



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:17 am GMT

PDB ID : 4KZZ
Title : Rabbit 40S ribosomal subunit in complex with mRNA, initiator tRNA and eIF1A
Authors : Lomakin, I.B.; Steitz, T.A.
Deposited on : 2013-05-30
Resolution : 7.03 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

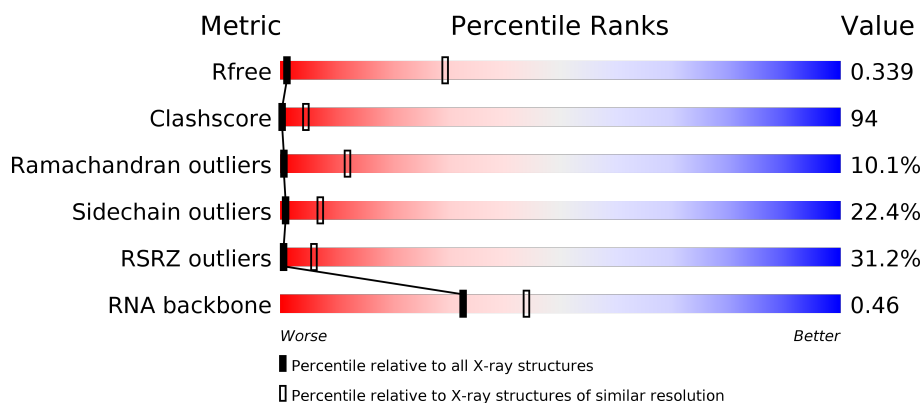
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.03 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}	100719	1100 (10.00-3.70)
Clashscore	112137	1035 (10.00-3.80)
Ramachandran outliers	110173	1003 (10.00-3.76)
Sidechain outliers	110143	1098 (10.00-3.70)
RSRZ outliers	101464	1003 (10.00-3.72)
RNA backbone	2435	1053 (10.00-2.90)

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 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 $\leq 5\%$. 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	295	<div> <div>14%</div> <div>9% 39% 19% • 29%</div> </div>
2	B	264	<div> <div>28%</div> <div>14% 45% 20% • 19%</div> </div>
3	C	278	<div> <div>39%</div> <div>14% 46% 18% • 19%</div> </div>
4	D	243	<div> <div>68%</div> <div>21% 45% 23% 5% 7%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	263	
6	F	204	
7	G	249	
8	H	194	
9	I	208	
10	J	194	
11	K	165	
12	L	158	
13	M	132	
14	N	151	
15	O	151	
16	P	145	
17	Q	146	
18	R	135	
19	S	152	
20	T	145	
21	U	119	
22	V	83	
23	W	130	
24	X	143	
25	Y	133	
26	Z	125	
27	a	115	
28	b	84	
29	c	69	

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Mol	Chain	Length	Quality of chain
30	d	56	<div><div></div><div>38%</div><div>66%</div><div>27%</div><div>5%</div></div>
31	e	133	<div><div></div><div>9%</div><div>18%</div><div>16%</div><div>10%</div><div>56%</div></div>
32	f	156	<div><div></div><div>19%</div><div>18%</div><div>8%</div><div>54%</div></div>
33	g	317	<div><div></div><div>12%</div><div>74%</div><div>20%</div></div>
34	i	1863	<div><div></div><div>25%</div><div>8%</div><div>64%</div><div>25%</div></div>
35	j	75	<div><div></div><div>28%</div><div>72%</div><div>27%</div></div>
36	k	24	<div><div></div><div>50%</div><div>42%</div><div>8%</div><div>46%</div></div>
37	n	144	<div><div></div><div>22%</div><div>44%</div><div>11%</div><div>43%</div></div>

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 79048 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 40S Ribosomal Protein SA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1642	1045	289	300	8			

- Molecule 2 is a protein called 40S Ribosomal Protein S3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1741	1107	309	310	15			

- Molecule 3 is a protein called 40S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	226	Total	C	N	O	S	0	0	0
			1742	1127	300	306	9			

- Molecule 4 is a protein called 40S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	227	Total	C	N	O	S	0	0	0
			1764	1124	317	315	8			

- Molecule 5 is a protein called 40S Ribosomal Protein S4X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	263	Total	C	N	O	S	0	0	0
			2083	1329	385	359	10			

- Molecule 6 is a protein called 40S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	191	Total	C	N	O	S	0	0	0
			1509	943	286	273	7			

- Molecule 7 is a protein called 40S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	237	Total	C	N	O	S	0	0	0
			1923	1200	387	329	7			

- Molecule 8 is a protein called 40S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	190	Total	C	N	O	S	0	0	0
			1530	975	281	273	1			

- Molecule 9 is a protein called 40S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	206	Total	C	N	O	S	0	0	0
			1679	1054	329	291	5			

- Molecule 10 is a protein called 40S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	182	Total	C	N	O	S	0	0	0
			1498	952	300	244	2			

- Molecule 11 is a protein called 40S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	98	Total	C	N	O	S	0	0	0
			827	539	148	134	6			

- Molecule 12 is a protein called 40S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	158	Total	C	N	O	S	0	0	0
			1296	827	241	221	7			

- Molecule 13 is a protein called 40S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	124	Total	C	N	O	S	0	0	0
			950	594	169	179	8			

- Molecule 14 is a protein called 40S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	150	Total	C	N	O	S	0	0	0
			1208	773	229	205	1			

- Molecule 15 is a protein called 40S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	136	Total	C	N	O	S	0	0	0
			1016	621	199	190	6			

- Molecule 16 is a protein called 40S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	127	Total	C	N	O	S	0	0	0
			1060	673	201	179	7			

- Molecule 17 is a protein called 40S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	141	Total	C	N	O	S	0	0	0
			1124	715	212	194	3			

- Molecule 18 is a protein called 40S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	126	Total	C	N	O	S	0	0	0
			1019	639	188	187	5			

- Molecule 19 is a protein called 40S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	137	Total	C	N	O	S	0	0	0
			1139	714	231	193	1			

- Molecule 20 is a protein called 40S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	141	Total	C	N	O	S	0	0	0
			1112	701	213	195	3			

- Molecule 21 is a protein called 40S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	104	Total	C	N	O	S	0	0	0
			822	514	156	148	4			

- Molecule 22 is a protein called 40S Ribosomal Protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	82	Total	C	N	O	S	0	0	0
			619	378	117	119	5			

- Molecule 23 is a protein called 40S Ribosomal Protein S15A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	129	Total	C	N	O	S	0	0	0
			1034	659	193	176	6			

- Molecule 24 is a protein called 40S Ribosomal Protein S23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	142	Total	C	N	O	S	0	0	0
			1106	698	220	184	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	ALA	SEE REMARK 999	UNP G1SZ47

- Molecule 25 is a protein called 40S Ribosomal Protein S24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	126	Total	C	N	O	S	0	0	0
			1021	645	198	173	5			

- Molecule 26 is a protein called 40S Ribosomal Protein S25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	75	Total	C	N	O	S	0	0	0
			598	382	111	104	1			

- Molecule 27 is a protein called 40S Ribosomal Protein S26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	a	107	Total	C	N	O	S	0	0	0
			844	527	173	138	6			

- Molecule 28 is a protein called 40S Ribosomal Protein S27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	b	84	Total	C	N	O	S	0	0	0
			659	413	122	116	8			

- Molecule 29 is a protein called 40S Ribosomal Protein S28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	c	64	Total	C	N	O	S	0	0	0
			506	308	102	94	2			

- Molecule 30 is a protein called 40S Ribosomal Protein S29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	d	53	Total	C	N	O	S	0	0	0
			445	278	90	72	5			

- Molecule 31 is a protein called 40S Ribosomal Protein S30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	e	59	Total	C	N	O	S	0	0	0
			473	293	104	75	1			

- Molecule 32 is a protein called 40S Ribosomal Protein S27A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	f	71	Total	C	N	O	S	0	0	0
			581	367	109	98	7			

- Molecule 33 is a protein called 40S Ribosomal Protein RACK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	g	313	Total	C	N	O	S	0	0	0
			2436	1535	424	465	12			

