



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:27 AM GMT

PDB ID : 2CV1  
Title : Glutamyl-tRNA synthetase from *Thermus thermophilus* in complex with tRNA(Glu), ATP, and an analog of L-glutamate: a quaternary complex  
Authors : Sekine, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-05-31  
Resolution : 2.41 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 (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

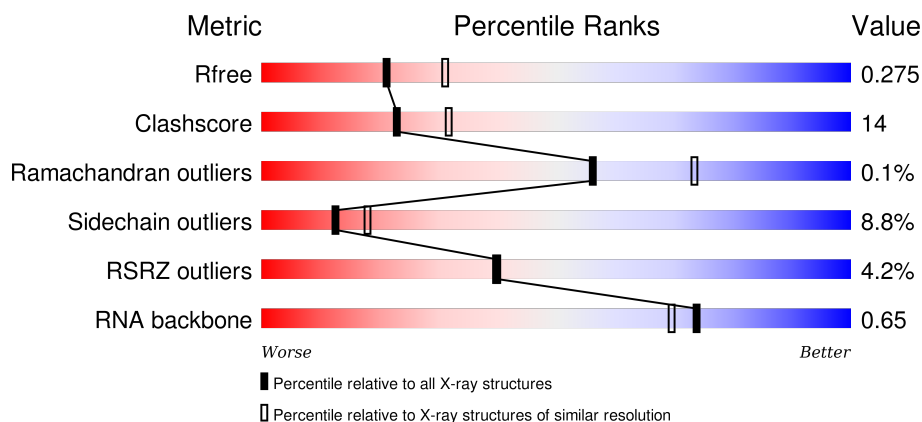
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)
RNA backbone	2183	1033 (2.90-1.94)

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	C	75	<div> <div>13%</div> <div> <div></div> <div>53%</div> <div>32%</div> <div>11%</div> <div>•</div> </div> </div>
1	D	75	<div> <div>11%</div> <div> <div></div> <div>51%</div> <div>37%</div> <div>7%</div> <div>5%</div> </div> </div>
2	A	468	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>28%</div> <div>•</div> </div> </div>
2	B	468	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>•</div> </div> </div>

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	ATP	A	601	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11088 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 tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	75	Total	C	N	O	P	0	0	0
			1597	711	284	527	75			
1	D	75	Total	C	N	O	P	0	0	0
			1597	711	284	527	75			

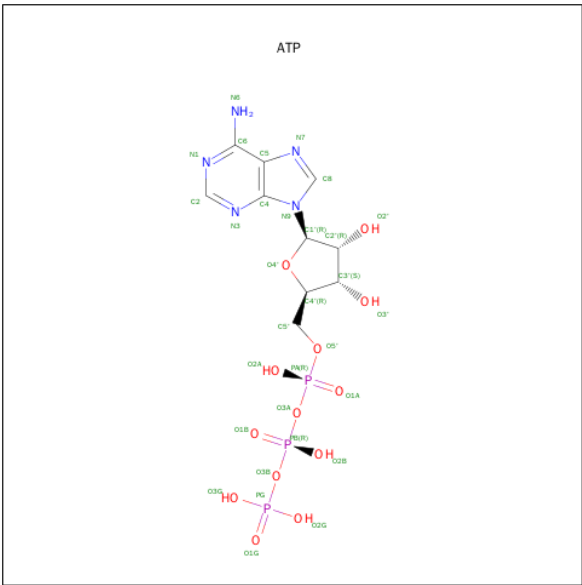
- Molecule 2 is a protein called glutamyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	468	Total	C	N	O	S	0	0	0
			3814	2443	676	687	8			
2	B	468	Total	C	N	O	S	0	0	0
			3814	2443	676	687	8			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

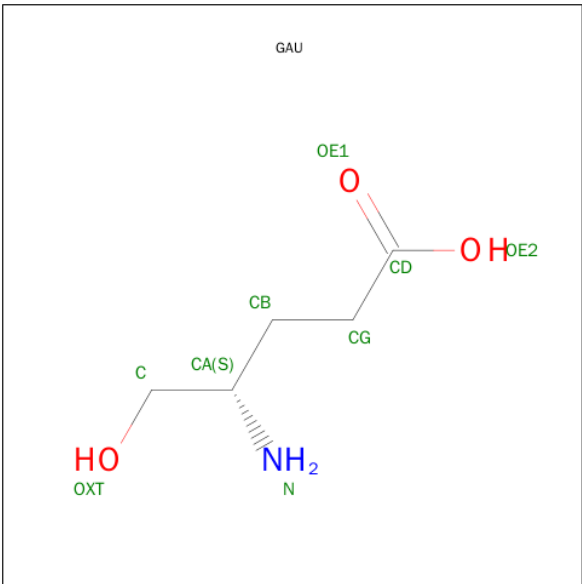
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 5 is (4S)-4-AMINO-5-HYDROXPENTANOIC ACID (three-letter code: GAU) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			18	10	2	6		

