Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:10 AM GMT

PDB ID	:	2ZUF
Title	:	Crystal structure of Pyrococcus horikoshii arginyl-tRNA synthetase complexed with tRNA(Arg)
Authors	:	Konno, M.; Sumida, T.; Uchikawa, E.; Mori, Y.; Yanagisawa, T.; Sekine, S.; Yokoyama, S.
Deposited on	:	2008-10-16
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

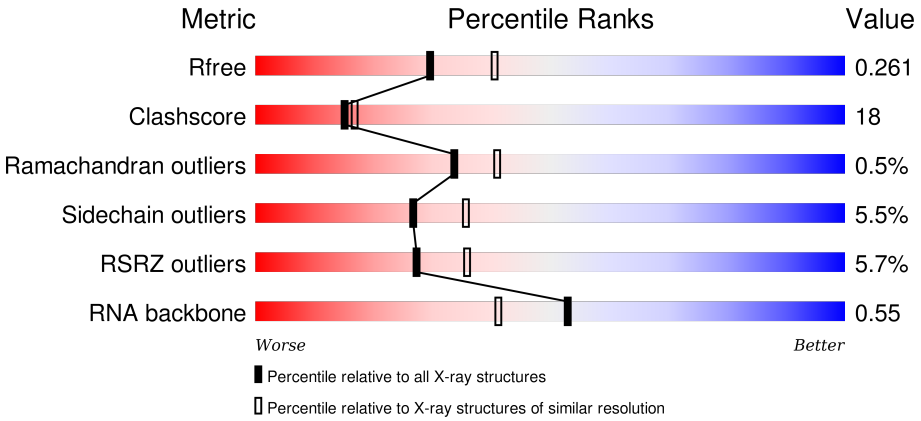
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)
RNA backbone	2183	1011 (2.84-1.76)

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	A	629	5% 64% 32% ·
2	B	78	10% 54% 26% 15% · ·

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6994 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 protein called Arginyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	0	0	0
			5097	3282	867	933	15			

- Molecule 2 is a RNA chain called tRNA-Arg.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	P	0	2	0
			1649	733	302	537	77			

- Molecule 3 is water.

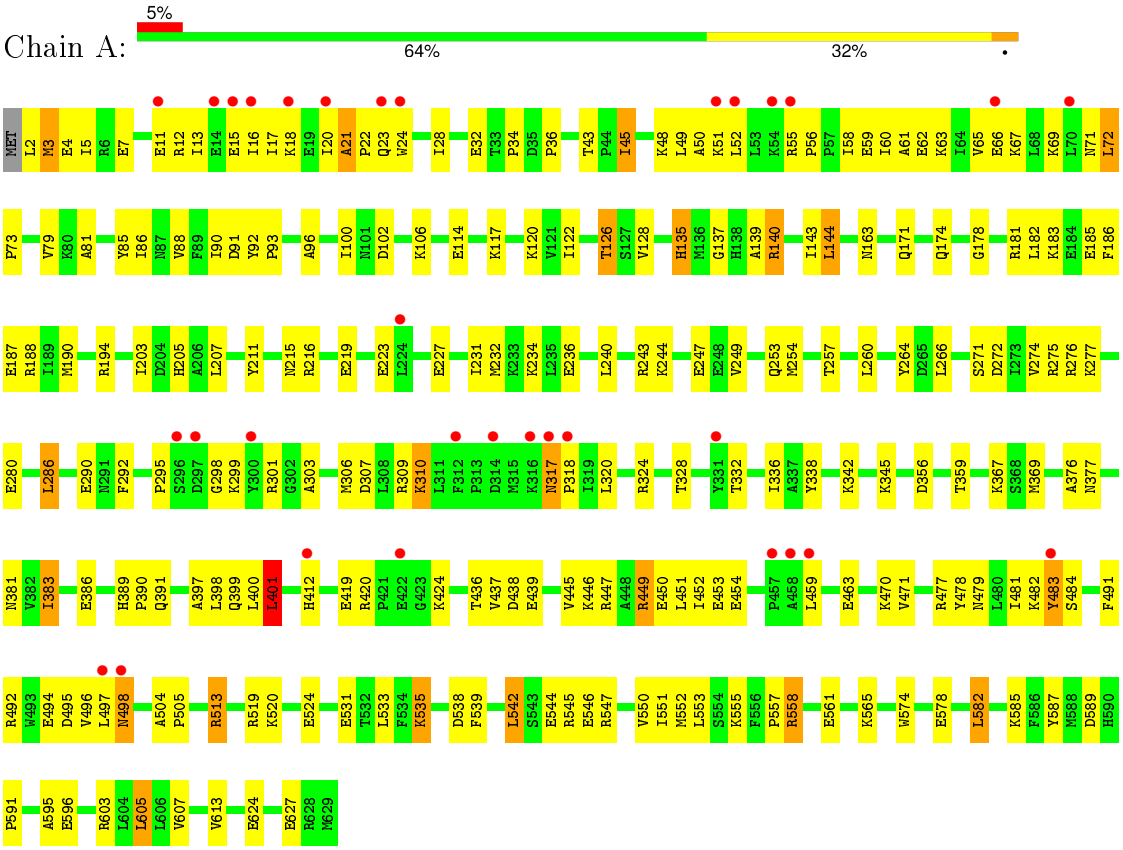
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total	O	0	0
			170	170		
3	B	78	Total	O	0	0
			78	78		

