wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2023 – 12:25 pm GMT

PDB ID	:	1W2B
Title	:	Trigger Factor ribosome binding domain in complex with 50S
Authors	:	Ferbitz, L.; Maier, T.; Patzelt, H.; Bukau, B.; Deuerling, E.; Ban, N.
Deposited on	:	2004-07-01
Resolution	:	3.50 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:

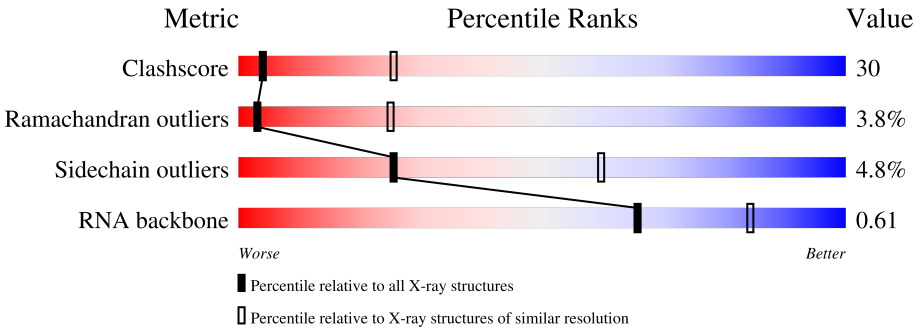
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2922	32% 43% 13% 6% 6%
2	1	48	38% 56%
3	2	92	39% 57%
4	5	144	9% 14% 76%
5	9	122	26% 51% 16% 7%
6	A	239	41% 51% 8%

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Mol	Chain	Length	Quality of chain
7	B	337	39% 55% 6%
8	C	246	46% 48% 6%
9	D	176	27% 44% 9% 20%
10	E	177	49% 45%
11	F	119	47% 50%
12	G	348	5% 91%
13	H	167	29% 56% 8% 7%
14	I	145	40% 52% 6%
15	J	132	52% 45%
16	K	164	40% 43% 6% 11%
17	L	194	26% 69% 5%
18	M	186	37% 57% 6%
19	N	115	58% 39%
20	O	148	56% 38%
21	P	95	48% 46%
22	Q	154	54% 39% 5%
23	R	84	48% 50%
24	S	119	42% 55%
25	T	66	36% 41% 5% 18%
26	U	70	37% 56% 6%
27	V	154	44% 51% 5%
28	W	91	41% 41% 10% 9%
29	X	240	27% 30% 40%
30	Y	73	34% 58% 8%
31	Z	56	36% 62%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	I	202	-	-	X	-
35	CL	L	202	-	-	X	-
35	CL	P	102	-	-	X	-
35	CL	X	301	-	-	X	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 98859 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 23S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2754	59017	26346	10878	19048	2745	0	0	0

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	1	46	394	238	86	69	1	0	0	0

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L44E LA, HLA, RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	2	92	755	458	153	137	7	0	0	0

- Molecule 4 is a protein called TRIGGER FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	5	35	273	173	52	47	1	0	0	0

- Molecule 5 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	9	122	2600	1160	472	847	121	0	0	0

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	A	238	Total	C	N	O	S	0	0	1
			1755	1072	353	325	5			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	ARG	PHE	conflict	UNP P20279

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L5P HMAL5, HL13, RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	141	Total	C	N	O	S	0	0	1
			1095	685	196	210	4			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	E	173	Total	C	N	O	S	0	0	1
			1358	840	225	289	4			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	F	119	Total	C	N	O	S	0	0	0
			886	552	141	192	1			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	G	30	Total	C	N	O	S	0	0	1
			241	149	40	51	1			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	H	156	Total	C	N	O	S	0	0	0
			1216	766	233	213	4			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	I	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	J	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	K	146	Total	C	N	O	0	0	1
			1115	668	223	224			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	L	194	Total	C	N	O	S	0	0	0
			1606	988	346	267	5			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	M	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	N	115	Total 865	C 529	N 161	O 175	0	0	0

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	O	144	Total 1134	C 680	N 231	O 223	0	0	1

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	P	95	Total 735	C 450	N 141	O 144	0	0	0

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L22P HMAL22, HL23, RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Q	151	Total 1150	C 713	N 210	O 223	S 4	0	0	1

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R	84	Total 664	C 405	N 114	O 142	S 3	0	0	0

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	S	119	Total 950	C 568	N 180	O 202	0	0	0

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	T	54	Total 411	C 244	N 76	O 86	S 5	0	0	1

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	U	66	Total	C	N	O	S	0	0	1
			500	304	95	100	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	V	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	W	83	Total	C	N	O	S	0	0	1
			655	402	130	122	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	X	143	Total	C	N	O	0	0	1
			1131	686	229	216			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	73	Total	C	N	O	S	0	0	0
			564	359	111	87	7			

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Z	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	105	Total	Mg	0	0
			105	105		
32	2	1	Total	Mg	0	0
			1	1		
32	9	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	3	Total Mg 3 3	0	0
32	B	3	Total Mg 3 3	0	0
32	J	1	Total Mg 1 1	0	0
32	S	1	Total Mg 1 1	0	0
32	X	1	Total Mg 1 1	0	0

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	74	Total Na 74 74	0	0
34	9	2	Total Na 2 2	0	0
34	A	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	I	1	Total Na 1 1	0	0
34	K	1	Total Na 1 1	0	0
34	L	1	Total Na 1 1	0	0
34	P	1	Total Na 1 1	0	0
34	Q	2	Total Na 2 2	0	0
34	R	1	Total Na 1 1	0	0
34	S	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	7	Total Cl 7 7	0	0
35	2	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	I	3	Total Cl 3 3	0	0
35	J	1	Total Cl 1 1	0	0
35	K	2	Total Cl 2 2	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	P	1	Total Cl 1 1	0	0
35	Q	1	Total Cl 1 1	0	0
35	X	1	Total Cl 1 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	2	1	Total Cd 1 1	0	0
36	N	1	Total Cd 1 1	0	0
36	T	1	Total Cd 1 1	0	0
36	Y	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	5875	Total O 5875 5875	0	0
37	1	49	Total O 49 49	0	0
37	2	69	Total O 69 69	0	0
37	9	153	Total O 153 153	0	0
37	A	135	Total O 135 135	0	0
37	B	156	Total O 156 156	0	0
37	C	169	Total O 169 169	0	0
37	D	52	Total O 52 52	0	0
37	E	41	Total O 41 41	0	0
37	F	30	Total O 30 30	0	0
37	G	20	Total O 20 20	0	0
37	H	80	Total O 80 80	0	0
37	I	52	Total O 52 52	0	0
37	J	61	Total O 61 61	0	0
37	K	98	Total O 98 98	0	0
37	L	155	Total O 155 155	0	0
37	M	60	Total O 60 60	0	0
37	N	38	Total O 38 38	0	0
37	O	67	Total O 67 67	0	0
37	P	53	Total O 53 53	0	0
37	Q	83	Total O 83 83	0	0
37	R	32	Total O 32 32	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	S	36	Total O 36 36	0	0
37	T	25	Total O 25 25	0	0
37	U	11	Total O 11 11	0	0
37	V	69	Total O 69 69	0	0
37	W	26	Total O 26 26	0	0
37	X	107	Total O 107 107	0	0
37	Y	35	Total O 35 35	0	0
37	Z	50	Total O 50 50	0	0

