wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:04 PM GMT

PDB ID	:	4K0K
Title	:	Crystal structure of the Thermus thermophilus 30S ribosomal subunit complexed with a serine-ASL and mRNA containing a stop codon
Authors	:	Fernandez, I.S.; Ng, C.L.; Kelley, A.C.; Guowei, W.; Yu, Y.T.; Ramakrishnan, V.
Deposited on	:	2013-04-04
Resolution	:	3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

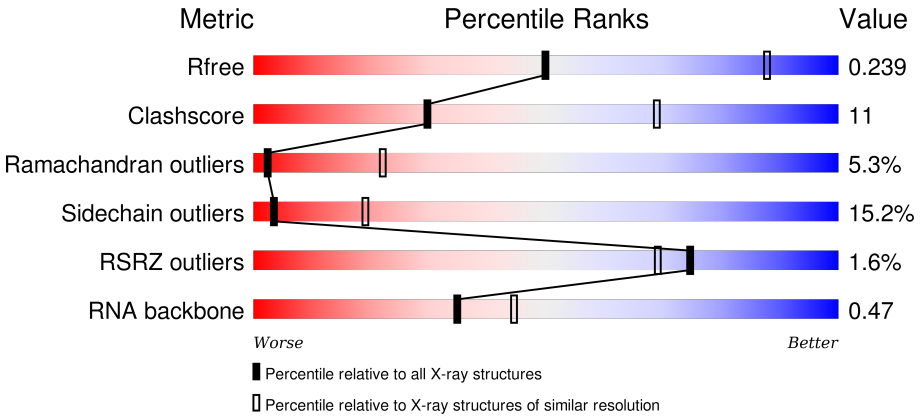
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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 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	1517	2% 54% 35% 10%
2	B	235	2% 49% 40% 10%
3	C	207	54% 37% 8%
4	D	208	% 54% 32% 13%

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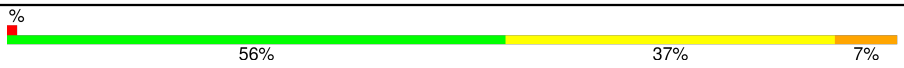
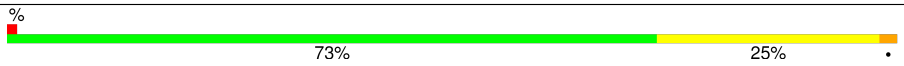
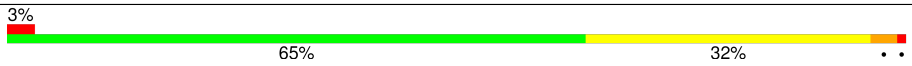
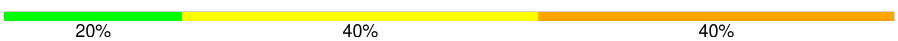
Mol	Chain	Length	Quality of chain
5	E	151	
6	F	101	
7	G	155	
8	H	138	
9	I	127	
10	J	99	
11	K	119	
12	L	126	
13	M	121	
14	N	60	
15	O	88	
16	P	84	
17	Q	100	
18	R	70	
19	S	79	
20	T	99	
21	U	25	
22	X	5	
23	Y	11	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51915 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1511	Total	C	N	O	P	0	0	0
			32468	14453	6008	10497	1510			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	A	G	CONFLICT	GB 55771382

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	126	Total	C	N	O	S	0	0	1
			976	614	197	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	121	Total	C	N	O	S	0	0	1
			956	591	198	165	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	5	Total	C	N	O	P	0	0	0
			104	48	19	33	4			

- Molecule 23 is a RNA chain called RNA-ASL.