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.

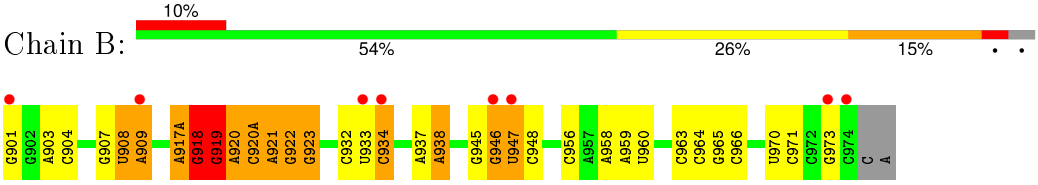
- Molecule 1: Arginyl-tRNA synthetase

Chain A:



- Molecule 2: tRNA-Arg

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.21Å 60.14Å 110.33Å 90.00° 107.06° 90.00°	Depositor
Resolution (Å)	39.65 – 2.30 39.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.7 (39.65-2.30) 90.7 (39.65-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.262 0.200 , 0.261	Depositor DCC
R_{free} test set	3892 reflections (10.03%)	DCC
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 38820 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6994	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	A	0.36	0/5202	0.58	1/7015 (0.0%)
2	B	0.44	1/1840 (0.1%)	0.83	2/2862 (0.1%)
All	All	0.38	1/7042 (0.0%)	0.67	3/9877 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	G	OP3-P	-6.97	1.52	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	918	G	N9-C1'-C2'	5.51	121.17	114.00
1	A	401	LEU	N-CA-C	-5.37	96.51	111.00
2	B	938	A	N9-C1'-C2'	5.12	120.65	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	919	G	Sidechain

