22	2.47	0.50
1:B:926:A:H2'	1:B:927:C:O4'	2.11	0.50
2:A:80:SER:O	2:A:83:ASN:HB3	2.12	0.50
2:A:534:GLU:O	2:A:536:PRO:HD3	2.12	0.50
1:B:943:G:C2'	1:B:944:C:H5'	2.42	0.50
2:A:46:SER:HB2	3:A:998:QSI:H1'	1.94	0.49
2:A:282:VAL:HG12	2:A:289:ARG:HH11	1.76	0.49
2:A:472:TYR:HA	2:A:495:SER:O	2.12	0.49
2:A:192:ARG:HD3	2:A:194:LYS:HE3	1.93	0.49
2:A:129:ILE:HG13	2:A:173:ARG:NH2	2.28	0.49
2:A:391:ASP:HA	2:A:402:ARG:HD2	1.95	0.49
2:A:500:GLN:HA	2:A:500:GLN:OE1	2.12	0.49
2:A:288:PRO:HG3	2:A:298:ARG:HG2	1.94	0.49
1:B:909:C:N3	1:B:947:A:C2	2.80	0.49
2:A:229:CYS:O	2:A:257:GLU:HA	2.12	0.48
1:B:902:G:H5''	4:B:48:HOH:O	2.12	0.48
1:B:974:C:N3	2:A:168:GLY:HA2	2.28	0.48
1:B:914:A:N6	1:B:915:G:C2	2.82	0.48
2:A:385:ILE:HA	2:A:460:SER:HA	1.95	0.48
2:A:260:ARG:HB2	3:A:998:QSI:C6	2.44	0.48
1:B:921:A:C2	1:B:947:A:C2	3.02	0.48
2:A:397:ASN:ND2	2:A:399:GLN:HB2	2.28	0.47
1:B:902:G:C5'	4:B:48:HOH:O	2.62	0.47
1:B:909:C:H5'	1:B:910:G:OP2	2.14	0.47
2:A:341:ARG:HD3	2:A:369:PRO:CD	2.37	0.47
2:A:347:ASP:O	2:A:388:ASP:HA	2.13	0.47
2:A:422:VAL:HG23	2:A:433:ILE:HG13	1.96	0.47
2:A:377:ARG:HH11	2:A:377:ARG:HG2	1.79	0.47
2:A:522:GLY:HA2	2:A:544:LEU:CD1	2.44	0.47
2:A:110:ALA:O	2:A:114:ILE:HG13	2.15	0.46
2:A:227:SER:O	2:A:255:GLN:HA	2.14	0.46
2:A:393:ARG:HG2	2:A:395:GLU:O	2.15	0.46
1:B:954:U:H2'	1:B:955:U:O4'	2.15	0.46
2:A:150:VAL:HG12	2:A:154:LEU:HD22	1.95	0.46
2:A:343:MET:HE3	2:A:458:TRP:H	1.80	0.46
2:A:71:VAL:HG23	2:A:72:LYS:NZ	2.31	0.46
1:B:974:C:H1'	2:A:192:ARG:HB3	1.97	0.46
2:A:236:ASN:HD22	2:A:236:ASN:H	1.62	0.46
1:B:936:G:C6	2:A:401:LYS:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:343:MET:HE1	2:A:412:ARG:HB3	1.98	0.46
2:A:422:VAL:HG21	2:A:430:ILE:HD13	1.98	0.46
2:A:231:LEU:HD22	2:A:259:SER:HA	1.98	0.46
1:B:952:G:C4	1:B:953:G:C8	3.03	0.46
2:A:335:LEU:HB3	2:A:523:TYR:CD1	2.51	0.46
1:B:921:A:N6	1:B:947:A:H2'	2.25	0.46
2:A:157:PHE:O	2:A:160:MET:HB2	2.16	0.46
2:A:377:ARG:NH1	2:A:377:ARG:HG2	2.30	0.45
2:A:82:LYS:O	2:A:86:GLU:HG3	2.15	0.45