- Molecule 34 is a RNA chain called 18S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	i	1797	Total	C	N	O	P	0	0	0
			37514	16712	6634	12372	1796			

- Molecule 35 is a RNA chain called initiator Met-RNA-i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	j	75	Total	C	N	O	P	0	0	0
			1607	717	298	517	75			

- Molecule 36 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	k	13	Total	C	N	O	P	0	0	0
			273	123	47	90	13			

- Molecule 37 is a protein called human initiation factor eIF1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	n	82	Total	C	N	O	S	0	0	0
			648	407	119	118	4			

Chain C:

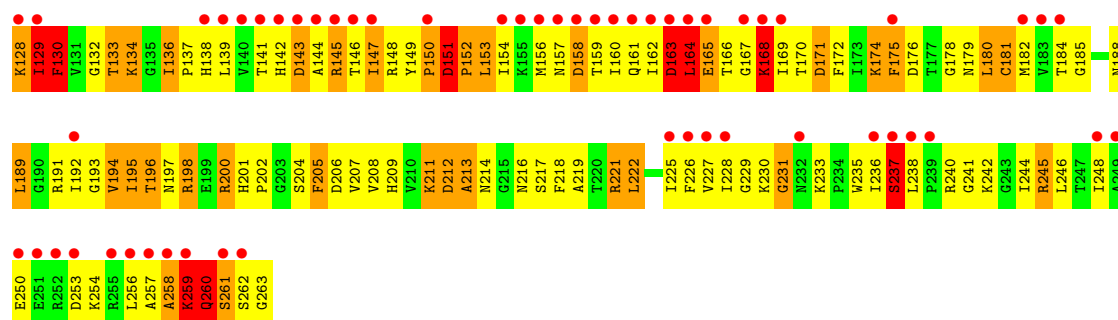
Amino Acid	Percentage
Met	14%
L63	39%
L64	46%
Val	18%
ASP	19%
ASP	
ALA	
GLY	
GLY	
PRO	
GLY	
PRO	
GLY	
GLY	
GLY	
ARG	
GLY	
GLY	
PHE	
ARG	
GLY	
PHE	
GLY	
SER	
GLY	
ILE	
ARG	
GLY	
CYS	
GLY	
G38	
D42	
K43	
E44	
L46	
P47	
V48	
T49	
K50	
L51	
G52	
R53	
L54	
V55	
K56	
D57	
M58	
K59	
L60	
K61	
R62	
L63	
E64	
E65	
T66	
V67	
L68	
F69	
S70	
L71	
P72	
I73	
K74	
E75	
S76	
E77	
I78	
L79	
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K93	
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K99	
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T101	
Q102	
A103	
G104	
Q105	
R106	
T107	
R108	
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K110	
A111	
F112	
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D117	
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G125	
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C128	
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K130	
E131	
V132	
A133	
T134	
A135	
P184	
R185	
G186	
T187	
K188	
I189	
I190	
S191	
A192	
P193	
V194	
P195	
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H197	
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A202	
G203	
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D205	
D206	
C207	
L208	
T209	
S210	
A211	
G212	
G213	
A214	
L215	
A216	
T217	
L218	
G219	
F220	
F221	
A222	
K223	
K224	
T225	
F226	
D227	
A228	
T229	
S230	
K231	
T232	
G233	
S234	
V235	
L236	
T237	
P238	
D239	
L240	
K241	
K242	
F243	
T244	
V245	
F246	
T247	
K248	
S249	
P250	
K251	
K252	
E253	
F254	
T255	
D256	
L257	
L258	
V259	
K260	
T261	
H262	
T263	
ARG	
VAL	
SER	
VAL	
GLN	
ARG	
THR	
GLN	
ALA	
PRO	
ALA	
VAL	
ALA	
THR	
THR	

Chain D:

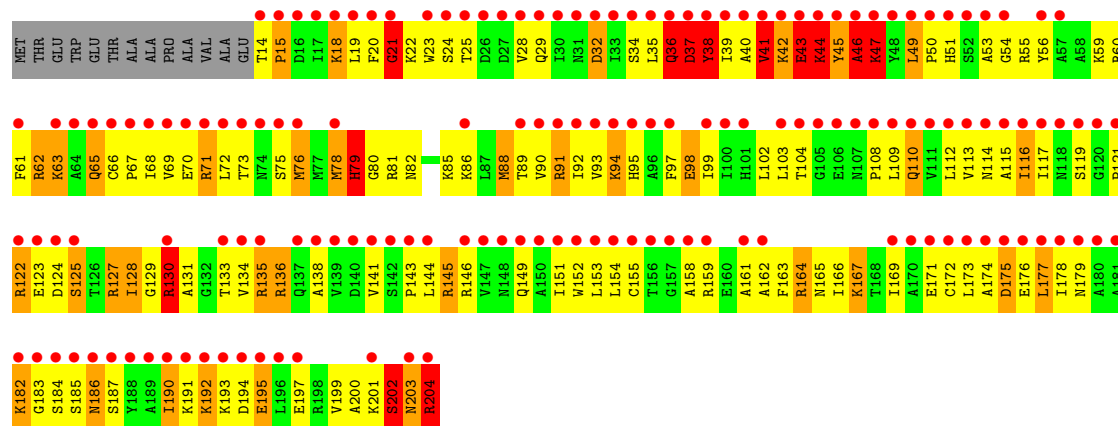
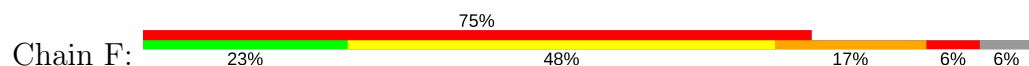
State	Category
M1	Green
B61	Green
G121	Green
G183	Green
I184	Green
K185	Green
L123	Green
L186	Green
L187	Green
L188	Green
L189	Green
L190	Green
L191	Green
L192	Green
L193	Green
L194	Green
S195	Green
G196	Green
K197	Green
I198	Green
G199	Green
P200	Green
K201	Green
K202	Green
P203	Green
L204	Green
P205	Green
D206	Green
H207	Green
S208	Green
S209	Green
I210	Green
V211	Green
E212	Green
P213	Green
K214	Green
D215	Green
E216	Green
D217	Green
L218	Green
P219	Green
T220	Green
T221	Green
P222	Green
T223	Green
S224	Green
E225	Green
Q226	Green
K227	Green
GLY	Green
GLY	Green
PRO	Green
GLU	Green
PRO	Green
PRO	Green
ALA	Green
MET	Green
PRO	Green
GLN	Green
PRO	Green
VAL	Green
THR	Green
B62	Orange
G63	Orange
R64	Orange
T65	Orange
I66	Orange
R67	Orange
E68	Orange
K69	Orange
L70	Orange
A71	Orange
V72	Orange
V73	Orange
Q74	Orange
K75	Orange
R76	Orange
F77	Orange
G78	Orange
F79	Orange
P80	Orange
E81	Orange
G82	Orange
S83	Orange
H84	Orange
E85	Orange
L86	Orange
H87	Orange
A88	Orange
E89	Orange
K90	Orange
V91	Orange
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T93	Orange
R94	Orange
G95	Orange
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C97	Orange
A98	Orange
I99	Orange
R100	Orange
A101	Orange
P102	Orange
Q101	Orange
A102	Orange
E103	Orange
S104	Orange
L105	Orange
R106	Orange
I107	Orange
K108	Orange
L109	Orange
L110	Orange
G111	Orange
G112	Orange
L113	Orange
A114	Orange
V115	Orange
R116	Orange
A117	Orange
R118	Orange
G119	Orange
V120	Orange
L121	Orange
N22	Orange
E23	Orange
F24	Orange
L25	Orange
T26	Orange
R27	Orange
E28	Orange
L29	Orange
A30	Orange
E31	Orange
D32	Orange
G33	Orange
G34	Orange
S35	Orange
G36	Orange
V37	Orange
E38	Orange
V39	Orange
R40	Orange
V41	Orange
T42	Orange
R43	Orange
R44	Orange
R45	Orange
T46	Orange
E47	Orange
L48	Orange
L49	Orange
L50	Orange
L51	Orange
A52	Orange
T53	Orange
R54	Orange
T55	Orange
Q56	Orange
N57	Orange
V58	Orange
L59	Orange
C60	Orange
B61	Yellow
G62	Yellow
R63	Yellow
T64	Yellow
I65	Yellow
R66	Yellow
E67	Yellow
K68	Yellow
L69	Yellow
A70	Yellow
V71	Yellow
V72	Yellow
Q73	Yellow
K74	Yellow
R75	Yellow
F76	Yellow
G77	Yellow
H78	Yellow
F79	Yellow
P80	Yellow
E81	Yellow
G82	Yellow
S83	Yellow
H84	Yellow
E85	Yellow
L86	Yellow
H87	Yellow
A88	Yellow
E89	Yellow
K90	Yellow
V91	Yellow
A92	Yellow
T93	Yellow
R94	Yellow
G95	Yellow
L96	Yellow
C97	Yellow
A98	Yellow
I99	Yellow
R100	Yellow
A101	Yellow
P102	Yellow
Q101	Yellow
A102	Yellow
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I107	Yellow
K108	Yellow
L109	Yellow
L110	Yellow