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	A	5097	0	5183	195	0
2	B	1649	0	840	34	0
3	A	170	0	0	10	0
3	B	78	0	0	2	0
All	All	6994	0	6023	223	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 (223) 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)
1:A:381:ASN:HD22	1:A:391:GLN:HE22	1.08	1.01
1:A:558:ARG:HD2	1:A:558:ARG:H	1.30	0.96
1:A:299:LYS:HD2	1:A:299:LYS:H	1.38	0.89
1:A:120:LYS:H	1:A:377:ASN:HD22	1.22	0.86
2:B:917(A):A:H5'	2:B:918:G:OP2	1.77	0.85
2:B:932:C:H4'	2:B:934:C:H41	1.42	0.84
2:B:920:A:H4'	2:B:920(A):C:OP2	1.79	0.81
2:B:932:C:H4'	2:B:934:C:N4	1.97	0.79
1:A:381:ASN:HD22	1:A:391:GLN:NE2	1.82	0.78
1:A:545:ARG:NH2	1:A:585:LYS:HD3	1.99	0.77
1:A:381:ASN:ND2	1:A:391:GLN:HE22	1.82	0.75
1:A:85:TYR:OH	2:B:919:G:H2'	1.89	0.73
1:A:34:PRO:HB3	2:B:920(A):C:H41	1.53	0.72
1:A:367:LYS:HE3	1:A:369:MET:SD	2.29	0.72
1:A:86:ILE:HD13	3:A:1001:HOH:O	1.90	0.71
1:A:16:ILE:HD12	1:A:67:LYS:HB3	1.72	0.71
1:A:420:ARG:HH22	1:A:492:ARG:NH1	1.88	0.71
1:A:391:GLN:HG3	1:A:412:HIS:ND1	2.06	0.70
1:A:383:ILE:HG13	1:A:412:HIS:CD2	2.26	0.70
1:A:183:LYS:O	1:A:187:GLU:HG2	1.92	0.70
1:A:298:GLY:H	1:A:301:ARG:HG2	1.57	0.70
1:A:65:VAL:HG13	1:A:79:VAL:HG23	1.73	0.69
1:A:561:GLU:O	1:A:565:LYS:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:LYS:O	1:A:535:LYS:HD3	1.93	0.69
2:B:947:U:H3'	3:B:1091:HOH:O	1.93	0.69
2:B:946:G:O2'	2:B:947:U:H5'	1.91	0.69
1:A:61:ALA:HA	1:A:86:ILE:HD11	1.75	0.69
1:A:555:LYS:HA	1:A:558:ARG:HD3	1.73	0.69
1:A:299:LYS:N	1:A:299:LYS:HD2	2.09	0.68
1:A:52:LEU:HD12	1:A:52:LEU:H	1.59	0.68
1:A:538:ASP:O	1:A:539:PHE:HB2	1.93	0.68
1:A:535:LYS:HD3	1:A:535:LYS:C	2.16	0.67
2:B:922:G:C3'	2:B:923:G:H5"	2.26	0.66
1:A:96:ALA:O	1:A:100:ILE:HG12	1.96	0.65
1:A:114:GLU:HB3	1:A:117:LYS:HD3	1.78	0.65
1:A:4:GLU:HB2	3:A:1158:HOH:O	1.97	0.64
1:A:232:MET:O	1:A:236:GLU:HG3	1.97	0.64
1:A:50:ALA:HA	1:A:60:ILE:CD1	2.27	0.64
1:A:277:LYS:HB3	1:A:280:GLU:CG	2.27	0.64
1:A:271:SER:O	1:A:275:ARG:HG3	1.99	0.63
1:A:596:GLU:HG2	3:A:1211:HOH:O	1.98	0.63
1:A:545:ARG:CZ	1:A:585:LYS:HD3	2.29	0.62
1:A:52:LEU:N	1:A:52:LEU:HD12	2.15	0.62
2:B:923:G:H5'	2:B:923:G:C8	2.35	0.61
1:A:11:GLU:O	1:A:15:GLU:HG3	2.00	0.61
1:A:391:GLN:HG3	1:A:412:HIS:CG	2.35	0.61
1:A:140:ARG:HG3	1:A:144:LEU:HD22	1.82	0.61
1:A:12:ARG:HH21	1:A:71:ASN:HD21	1.48	0.61
1:A:22:PRO:HG2	1:A:23:GLN:HE21	1.65	0.61
1:A:92:TYR:CZ	1:A:547:ARG:HG2	2.36	0.61
1:A:307:ASP:OD1	1:A:309:ARG:HG2	2.00	0.60
1:A:69:LYS:HA	1:A:72:LEU:HD13	1.83	0.60
