



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:41 AM GMT

PDB ID : 2DXI
Title : 2.2 Å crystal structure of glutamyl-tRNA synthetase from *Thermus thermophilus* complexed with tRNA(Glu), ATP, and L-glutamol
Authors : Sekine, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-08-28
Resolution : 2.20 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

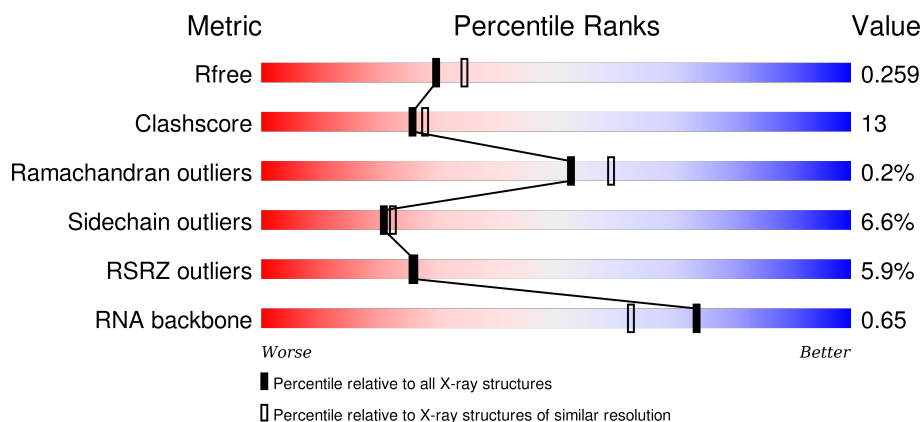
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)
RNA backbone	2183	1062 (2.80-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>9%</div> <div> <div></div> <div>55%</div> <div>29%</div> <div>9%</div> <div>7%</div> </div> </div>
1	D	75	<div> <div>17%</div> <div> <div></div> <div>56%</div> <div>28%</div> <div>11%</div> <div>5%</div> </div> </div>
2	A	468	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>.</div> </div> </div>
2	B	468	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>26%</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 11272 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			

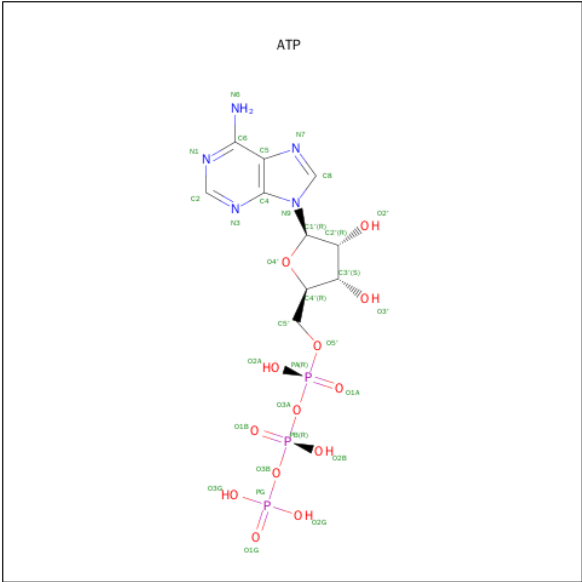
- Molecule 2 is a protein called glutamyl-tRNA synthetase.

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).

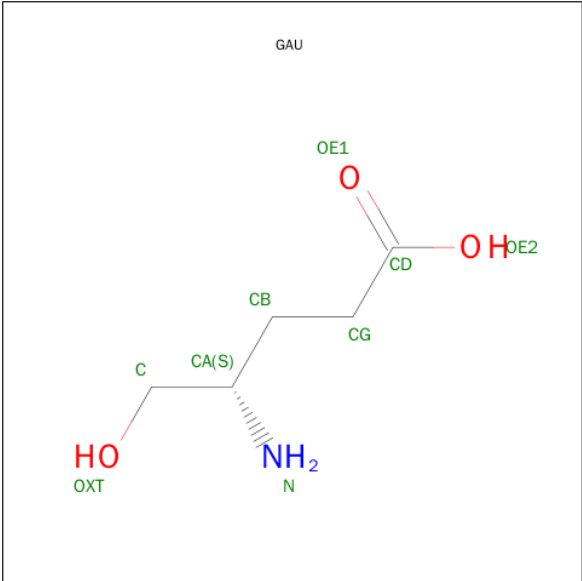
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 5 is (4S)-4-AMINO-5-HYDROXYPENTANOIC ACID (three-letter code: GAU) (formula: C₅H₁₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			18	10	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total	O	0	0
			147	147		
6	B	130	Total	O	0	0
			130	130		
6	C	38	Total	O	0	0
			38	38		
6	D	44	Total	O	0	0
			44	44		

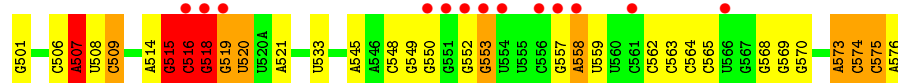
3 Residue-property plots [i](#)

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.

