Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:22 PM GMT

PDB ID	:	1F7V
Title	:	CRYSTAL STRUCTURE OF YEAST ARGINYL-TRNA SYNTHETASE COMPLEXED WITH THE TRNAARG
Authors	:	Delagoutte, B.; Moras, D.; Cavarelli, J.
Deposited on	:	2000-06-28
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references (1)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		18
Ramachandran outliers		1.0%
Sidechain outliers		3.4%
RSRZ outliers		3.5%
RNA backbone		0.68

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
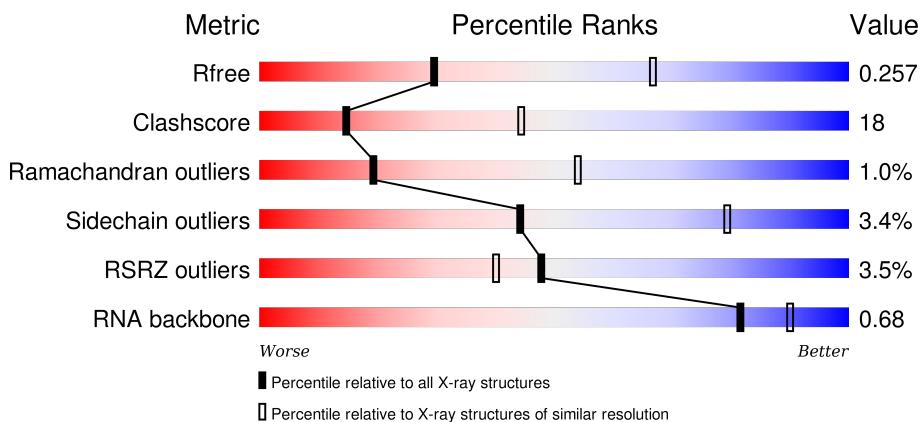
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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 <=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	76	% 57% 36% · ·
2	A	607	4% 62% 36% ·
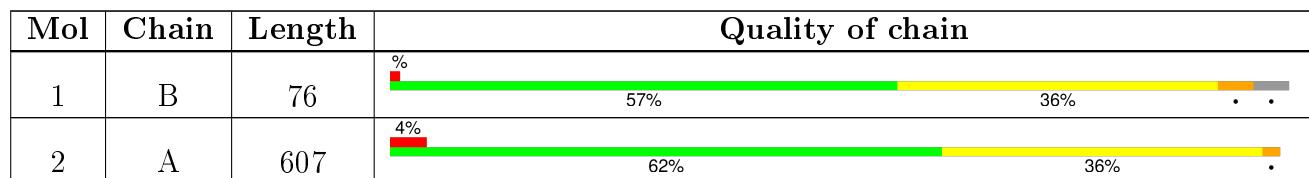
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6503 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(ARG).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	73	Total	C	N	O	P	0	0	0
			1567	702	279	513	73			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	606	Total	C	N	O	S	0	0	0
			4892	3138	828	905	21			

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	9	Total	O	0	0
			9	9		

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(ARG)

- Molecule 2: ARGINYL-TRNA SYNTHETASE
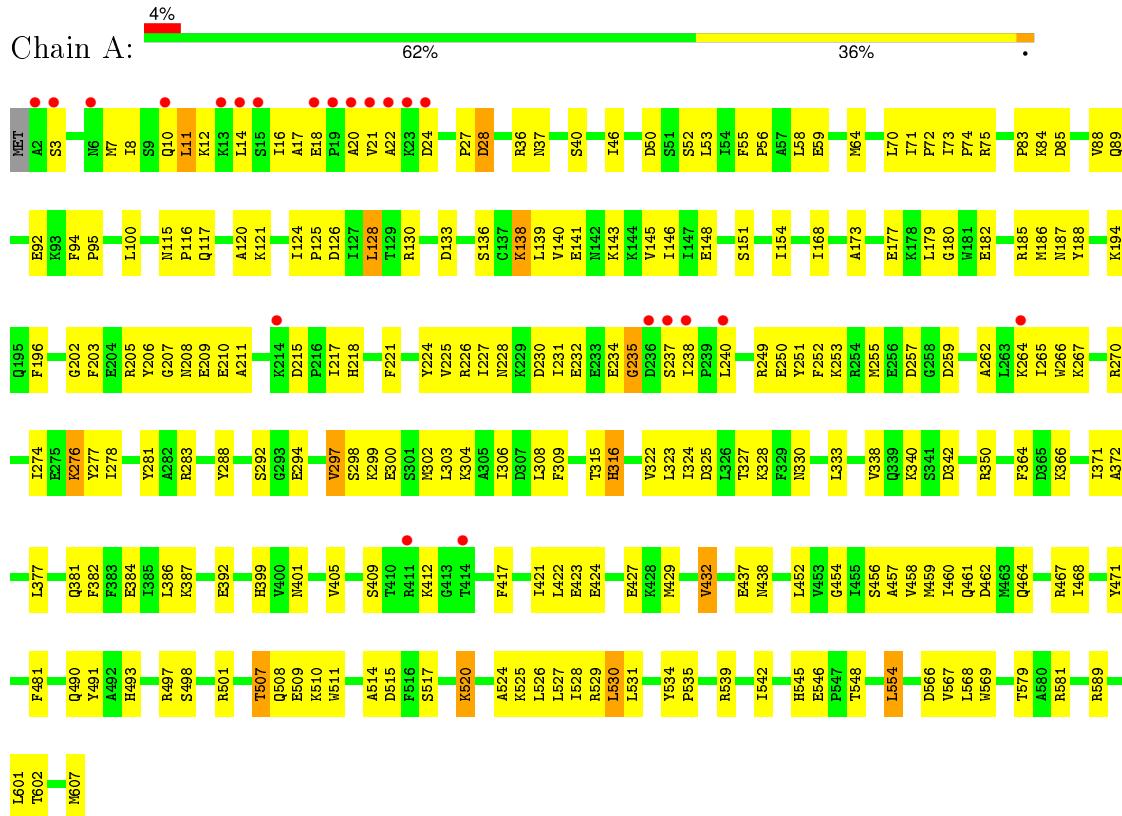
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	107.72Å 129.61Å 184.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.87 – 2.90 29.58 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.87-2.90) 99.9 (29.58-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	6.92 (at 2.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.245 0.210 , 0.257	Depositor DCC
R_{free} test set	2875 reflections (9.96%)	DCC
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.895	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]	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Outliers	1 of 28892 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6503	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, H2U, 2MG, 5MC, 1MA, M2G, 1MG, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	B	0.42	0/1463	0.69	0/2280