Chain E:

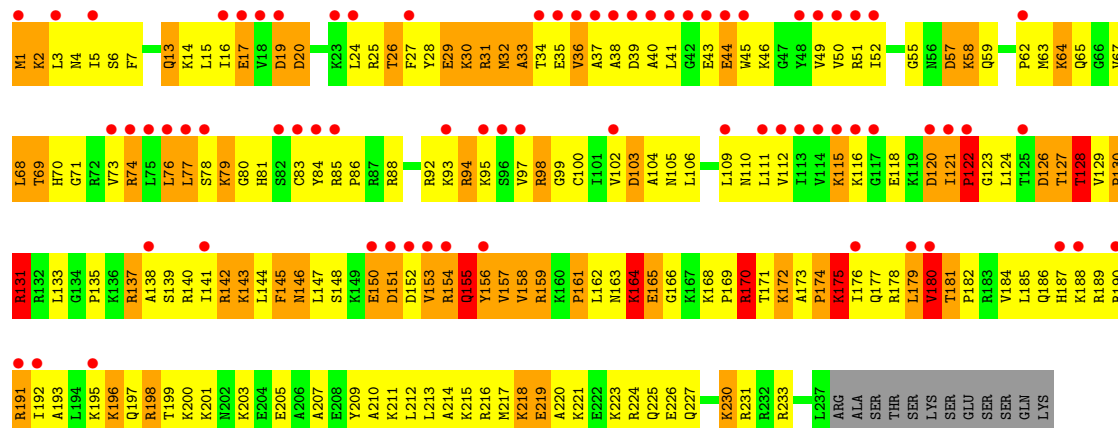
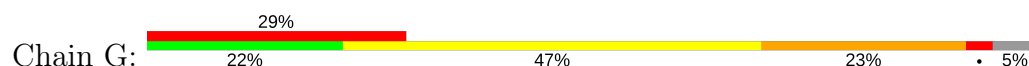
Segment	Percentage
Green	23%
Red	47%
Orange	25%



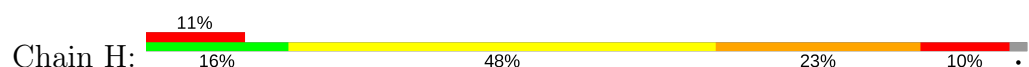
• Molecule 6: 40S Ribosomal Protein S5

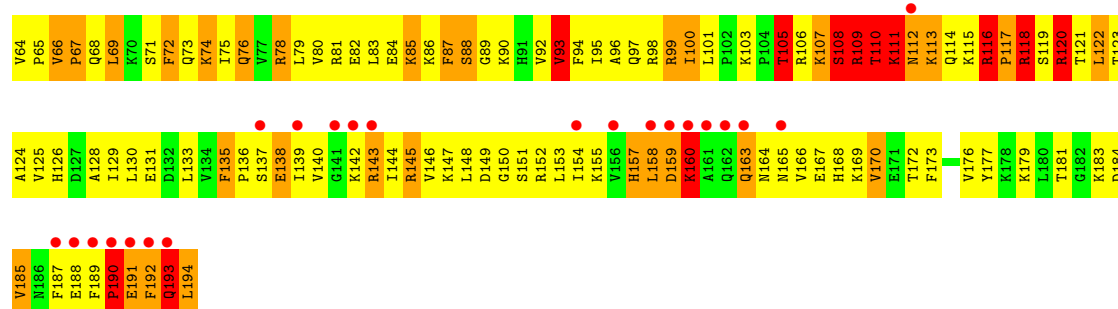


• Molecule 7: 40S Ribosomal Protein S6

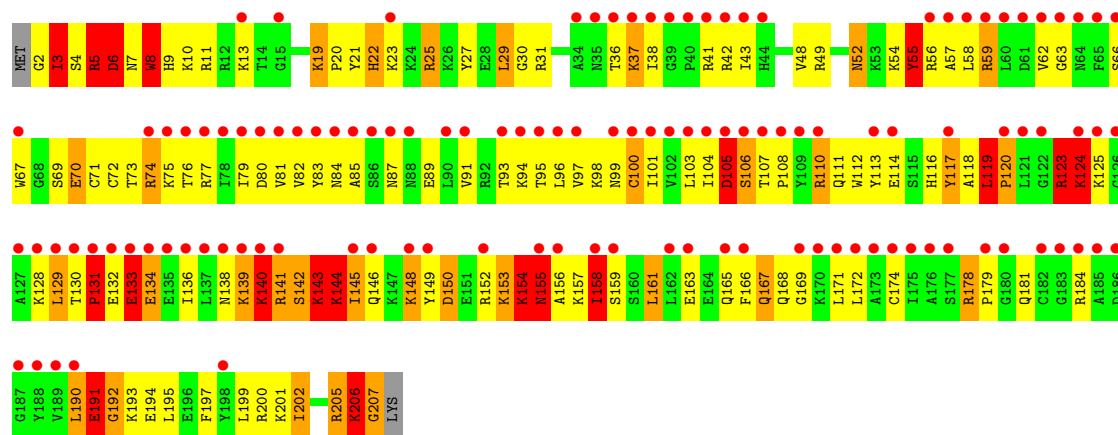


• Molecule 8: 40S Ribosomal Protein S7

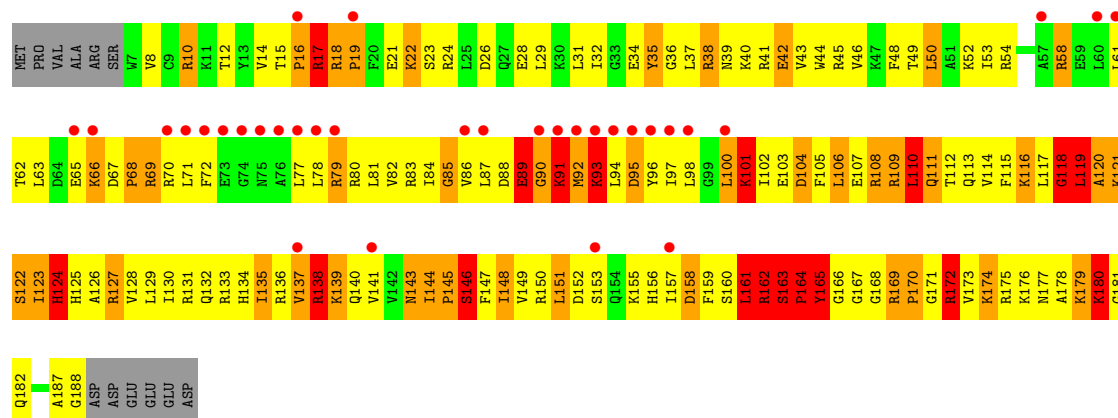
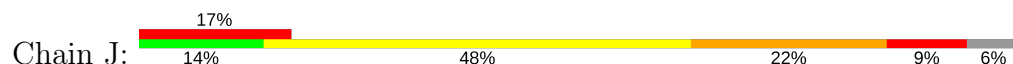