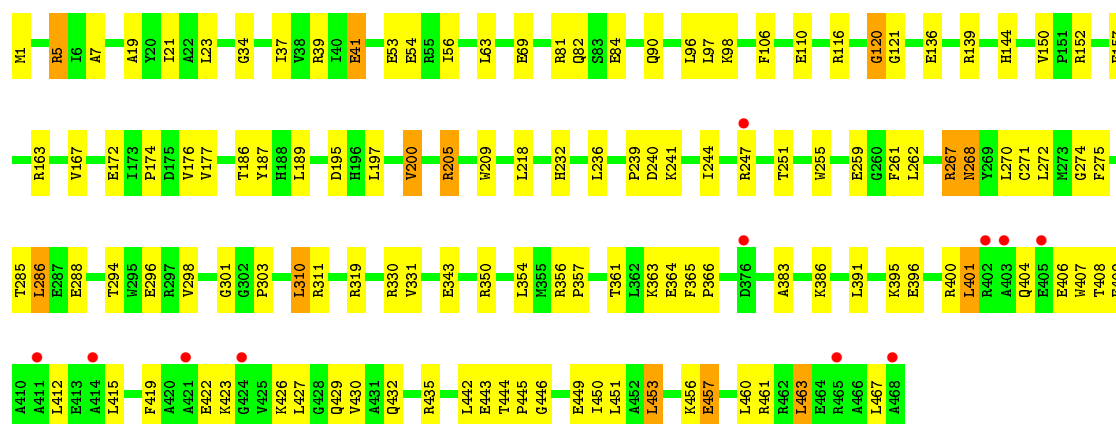
• Molecule 1: tRNA



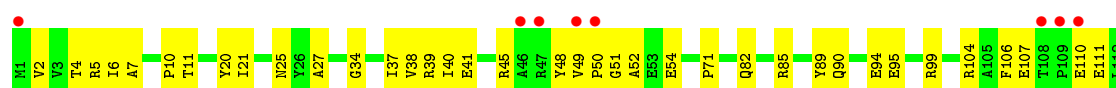
• Molecule 1: tRNA

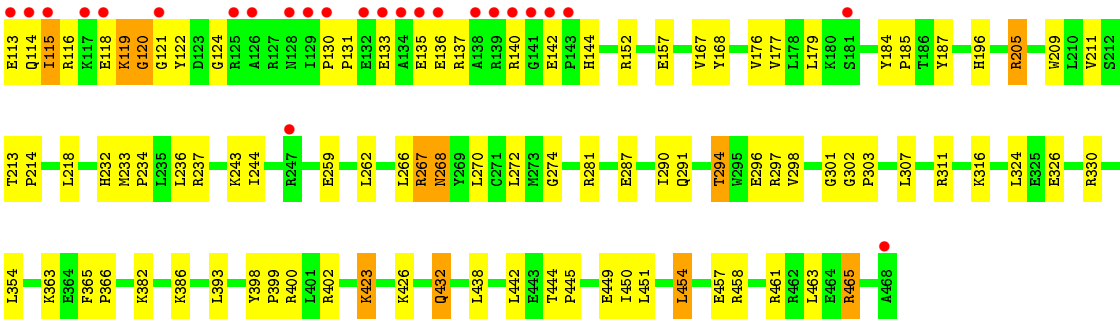


• Molecule 2: glutamyl-tRNA synthetase



• 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, α , β , γ	110.61Å 219.12Å 135.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.20 49.37 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.97-2.20) 99.2 (49.37-2.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.257 0.215 , 0.259	Depositor DCC
R_{free} test set	4167 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 96114 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11272	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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%)	0.89	11/2774 (0.4%)
1	D	0.50	1/1782 (0.1%)	0.87	11/2774 (0.4%)
2	A	0.57	0/3910	0.72	0/5293
2	B	0.54	0/3910	0.69	1/5293 (0.0%)
All	All	0.54	2/11384 (0.0%)	0.77	23/16134 (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	C	0	2
1	D	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	501	G	OP3-P	-7.81	1.51	1.61
1	D	501	G	OP3-P	-5.33	1.54	1.61

