wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 08:31 PM GMT

PDB ID	:	4WFN
Title	:	Crystal structure of the large ribosomal subunit (50S) of Deinococcus radiodurans containing a three residue insertion in L22 in complex with erythromycin
Authors	:	Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on	:	2014-09-16
Resolution	:	3.54 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:

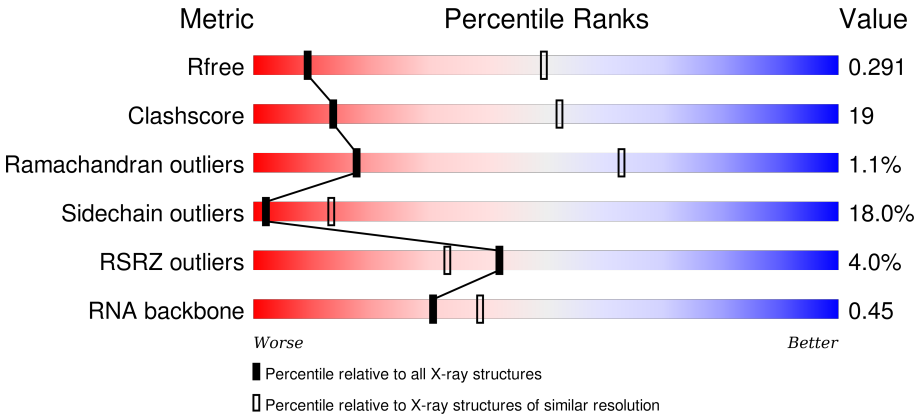
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.54 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.



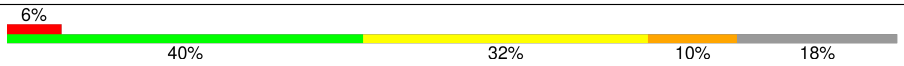
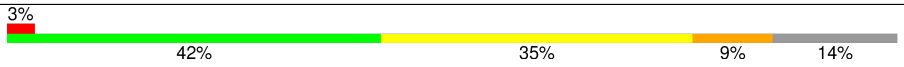
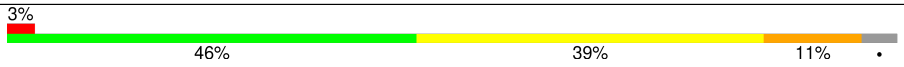
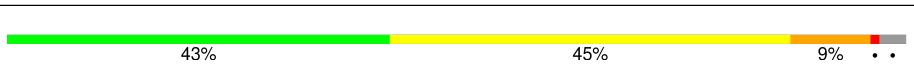
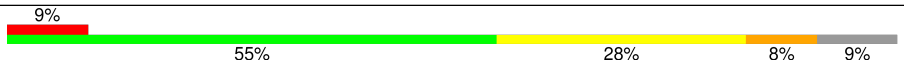
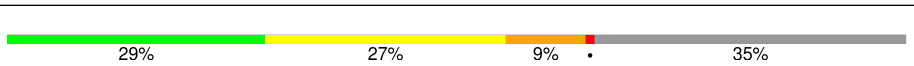
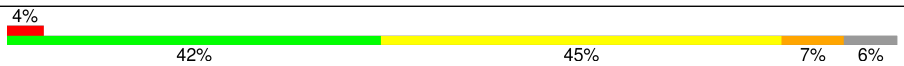
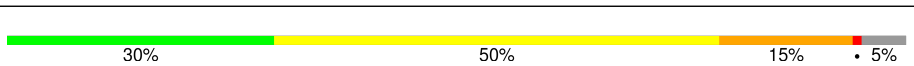
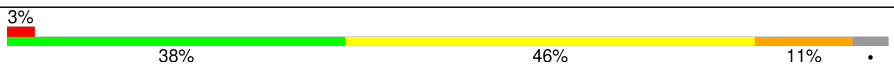
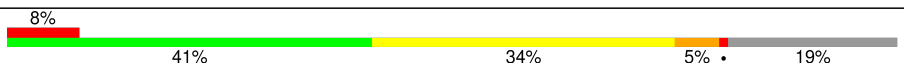
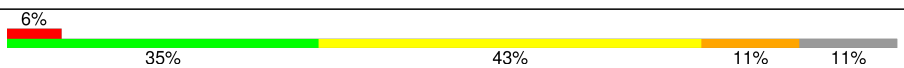
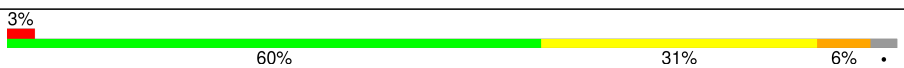
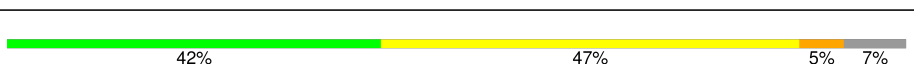
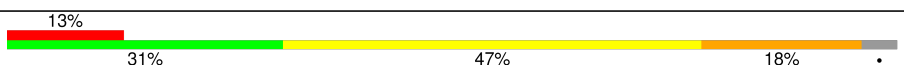
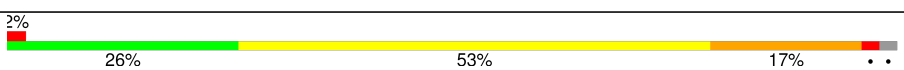
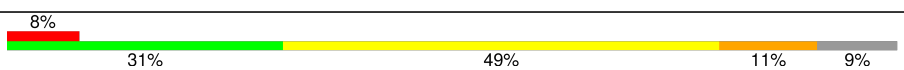
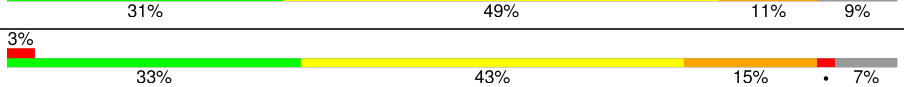
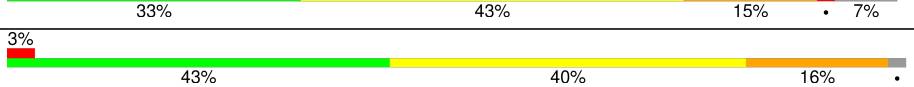
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1136 (3.68-3.40)
Clashscore	102246	1248 (3.68-3.40)
Ramachandran outliers	100387	1208 (3.68-3.40)
Sidechain outliers	100360	1208 (3.68-3.40)
RSRZ outliers	91569	1143 (3.68-3.40)
RNA backbone	2183	1052 (4.26-2.80)

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	275	3% 40% 45% 10% 5%
2	B	211	2% 45% 43% 10% •
3	C	205	7% 42% 44% 8% 5%
4	D	180	8% 48% 46% 5% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	185	
6	G	174	
7	H	134	
8	I	156	
9	J	141	
10	K	116	
11	L	114	
12	M	165	
13	N	118	
14	O	100	
15	P	137	
16	Q	95	
17	R	115	
18	S	237	
19	T	91	
20	U	81	
21	V	67	
22	W	55	
23	Z	60	
24	1	55	
25	2	47	
26	3	65	
27	X	2880	
28	Y	124	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MG	K	201	-	-	-	X
29	MG	K	202	-	-	-	X
29	MG	X	2903	-	-	-	X
29	MG	X	2909	-	-	-	X
29	MG	X	2910	-	-	-	X
29	MG	X	2913	-	-	-	X
29	MG	X	2914	-	-	-	X
29	MG	X	2916	-	-	-	X
29	MG	X	2922	-	-	-	X
29	MG	X	2923	-	-	-	X
29	MG	X	2926	-	-	-	X
29	MG	X	2939	-	-	-	X
29	MG	X	2942	-	-	-	X
29	MG	X	2944	-	-	-	X
29	MG	X	2947	-	-	-	X
29	MG	X	2948	-	-	-	X
29	MG	X	2954	-	-	-	X
29	MG	X	2957	-	-	-	X
29	MG	X	2959	-	-	-	X
29	MG	X	2961	-	-	-	X
29	MG	X	2965	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 84118 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1987	1235	399	350	3			

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L13.

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

- Molecule 7 is a protein called 50S ribosomal protein L14.

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

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	134	Total	C	N	O	0	0	0
			1011	619	206	186			

- Molecule 9 is a protein called 50S ribosomal protein L16.

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

- Molecule 10 is a protein called 50S ribosomal protein L17.

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

- Molecule 11 is a protein called 50S ribosomal protein L18.

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

- Molecule 12 is a protein called 50S ribosomal protein L19.

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

- Molecule 13 is a protein called 50S ribosomal protein L20.

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

- Molecule 14 is a protein called 50S ribosomal protein L21.