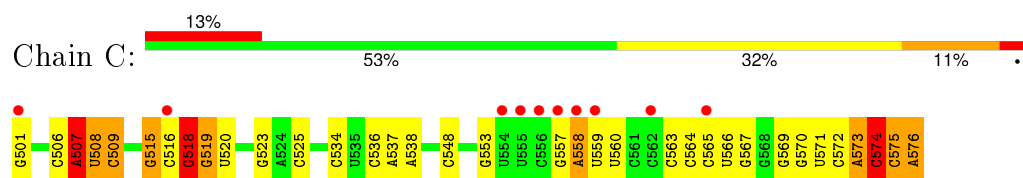
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total 75	O 75	0	0
6	B	61	Total 61	O 61	0	0
6	C	23	Total 23	O 23	0	0
6	D	23	Total 23	O 23	0	0

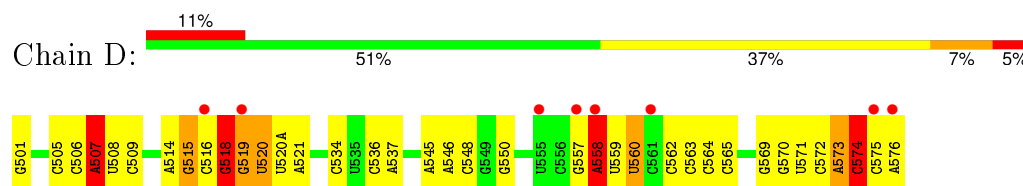
### 3 Residue-property plots

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

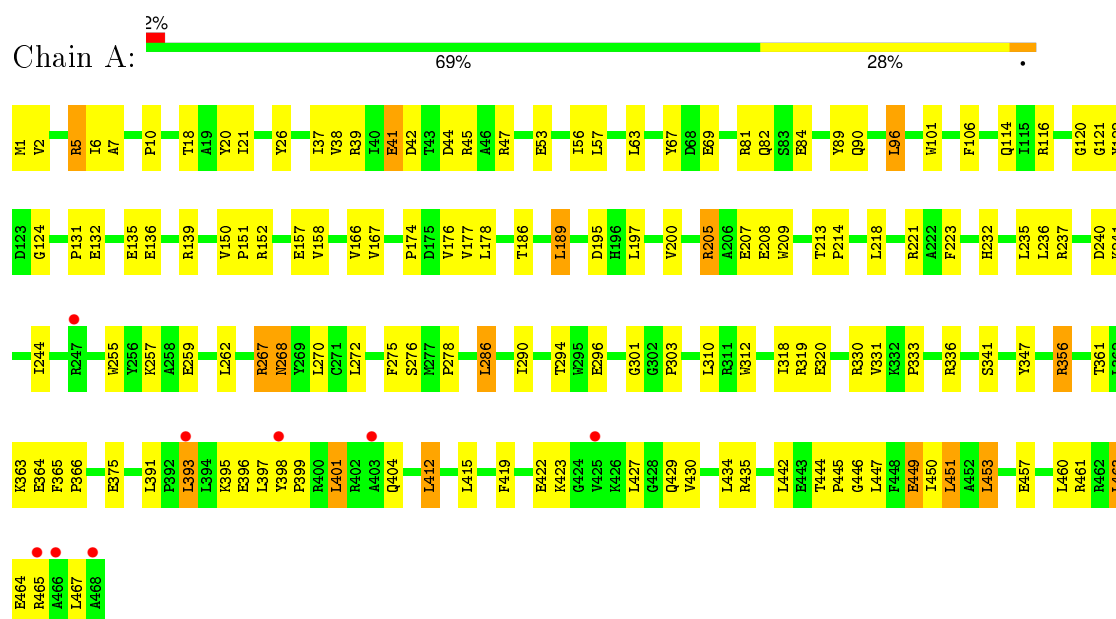
#### • Molecule 1: tRNA



#### • Molecule 1: tRNA



#### • Molecule 2: glutamyl-tRNA synthetase



#### • Molecule 2: glutamyl-tRNA synthetase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.62Å 218.82Å 134.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.41 49.36 – 2.41	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.36-2.41) 96.1 (49.36-2.41)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.221 , 0.277 0.222 , 0.275	Depositor DCC
$R_{free}$ test set	3084 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 61079 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, GAU, 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	C	0.51	1/1782 (0.1%)	0.88	9/2774 (0.3%)
1	D	0.51	1/1782 (0.1%)	0.85	9/2774 (0.3%)
2	A	0.53	0/3910	0.70	0/5293
2	B	0.51	0/3910	0.68	0/5293
All	All	0.52	2/11384 (0.0%)	0.75	18/16134 (0.1%)

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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	501	G	OP3-P	-7.00	1.52	1.61
1	D	501	G	OP3-P	-6.74	1.53	1.61