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	558	A	C2'-C3'-O3'	8.09	127.29	109.50
1	D	558	A	C2'-C3'-O3'	8.06	127.24	109.50
1	C	573	A	C2'-C3'-O3'	7.74	126.53	109.50
1	D	518	G	C2'-C3'-O3'	7.72	126.48	109.50
1	C	518	G	C2'-C3'-O3'	7.67	126.37	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	519	G	C2'-C3'-O3'	7.55	126.11	109.50
1	D	573	A	C2'-C3'-O3'	7.31	125.58	109.50
1	D	519	G	C2'-C3'-O3'	7.15	125.22	109.50
1	D	507	A	C2'-C3'-O3'	6.80	124.58	113.70
1	C	516	C	C2'-C3'-O3'	6.41	123.96	113.70
2	B	267	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	D	516	C	C2'-C3'-O3'	6.21	123.64	113.70
1	D	509	C	N1-C1'-C2'	6.15	122.00	114.00
1	C	548	C	N1-C1'-C2'	6.14	121.99	114.00
1	D	558	A	C4'-C3'-C2'	5.67	108.27	102.60
1	C	576	A	C2'-C3'-O3'	5.65	122.74	113.70
1	C	558	A	C4'-C3'-C2'	5.64	108.24	102.60
1	C	516	C	C4'-C3'-C2'	5.54	108.14	102.60
1	C	509	C	N1-C1'-C2'	5.50	121.15	114.00
1	D	516	C	C4'-C3'-C2'	5.43	108.03	102.60
1	D	507	A	C4'-C3'-C2'	5.39	107.99	102.60
1	D	518	G	C4'-C3'-C2'	5.08	107.68	102.60
1	C	518	G	C4'-C3'-O3'	5.07	123.14	113.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	515	G	Sidechain
1	C	545	A	Sidechain
1	D	515	G	Sidechain
1	D	533	U	Sidechain
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	28	0
1	D	1597	0	813	27	0
2	A	3814	0	3818	103	1
2	B	3814	0	3818	108	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	3	0
4	B	31	0	12	2	0
5	A	18	0	20	6	0
5	B	9	0	10	4	0
6	A	147	0	0	2	0
6	B	130	0	0	4	0
6	C	38	0	0	4	0
6	D	44	0	0	0	0
All	All	11272	0	9316	253	1

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 13.