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

- Molecule 15 is a protein called 50S ribosomal protein L22,50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	130	Total	C	N	O	S	0	0	0
			1038	655	205	176	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	110	VAL	-	linker	UNP Q9RXJ7
P	111	PRO	-	linker	UNP Q9RXJ7
P	112	ARG	-	linker	UNP Q9RXJ7

- Molecule 16 is a protein called 50S ribosomal protein L23.

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

- Molecule 17 is a protein called 50S ribosomal protein L24.

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

- Molecule 18 is a protein called 50S ribosomal protein L25.

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

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

- Molecule 20 is a protein called 50S ribosomal protein L28.

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

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- Molecule 22 is a protein called 50S ribosomal protein L30.

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

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	56	Total	C	N	O	S	0	0	0
			443	272	91	75	5			

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	2680	Total 57533	C 25663	N 10626	O 18564	P 2680	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

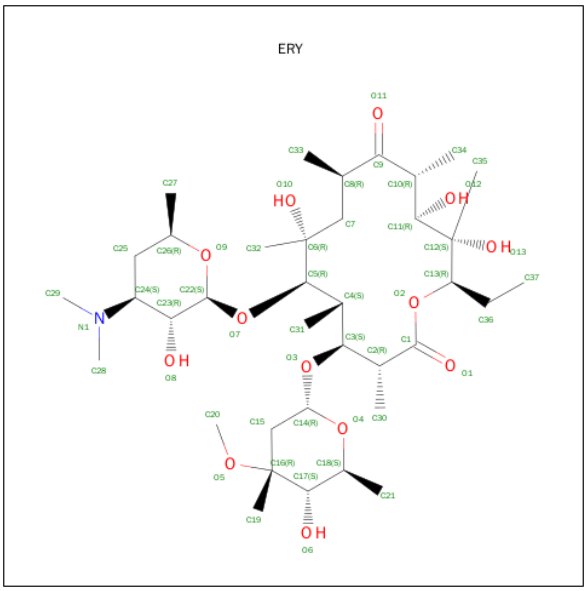
- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	122	Total 2602	C 1161	N 476	O 843	P 122	0	0	0

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	X	64	Total 64	Mg 64	0	0
29	B	1	Total 1	Mg 1	0	0
29	A	1	Total 1	Mg 1	0	0
29	K	2	Total 2	Mg 2	0	0
29	M	2	Total 2	Mg 2	0	0

- Molecule 30 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



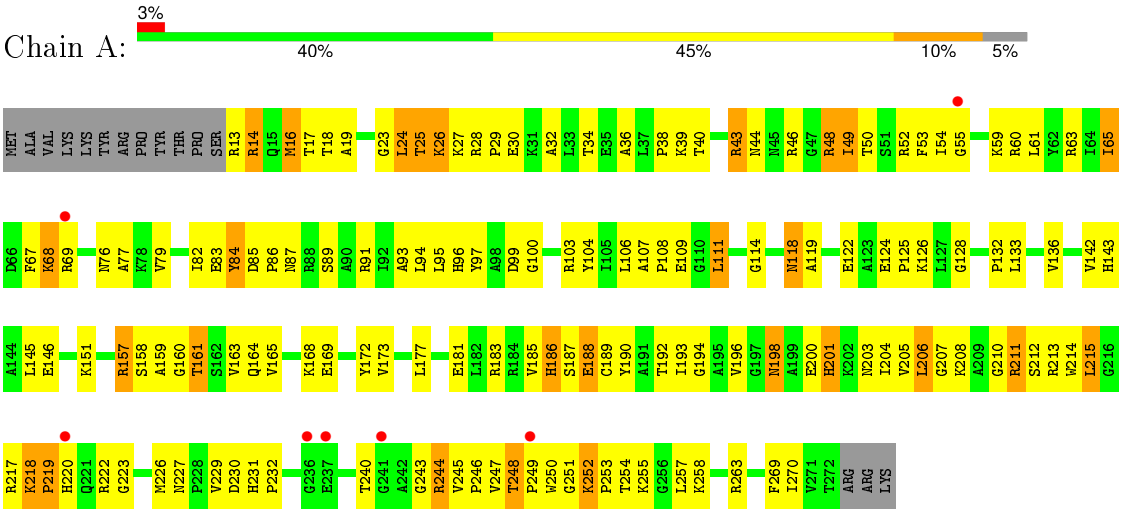
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
30	X	1	51	37	1	13	0	0

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.

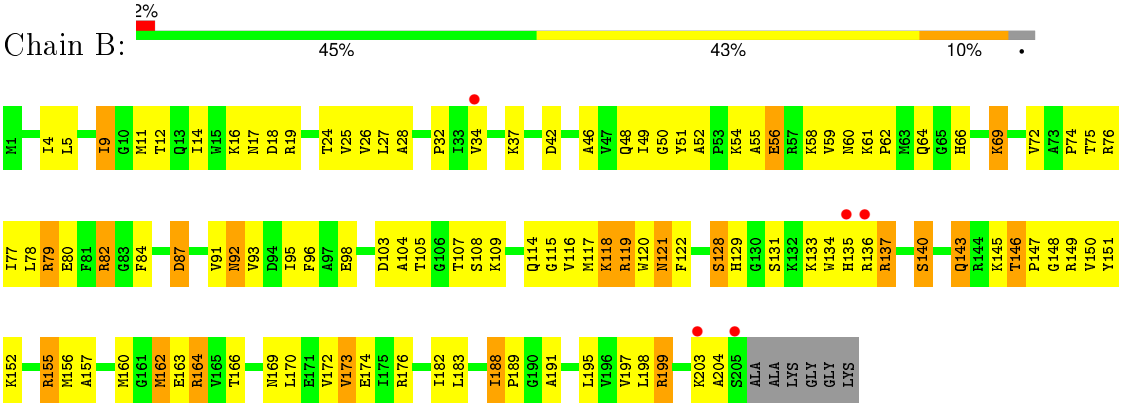
- Molecule 1: 50S ribosomal protein L2

Chain A:



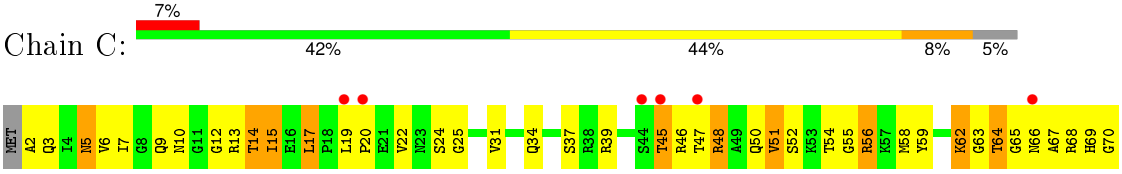
- Molecule 2: 50S ribosomal protein L3

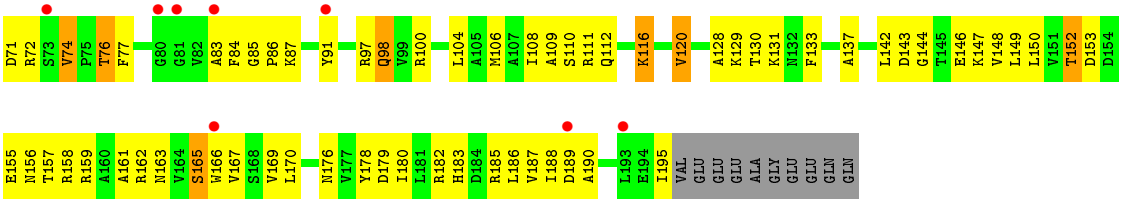
Chain B:



- Molecule 3: 50S ribosomal protein L4

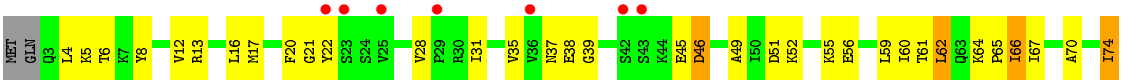
Chain C:

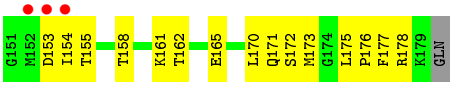




• Molecule 4: 50S ribosomal protein L5

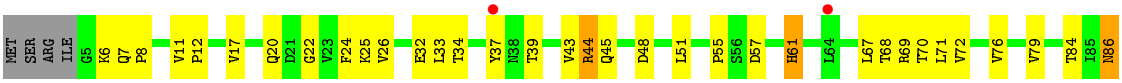
Chain D:

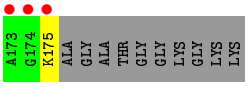




• Molecule 5: 50S ribosomal protein L6

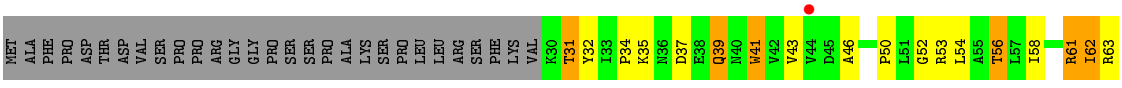
Chain E:

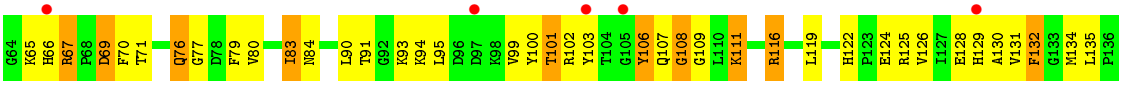


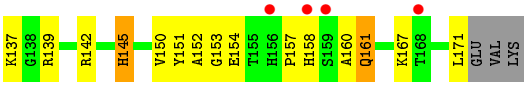


• Molecule 6: 50S ribosomal protein L13

Chain G:

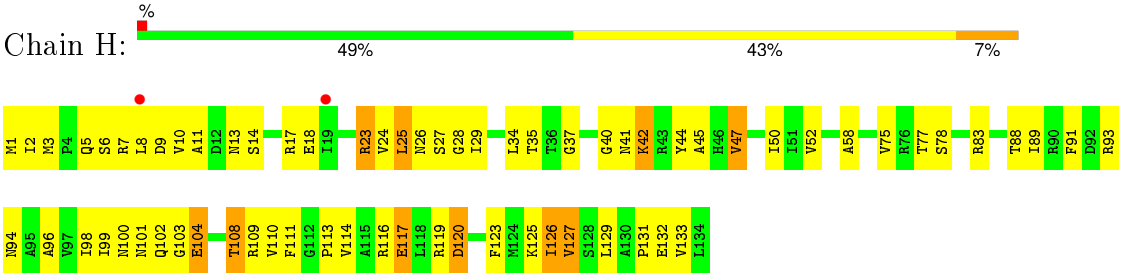






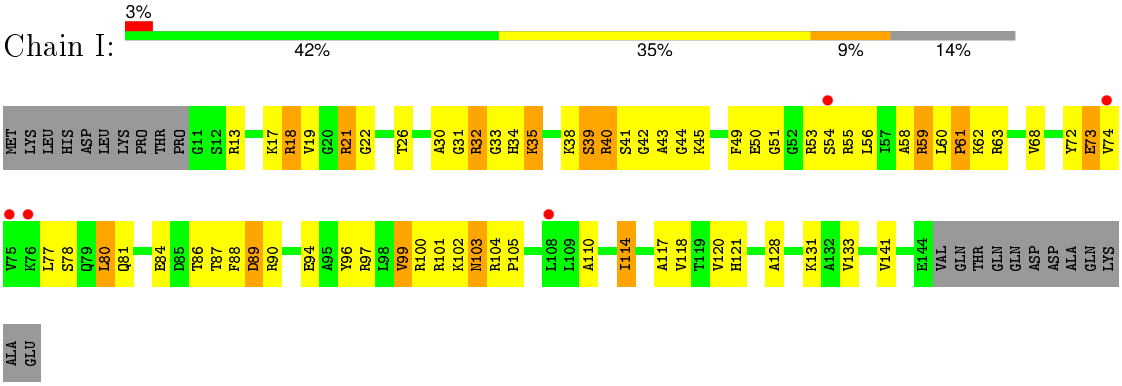
• Molecule 7: 50S ribosomal protein L14

Chain H:



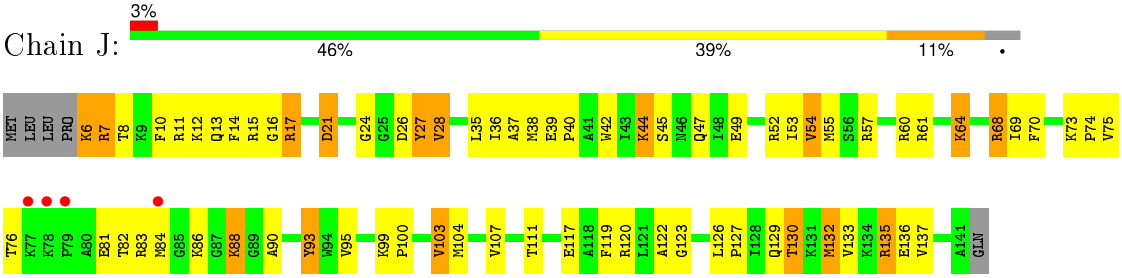
- Molecule 8: 50S ribosomal protein L15

Chain I:



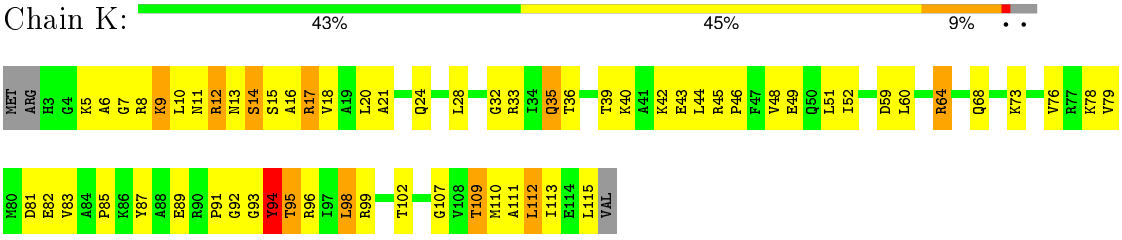
- Molecule 9: 50S ribosomal protein L16

Chain J:



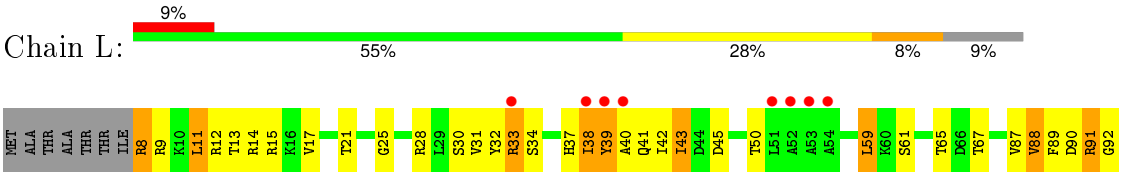
- Molecule 10: 50S ribosomal protein L17

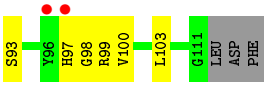
Chain K:



- Molecule 11: 50S ribosomal protein L18

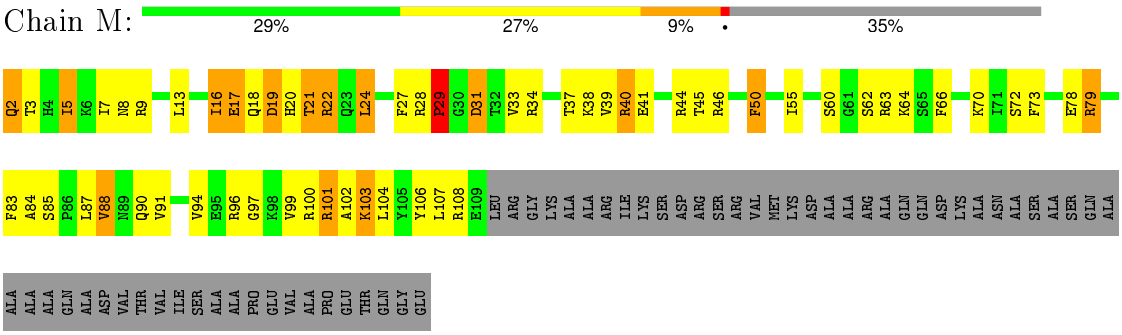
Chain L:





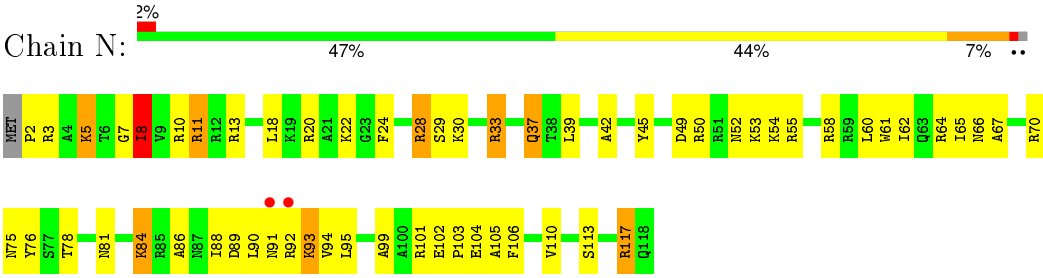
• Molecule 12: 50S ribosomal protein L19

Chain M:



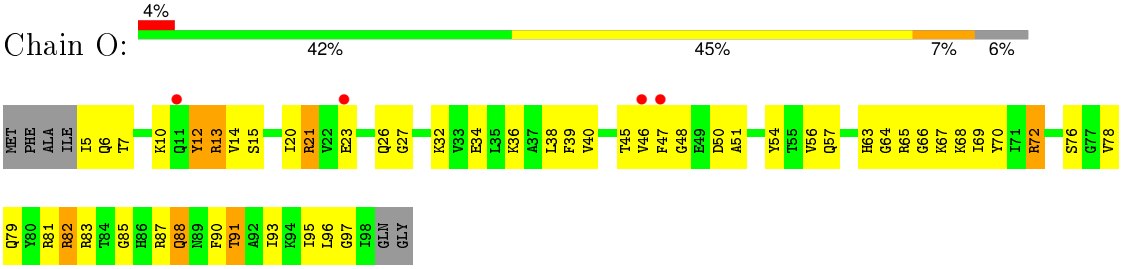
• Molecule 13: 50S ribosomal protein L20

Chain N:



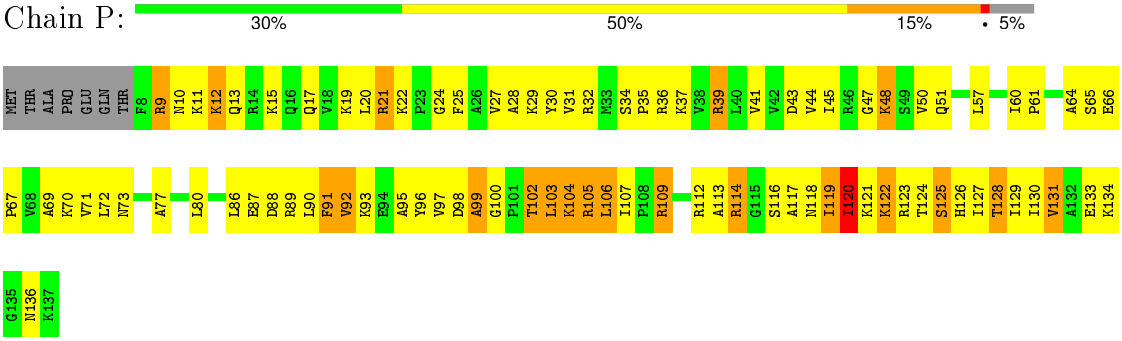
• Molecule 14: 50S ribosomal protein L21

Chain O:



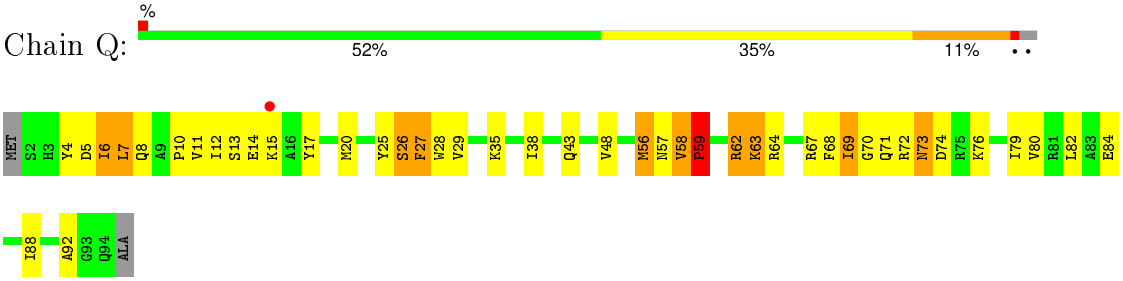
• Molecule 15: 50S ribosomal protein L22,50S ribosomal protein L22

Chain P:



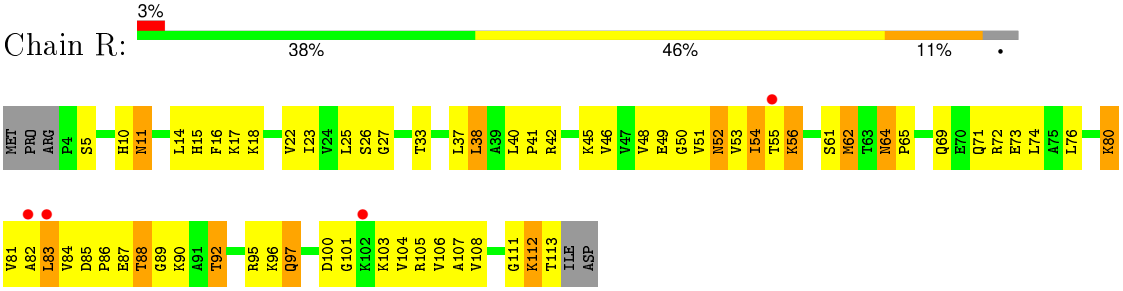
• Molecule 16: 50S ribosomal protein L23

Chain Q:



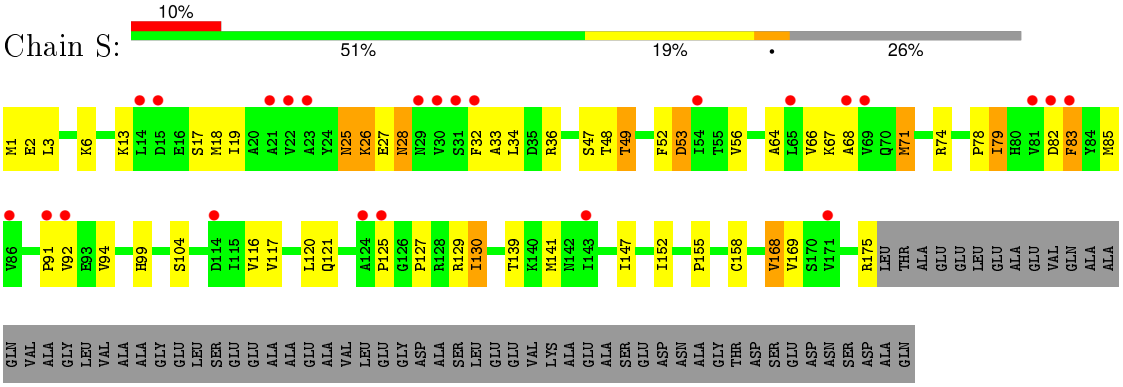
• Molecule 17: 50S ribosomal protein L24

Chain R:



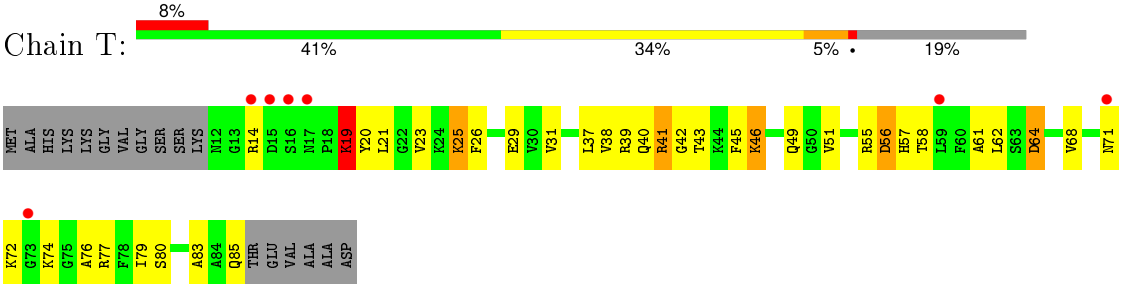
• Molecule 18: 50S ribosomal protein L25

Chain S:



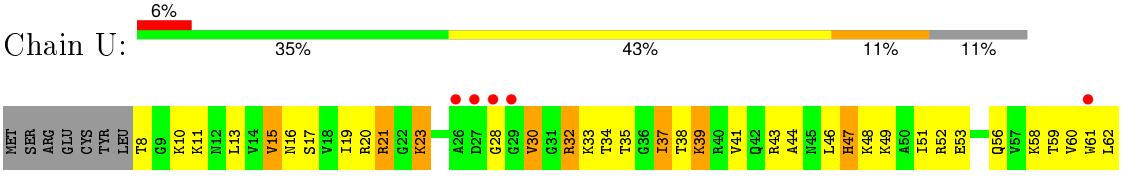
• Molecule 19: 50S ribosomal protein L27

Chain T:



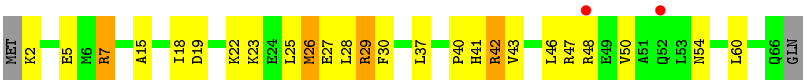
• Molecule 20: 50S ribosomal protein L28

Chain U:



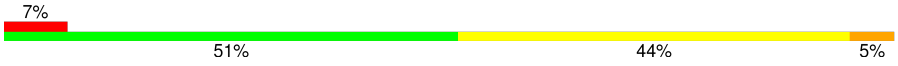
- Molecule 21: 50S ribosomal protein L29

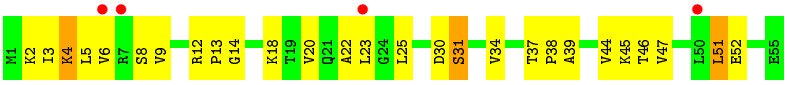
Chain V:



- Molecule 22: 50S ribosomal protein L30

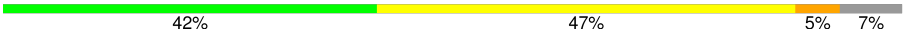
Chain W:

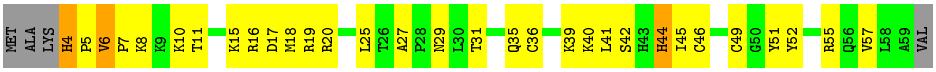




- Molecule 23: 50S ribosomal protein L32

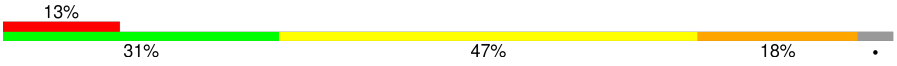
Chain Z:

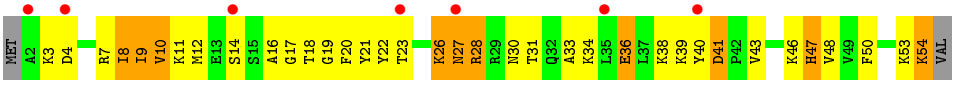




- Molecule 24: 50S ribosomal protein L33

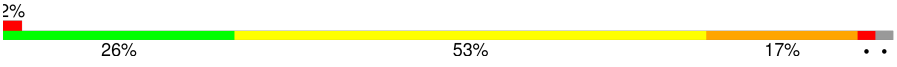
Chain 1:

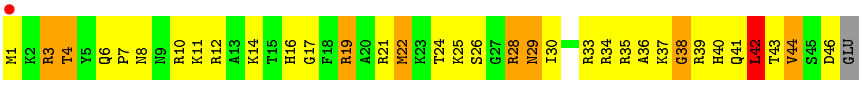




- Molecule 25: 50S ribosomal protein L34

Chain 2:



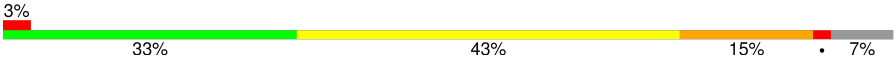


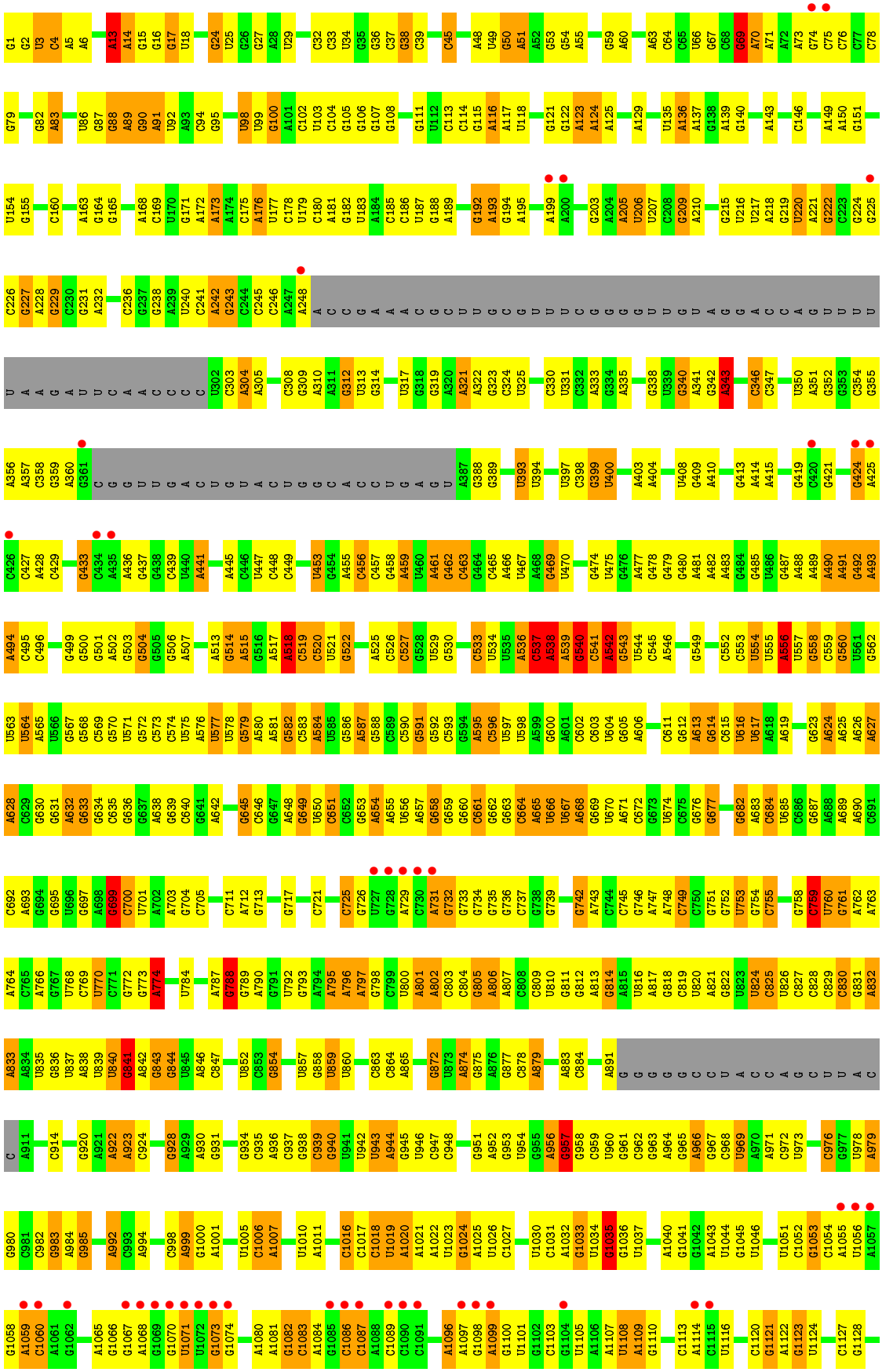
- Molecule 26: 50S ribosomal protein L35

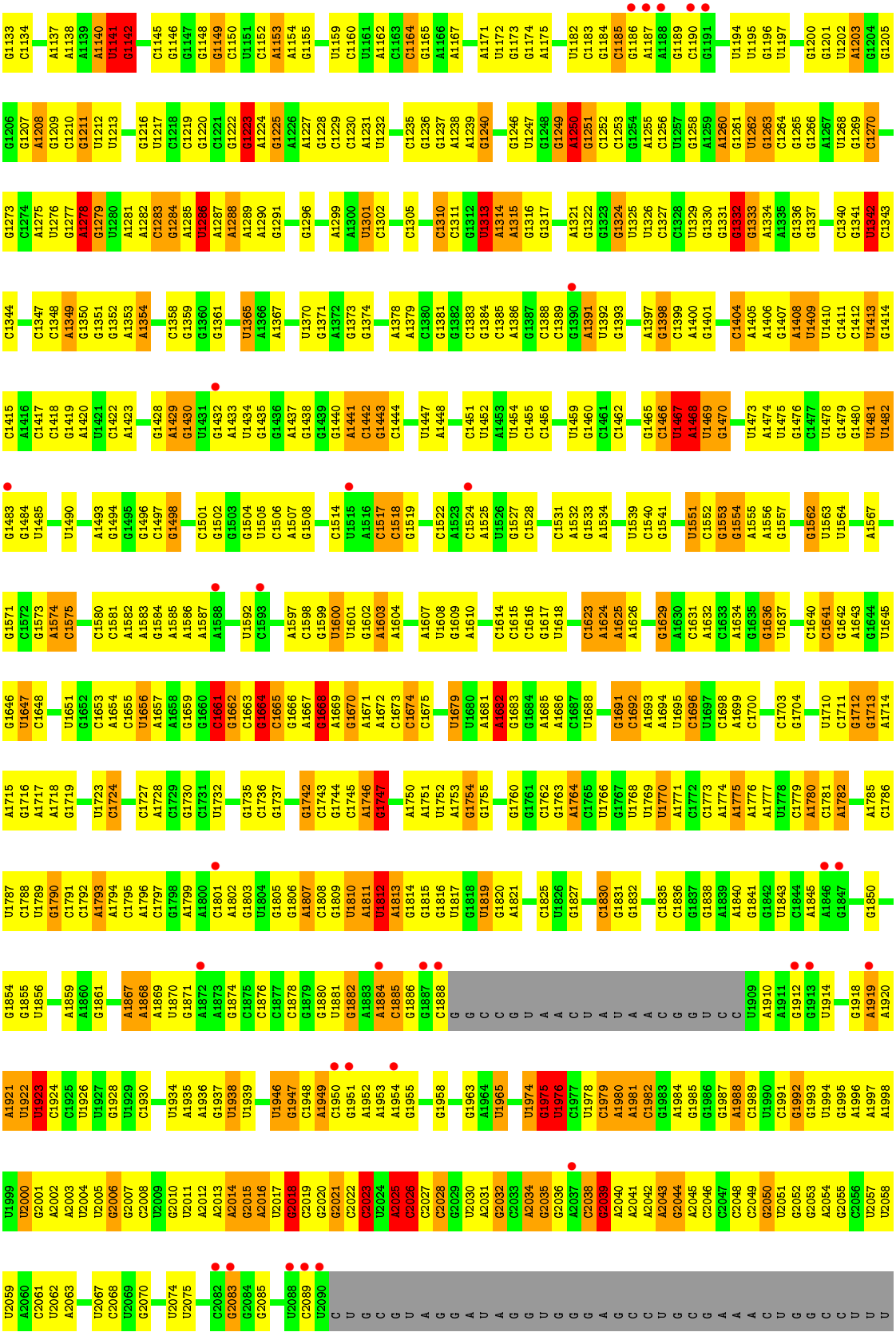
Chain 3:

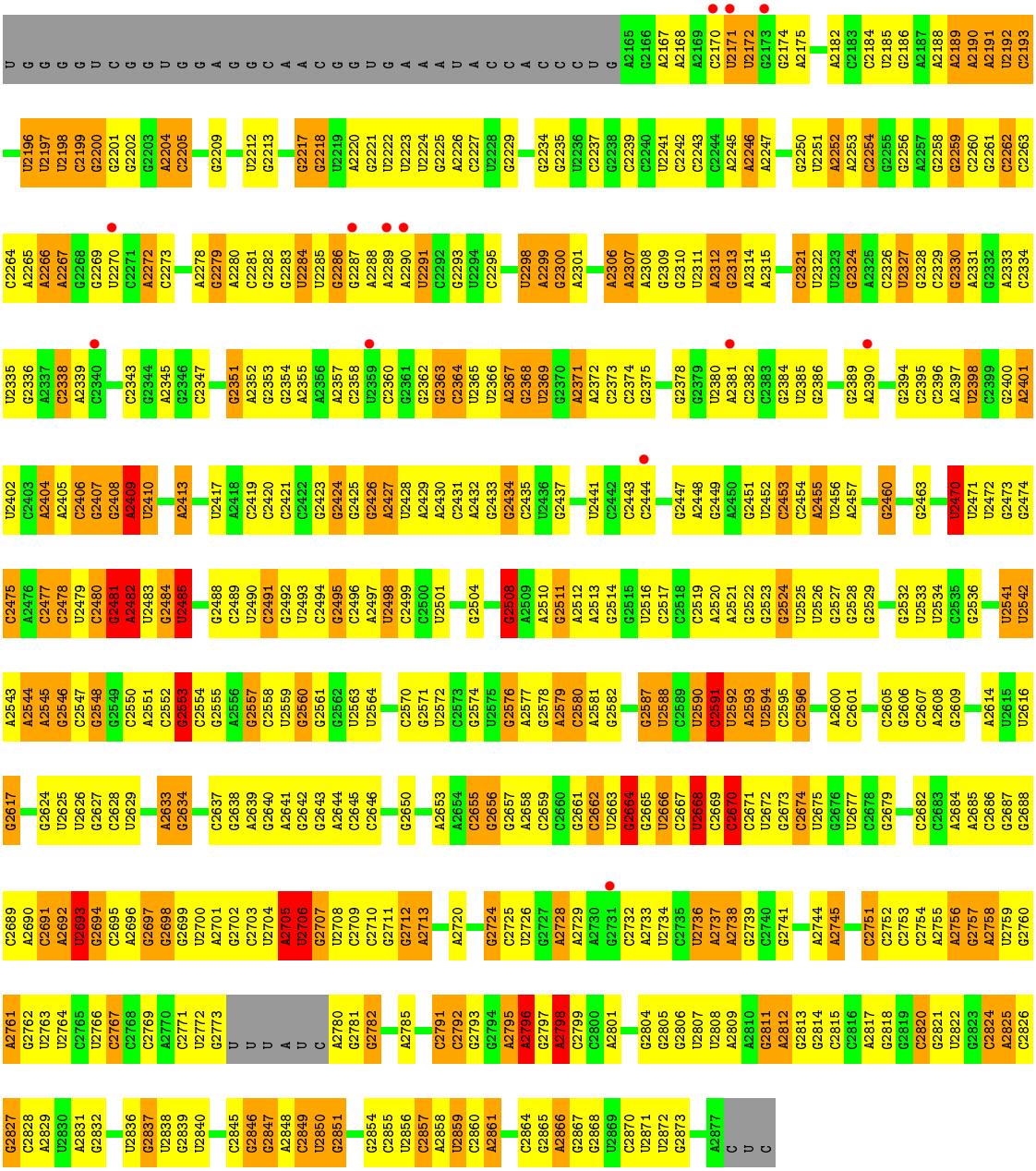
- Molecule 27: 23S ribosomal RNA

Chain X:



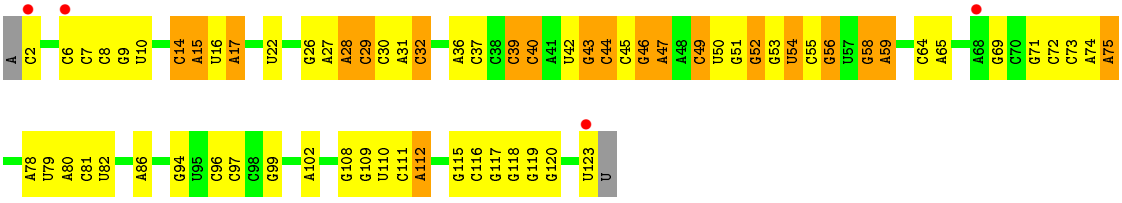






- Molecule 28: 5S ribosomal RNA

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	170.09Å 411.59Å 695.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.54 49.53 – 3.52	Depositor EDS
% Data completeness (in resolution range)	90.4 (19.99-3.54) 89.6 (49.53-3.52)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.234 , 0.282 0.243 , 0.291	Depositor DCC
R_{free} test set	13480 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	100.0	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.16 , 13.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 268448 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	84118	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ERY

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	0/2025	0.70	0/2726
2	B	0.55	0/1567	0.76	0/2105
3	C	0.47	0/1504	0.72	1/2036 (0.0%)
4	D	0.29	0/1419	0.52	0/1903
5	E	0.29	0/1308	0.51	0/1771
6	G	0.47	0/1138	0.78	1/1539 (0.1%)
7	H	0.61	0/1007	0.80	0/1352
8	I	0.46	0/1022	0.76	0/1366
9	J	0.52	0/1113	0.75	0/1486
10	K	0.67	0/886	0.90	1/1188 (0.1%)
11	L	0.32	0/785	0.60	0/1048
12	M	0.61	0/884	0.87	1/1186 (0.1%)
13	N	0.45	0/994	0.68	0/1323
14	O	0.44	0/750	0.74	1/1000 (0.1%)
15	P	0.58	0/1052	0.79	1/1409 (0.1%)
16	Q	0.42	0/737	0.67	1/988 (0.1%)
17	R	0.45	0/835	0.72	0/1121
18	S	0.30	0/1370	0.53	0/1862
19	T	0.44	0/563	0.70	0/747
20	U	0.41	0/556	0.69	0/741
21	V	0.31	0/529	0.51	0/704
22	W	0.36	0/426	0.61	0/568
23	Z	0.52	0/455	0.87	0/611
24	1	0.47	0/438	0.74	0/583
25	2	0.46	0/387	0.79	1/509 (0.2%)
26	3	0.53	0/468	0.85	0/614
27	X	0.63	3/64429 (0.0%)	1.22	424/100499 (0.4%)
28	Y	0.44	1/2908 (0.0%)	0.96	1/4529 (0.0%)
All	All	0.58	4/91555 (0.0%)	1.11	433/137514 (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
2	B	0	1
6	G	0	1
7	H	0	1
8	I	0	3
10	K	0	2
16	Q	0	1
17	R	0	1
19	T	0	1
20	U	0	1
23	Z	0	1
25	2	0	1
26	3	0	1
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	2	C	OP3-P	-10.49	1.48	1.61
27	X	1	G	OP3-P	-10.37	1.48	1.61
27	X	1981	A	N3-C4	-5.23	1.31	1.34
27	X	774	A	N3-C4	5.08	1.37	1.34