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	507	A	C2'-C3'-O3'	7.81	126.68	109.50
1	C	573	A	C2'-C3'-O3'	7.73	126.50	109.50
1	D	558	A	C2'-C3'-O3'	7.72	126.49	109.50
1	C	558	A	C2'-C3'-O3'	7.68	126.40	109.50
1	C	519	G	C2'-C3'-O3'	7.48	125.96	109.50
1	D	573	A	C2'-C3'-O3'	7.06	125.03	109.50
1	D	519	G	C2'-C3'-O3'	7.02	124.95	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	518	G	C2'-C3'-O3'	6.92	124.77	113.70
1	C	574	C	C2'-C3'-O3'	6.87	124.69	113.70
1	C	518	G	C2'-C3'-O3'	6.34	123.85	113.70
1	D	574	C	C2'-C3'-O3'	6.28	123.75	113.70
1	C	576	A	C2'-C3'-O3'	6.15	123.55	113.70
1	D	507	A	C4'-C3'-C2'	5.66	108.26	102.60
1	D	558	A	C4'-C3'-C2'	5.59	108.19	102.60
1	C	558	A	C4'-C3'-C2'	5.57	108.17	102.60
1	C	574	C	C4'-C3'-C2'	5.04	107.64	102.60
1	D	518	G	C4'-C3'-C2'	5.04	107.64	102.60
1	C	507	A	C4'-C3'-O3'	5.01	123.02	113.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	545	A	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	C	1597	0	813	19	0
1	D	1597	0	813	27	0
2	A	3814	0	3818	104	0
2	B	3814	0	3818	131	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	31	0	12	3	0
4	B	31	0	12	3	0
5	A	18	0	20	6	0
6	A	75	0	0	3	0
6	B	61	0	0	3	0
6	C	23	0	0	2	0
6	D	23	0	0	2	0
All	All	11088	0	9306	272	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 (272) 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:294:THR:HG22	2:A:296:GLU:H	1.32	0.95
2:B:205:ARG:HD3	2:B:232:HIS:CE1	2.00	0.95
1:D:570:G:H21	2:B:211:VAL:HG21	1.40	0.86
2:A:205:ARG:HD3	2:A:232:HIS:CE1	2.10	0.86
2:A:393:LEU:H	2:A:393:LEU:HD23	1.44	0.82
2:A:41:GLU:HG3	2:A:82:GLN:OE1	1.79	0.81
1:D:506:C:O2'	1:D:507:A:H5'	1.84	0.77
2:A:177:VAL:HG23	2:A:186:THR:HG21	1.65	0.77
2:A:37:ILE:HD12	2:A:69:GLU:HB2	1.68	0.75
2:B:10:PRO:CB	2:B:52:ALA:HB3	2.17	0.75
2:B:454:LEU:HD13	2:B:454:LEU:H	1.52	0.74
1:D:576:A:H5''	2:B:187:TYR:HB2	1.70	0.74
2:A:21:ILE:HG13	4:A:601:ATP:H1'	1.70	0.74
2:B:435:ARG:HD3	2:B:444:THR:HG22	1.68	0.73
2:B:10:PRO:HB3	2:B:52:ALA:HB3	1.70	0.73
2:A:114:GLN:HG3	6:A:1045:HOH:O	1.87	0.73
2:A:205:ARG:HD3	2:A:232:HIS:HE1	1.52	0.73
2:A:412:LEU:HG	2:A:451:LEU:HD13	1.71	0.72
1:C:518:G:O2'	1:C:557:G:N2	2.23	0.70
2:A:157:GLU:HG2	2:A:167:VAL:HG22	1.74	0.70
2:B:358:ARG:O	2:B:368:LYS:HE2	1.93	0.69
2:A:361:THR:OG1	2:A:364:GLU:HG3	1.93	0.69
2:A:255:TRP:CZ2	2:A:259:GLU:HG3	2.28	0.68
2:B:398:TYR:HB3	2:B:399:PRO:HD3	1.75	0.68
2:B:454:LEU:N	2:B:454:LEU:HD13	2.09	0.68
5:A:702:GAU:HO2	4:B:602:ATP:H3'	1.76	0.67
1:C:563:C:H2'	1:C:564:C:C6	2.29	0.67
2:B:391:LEU:O	2:B:395:LYS:HG3	1.93	0.67
2:A:116:ARG:O	2:A:120:GLY:HA2	1.96	0.66
1:D:572:C:OP2	6:D:1228:HOH:O	2.14	0.66
2:B:454:LEU:H	2:B:454:LEU:HD22	1.60	0.65
2:B:95:GLU:HG3	2:B:99:ARG:HD2	1.79	0.65
1:C:538:A:OP1	6:C:1006:HOH:O	2.14	0.65
2:B:137:ARG:HB3	2:B:142:GLU:OE1	1.96	0.65
2:A:463:LEU:HD22	2:A:463:LEU:O	1.96	0.65
1:C:506:C:O2'	1:C:507:A:H5'	1.96	0.65
2:A:294:THR:HG22	2:A:296:GLU:N	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:454:LEU:N	2:B:454:LEU:HD22	2.12	0.65
2:A:18:THR:HG21	2:A:56:ILE:HD11	1.79	0.65
2:B:51:GLY:O	2:B:54:GLU:HG2	1.98	0.64
2:A:404:GLN:HG3	2:A:415:LEU:HD22	1.80	0.64
2:B:444:THR:HG23	2:B:445:PRO:O	1.97	0.64
2:B:4:THR:HB	2:B:25:ASN:HD22	1.64	0.63
2:B:116:ARG:O	2:B:120:GLY:HA2	1.98	0.63
2:B:41:GLU:HG2	2:B:82:GLN:CD	2.19	0.63