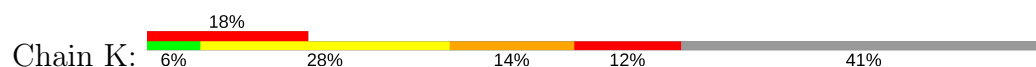
• Molecule 9: 40S Ribosomal Protein S8

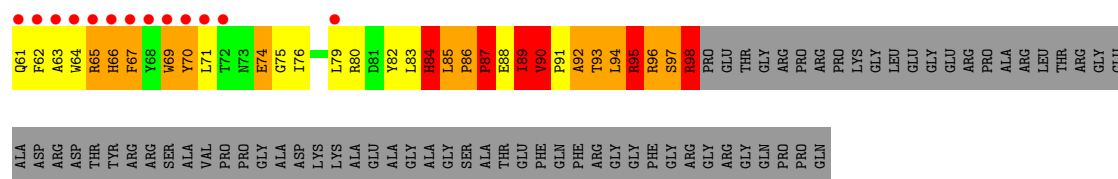


• Molecule 10: 40S Ribosomal Protein S9

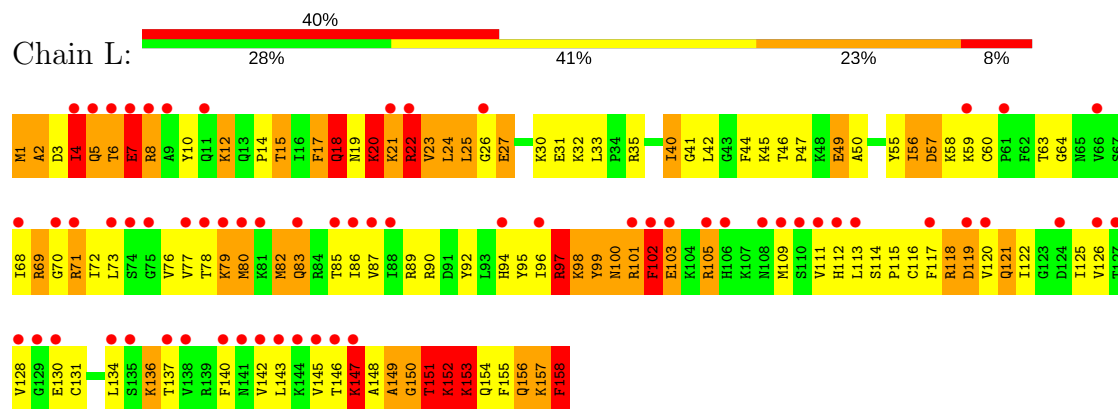


• Molecule 11: 40S Ribosomal Protein S10

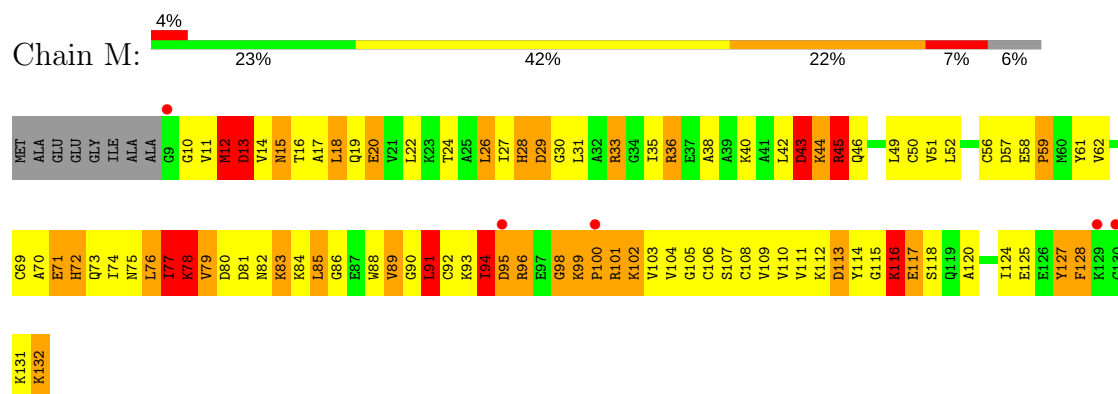




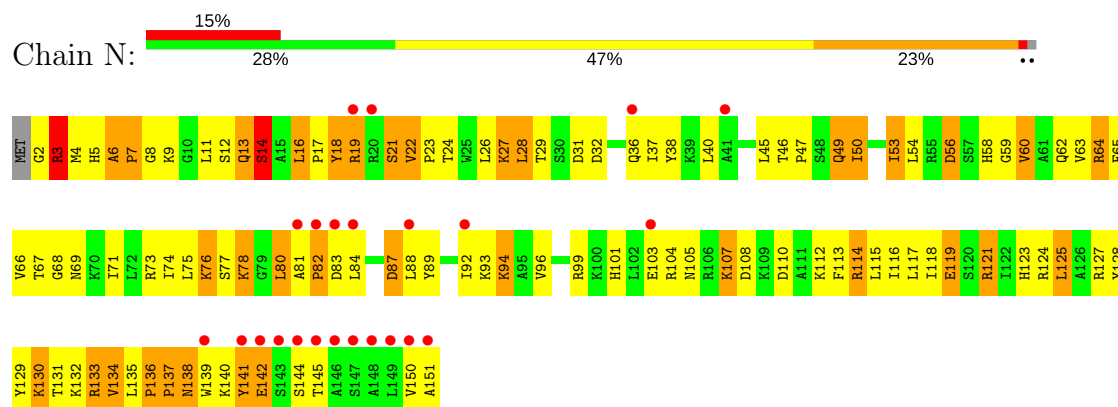
• Molecule 12: 40S Ribosomal Protein S11



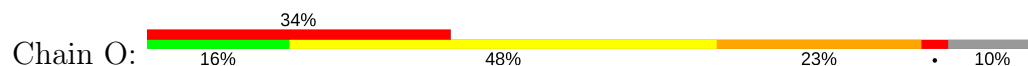
• Molecule 13: 40S Ribosomal Protein S12



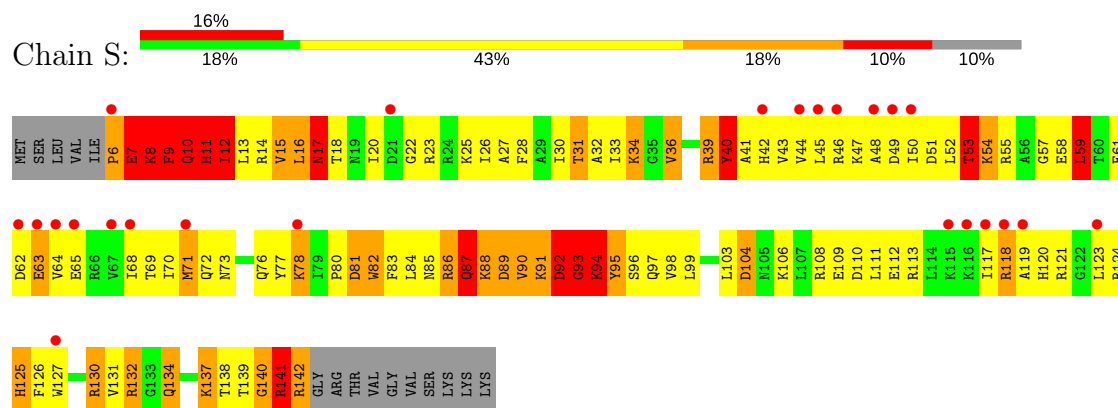
• Molecule 14: 40S Ribosomal Protein S13