The worst 5 of 433 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	1468	A	C8-N9-C4	-12.74	100.70	105.80
27	X	1746	A	O5'-P-OP1	-12.19	94.73	105.70
27	X	1670	G	C8-N9-C4	11.14	110.86	106.40
27	X	537	C	C6-N1-C2	-10.97	115.91	120.30
27	X	774	A	N7-C8-N9	10.55	119.08	113.80

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	146	THR	Peptide
6	G	108	GLY	Peptide
7	H	26	ASN	Peptide
8	I	35	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	I	40	ARG	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	1987	0	2056	145	0
2	B	1539	0	1600	109	0
3	C	1481	0	1504	99	0
4	D	1400	0	1481	55	0
5	E	1286	0	1336	54	0
6	G	1114	0	1144	73	0
7	H	997	0	1046	56	0
8	I	1011	0	1047	72	0
9	J	1090	0	1125	64	0
10	K	878	0	930	45	0
11	L	779	0	820	36	0
12	M	871	0	894	61	0
13	N	978	0	1020	52	0
14	O	741	0	756	51	0
15	P	1038	0	1125	85	0
16	Q	726	0	753	32	0
17	R	825	0	881	52	0
18	S	1345	0	1372	37	0
19	T	556	0	579	30	0
20	U	552	0	604	35	0
21	V	525	0	546	19	0
22	W	424	0	470	16	0
23	Z	443	0	444	26	0
24	1	431	0	456	29	0
25	2	383	0	414	26	0
26	3	462	0	506	53	0
27	X	57533	0	28987	1351	0
28	Y	2602	0	1327	61	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	K	2	0	0	0	0
29	M	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	X	64	0	0	0	0
30	X	51	0	67	9	0
All	All	84118	0	55290	2473	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 19.

The worst 5 of 2473 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:VAL:HG22	2:B:136:ARG:HG3	1.32	1.11
23:Z:19:ARG:NH2	27:X:1277:G:OP1	1.90	1.04
13:N:66:ASN:HB3	13:N:76:TYR:HB2	1.46	0.97
27:X:854:G:H1	27:X:948:C:H42	1.04	0.96
7:H:40:GLY:HA3	27:X:2545:A:H61	1.29	0.95

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	258/275 (94%)	221 (86%)	34 (13%)	3 (1%)	16 61
2	B	203/211 (96%)	178 (88%)	24 (12%)	1 (0%)	34 77
3	C	192/205 (94%)	164 (85%)	26 (14%)	2 (1%)	19 65
4	D	175/180 (97%)	155 (89%)	19 (11%)	1 (1%)	30 74
5	E	169/185 (91%)	157 (93%)	11 (6%)	1 (1%)	30 74
6	G	140/174 (80%)	127 (91%)	13 (9%)	0	100 100
7	H	132/134 (98%)	120 (91%)	11 (8%)	1 (1%)	24 69
8	I	132/156 (85%)	102 (77%)	26 (20%)	4 (3%)	5 41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	J	134/141 (95%)	113 (84%)	21 (16%)	0	100 100
10	K	111/116 (96%)	102 (92%)	8 (7%)	1 (1%)	21 67
11	L	102/114 (90%)	86 (84%)	16 (16%)	0	100 100
12	M	106/165 (64%)	99 (93%)	6 (6%)	1 (1%)	21 67
13	N	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	11 53
14	O	92/100 (92%)	82 (89%)	10 (11%)	0	100 100
15	P	128/137 (93%)	109 (85%)	15 (12%)	4 (3%)	5 41
16	Q	91/95 (96%)	76 (84%)	12 (13%)	3 (3%)	5 39
17	R	108/115 (94%)	91 (84%)	16 (15%)	1 (1%)	21 67
18	S	173/237 (73%)	154 (89%)	19 (11%)	0	100 100
19	T	72/91 (79%)	62 (86%)	9 (12%)	1 (1%)	14 57
20	U	70/81 (86%)	52 (74%)	14 (20%)	4 (6%)	2 24
21	V	63/67 (94%)	58 (92%)	5 (8%)	0	100 100
22	W	53/55 (96%)	48 (91%)	5 (9%)	0	100 100
23	Z	54/60 (90%)	48 (89%)	6 (11%)	0	100 100
24	1	51/55 (93%)	38 (74%)	10 (20%)	3 (6%)	2 23
25	2	44/47 (94%)	41 (93%)	3 (7%)	0	100 100
26	3	57/65 (88%)	46 (81%)	10 (18%)	1 (2%)	11 52
All	All	3025/3379 (90%)	2632 (87%)	359 (12%)	34 (1%)	17 63

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	120	ILE
16	Q	6	ILE
16	Q	69	ILE
1	A	24	LEU
1	A	25	THR

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	202/216 (94%)	163 (81%)	39 (19%)	2 11
2	B	155/157 (99%)	127 (82%)	28 (18%)	2 13
3	C	154/163 (94%)	131 (85%)	23 (15%)	4 22
4	D	153/156 (98%)	140 (92%)	13 (8%)	13 50
5	E	136/144 (94%)	115 (85%)	21 (15%)	3 21
6	G	118/146 (81%)	93 (79%)	25 (21%)	1 8
7	H	103/103 (100%)	88 (85%)	15 (15%)	4 23
8	I	101/121 (84%)	82 (81%)	19 (19%)	2 11
9	J	110/115 (96%)	87 (79%)	23 (21%)	1 9
10	K	90/93 (97%)	70 (78%)	20 (22%)	1 7
11	L	74/82 (90%)	57 (77%)	17 (23%)	1 6
12	M	94/133 (71%)	71 (76%)	23 (24%)	1 5
13	N	96/97 (99%)	81 (84%)	15 (16%)	3 20
14	O	75/79 (95%)	61 (81%)	14 (19%)	2 11
15	P	112/118 (95%)	87 (78%)	25 (22%)	1 7
16	Q	75/76 (99%)	61 (81%)	14 (19%)	2 11
17	R	91/96 (95%)	72 (79%)	19 (21%)	1 9
18	S	149/192 (78%)	135 (91%)	14 (9%)	11 45
19	T	55/67 (82%)	44 (80%)	11 (20%)	1 10
20	U	57/66 (86%)	45 (79%)	12 (21%)	1 9
21	V	53/55 (96%)	46 (87%)	7 (13%)	5 27
22	W	48/48 (100%)	39 (81%)	9 (19%)	2 11
23	Z	50/53 (94%)	44 (88%)	6 (12%)	6 31
24	1	46/48 (96%)	32 (70%)	14 (30%)	0 3
25	2	39/40 (98%)	28 (72%)	11 (28%)	0 3
26	3	46/51 (90%)	36 (78%)	10 (22%)	1 8
All	All	2482/2715 (91%)	2035 (82%)	447 (18%)	2 13

5 of 447 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	130	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	M	29	PRO
24	1	8	ILE
10	K	9	LYS
11	L	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	3	HIS
13	N	41	ASN
19	T	85	GLN
10	K	11	ASN
12	M	2	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2673/2880 (92%)	638 (23%)	40 (1%)
28	Y	121/124 (97%)	29 (23%)	1 (0%)
All	All	2794/3004 (93%)	667 (23%)	41 (1%)

5 of 667 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	X	3	U
27	X	4	C
27	X	13	A
27	X	14	A
27	X	17	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	X	1391	A
27	X	1625	A
27	X	2756	A
27	X	1441	A
27	X	1496	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 (i)

Of 71 ligands modelled in this entry, 70 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	ERY	X	2902	-	53,53,53	0.85	1 (1%)	82,82,82	1.29	10 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	ERY	X	2902	-	-	0/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	X	2902	ERY	C4-C3	-2.20	1.49	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	X	2902	ERY	O8-C23-C22	-2.72	103.96	110.01
30	X	2902	ERY	C2-C3-C4	-2.41	105.94	112.77
30	X	2902	ERY	C30-C2-C1	-2.26	103.83	109.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	X	2902	ERY	C13-O2-C1	-2.23	114.36	118.10
30	X	2902	ERY	C16-C15-C14	-2.17	111.25	115.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	2902	ERY	9	0