2:A:136:LEU:HD23	2:A:183:ILE:CD1	2.47	0.45
1:B:935:U:C5	1:B:937:A:C2	3.04	0.45
1:B:919:G:C4	1:B:957:G:N2	2.84	0.45
2:A:238:ARG:HD2	2:A:238:ARG:N	2.32	0.45
1:B:954:U:C2'	1:B:955:U:H5'	2.46	0.45
2:A:346:ILE:HG13	2:A:469:ILE:CD1	2.46	0.45
1:B:934:C:N4	2:A:410:ARG:HH21	2.14	0.45
2:A:386:TRP:N	2:A:459:VAL:O	2.49	0.45
2:A:43:HIS:CE1	2:A:270:LYS:HE3	2.51	0.45
2:A:397:ASN:ND2	2:A:399:GLN:H	2.15	0.45
2:A:192:ARG:NE	2:A:194:LYS:HE3	2.32	0.45
2:A:230:THR:HG21	2:A:260:ARG:HB3	1.99	0.44
1:B:916:C:C5'	1:B:960:U:O2	2.63	0.44
2:A:393:ARG:HB2	2:A:400:TYR:CZ	2.53	0.44
2:A:522:GLY:HA2	2:A:544:LEU:HD13	1.97	0.44
1:B:959:A:C6	1:B:960:U:C2	3.06	0.44
2:A:340:PRO:HA	2:A:367:ASN:O	2.15	0.44
1:B:907:A:C5'	1:B:908:U:OP2	2.61	0.44
2:A:44:ALA:HB2	2:A:293:ILE:HD11	2.00	0.44
2:A:43:HIS:HE1	2:A:270:LYS:HE3	1.82	0.44
2:A:411:LEU:HD23	2:A:411:LEU:HA	1.82	0.44
1:B:963:U:O2'	1:B:964:C:H5'	2.18	0.44
2:A:184:VAL:HG22	2:A:239:LEU:HD22	1.99	0.44
1:B:909:C:H5''	1:B:910:G:OP2	2.18	0.44
2:A:114:ILE:CG2	2:A:154:LEU:HD13	2.47	0.44
2:A:286:ASP:O	2:A:298:ARG:HD3	2.18	0.44
1:B:914:A:N6	1:B:915:G:N1	2.66	0.44
2:A:159:LYS:HD2	2:A:165:PHE:CE2	2.52	0.43
2:A:38:TYR:HB2	2:A:285:TRP:CE3	2.53	0.43
2:A:341:ARG:HD2	2:A:341:ARG:H	1.84	0.43
1:B:934:C:O2'	2:A:412:ARG:NH2	2.51	0.43
1:B:907:A:C4'	1:B:908:U:OP2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:929:G:C6	1:B:942:G:C6	3.06	0.43
1:B:968:C:H2'	1:B:969:C:H6	1.83	0.43
2:A:183:ILE:HA	2:A:186:ARG:HG3	1.99	0.43
1:B:903:G:C2'	1:B:904:G:H5'	2.49	0.43
2:A:11:ILE:HD13	2:A:228:LEU:HD22	2.00	0.43
1:B:937:A:H2'	1:B:938:U:C5'	2.48	0.43
1:B:939:U:C2'	1:B:940:C:H5'	2.49	0.43
1:B:976:A:C2	2:A:233:PHE:CZ	3.07	0.43
2:A:192:ARG:HE	2:A:194:LYS:HE3	1.83	0.43
2:A:32:PRO:HG3	2:A:215:HIS:HE1	1.84	0.43
2:A:403:LEU:HD21	2:A:419:ALA:HB2	2.00	0.43
1:B:952:G:C6	1:B:953:G:C5	3.07	0.43
2:A:173:ARG:HD2	2:A:187:ASP:O	2.18	0.43
2:A:524:PHE:HA	2:A:539:ASN:O	2.19	0.43
2:A:343:MET:CE	2:A:458:TRP:H	2.32	0.42
1:B:938:U:H4'	2:A:336:ASN:OD1	2.19	0.42