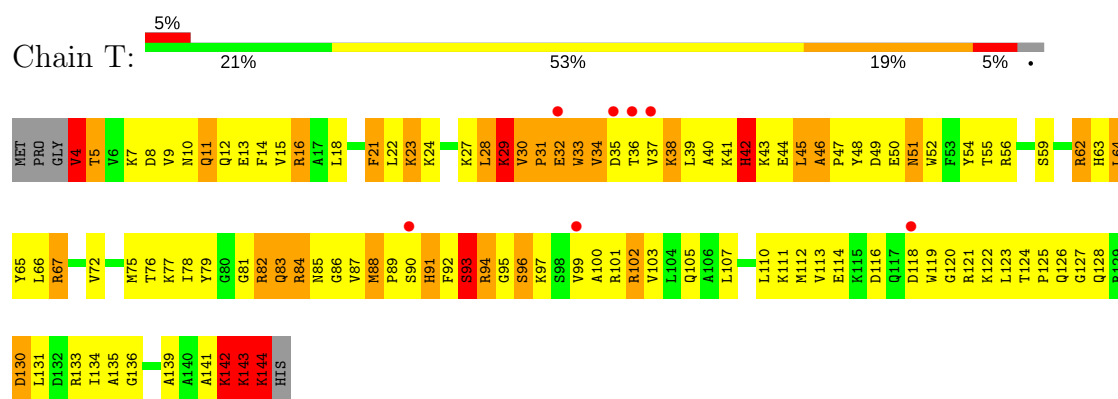
• Molecule 15: 40S Ribosomal Protein S14



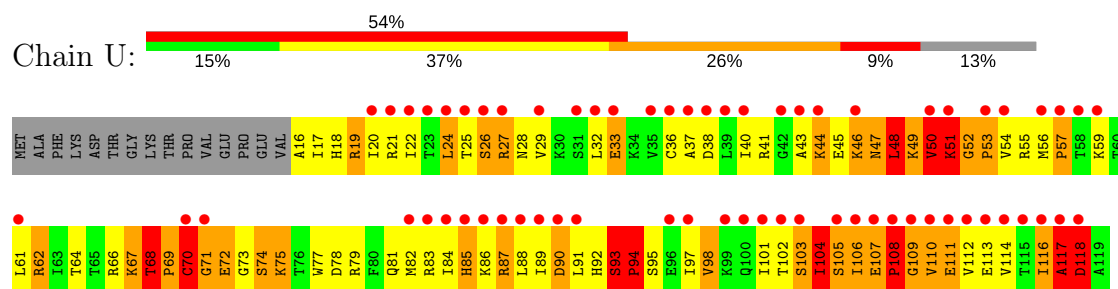
• Molecule 19: 40S Ribosomal Protein S18



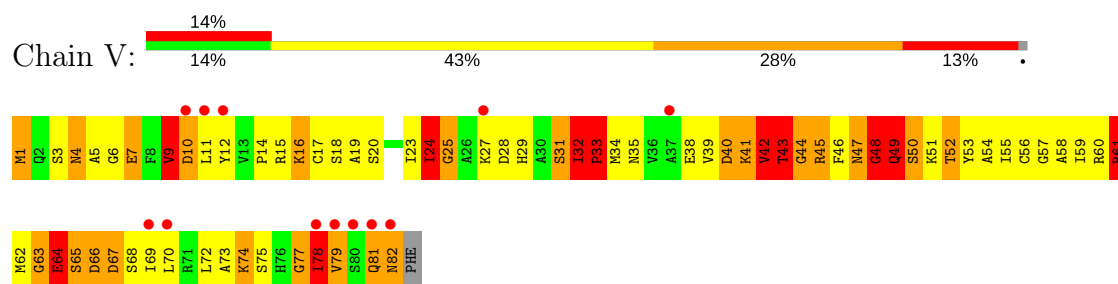
• Molecule 20: 40S Ribosomal Protein S19



• Molecule 21: 40S Ribosomal Protein S20

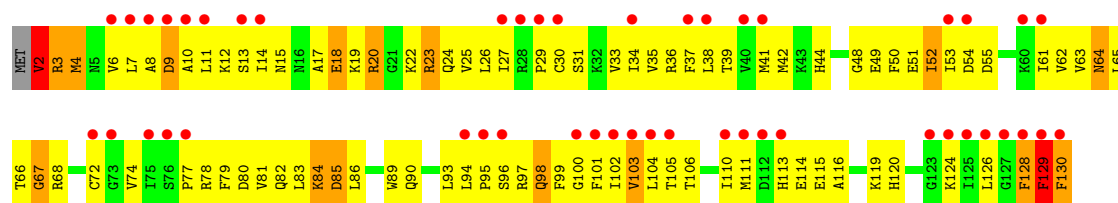


• Molecule 22: 40S Ribosomal Protein S21

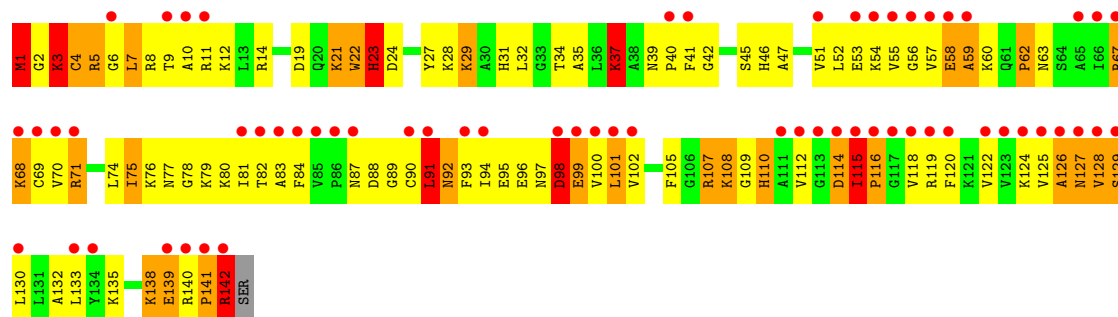


• Molecule 23: 40S Ribosomal Protein S15A

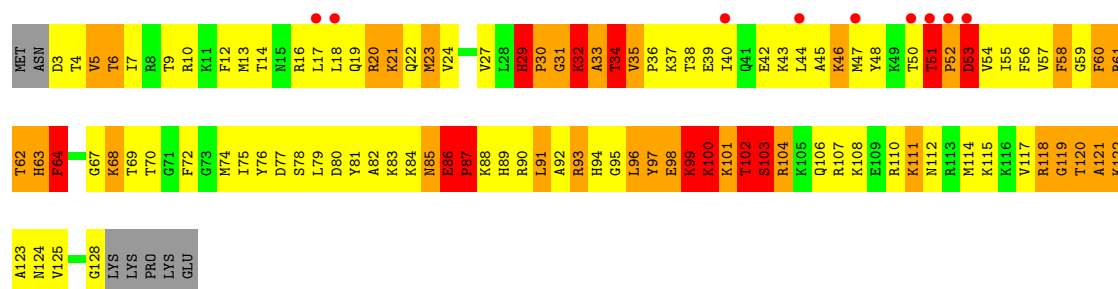
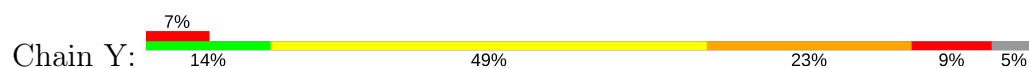




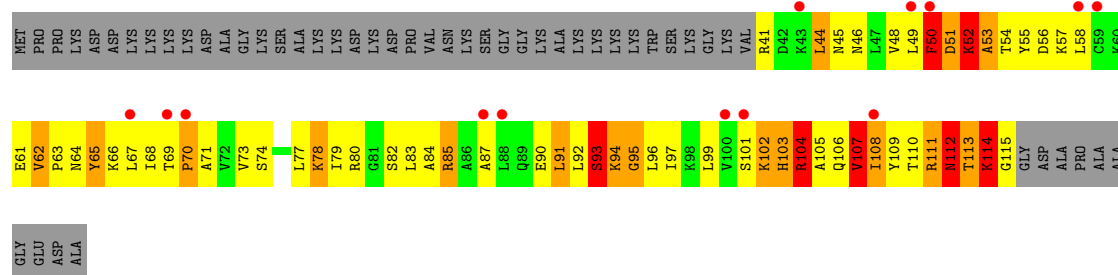
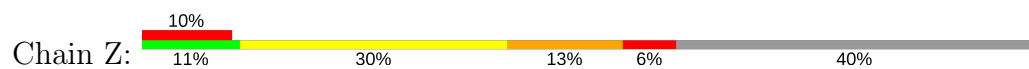
• Molecule 24: 40S Ribosomal Protein S23