1:A:557:PRO:HG2	1:A:558:ARG:NH1	2.16	0.60
1:A:299:LYS:CD	1:A:299:LYS:H	2.12	0.60
1:A:17:ILE:HG21	1:A:24:TRP:CD1	2.37	0.60
1:A:451:LEU:HD23	2:B:938:A:C2	2.37	0.60
1:A:205:HIS:HE1	1:A:438:ASP:OD1	1.86	0.59
1:A:178:GLY:O	1:A:182:LEU:HB2	2.03	0.58
2:B:973[B]:G:N3	2:B:973[B]:G:H3'	2.18	0.58
1:A:397:ALA:O	1:A:401:LEU:HD22	2.04	0.58
1:A:135:HIS:CD2	1:A:137:GLY:H	2.21	0.58
2:B:923:G:H5'	2:B:923:G:H8	1.68	0.57
1:A:449:ARG:O	1:A:452:ILE:HG22	2.04	0.57
1:A:216:ARG:HG2	1:A:216:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:H	1:A:52:LEU:CD1	2.18	0.57
1:A:419:GLU:CD	1:A:424:LYS:HG2	2.25	0.57
1:A:533:LEU:CB	1:A:605:LEU:HD11	2.35	0.57
1:A:51:LYS:HE3	2:B:956:C:C6	2.39	0.57
1:A:181:ARG:HH11	1:A:181:ARG:HG2	1.69	0.56
1:A:553:LEU:HD22	1:A:613:VAL:HG21	1.87	0.56
1:A:552:MET:HE3	1:A:555:LYS:HD2	1.87	0.56
1:A:492:ARG:HG3	1:A:494:GLU:HG2	1.87	0.56
1:A:399:GLN:O	1:A:401:LEU:O	2.23	0.56
1:A:215:ASN:O	1:A:219:GLU:HG3	2.06	0.56
1:A:3:MET:HG2	1:A:5:ILE:HG22	1.86	0.56
1:A:244:LYS:HB3	3:A:1159:HOH:O	2.05	0.56
1:A:56:PRO:HB2	1:A:59:GLU:HG2	1.87	0.56
1:A:558:ARG:H	1:A:558:ARG:CD	2.05	0.56
2:B:923:G:C5'	2:B:923:G:H8	2.18	0.56
1:A:324:ARG:HD2	1:A:328:THR:OG1	2.07	0.55
1:A:412:HIS:HB3	3:A:1027:HOH:O	2.05	0.55
1:A:533:LEU:HB3	1:A:605:LEU:CD1	2.36	0.55
2:B:958:A:O2'	2:B:960:U:OP2	2.17	0.55
1:A:482:LYS:HE3	1:A:483:TYR:CE2	2.42	0.55
1:A:243:ARG:NH1	1:A:247:GLU:OE2	2.40	0.54
1:A:20:ILE:O	1:A:20:ILE:HG22	2.06	0.54
1:A:122:ILE:HG13	1:A:376:ALA:HB2	1.90	0.54
1:A:260:LEU:O	1:A:477:ARG:HD2	2.09	0.53
1:A:32:GLU:H	1:A:32:GLU:CD	2.11	0.53
1:A:102:ASP:OD2	1:A:106:LYS:HE2	2.08	0.53
1:A:2:LEU:HD22	1:A:558:ARG:NH2	2.22	0.53
1:A:449:ARG:HH11	1:A:453:GLU:HG2	1.74	0.53
1:A:383:ILE:HG13	1:A:412:HIS:NE2	2.23	0.53
1:A:12:ARG:HG3	1:A:73:PRO:HG3	1.90	0.53
1:A:69:LYS:HA	1:A:72:LEU:CD1	2.39	0.53
1:A:504:ALA:HB3	1:A:505:PRO:HD3	1.91	0.53
1:A:557:PRO:HG2	1:A:558:ARG:HH11	1.72	0.53
1:A:298:GLY:O	1:A:301:ARG:HG3	2.08	0.53
1:A:513:ARG:HH11	1:A:513:ARG:CG	2.22	0.53
1:A:36:PRO:HB2	1:A:544:GLU:OE2	2.08	0.52
2:B:922:G:H3'	2:B:923:G:H5"	1.91	0.52
1:A:542:LEU:HB2	3:A:1079:HOH:O	2.09	0.52
1:A:12:ARG:HH21	1:A:71:ASN:ND2	2.08	0.52
1:A:92:TYR:CE1	1:A:547:ARG:HG2	2.45	0.52
1:A:277:LYS:HB3	1:A:280:GLU:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HD12	1:A:551:ILE:HD11	1.91	0.51
1:A:15:GLU:O	1:A:18:LYS:HB3	2.10	0.51
1:A:555:LYS:O	1:A:558:ARG:HG2	2.10	0.51
1:A:174:GLN:NE2	1:A:211:TYR:HE1	2.08	0.51
1:A:249:VAL:O	1:A:253:GLN:HG3	2.10	0.51