2:A:363:LYS:O	2:A:366:PRO:HD2	1.99	0.63
2:A:427:LEU:O	2:A:430:VAL:HG12	1.99	0.63
2:B:262:LEU:HD22	2:B:330:ARG:HH11	1.64	0.62
2:A:152:ARG:HG2	6:A:1035:HOH:O	1.98	0.62
1:D:563:C:H2'	1:D:564:C:C6	2.34	0.62
2:B:412:LEU:HG	2:B:451:LEU:HD23	1.81	0.61
2:B:157:GLU:HG2	2:B:167:VAL:HG22	1.81	0.61
1:D:574:C:H5'	2:B:177:VAL:HG21	1.80	0.61
2:B:104:ARG:HB3	2:B:144:HIS:HD2	1.64	0.61
2:B:115:ILE:HD13	2:B:116:ARG:N	2.16	0.61
2:A:391:LEU:O	2:A:395:LYS:HG2	2.00	0.61
2:A:81:ARG:HD2	2:A:84:GLU:OE2	2.00	0.61
1:C:534:C:O2	2:A:435:ARG:NH2	2.33	0.61
2:A:435:ARG:HD3	2:A:444:THR:OG1	2.00	0.61
1:D:563:C:H2'	1:D:564:C:H6	1.64	0.60
2:B:114:GLN:O	2:B:118:GLU:HG2	2.02	0.60
2:A:446:GLY:O	2:A:449:GLU:HG2	2.01	0.60
2:B:363:LYS:O	2:B:366:PRO:HD2	2.02	0.59
2:B:205:ARG:HD3	2:B:232:HIS:HE1	1.67	0.59
2:B:111:GLU:O	2:B:114:GLN:HB2	2.03	0.59
2:B:423:LYS:HZ2	2:B:423:LYS:HB2	1.68	0.59
2:B:122:TYR:CE2	2:B:124:GLY:HA2	2.37	0.58
2:A:333:PRO:HA	2:A:336:ARG:NH1	2.19	0.58
1:D:534:C:O2	2:B:435:ARG:NH2	2.31	0.58
2:B:317:TYR:HA	2:B:321:VAL:HG23	1.85	0.57
2:A:255:TRP:CH2	2:A:259:GLU:HG3	2.39	0.57
1:D:518:G:O2'	1:D:557:G:N2	2.37	0.57
2:A:157:GLU:CG	2:A:167:VAL:HG22	2.35	0.57
2:A:213:THR:N	2:A:214:PRO:HD2	2.19	0.57
2:B:319:ARG:HD2	6:B:1180:HOH:O	2.04	0.57
2:A:136:GLU:HG2	2:A:139:ARG:HH21	1.70	0.57
2:A:116:ARG:HA	2:A:121:GLY:H	1.69	0.56
2:A:208:GLU:H	2:A:235:LEU:HD21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:HD12	2:B:102:ALA:HB3	1.87	0.56
2:B:104:ARG:HE	2:B:144:HIS:CD2	2.23	0.56
2:A:460:LEU:O	2:A:464:GLU:HG3	2.05	0.56
2:B:118:GLU:HB2	2:B:119:LYS:HD2	1.88	0.56
2:A:177:VAL:HG23	2:A:186:THR:CG2	2.35	0.55
2:B:131:PRO:O	2:B:135:GLU:HG2	2.07	0.55
2:A:195:ASP:HB3	2:A:200:VAL:HG22	1.87	0.55
2:A:5:ARG:HB3	2:A:37:ILE:HB	1.89	0.55
2:A:177:VAL:CG2	2:A:186:THR:HG21	2.35	0.55
1:D:521:A:H61	1:D:546:A:H2'	1.70	0.55
2:B:7:ALA:HA	2:B:39:ARG:O	2.06	0.55
2:B:294:THR:HG23	2:B:297:ARG:HG2	1.89	0.54
2:A:244:ILE:HG22	4:A:601:ATP:HN62	1.73	0.54
2:B:116:ARG:HD2	2:B:121:GLY:H	1.72	0.54
1:C:563:C:H2'	1:C:564:C:H6	1.70	0.54
2:A:1:MET:HE3	2:A:2:VAL:O	2.07	0.54
2:B:244:ILE:HG12	2:B:251:THR:HG22	1.89	0.54
2:B:133:GLU:O	2:B:137:ARG:HG3	2.08	0.54
2:B:115:ILE:HD11	2:B:122:TYR:HA	1.89	0.54
2:B:10:PRO:CA	2:B:52:ALA:HB3	2.38	0.54
2:A:419:PHE:HA	2:A:422:GLU:HG2	1.90	0.53
2:B:393:LEU:HD21	2:B:423:LYS:HG2	1.90	0.53
2:B:106:PHE:CD2	2:B:144:HIS:HB3	2.43	0.53
2:A:205:ARG:HG3	2:A:209:TRP:CD1	2.44	0.53
6:C:1046:HOH:O	2:A:41:GLU:HG2	2.07	0.53
2:A:53:GLU:O	2:A:56:ILE:HG22	2.08	0.53
2:A:158:VAL:HB	2:A:166:VAL:HG23	1.90	0.53
2:B:152:ARG:HH11	2:B:152:ARG:HG2	1.74	0.52
2:B:454:LEU:HB2	2:B:458:ARG:HD2	1.90	0.52
2:A:404:GLN:CG	2:A:415:LEU:HD22	2.40	0.52
2:B:311:ARG:HB3	2:B:311:ARG:NH1	2.24	0.52
2:B:37:ILE:HG22	2:B:38:VAL:N	2.23	0.52
1:D:550:G:N2	1:D:565:C:H1'	2.25	0.52
2:B:255:TRP:CZ2	2:B:259:GLU:HG2	2.45	0.52
2:A:207:GLU:HB3	2:A:235:LEU:HD23	1.91	0.51
1:D:520(A):U:OP2	6:D:1227:HOH:O	2.19	0.51
2:A:122:TYR:CE2	2:A:124:GLY:HA2	2.46	0.51
2:A:240:ASP:O	2:A:241:LYS:HB2	2.11	0.51
1:D:576:A:O3'	5:A:702:GAU:N	2.44	0.51
2:A:208:GLU:N	2:A:235:LEU:HD21	2.26	0.51
1:D:558:A:O2'	1:D:560:U:OP2	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:ALA:O	2:B:56:ILE:HG22	2.12	0.50
1:C:571:U:H2'	1:C:572:C:C6	2.47	0.49
2:B:435:ARG:HD3	2:B:444:THR:CG2	2.37	0.49