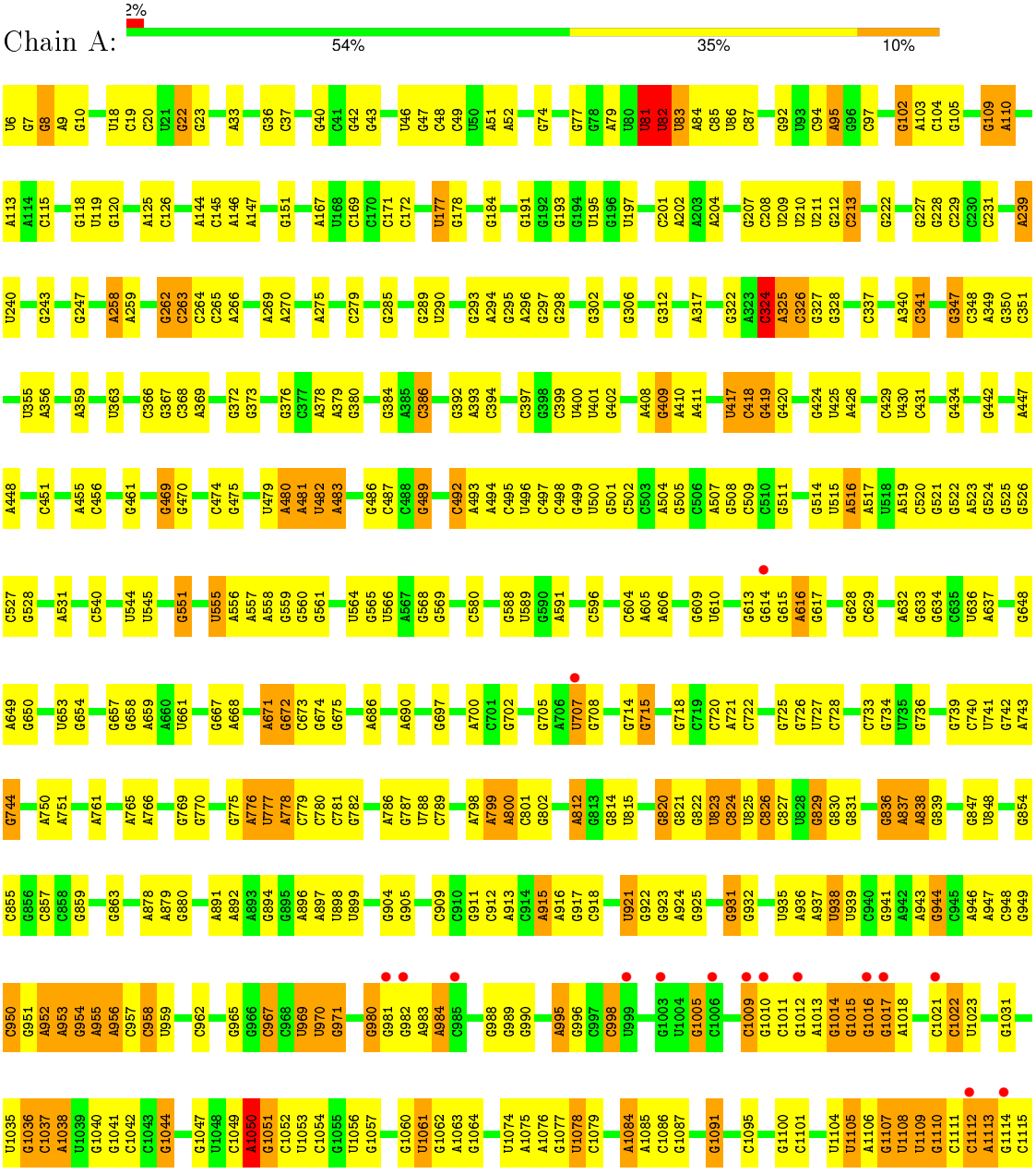
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	10	Total	C	N	O	P	0	0	0
			213	96	38	69	10			

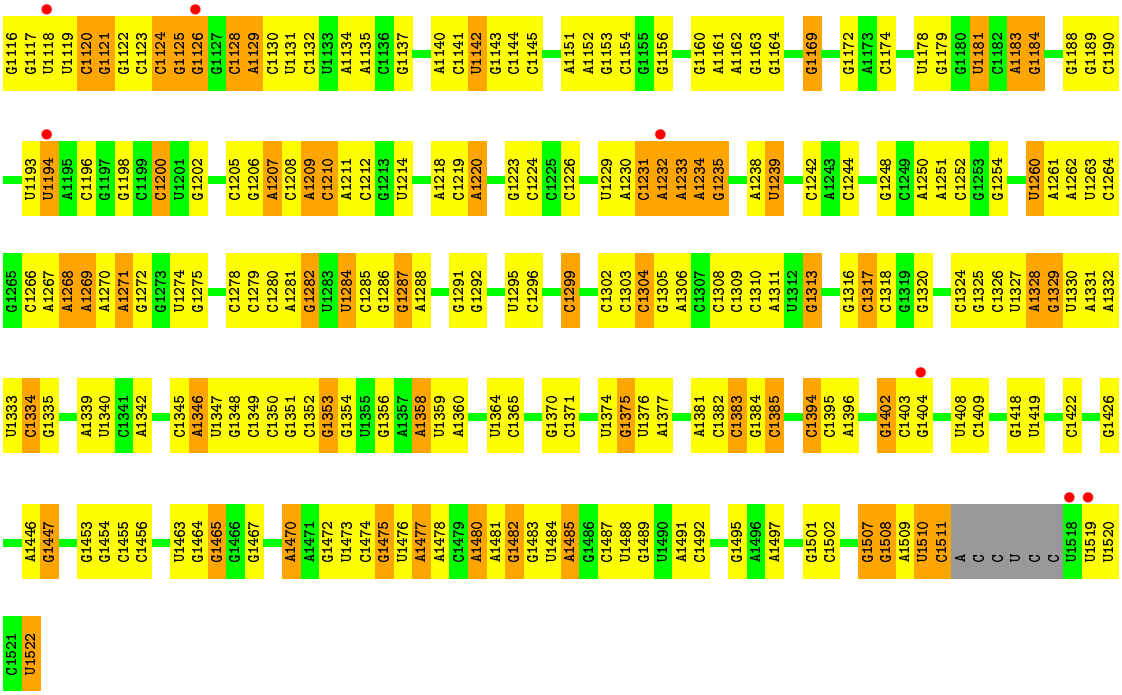
3 Residue-property plots (i)