2:A:41:ILE:HG22	2:A:268:MET:SD	2.59	0.42
2:A:51:PHE:O	2:A:55:GLN:HG2	2.19	0.42
1:B:929:G:C2	1:B:942:G:C4	3.07	0.42
2:A:505:PRO:O	2:A:508:LYS:HB3	2.20	0.42
1:B:909:C:H5	1:B:912:C:H41	1.67	0.42
1:B:937:A:C2'	1:B:938:U:H5'	2.49	0.42
1:B:954:U:C2	1:B:955:U:C6	3.08	0.42
2:A:43:HIS:O	2:A:47:ILE:HG13	2.20	0.42
1:B:964:C:H2'	1:B:965:G:O4'	2.20	0.42
2:A:340:PRO:CD	2:A:514:LYS:HE3	2.50	0.42
1:B:948:G:HO2'	1:B:949:C:P	2.43	0.42
2:A:341:ARG:HD2	2:A:341:ARG:N	2.35	0.42
2:A:121:VAL:H	2:A:153:ASN:ND2	2.18	0.42
2:A:362:MET:HG2	2:A:378:GLN:CG	2.45	0.42
2:A:427:GLU:HG2	2:A:427:GLU:O	2.19	0.42
1:B:968:C:H2'	1:B:969:C:C6	2.55	0.42
2:A:524:PHE:CE2	2:A:540:ARG:HB2	2.55	0.41
2:A:353:ILE:HG21	2:A:437:TYR:HB3	2.02	0.41
1:B:966:U:O2'	1:B:967:A:H5'	2.20	0.41
2:A:407:LYS:HG3	2:A:408:GLU:N	2.35	0.41
2:A:464:ALA:O	2:A:466:PRO:HD3	2.21	0.41
2:A:263:LEU:HB2	2:A:268:MET:HE1	2.02	0.41
2:A:64:ARG:HA	2:A:97:ARG:O	2.20	0.41
1:B:934:C:O2'	2:A:412:ARG:CZ	2.69	0.41
2:A:50:ASN:OD1	2:A:228:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:236:ASN:N	2:A:236:ASN:HD22	2.18	0.41
2:A:351:LEU:C	2:A:351:LEU:HD23	2.41	0.41
2:A:231:LEU:O	2:A:234:GLN:HG3	2.21	0.41
2:A:254:ARG:HD3	2:A:254:ARG:HA	1.86	0.41
1:B:967:A:H2'	1:B:968:C:C6	2.56	0.41
2:A:457:HIS:HD2	2:A:520:ARG:HE	1.69	0.41
2:A:512:ALA:N	2:A:526:LEU:HD23	2.35	0.41
2:A:368:HIS:HB2	2:A:374:MET:SD	2.61	0.41
2:A:53:ILE:O	2:A:57:TYR:HD1	2.05	0.41
2:A:75:ILE:O	2:A:79:GLU:HG3	2.21	0.41
2:A:45:LYS:HD2	2:A:261:LEU:HB2	2.02	0.40
2:A:41:ILE:CG2	2:A:268:MET:SD	3.09	0.40
2:A:425:ASP:OD1	2:A:429:ASN:HB2	2.22	0.40
2:A:60:GLN:HB3	2:A:93:SER:HB2	2.04	0.40
2:A:166:GLU:HB2	2:A:169:LYS:HD3	2.02	0.40
2:A:225:THR:OG1	2:A:226:HIS:HD2	2.04	0.40
2:A:402:ARG:HD3	2:A:520:ARG:HH22	1.85	0.40
1:B:939:U:C4	1:B:940:C:C4	3.09	0.40
1:B:954:U:HO2'	1:B:955:U:H5'	1.80	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
2	A	525/548 (96%)	488 (93%)	30 (6%)	7 (1%)	14 29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	32	PRO
2	A	405	LEU