2:B:391:LEU:N	2:B:392:PRO:HD2	2.28	0.49
2:B:48:TYR:OH	2:B:50:PRO:HB3	2.13	0.49
1:C:569:G:O2'	1:C:570:G:H5'	2.11	0.49
2:B:113:GLU:HA	2:B:113:GLU:OE1	2.11	0.49
2:B:446:GLY:O	2:B:449:GLU:HG2	2.12	0.49
2:A:301:GLY:O	2:A:303:PRO:HD3	2.13	0.49
2:A:44:ASP:OD1	2:A:47:ARG:HG3	2.12	0.49
1:C:574:C:H5'	2:A:177:VAL:HG11	1.94	0.49
2:B:89:TYR:CD2	2:B:185:PRO:HG3	2.48	0.49
2:B:213:THR:N	2:B:214:PRO:CD	2.75	0.48
2:B:140:ARG:HA	2:B:140:ARG:NE	2.28	0.48
1:C:574:C:O2'	1:C:575:C:OP1	2.25	0.48
2:B:116:ARG:HA	2:B:121:GLY:H	1.78	0.48
2:A:347:TYR:CE1	2:A:453:LEU:HD22	2.48	0.48
2:B:145:VAL:HG12	2:B:181:SER:N	2.28	0.48
2:A:116:ARG:HD3	6:A:1136:HOH:O	2.13	0.48
2:B:40:ILE:HG13	2:B:53:GLU:HG3	1.96	0.48
1:D:536:C:H2'	1:D:537:A:O4'	2.14	0.48
2:A:463:LEU:O	2:A:467:LEU:HG	2.13	0.48
2:A:404:GLN:HE21	2:A:415:LEU:HD13	1.79	0.48
2:B:25:ASN:ND2	6:B:1059:HOH:O	2.47	0.48
2:B:454:LEU:CB	2:B:458:ARG:HD2	2.44	0.48
2:B:465:ARG:HH11	2:B:465:ARG:HB3	1.78	0.47
2:A:461:ARG:NH1	2:A:465:ARG:HD3	2.29	0.47
1:D:576:A:H2'	2:B:209:TRP:HH2	1.80	0.47
2:B:444:THR:OG1	2:B:445:PRO:HD2	2.14	0.47
1:D:520:U:H2'	1:D:521:A:H5'	1.96	0.47
2:B:179:LEU:HD21	2:B:183:GLY:O	2.15	0.47
2:B:45:ARG:HD3	2:B:184:TYR:CZ	2.49	0.47
2:B:119:LYS:HD2	2:B:119:LYS:N	2.30	0.47
2:B:168:TYR:CD2	2:B:214:PRO:HG3	2.50	0.47
1:D:569:G:O2'	1:D:570:G:H5'	2.15	0.47
2:A:38:VAL:HG11	2:A:57:LEU:HD21	1.97	0.47
2:B:152:ARG:HG2	2:B:152:ARG:NH1	2.29	0.47
2:B:48:TYR:CE1	2:B:50:PRO:HD3	2.50	0.47
2:A:375:GLU:CD	2:A:461:ARG:HH22	2.18	0.46
2:A:174:PRO:HG2	2:A:176:VAL:CG1	2.46	0.46
2:A:106:PHE:CD1	2:A:106:PHE:N	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:601:ATP:O1A	5:A:701:GAU:HO1	2.15	0.46
1:D:505:C:H4'	2:B:163:ARG:HD3	1.97	0.46
2:A:444:THR:HB	2:A:445:PRO:HD2	1.97	0.46
2:B:398:TYR:HD1	2:B:463:LEU:HD13	1.80	0.46
2:B:416:LEU:HD12	2:B:448:PHE:CE1	2.51	0.46
2:A:262:LEU:HD22	2:A:330:ARG:HH11	1.81	0.46
2:A:330:ARG:O	2:A:333:PRO:HD2	2.16	0.46
2:A:26:TYR:CE1	2:A:286:LEU:HD21	2.51	0.46
2:B:107:GLU:H	2:B:107:GLU:CD	2.18	0.46
2:B:98:LYS:HD2	2:B:98:LYS:N	2.31	0.46
2:B:112:LEU:O	2:B:115:ILE:HD13	2.16	0.45
2:A:267:ARG:HD2	2:A:286:LEU:HG	1.97	0.45
2:B:111:GLU:O	2:B:115:ILE:HG23	2.16	0.45
2:B:371:TYR:OH	2:B:444:THR:OG1	2.30	0.45
2:B:412:LEU:HG	2:B:451:LEU:CD2	2.46	0.45
1:C:536:C:H2'	1:C:537:A:O4'	2.16	0.45
2:A:398:TYR:N	2:A:399:PRO:HD2	2.32	0.45
5:A:702:GAU:CD	2:B:5:ARG:HH12	2.30	0.45
2:B:205:ARG:O	2:B:232:HIS:HA	2.17	0.45
2:B:238:ASN:CG	2:B:244:ILE:HA	2.37	0.45
2:B:14:PRO:HB3	2:B:56:ILE:HA	1.97	0.45
2:B:203:VAL:HG12	2:B:205:ARG:HD2	1.99	0.45
1:D:550:G:C2	1:D:565:C:C2	3.05	0.45
2:A:131:PRO:O	2:A:135:GLU:HG2	2.17	0.45
2:A:20:TYR:CE2	2:A:236:LEU:HD13	2.51	0.45
1:C:525:C:H5''	2:A:312:TRP:CE2	2.51	0.45
2:B:146:ILE:HD12	2:B:179:LEU:HD12	1.99	0.45
2:B:423:LYS:NZ	2:B:423:LYS:HB2	2.32	0.45
2:A:26:TYR:CE1	2:A:290:ILE:HD11	2.52	0.45
2:B:268:ASN:HD22	2:B:268:ASN:C	2.19	0.45
2:A:116:ARG:O	2:A:120:GLY:CA	2.63	0.44
2:B:244:ILE:HG22	4:B:602:ATP:HN62	1.81	0.44
2:A:262:LEU:HD22	2:A:330:ARG:NH1	2.32	0.44
2:A:393:LEU:CD2	2:A:393:LEU:H	2.24	0.44
2:A:445:PRO:HG2	2:A:450:ILE:HG12	1.99	0.44
2:B:371:TYR:HH	2:B:444:THR:HG1	1.57	0.44
2:B:363:LYS:O	2:B:367:GLU:HG3	2.18	0.44
1:C:509:C:H5	1:C:523:G:O6	2.01	0.44
2:B:144:HIS:O	2:B:181:SER:HA	2.18	0.44
2:A:319:ARG:HG3	2:A:320:GLU:HG3	1.99	0.44