1:A:338:TYR:CE2	1:A:342:LYS:HE3	2.45	0.51
2:B:923:G:C5'	2:B:923:G:C8	2.93	0.51
1:A:533:LEU:HB2	1:A:605:LEU:HD11	1.93	0.51
1:A:446:LYS:O	1:A:450:GLU:HG2	2.09	0.51
1:A:306:MET:CE	1:A:320:LEU:HD12	2.41	0.51
1:A:190:MET:O	1:A:194:ARG:HG3	2.09	0.51
1:A:135:HIS:HD2	1:A:137:GLY:N	2.08	0.51
1:A:45:ILE:O	1:A:45:ILE:HD13	2.11	0.51
2:B:903:A:O2'	2:B:904:C:H5'	2.11	0.51
1:A:12:ARG:HA	1:A:15:GLU:OE1	2.11	0.50
1:A:298:GLY:H	1:A:301:ARG:CG	2.22	0.50
1:A:28:ILE:CD1	1:A:45:ILE:HG13	2.41	0.50
1:A:551:ILE:HG22	1:A:555:LYS:HE3	1.93	0.50
1:A:223:GLU:HB3	3:A:1119:HOH:O	2.11	0.49
1:A:139:ALA:O	1:A:143:ILE:HG12	2.12	0.49
1:A:574:TRP:CZ2	1:A:578:GLU:HG3	2.47	0.49
1:A:55:ARG:HH12	1:A:63:LYS:HE2	1.77	0.49
1:A:286:LEU:HG	1:A:292:PHE:CD2	2.48	0.49
1:A:295:PRO:HD2	1:A:303:ALA:O	2.12	0.49
1:A:13:ILE:O	1:A:17:ILE:HG13	2.13	0.49
1:A:533:LEU:HB3	1:A:605:LEU:HD13	1.94	0.49
1:A:58:ILE:O	1:A:62:GLU:HG3	2.12	0.49
1:A:34:PRO:CB	2:B:920(A):C:H41	2.24	0.49
1:A:254:MET:HA	1:A:257:THR:OG1	2.13	0.49
2:B:970:U:H2'	2:B:971:C:C6	2.47	0.49
1:A:538:ASP:O	3:A:1166:HOH:O	2.20	0.48
1:A:43:THR:OG1	1:A:45:ILE:HB	2.12	0.48
1:A:494:GLU:HG3	1:A:495:ASP:OD2	2.14	0.48
1:A:45:ILE:HD12	1:A:49:LEU:HG	1.96	0.48
2:B:920(A):C:H2'	2:B:921:A:OP1	2.13	0.48
2:B:917(A):A:OP1	2:B:917(A):A:H8	1.97	0.48
1:A:135:HIS:CD2	1:A:137:GLY:N	2.81	0.48
2:B:945:G:H2'	2:B:946:G:H5'	1.96	0.47
1:A:400:LEU:C	1:A:401:LEU:O	2.50	0.47
1:A:471:VAL:HG13	1:A:505:PRO:HG3	1.96	0.47
1:A:531:GLU:CD	1:A:531:GLU:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:SER:HB3	3:B:1157:HOH:O	2.14	0.47
1:A:519:ARG:NH2	1:A:627:GLU:O	2.47	0.47
1:A:280:GLU:H	1:A:280:GLU:CD	2.18	0.47
1:A:277:LYS:HB3	1:A:280:GLU:HG3	1.97	0.46
1:A:513:ARG:HG2	1:A:587:TYR:CE1	2.50	0.46
1:A:234:LYS:HB2	1:A:240:LEU:HD12	1.98	0.46
1:A:436:THR:OG1	1:A:439:GLU:HG3	2.16	0.46
1:A:459:LEU:HD22	1:A:463:GLU:OE1	2.16	0.46
1:A:126:THR:HG22	1:A:128:VAL:HG23	1.96	0.46
1:A:513:ARG:HH11	1:A:513:ARG:HG3	1.81	0.46
1:A:492:ARG:HD2	1:A:492:ARG:HA	1.56	0.45
1:A:185:GLU:OE2	1:A:188:ARG:HD2	2.16	0.45
1:A:50:ALA:HA	1:A:60:ILE:HD11	1.97	0.45
1:A:547:ARG:O	1:A:550:VAL:HG22	2.15	0.45
1:A:478:TYR:HB2	1:A:504:ALA:HB2	1.98	0.45
1:A:504:ALA:N	1:A:505:PRO:CD	2.80	0.45
1:A:386:GLU:HB3	3:A:1182:HOH:O	2.16	0.45
1:A:65:VAL:HG21	1:A:81:ALA:HB2	1.98	0.45
1:A:186:PHE:HZ	1:A:203:ILE:CD1	2.29	0.45
1:A:227:GLU:O	1:A:231:ILE:HG12	2.16	0.45
1:A:533:LEU:HB3	1:A:605:LEU:HD11	1.98	0.45
2:B:965:G:O2'	2:B:966:C:H5'	2.17	0.45
