wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2023 – 06:12 AM EDT

PDB ID	:	2ZJQ
Title	:	Interaction of L7 with L11 induced by Microccocin binding to the Deinococcus radiodurans 50S subunit
Authors	:	Harms, J.M.; Wilson, D.N.; Schluenzen, F.; Connell, S.R.; Stachelhaus, T.; Zaborowska, Z.; Spahn, C.M.T.; Fucini, P.
Deposited on	:	2008-03-08
Resolution	:	3.30 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
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 (i)) were used in the production of this report:

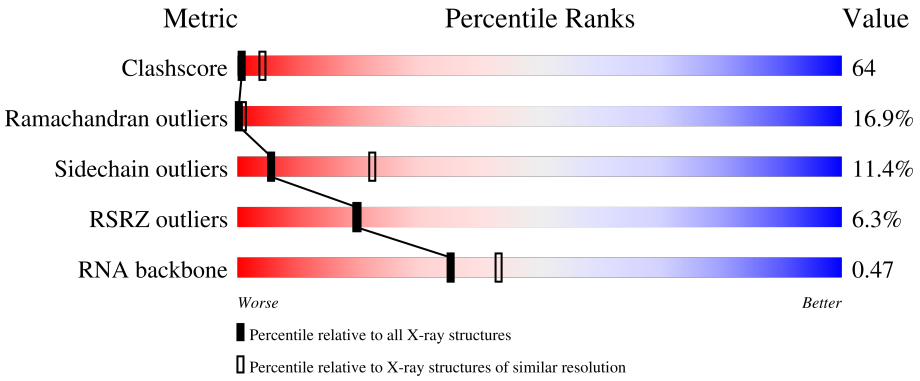
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 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))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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	X	2880	11% 50% 23% 10% 7%
2	Y	122	16% 69% 14%
3	A	274	19% 55% 14% 12%
4	B	211	25% 56% 13%
5	C	205	14% 54% 24% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	D	180	3% 9% 71% 16%
7	E	185	% 18% 59% 14% 8%
8	F	144	51% 60% 35% 5%
9	G	174	2% 7% 52% 18% 18%
10	H	134	28% 61% 10%
11	I	156	8% 16% 45% 27% 10%
12	J	142	% 18% 61% 14%
13	K	116	22% 59% 15%
14	L	114	5% 12% 54% 22% 9%
15	M	166	13% 36% 15% 35%
16	N	118	11% 67% 20%
17	O	100	11% 50% 32% 6%
18	P	134	18% 62% 14% 5%
19	Q	95	8% 65% 20%
20	R	115	3% 10% 57% 23%
21	S	237	3% 13% 47% 12% 26%
22	T	91	12% 27% 55% 8% 8%
23	U	81	4% 10% 52% 21% 6% 11%
24	V	67	13% 64% 21%
25	W	55	15% 65% 20%
26	Z	60	2% 20% 52% 22%
27	1	55	64% 96%
28	2	47	98% 98%
29	3	66	88% 92% 5%
30	4	37	11% 16% 73% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	5	122	

2 Entry composition (i)

There are 31 unique types of molecules in this entry. The entry contains 84395 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 ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2686	57651	25718	10642	18606	2685	0	0	0

- Molecule 2 is a RNA chain called ribosomal 5S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	122	2598	1161	476	840	121	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	240	1826	1137	366	321	2	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	205	1539	965	295	271	8	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	197	1506	935	287	282	2	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	177	1400	892	247	254	7	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	144	Total	C	N	O	S	0	0	0
			1043	663	179	196	5			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	initiating methionine	UNP Q9RXJ5

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total 878	C 541	N 178	O 157	S 2	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total 779	C 476	N 161	O 142	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total 871	C 543	N 172	O 156	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total 978	C 608	N 210	O 159	S 1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total 741	C 465	N 139	O 137	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total 1014	C 639	N 199	O 174	S 2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total 726	C 458	N 136	O 130	S 2	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O	0	0	0
			552	341	116	95			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C 53 53	0	0	53

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
30	4	37	Total 297	C 179	N 66	O 47	S 5	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L7/L12.

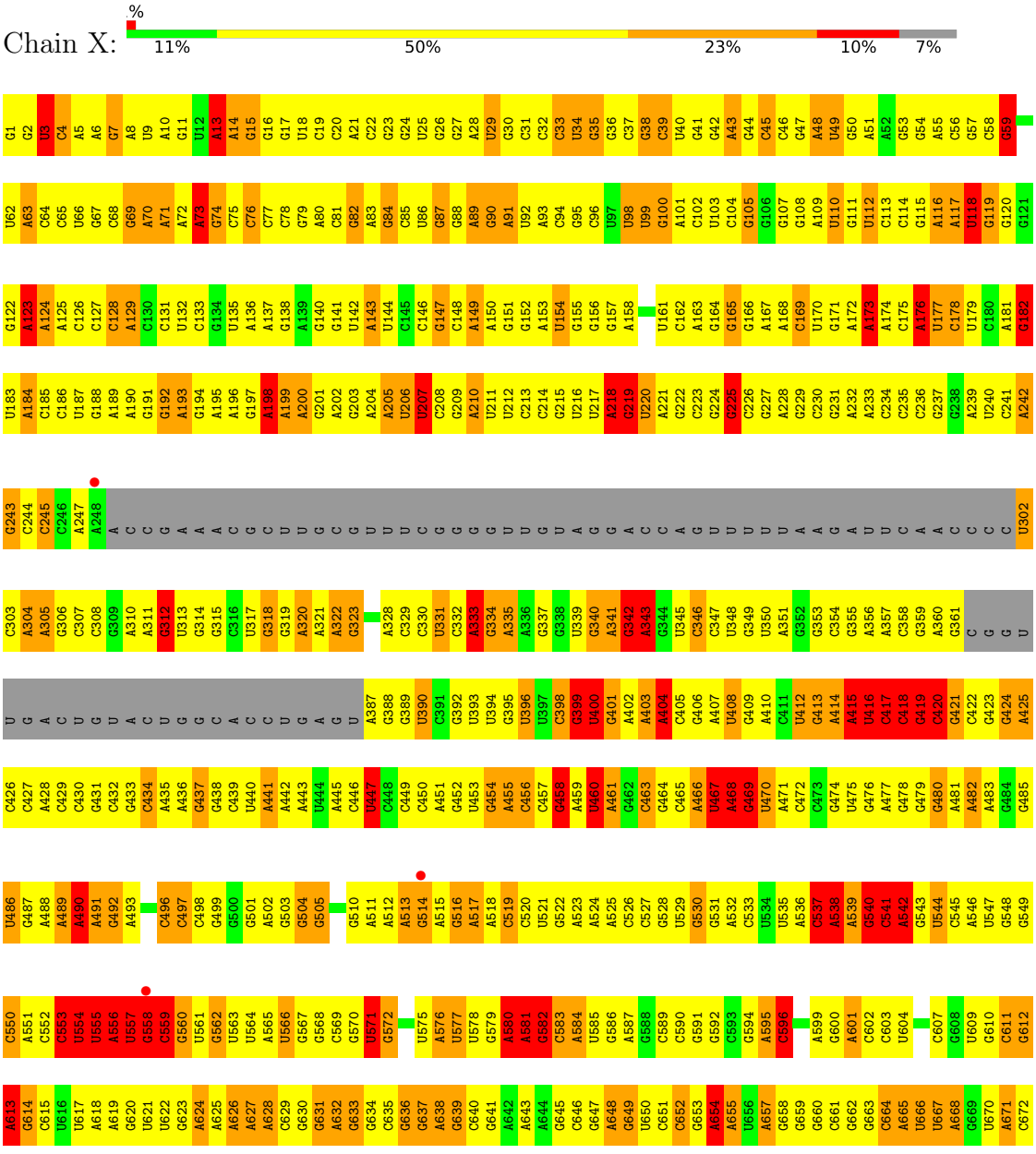
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	5	71	Total C 71 71	0	0	71

