Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 09:28 PM EDT

PDB ID	:	4NL3
Title	:	Crystal Structure of Listeria monocytogenes Hfq in complex with U6 RNA
Authors	:	Kovach, A.R.; Brennan, R.G.
Deposited on	:	2013-11-13
Resolution	:	3.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

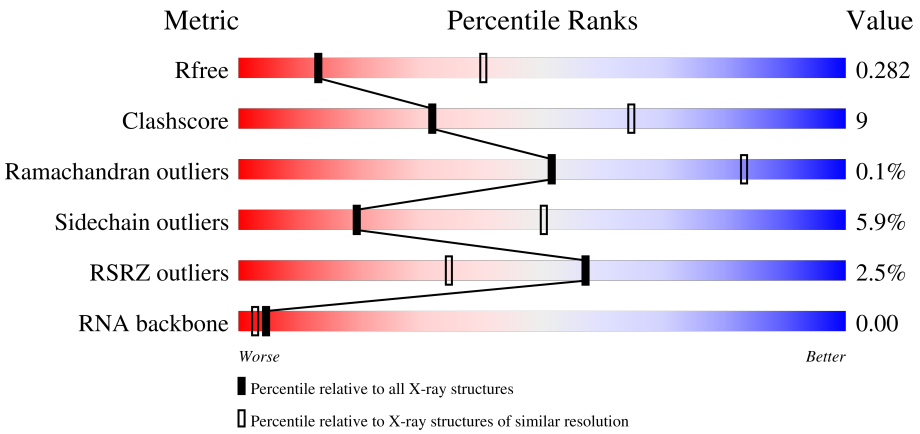
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	77	71% 21% • 6%
1	B	77	65% 27% 8%
1	C	77	.% 74% 18% • •
1	D	77	6% 79% 14% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	77	6% 66% 25% 6%
1	F	77	74% 22%
1	G	77	% 73% 22% 5%
1	H	77	3% 69% 22% 8%
1	I	77	79% 14%
1	J	77	5% 70% 22% 5%
1	K	77	5% 68% 23% 5%
1	L	77	70% 25%
2	R	6	33% 67%
2	Z	6	33% 67%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7168 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 Protein hfq.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	D	73	Total C N O S 577 371 101 104 1	0	0	0
1	A	72	Total C N O 578 372 102 104	0	0	0
1	B	71	Total C N O 570 368 100 102	0	0	0
1	C	74	Total C N O S 583 374 103 105 1	0	0	0
1	E	72	Total C N O 565 361 100 104	0	0	0
1	F	75	Total C N O S 596 381 105 109 1	0	0	0
1	J	73	Total C N O 575 371 100 104	0	0	0
1	G	73	Total C N O S 581 372 103 105 1	0	0	0
1	H	71	Total C N O 570 368 100 102	0	0	0
1	I	74	Total C N O 580 372 103 105	0	0	0
1	K	73	Total C N O S 573 366 101 105 1	0	0	0
1	L	74	Total C N O 584 374 104 106	0	0	0

- Molecule 2 is a RNA chain called 5'-R(*UP*UP*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	R	6	Total C N O P 117 54 12 46 5	0	0	0
2	Z	6	Total C N O P 117 54 12 46 5	0	0	0

- Molecule 3 is water.

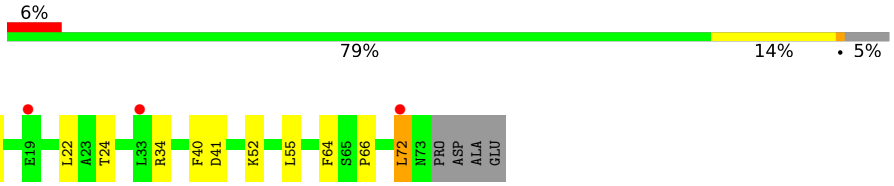
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	J	1	1	1	0	0
			Total	O		
3	R	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