• Molecule 25: 40S Ribosomal Protein S24

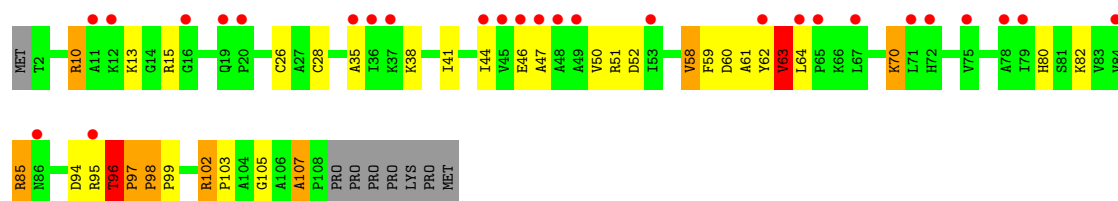


• Molecule 26: 40S Ribosomal Protein S25

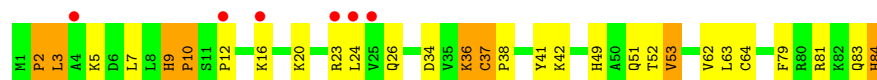


• Molecule 27: 40S Ribosomal Protein S26

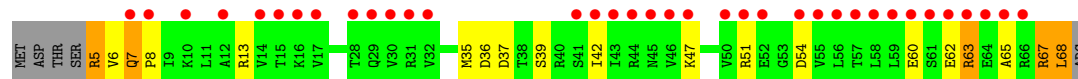




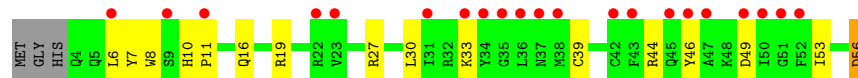
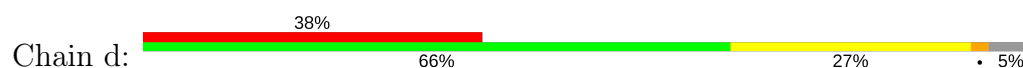
• Molecule 28: 40S Ribosomal Protein S27



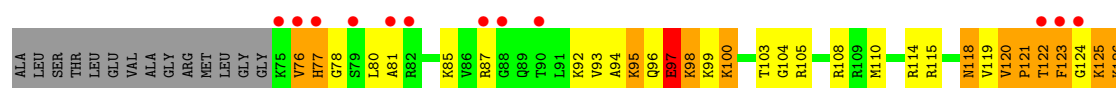
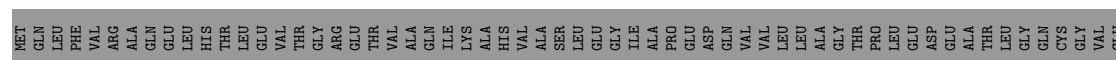
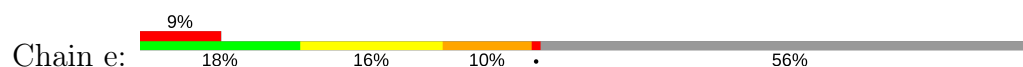
• Molecule 29: 40S Ribosomal Protein S28



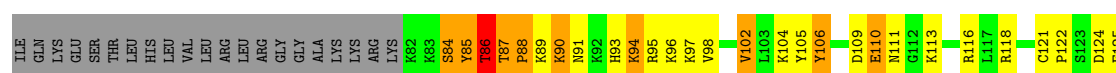
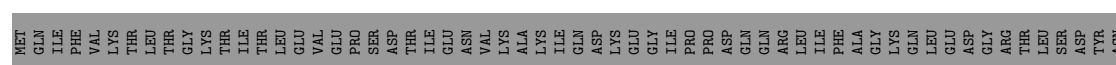
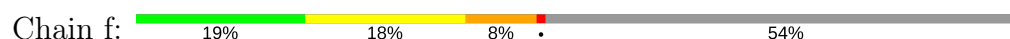
• Molecule 30: 40S Ribosomal Protein S29