All (253) 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	1.20	1.04
2:A:37:ILE:HD12	2:A:69:GLU:HB2	1.39	1.00
2:A:426:LYS:HG3	2:A:429:GLN:HE21	1.28	0.96
2:A:41:GLU:HG3	2:A:82:GLN:OE1	1.69	0.92
2:B:454:LEU:H	2:B:454:LEU:HD22	1.36	0.90
2:A:157:GLU:HG2	2:A:167:VAL:HG22	1.57	0.86
1:D:506:C:O2'	1:D:507:A:H5'	1.76	0.84
2:A:177:VAL:HG23	2:A:186:THR:HG21	1.56	0.84
2:B:465:ARG:HB3	2:B:465:ARG:HH11	1.43	0.82
2:A:294:THR:HG22	2:A:296:GLU:N	1.93	0.82
2:A:54:GLU:HG2	6:A:1241:HOH:O	1.80	0.82
2:B:4:THR:HB	2:B:25:ASN:HD22	1.48	0.79
1:C:572:C:H5'	6:C:1189:HOH:O	1.85	0.77
2:B:402:ARG:HH11	2:B:402:ARG:HG2	1.49	0.76
2:B:262:LEU:HD22	2:B:330:ARG:HH11	1.49	0.76
1:D:570:G:H5''	2:B:243:LYS:HD2	1.68	0.75
2:A:445:PRO:HG2	2:A:450:ILE:HD11	1.70	0.74
2:A:408:THR:O	2:A:412:LEU:HD23	1.88	0.73
2:B:104:ARG:HB3	2:B:144:HIS:HD2	1.55	0.72
2:A:1:MET:HE3	2:A:34:GLY:HA2	1.72	0.71
2:A:386:LYS:HE3	2:A:432:GLN:HG2	1.70	0.71
2:B:454:LEU:N	2:B:454:LEU:HD22	2.03	0.70
2:B:10:PRO:HB3	2:B:52:ALA:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365:PHE:HB3	2:B:366:PRO:HD3	1.75	0.69
1:D:574:C:H5''	2:B:177:VAL:HG21	1.73	0.68
1:D:576:A:H5''	2:B:187:TYR:HB2	1.75	0.68
2:B:10:PRO:CB	2:B:52:ALA:HB3	2.23	0.68
1:C:518:G:O2'	1:C:557:G:N2	2.27	0.68
2:A:244:ILE:HG22	4:A:601:ATP:HN62	1.56	0.68
2:B:116:ARG:O	2:B:120:GLY:HA2	1.93	0.68
2:B:465:ARG:NH1	2:B:465:ARG:HB3	2.10	0.67
1:D:563:C:H2'	1:D:564:C:C6	2.29	0.67
2:A:294:THR:CG2	2:A:296:GLU:H	2.03	0.66
6:C:1009:HOH:O	2:A:41:GLU:HG2	1.95	0.66
1:D:518:G:O2'	1:D:557:G:N2	2.28	0.66
1:C:506:C:O2'	1:C:507:A:H5'	1.95	0.65
2:B:454:LEU:N	2:B:454:LEU:HD13	2.11	0.65
2:B:27:ALA:HA	2:B:290:ILE:HG22	1.78	0.65
2:A:1:MET:CE	2:A:34:GLY:HA2	2.27	0.65
2:A:255:TRP:CZ2	2:A:259:GLU:HG3	2.33	0.64
2:B:294:THR:HG23	2:B:297:ARG:HG2	1.79	0.64
2:A:116:ARG:O	2:A:120:GLY:HA2	1.97	0.64
2:A:404:GLN:CG	2:A:415:LEU:HD22	2.28	0.63
2:A:365:PHE:HB3	2:A:366:PRO:HD3	1.79	0.63
2:B:152:ARG:HH11	2:B:152:ARG:HG2	1.63	0.63
2:B:454:LEU:CD2	2:B:454:LEU:H	2.06	0.63
2:B:205:ARG:HD3	2:B:232:HIS:NE2	2.13	0.63
2:A:261:PHE:CE2	2:A:310:LEU:HD13	2.33	0.63
2:A:383:ALA:HA	2:A:442:LEU:CD1	2.28	0.63
2:A:354:LEU:HD12	2:A:453:LEU:HD12	1.81	0.61
1:C:563:C:H2'	1:C:564:C:C6	2.35	0.61
2:B:114:GLN:O	2:B:118:GLU:HG2	2.01	0.61
2:A:205:ARG:HD3	2:A:232:HIS:NE2	2.15	0.61
2:B:106:PHE:CD2	2:B:144:HIS:HB3	2.36	0.61
2:A:361:THR:OG1	2:A:364:GLU:HG3	2.01	0.61
1:D:563:C:H2'	1:D:564:C:H6	1.66	0.61
2:A:21:ILE:HG13	4:A:601:ATP:H1'	1.83	0.60
2:A:400:ARG:HH22	2:A:422:GLU:CD	2.04	0.60
2:B:136:GLU:O	2:B:140:ARG:HG2	2.01	0.60
2:A:209:TRP:CZ2	5:A:701[B]:GAU:HO1	2.37	0.60
4:A:601:ATP:H3'	5:A:701[B]:GAU:OXT	2.02	0.59
2:B:386:LYS:NZ	2:B:432:GLN:HG2	2.17	0.59
2:B:45:ARG:HD3	2:B:184:TYR:CZ	2.37	0.59
2:A:391:LEU:O	2:A:395:LYS:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:LEU:HD11	2:B:451:LEU:HD13	1.84	0.59
2:A:267:ARG:HD2	2:A:286:LEU:HG	1.84	0.58
2:B:137:ARG:HB3	2:B:142:GLU:OE1	2.04	0.58
2:B:130:PRO:HD2	2:B:133:GLU:OE2	2.03	0.58
2:A:404:GLN:HG3	2:A:415:LEU:HD22	1.85	0.58
2:A:116:ARG:HA	2:A:121:GLY:H	1.69	0.57
2:A:177:VAL:HG23	2:A:186:THR:CG2	2.33	0.57
2:B:104:ARG:HE	2:B:144:HIS:CD2	2.23	0.56
2:A:53:GLU:O	2:A:56:ILE:HG22	2.05	0.56
1:D:562:C:H2'	1:D:563:C:C6	2.41	0.56
2:B:402:ARG:NH1	2:B:402:ARG:HG2	2.18	0.56
2:B:423:LYS:NZ	2:B:423:LYS:HB2	2.21	0.56
2:B:196:HIS:HD2	6:B:1043:HOH:O	1.87	0.56
1:D:514:A:C2'	1:D:515:G:H5'	2.36	0.56
2:B:95:GLU:HG3	2:B:99:ARG:HD2	1.89	0.55
2:B:287:GLU:OE1	2:B:290:ILE:HD11	2.06	0.55
2:A:240:ASP:O	2:A:241:LYS:HB2	2.06	0.55
2:A:350:ARG:NH2	2:A:409:GLU:OE1	2.39	0.55
2:A:41:GLU:OE2	5:A:701[B]:GAU:N	2.40	0.54
2:B:116:ARG:HA	2:B:121:GLY:H	1.72	0.54