2	A	0.35	0/4996	0.58	1/6736 (0.0%)
All	All	0.37	0/6459	0.61	1/9016 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	182	GLU	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1567	0	801	21	0
2	A	4892	0	4906	198	0
3	A	35	0	0	0	0
3	B	9	0	0	0	0
All	All	6503	0	5707	216	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 18.

All (216) 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:17:ALA:HB1	2:A:21:VAL:HG13	1.37	1.01
2:A:520:LYS:HD3	2:A:520:LYS:H	1.25	0.98
2:A:238:ILE:HD12	2:A:238:ILE:H	1.28	0.95
2:A:138:LYS:H	2:A:138:LYS:HD3	1.33	0.93
2:A:217:ILE:HD11	2:A:276:LYS:HD3	1.52	0.90
1:B:947:H2U:H1'	1:B:948:U:OP2	1.75	0.86
2:A:507:THR:HB	2:A:509:GLU:OE2	1.77	0.85
2:A:14:LEU:HG	2:A:16:ILE:HG23	1.62	0.81
2:A:252:PHE:HA	2:A:255:MET:HE3	1.66	0.77
1:B:920:C:H2'	1:B:920:C:O2	1.85	0.75
2:A:230:ASP:O	2:A:234:GLU:HG2	1.85	0.75
2:A:194:LYS:HZ3	2:A:249:ARG:HH12	1.36	0.73
2:A:520:LYS:H	2:A:520:LYS:CD	2.01	0.72
2:A:520:LYS:HD3	2:A:520:LYS:N	2.00	0.72
2:A:253:LYS:O	2:A:257:ASP:HB2	1.90	0.71
2:A:509:GLU:H	2:A:509:GLU:CD	1.92	0.71
2:A:18:GLU:HG2	2:A:21:VAL:HG12	1.72	0.70
2:A:270:ARG:HH11	2:A:270:ARG:HG3	1.56	0.70
2:A:138:LYS:CD	2:A:138:LYS:H	2.02	0.70
2:A:330:ASN:HB3	2:A:333:LEU:HG	1.73	0.70
2:A:490:GLN:HB3	2:A:607:MET:HE1	1.74	0.69
2:A:238:ILE:CD1	2:A:238:ILE:H	2.04	0.69
2:A:16:ILE:CD1	2:A:37:ASN:HA	2.25	0.67
2:A:371:ILE:HG22	2:A:372:ALA:H	1.59	0.67
2:A:546:GLU:HB3	2:A:548:THR:HG22	1.77	0.67
2:A:409:SER:HB3	2:A:412:LYS:HB2	1.76	0.67
2:A:215:ASP:OD2	2:A:218:HIS:HB2	1.95	0.67
2:A:234:GLU:HB2	2:A:238:ILE:HD13	1.75	0.66
2:A:302:MET:HE3	2:A:350:ARG:HB2	1.77	0.65
1:B:947:H2U:C1'	1:B:948:U:OP2	2.44	0.65
2:A:304:LYS:O	2:A:308:LEU:HD23	1.97	0.64
2:A:126:ASP:OD1	2:A:130:ARG:HD3	1.99	0.63
2:A:133:ASP:O	2:A:136:SER:HB3	1.98	0.63
2:A:88:VAL:O	2:A:92:GLU:HG3	2.00	0.62
2:A:493:HIS:NE2	2:A:589:ARG:NH1	2.48	0.62
2:A:461:GLN:HA	2:A:464:GLN:HE21	1.65	0.61
2:A:452:LEU:HD22	2:A:602:THR:HB	1.82	0.61
2:A:10:GLN:HE22	2:A:14:LEU:HD13	1.66	0.61
2:A:124:ILE:HB	2:A:125:PRO:HD3	1.81	0.61
2:A:238:ILE:HD12	2:A:238:ILE:N	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:U:H2'	1:B:906:C:C6	2.35	0.61
2:A:252:PHE:HD1	2:A:255:MET:HE3	1.66	0.61
2:A:16:ILE:HD12	2:A:40:SER:HB2	1.83	0.60