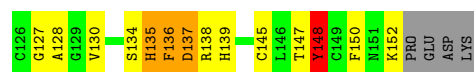


• Molecule 31: 40S Ribosomal Protein S30

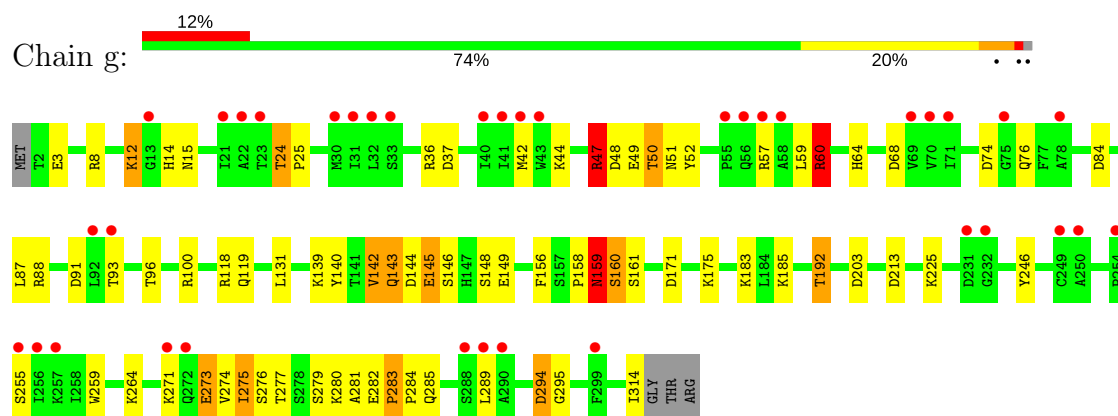


• Molecule 32: 40S Ribosomal Protein S27A

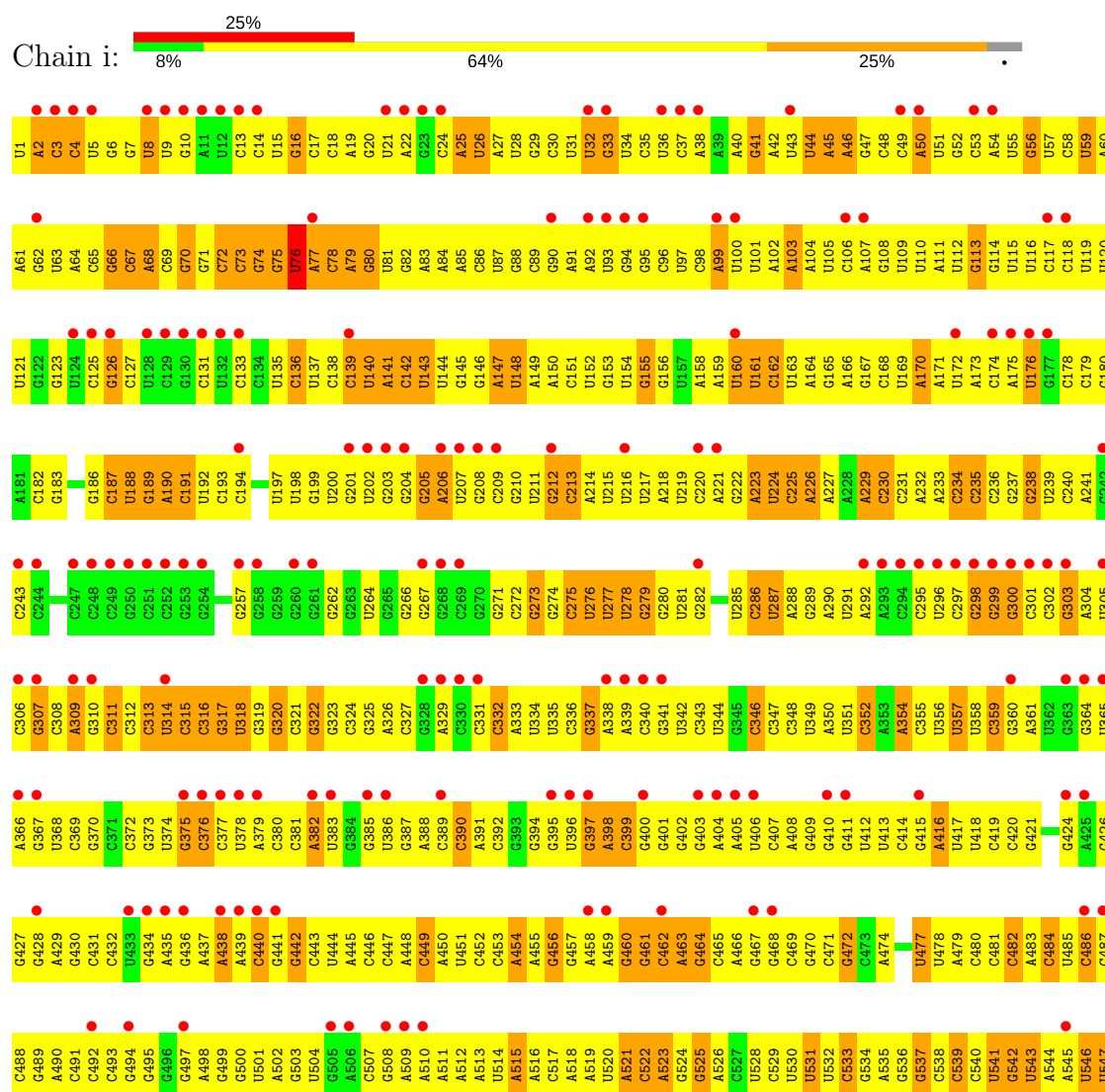




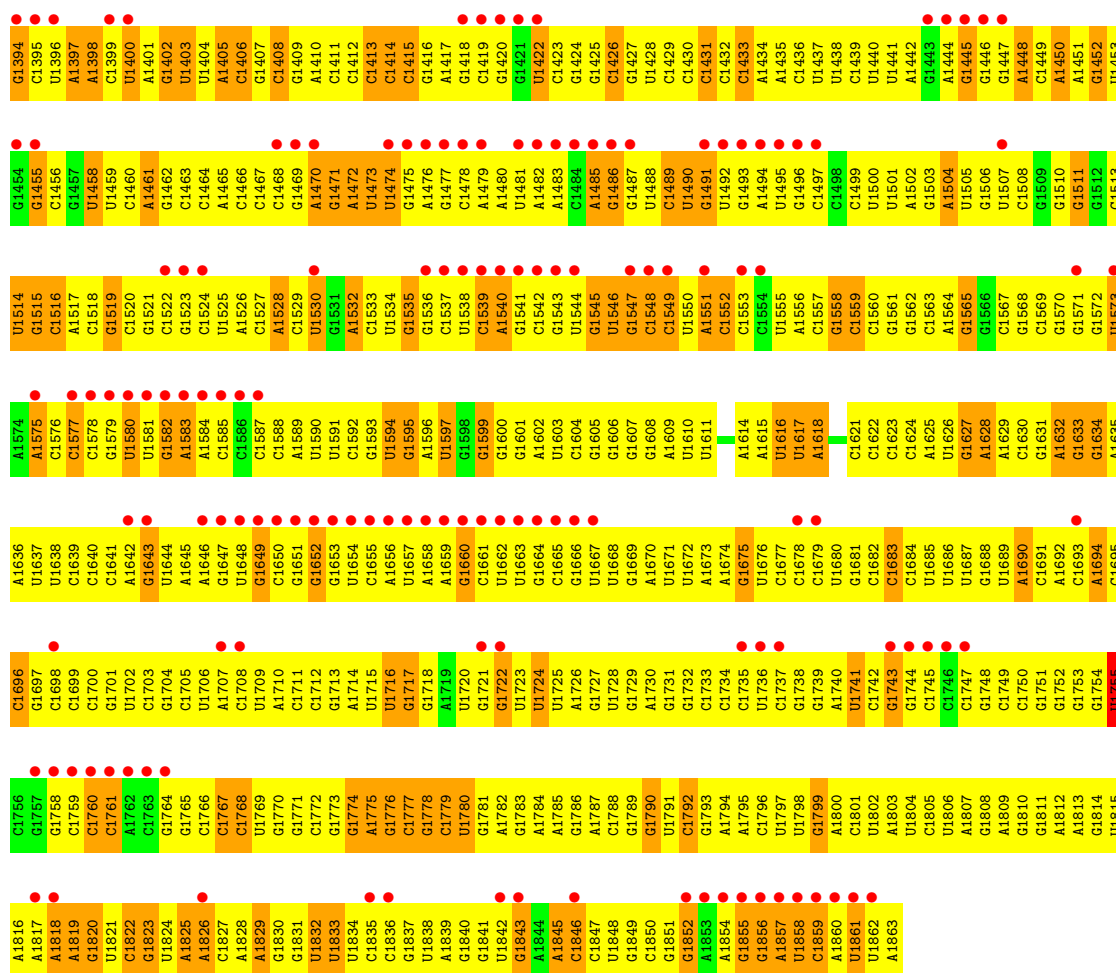
● Molecule 33: 40S Ribosomal Protein RACK1