4:B:602:ATP:H3'	5:B:702:GAU:OXT	2.08	0.54
2:B:274:GLY:O	2:B:298:VAL:HA	2.07	0.54
1:D:568:G:O2'	1:D:569:G:H5'	2.08	0.54
2:B:444:THR:HB	2:B:445:PRO:HD2	1.90	0.53
2:A:383:ALA:HA	2:A:442:LEU:HD13	1.89	0.53
2:B:454:LEU:H	2:B:454:LEU:HD13	1.72	0.53
2:B:133:GLU:O	2:B:137:ARG:HG3	2.08	0.53
2:B:423:LYS:HZ3	2:B:423:LYS:HB2	1.73	0.53
2:B:244:ILE:HG22	4:B:602:ATP:N6	2.23	0.53
2:A:407:TRP:CZ3	2:A:456:LYS:HG3	2.43	0.53
2:B:41:GLU:HG2	2:B:82:GLN:CD	2.29	0.53
2:A:311:ARG:NH1	2:A:311:ARG:HB3	2.23	0.53
1:D:562:C:H2'	1:D:563:C:H6	1.73	0.52
2:A:174:PRO:HG2	2:A:176:VAL:HG13	1.91	0.52
2:A:294:THR:HG21	2:A:296:GLU:HB2	1.92	0.52
2:A:396:GLU:OE1	2:A:423:LYS:NZ	2.43	0.52
2:B:382:LYS:HB3	2:B:382:LYS:NZ	2.23	0.52
2:B:398:TYR:HB3	2:B:399:PRO:HD3	1.92	0.52
2:B:115:ILE:HD11	2:B:122:TYR:HA	1.91	0.52
1:C:562:C:H2'	1:C:563:C:C6	2.44	0.52
2:A:311:ARG:NH2	2:A:364:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:576:A:H2'	2:B:209:TRP:CH2	2.45	0.52
2:B:311:ARG:HB3	2:B:311:ARG:NH1	2.25	0.52
2:A:294:THR:CG2	2:A:296:GLU:HB2	2.40	0.52
1:D:570:G:H21	2:B:211:VAL:HG21	1.75	0.52
1:C:562:C:H2'	1:C:563:C:H6	1.74	0.51
2:A:268:ASN:C	2:A:268:ASN:HD22	2.13	0.51
2:B:393:LEU:HD21	2:B:423:LYS:HG2	1.93	0.51
2:A:354:LEU:CD1	2:A:453:LEU:HD12	2.39	0.51
2:A:400:ARG:NH2	2:A:422:GLU:OE2	2.39	0.51
1:C:574:C:H4'	2:A:177:VAL:HG21	1.93	0.51
2:A:7:ALA:HA	2:A:39:ARG:O	2.11	0.51
2:B:157:GLU:HG2	2:B:167:VAL:HG22	1.92	0.51
2:B:294:THR:CG2	2:B:297:ARG:HG2	2.41	0.51
2:A:427:LEU:O	2:A:430:VAL:HG12	2.11	0.51
1:D:576:A:H2'	2:B:209:TRP:HH2	1.75	0.50
1:C:563:C:H2'	1:C:564:C:H6	1.74	0.50
2:A:301:GLY:O	2:A:303:PRO:HD3	2.10	0.50
2:A:426:LYS:HG3	2:A:429:GLN:NE2	2.11	0.50
2:B:6:ILE:CD1	2:B:21:ILE:HG22	2.42	0.50
1:C:574:C:H5''	2:A:177:VAL:HG11	1.92	0.50
2:B:115:ILE:HD13	2:B:116:ARG:N	2.27	0.50
2:B:48:TYR:OH	2:B:50:PRO:HB3	2.12	0.50
2:B:107:GLU:H	2:B:107:GLU:CD	2.15	0.50
2:A:457:GLU:O	2:A:461:ARG:HB2	2.12	0.50
2:B:301:GLY:O	2:B:303:PRO:HD3	2.13	0.49
2:B:465:ARG:NH1	6:B:1216:HOH:O	2.42	0.49
2:A:404:GLN:HG2	2:A:415:LEU:HD22	1.93	0.49
1:C:576:A:H5'	6:C:1009:HOH:O	2.13	0.49
2:A:383:ALA:HA	2:A:442:LEU:HD11	1.95	0.49
2:B:7:ALA:HA	2:B:39:ARG:O	2.12	0.49
1:C:505:C:O2'	2:A:163:ARG:NH1	2.46	0.49
2:B:326:GLU:O	2:B:330:ARG:HG3	2.13	0.48
2:A:41:GLU:OE2	5:A:701[A]:GAU:N	2.42	0.48
2:B:118:GLU:HB2	2:B:119:LYS:HD2	1.96	0.48
2:B:110:GLU:H	2:B:110:GLU:CD	2.17	0.48
2:A:5:ARG:HB3	2:A:37:ILE:HB	1.96	0.48
2:A:311:ARG:CB	2:A:311:ARG:HH11	2.27	0.48
1:C:576:A:H5''	2:A:187:TYR:HB2	1.96	0.48
2:B:262:LEU:HD22	2:B:330:ARG:NH1	2.23	0.48
2:B:296:GLU:OE1	2:B:296:GLU:N	2.47	0.47
2:A:445:PRO:CG	2:A:450:ILE:HD11	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:ASN:HD22	2:B:268:ASN:C	2.17	0.47
1:C:518:G:N2	1:C:558:A:OP2	2.48	0.47
2:A:419:PHE:HA	2:A:422:GLU:HG2	1.97	0.47
2:B:89:TYR:CD2	2:B:185:PRO:HG3	2.50	0.47
2:A:255:TRP:CE2	2:A:259:GLU:HG3	2.49	0.47
2:B:115:ILE:O	2:B:119:LYS:HG2	2.15	0.47
2:A:445:PRO:HG2	2:A:450:ILE:CD1	2.43	0.46
2:B:213:THR:N	2:B:214:PRO:CD	2.78	0.46
2:A:311:ARG:HB3	2:A:311:ARG:HH11	1.79	0.46
2:B:111:GLU:O	2:B:115:ILE:HG23	2.16	0.46
2:B:113:GLU:HA	2:B:113:GLU:OE1	2.14	0.46
2:A:426:LYS:CG	2:A:429:GLN:HE21	2.15	0.46
2:A:106:PHE:CD2	2:A:144:HIS:HB3	2.51	0.46
1:C:514:A:C2'	1:C:515:G:H5'	2.46	0.46
2:B:2:VAL:O	2:B:34:GLY:HA3	2.16	0.46
2:A:435:ARG:HD3	2:A:444:THR:OG1	2.16	0.46
2:B:51:GLY:O	2:B:54:GLU:HG2	2.16	0.46
2:B:37:ILE:HG22	2:B:38:VAL:N	2.31	0.46
1:D:564:C:O2'	1:D:565:C:H5'	2.16	0.46
1:C:562:C:O2'	1:C:563:C:H5'	2.16	0.46
2:B:205:ARG:HG3	2:B:209:TRP:CD1	2.51	0.45
2:A:444:THR:HB	2:A:445:PRO:HD2	1.98	0.45
2:A:463:LEU:HD23	2:A:463:LEU:O	2.16	0.45