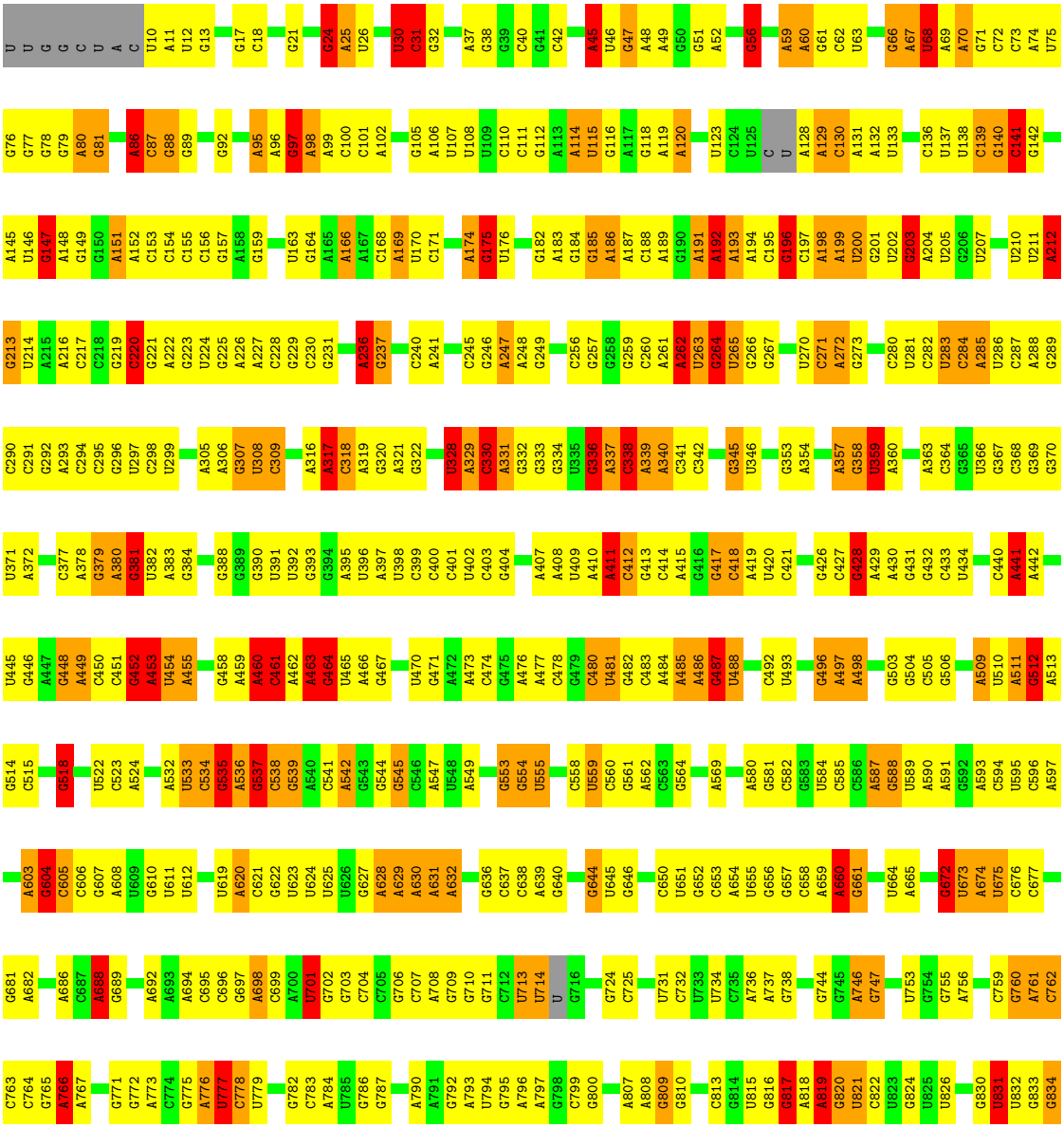
3 Residue-property plots (i)

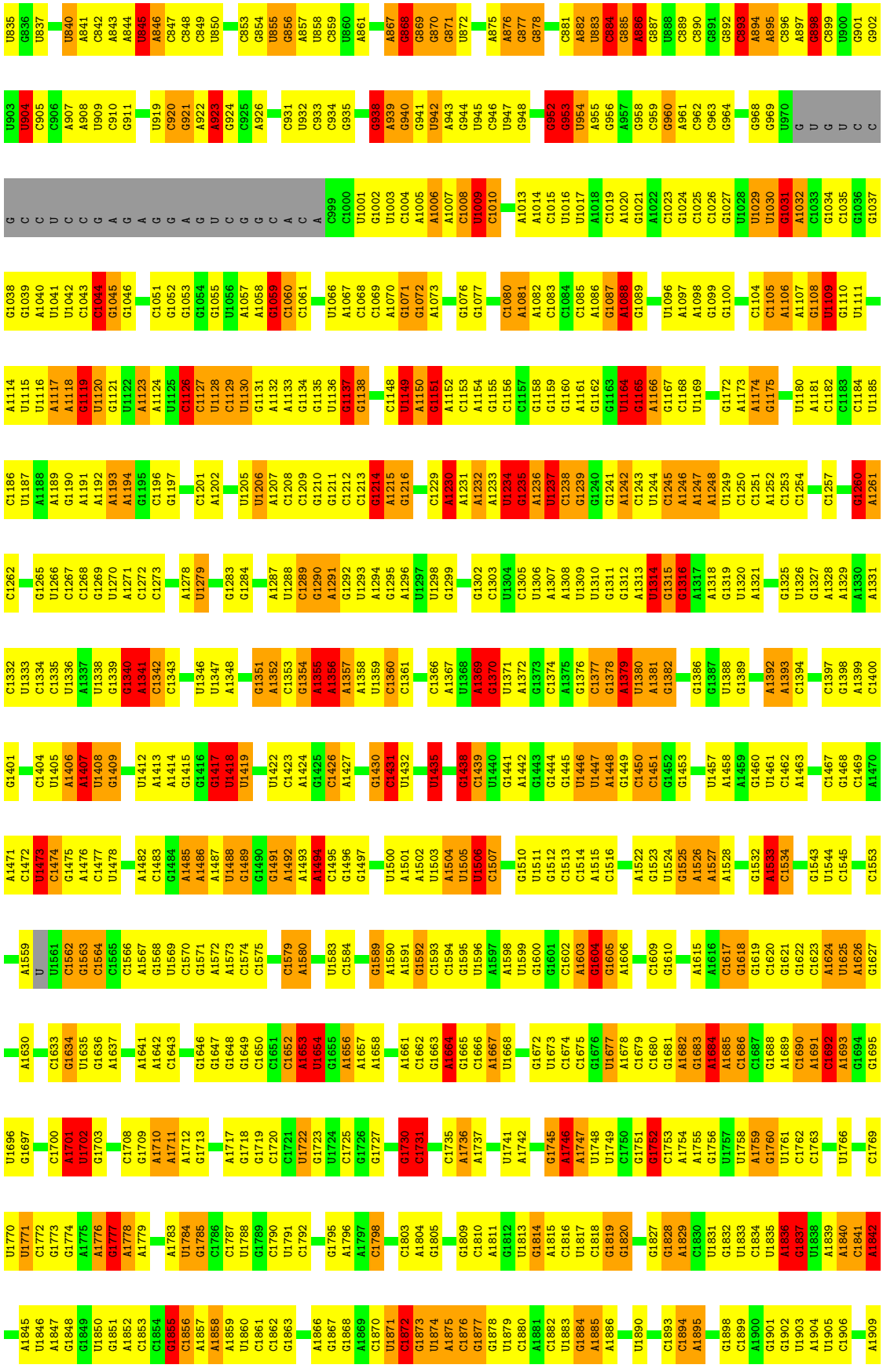
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