2:B:325:GLU:O	2:B:329:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:237:ARG:NH1	2:A:241:LYS:O	2.49	0.44
1:D:570:G:H2'	1:D:571:U:C6	2.52	0.43
2:B:25:ASN:ND2	2:B:204:ILE:HB	2.33	0.43
2:B:148:LEU:HB2	2:B:178:LEU:HD21	1.99	0.43
2:A:275:PHE:CG	2:A:276:SER:N	2.86	0.43
2:B:40:ILE:HG13	2:B:53:GLU:OE2	2.17	0.43
2:B:324:LEU:HD11	2:B:353:GLU:HB2	1.99	0.43
2:B:5:ARG:HD2	2:B:5:ARG:O	2.18	0.43
2:A:205:ARG:CD	2:A:232:HIS:CE1	2.93	0.43
2:B:55:ARG:HD3	6:B:1198:HOH:O	2.19	0.43
2:A:37:ILE:HG22	2:A:38:VAL:N	2.32	0.43
2:B:365:PHE:HB3	2:B:366:PRO:HD3	2.01	0.43
2:A:195:ASP:HB3	2:A:200:VAL:CG2	2.49	0.43
2:A:259:GLU:OE1	2:A:363:LYS:HE3	2.19	0.43
2:B:94:GLU:O	2:B:97:LEU:HB2	2.19	0.43
2:B:44:ASP:OD2	2:B:47:ARG:HB2	2.19	0.43
2:B:82:GLN:NE2	2:B:190:ALA:HB1	2.34	0.43
2:A:96:LEU:HD13	2:A:223:PHE:CE1	2.54	0.43
2:A:365:PHE:HB3	2:A:366:PRO:HD3	2.00	0.43
1:C:566:U:O2'	1:C:567:G:H5'	2.19	0.43
5:A:702:GAU:N	2:B:41:GLU:OE2	2.51	0.43
1:C:508:U:C2	1:C:515:G:O6	2.72	0.43
2:B:275:PHE:CD1	2:B:276:SER:N	2.87	0.43
1:D:570:G:H21	2:B:211:VAL:CG2	2.22	0.42
1:D:569:G:O4'	2:B:237:ARG:NH2	2.53	0.42
2:B:115:ILE:O	2:B:119:LYS:HG2	2.19	0.42
2:A:81:ARG:NH1	2:A:84:GLU:OE2	2.32	0.42
2:A:101:TRP:CH2	2:A:221:ARG:HD2	2.54	0.42
1:D:514:A:C2'	1:D:515:G:H5'	2.49	0.42
2:A:419:PHE:O	2:A:423:LYS:HB2	2.19	0.42
2:B:136:GLU:O	2:B:140:ARG:HG2	2.19	0.42
2:B:296:GLU:OE1	2:B:296:GLU:N	2.52	0.42
2:A:7:ALA:HA	2:A:39:ARG:O	2.19	0.42
1:C:575:C:H2'	1:C:576:A:O4'	2.19	0.42
2:A:268:ASN:C	2:A:268:ASN:HD22	2.22	0.42
2:B:86:LEU:HB2	2:B:87:PRO:HD3	2.01	0.42
2:A:318:ILE:O	2:A:356:ARG:HD3	2.19	0.42
2:B:61:LYS:HE3	2:B:67:TYR:OH	2.20	0.42
2:A:397:LEU:HG	2:A:401:LEU:HD13	2.02	0.42
2:A:450:ILE:HA	2:A:450:ILE:HD13	1.96	0.42
2:B:238:ASN:O	2:B:304:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:240:ASP:C	2:A:240:ASP:OD1	2.57	0.41
2:B:213:THR:N	2:B:214:PRO:HD2	2.34	0.41
1:D:562:C:H2'	1:D:563:C:C6	2.55	0.41
2:B:261:PHE:CE2	2:B:310:LEU:HD13	2.54	0.41
2:A:6:ILE:HD12	2:A:6:ILE:HA	1.96	0.41
2:B:425:VAL:HG13	2:B:429:GLN:HB2	2.02	0.41
1:C:565:C:O2'	1:C:566:U:H5'	2.21	0.41
2:B:269:TYR:CE1	2:B:309:LYS:HB3	2.55	0.41
2:A:10:PRO:HG3	2:A:42:ASP:HB3	2.01	0.41
2:B:19:ALA:HB1	2:B:63:LEU:CD1	2.50	0.41
1:D:506:C:C2'	1:D:507:A:H5'	2.50	0.41
2:A:89:TYR:HB3	2:A:189:LEU:HD13	2.01	0.41
1:C:576:A:O3'	5:A:701:GAU:N	2.54	0.41
2:B:355:MET:HE3	2:B:358:ARG:HB2	2.01	0.41
1:C:565:C:H2'	1:C:566:U:C6	2.56	0.41
1:D:514:A:H2'	1:D:515:G:O4'	2.20	0.41
2:A:45:ARG:H	2:A:45:ARG:HG2	1.73	0.41
2:A:398:TYR:HB3	2:A:399:PRO:CD	2.51	0.41
2:B:205:ARG:HG3	2:B:209:TRP:HB2	2.03	0.41
2:B:244:ILE:HG22	4:B:602:ATP:N6	2.36	0.41
2:A:461:ARG:HH11	2:A:465:ARG:HD3	1.85	0.41
2:B:73:VAL:O	2:B:73:VAL:HG12	2.20	0.41
2:A:150:VAL:HA	2:A:151:PRO:HD3	1.89	0.41
2:B:130:PRO:HD2	2:B:133:GLU:OE2	2.22	0.40
2:B:116:ARG:HD2	2:B:121:GLY:N	2.35	0.40
2:B:240:ASP:O	2:B:241:LYS:HB2	2.21	0.40
2:A:396:GLU:OE1	2:A:423:LYS:NZ	2.53	0.40
2:B:311:ARG:NH1	2:B:311:ARG:CB	2.85	0.40
2:A:178:LEU:HA	2:A:178:LEU:HD23	1.94	0.40
2:A:434:LEU:HD23	2:A:447:LEU:HD21	2.04	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	466/468 (100%)	456 (98%)	10 (2%)	0	100	100
2	B	466/468 (100%)	454 (97%)	11 (2%)	1 (0%)	52	69
All	All	932/936 (100%)	910 (98%)	21 (2%)	1 (0%)	56	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	120	GLY