2:B:454:LEU:HB3	2:B:458:ARG:HD2	1.99	0.45
2:B:363:LYS:O	2:B:366:PRO:HD2	2.16	0.45
2:A:262:LEU:HD22	2:A:330:ARG:HH11	1.82	0.45
2:B:294:THR:HG23	2:B:297:ARG:CG	2.44	0.45
2:A:401:LEU:HB3	2:A:460:LEU:HD21	1.99	0.45
1:C:535:U:C4'	2:A:432:GLN:HE22	2.30	0.45
2:A:406:GLU:O	2:A:406:GLU:HG3	2.17	0.45
2:A:110:GLU:H	2:A:110:GLU:CD	2.19	0.45
2:A:205:ARG:HD3	2:A:232:HIS:CD2	2.52	0.45
2:A:244:ILE:HG12	2:A:251:THR:HG22	1.99	0.45
2:A:363:LYS:O	2:A:366:PRO:HD2	2.17	0.45
2:B:90:GLN:O	2:B:94:GLU:HG3	2.17	0.45
2:B:423:LYS:NZ	2:B:423:LYS:CB	2.79	0.44
2:B:211:VAL:HG23	6:B:1110:HOH:O	2.16	0.44
1:C:535:U:H4'	2:A:432:GLN:HE22	1.82	0.44
1:C:574:C:C4'	2:A:177:VAL:HG21	2.47	0.44
1:D:569:G:O2'	1:D:570:G:H5'	2.16	0.44
2:B:48:TYR:CE1	2:B:50:PRO:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:VAL:HB	6:B:1316:HOH:O	2.17	0.44
2:B:237:ARG:NH1	2:B:302:GLY:HA3	2.32	0.44
2:A:23:LEU:HD21	2:A:271:CYS:SG	2.58	0.44
2:B:40:ILE:HG12	2:B:71:PRO:HG2	1.99	0.44
2:B:10:PRO:CA	2:B:52:ALA:HB3	2.48	0.44
1:D:516:C:H5'	1:D:516:C:H6	1.83	0.44
2:B:11:THR:HA	2:B:49:VAL:HG23	2.00	0.44
2:B:209:TRP:CZ2	5:B:702:GAU:HO1	2.53	0.44
1:D:575:C:H2'	1:D:576:A:O4'	2.18	0.44
2:B:20:TYR:CD2	2:B:21:ILE:HD12	2.53	0.44
2:B:354:LEU:HD22	2:B:449:GLU:HG3	1.99	0.44
1:C:568:G:O2'	1:C:569:G:H5'	2.18	0.44
2:B:41:GLU:OE2	5:B:702:GAU:N	2.51	0.43
2:A:239:PRO:HD2	6:A:1202:HOH:O	2.18	0.43
2:A:150:VAL:O	2:A:152:ARG:HG3	2.19	0.43
1:C:519:G:C6	1:C:557:G:N2	2.86	0.43
2:A:136:GLU:HA	2:A:139:ARG:HE	1.83	0.43
1:D:562:C:O2'	1:D:563:C:H5'	2.19	0.43
1:C:576:A:O3'	5:A:701[B]:GAU:N	2.48	0.43
1:C:519:G:C5	1:C:557:G:N2	2.86	0.43
2:A:271:CYS:O	2:A:275:PHE:HB3	2.19	0.43
2:A:136:GLU:HG2	2:A:139:ARG:HH21	1.84	0.43
1:D:552:G:H5'	1:D:553:G:OP2	2.19	0.43
2:A:274:GLY:O	2:A:298:VAL:HA	2.19	0.43
1:D:576:A:O3'	5:B:702:GAU:N	2.51	0.43
2:B:104:ARG:HB3	2:B:144:HIS:CD2	2.45	0.42
2:B:152:ARG:HG2	2:B:152:ARG:NH1	2.32	0.42
1:C:509:C:H5	1:C:523:G:O6	2.02	0.42
2:B:465:ARG:CB	2:B:465:ARG:NH1	2.80	0.42
2:B:402:ARG:NH1	2:B:402:ARG:CG	2.82	0.42
2:B:122:TYR:CE2	2:B:124:GLY:HA2	2.54	0.42
1:C:576:A:O3'	5:A:701[A]:GAU:N	2.51	0.42
2:A:261:PHE:CD2	2:A:310:LEU:HD13	2.54	0.42
2:A:195:ASP:HB3	2:A:200:VAL:HG22	2.01	0.42
2:B:85:ARG:HD2	2:B:89:TYR:OH	2.19	0.42
1:D:514:A:H2'	1:D:515:G:O4'	2.19	0.42
2:B:281:ARG:O	2:B:281:ARG:HG3	2.20	0.42
2:A:37:ILE:HD12	2:A:69:GLU:CB	2.29	0.42
1:D:514:A:O2'	1:D:515:G:H5'	2.20	0.42
2:A:463:LEU:O	2:A:467:LEU:HG	2.20	0.42
2:A:446:GLY:O	2:A:449:GLU:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:205:ARG:HG3	2:A:209:TRP:CD1	2.55	0.41
2:B:131:PRO:O	2:B:135:GLU:HG2	2.20	0.41
2:A:319:ARG:HD3	2:A:357:PRO:HA	2.03	0.41
2:B:7:ALA:HB1	2:B:41:GLU:HG3	2.02	0.41
2:B:386:LYS:HZ3	2:B:432:GLN:HG2	1.86	0.41
2:A:136:GLU:HG2	2:A:139:ARG:NH2	2.35	0.41
2:B:45:ARG:HD3	2:B:184:TYR:CE2	2.54	0.41
6:C:1198:HOH:O	2:A:172:GLU:HG2	2.21	0.41
1:D:549:G:C2	1:D:550:G:C8	3.09	0.41
2:A:19:ALA:HB1	2:A:63:LEU:CD1	2.51	0.41
2:B:233:MET:HA	2:B:234:PRO:HD3	1.91	0.41
1:D:514:A:H2'	1:D:515:G:H5'	2.02	0.41
1:C:536:C:H2'	1:C:537:A:O4'	2.20	0.41
1:C:550:G:O2'	1:C:551:G:H5'	2.21	0.41
2:B:450:ILE:HA	2:B:450:ILE:HD13	1.97	0.41
1:D:520:U:H2'	1:D:521:A:H5'	2.03	0.41
2:B:168:TYR:CD2	2:B:214:PRO:HG3	2.56	0.40
1:C:536:C:H4'	2:A:443:GLU:HG2	2.02	0.40
1:C:574:C:O2'	1:C:575:C:OP1	2.34	0.40
1:D:569:G:H4'	2:B:237:ARG:NH2	2.37	0.40
2:A:354:LEU:HD22	2:A:449:GLU:HG3	2.04	0.40
2:A:81:ARG:HD2	2:A:84:GLU:OE2	2.21	0.40
2:B:457:GLU:O	2:B:461:ARG:HG2	2.21	0.40
2:B:37:ILE:CG2	2:B:38:VAL:N	2.84	0.40
2:A:285:THR:OG1	2:A:288:GLU:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:343:GLU:O	2:B:50:PRO:O[6_654]	2.19	0.01