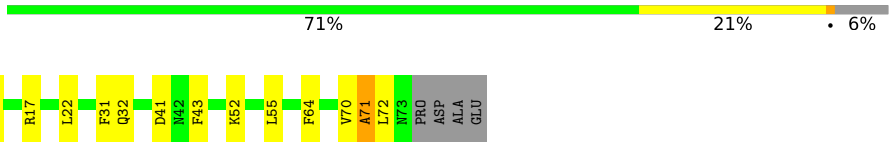
- Molecule 1: Protein hfq

Chain D:



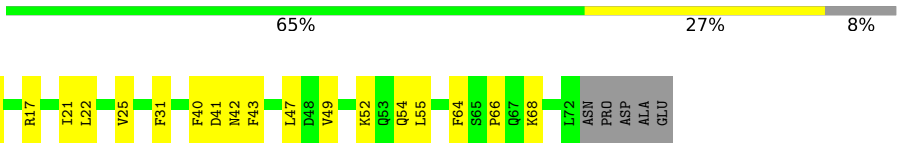
- Molecule 1: Protein hfq

Chain A:



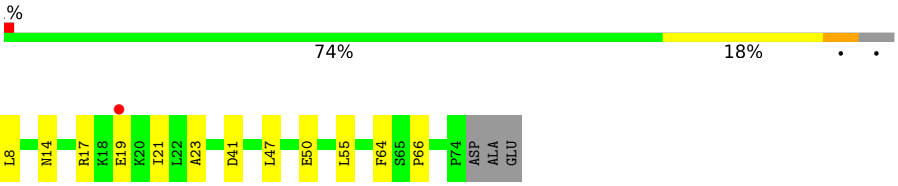
- Molecule 1: Protein hfq

Chain B:



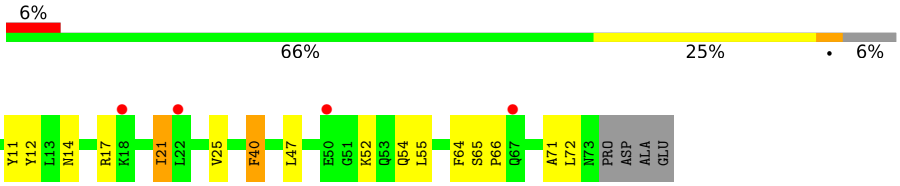
- Molecule 1: Protein hfq

Chain C:



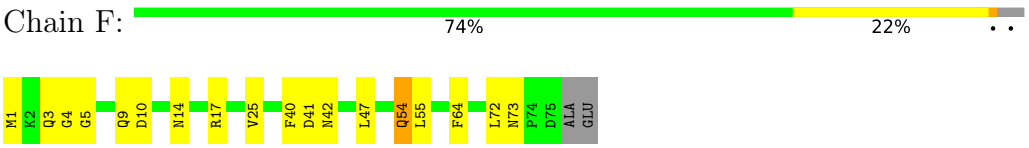
- Molecule 1: Protein hfq

Chain E:



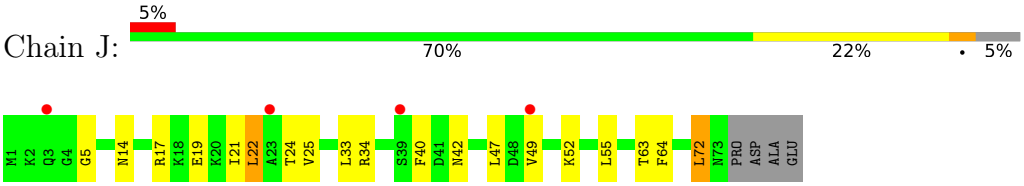
- Molecule 1: Protein hfq

Chain F:



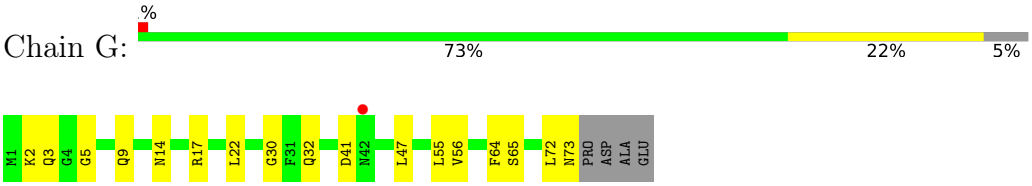
• Molecule 1: Protein hfq

Chain J:



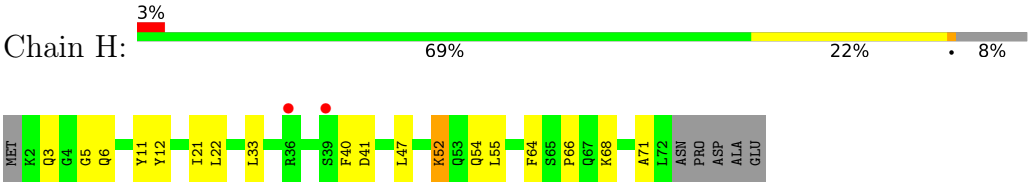
• Molecule 1: Protein hfq

Chain G:



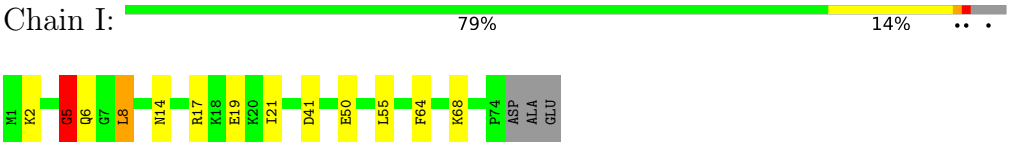
• Molecule 1: Protein hfq

Chain H:



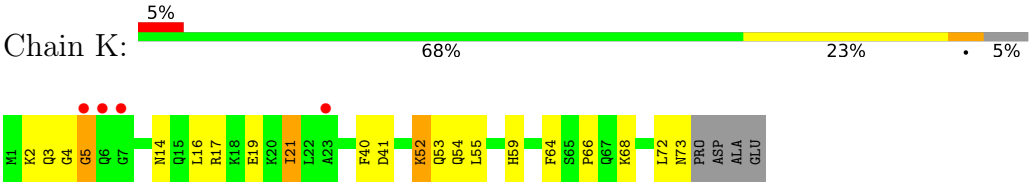
• Molecule 1: Protein hfq

Chain I:



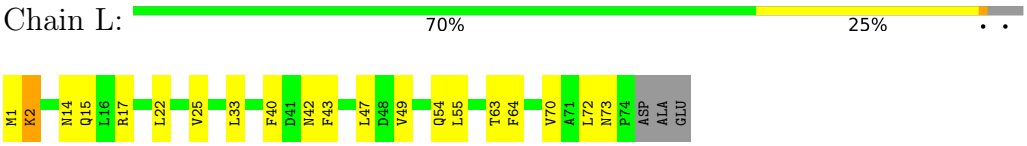
• Molecule 1: Protein hfq

Chain K:



• Molecule 1: Protein hfq

Chain L:



• Molecule 2: 5'-R(*UP*UP*UP*UP*UP*U)-3'

Chain R: 33% 67%

U17 U18 U19 U20 U21 U22

• Molecule 2: 5'-R(*UP*UP*UP*UP*UP*U)-3'