2:A:21:VAL:O	2:A:24:ASP:HB2	2.01	0.60
2:A:117:GLN:NE2	2:A:517:SER:HA	2.16	0.60
2:A:17:ALA:HB3	2:A:22:ALA:HA	1.83	0.60
2:A:460:ILE:O	2:A:464:GLN:HG3	2.02	0.60
1:B:928:C:O2'	1:B:929:U:H5'	2.01	0.60
2:A:202:GLY:HA2	2:A:227:ILE:HD13	1.84	0.60
2:A:205:ARG:HG2	2:A:206:TYR:CE1	2.37	0.60
2:A:138:LYS:HD3	2:A:138:LYS:N	2.10	0.59
2:A:221:PHE:O	2:A:225:VAL:HG23	2.02	0.59
2:A:16:ILE:HD11	2:A:37:ASN:HA	1.85	0.59
2:A:139:LEU:HD12	2:A:179:LEU:HD13	1.84	0.58
2:A:456:SER:HA	2:A:601:LEU:HD22	1.84	0.58
2:A:217:ILE:HD11	2:A:276:LYS:CD	2.31	0.58
2:A:16:ILE:HD12	2:A:40:SER:CB	2.34	0.58
2:A:46:ILE:HD11	2:A:95:PRO:HD3	1.86	0.57
2:A:298:SER:O	2:A:302:MET:HG3	2.03	0.57
1:B:942:G:O2'	1:B:943:A:H5'	2.05	0.57
2:A:36:ARG:HB3	2:A:55:PHE:CE1	2.40	0.57
2:A:252:PHE:HA	2:A:255:MET:CE	2.34	0.57
2:A:371:ILE:O	2:A:401:ASN:HA	2.05	0.56
2:A:299:LYS:O	2:A:303:LEU:HD13	2.05	0.55
2:A:173:ALA:O	2:A:177:GLU:HG3	2.06	0.55
2:A:382:PHE:CE1	2:A:386:LEU:HD21	2.41	0.55
2:A:371:ILE:HG22	2:A:372:ALA:N	2.20	0.55
2:A:10:GLN:NE2	2:A:14:LEU:HD13	2.22	0.55
2:A:84:LYS:O	2:A:88:VAL:HG23	2.07	0.54
2:A:270:ARG:HH11	2:A:270:ARG:CG	2.20	0.54
2:A:208:ASN:HD22	2:A:211:ALA:HB2	1.73	0.54
2:A:309:PHE:HB3	2:A:315:THR:HG23	1.89	0.54
2:A:491:TYR:HA	2:A:607:MET:HE3	1.89	0.54
2:A:510:LYS:HD2	2:A:510:LYS:N	2.23	0.54
2:A:274:ILE:O	2:A:278:ILE:HG13	2.08	0.54
2:A:16:ILE:HD13	2:A:37:ASN:HA	1.89	0.53
2:A:206:TYR:CD2	2:A:226:ARG:HD3	2.42	0.53
2:A:17:ALA:HB3	2:A:22:ALA:CA	2.37	0.53
2:A:283:ARG:HD3	2:A:422:LEU:HD23	1.88	0.53
2:A:3:SER:O	2:A:7:MET:HG3	2.09	0.53
2:A:228:ASN:O	2:A:231:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:231:ILE:HG13	2:A:232:GLU:N	2.22	0.53
2:A:194:LYS:HZ3	2:A:249:ARG:NH1	2.06	0.52
1:B:906:C:O2'	1:B:907:G:H5'	2.08	0.52
2:A:459:MET:SD	2:A:601:LEU:HD23	2.50	0.52
1:B:935:C:N4	2:A:569:TRP:HA	2.25	0.51
2:A:64:MET:HE1	2:A:526:LEU:HA	1.92	0.51
2:A:322:VAL:C	2:A:323:LEU:HD12	2.31	0.51
2:A:509:GLU:HG2	2:A:510:LYS:HD2	1.93	0.51
2:A:340:LYS:HE2	2:A:342:ASP:OD2	2.11	0.51
2:A:59:GLU:OE2	2:A:75:ARG:NH1	2.44	0.50
2:A:141:GLU:HG3	2:A:143:LYS:HE2	1.92	0.50
2:A:64:MET:SD	2:A:530:LEU:HD13	2.52	0.50
2:A:508:GLN:HG2	2:A:511:TRP:CZ3	2.47	0.50
2:A:194:LYS:NZ	2:A:249:ARG:NH1	2.60	0.50