### 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	393/393 (100%)	361 (92%)	32 (8%)	15	21
2	B	393/393 (100%)	356 (91%)	37 (9%)	11	15
All	All	786/786 (100%)	717 (91%)	69 (9%)	12	18

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	ARG
2	A	41	GLU
2	A	63	LEU
2	A	67	TYR
2	A	90	GLN
2	A	96	LEU
2	A	132	GLU
2	A	189	LEU
2	A	197	LEU
2	A	205	ARG
2	A	218	LEU
2	A	257	LYS

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Mol	Chain	Res	Type
2	A	267	ARG
2	A	268	ASN
2	A	270	LEU
2	A	272	LEU
2	A	278	PRO
2	A	286	LEU
2	A	310	LEU
2	A	331	VAL
2	A	341	SER
2	A	356	ARG
2	A	393	LEU
2	A	401	LEU
2	A	412	LEU
2	A	429	GLN
2	A	442	LEU
2	A	449	GLU
2	A	451	LEU
2	A	453	LEU
2	A	457	GLU
2	A	463	LEU
2	B	1	MET
2	B	86	LEU
2	B	90	GLN
2	B	115	ILE
2	B	116	ARG
2	B	119	LYS
2	B	171	GLN
2	B	179	LEU
2	B	185	PRO
2	B	189	LEU
2	B	205	ARG
2	B	218	LEU
2	B	236	LEU
2	B	243	LYS
2	B	259	GLU
2	B	266	LEU
2	B	267	ARG
2	B	268	ASN
2	B	270	LEU
2	B	272	LEU
2	B	296	GLU
2	B	308	GLU