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Mol	Chain	Res	Type
2	A	527	ASP
2	A	531	SER
2	A	426	ALA
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	462/478 (97%)	425 (92%)	37 (8%)	14	27

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	30	ARG
2	A	32	PRO
2	A	39	LEU
2	A	49	LEU
2	A	66	ASP
2	A	105	GLN
2	A	106	LEU
2	A	124	LEU
2	A	126	PRO
2	A	154	LEU
2	A	156	LEU
2	A	159	LYS
2	A	180	SER
2	A	186	ARG
2	A	190	LEU
2	A	192	ARG
2	A	231	LEU
2	A	263	LEU
2	A	266	THR
2	A	327	LEU
2	A	335	LEU

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Mol	Chain	Res	Type
2	A	341	ARG
2	A	352	VAL
2	A	369	PRO
2	A	395	GLU
2	A	408	GLU
2	A	412	ARG
2	A	432	THR
2	A	437	TYR
2	A	441	THR
2	A	442	LEU
2	A	463	HIS
2	A	474	ARG
2	A	475	LEU
2	A	497	VAL
2	A	511	VAL
2	A	529	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	28	HIS
2	A	105	GLN
2	A	115	ASN
2	A	142	ASN
2	A	153	ASN
2	A	226	HIS
2	A	236	ASN
2	A	281	HIS
2	A	355	ASN
2	A	368	HIS
2	A	397	ASN
2	A	413	ASN
2	A	457	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	72/74 (97%)	19 (26%)	0

All (19) RNA backbone outliers are listed below:



Mol	Chain	Res	Type
1	B	907	A
1	B	908	U
1	B	909	C
1	B	910	G
1	B	916	C
1	B	918	G
1	B	919	G
1	B	920	U
1	B	921	A
1	B	935	U
1	B	936	G
1	B	937	A
1	B	941	C
1	B	949	C
1	B	956	C
1	B	961	C
1	B	965	G
1	B	973	G
1	B	974	C

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	QSI	A	998	-	30,34,34	2.68	5 (16%)	32,50,50	0.86	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	QSI	A	998	-	-	0/19/40/40	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	QSI	O5'-S	-5.49	1.51	1.59
3	A	998	QSI	CA-N	-2.85	1.33	1.48
3	A	998	QSI	CD-NE2	4.33	1.46	1.32
3	A	998	QSI	S-N10	7.69	1.68	1.59
3	A	998	QSI	O1S-S	9.57	1.50	1.42

There are no bond angle outliers.

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	998	QSI	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	73/74 (98%)	1.47	21 (28%) <b>1</b> <b>0</b>	0, 55, 85, 87	0
2	A	529/548 (96%)	0.33	37 (6%) <b>17</b> <b>12</b>	6, 28, 67, 94	0
All	All	602/622 (96%)	0.47	58 (9%) <b>9</b> <b>5</b>	0, 30, 75, 94	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	920	U	7.7
1	B	945	A	7.0
1	B	953	G	6.8
1	B	916	C	6.4
1	B	954	U	5.5
2	A	426	ALA	5.3
1	B	955	U	5.1
1	B	909	C	5.0
2	A	398	LYS	4.8
2	A	399	GLN	4.6
1	B	963	U	4.6
2	A	439	ALA	4.6
2	A	440	ASP	4.3
2	A	529	ARG	4.2
1	B	957	G	4.1
2	A	427	GLU	3.8
2	A	393	ARG	3.8
2	A	456	ILE	3.7
2	A	441	THR	3.7
1	B	951	A	3.6
1	B	952	G	3.6
2	A	528	SER	3.5
1	B	964	C	3.4
2	A	354	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	956	C	3.2
1	B	921	A	3.1
1	B	942	G	3.1
2	A	431	THR	3.0
2	A	532	THR	3.0
2	A	404	VAL	2.9
1	B	947	A	2.9
2	A	189	VAL	2.7
2	A	512	ALA	2.7
2	A	376	SER	2.7
1	B	931	A	2.6
2	A	419	ALA	2.5
2	A	397	ASN	2.5
2	A	534	GLU	2.5
2	A	230	THR	2.4
2	A	425	ASP	2.4
1	B	930	G	2.4
2	A	483	ALA	2.3
2	A	535	LYS	2.3
2	A	271	ARG	2.2
1	B	918	G	2.2
2	A	455	VAL	2.2
2	A	454	GLY	2.2
1	B	929	G	2.2
2	A	458	TRP	2.1
2	A	408	GLU	2.1
2	A	526	LEU	2.1
2	A	531	SER	2.1
2	A	365	MET	2.1
2	A	374	MET	2.1
2	A	72	LYS	2.0
2	A	344	ALA	2.0
2	A	136	LEU	2.0
1	B	958	A	2.0

## 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 [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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	QSI	A	998	32/32	0.88	0.29	1.71	25,44,56,59	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.