2:A:151:SER:HB3	2:A:188:TYR:O	2.11	0.50
2:A:567:VAL:HG23	2:A:568:LEU:HG	1.93	0.49
2:A:297:VAL:HG11	2:A:350:ARG:HG2	1.94	0.49
2:A:322:VAL:O	2:A:338:VAL:HG22	2.11	0.49
2:A:251:TYR:OH	2:A:265:ILE:HG21	2.12	0.49
2:A:10:GLN:O	2:A:14:LEU:HB2	2.11	0.49
2:A:423:GLU:O	2:A:427:GLU:HG3	2.12	0.49
1:B:950:C:O2'	1:B:951:A:H5'	2.13	0.49
2:A:267:LYS:HB2	2:A:267:LYS:NZ	2.29	0.48
2:A:18:GLU:HG3	2:A:20:ALA:H	1.78	0.48
2:A:64:MET:HE3	2:A:529:ARG:NE	2.28	0.48
2:A:168:ILE:HD13	2:A:467:ARG:HD2	1.96	0.48
2:A:85:ASP:O	2:A:89:GLN:HG3	2.13	0.48
2:A:315:THR:HG22	2:A:324:ILE:HG12	1.94	0.48
2:A:194:LYS:NZ	2:A:249:ARG:HH12	2.08	0.48
2:A:330:ASN:HB3	2:A:333:LEU:CG	2.41	0.48
2:A:124:ILE:HG22	2:A:128:LEU:HD22	1.96	0.48
2:A:325:ASP:OD1	2:A:327:THR:HB	2.14	0.47
2:A:467:ARG:NH1	2:A:545:HIS:O	2.47	0.47
2:A:64:MET:HE2	2:A:526:LEU:HD13	1.96	0.47
1:B:904:C:H2'	1:B:905:U:C6	2.50	0.47
1:B:935:C:H42	2:A:569:TRP:HA	1.79	0.47
2:A:401:ASN:HD21	2:A:468:ILE:HD13	1.80	0.47
2:A:458:VAL:O	2:A:461:GLN:HG3	2.15	0.47
2:A:490:GLN:O	2:A:607:MET:HE3	2.13	0.47
2:A:141:GLU:O	2:A:141:GLU:HG3	2.14	0.47
2:A:384:GLU:O	2:A:387:LYS:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:117:GLN:HE22	2:A:517:SER:HA	1.80	0.46
2:A:55:PHE:HB3	2:A:56:PRO:HD3	1.98	0.46
2:A:116:PRO:HG2	2:A:525:LYS:HD3	1.97	0.46
2:A:515:ASP:OD1	2:A:517:SER:OG	2.27	0.46
2:A:55:PHE:HB3	2:A:56:PRO:CD	2.44	0.46
2:A:12:LYS:HA	2:A:27:PRO:HB2	1.98	0.46
2:A:139:LEU:HD11	2:A:539:ARG:HG3	1.98	0.46
2:A:539:ARG:O	2:A:542:ILE:HG22	2.15	0.46
2:A:497:ARG:HG2	2:A:589:ARG:HD2	1.98	0.46
1:B:901:PSU:H2'	1:B:902:U:H6	1.79	0.46
2:A:250:GLU:O	2:A:253:LYS:HB3	2.14	0.46
2:A:270:ARG:NH1	2:A:274:ILE:HD11	2.30	0.46
2:A:294:GLU:O	2:A:350:ARG:NH1	2.49	0.46
2:A:11:LEU:HD12	2:A:11:LEU:HA	1.78	0.46
2:A:117:GLN:O	2:A:121:LYS:HG3	2.16	0.46
2:A:405:VAL:HG22	2:A:471:TYR:CZ	2.51	0.45
2:A:297:VAL:HG13	2:A:350:ARG:HH11	1.81	0.45
2:A:138:LYS:HG2	2:A:138:LYS:O	2.17	0.45
2:A:490:GLN:C	2:A:607:MET:HE3	2.37	0.45
2:A:554:LEU:HD12	2:A:554:LEU:HA	1.74	0.45
2:A:306:ILE:HA	2:A:309:PHE:CD2	2.51	0.45
2:A:73:ILE:HB	2:A:83:PRO:HB3	1.98	0.45
2:A:203:PHE:CD1	2:A:207:GLY:HA3	2.52	0.45
2:A:154:ILE:HG22	2:A:277:TYR:CE2	2.52	0.45
2:A:534:TYR:HB3	2:A:535:PRO:HD3	1.99	0.45