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: 16S ribosomal RNA

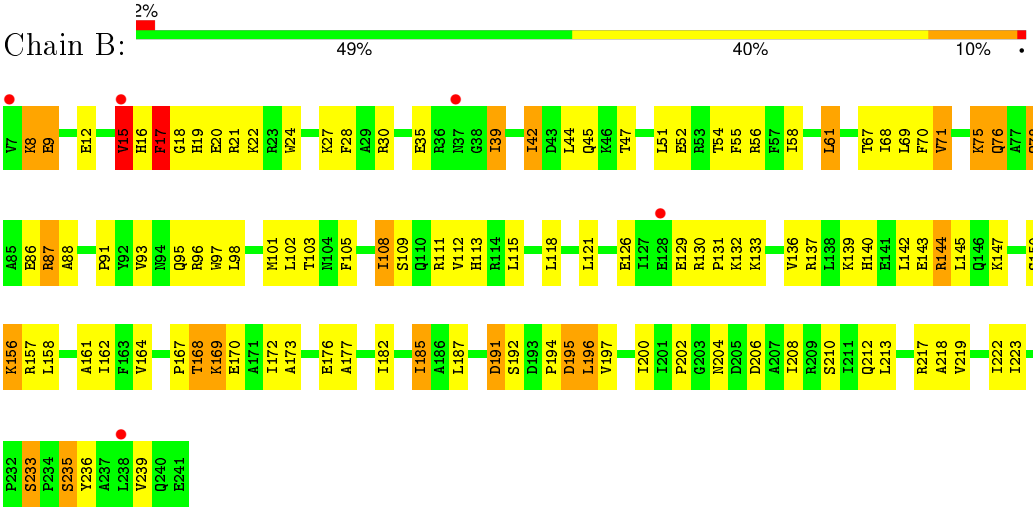
Chain A:





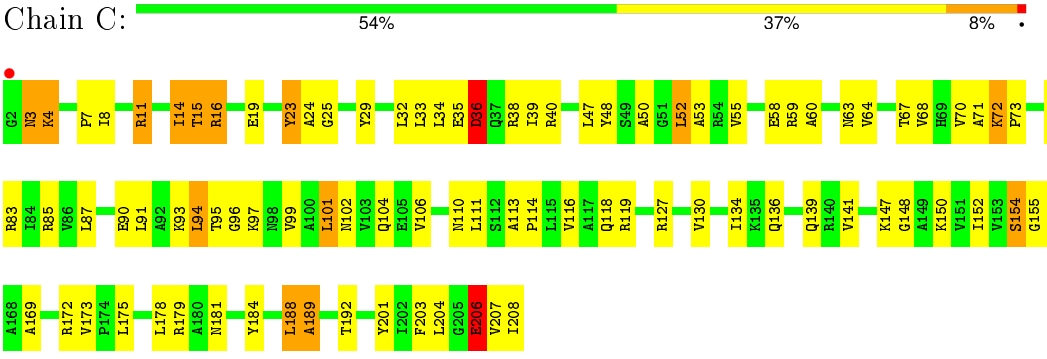
• Molecule 2: 30S ribosomal protein S2

Chain B:



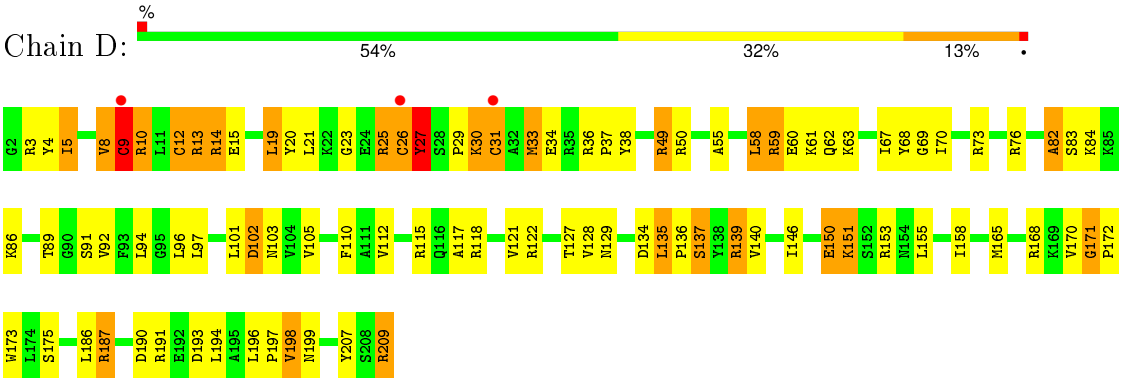
• Molecule 3: 30S ribosomal protein S3

Chain C:



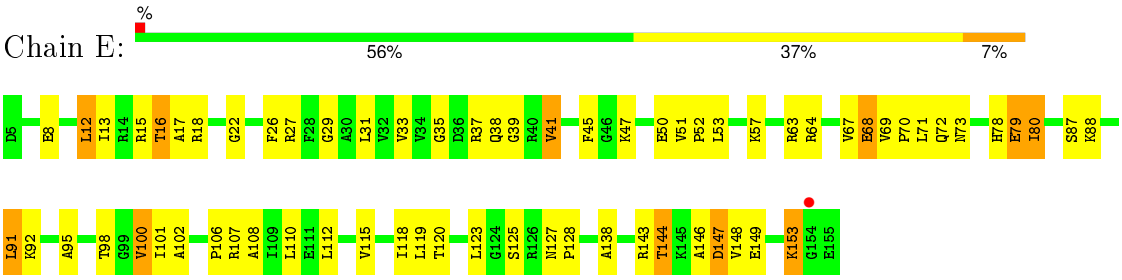
- Molecule 4: 30S ribosomal protein S4

Chain D:



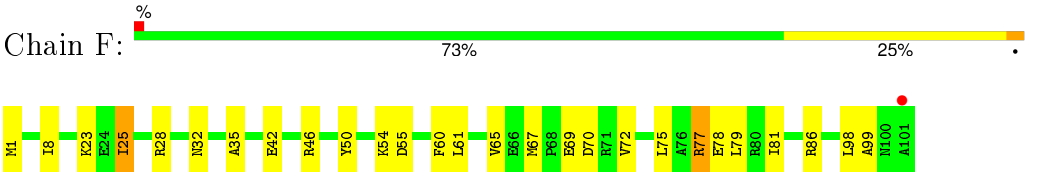
- Molecule 5: 30S ribosomal protein S5

Chain E:



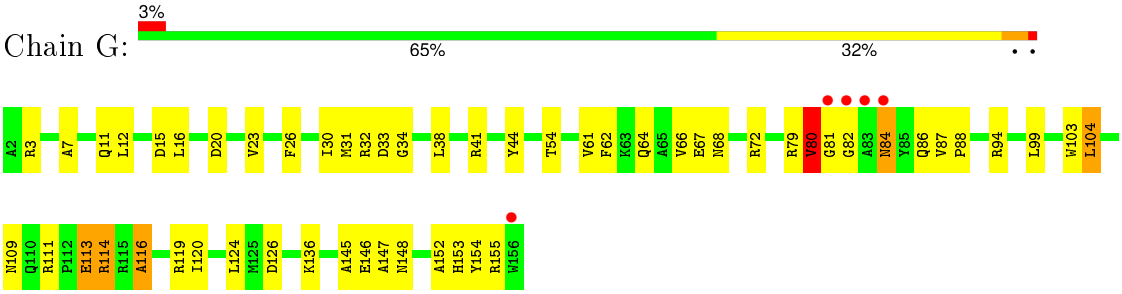
- Molecule 6: 30S ribosomal protein S6

Chain F:



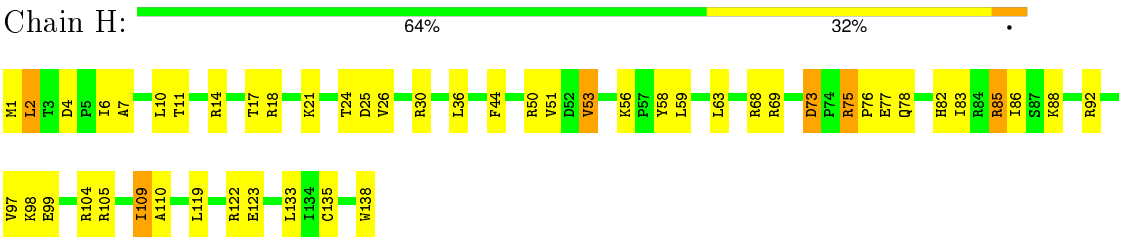
- Molecule 7: 30S ribosomal protein S7

Chain G:



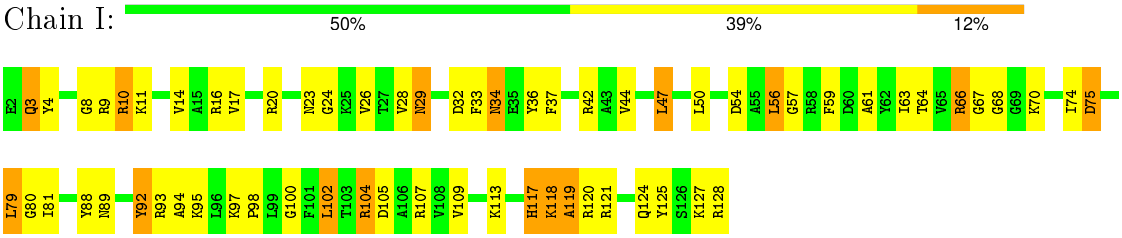
- Molecule 8: 30S ribosomal protein S8

Chain H:



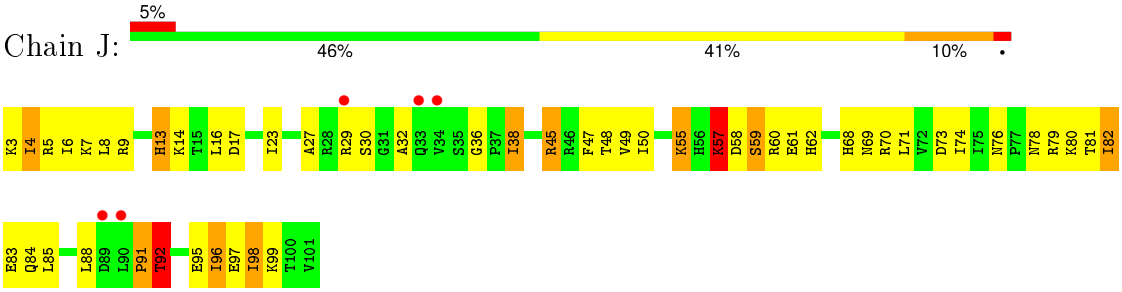
- Molecule 9: 30S ribosomal protein S9

Chain I:



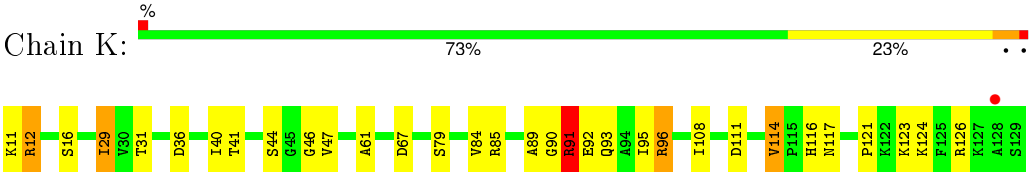
- Molecule 10: 30S ribosomal protein S10

Chain J:



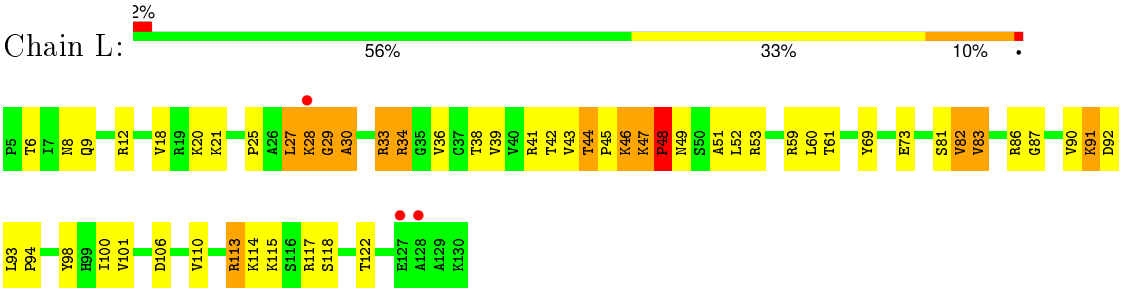
- Molecule 11: 30S ribosomal protein S11

Chain K:



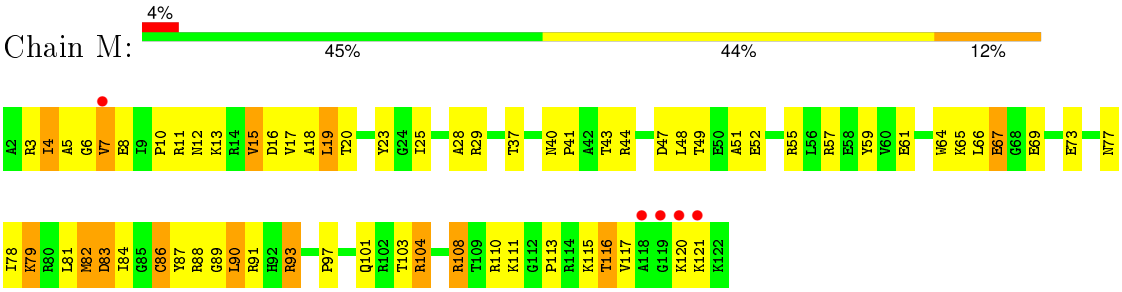
- Molecule 12: 30S ribosomal protein S12

Chain L:



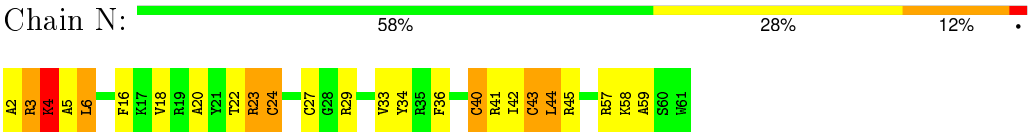
- Molecule 13: 30S ribosomal protein S13

Chain M:



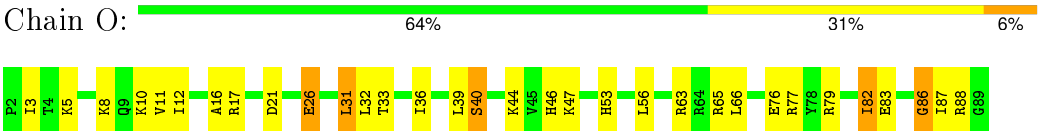
- Molecule 14: 30S ribosomal protein S14

Chain N:



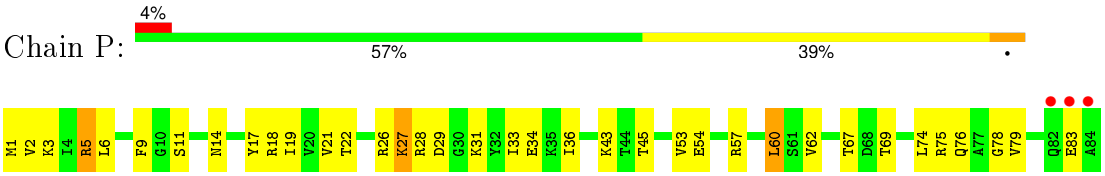
• Molecule 15: 30S ribosomal protein S15

Chain O:



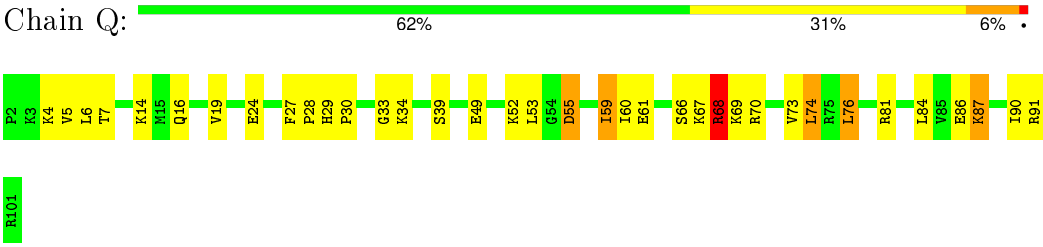
• Molecule 16: 30S ribosomal protein S16

Chain P:



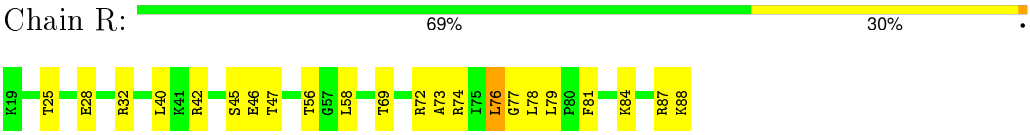
• Molecule 17: 30S ribosomal protein S17

Chain Q:



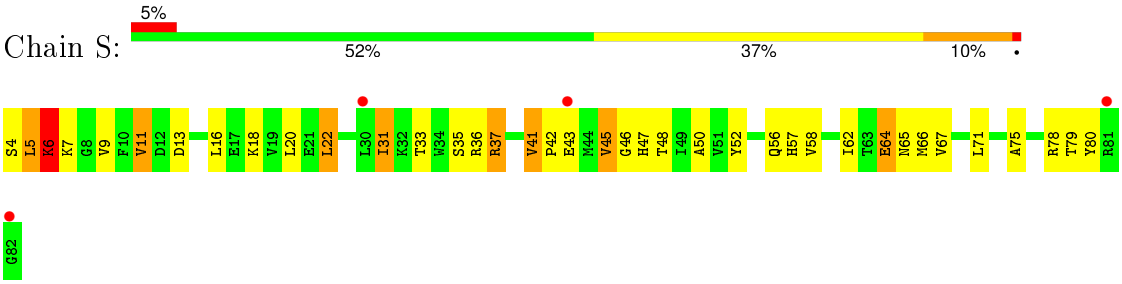
• Molecule 18: 30S ribosomal protein S18

Chain R:



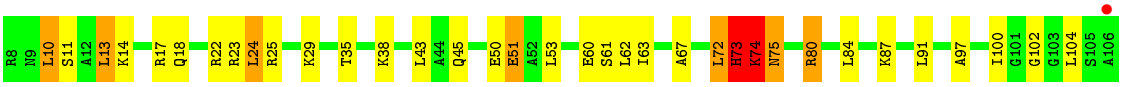
• Molecule 19: 30S ribosomal protein S19

Chain S:



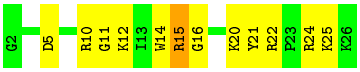
• Molecule 20: 30S ribosomal protein S20

Chain T:



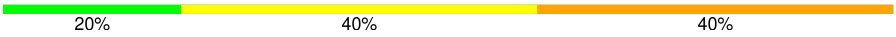
- Molecule 21: 30S ribosomal protein THX

Chain U:



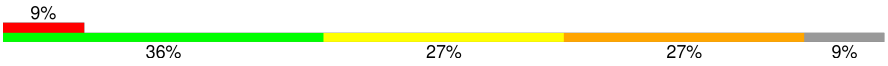
- Molecule 22: mRNA

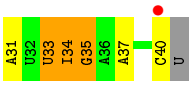
Chain X:



- Molecule 23: RNA-ASL

Chain Y:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.30Å 401.30Å 173.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-3.40) 98.7 (20.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 3.36Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.187 , 0.242 0.189 , 0.239	Depositor DCC
R_{free} test set	9471 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	95.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 64.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 189418 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	51915	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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	0.45	3/36342 (0.0%)	0.74	17/56718 (0.0%)
2	B	0.46	0/1936	0.74	0/2611
3	C	0.51	0/1637	0.77	1/2207 (0.0%)
4	D	0.54	1/1733 (0.1%)	0.83	2/2318 (0.1%)
5	E	0.58	0/1163	0.84	1/1566 (0.1%)
6	F	0.41	0/856	0.65	0/1154
7	G	0.43	0/1276	0.71	0/1709
8	H	0.57	0/1136	0.81	0/1527
9	I	0.47	0/1029	0.73	0/1378
10	J	0.50	0/808	0.75	0/1087
11	K	0.51	0/900	0.75	0/1213
12	L	0.57	0/992	0.87	1/1329 (0.1%)
13	M	0.50	0/966	0.79	0/1294
14	N	0.66	1/501 (0.2%)	0.94	1/664 (0.2%)
15	O	0.45	0/745	0.73	0/992
16	P	0.55	0/717	0.83	1/965 (0.1%)
17	Q	0.55	0/837	0.81	1/1119 (0.1%)
18	R	0.45	0/579	0.73	0/768
19	S	0.47	0/643	0.73	0/867
20	T	0.51	0/765	0.81	0/1007
21	U	0.55	0/213	0.83	0/279
22	X	1.72	3/116 (2.6%)	1.95	5/179 (2.8%)
23	Y	2.48	1/237 (0.4%)	1.39	4/364 (1.1%)
All	All	0.51	9/56127 (0.0%)	0.76	34/83315 (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
3	C	0	1
9	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	T	0	2
23	Y	1	0
All	All	1	4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	34	I	O3'-P	37.06	2.05	1.61
22	X	4	U	C4-C5	-10.47	1.34	1.43
22	X	4	U	N1-C2	10.39	1.47	1.38
1	A	82	U	O3'-P	7.11	1.69	1.61
1	A	81	U	O3'-P	6.22	1.68	1.61

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Y	34	I	OP1-P-O3'	13.34	134.54	105.20
22	X	4	U	C5-C4-O4	-13.18	117.99	125.90
22	X	4	U	N3-C4-C5	10.84	121.10	114.60
23	Y	34	I	P-O3'-C3'	-10.75	106.80	119.70
23	Y	34	I	OP2-P-O3'	-10.19	82.79	105.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	Y	34	I	C4'

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	206	GLU	Peptide
9	I	117	HIS	Peptide
20	T	74	LYS	Peptide
20	T	75	ASN	Peptide

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	32468	0	16391	481	0
2	B	1901	0	1951	66	0
3	C	1613	0	1677	58	0
4	D	1703	0	1763	55	0
5	E	1147	0	1207	44	0
6	F	843	0	857	15	0
7	G	1257	0	1296	32	0
8	H	1116	0	1177	29	0
9	I	1011	0	1043	49	0
10	J	795	0	840	38	0
11	K	885	0	904	20	0
12	L	976	0	1062	38	0
13	M	956	0	1021	36	0
14	N	492	0	529	18	0
15	O	734	0	771	12	0
16	P	701	0	720	18	0
17	Q	824	0	891	24	0
18	R	574	0	644	12	0
19	S	630	0	652	25	0
20	T	763	0	861	18	0
21	U	209	0	221	7	0
22	X	104	0	55	5	0
23	Y	213	0	109	18	0
All	All	51915	0	36642	984	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 11.

The worst 5 of 984 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)
23:Y:34:I:O3'	23:Y:35:G:P	2.05	1.15
1:A:1231:C:N4	1:A:1269:A:N7	2.00	1.07
1:A:1522:U:O3'	22:X:4:U:O5'	1.72	1.05
1:A:951:G:OP1	10:J:57:LYS:NZ	1.99	0.95
3:C:154:SER:OG	3:C:155:GLY:N	1.96	0.93

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	B	233/235 (99%)	168 (72%)	48 (21%)	17 (7%)	1 14
3	C	205/207 (99%)	151 (74%)	39 (19%)	15 (7%)	1 14
4	D	206/208 (99%)	165 (80%)	24 (12%)	17 (8%)	1 11
5	E	149/151 (99%)	132 (89%)	14 (9%)	3 (2%)	9 48
6	F	99/101 (98%)	85 (86%)	13 (13%)	1 (1%)	19 63
7	G	153/155 (99%)	122 (80%)	22 (14%)	9 (6%)	2 19
8	H	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	13 54
9	I	125/127 (98%)	99 (79%)	20 (16%)	6 (5%)	3 25
10	J	97/99 (98%)	74 (76%)	15 (16%)	8 (8%)	1 11
11	K	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	11 51
12	L	124/126 (98%)	98 (79%)	17 (14%)	9 (7%)	1 14
13	M	119/121 (98%)	84 (71%)	26 (22%)	9 (8%)	1 13
14	N	58/60 (97%)	49 (84%)	3 (5%)	6 (10%)	1 7
15	O	86/88 (98%)	68 (79%)	15 (17%)	3 (4%)	4 35
16	P	82/84 (98%)	70 (85%)	11 (13%)	1 (1%)	16 59
17	Q	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	9 48
18	R	68/70 (97%)	66 (97%)	1 (2%)	1 (2%)	13 54
19	S	77/79 (98%)	60 (78%)	11 (14%)	6 (8%)	1 12
20	T	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1 14
21	U	23/25 (92%)	18 (78%)	4 (17%)	1 (4%)	3 29
All	All	2352/2392 (98%)	1895 (81%)	332 (14%)	125 (5%)	2 22