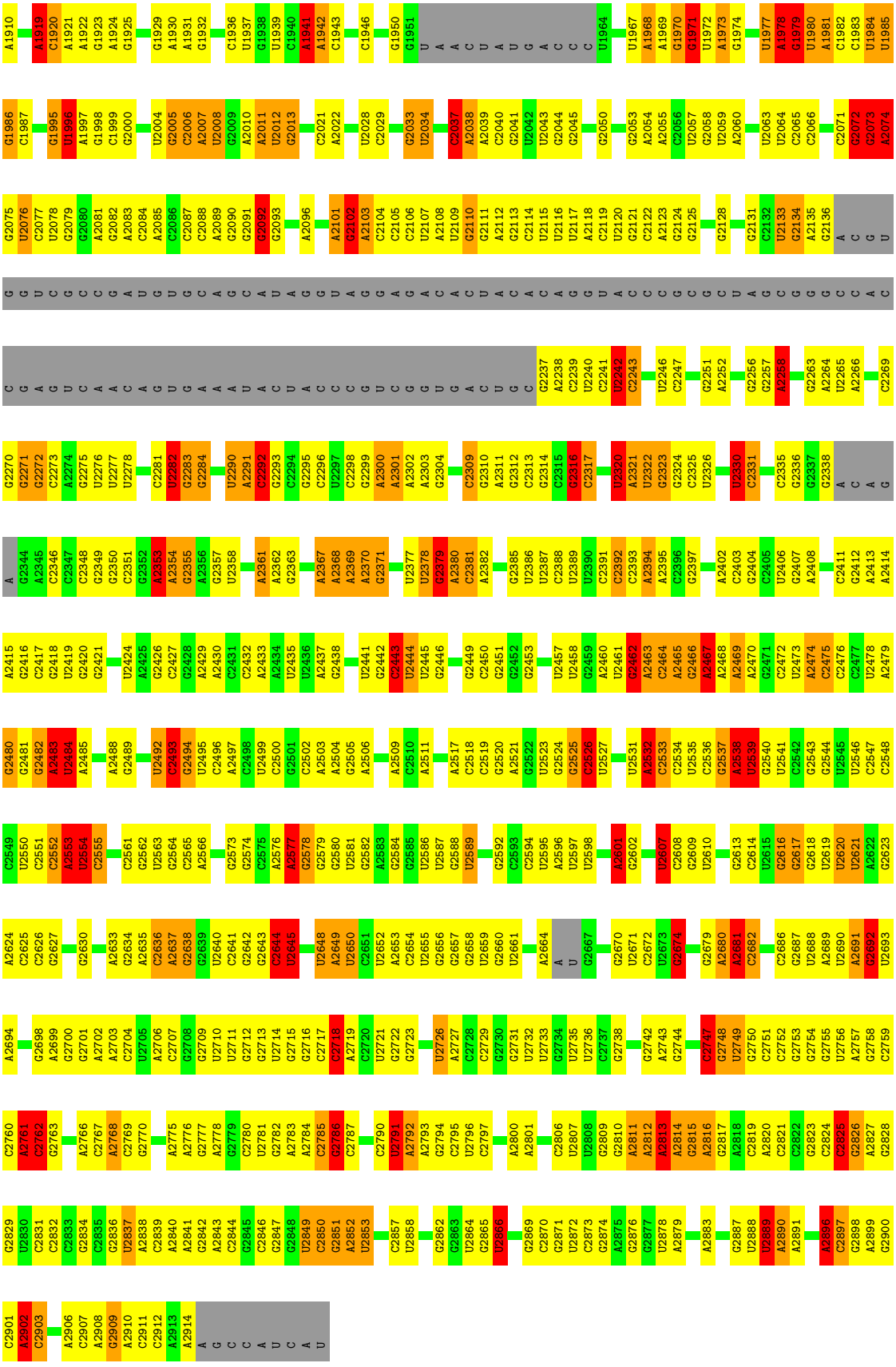
Note EDS was not executed.

- Molecule 1: 23S RRNA

Chain 0: 32% 43% 13% 6% 6%

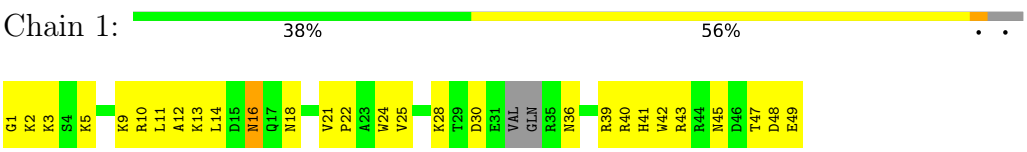






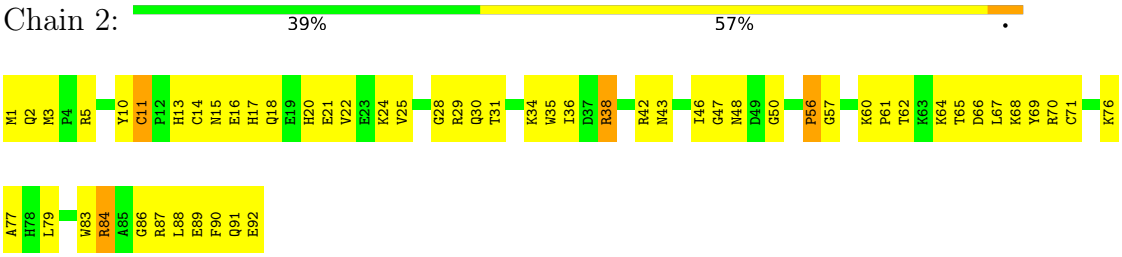
• Molecule 2: 50S RIBOSOMAL PROTEIN L39E

Chain 1:



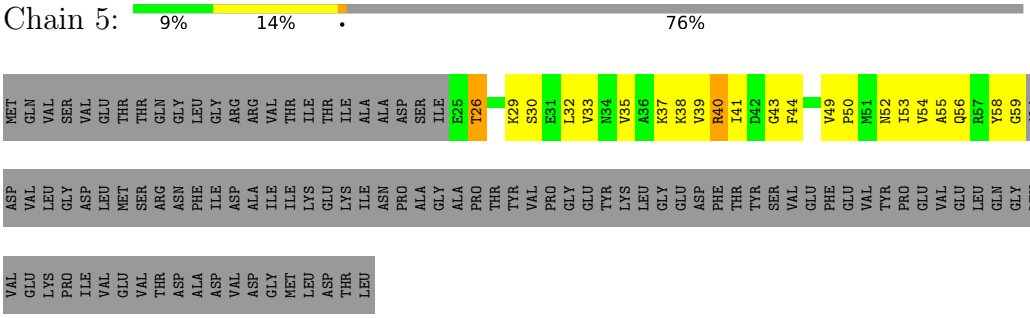
• Molecule 3: 50S RIBOSOMAL PROTEIN L44E LA, HLA, RIBOSOMAL PROTEIN L44E

Chain 2:



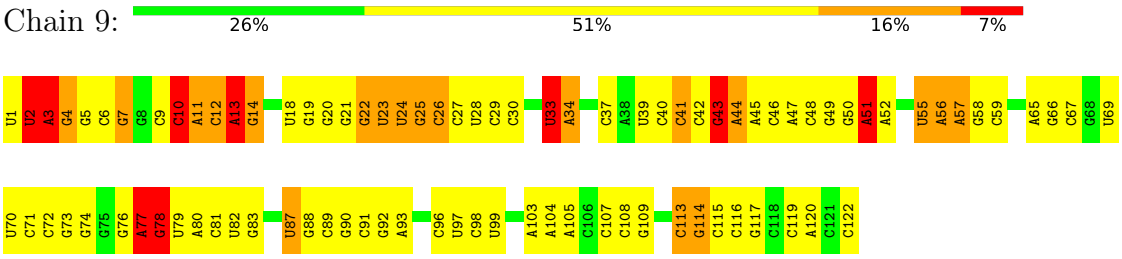
• Molecule 4: TRIGGER FACTOR

Chain 5:



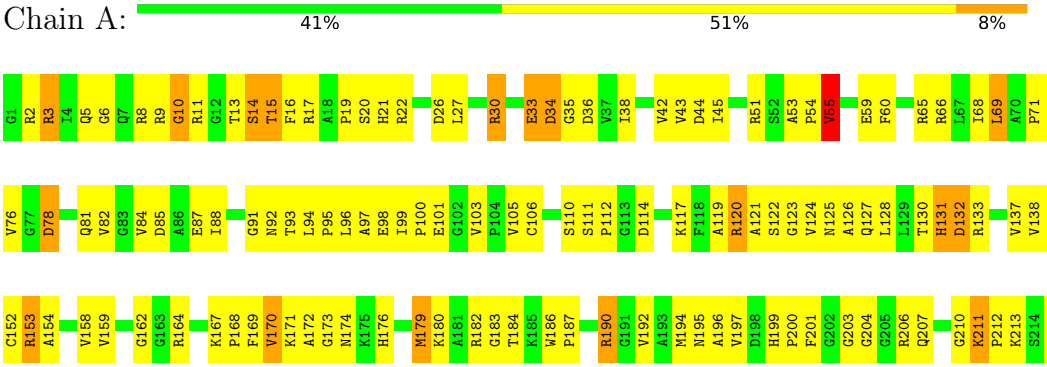
• Molecule 5: 5S RRNA

Chain 9:



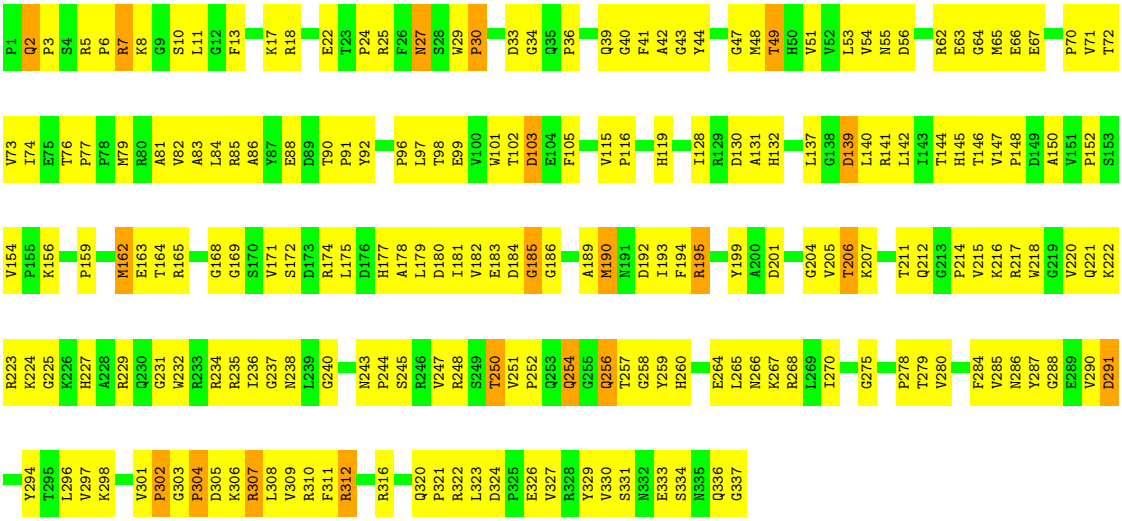
• Molecule 6: 50S RIBOSOMAL PROTEIN L2P

Chain A:



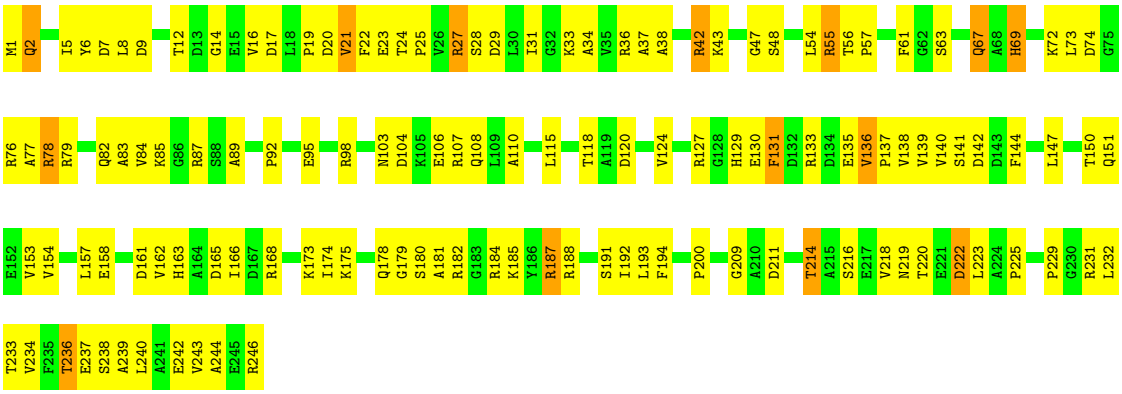
• Molecule 7: 50S RIBOSOMAL PROTEIN L3P

Chain B:



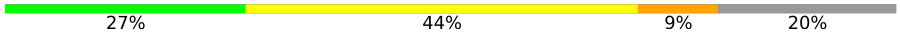
• Molecule 8: 50S RIBOSOMAL PROTEIN L4P

Chain C:



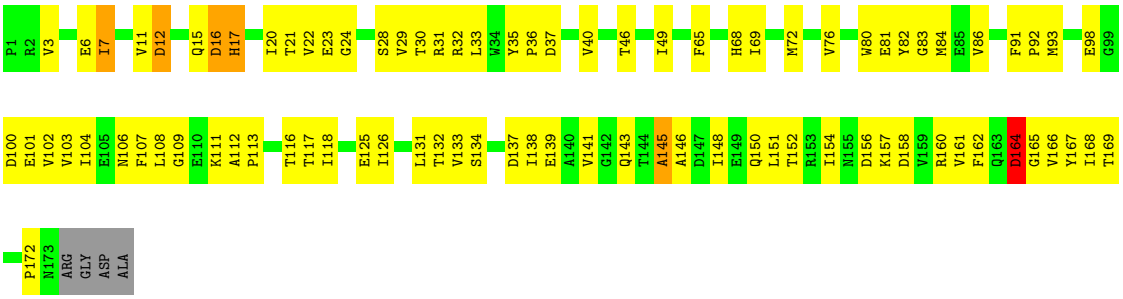
• Molecule 9: 50S RIBOSOMAL PROTEIN L5P HMAL5, HL13, RIBOSOMAL PROTEIN L5

Chain D:



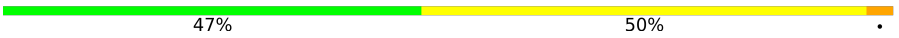
• Molecule 10: 50S RIBOSOMAL PROTEIN L6P

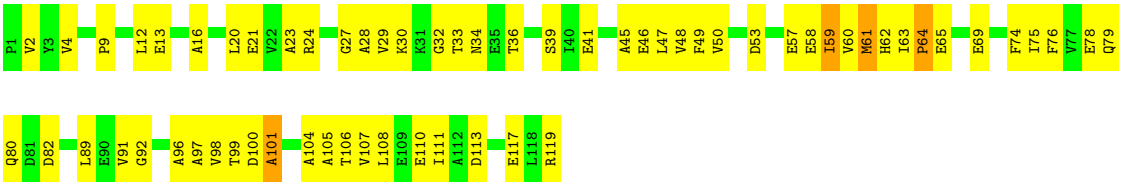
Chain E:



• Molecule 11: 50S RIBOSOMAL PROTEIN L7AE

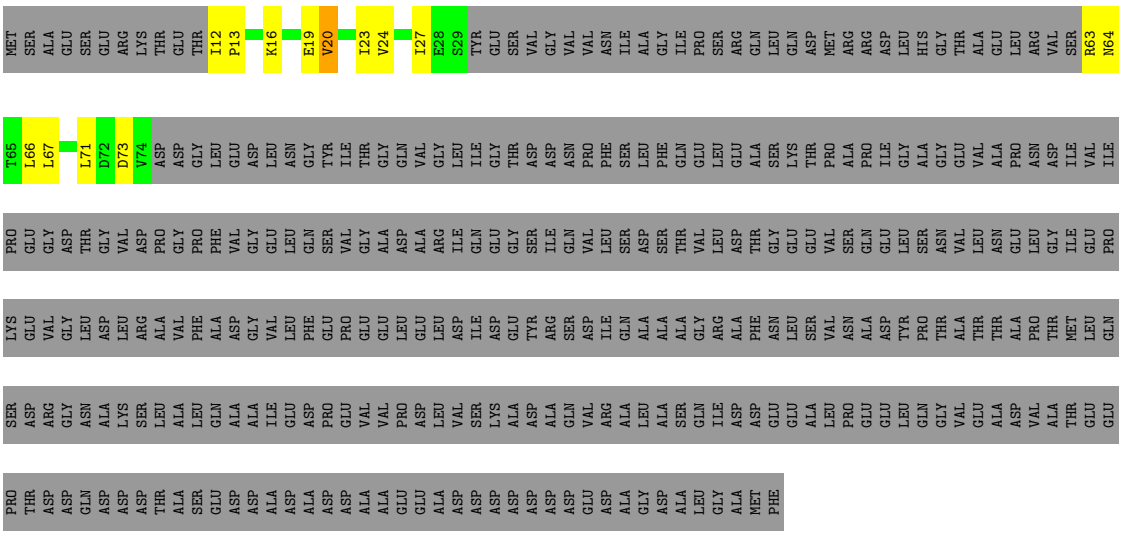
Chain F:





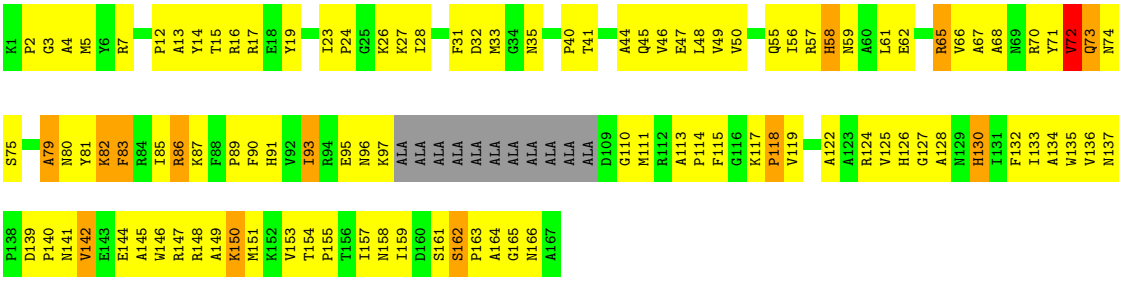
• Molecule 12: 50S RIBOSOMAL PROTEIN L10E

Chain G:



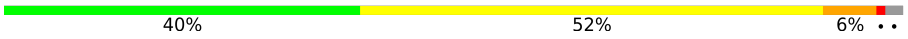
• Molecule 13: 50S RIBOSOMAL PROTEIN L10E

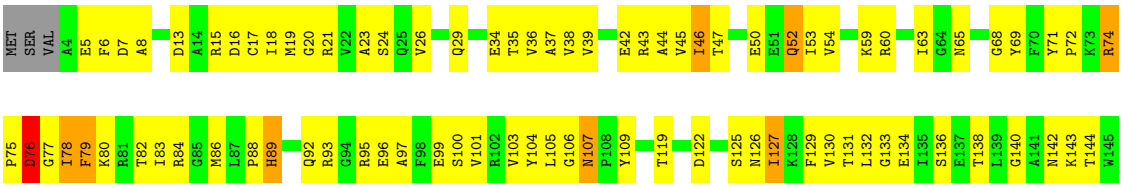
Chain H:



• Molecule 14: 50S RIBOSOMAL PROTEIN L13P

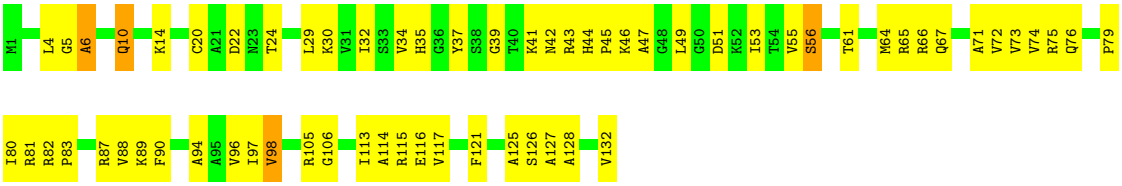
Chain I:





• Molecule 15: 50S RIBOSOMAL PROTEIN L14P

Chain J:

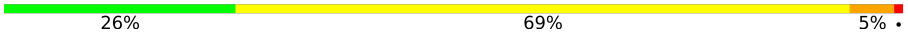


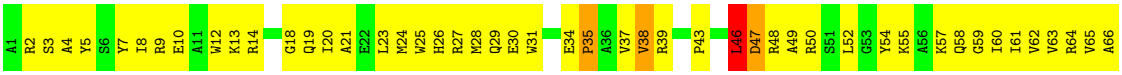
• Molecule 16: 50S RIBOSOMAL PROTEIN L15P

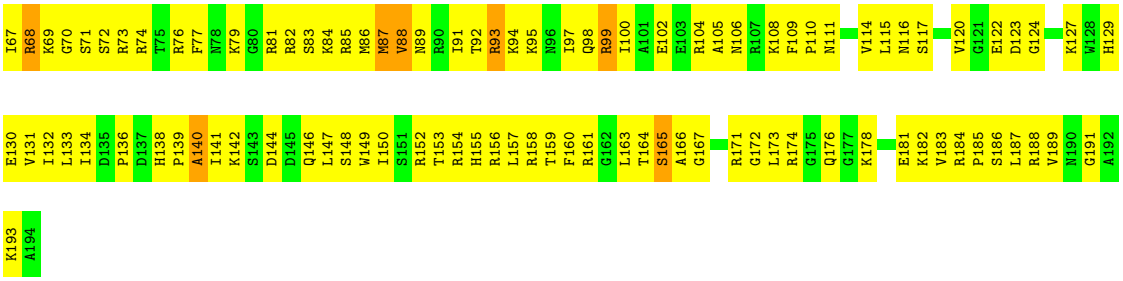
Chain K:

• Molecule 17: 50S RIBOSOMAL PROTEIN L15E

Chain L:

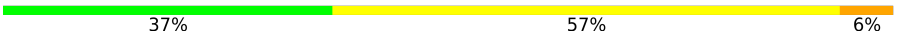


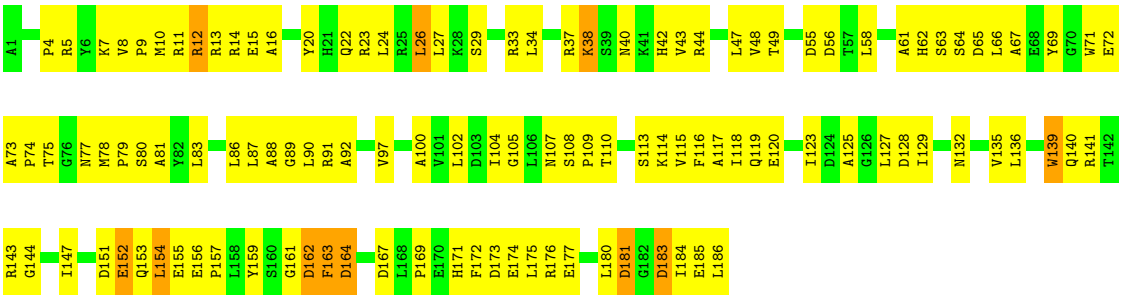




• Molecule 18: 50S RIBOSOMAL PROTEIN L18P

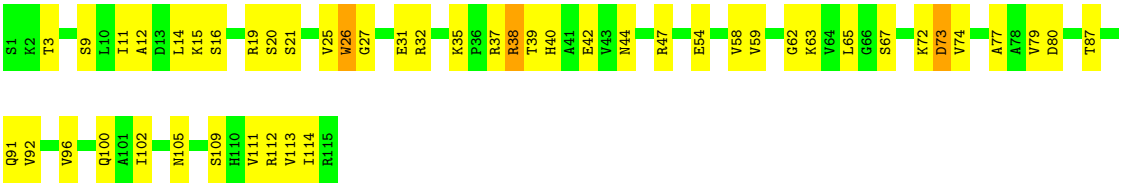
Chain M:





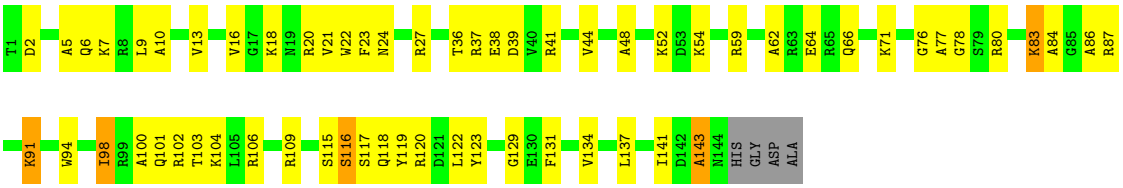
• Molecule 19: 50S RIBOSOMAL PROTEIN L18E

Chain N:



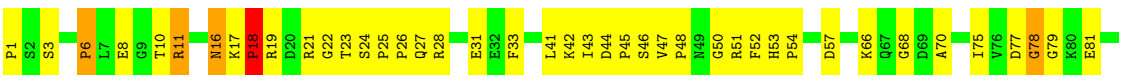
• Molecule 20: 50S RIBOSOMAL PROTEIN L19E

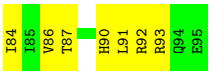
Chain O:



• Molecule 21: 50S RIBOSOMAL PROTEIN L21E

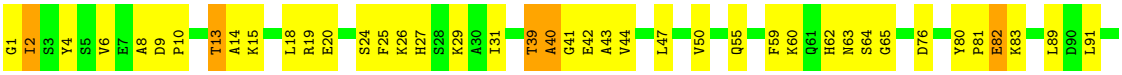
Chain P:

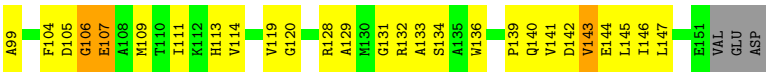




• Molecule 22: 50S RIBOSOMAL PROTEIN L22P HMAL22, HL23, RIBOSOMAL PROTEIN L22

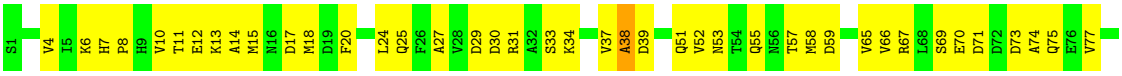
Chain Q:





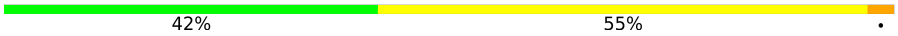
• Molecule 23: 50S RIBOSOMAL PROTEIN L23P

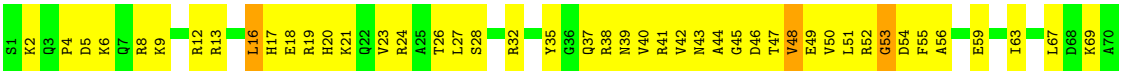
Chain R:

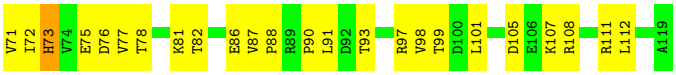


• Molecule 24: RIBOSOMAL PROTEIN L24

Chain S:

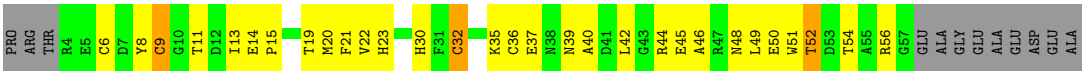






• Molecule 25: 50S RIBOSOMAL PROTEIN L24P

Chain T:

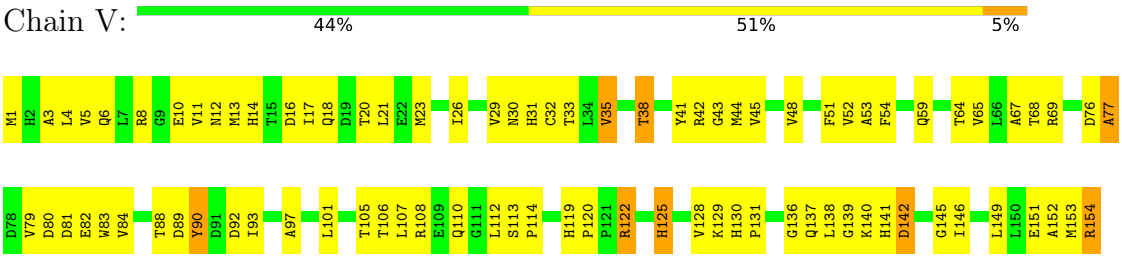


• Molecule 26: 50S RIBOSOMAL PROTEIN L24E

Chain U:

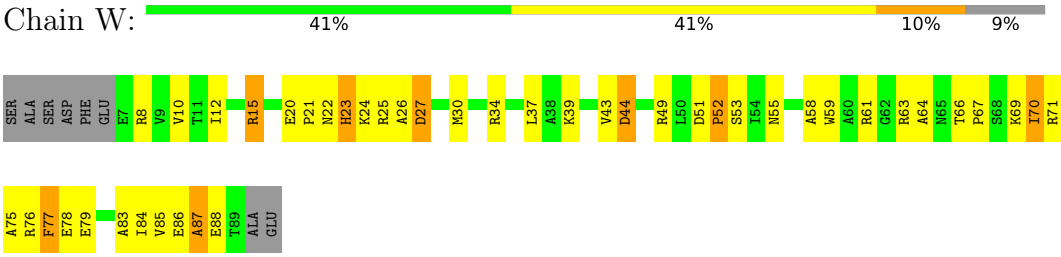
• Molecule 27: 50S RIBOSOMAL PROTEIN L30P

Chain V:



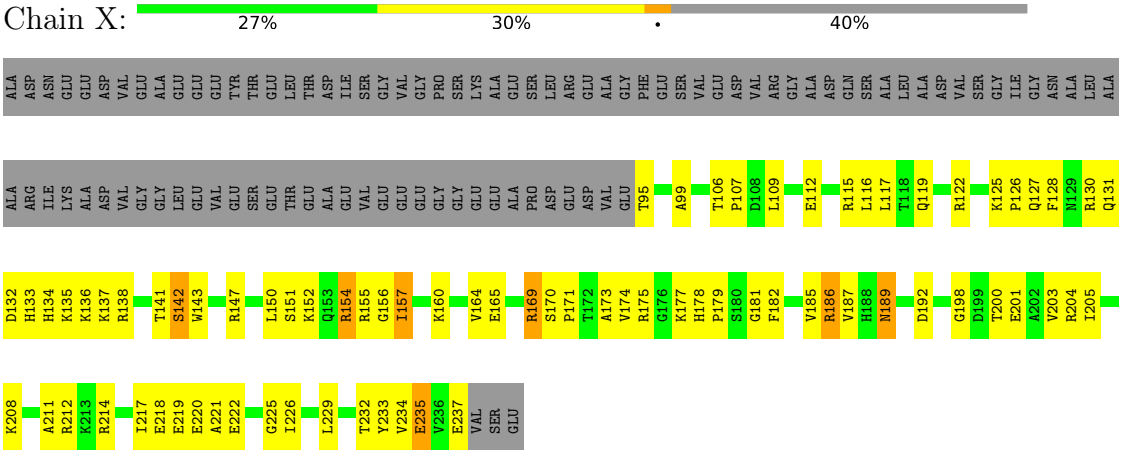
• Molecule 28: 50S RIBOSOMAL PROTEIN L31E

Chain W:



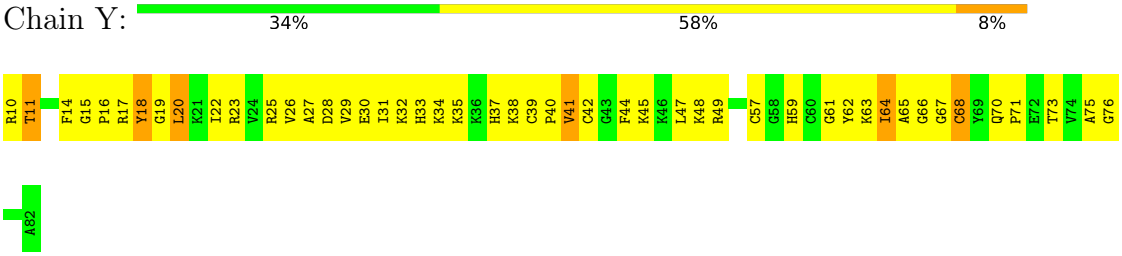
• Molecule 29: 50S RIBOSOMAL PROTEIN L32E

Chain X:



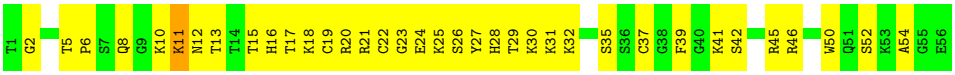
• Molecule 30: 50S RIBOSOMAL PROTEIN L37AE

Chain Y:



• Molecule 31: RIBOSOMAL PROTEIN L37E

Chain Z:


T1
G2
T5
P6
S7
Q8
G9
K10
K11
N12
T13
T14
T15
H16
T17
K18
C19
R20
R21
C22
G23
E24
K25
S26
Y27
H28
T29
K30
K31
K32
S35
S36
C37
G38
F39
G40
K41
S42
R45
R46
W50
Q51
S52
K53
A54
G55
E56

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	210.75Å 298.87Å 574.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50	Depositor
% Data completeness (in resolution range)	80.3 (30.00-3.50)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	98859	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, CD, K

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	0	0.49	0/66076	0.85	218/103052 (0.2%)
2	1	0.34	0/399	0.56	0/527
3	2	0.34	0/771	0.55	0/1024
4	5	0.38	0/275	0.77	0/366
5	9	0.44	0/2905	0.84	11/4528 (0.2%)
6	A	0.36	0/1788	0.65	0/2411
7	B	0.36	0/2690	0.65	0/3652
8	C	0.37	0/1884	0.62	0/2551
9	D	0.35	0/1112	0.59	0/1500
10	E	0.38	0/1383	0.63	0/1882
11	F	0.35	0/897	0.59	0/1219
12	G	0.41	0/242	0.53	0/326
13	H	0.38	0/1247	0.68	0/1686
14	I	0.37	0/1136	0.63	0/1530
15	J	0.39	0/1004	0.68	0/1351
16	K	0.34	0/1127	0.64	0/1506
17	L	0.40	0/1634	0.66	0/2180
18	M	0.32	0/1474	0.66	0/1999
19	N	0.35	0/874	0.65	0/1181
20	O	0.37	0/1144	0.55	0/1523
21	P	0.37	0/749	0.67	0/1005
22	Q	0.41	0/1173	0.63	0/1580
23	R	0.53	0/672	0.69	0/906
24	S	0.34	0/958	0.65	0/1289
25	T	0.40	0/418	0.57	0/564
26	U	0.36	0/503	0.59	0/677
27	V	0.37	0/1219	0.64	0/1655
28	W	0.37	0/665	0.61	0/897
29	X	0.38	0/1147	0.65	0/1538
30	Y	0.34	0/576	0.58	0/763
31	Z	0.40	0/438	0.63	0/578
All	All	0.45	0/98580	0.80	229/147446 (0.2%)

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	0	0	65
5	9	0	4
27	V	0	1
All	All	0	70

There are no bond length outliers.

The worst 5 of 229 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	535	G	N9-C1'-C2'	10.05	127.07	114.00
1	0	537	G	N9-C1'-C2'	9.91	126.88	114.00
1	0	1235	G	O4'-C1'-N9	8.50	115.00	108.20
1	0	1702	U	N1-C1'-C2'	8.48	125.03	114.00
1	0	337	A	N9-C1'-C2'	8.44	124.97	114.00

There are no chirality outliers.

5 of 70 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	203	G	Sidechain
1	0	224	U	Sidechain
1	0	30	U	Sidechain
1	0	68	U	Sidechain
1	0	86	A	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	0	59017	0	29808	2081	0
2	1	394	0	406	38	0
3	2	755	0	732	81	0
4	5	273	0	296	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	9	2600	0	1326	119	0
6	A	1755	0	1763	185	0
7	B	2625	0	2533	240	0
8	C	1859	0	1816	166	0
9	D	1095	0	1085	125	0
10	E	1358	0	1266	95	0
11	F	886	0	854	75	0
12	G	241	0	231	20	0
13	H	1216	0	1215	169	0
14	I	1120	0	1098	92	0
15	J	994	0	1027	82	0
16	K	1115	0	1072	91	0
17	L	1606	0	1676	241	0
18	M	1445	0	1401	149	0
19	N	865	0	873	52	0
20	O	1134	0	1127	65	0
21	P	735	0	729	49	0
22	Q	1150	0	1122	76	0
23	R	664	0	626	50	0
24	S	950	0	924	80	0
25	T	411	0	368	35	0
26	U	500	0	511	45	0
27	V	1196	0	1137	120	0
28	W	655	0	653	55	0
29	X	1131	0	1133	100	0
30	Y	564	0	601	85	0
31	Z	431	0	426	45	0
32	0	105	0	0	0	0
32	2	1	0	0	0	0
32	9	2	0	0	0	0
32	A	3	0	0	0	0
32	B	3	0	0	0	0
32	J	1	0	0	0	0
32	S	1	0	0	0	0
32	X	1	0	0	0	0
33	0	2	0	0	0	0
34	0	74	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	I	1	0	0	0	0
34	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	L	1	0	0	0	0
34	P	1	0	0	0	0
34	Q	2	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	7	0	0	2	0
35	2	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	I	3	0	0	3	0
35	J	1	0	0	0	0
35	K	2	0	0	0	0
35	L	1	0	0	2	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	P	1	0	0	2	0
35	Q	1	0	0	0	0
35	X	1	0	0	2	0
36	2	1	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	Y	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5875	0	0	346	0
37	1	49	0	0	8	0
37	2	69	0	0	7	0
37	9	153	0	0	16	0
37	A	135	0	0	29	0
37	B	156	0	0	31	0
37	C	169	0	0	43	0
37	D	52	0	0	15	0
37	E	41	0	0	8	0
37	F	30	0	0	6	0
37	G	20	0	0	3	0
37	H	80	0	0	19	0
37	I	52	0	0	4	0
37	J	61	0	0	18	0
37	K	98	0	0	23	0
37	L	155	0	0	34	0
37	M	60	0	0	18	0
37	N	38	0	0	5	0
37	O	67	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	P	53	0	0	6	0
37	Q	83	0	0	6	0
37	R	32	0	0	6	0
37	S	36	0	0	4	0
37	T	25	0	0	6	0
37	U	11	0	0	2	0
37	V	69	0	0	10	0
37	W	26	0	0	6	0
37	X	107	0	0	13	0
37	Y	35	0	0	10	0
37	Z	50	0	0	2	0
All	All	98859	0	59835	4534	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 30.