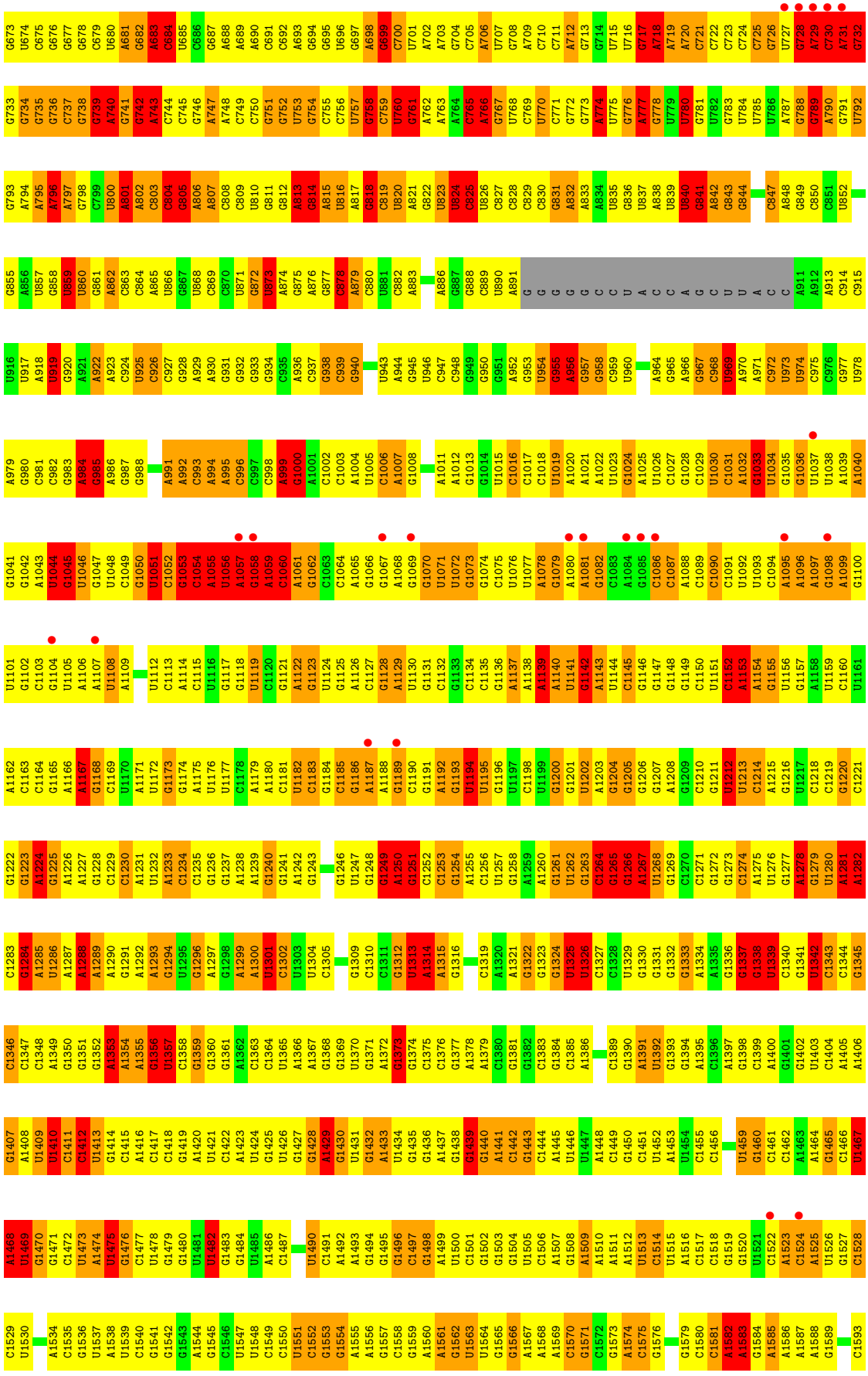
3 Residue-property plots (i)

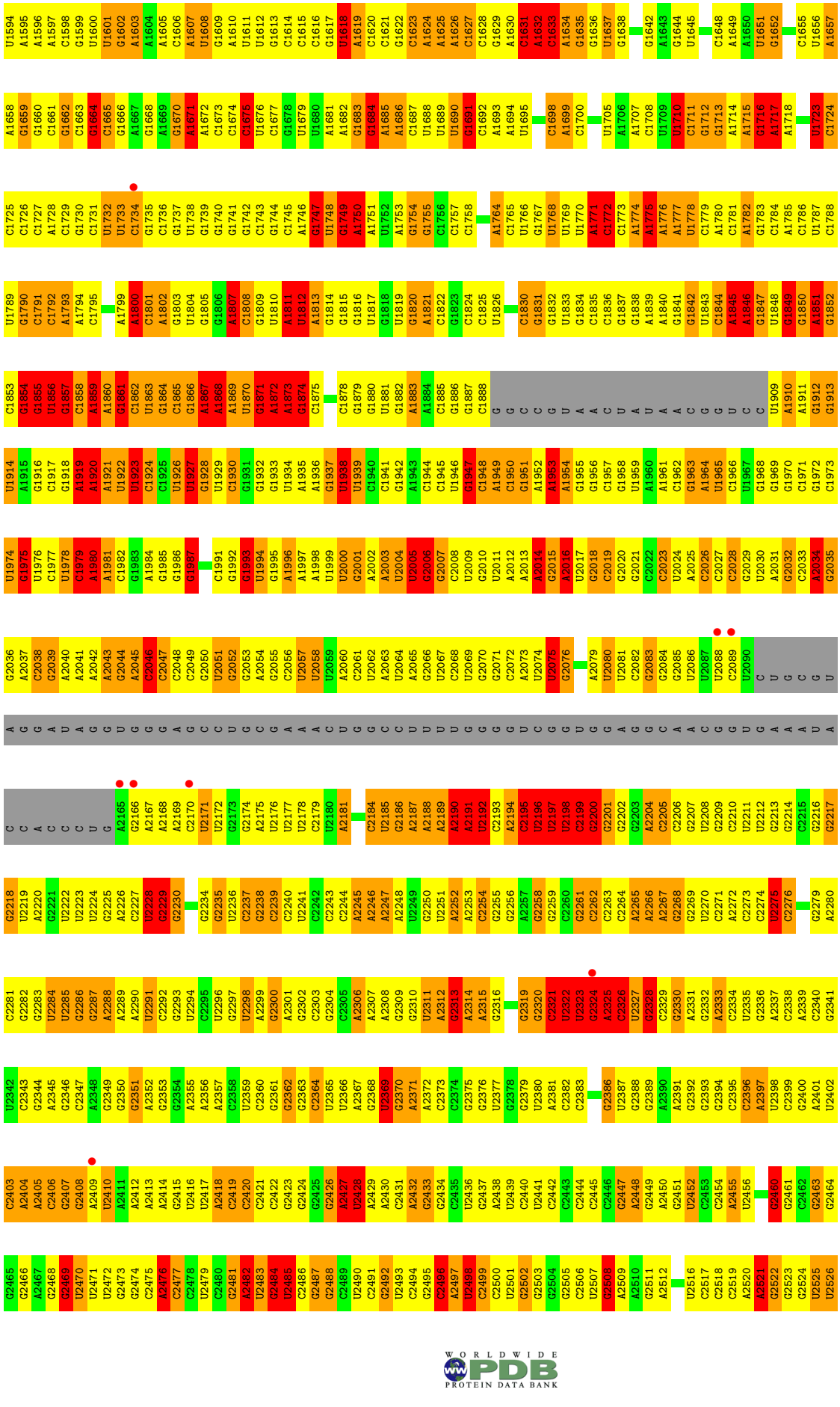
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