2:A:10:GLN:HE21	2:A:14:LEU:HD22	1.82	0.45
2:A:454:GLY:O	2:A:457:ALA:HB3	2.17	0.44
2:A:377:LEU:O	2:A:381:GLN:HG3	2.17	0.44
2:A:16:ILE:CD1	2:A:40:SER:HB2	2.48	0.44
2:A:115:ASN:OD1	2:A:117:GLN:HB2	2.16	0.44
2:A:148:GLU:HA	2:A:186:MET:O	2.18	0.44
2:A:514:ALA:HB2	2:A:579:THR:HG22	2.00	0.44
2:A:508:GLN:HG2	2:A:511:TRP:CE3	2.53	0.44
2:A:120:ALA:HB2	2:A:528:ILE:HD13	2.00	0.44
1:B:914:A:O2'	1:B:915:A:H5'	2.17	0.44
2:A:8:ILE:CG2	2:A:12:LYS:HE3	2.47	0.44
2:A:281:TYR:CD2	2:A:288:TYR:HE2	2.36	0.44
2:A:224:TYR:O	2:A:227:ILE:HG22	2.17	0.44
2:A:179:LEU:HD12	2:A:542:ILE:CD1	2.48	0.44
2:A:315:THR:HA	2:A:323:LEU:O	2.17	0.44
2:A:322:VAL:HB	2:A:338:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:151:SER:HA	2:A:187:ASN:OD1	2.18	0.44
2:A:117:GLN:CD	2:A:517:SER:HA	2.38	0.43
2:A:28:ASP:OD1	2:A:138:LYS:NZ	2.51	0.43
2:A:140:VAL:HG23	2:A:180:GLY:O	2.18	0.43
1:B:901:PSU:H2'	1:B:902:U:C6	2.53	0.43
2:A:371:ILE:HB	2:A:399:HIS:CE1	2.54	0.43
2:A:270:ARG:NH1	2:A:270:ARG:CG	2.79	0.43
2:A:461:GLN:NE2	2:A:462:ASP:HB2	2.34	0.43
2:A:179:LEU:HD12	2:A:542:ILE:HD12	2.01	0.43
2:A:467:ARG:HG3	2:A:546:GLU:OE1	2.19	0.43
2:A:524:ALA:O	2:A:528:ILE:HG13	2.19	0.43
2:A:429:MET:O	2:A:432:VAL:HG13	2.19	0.43
2:A:11:LEU:HD12	2:A:14:LEU:CD2	2.49	0.42
2:A:17:ALA:HB3	2:A:22:ALA:HB2	2.00	0.42
2:A:417:PHE:O	2:A:421:ILE:HG12	2.18	0.42
2:A:71:ILE:HA	2:A:72:PRO:HD3	1.87	0.42
1:B:905:U:H2'	1:B:906:C:H6	1.83	0.42
2:A:437:GLU:O	2:A:438:ASN:C	2.56	0.42
2:A:234:GLU:O	2:A:235:GLY:C	2.58	0.42
2:A:94:PHE:HA	2:A:95:PRO:HD3	1.67	0.42
2:A:498:SER:HA	2:A:501:ARG:NH1	2.34	0.42
1:B:965:G:O2'	1:B:966:C:H5'	2.20	0.42
1:B:938:A:N3	2:A:481:PHE:HB2	2.34	0.42
2:A:185:ARG:HH11	2:A:185:ARG:HG3	1.83	0.42
2:A:530:LEU:HD12	2:A:530:LEU:HA	1.81	0.42
2:A:327:THR:O	2:A:328:LYS:C	2.58	0.42
1:B:913:C:O2'	1:B:914:A:H5'	2.20	0.41
2:A:146:ILE:HD12	2:A:364:PHE:CD2	2.55	0.41
2:A:50:ASP:OD2	2:A:52:SER:HB2	2.19	0.41
2:A:227:ILE:HD12	2:A:227:ILE:HA	1.91	0.41
2:A:17:ALA:HB3	2:A:22:ALA:CB	2.49	0.41
2:A:294:GLU:O	2:A:297:VAL:HG13	2.20	0.41
2:A:264:LYS:HA	2:A:264:LYS:HD3	1.90	0.41
1:B:926:M2G:HN1	1:B:944:A:H2	1.68	0.41
2:A:302:MET:HE3	2:A:350:ARG:CB	2.47	0.41
2:A:73:ILE:N	2:A:74:PRO:CD	2.83	0.41
2:A:262:ALA:C	2:A:264:LYS:H	2.23	0.41