Chain Z: 33% 67%

U27 U28 U29 U30 U31 U32

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	124.03Å 123.93Å 67.59Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	45.67 – 3.10 45.68 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (45.67-3.10) 91.4 (45.68-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.221 , 0.283 0.221 , 0.282	Depositor DCC
R_{free} test set	910 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 9.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.420 for k,h,-l 0.418 for -k,-h,-l 0.447 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7168	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.43	0/587	0.57	1/789 (0.1%)
1	B	0.45	0/579	0.54	0/778
1	C	0.54	0/592	0.67	3/797 (0.4%)
1	D	0.44	0/585	0.62	1/785 (0.1%)
1	E	0.45	0/573	0.55	1/773 (0.1%)
1	F	0.45	0/605	0.73	2/814 (0.2%)
1	G	0.44	0/589	0.55	1/791 (0.1%)
1	H	0.50	0/579	0.52	0/778
1	I	0.70	1/589 (0.2%)	0.66	1/794 (0.1%)
1	J	0.39	0/584	0.55	1/786 (0.1%)
1	K	0.47	0/581	0.68	2/783 (0.3%)
1	L	0.44	0/593	0.62	1/799 (0.1%)
2	R	0.49	0/128	0.88	0/196
2	Z	0.62	0/128	0.87	0/196
All	All	0.48	1/7292 (0.0%)	0.62	14/9859 (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	F	0	1
1	I	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	5	GLY	C-N	12.90	1.63	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	4	GLY	N-CA-C	-9.94	88.26	113.10
1	L	73	ASN	N-CA-CB	-6.82	98.33	110.60
1	D	72	LEU	CB-CA-C	-6.64	97.58	110.20
1	I	5	GLY	CA-C-N	-6.16	103.66	117.20
1	K	5	GLY	N-CA-C	-6.08	97.89	113.10
1	A	71	ALA	CB-CA-C	5.91	118.96	110.10
1	F	73	ASN	N-CA-CB	-5.74	100.27	110.60
1	J	72	LEU	CB-CA-C	-5.68	99.40	110.20
1	C	3	GLN	N-CA-C	5.46	125.73	111.00
1	C	7	GLY	N-CA-C	-5.25	99.98	113.10
1	E	72	LEU	CB-CA-C	-5.21	100.30	110.20
1	K	73	ASN	N-CA-CB	-5.12	101.38	110.60
1	C	5	GLY	N-CA-C	5.07	125.76	113.10
1	G	73	ASN	N-CA-CB	-5.02	101.57	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	5	GLY	Peptide
1	I	5	GLY	Mainchain

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	578	0	591	18	0
1	B	570	0	585	16	0
1	C	583	0	597	15	0
1	D	577	0	591	11	0
1	E	565	0	564	19	0
1	F	596	0	609	13	0
1	G	581	0	598	13	0
1	H	570	0	585	11	0
1	I	580	0	590	8	0
1	J	575	0	578	12	0
1	K	573	0	576	17	0
1	L	584	0	596	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	117	0	62	9	0
2	Z	117	0	62	5	0
3	J	1	0	0	1	0
3	R	1	0	0	0	0
All	All	7168	0	7184	127	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 9.