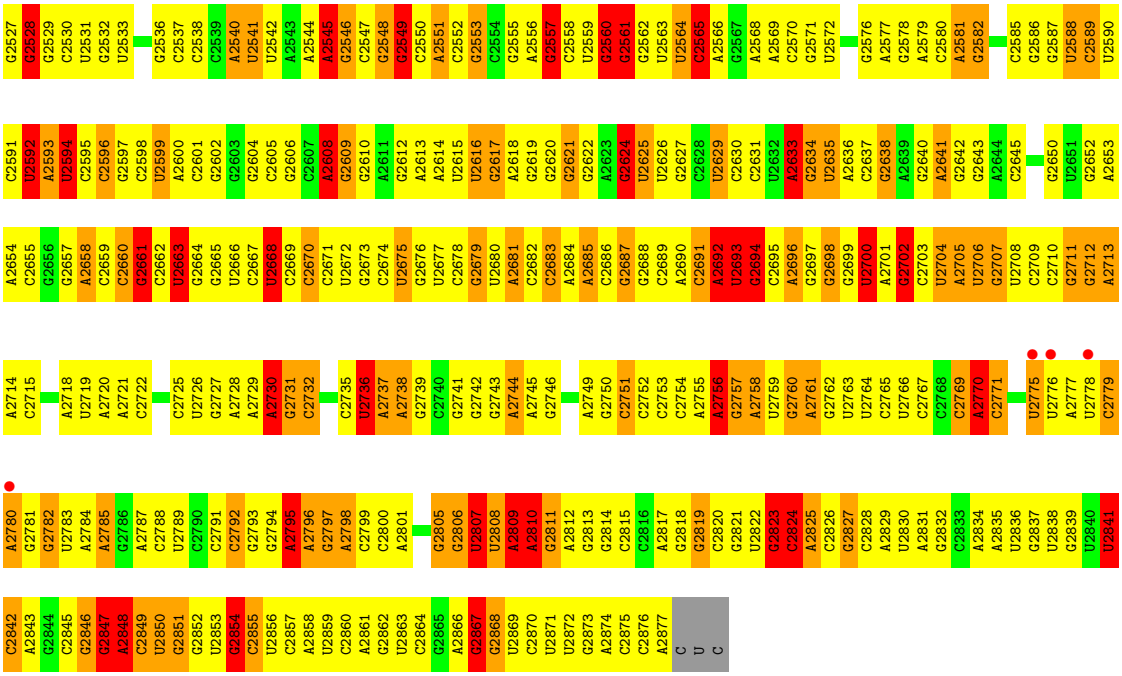
- Molecule 1: ribosomal 23S RNA

Chain X:

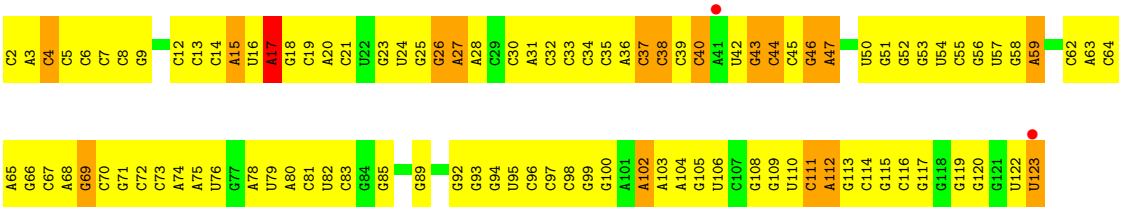




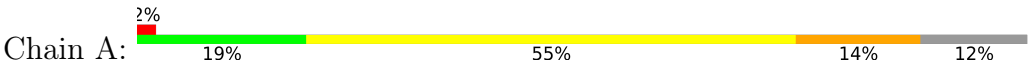


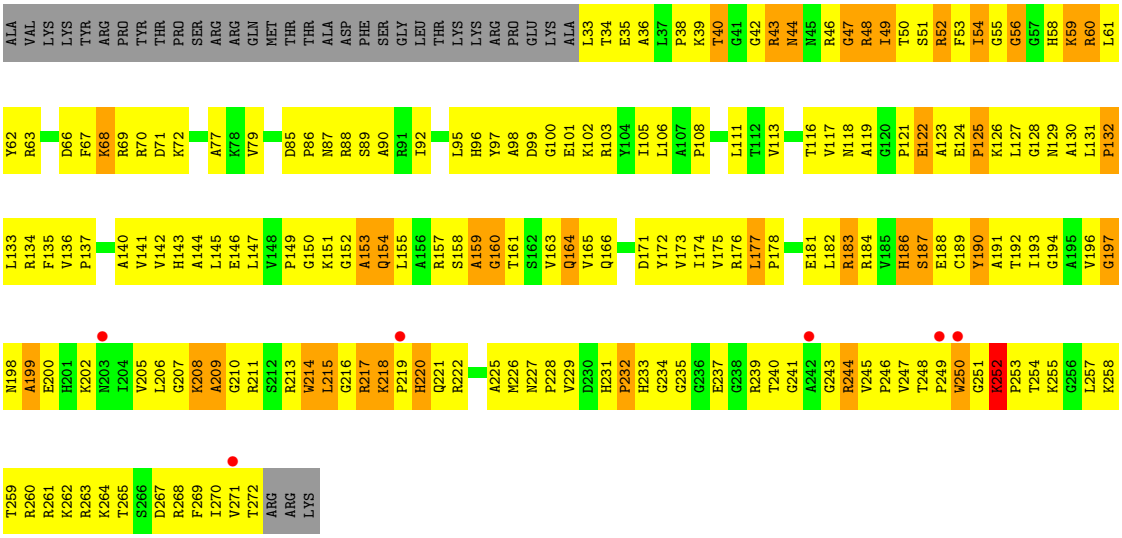


• Molecule 2: ribosomal 5S RNA



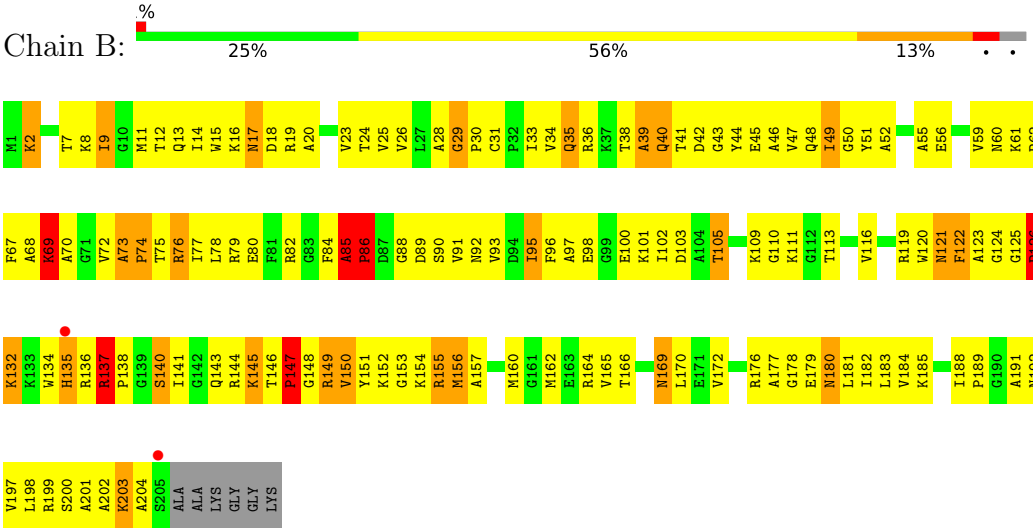
• Molecule 3: 50S ribosomal protein L2





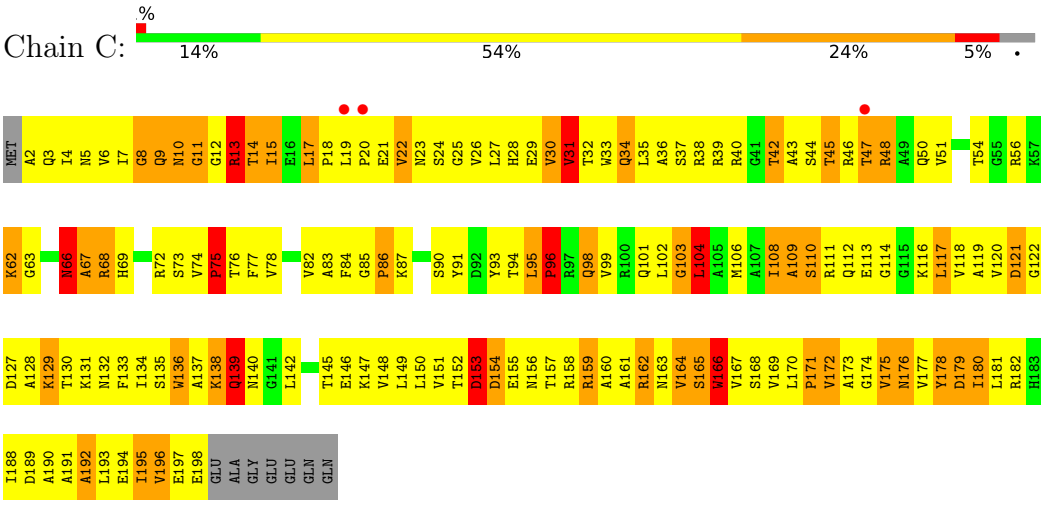
• Molecule 4: 50S ribosomal protein L3

Chain B:



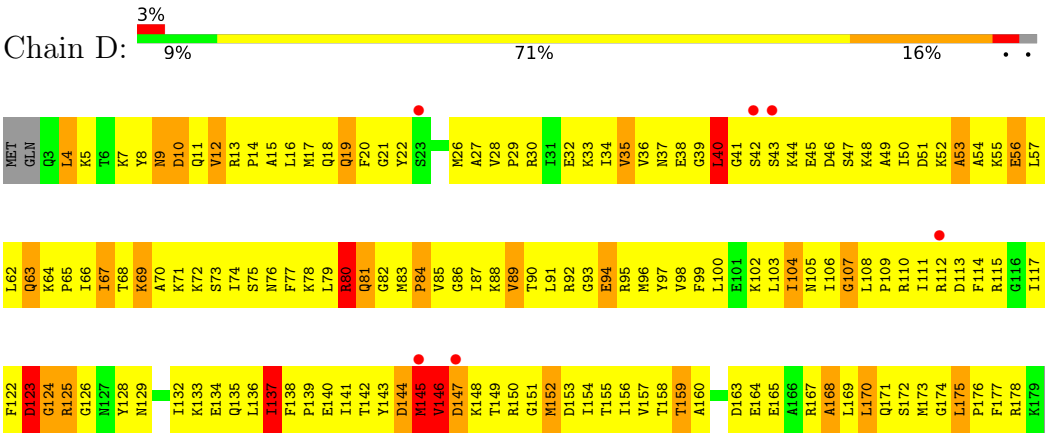
• Molecule 5: 50S ribosomal protein L4

Chain C:



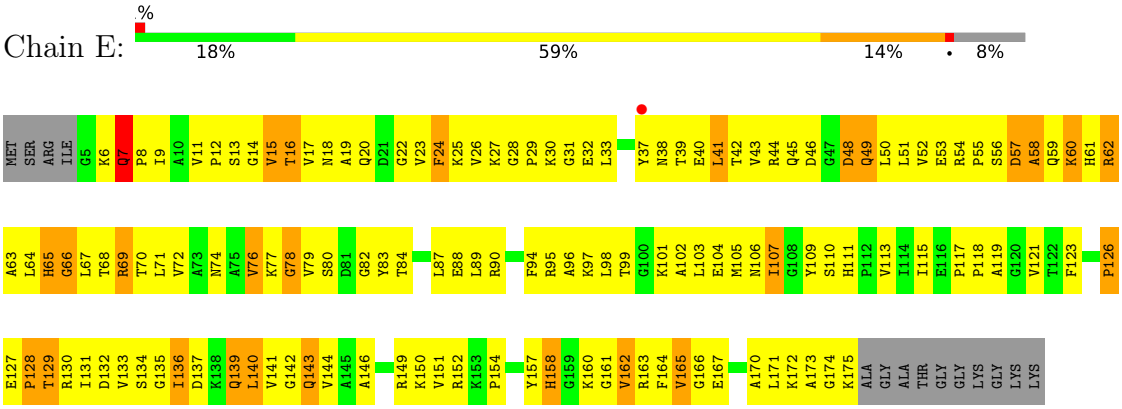
• Molecule 6: 50S ribosomal protein L5

Chain D:



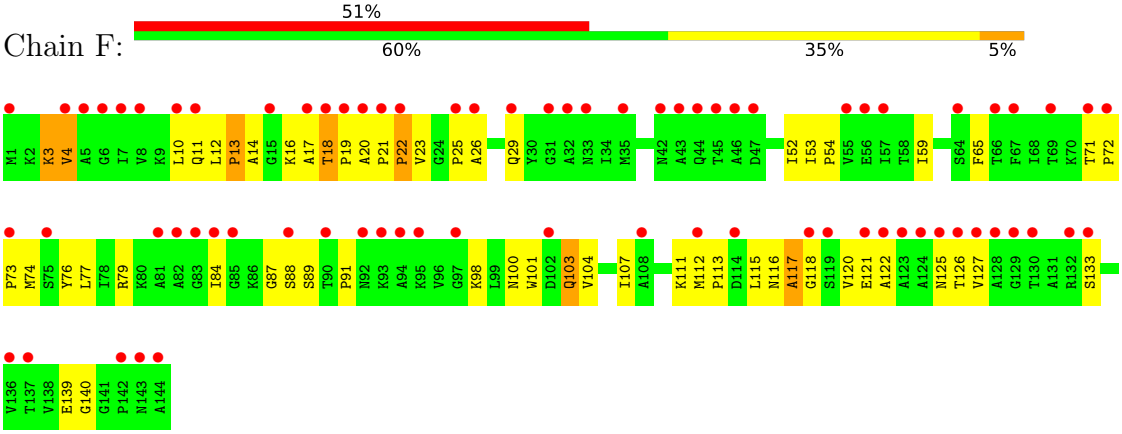
• Molecule 7: 50S ribosomal protein L6

Chain E:



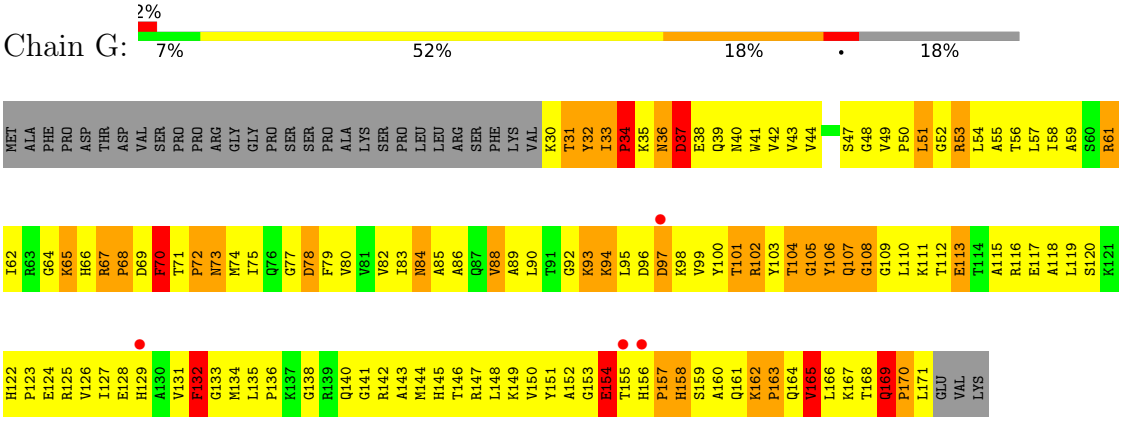
• Molecule 8: 50S ribosomal protein L11

Chain F:



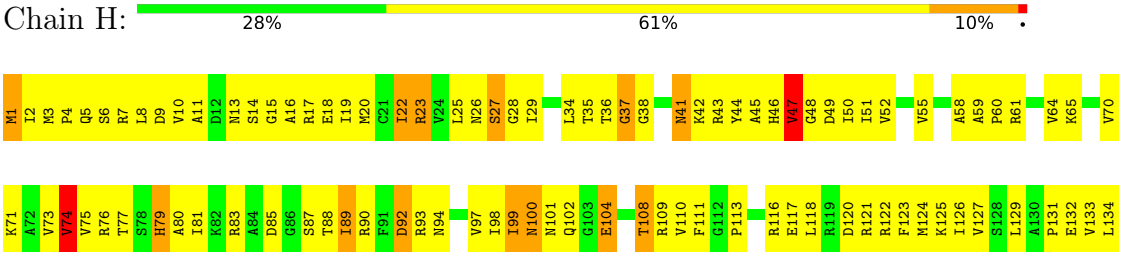
• Molecule 9: 50S ribosomal protein L13

Chain G:



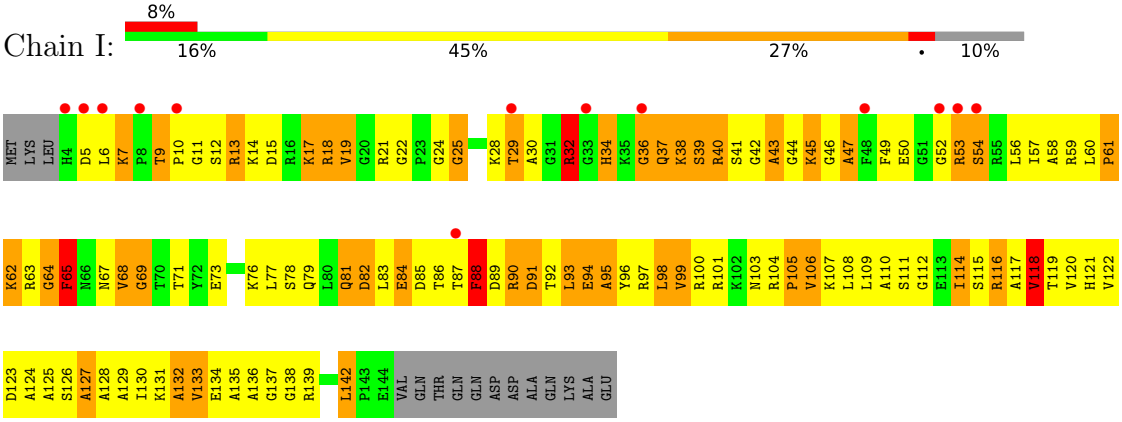
• Molecule 10: 50S ribosomal protein L14

Chain H:



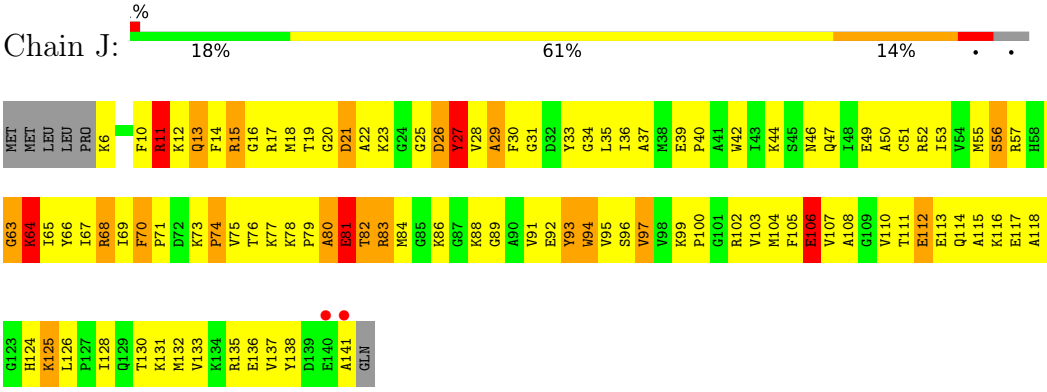
• Molecule 11: 50S ribosomal protein L15

Chain I:



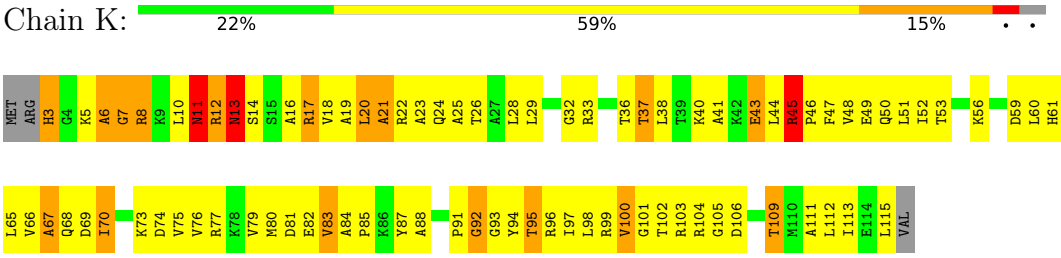
• Molecule 12: 50S ribosomal protein L16

Chain J:



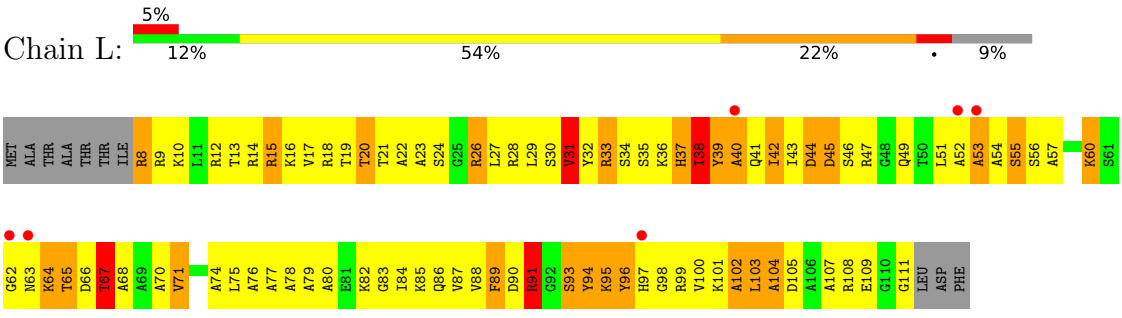
• Molecule 13: 50S ribosomal protein L17

Chain K:



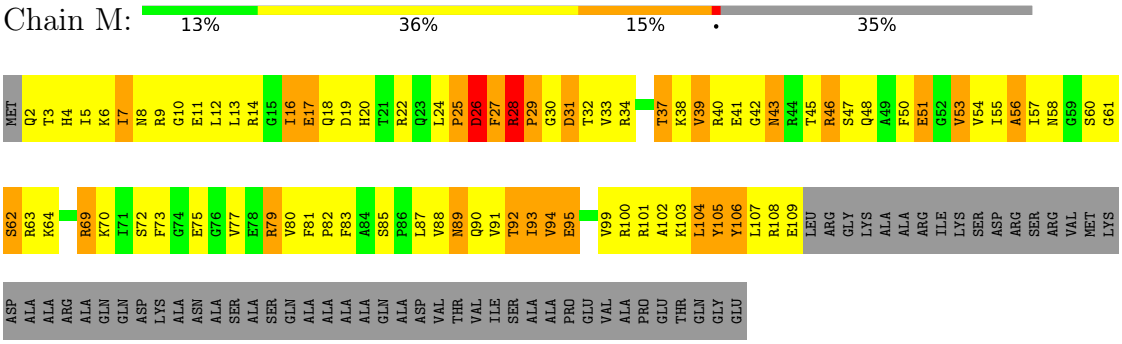
• Molecule 14: 50S ribosomal protein L18

Chain L:



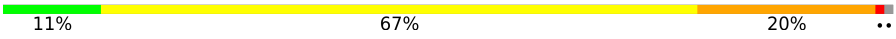
• Molecule 15: 50S ribosomal protein L19

Chain M:



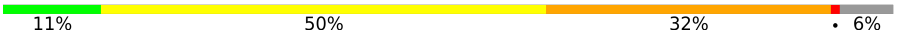
• Molecule 16: 50S ribosomal protein L20

Chain N:



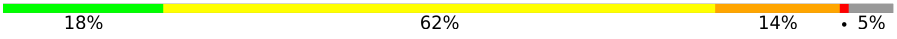
• Molecule 17: 50S ribosomal protein L21

Chain O:



• Molecule 18: 50S ribosomal protein L22

Chain P:

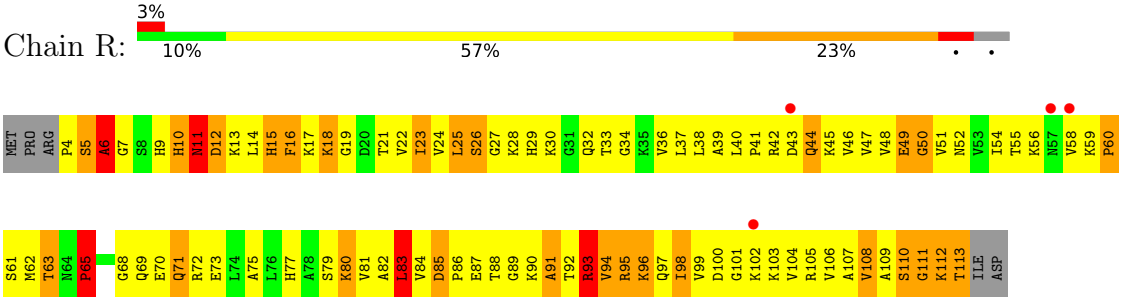


• Molecule 19: 50S ribosomal protein L23

Chain Q:

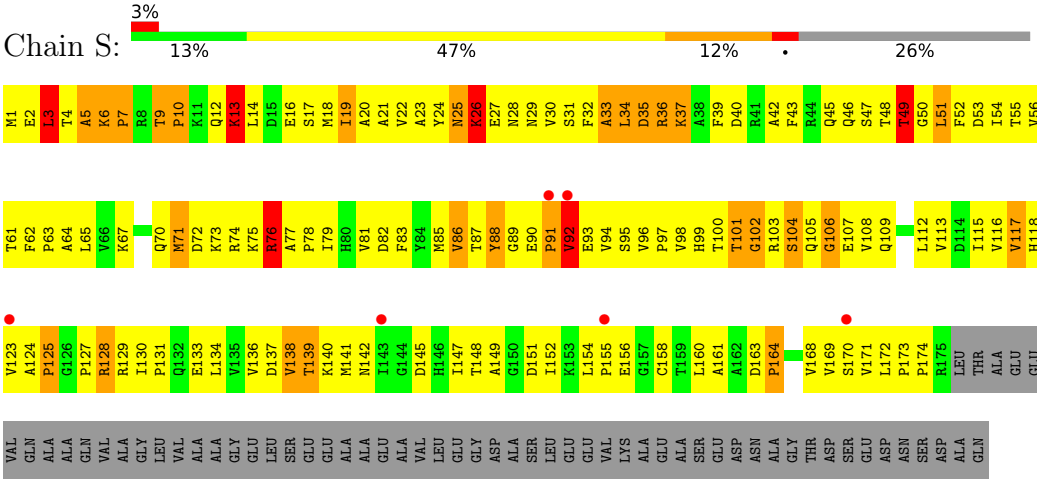
• Molecule 20: 50S ribosomal protein L24

Chain R:



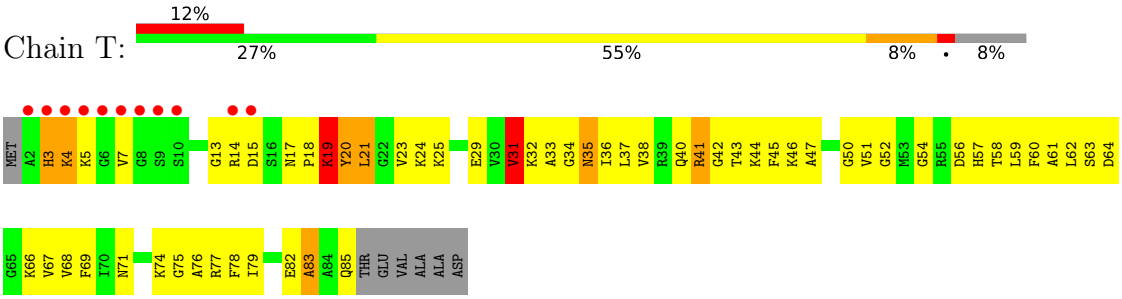
• Molecule 21: 50S ribosomal protein L25

Chain S:



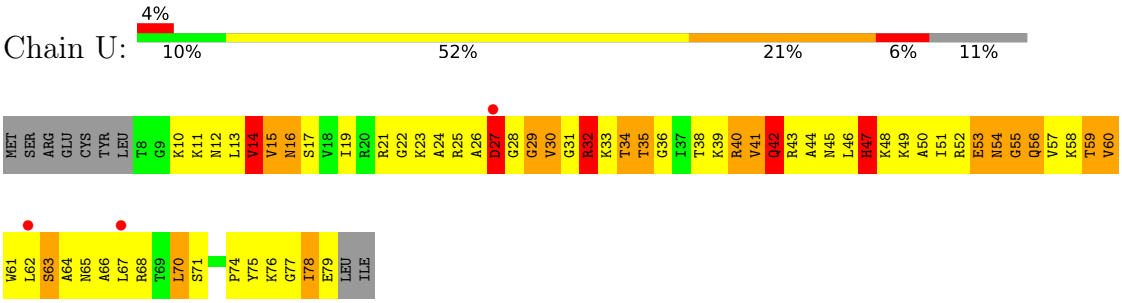
• Molecule 22: 50S ribosomal protein L27

Chain T:



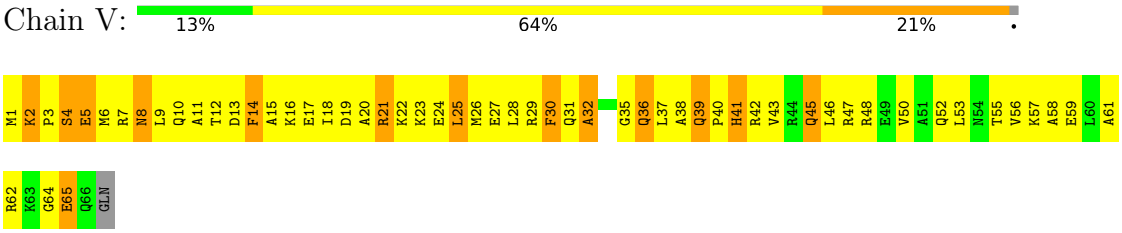
• Molecule 23: 50S ribosomal protein L28

Chain U:



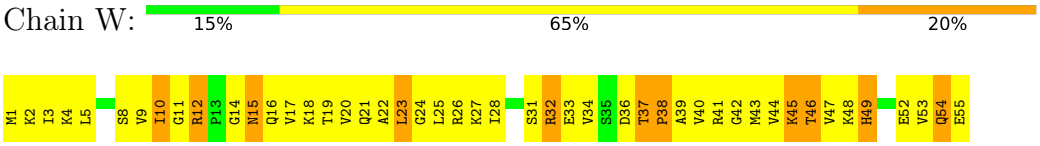
• Molecule 24: 50S ribosomal protein L29

Chain V:



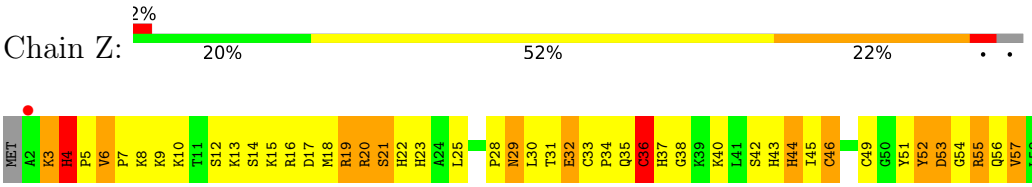
• Molecule 25: 50S ribosomal protein L30

Chain W:



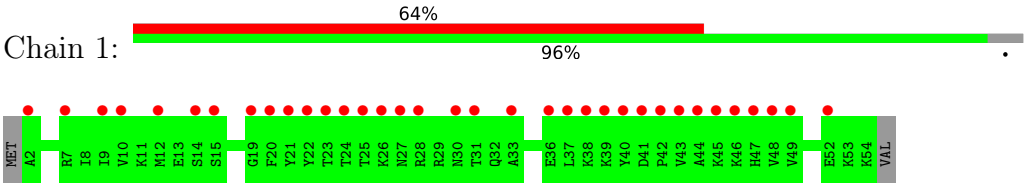
• Molecule 26: 50S ribosomal protein L32

Chain Z:



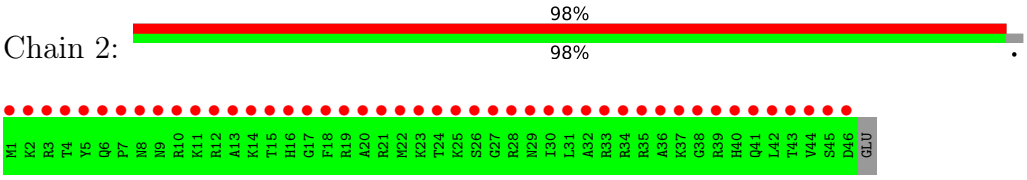
• Molecule 27: 50S ribosomal protein L33

Chain 1:



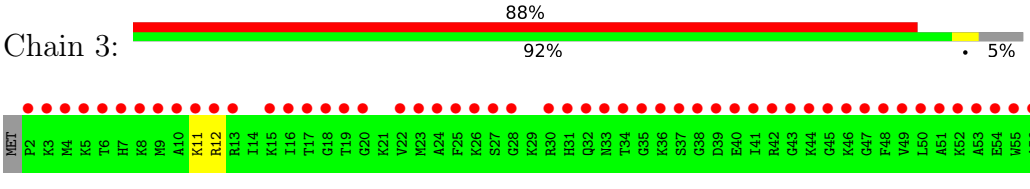
• Molecule 28: 50S ribosomal protein L34

Chain 2:



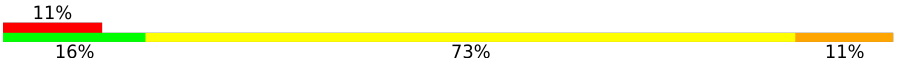
• Molecule 29: 50S ribosomal protein L35

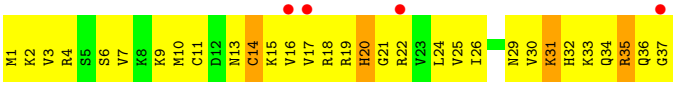
Chain 3:



• Molecule 30: 50S ribosomal protein L36

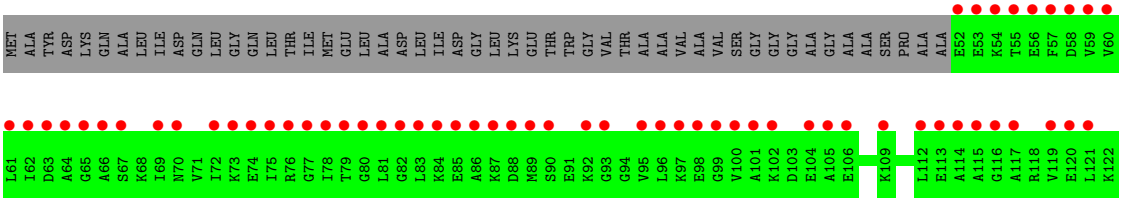
Chain 4:





• Molecule 31: 50S ribosomal protein L7/L12

Chain 5:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	169.90Å 408.90Å 694.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.92 – 3.31	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-3.30) 97.2 (29.92-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.302 , 0.339 0.274 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	73.4	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 64.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	84395	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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	X	0.90	77/64561 (0.1%)	1.04	462/100708 (0.5%)
2	Y	0.60	0/2904	0.77	0/4525
3	A	0.60	0/1862	0.83	0/2510
4	B	0.72	0/1567	0.95	2/2105 (0.1%)
5	C	0.63	0/1529	0.86	0/2070
6	D	0.60	0/1419	0.77	0/1903
7	E	0.55	0/1308	0.82	0/1771
8	F	0.23	0/1062	0.41	0/1440
9	G	0.65	0/1138	0.93	2/1539 (0.1%)
10	H	0.77	0/1007	0.85	0/1352
11	I	0.65	0/1081	0.93	1/1448 (0.1%)
12	J	0.68	0/1113	0.87	0/1486
13	K	0.80	0/886	0.95	0/1188
14	L	0.56	0/785	0.83	0/1048
15	M	0.73	0/884	0.97	2/1186 (0.2%)
16	N	0.60	0/994	0.81	0/1323
17	O	0.62	0/750	0.85	1/1000 (0.1%)
18	P	0.78	0/1027	0.89	0/1373
19	Q	0.67	0/737	0.94	1/988 (0.1%)
20	R	0.57	0/835	0.90	1/1121 (0.1%)
21	S	0.56	0/1370	0.79	0/1862
22	T	0.62	0/633	0.81	1/838 (0.1%)
23	U	0.58	0/556	0.94	0/741
24	V	0.54	0/537	0.75	0/714
25	W	0.55	0/426	0.82	0/568
26	Z	0.62	0/469	0.87	0/629
30	4	0.54	0/298	0.75	0/390
All	All	0.83	77/91738 (0.1%)	0.99	473/137826 (0.3%)

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	X	2	281
2	Y	0	2
5	C	0	1
9	G	0	1
16	N	0	1
17	O	0	1
22	T	0	1
All	All	2	288

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1056	U	P-O5'	8.88	1.68	1.59
1	X	1750	A	C5-C6	-7.65	1.34	1.41
1	X	1688	U	C4-O4	7.39	1.29	1.23
1	X	2189	A	N9-C4	7.30	1.42	1.37
1	X	1981	A	C5-C6	-7.18	1.34	1.41

The worst 5 of 473 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1055	A	N9-C1'-C2'	-32.03	72.36	114.00
1	X	557	U	N1-C1'-C2'	19.61	139.50	114.00
1	X	417	C	N1-C1'-C2'	17.87	137.24	114.00
1	X	2323	U	O4'-C1'-N1	13.98	119.39	108.20
1	X	558	G	C3'-C2'-C1'	-13.92	90.37	101.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	1278	A	C1'
1	X	2592	U	C1'

5 of 288 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	13	A	Sidechain
1	X	15	G	Sidechain
1	X	29	U	Sidechain
1	X	43	A	Sidechain
1	X	59	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	X	57651	0	29046	4354	0
2	Y	2598	0	1328	184	0
3	A	1826	0	1885	379	0
4	B	1539	0	1600	236	0
5	C	1506	0	1525	356	0
6	D	1400	0	1481	400	0
7	E	1286	0	1336	249	0
8	F	1043	0	1088	71	0
9	G	1114	0	1144	282	0
10	H	997	0	1046	167	1
11	I	1067	0	1103	286	0
12	J	1090	0	1125	268	0
13	K	878	0	930	131	1
14	L	779	0	820	227	0
15	M	871	0	894	183	0
16	N	978	0	1020	234	0
17	O	741	0	756	200	0
18	P	1014	0	1096	184	0
19	Q	726	0	753	159	0
20	R	825	0	881	266	0
21	S	1345	0	1372	276	0
22	T	625	0	655	99	0
23	U	552	0	604	209	0
24	V	533	0	558	86	0
25	W	424	0	470	84	0
26	Z	457	0	464	81	0
27	1	53	0	0	0	0
28	2	46	0	0	0	0
29	3	63	0	0	2	0
30	4	297	0	330	69	0
31	5	71	0	0	0	0
All	All	84395	0	55310	8913	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

The worst 5 of 8913 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:X:1854:G:O2'	1:X:1855:G:H5'	1.31	1.28
1:X:2195:C:C5	1:X:2196:U:C5	2.22	1.28
1:X:729:A:H2'	1:X:730:C:O4'	1.19	1.25
1:X:2196:U:H2'	1:X:2197:U:C6	1.74	1.21
1:X:731:A:H2'	1:X:732:G:O4'	1.34	1.21

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:125:LYS:NZ	13:K:82:GLU:OE2[8_555]	2.08	0.12