The worst 5 of 4534 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)
1:0:156:C:H5"	17:L:171:ARG:HD3	1.28	1.14
3:2:46:ILE:HG21	17:L:87:MET:HG2	1.24	1.14
26:U:12:THR:HG22	26:U:15:GLU:HG3	1.28	1.14
11:F:91:VAL:HG12	11:F:92:GLY:H	1.09	1.13
5:9:6:C:H5"	18:M:37:ARG:HH12	1.08	1.11

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	1	42/48 (88%)	37 (88%)	5 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	2	90/92 (98%)	82 (91%)	5 (6%)	3 (3%)	4 28
4	5	33/144 (23%)	24 (73%)	9 (27%)	0	100 100
6	A	236/239 (99%)	197 (84%)	27 (11%)	12 (5%)	2 19
7	B	335/337 (99%)	281 (84%)	40 (12%)	14 (4%)	3 23
8	C	244/246 (99%)	201 (82%)	37 (15%)	6 (2%)	5 34
9	D	135/176 (77%)	90 (67%)	31 (23%)	14 (10%)	0 7
10	E	171/177 (97%)	147 (86%)	21 (12%)	3 (2%)	8 41
11	F	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	3 28
12	G	26/348 (8%)	23 (88%)	2 (8%)	1 (4%)	3 25
13	H	152/167 (91%)	123 (81%)	21 (14%)	8 (5%)	2 17
14	I	140/145 (97%)	117 (84%)	17 (12%)	6 (4%)	2 22
15	J	130/132 (98%)	115 (88%)	13 (10%)	2 (2%)	10 45
16	K	142/164 (87%)	116 (82%)	20 (14%)	6 (4%)	3 23
17	L	192/194 (99%)	144 (75%)	40 (21%)	8 (4%)	3 23
18	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	3 25
19	N	113/115 (98%)	92 (81%)	17 (15%)	4 (4%)	3 27
20	O	142/148 (96%)	126 (89%)	12 (8%)	4 (3%)	5 32
21	P	93/95 (98%)	72 (77%)	16 (17%)	5 (5%)	2 17
22	Q	149/154 (97%)	127 (85%)	18 (12%)	4 (3%)	5 33
23	R	82/84 (98%)	68 (83%)	9 (11%)	5 (6%)	1 15
24	S	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	5 33
25	T	52/66 (79%)	49 (94%)	3 (6%)	0	100 100
26	U	64/70 (91%)	49 (77%)	13 (20%)	2 (3%)	4 30
27	V	152/154 (99%)	132 (87%)	19 (12%)	1 (1%)	22 61
28	W	81/91 (89%)	65 (80%)	11 (14%)	5 (6%)	1 15
29	X	141/240 (59%)	126 (89%)	12 (8%)	3 (2%)	7 38
30	Y	71/73 (97%)	59 (83%)	7 (10%)	5 (7%)	1 12
31	Z	54/56 (96%)	43 (80%)	7 (13%)	4 (7%)	1 11
All	All	3680/4379 (84%)	3056 (83%)	485 (13%)	139 (4%)	3 25

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	D	20	LYS
9	D	93	LEU
9	D	95	THR
9	D	144	ARG
9	D	173	GLU

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	1	42/44 (96%)	40 (95%)	2 (5%)	25 60
3	2	79/79 (100%)	75 (95%)	4 (5%)	24 57
4	5	29/122 (24%)	26 (90%)	3 (10%)	7 32
6	A	179/181 (99%)	167 (93%)	12 (7%)	16 48
7	B	282/282 (100%)	268 (95%)	14 (5%)	24 58
8	C	193/193 (100%)	181 (94%)	12 (6%)	18 51
9	D	117/147 (80%)	109 (93%)	8 (7%)	16 48
10	E	152/155 (98%)	147 (97%)	5 (3%)	38 68
11	F	92/92 (100%)	91 (99%)	1 (1%)	73 88
12	G	27/283 (10%)	27 (100%)	0	100 100
13	H	122/122 (100%)	111 (91%)	11 (9%)	9 37
14	I	118/121 (98%)	111 (94%)	7 (6%)	19 53
15	J	106/106 (100%)	102 (96%)	4 (4%)	33 65
16	K	112/126 (89%)	106 (95%)	6 (5%)	22 55
17	L	166/166 (100%)	160 (96%)	6 (4%)	35 66
18	M	149/149 (100%)	142 (95%)	7 (5%)	26 60
19	N	93/93 (100%)	90 (97%)	3 (3%)	39 69
20	O	113/116 (97%)	109 (96%)	4 (4%)	36 67
21	P	79/79 (100%)	74 (94%)	5 (6%)	18 51
22	Q	117/121 (97%)	113 (97%)	4 (3%)	37 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	R	73/73 (100%)	72 (99%)	1 (1%)	67 85
24	S	105/105 (100%)	101 (96%)	4 (4%)	33 65
25	T	44/52 (85%)	41 (93%)	3 (7%)	16 48
26	U	51/56 (91%)	51 (100%)	0	100 100
27	V	130/130 (100%)	124 (95%)	6 (5%)	27 61
28	W	66/73 (90%)	61 (92%)	5 (8%)	13 43
29	X	120/195 (62%)	115 (96%)	5 (4%)	30 63
30	Y	56/56 (100%)	51 (91%)	5 (9%)	9 37
31	Z	46/46 (100%)	46 (100%)	0	100 100
All	All	3058/3563 (86%)	2911 (95%)	147 (5%)	25 60

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	Q	39	THR
30	Y	28	ASP
24	S	5	ASP
27	V	142	ASP
9	D	50	VAL

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

Mol	Chain	Res	Type
19	N	105	ASN
26	U	60	GLN
20	O	66	GLN
22	Q	113	HIS
27	V	110	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	542 (19%)	360 (13%)
5	9	121/122 (99%)	27 (22%)	14 (11%)
All	All	2866/3044 (94%)	569 (19%)	374 (13%)

5 of 569 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	24	G
1	0	25	A
1	0	31	C
1	0	32	G
1	0	46	U

5 of 374 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1722	U
1	0	2282	U
1	0	1771	U
1	0	1977	U
1	0	2370	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 232 ligands modelled in this entry, 232 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.