All (127) 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:C:1:MET:HB2	1:C:2:LYS:HE3	1.39	1.04
1:A:31:PHE:CE1	1:E:3:GLN:OE1	2.25	0.90
1:C:2:LYS:HB2	1:C:2:LYS:NZ	1.85	0.90
1:A:31:PHE:HA	1:E:3:GLN:HB2	1.54	0.87
1:C:1:MET:O	1:C:2:LYS:HG3	1.78	0.83
1:K:3:GLN:CG	1:K:4:GLY:HA3	2.12	0.80
1:K:3:GLN:HG2	1:K:4:GLY:HA3	1.63	0.78
3:J:101:HOH:O	2:R:20:U:H5"	1.84	0.78
1:A:14:ASN:OD1	1:A:17:ARG:NH1	2.21	0.74
1:C:1:MET:HB2	1:C:2:LYS:CE	2.17	0.73
1:C:1:MET:C	1:C:2:LYS:HG3	2.08	0.73
1:F:9:GLN:NE2	2:Z:30:U:O2	2.20	0.72
1:K:21:ILE:HD11	1:K:66:PRO:HB2	1.72	0.71
1:G:14:ASN:OD1	1:G:17:ARG:NH1	2.23	0.71
1:E:21:ILE:HD11	1:E:66:PRO:HB2	1.73	0.68
1:I:14:ASN:OD1	1:I:17:ARG:NH1	2.29	0.66
1:G:64:PHE:HB2	1:H:55:LEU:HB3	1.78	0.66
1:K:3:GLN:HG2	1:K:4:GLY:CA	2.25	0.66
1:C:5:GLY:O	1:K:41:ASP:HB2	1.96	0.65
1:F:14:ASN:OD1	1:F:17:ARG:NH1	2.30	0.64
1:B:41:ASP:OD1	1:B:41:ASP:C	2.36	0.64
1:D:55:LEU:HB3	1:H:64:PHE:HB2	1.80	0.64
1:I:5:GLY:HA2	1:I:6:GLN:C	2.19	0.63
1:C:2:LYS:HB2	1:C:2:LYS:HZ2	1.64	0.62
2:R:17:U:O2'	2:R:18:U:OP1	2.16	0.62
1:A:64:PHE:HB2	1:B:55:LEU:HB3	1.81	0.62
1:E:55:LEU:HB3	1:I:64:PHE:HB2	1.81	0.62
1:D:64:PHE:HB2	1:A:55:LEU:HB3	1.80	0.61
1:C:2:LYS:HB2	1:C:2:LYS:HZ1	1.63	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:LEU:HB3	1:L:64:PHE:HB2	1.83	0.60
1:D:52:LYS:NZ	1:H:66:PRO:O	2.31	0.60
1:C:55:LEU:HB3	1:F:64:PHE:HB2	1.84	0.60
1:C:14:ASN:OD1	1:C:17:ARG:NH1	2.34	0.60
1:B:14:ASN:OD1	1:B:17:ARG:NH1	2.35	0.59
1:E:4:GLY:C	1:E:6:GLN:H	2.05	0.59
1:B:64:PHE:HB2	1:J:55:LEU:HB3	1.85	0.58
1:D:24:THR:OG1	1:D:34:ARG:NH1	2.36	0.58
1:D:41:ASP:OD1	1:D:41:ASP:C	2.42	0.58
1:A:2:LYS:HG3	1:A:3:GLN:N	2.17	0.58
1:J:64:PHE:HB2	1:G:55:LEU:HB3	1.86	0.58
1:C:64:PHE:HB2	1:K:55:LEU:HB3	1.86	0.58
1:L:1:MET:O	1:L:2:LYS:HG2	2.04	0.57
1:K:21:ILE:HD12	1:K:68:LYS:HB2	1.86	0.57
1:K:64:PHE:HB2	1:L:55:LEU:HB3	1.85	0.57
1:C:19:GLU:HB2	1:C:21:ILE:HG12	1.87	0.56
1:A:5:GLY:O	1:B:41:ASP:HB2	2.06	0.56
1:D:41:ASP:HB2	1:H:5:GLY:O	2.05	0.56
1:B:21:ILE:HD12	1:B:68:LYS:HB2	1.88	0.56
1:L:14:ASN:OD1	1:L:17:ARG:NH1	2.39	0.56
1:A:43:PHE:HD1	2:R:18:U:H5'	1.71	0.56
1:A:3:GLN:CD	1:A:4:GLY:H	2.10	0.55
1:L:43:PHE:CD1	2:Z:32:U:H2'	2.42	0.54
1:C:1:MET:CB	1:C:2:LYS:HE3	2.27	0.53
1:E:14:ASN:OD1	1:E:17:ARG:NH1	2.41	0.52
1:D:66:PRO:O	1:A:52:LYS:NZ	2.39	0.52
1:E:5:GLY:O	1:F:41:ASP:HB2	2.10	0.51
1:C:41:ASP:OD1	1:C:41:ASP:C	2.49	0.51
1:K:52:LYS:HD2	1:K:53:GLN:N	2.25	0.51
1:L:25:VAL:HG21	1:L:47:LEU:HD21	1.93	0.51
1:J:22:LEU:HD22	1:J:34:ARG:NH2	2.26	0.51
1:G:2:LYS:HG2	1:G:3:GLN:N	2.27	0.50
1:B:43:PHE:HE1	2:R:19:U:H5"	1.76	0.50
1:E:40:PHE:C	1:I:8:LEU:HD21	2.32	0.50
2:R:17:U:HO2'	2:R:18:U:P	2.34	0.50
1:F:25:VAL:HG21	1:F:47:LEU:HD21	1.94	0.49
1:I:21:ILE:HD12	1:I:68:LYS:HB3	1.94	0.49
1:I:19:GLU:HB2	1:I:21:ILE:HG12	1.93	0.49
1:K:41:ASP:OD1	1:K:41:ASP:C	2.50	0.49
1:G:5:GLY:O	1:H:41:ASP:HB2	2.12	0.49
1:G:32:GLN:N	1:K:2:LYS:O	2.36	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LEU:HD22	1:H:12:TYR:CD1	2.48	0.48