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%)	455 (98%)	10 (2%)	1 (0%)	52	59
2	B	466/468 (100%)	460 (99%)	5 (1%)	1 (0%)	52	59
All	All	932/936 (100%)	915 (98%)	15 (2%)	2 (0%)	52	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	120	GLY
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%)	367 (93%)	26 (7%)	21	22
2	B	393/393 (100%)	367 (93%)	26 (7%)	21	22
All	All	786/786 (100%)	734 (93%)	52 (7%)	21	22

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	ARG
2	A	41	GLU
2	A	90	GLN
2	A	96	LEU
2	A	97	LEU
2	A	98	LYS
2	A	189	LEU
2	A	197	LEU
2	A	200	VAL
2	A	205	ARG
2	A	218	LEU

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Mol	Chain	Res	Type
2	A	236	LEU
2	A	247	ARG
2	A	267	ARG
2	A	268	ASN
2	A	270	LEU
2	A	272	LEU
2	A	286	LEU
2	A	310	LEU
2	A	331	VAL
2	A	356	ARG
2	A	401	LEU
2	A	451	LEU
2	A	453	LEU
2	A	457	GLU
2	A	463	LEU
2	B	5	ARG
2	B	115	ILE
2	B	119	LYS
2	B	179	LEU
2	B	205	ARG
2	B	218	LEU
2	B	236	LEU
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	291	GLN
2	B	294	THR
2	B	307	LEU
2	B	316	LYS
2	B	324	LEU
2	B	400	ARG
2	B	423	LYS
2	B	426	LYS
2	B	432	GLN
2	B	442	LEU
2	B	454	LEU
2	B	463	LEU
2	B	465	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such

sidechains are listed below:

Mol	Chain	Res	Type
2	A	32	ASN
2	A	90	GLN
2	A	114	GLN
2	A	429	GLN
2	B	25	ASN
2	B	171	GLN
2	B	191	ASN
2	B	196	HIS
2	B	404	GLN
2	B	432	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	14 (18%)	7 (9%)
1	D	74/75 (98%)	14 (18%)	7 (9%)
All	All	148/150 (98%)	28 (18%)	14 (9%)

All (28) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	507	A
1	C	508	U
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	507	A
1	D	508	U
1	D	509	C
1	D	516	C
1	D	518	G
1	D	519	G