1:A:479:ASN:HD22	1:A:496:VAL:HG12	1.82	0.45
1:A:12:ARG:HG2	1:A:12:ARG:HH11	1.82	0.45
1:A:520:LYS:NZ	1:A:524:GLU:OE2	2.48	0.45
1:A:389:HIS:HB2	1:A:390:PRO:HD3	1.99	0.45
1:A:90:ILE:HG22	1:A:91:ASP:N	2.32	0.44
1:A:449:ARG:NH1	1:A:453:GLU:HG2	2.32	0.44
1:A:86:ILE:HD12	1:A:86:ILE:N	2.33	0.44
1:A:546:GLU:O	1:A:550:VAL:HG13	2.18	0.44
1:A:491:PHE:CD1	1:A:491:PHE:C	2.92	0.44
2:B:917(A):A:C5'	2:B:918:G:OP2	2.59	0.44
2:B:920:A:O2'	2:B:920(A):C:P	2.76	0.43
1:A:400:LEU:HA	1:A:400:LEU:HD23	1.90	0.43
1:A:260:LEU:HD11	1:A:437:VAL:HG11	2.01	0.43
1:A:257:THR:HG21	1:A:264:TYR:OH	2.18	0.43
1:A:591:PRO:O	1:A:595:ALA:HB2	2.18	0.43
1:A:494:GLU:O	1:A:498:ASN:HB3	2.18	0.43
1:A:135:HIS:CD2	1:A:135:HIS:C	2.92	0.43
1:A:533:LEU:HD13	1:A:605:LEU:CD1	2.49	0.43
1:A:92:TYR:CE2	1:A:547:ARG:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:HD2	3:A:1238:HOH:O	2.18	0.43
1:A:496:VAL:O	1:A:497:LEU:HD12	2.19	0.42
1:A:470:LYS:HG2	1:A:624:GLU:OE1	2.19	0.42
1:A:552:MET:CE	1:A:552:MET:HA	2.49	0.42
2:B:959:A:C2'	2:B:960:U:H5'	2.49	0.42
1:A:45:ILE:CD1	1:A:49:LEU:HG	2.49	0.42
1:A:274:VAL:CG2	1:A:275:ARG:N	2.82	0.42
1:A:520:LYS:HE3	1:A:524:GLU:OE2	2.19	0.42
1:A:558:ARG:HD2	1:A:558:ARG:N	2.14	0.42
1:A:163:ASN:HB2	1:A:264:TYR:CD2	2.54	0.42
1:A:16:ILE:HD12	1:A:67:LYS:CB	2.46	0.42
1:A:603:ARG:O	1:A:607:VAL:HG23	2.20	0.42
1:A:51:LYS:HA	1:A:51:LYS:HD2	1.81	0.42
1:A:79:VAL:HG12	1:A:88:VAL:HG12	2.02	0.42
2:B:908:U:H5"	2:B:909:A:OP1	2.19	0.42
1:A:533:LEU:CB	1:A:605:LEU:CD1	2.97	0.41
2:B:922:G:C2'	2:B:923:G:H5"	2.50	0.41
2:B:963:C:O2'	2:B:964:C:H5'	2.20	0.41
1:A:272:ASP:O	1:A:276:ARG:HG2	2.20	0.41
1:A:48:LYS:HG3	2:B:919:G:O6	2.21	0.41
1:A:181:ARG:O	1:A:182:LEU:HD23	2.21	0.41
1:A:5:ILE:HG12	1:A:5:ILE:O	2.19	0.41
2:B:959:A:H2'	2:B:960:U:H5'	2.02	0.41
1:A:582:LEU:HD12	1:A:582:LEU:HA	1.92	0.41
1:A:317:ASN:N	1:A:318:PRO:HD3	2.34	0.41
1:A:332:THR:O	1:A:336:ILE:HD13	2.21	0.41
2:B:922:G:H2'	2:B:923:G:H5"	2.03	0.41
1:A:144:LEU:HD13	1:A:481:ILE:HG22	2.02	0.41
1:A:420:ARG:HH22	1:A:492:ARG:HH11	1.62	0.41
1:A:63:LYS:O	1:A:66:GLU:HB3	2.21	0.41
1:A:483:TYR:CD1	1:A:483:TYR:N	2.89	0.41
1:A:356:ASP:HB2	1:A:359:THR:HB	2.02	0.41
1:A:445:VAL:O	1:A:449:ARG:HB2	2.21	0.40
1:A:20:ILE:O	1:A:21:ALA:HB2	2.21	0.40
1:A:4:GLU:OE2	1:A:4:GLU:HA	2.21	0.40
1:A:72:LEU:HA	1:A:73:PRO:HD3	1.97	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
1	A	626/629 (100%)	601 (96%)	22 (4%)	3 (0%)	34 41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	THR
1	A	21	ALA
1	A	93	PRO