1:K:19:GLU:HB2	1:K:21:ILE:HG22	1.96	0.48
1:B:49:VAL:HG11	1:F:1:MET:HB3	1.96	0.48
1:J:5:GLY:O	1:G:41:ASP:HB2	2.14	0.48
1:G:2:LYS:HG2	1:G:3:GLN:H	1.79	0.47
1:A:43:PHE:CD1	2:R:18:U:H5'	2.49	0.47
1:K:59:HIS:ND1	2:Z:31:U:O2'	2.45	0.47
1:D:12:TYR:CD1	1:A:55:LEU:HD22	2.50	0.47
1:E:65:SER:OG	1:F:54:GLN:OE1	2.33	0.47
1:A:70:VAL:HG12	1:A:71:ALA:O	2.15	0.46
1:J:14:ASN:OD1	1:J:17:ARG:NH1	2.47	0.46
1:J:25:VAL:HG21	1:J:47:LEU:HD11	1.97	0.46
1:D:5:GLY:O	1:A:41:ASP:HB2	2.15	0.46
1:J:33:LEU:HD23	1:J:49:VAL:HG21	1.97	0.46
1:K:16:LEU:HA	1:K:21:ILE:HG23	1.96	0.46
1:I:41:ASP:C	1:I:41:ASP:OD1	2.53	0.45
1:A:32:GLN:N	1:E:2:LYS:O	2.34	0.45
1:B:43:PHE:CE1	2:R:19:U:H5"	2.51	0.45
1:J:19:GLU:HB2	1:J:21:ILE:HG12	1.99	0.45
1:A:31:PHE:CA	1:E:3:GLN:HB2	2.36	0.45
1:J:63:THR:HG22	1:G:56:VAL:HG22	1.99	0.45
1:B:66:PRO:O	1:J:52:LYS:NZ	2.45	0.45
1:K:14:ASN:OD1	1:K:17:ARG:NH1	2.50	0.45
1:B:25:VAL:HG21	1:B:47:LEU:HD21	1.98	0.44
1:E:25:VAL:HG21	1:E:47:LEU:HD21	1.99	0.44
1:E:11:TYR:OH	1:E:71:ALA:O	2.20	0.44
1:K:5:GLY:O	1:L:42:ASN:HB2	2.17	0.44
1:B:2:LYS:HG2	1:B:3:GLN:H	1.83	0.44
1:B:31:PHE:HA	1:F:3:GLN:O	2.17	0.43
2:R:19:U:O2'	2:R:20:U:OP1	2.25	0.43
1:G:30:GLY:O	1:K:3:GLN:HG3	2.18	0.43
1:H:11:TYR:OH	1:H:71:ALA:O	2.23	0.43
1:E:12:TYR:CD1	1:F:55:LEU:HD22	2.54	0.43
1:L:33:LEU:HD22	1:L:49:VAL:HG21	2.00	0.43
1:F:9:GLN:HG3	1:F:10:ASP:N	2.34	0.43
1:A:72:LEU:HD13	1:A:72:LEU:HA	1.87	0.43
1:E:4:GLY:C	1:E:6:GLN:N	2.71	0.43
1:C:23:ALA:HA	1:C:66:PRO:HA	2.00	0.42
1:L:15:GLN:HG2	1:L:70:VAL:HG13	2.01	0.42
1:E:64:PHE:HB2	1:F:55:LEU:HB3	2.00	0.42
1:A:41:ASP:OD1	1:A:41:ASP:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:TYR:OH	1:E:66:PRO:HG3	2.20	0.42
1:H:21:ILE:HD12	1:H:68:LYS:HB2	2.02	0.42
1:H:3:GLN:HB3	1:H:6:GLN:HE21	1.84	0.42
1:E:3:GLN:HA	1:E:4:GLY:HA3	1.82	0.41
1:G:65:SER:OG	1:H:52:LYS:HE2	2.20	0.41
2:Z:29:U:H4'	2:Z:30:U:OP1	2.20	0.41
1:J:24:THR:OG1	1:J:34:ARG:NH1	2.54	0.41
1:G:17:ARG:HH11	1:G:17:ARG:HB3	1.86	0.41
1:D:22:LEU:HD22	1:D:34:ARG:NH2	2.36	0.41
1:B:49:VAL:HG11	1:F:1:MET:CB	2.50	0.41
1:E:5:GLY:HA3	1:F:42:ASN:ND2	2.36	0.41
2:Z:29:U:H4'	2:Z:29:U:OP2	2.20	0.41
1:B:42:ASN:OD1	2:R:19:U:O4	2.40	0.41
1:H:33:LEU:HD11	1:L:2:LYS:HD2	2.02	0.40
1:B:5:GLY:O	1:J:42:ASN:HB2	2.20	0.40
1:G:9:GLN:HE21	1:G:9:GLN:HB3	1.66	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	
1	A	70/77 (91%)	66 (94%)	4 (6%)	0	100	100
1	B	69/77 (90%)	66 (96%)	3 (4%)	0	100	100
1	C	72/77 (94%)	68 (94%)	4 (6%)	0	100	100
1	D	71/77 (92%)	66 (93%)	5 (7%)	0	100	100
1	E	70/77 (91%)	63 (90%)	7 (10%)	0	100	100
1	F	73/77 (95%)	68 (93%)	5 (7%)	0	100	100
1	G	71/77 (92%)	68 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	69/77 (90%)	67 (97%)	2 (3%)	0	100	100
1	I	72/77 (94%)	66 (92%)	5 (7%)	1 (1%)	11	40
1	J	71/77 (92%)	66 (93%)	5 (7%)	0	100	100
1	K	71/77 (92%)	65 (92%)	6 (8%)	0	100	100
1	L	72/77 (94%)	68 (94%)	4 (6%)	0	100	100
All	All	851/924 (92%)	797 (94%)	53 (6%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	5	GLY