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
3	A	238/274 (87%)	150 (63%)	62 (26%)	26 (11%)	0 2
4	B	203/211 (96%)	143 (70%)	29 (14%)	31 (15%)	0 1
5	C	195/205 (95%)	89 (46%)	60 (31%)	46 (24%)	0 0
6	D	175/180 (97%)	101 (58%)	44 (25%)	30 (17%)	0 1
7	E	169/185 (91%)	98 (58%)	43 (25%)	28 (17%)	0 1
8	F	142/144 (99%)	113 (80%)	22 (16%)	7 (5%)	2 14
9	G	140/174 (80%)	76 (54%)	35 (25%)	29 (21%)	0 0
10	H	132/134 (98%)	108 (82%)	16 (12%)	8 (6%)	1 10
11	I	139/156 (89%)	63 (45%)	36 (26%)	40 (29%)	0 0
12	J	134/142 (94%)	74 (55%)	39 (29%)	21 (16%)	0 1
13	K	111/116 (96%)	75 (68%)	20 (18%)	16 (14%)	0 1
14	L	102/114 (90%)	52 (51%)	31 (30%)	19 (19%)	0 1
15	M	106/166 (64%)	57 (54%)	32 (30%)	17 (16%)	0 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	N	115/118 (98%)	68 (59%)	30 (26%)	17 (15%)	0 1
17	O	92/100 (92%)	53 (58%)	14 (15%)	25 (27%)	0 0
18	P	125/134 (93%)	87 (70%)	20 (16%)	18 (14%)	0 1
19	Q	91/95 (96%)	46 (50%)	23 (25%)	22 (24%)	0 0
20	R	108/115 (94%)	57 (53%)	28 (26%)	23 (21%)	0 0
21	S	173/237 (73%)	99 (57%)	43 (25%)	31 (18%)	0 1
22	T	82/91 (90%)	48 (58%)	24 (29%)	10 (12%)	0 1
23	U	70/81 (86%)	35 (50%)	18 (26%)	17 (24%)	0 0
24	V	64/67 (96%)	32 (50%)	19 (30%)	13 (20%)	0 0
25	W	53/55 (96%)	36 (68%)	11 (21%)	6 (11%)	0 2
26	Z	56/60 (93%)	35 (62%)	13 (23%)	8 (14%)	0 1
30	4	35/37 (95%)	23 (66%)	6 (17%)	6 (17%)	0 1
All	All	3050/3391 (90%)	1818 (60%)	718 (24%)	514 (17%)	0 1

5 of 514 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	54	ILE
3	A	59	LYS
3	A	60	ARG
3	A	153	ALA
3	A	154	GLN

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
3	A	185/215 (86%)	165 (89%)	20 (11%)	6 24
4	B	155/157 (99%)	140 (90%)	15 (10%)	8 29
5	C	157/163 (96%)	133 (85%)	24 (15%)	2 12
6	D	153/156 (98%)	137 (90%)	16 (10%)	7 25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	E	136/144 (94%)	126 (93%)	10 (7%)	13 40
8	F	107/107 (100%)	105 (98%)	2 (2%)	57 77
9	G	118/146 (81%)	102 (86%)	16 (14%)	3 16
10	H	103/103 (100%)	90 (87%)	13 (13%)	4 19
11	I	108/121 (89%)	95 (88%)	13 (12%)	5 20
12	J	110/116 (95%)	99 (90%)	11 (10%)	7 27
13	K	90/93 (97%)	79 (88%)	11 (12%)	5 20
14	L	74/82 (90%)	57 (77%)	17 (23%)	1 3
15	M	94/134 (70%)	82 (87%)	12 (13%)	4 18
16	N	96/97 (99%)	87 (91%)	9 (9%)	8 30
17	O	75/79 (95%)	65 (87%)	10 (13%)	4 17
18	P	109/115 (95%)	103 (94%)	6 (6%)	21 52
19	Q	75/76 (99%)	66 (88%)	9 (12%)	5 20
20	R	91/96 (95%)	76 (84%)	15 (16%)	2 10
21	S	149/192 (78%)	131 (88%)	18 (12%)	5 20
22	T	62/67 (92%)	57 (92%)	5 (8%)	11 36
23	U	57/66 (86%)	46 (81%)	11 (19%)	1 6
24	V	54/55 (98%)	50 (93%)	4 (7%)	13 40
25	W	48/48 (100%)	42 (88%)	6 (12%)	4 19
26	Z	51/53 (96%)	41 (80%)	10 (20%)	1 5
30	4	35/35 (100%)	35 (100%)	0	100 100
All	All	2492/2716 (92%)	2209 (89%)	283 (11%)	5 22

5 of 283 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	S	9	THR
21	S	71	MET
23	U	63	SER
9	G	113	GLU
9	G	101	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
16	N	81	ASN
21	S	70	GLN
17	O	88	GLN
19	Q	71	GLN
22	T	57	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	695 (25%)	301 (11%)
2	Y	121/122 (99%)	23 (19%)	0
All	All	2801/3002 (93%)	718 (25%)	301 (10%)

5 of 718 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	13	A
1	X	14	A
1	X	34	U
1	X	35	G

5 of 301 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	2045	A
1	X	2712	G
1	X	2204	A
1	X	2427	A
1	X	2867	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 monosaccharides 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	X	2686/2880 (93%)	-0.29	38 (1%) 75 75	11, 57, 103, 131	0
2	Y	122/122 (100%)	-0.04	2 (1%) 72 70	29, 81, 102, 108	0
3	A	240/274 (87%)	-0.04	6 (2%) 57 54	35, 65, 77, 90	0
4	B	205/211 (97%)	-0.27	2 (0%) 82 82	30, 53, 64, 77	0
5	C	197/205 (96%)	-0.25	3 (1%) 73 72	38, 60, 71, 83	0
6	D	177/180 (98%)	0.07	6 (3%) 45 43	54, 67, 76, 84	0
7	E	171/185 (92%)	-0.40	1 (0%) 89 90	50, 64, 75, 80	0
8	F	144/144 (100%)	2.13	74 (51%) 0 0	0, 0, 83, 88	0
9	G	142/174 (81%)	-0.15	4 (2%) 53 51	47, 59, 69, 77	0
10	H	134/134 (100%)	-0.29	0 100 100	27, 52, 62, 69	0
11	I	141/156 (90%)	0.34	13 (9%) 9 9	40, 63, 75, 83	0
12	J	136/142 (95%)	-0.22	2 (1%) 73 72	45, 61, 72, 78	0
13	K	113/116 (97%)	-0.24	0 100 100	37, 50, 60, 63	0
14	L	104/114 (91%)	0.04	6 (5%) 23 22	52, 63, 73, 78	0
15	M	108/166 (65%)	-0.33	0 100 100	23, 53, 65, 73	0
16	N	117/118 (99%)	-0.36	0 100 100	39, 57, 69, 75	0
17	O	94/100 (94%)	-0.40	0 100 100	42, 61, 72, 79	0
18	P	127/134 (94%)	-0.38	0 100 100	34, 52, 66, 76	0
19	Q	93/95 (97%)	-0.33	0 100 100	47, 58, 73, 78	0
20	R	110/115 (95%)	-0.05	4 (3%) 42 40	49, 62, 73, 85	0
21	S	175/237 (73%)	0.04	6 (3%) 45 43	55, 65, 76, 87	0
22	T	84/91 (92%)	0.27	11 (13%) 3 3	50, 61, 74, 80	0
23	U	72/81 (88%)	0.10	3 (4%) 36 34	52, 64, 73, 78	0
24	V	66/67 (98%)	-0.31	0 100 100	54, 63, 75, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	55/55 (100%)	-0.51	0 100 100	48, 58, 70, 79	0
26	Z	58/60 (96%)	-0.26	1 (1%) 70 68	35, 53, 66, 69	0
27	1	53/55 (96%)	3.19	35 (66%) 0 0	53, 61, 68, 71	0
28	2	46/47 (97%)	6.59	46 (100%) 0 0	43, 56, 62, 63	0
29	3	63/66 (95%)	5.23	58 (92%) 0 0	50, 58, 65, 67	0
30	4	37/37 (100%)	0.34	4 (10%) 5 5	52, 63, 71, 76	0
31	5	71/122 (58%)	4.99	60 (84%) 0 0	0, 0, 0, 0	0
All	All	6141/6683 (91%)	0.04	385 (6%) 20 20	0, 60, 91, 131	0

The worst 5 of 385 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	5	101	ALA	22.2
29	3	37	SER	16.3
28	2	4	THR	13.3
31	5	97	LYS	12.9
31	5	104	GLU	12.8

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.