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
1	A	542/543 (100%)	512 (94%)	30 (6%)	27 36

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	7	GLU
1	A	45	ILE
1	A	72	LEU
1	A	135	HIS
1	A	140	ARG
1	A	144	LEU
1	A	171	GLN

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Mol	Chain	Res	Type
1	A	207	LEU
1	A	266	LEU
1	A	286	LEU
1	A	290	GLU
1	A	310	LYS
1	A	317	ASN
1	A	345	LYS
1	A	383	ILE
1	A	398	LEU
1	A	401	LEU
1	A	447	ARG
1	A	449	ARG
1	A	454	GLU
1	A	483	TYR
1	A	498	ASN
1	A	513	ARG
1	A	535	LYS
1	A	542	LEU
1	A	558	ARG
1	A	582	LEU
1	A	589	ASP
1	A	605	LEU

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

Mol	Chain	Res	Type
1	A	23	GLN
1	A	71	ASN
1	A	129	ASN
1	A	135	HIS
1	A	171	GLN
1	A	174	GLN
1	A	205	HIS
1	A	226	ASN
1	A	377	ASN
1	A	391	GLN
1	A	399	GLN
1	A	584	ASN
1	A	590	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	73/78 (93%)	16 (21%)	5 (6%)

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	908	U
2	B	909	A
2	B	917(A)	A
2	B	918	G
2	B	919	G
2	B	920	A
2	B	920(A)	C
2	B	921	A
2	B	922	G
2	B	923	G
2	B	933	U
2	B	934	C
2	B	937	A
2	B	946	G
2	B	947	U
2	B	948	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	907	G
2	B	909	A
2	B	919	G
2	B	920	A
2	B	946	G

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	A	628/629 (99%)	0.33	32 (5%) 32 41	14, 31, 64, 88	0
2	B	76/78 (97%)	0.39	8 (10%) 8 12	26, 39, 83, 90	1 (1%)
All	All	704/707 (99%)	0.34	40 (5%) 27 36	14, 32, 67, 90	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	947	U	5.5
2	B	974[B]	C	5.5
1	A	20	ILE	4.7
1	A	317	ASN	4.4
1	A	23	GLN	4.3
1	A	316	LYS	4.0
1	A	483	TYR	4.0
1	A	458	ALA	3.9
2	B	934	C	3.9
2	B	946	G	3.8
1	A	297	ASP	3.7
2	B	901	G	3.6
2	B	909	A	3.4
1	A	51	LYS	3.3
1	A	318	PRO	3.3
1	A	16	ILE	3.2
2	B	973[A]	G	3.1
1	A	11	GLU	3.0
1	A	70	LEU	3.0
1	A	497	LEU	2.9
1	A	314	ASP	2.9
1	A	15	GLU	2.9
1	A	66	GLU	2.7
1	A	331	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	14	GLU	2.5
1	A	55	ARG	2.5
1	A	18	LYS	2.5
1	A	498	ASN	2.4
1	A	422	GLU	2.3
1	A	52	LEU	2.3
1	A	224	LEU	2.3
1	A	54	LYS	2.3
1	A	459	LEU	2.3
1	A	457	PRO	2.3
1	A	296	SER	2.3
1	A	300	TYR	2.3
1	A	412	HIS	2.1
1	A	24	TRP	2.1
1	A	312	PHE	2.0
2	B	933	U	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.