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Mol	Chain	Res	Type
2	B	310	LEU
2	B	324	LEU
2	B	331	VAL
2	B	355	MET
2	B	356	ARG
2	B	375	GLU
2	B	402	ARG
2	B	412	LEU
2	B	423	LYS
2	B	425	VAL
2	B	432	GLN
2	B	442	LEU
2	B	444	THR
2	B	454	LEU
2	B	463	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	90	GLN
2	A	232	HIS
2	B	25	ASN
2	B	171	GLN
2	B	188	HIS
2	B	191	ASN
2	B	232	HIS
2	B	404	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	14 (18%)	8 (10%)
1	D	74/75 (98%)	12 (16%)	8 (10%)
All	All	148/150 (98%)	26 (17%)	16 (10%)

All (26) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	507	A
1	C	508	U

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Mol	Chain	Res	Type
1	C	509	C
1	C	516	C
1	C	518	G
1	C	519	G
1	C	520	U
1	C	548	C
1	C	553	G
1	C	558	A
1	C	559	U
1	C	573	A
1	C	574	C
1	C	575	C
1	D	508	U
1	D	509	C
1	D	516	C
1	D	518	G
1	D	519	G
1	D	520	U
1	D	548	C
1	D	558	A
1	D	559	U
1	D	573	A
1	D	574	C
1	D	575	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	507	A
1	C	515	G
1	C	518	G
1	C	519	G
1	C	558	A
1	C	560	U
1	C	573	A
1	C	574	C
1	D	507	A
1	D	515	G
1	D	518	G
1	D	519	G
1	D	558	A
1	D	560	U

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Mol	Chain	Res	Type
1	D	573	A
1	D	574	C

## 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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ATP	A	601	-	24,33,33	0.94	2 (8%)	31,52,52	0.91	1 (3%)
5	GAU	A	701	-	5,8,8	0.61	0	3,9,9	0.37	0
5	GAU	A	702	-	5,8,8	0.36	0	3,9,9	0.39	0
4	ATP	B	602	-	24,33,33	0.83	0	31,52,52	0.94	2 (6%)

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
4	ATP	A	601	-	-	0/18/38/38	0/3/3/3
5	GAU	A	701	-	-	0/5/7/7	0/0/0/0
5	GAU	A	702	-	-	0/5/7/7	0/0/0/0
4	ATP	B	602	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	ATP	C2-N3	2.00	1.35	1.32
4	A	601	ATP	O4'-C1'	2.03	1.43	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	ATP	PA-O3A-PB	-2.42	125.93	132.73
4	A	601	ATP	PA-O3A-PB	-2.31	126.25	132.73
4	B	602	ATP	PB-O3B-PG	-2.05	125.79	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	ATP	3	0
5	A	701	GAU	2	0
5	A	702	GAU	4	0
4	B	602	ATP	3	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	C	75/75 (100%)	0.61	10 (13%) <b>4</b> <b>4</b>	37, 60, 101, 105	0
1	D	75/75 (100%)	0.52	8 (10%) <b>8</b> <b>7</b>	35, 55, 95, 112	0
2	A	468/468 (100%)	-0.06	8 (1%) <b>73</b> <b>72</b>	22, 37, 70, 83	0
2	B	468/468 (100%)	0.10	20 (4%) <b>39</b> <b>39</b>	24, 41, 90, 107	0
All	All	1086/1086 (100%)	0.10	46 (4%) <b>40</b> <b>40</b>	22, 41, 90, 112	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	516	C	5.9
1	C	516	C	5.0
1	C	555	U	5.0
1	C	556	C	5.0
2	B	139	ARG	4.8
1	D	561	C	4.8
2	B	117	LYS	4.7
1	C	554	U	4.2
2	B	108	THR	3.9
2	A	468	ALA	3.8
2	B	141	GLY	3.5
1	D	519	G	3.5
2	B	140	ARG	3.4
2	B	122	TYR	3.3
1	C	558	A	3.3
2	B	11	THR	3.2
2	B	109	PRO	3.2
1	D	576	A	3.2
2	B	128	ASN	3.0
1	D	558	A	3.0
2	B	112	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	A	466	ALA	2.9
1	D	575	C	2.9
2	B	50	PRO	2.6
2	A	398	TYR	2.6
2	B	181	SER	2.5
2	A	393	LEU	2.5
2	A	425	VAL	2.5
1	C	565	C	2.4
2	B	110	GLU	2.4
1	D	557	G	2.4
1	C	562	C	2.3
1	D	555	U	2.3
1	C	557	G	2.3
2	B	138	ALA	2.3
2	A	465	ARG	2.3
2	B	114	GLN	2.3
2	B	184	TYR	2.3
1	C	559	U	2.3
2	A	247	ARG	2.3
2	B	135	GLU	2.2
2	A	403	ALA	2.2
2	B	367	GLU	2.2
2	B	113	GLU	2.1
1	C	501	G	2.1
2	B	10	PRO	2.1

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

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
4	ATP	A	601	31/31	0.76	0.28	3.52	83,104,127,127	0
4	ATP	B	602	31/31	0.75	0.24	0.91	84,110,136,137	0
5	GAU	A	702	9/9	0.90	0.21	0.40	50,54,60,66	0
5	GAU	A	701	9/9	0.96	0.18	-0.04	24,29,39,45	0
3	MG	C	901	1/1	0.95	0.14	-	55,55,55,55	0
3	MG	C	902	1/1	0.95	0.28	-	24,24,24,24	0
3	MG	D	904	1/1	0.92	0.32	-	24,24,24,24	0
3	MG	D	903	1/1	0.95	0.23	-	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.