2:A:460:ILE:O	2:A:464:GLN:CG	2.68	0.41
2:A:315:THR:HG22	2:A:324:ILE:CG1	2.51	0.41
2:A:316:HIS:C	2:A:316:HIS:CD2	2.93	0.41
2:A:210:GLU:HG3	2:A:211:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:58:LEU:HD23	2:A:71:ILE:HB	2.03	0.41
1:B:958:1MA:HM12	1:B:961:C:O4'	2.20	0.41
2:A:196:PHE:CZ	2:A:266:TRP:HA	2.55	0.41
2:A:22:ALA:C	2:A:24:ASP:H	2.23	0.41
2:A:145:VAL:HA	2:A:366:LYS:O	2.21	0.41
2:A:527:LEU:O	2:A:531:LEU:HG	2.20	0.41
2:A:300:GLU:N	2:A:300:GLU:OE1	2.52	0.41
2:A:371:ILE:HB	2:A:399:HIS:HE1	1.85	0.41
2:A:196:PHE:CE2	2:A:266:TRP:HD1	2.38	0.40
2:A:392:GLU:H	2:A:392:GLU:CD	2.24	0.40
2:A:467:ARG:HG3	2:A:467:ARG:HH11	1.85	0.40
1:B:964:G:O2'	1:B:965:G:H5'	2.22	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	604/607 (100%)	547 (91%)	51 (8%)	6 (1%)	19 54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	209	GLU
2	A	235	GLY
2	A	237	SER
2	A	240	LEU
2	A	259	ASP
2	A	292	SER

5.3.2 Protein sidechains (i)

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	525/526 (100%)	507 (97%)	18 (3%)	44	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	11	LEU
2	A	28	ASP
2	A	53	LEU
2	A	70	LEU
2	A	100	LEU
2	A	128	LEU
2	A	138	LYS
2	A	276	LYS
2	A	297	VAL
2	A	316	HIS
2	A	424	GLU
2	A	432	VAL
2	A	507	THR
2	A	520	LYS
2	A	530	LEU
2	A	554	LEU
2	A	566	ASP
2	A	581	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	10	GLN
2	A	62	ASN
2	A	89	GLN
2	A	162	HIS
2	A	208	ASN
2	A	242	GLN
2	A	316	HIS

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Mol	Chain	Res	Type
2	A	374	GLN
2	A	375	GLN
2	A	406	GLN
2	A	420	ASN
2	A	464	GLN
2	A	502	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	72/76 (94%)	6 (8%)	1 (1%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	909	1MG
1	B	917	G
1	B	920	C
1	B	921	A
1	B	947	H2U
1	B	948	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	947	H2U

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	PSU	B	901	1	18,22,22	1.82	4 (22%)	24,33,33	5.16	4 (16%)
1	1MG	B	909	1	16,26,27	0.74	0	19,39,42	1.49	1 (5%)
1	2MG	B	910	1	17,26,27	1.21	2 (11%)	21,38,41	3.82	5 (23%)
1	H2U	B	916	1	17,21,22	0.65	0	23,30,33	1.43	2 (8%)
1	H2U	B	919	1	17,21,22	0.74	0	23,30,33	1.20	1 (4%)
1	M2G	B	926	1	17,27,28	1.24	1 (5%)	22,40,43	3.80	7 (31%)