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Mol	Chain	Res	Type
1	D	520	U
1	D	548	C
1	D	553	G
1	D	558	A
1	D	559	U
1	D	573	A
1	D	574	C
1	D	575	C

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	507	A
1	C	515	G
1	C	516	C
1	C	518	G
1	C	519	G
1	C	558	A
1	C	573	A
1	D	507	A
1	D	515	G
1	D	516	C
1	D	518	G
1	D	519	G
1	D	558	A
1	D	573	A

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	1.04	1 (4%)	31,52,52	1.02	1 (3%)
5	GAU	A	701[A]	-	5,8,8	0.35	0	3,9,9	0.78	0
5	GAU	A	701[B]	-	5,8,8	0.63	0	3,9,9	0.48	0
4	ATP	B	602	-	24,33,33	0.81	1 (4%)	31,52,52	0.92	1 (3%)
5	GAU	B	702	-	5,8,8	0.38	0	3,9,9	0.27	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
4	ATP	A	601	-	-	0/18/38/38	0/3/3/3
5	GAU	A	701[A]	-	-	0/5/7/7	0/0/0/0
5	GAU	A	701[B]	-	-	0/5/7/7	0/0/0/0
4	ATP	B	602	-	-	0/18/38/38	0/3/3/3
5	GAU	B	702	-	-	0/5/7/7	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	ATP	C2-N3	2.18	1.36	1.32
4	A	601	ATP	C2-N3	2.54	1.36	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	ATP	PB-O3B-PG	-2.36	124.76	132.67
4	A	601	ATP	O5'-C5'-C4'	2.13	116.99	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	ATP	3	0
5	A	701[A]	GAU	2	0
5	A	701[B]	GAU	4	0
4	B	602	ATP	2	0
5	B	702	GAU	4	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, 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	C	75/75 (100%)	0.13	7 (9%) 11 10	35, 52, 90, 92	0
1	D	75/75 (100%)	0.44	13 (17%) 2 2	30, 51, 97, 102	0
2	A	468/468 (100%)	-0.12	11 (2%) 62 61	19, 33, 68, 81	0
2	B	468/468 (100%)	0.01	33 (7%) 19 18	20, 36, 82, 96	0
All	All	1086/1086 (100%)	-0.01	64 (5%) 26 25	19, 37, 83, 102	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	140	ARG	6.8
2	B	141	GLY	5.5
1	D	516	C	5.4
2	B	136	GLU	5.3
2	B	50	PRO	4.9
2	B	128	ASN	4.8
2	B	46	ALA	4.8
2	B	1	MET	4.6
2	B	129	ILE	4.6
2	A	468	ALA	4.6
2	B	138	ALA	4.4
2	B	134	ALA	4.3
2	B	110	GLU	4.2
2	B	130	PRO	4.1
2	B	143	PRO	4.1
2	B	139	ARG	4.0
2	B	135	GLU	3.9
2	B	118	GLU	3.9
2	B	133	GLU	3.7
1	C	516	C	3.7
2	B	142	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	558	A	3.4
1	D	551	G	3.3
1	D	558	A	3.3
1	D	557	G	3.2
1	D	553	G	3.1
1	D	518	G	3.1
2	B	109	PRO	3.0
2	A	414	ALA	3.0
2	B	468	ALA	3.0
2	B	126	ALA	2.9
2	A	411	ALA	2.9
1	D	519	G	2.9
1	D	556	C	2.8
2	B	114	GLN	2.7
2	A	247	ARG	2.7
2	B	115	ILE	2.7
1	D	550	G	2.6
1	D	552	G	2.6
1	C	554	U	2.6
2	A	465	ARG	2.6
1	C	556	C	2.5
1	C	563	C	2.5
1	D	554	U	2.5
1	D	561	C	2.4
2	A	376	ASP	2.4
2	A	421	ALA	2.4
2	B	247	ARG	2.3
2	B	125	ARG	2.3
2	A	402	ARG	2.3
1	C	564	C	2.3
2	B	108	THR	2.3
2	A	424	GLY	2.2
2	B	113	GLU	2.2
2	A	403	ALA	2.2
1	D	566	U	2.2
2	B	132	GLU	2.2
2	B	49	VAL	2.2
2	B	117	LYS	2.2
2	B	121	GLY	2.1
2	B	47	ARG	2.1
1	C	557	G	2.1
2	B	181	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	405	GLU	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ATP	A	601	31/31	0.73	0.30	6.85	72,90,98,101	0
4	ATP	B	602	31/31	0.76	0.23	1.69	60,94,112,122	0
5	GAU	B	702	9/9	0.91	0.17	0.41	31,39,42,44	0
5	GAU	A	701[A]	9/9	0.97	0.14	-1.19	25,29,40,48	9
5	GAU	A	701[B]	9/9	0.97	0.14	-1.19	25,29,35,51	9
3	MG	C	901	1/1	0.70	0.25	-	49,49,49,49	0
3	MG	D	902	1/1	0.82	0.26	-	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.