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	PHE

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Mol	Chain	Res	Type
3	C	15	THR
3	C	82	GLU
3	C	189	ALA
3	C	207	VAL

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	B	202/203 (100%)	160 (79%)	42 (21%)	1 6
3	C	160/161 (99%)	140 (88%)	20 (12%)	6 27
4	D	180/180 (100%)	152 (84%)	28 (16%)	3 18
5	E	115/116 (99%)	95 (83%)	20 (17%)	2 13
6	F	90/90 (100%)	82 (91%)	8 (9%)	12 45
7	G	126/126 (100%)	113 (90%)	13 (10%)	9 37
8	H	119/119 (100%)	103 (87%)	16 (13%)	5 24
9	I	98/98 (100%)	82 (84%)	16 (16%)	3 16
10	J	88/89 (99%)	70 (80%)	18 (20%)	1 7
11	K	90/90 (100%)	80 (89%)	10 (11%)	8 33
12	L	104/105 (99%)	90 (86%)	14 (14%)	5 24
13	M	96/97 (99%)	76 (79%)	20 (21%)	1 6
14	N	49/49 (100%)	42 (86%)	7 (14%)	4 22
15	O	79/79 (100%)	66 (84%)	13 (16%)	3 15
16	P	72/72 (100%)	60 (83%)	12 (17%)	3 14
17	Q	94/95 (99%)	80 (85%)	14 (15%)	4 20
18	R	61/61 (100%)	56 (92%)	5 (8%)	14 50
19	S	69/69 (100%)	59 (86%)	10 (14%)	4 21
20	T	76/76 (100%)	62 (82%)	14 (18%)	2 10
21	U	19/20 (95%)	16 (84%)	3 (16%)	3 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1987/1995 (100%)	1684 (85%)	303 (15%)	3 19

5 of 303 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	56	LYS
10	J	38	ILE
19	S	13	ASP
8	H	97	VAL
9	I	47	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	129	ASN
19	S	65	ASN
11	K	99	GLN
4	D	116	GLN
4	D	161	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1509/1517 (99%)	306 (20%)	33 (2%)
22	X	4/5 (80%)	2 (50%)	0
23	Y	8/11 (72%)	3 (37%)	0
All	All	1521/1533 (99%)	311 (20%)	33 (2%)

5 of 311 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	G
1	A	10	G
1	A	33	A
1	A	40	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	671	A
1	A	938	U
1	A	1317	C
1	A	707	U
1	A	777	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 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

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	1511/1517 (99%)	-0.18	23 (1%) 76 71	49, 80, 148, 246	0
2	B	235/235 (100%)	-0.09	5 (2%) 67 61	65, 115, 172, 216	0
3	C	207/207 (100%)	-0.26	1 (0%) 91 89	73, 106, 146, 172	0
4	D	208/208 (100%)	-0.27	3 (1%) 78 73	69, 98, 133, 149	0
5	E	151/151 (100%)	-0.42	1 (0%) 89 85	57, 77, 105, 134	0
6	F	101/101 (100%)	-0.29	1 (0%) 84 79	80, 110, 133, 149	0
7	G	155/155 (100%)	-0.16	5 (3%) 51 47	76, 103, 158, 199	0
8	H	138/138 (100%)	-0.54	0 100 100	51, 73, 95, 118	0
9	I	127/127 (100%)	-0.18	0 100 100	66, 115, 149, 166	0
10	J	99/99 (100%)	0.17	5 (5%) 32 28	68, 142, 187, 196	0
11	K	119/119 (100%)	-0.29	1 (0%) 87 83	52, 87, 121, 160	0
12	L	126/126 (100%)	-0.31	3 (2%) 62 57	51, 84, 122, 176	0
13	M	121/121 (100%)	-0.24	5 (4%) 41 36	66, 104, 147, 176	0
14	N	60/60 (100%)	-0.27	0 100 100	78, 99, 124, 133	0
15	O	88/88 (100%)	-0.49	0 100 100	58, 87, 124, 152	0
16	P	84/84 (100%)	-0.35	3 (3%) 46 41	59, 75, 101, 142	0
17	Q	100/100 (100%)	-0.46	0 100 100	56, 78, 110, 127	0
18	R	70/70 (100%)	-0.42	0 100 100	74, 96, 128, 134	0
19	S	79/79 (100%)	-0.19	4 (5%) 32 28	85, 122, 170, 196	0
20	T	99/99 (100%)	-0.46	1 (1%) 84 79	58, 84, 120, 148	0
21	U	25/25 (100%)	-0.26	0 100 100	71, 91, 120, 137	0
22	X	5/5 (100%)	0.47	0 100 100	65, 81, 128, 129	0
23	Y	9/11 (81%)	0.53	1 (11%) 7 7	73, 84, 116, 137	0
All	All	3917/3925 (99%)	-0.24	62 (1%) 74 69	49, 90, 150, 246	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	82	GLY	7.9
1	A	1518	U	7.0
10	J	33	GLN	5.9
7	G	82	GLY	5.5
1	A	1017	G	5.2

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.