1	PSU	B	927	1	13,21,22	2.42	4 (30%)	18,30,33	5.89	3 (16%)
1	H2U	B	947	1	17,21,22	0.77	1 (5%)	23,30,33	1.16	1 (4%)
1	5MC	B	949	1	13,22,23	1.09	2 (15%)	15,32,35	0.58	0
1	5MU	B	954	1	12,22,23	1.21	2 (16%)	14,32,35	4.44	3 (21%)
1	PSU	B	955	1	13,21,22	2.42	4 (30%)	18,30,33	5.87	4 (22%)
1	1MA	B	958	1	14,25,26	0.95	1 (7%)	15,37,40	1.18	1 (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
1	PSU	B	901	1	-	0/10/26/26	0/2/2/2
1	1MG	B	909	1	-	0/3/25/26	0/3/3/3
1	2MG	B	910	1	-	0/5/27/28	0/3/3/3
1	H2U	B	916	1	-	0/7/38/39	0/2/2/2
1	H2U	B	919	1	-	0/7/38/39	0/2/2/2
1	M2G	B	926	1	-	0/7/29/30	0/3/3/3
1	PSU	B	927	1	-	0/7/25/26	0/2/2/2
1	H2U	B	947	1	-	0/7/38/39	0/2/2/2
1	5MC	B	949	1	-	0/3/25/26	0/2/2/2
1	5MU	B	954	1	-	0/3/25/26	0/2/2/2
1	PSU	B	955	1	-	0/7/25/26	0/2/2/2
1	1MA	B	958	1	-	0/3/25/26	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	955	PSU	C5-C1'	-6.22	1.46	1.52
1	B	927	PSU	C5-C1'	-6.11	1.46	1.52
1	B	927	PSU	C6-N1	-4.62	1.24	1.34
1	B	901	PSU	C6-N1	-4.59	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	901	PSU	C5-C1'	-4.58	1.48	1.52
1	B	955	PSU	C6-N1	-4.54	1.24	1.34
1	B	927	PSU	C6-C5	-2.71	1.34	1.38
1	B	901	PSU	C6-C5	-2.63	1.34	1.38
1	B	955	PSU	C6-C5	-2.62	1.34	1.38
1	B	949	5MC	C6-C5	-2.40	1.33	1.40
1	B	954	5MU	C6-C5	-2.16	1.34	1.40
1	B	910	2MG	CM2-N2	2.10	1.49	1.45
1	B	927	PSU	C4-N3	2.17	1.37	1.33
1	B	949	5MC	C5-C4	2.24	1.44	1.41
1	B	955	PSU	C4-N3	2.29	1.37	1.33
1	B	958	1MA	C6-N6	2.32	1.33	1.29
1	B	901	PSU	C4-N3	2.36	1.37	1.33
1	B	947	H2U	C2-N1	2.50	1.39	1.35
1	B	954	5MU	C4-N3	2.73	1.38	1.33
1	B	926	M2G	C6-N1	3.48	1.39	1.33
1	B	910	2MG	C6-N1	3.49	1.39	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	901	PSU	N1-C2-N3	-21.54	114.59	128.33
1	B	927	PSU	N1-C2-N3	-21.40	114.68	128.33
1	B	955	PSU	N1-C2-N3	-21.22	114.79	128.33
1	B	910	2MG	CM2-N2-C2	-12.37	109.11	123.07
1	B	926	M2G	CM1-N2-C2	-9.26	111.82	121.34
1	B	926	M2G	CM2-N2-C2	-9.11	111.97	121.34
1	B	954	5MU	C5-C4-N3	-8.81	115.33	125.14
1	B	926	M2G	C5-C6-N1	-8.80	111.56	123.59
1	B	910	2MG	C5-C6-N1	-8.75	111.62	123.59
1	B	909	1MG	C5-C6-N1	-5.11	111.84	118.33
1	B	958	1MA	C2-N3-C4	-3.82	110.48	116.40
1	B	926	M2G	C2'-C1'-N9	-3.49	108.96	114.29
1	B	926	M2G	C2-N3-C4	-2.66	111.89	115.09