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	260/275 (94%)	0.07	7 (2%) 58 48	48, 104, 163, 221	0
2	B	205/211 (97%)	-0.28	5 (2%) 62 52	27, 50, 107, 233	0
3	C	194/205 (94%)	0.12	14 (7%) 18 14	39, 102, 180, 292	0
4	D	177/180 (98%)	0.28	15 (8%) 13 11	114, 175, 232, 282	0
5	E	171/185 (92%)	-0.18	6 (3%) 48 37	57, 131, 192, 243	0
6	G	142/174 (81%)	0.03	10 (7%) 19 15	38, 77, 160, 339	0
7	H	134/134 (100%)	-0.35	2 (1%) 76 68	33, 45, 87, 135	0
8	I	134/156 (85%)	0.27	5 (3%) 45 36	55, 126, 192, 315	0
9	J	136/141 (96%)	0.05	4 (2%) 55 45	56, 94, 163, 214	0
10	K	113/116 (97%)	-0.46	0 100 100	27, 32, 67, 100	0
11	L	104/114 (91%)	0.15	10 (9%) 10 9	130, 161, 200, 243	0
12	M	108/165 (65%)	-0.43	0 100 100	30, 43, 95, 242	0
13	N	117/118 (99%)	-0.15	2 (1%) 73 64	41, 76, 133, 232	0
14	O	94/100 (94%)	-0.21	4 (4%) 39 30	52, 94, 178, 204	0
15	P	130/137 (94%)	-0.37	0 100 100	33, 51, 147, 188	0
16	Q	93/95 (97%)	-0.35	1 (1%) 82 74	49, 94, 162, 192	0
17	R	110/115 (95%)	0.06	4 (3%) 46 37	65, 100, 189, 259	0
18	S	175/237 (73%)	0.55	24 (13%) 4 4	93, 144, 224, 285	0
19	T	74/91 (81%)	0.21	7 (9%) 10 9	72, 112, 158, 228	0
20	U	72/81 (88%)	0.49	5 (6%) 20 15	75, 119, 185, 238	0
21	V	65/67 (97%)	-0.19	2 (3%) 52 43	76, 115, 164, 208	0
22	W	55/55 (100%)	0.32	4 (7%) 18 14	72, 91, 128, 190	0
23	Z	56/60 (93%)	-0.39	0 100 100	32, 40, 80, 152	0
24	1	53/55 (96%)	0.59	7 (13%) 4 5	102, 129, 217, 266	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	2	46/47 (97%)	0.18	1 (2%) 65 55	38, 67, 122, 169	0
26	3	59/65 (90%)	0.45	5 (8%) 13 11	81, 100, 172, 278	0
27	X	2680/2880 (93%)	-0.14	88 (3%) 50 40	26, 76, 186, 299	0
28	Y	122/124 (98%)	-0.10	4 (3%) 50 40	74, 153, 190, 332	0
All	All	5879/6383 (92%)	-0.06	236 (4%) 42 33	26, 89, 188, 339	0

The worst 5 of 236 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	S	23	ALA	8.1
18	S	22	VAL	8.0
18	S	15	ASP	7.6
27	X	1072	U	7.4
27	X	731	A	6.9

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MG	X	2957	1/1	0.94	0.82	88.73	52,52,52,52	0
29	MG	X	2903	1/1	0.95	0.67	34.47	30,30,30,30	0
29	MG	X	2961	1/1	0.93	1.06	30.91	56,56,56,56	0
29	MG	X	2916	1/1	0.93	0.88	29.58	41,41,41,41	0
29	MG	X	2965	1/1	0.91	0.91	24.90	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MG	X	2926	1/1	0.93	0.91	20.54	44,44,44,44	0
29	MG	X	2914	1/1	0.99	0.57	18.26	27,27,27,27	0
29	MG	X	2909	1/1	0.97	0.46	16.41	28,28,28,28	0
29	MG	X	2942	1/1	0.97	0.67	15.69	46,46,46,46	0
29	MG	K	202	1/1	0.76	0.82	10.86	27,27,27,27	0
29	MG	X	2910	1/1	0.96	0.62	10.67	56,56,56,56	0
29	MG	X	2922	1/1	0.97	0.35	10.03	29,29,29,29	0
29	MG	X	2944	1/1	0.97	0.40	8.85	35,35,35,35	0
29	MG	X	2939	1/1	0.93	0.62	8.75	50,50,50,50	0
29	MG	X	2959	1/1	0.97	0.66	8.48	41,41,41,41	0
29	MG	X	2954	1/1	0.97	0.45	8.37	45,45,45,45	0
29	MG	X	2913	1/1	0.96	0.47	6.57	43,43,43,43	0
29	MG	X	2923	1/1	0.94	0.39	6.22	40,40,40,40	0
29	MG	X	2947	1/1	0.96	0.26	2.58	34,34,34,34	0
29	MG	X	2948	1/1	0.96	0.29	2.26	34,34,34,34	0
29	MG	K	201	1/1	0.86	0.46	2.24	27,27,27,27	0
30	ERY	X	2902	51/51	0.94	0.24	0.92	31,34,36,36	0
29	MG	A	301	1/1	0.93	0.39	0.54	54,54,54,54	0
29	MG	X	2915	1/1	0.83	0.18	-0.69	63,63,63,63	0
29	MG	X	2929	1/1	0.98	0.13	-1.42	30,30,30,30	0
29	MG	X	2931	1/1	0.87	0.56	-	46,46,46,46	0
29	MG	X	2937	1/1	0.95	0.70	-	44,44,44,44	0
29	MG	X	2952	1/1	0.91	0.43	-	29,29,29,29	0
29	MG	X	2956	1/1	0.93	0.52	-	27,27,27,27	0
29	MG	X	2921	1/1	0.95	0.33	-	28,28,28,28	0
29	MG	B	301	1/1	0.80	0.77	-	34,34,34,34	0
29	MG	X	2960	1/1	0.92	0.32	-	61,61,61,61	0
29	MG	X	2949	1/1	0.98	0.44	-	42,42,42,42	0
29	MG	X	2924	1/1	0.99	0.23	-	38,38,38,38	0
29	MG	X	2936	1/1	0.96	0.65	-	45,45,45,45	0
29	MG	X	2911	1/1	0.91	0.53	-	56,56,56,56	0
29	MG	X	2938	1/1	0.98	0.79	-	31,31,31,31	0
29	MG	X	2927	1/1	0.95	0.35	-	29,29,29,29	0
29	MG	X	2904	1/1	0.95	0.55	-	32,32,32,32	0
29	MG	X	2920	1/1	0.96	0.45	-	52,52,52,52	0
29	MG	X	2932	1/1	0.98	0.40	-	37,37,37,37	0
29	MG	X	2901	1/1	0.94	0.39	-	69,69,69,69	0
29	MG	X	2946	1/1	0.91	0.19	-	46,46,46,46	0
29	MG	X	2943	1/1	0.93	0.97	-	42,42,42,42	0
29	MG	X	2906	1/1	0.85	0.85	-	28,28,28,28	0
29	MG	X	2962	1/1	0.94	0.13	-	69,69,69,69	0
29	MG	X	2945	1/1	0.97	0.14	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MG	X	2958	1/1	0.82	0.49	-	44,44,44,44	0
29	MG	X	2917	1/1	0.91	0.86	-	40,40,40,40	0
29	MG	X	2930	1/1	0.80	1.01	-	29,29,29,29	0
29	MG	X	2919	1/1	0.82	0.10	-	62,62,62,62	0
29	MG	X	2925	1/1	0.91	1.08	-	31,31,31,31	0
29	MG	X	2953	1/1	0.99	0.38	-	56,56,56,56	0
29	MG	M	201	1/1	0.97	0.36	-	35,35,35,35	0
29	MG	X	2912	1/1	0.96	0.14	-	27,27,27,27	0
29	MG	X	2940	1/1	0.98	0.37	-	36,36,36,36	0
29	MG	X	2934	1/1	0.95	0.26	-	29,29,29,29	0
29	MG	X	2907	1/1	0.90	0.78	-	28,28,28,28	0
29	MG	M	202	1/1	0.97	0.36	-	35,35,35,35	0
29	MG	X	2955	1/1	0.97	0.47	-	30,30,30,30	0
29	MG	X	2935	1/1	0.97	0.49	-	34,34,34,34	0
29	MG	X	2950	1/1	0.95	0.40	-	32,32,32,32	0
29	MG	X	2905	1/1	0.95	0.50	-	31,31,31,31	0
29	MG	X	2941	1/1	0.97	0.46	-	38,38,38,38	0
29	MG	X	2908	1/1	0.94	0.60	-	32,32,32,32	0
29	MG	X	2918	1/1	0.98	0.82	-	43,43,43,43	0
29	MG	X	2951	1/1	0.92	0.75	-	32,32,32,32	0
29	MG	X	2964	1/1	0.93	0.88	-	28,28,28,28	0
29	MG	X	2933	1/1	0.86	0.65	-	36,36,36,36	0
29	MG	X	2963	1/1	0.90	0.31	-	56,56,56,56	0
29	MG	X	2928	1/1	0.98	0.39	-	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.