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	
1	A	63/67 (94%)	62 (98%)	1 (2%)	62	84
1	B	62/67 (92%)	58 (94%)	4 (6%)	17	47
1	C	63/67 (94%)	58 (92%)	5 (8%)	12	40
1	D	61/67 (91%)	59 (97%)	2 (3%)	38	69
1	E	60/67 (90%)	56 (93%)	4 (7%)	16	46
1	F	65/67 (97%)	62 (95%)	3 (5%)	27	59
1	G	63/67 (94%)	60 (95%)	3 (5%)	25	58
1	H	62/67 (92%)	57 (92%)	5 (8%)	11	39
1	I	62/67 (92%)	59 (95%)	3 (5%)	25	58
1	J	60/67 (90%)	57 (95%)	3 (5%)	24	57
1	K	61/67 (91%)	56 (92%)	5 (8%)	11	38
1	L	63/67 (94%)	57 (90%)	6 (10%)	8	31
All	All	745/804 (93%)	701 (94%)	44 (6%)	19	50

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	40	PHE
1	D	72	LEU
1	A	22	LEU
1	B	22	LEU
1	B	40	PHE
1	B	52	LYS
1	B	54	GLN
1	C	1	MET
1	C	2	LYS
1	C	8	LEU
1	C	47	LEU
1	C	50	GLU
1	E	21	ILE
1	E	40	PHE
1	E	52	LYS
1	E	54	GLN
1	F	40	PHE
1	F	54	GLN
1	F	72	LEU
1	J	22	LEU
1	J	40	PHE
1	J	72	LEU
1	G	22	LEU
1	G	47	LEU
1	G	72	LEU
1	H	22	LEU
1	H	40	PHE
1	H	47	LEU
1	H	52	LYS
1	H	54	GLN
1	I	2	LYS
1	I	8	LEU
1	I	50	GLU
1	K	21	ILE
1	K	40	PHE
1	K	52	LYS
1	K	54	GLN
1	K	72	LEU
1	L	2	LYS
1	L	22	LEU
1	L	40	PHE
1	L	54	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	63	THR
1	L	72	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	54	GLN
1	E	54	GLN
1	K	54	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	6/6 (100%)	5 (83%)	2 (33%)
2	Z	5/6 (83%)	4 (80%)	1 (20%)
All	All	11/12 (91%)	9 (81%)	3 (27%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	18	U
2	R	19	U
2	R	20	U
2	R	21	U
2	R	22	U
2	Z	29	U
2	Z	30	U
2	Z	31	U
2	Z	32	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	17	U
2	R	19	U
2	Z	29	U