1	B	910	2MG	C2-N3-C4	-2.60	111.95	115.09
1	B	955	PSU	O4'-C1'-C2'	2.02	106.78	104.73
1	B	954	5MU	C5M-C5-C6	2.19	123.02	118.62
1	B	916	H2U	C4-N3-C2	2.23	127.62	125.79
1	B	926	M2G	N3-C2-N2	2.55	120.05	117.16
1	B	901	PSU	O4'-C1'-C2'	2.67	107.45	104.73
1	B	910	2MG	N2-C2-N3	3.42	120.91	116.94
1	B	947	H2U	C5-C6-N1	4.39	115.45	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	901	PSU	C6-N1-C2	4.45	122.62	115.47
1	B	955	PSU	C6-N1-C2	4.47	122.66	115.47
1	B	927	PSU	C6-N1-C2	4.52	122.74	115.47
1	B	919	H2U	C5-C6-N1	4.75	115.85	110.70
1	B	916	H2U	C5-C6-N1	5.82	117.00	110.70
1	B	926	M2G	CM2-N2-CM1	6.13	136.21	115.96
1	B	910	2MG	C6-N1-C2	6.93	125.39	115.31
1	B	927	PSU	C4-N3-C2	11.76	125.41	115.25
1	B	901	PSU	C4-N3-C2	11.93	125.56	115.25
1	B	955	PSU	C4-N3-C2	11.93	125.56	115.25
1	B	954	5MU	C4-N3-C2	13.84	127.22	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	901	PSU	2	0
1	B	926	M2G	1	0
1	B	947	H2U	2	0
1	B	958	1MA	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	B	60/76 (78%)	-0.07	1 (1%)	73	70	17, 28, 49, 82	0
2	A	606/607 (99%)	-0.12	22 (3%)	46	38	9, 38, 74, 114	0
All	All	666/683 (97%)	-0.12	23 (3%)	48	40	9, 36, 74, 114	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	21	VAL	5.7
2	A	20	ALA	5.4
2	A	236	ASP	4.3
2	A	19	PRO	4.2
2	A	14	LEU	4.0
2	A	2	ALA	3.9
2	A	414	THR	3.5
2	A	3	SER	3.1
2	A	13	LYS	3.0
2	A	23	LYS	2.9
2	A	22	ALA	2.9
1	B	973	G	2.8
2	A	15	SER	2.7
2	A	18	GLU	2.6
2	A	24	ASP	2.6
2	A	240	LEU	2.5
2	A	214	LYS	2.5
2	A	6	ASN	2.4
2	A	264	LYS	2.3
2	A	238	ILE	2.2
2	A	411	ARG	2.1
2	A	10	GLN	2.1
2	A	237	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	H2U	B	947	20/21	0.85	0.45	-	64,85,100,100	0
1	PSU	B	901	21/21	0.88	0.31	-	67,74,91,94	0
1	H2U	B	916	20/21	0.98	0.11	-	16,24,34,34	0
1	H2U	B	919	20/21	0.97	0.16	-	23,40,49,52	0
1	PSU	B	927	20/21	0.97	0.16	-	22,31,40,41	0
1	5MU	B	954	21/22	0.98	0.15	-	16,25,30,32	0
1	M2G	B	926	25/26	0.98	0.15	-	10,21,28,33	0
1	1MG	B	909	24/25	0.98	0.15	-	9,18,30,37	0
1	2MG	B	910	24/25	0.99	0.12	-	1,17,23,28	0
1	1MA	B	958	23/24	0.98	0.15	-	12,20,27,32	0
1	5MC	B	949	21/22	0.99	0.12	-	7,19,25,26	0
1	PSU	B	955	20/21	0.98	0.15	-	18,29,34,35	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.