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 monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	5:GLY	C	6:GLN	N	1.63

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(Å^2)	Q<0.9
1	A	72/77 (93%)	0.09	0	100	100	17, 35, 61, 72	0
1	B	71/77 (92%)	0.08	0	100	100	19, 32, 50, 68	0
1	C	74/77 (96%)	0.09	1 (1%)	75	56	17, 34, 65, 88	0
1	D	73/77 (94%)	0.31	5 (6%)	17	7	18, 32, 59, 70	0
1	E	72/77 (93%)	0.40	5 (6%)	16	7	18, 33, 57, 66	0
1	F	75/77 (97%)	0.14	0	100	100	19, 33, 63, 72	0
1	G	73/77 (94%)	0.10	1 (1%)	75	56	17, 34, 64, 69	0
1	H	71/77 (92%)	0.14	2 (2%)	53	30	19, 32, 52, 60	0
1	I	74/77 (96%)	0.16	0	100	100	17, 34, 55, 83	0
1	J	73/77 (94%)	0.25	4 (5%)	25	11	19, 32, 55, 76	0
1	K	73/77 (94%)	0.39	4 (5%)	25	11	18, 33, 56, 62	0
1	L	74/77 (96%)	0.09	0	100	100	17, 32, 53, 71	0
2	R	6/6 (100%)	1.04	0	100	100	35, 41, 44, 48	0
2	Z	6/6 (100%)	0.57	0	100	100	34, 40, 42, 47	0
All	All	887/936 (94%)	0.19	22 (2%)	57	34	17, 34, 59, 88	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	7	GLY	4.4
1	J	39	SER	3.8
1	D	7	GLY	3.6
1	J	49	VAL	3.3
1	D	72	LEU	3.2
1	E	18	LYS	2.9
1	D	6	GLN	2.6
1	K	6	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	23	ALA	2.6
1	H	39	SER	2.6
1	J	3	GLN	2.5
1	C	19	GLU	2.3
1	E	5	GLY	2.3
1	K	5	GLY	2.3
1	J	23	ALA	2.2
1	E	50	GLU	2.2
1	D	33	LEU	2.2
1	E	22	LEU	2.1
1	E	67	GLN	2.1
1	G	42	ASN	2.1
1	D	19	GLU	2.1
1	H	36	ARG	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 monosaccharides 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.