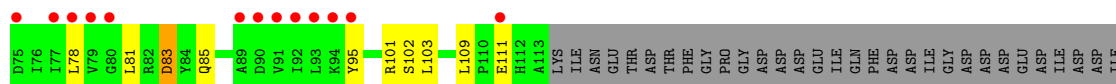


● Molecule 34: 18S Ribosomal RNA



G1334	A1274	G1214	U1152	G1092	A1032	G971	A909	C849	C788	U728	U668	C608	G548
U1335	C1275	C1215	G1153	G1093	G1033	G972	U910	A850	G789	C729	A669	A609	G549
C1337	G1276	A1216	C1094	C1095	U1034	C973	G911	G851	A790	C730	G670	G610	A550
U1338	G1277	G1217	G1095	G1096	C1035	G974	A912	C852	A791	C731	A671	C611	A551
A1339	C1278	C1218	U1097	U1097	U1036	A976	U913	U853	G792	C732	G672	G612	U552
A1340	A1279	A1219	U1098	U1098	G1037	A977	U914	A854	U793	G733	G673	G613	G553
G1341	C1159	G1220	C1098	C1098	A1038	A977	A915	G855	G794	C734	G674	C614	A554
U1342	G1160	U1221	C1099	C1099	G1039	G978	A916	G856	U795	C735	A675	G615	G555
G1343	G1161	G1222	G1100	G1100	U1040	A979	G917	A857	U796	C736	U676	G616	G556
U1344	G1162	A1223	U1041	U1041	U1041	C980	A918	A858	U797	C	U677	U617	C557
G1344	G1163	G1224	C1102	C1102	U1042	G981	G919	U859	A798	U678	U678	A618	C558
G1345	G1164	G1225	G1103	G1103	C1043	G982	G920	A860	C799	U739	U679	A619	A559
U1346	G1165	G1226	G1044	G1044	G1044	A983	G923	A861	U800	U740	G	U620	C560
G1347	A1166	C1227	A1045	C1105	A1045	C984	C924	U862	U801	C741	U	U621	U561
U1348	G1167	U1228	A1046	G1106	A1046	C985	G927	G864	A804	U742	G682	C622	U562
A1349	U1168	G1229	U1047	U1107	U1047	A986	C927	A865	A805	U743	G683	C623	U563
G1350	A1169	U1230	A1048	U1108	A1048	G987	G928	A866	A806	C744	A684	A624	A564
C1351	U1170	G1231	U1049	U1109	C1049	A988	G929	U867	A807	C	G685	G625	A565
G1352	G1171	C1232	G1050	U1110	G1050	G989	G930	A868	A808	C	G686	C626	A566
A1353	G1172	G1233	A1051	U1111	A1051	C990	G931	U869	A809	C	G687	U627	U567
U1354	U1173	U1234	U1052	C1112	U1052	A994	G932	A870	A810	C	U688	C628	C568
U1355	A1295	U1235	C1113	C1113	C1053	G995	G933	A871	U811	C	G689	C629	C569
U1356	G1175	A1236	U1114	C1114	A1054	C996	G934	C872	A812	C	C690	A630	U570
G1357	A1176	U1237	U1115	U1115	C1055	C997	U935	C873	G813	C	G691	A631	U571
A1358	A1177	U1238	U1056	U1116	A1056	C998	U936	C874	A814	C	U692	U632	U572
C1359	A1178	U1239	U1057	G1117	U1057	A997	U937	C875	G815	C	A693	A633	A573
U1360	C1181	G1240	A1058	A1118	A1058	U998	C937	C876	U816	C	G694	G634	A574
G1361	U1300	U1241	C1059	C1119	C1059	U999	G938	C877	U817	C	G695	C635	C575
G1362	C1301	G1242	U1060	C1120	U1060	U1000	U939	U878	U818	C	G696	G636	G576
U1363	U1302	C1243	G1183	C1121	G1061	G1001	A940	U879	U819	C	G697	U637	A577
A1364	U1303	U1244	A1184	C1122	U1062	C1002	U941	C880	C820	C	G698	A638	G578
A1365	C1305	C1245	A1185	C1123	C1063	C1003	U942	U881	A821	U	G699	U639	G579
A1366	U1186	A1246	G1186	C1124	G1064	A1004	G943	U882	A822	G	G	A640	A580
U1367	C1307	U1247	G1187	G1125	U1065	A1005	G944	U883	A823	C	U	U641	U581
U1368	U1188	C1248	U1188	G1126	A1066	G1006	G945	U884	C824	C	U	U642	C582
C1369	U1189	U1249	G1127	G1127	G1067	A1007	C946	U885	C825	C	C	A643	C583
C1370	U1310	G1250	U1068	C1128	U1068	A1008	C947	U886	A826	C	G	A644	A584
G1371	A1190	G1251	U1069	A1129	U1069	U1009	G948	U887	G827	U	C	A645	U585
A1372	A1191	G1252	C1070	G1130	C1070	G1010	C949	U888	G828	A	C	G646	U586
U1373	G1192	G1253	C1071	C1131	U1011	U1011	U950	U889	C829	C	C	U647	G587
A1374	G1193	A1254	U1012	U1132	U1012	A951	G952	U890	C830	C	C	U648	G588
A1375	U1194	C1255	A1073	U1133	A1073	U1013	G953	U891	C831	C	C	G649	A589
C1376	A1195	A1256	C1074	C1134	U1074	U1014	A954	U892	G832	U	A	C650	G590
G1377	U1197	C1257	C1075	C1135	C1075	C1015	G955	U893	A833	G	G	U651	G591
A1378	U1198	C1258	A1076	G1136	A1076	A1016	G956	U894	A834	A	G	G652	G592
A1379	G1199	U1259	U1077	G1137	U1077	U1017	U956	U895	C835	G	C	C653	C593
C1380	A1200	C1260	A1078	G1138	A1078	U1018	U957	U896	C836	U	C	A654	A594
G1381	C1201	C1261	A1079	A1139	A1079	A1019	A958	G897	C837	G	A	G655	A595
A1382	G1202	C1262	A1080	A1140	A1080	A1020	A959	G898	C838	U	C	U656	G596
G1383	G1203	C1263	C1081	A1141	C1081	U1021	A960	U899	C839	C	C	U657	U597
A1384	A1204	C1264	G1082	C1142	G1082	C1022	U961	A900	U840	C	C	A658	C598
C1385	U1205	G1265	A1083	C1143	A1083	A1023	U962	A901	U841	C	C	A659	U599
U1386	G1206	G1266	U1084	A1144	U1084	A1024	C963	C901	G842	G	C	U660	G600
C1387	G1207	C1267	G1085	A1145	G1085	G1025	U964	U902	G843	C	C	A661	G601
U1388	G1208	A1146	C1086	A1146	C1086	A1026	U965	G903	U844	G	C	U662	U602
G1389	C1209	G1268	C1087	U1147	C1087	A1027	G967	A904	U845	G	C	G723	G603
G1390	A1210	U1270	G1088	C1028	C1088	C1028	G967	G905	A846	G	C	G724	G604
C1391	C1211	G1271	A1089	U1148	A1089	U1029	A968	G906	C847	G	C	G725	C605
A1392	C1212	A1272	U1090	C1149	U1090	A1030	C969	C907	C847	C	C	C726	C606
U1393	C1333	C1273	U1091	U1151	U1091	A1031	C970	C908	G848	C	C	G667	G607





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	297.75Å 297.75Å 485.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.53 – 7.03 77.53 – 7.03	Depositor EDS
% Data completeness (in resolution range)	98.3 (77.53-7.03) 98.7 (77.53-7.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 6.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.345 , 0.359 0.332 , 0.339	Depositor DCC
R_{free} test set	1942 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	566.4	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 125.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	79048	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	2/1679 (0.1%)	1.06	17/2283 (0.7%)
2	B	0.79	7/1769 (0.4%)	1.08	22/2367 (0.9%)
3	C	0.97	7/1778 (0.4%)	1.19	18/2399 (0.8%)
4	D	1.03	6/1792 (0.3%)	1.30	22/2412 (0.9%)
5	E	0.76	5/2125 (0.2%)	0.98	23/2856 (0.8%)
6	F	0.99	5/1531 (0.3%)	1.21	17/2059 (0.8%)
7	G	0.97	15/1946 (0.8%)	1.23	25/2590 (1.0%)
8	H	1.09	7/1553 (0.5%)	2.19	29/2079 (1.4%)
9	I	1.11	7/1708 (0.4%)	1.51	33/2278 (1.4%)
10	J	1.27	19/1522 (1.2%)	1.51	42/2031 (2.1%)
11	K	1.21	6/851 (0.7%)	1.78	31/1147 (2.7%)
12	L	1.10	6/1319 (0.5%)	1.40	17/1761 (1.0%)
13	M	1.00	3/960 (0.3%)	1.23	7/1287 (0.5%)
14	N	0.83	4/1232 (0.3%)	1.01	12/1656 (0.7%)
15	O	0.61	0/1029	1.05	12/1380 (0.9%)
16	P	0.75	1/1079 (0.1%)	1.43	32/1437 (2.2%)
17	Q	0.71	3/1142 (0.3%)	1.11	15/1528 (1.0%)
18	R	1.23	10/1031 (1.0%)	1.64	30/1383 (2.2%)
19	S	1.21	10/1157 (0.9%)	1.61	36/1548 (2.3%)
20	T	0.95	3/1132 (0.3%)	1.26	13/1517 (0.9%)
21	U	0.96	1/832 (0.1%)	1.59	29/1117 (2.6%)
22	V	0.75	1/626 (0.2%)	1.39	15/839 (1.8%)
23	W	0.85	4/1051 (0.4%)	0.86	9/1406 (0.6%)
24	X	1.00	8/1124 (0.7%)	1.24	21/1500 (1.4%)
25	Y	0.93	3/1038 (0.3%)	1.42	21/1380 (1.5%)
26	Z	1.04	5/604 (0.8%)	1.35	17/810 (2.1%)
27	a	0.89	4/860 (0.5%)	1.60	21/1156 (1.8%)
28	b	1.02	2/673 (0.3%)	1.36	12/902 (1.3%)
29	c	0.80	1/508 (0.2%)	1.18	8/680 (1.2%)
30	d	0.90	2/455 (0.4%)	0.79	3/603 (0.5%)
31	e	1.47	5/478 (1.0%)	1.43	11/628 (1.8%)
32	f	1.10	4/593 (0.7%)	1.49	16/786 (2.0%)
33	g	0.91	1/2493 (0.0%)	1.29	27/3394 (0.8%)
34	i	2.41	1848/41879 (4.4%)	2.21	2565/65157 (3.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
35	j	0.67	5/1798 (0.3%)	0.82	0/2802
36	k	1.64	1/304 (0.3%)	1.35	3/470 (0.6%)
37	n	0.40	0/657	0.38	0/881
All	All	1.83	2021/84308 (2.4%)	1.84	3231/122509 (2.6%)

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	A	0	11
2	B	0	4
3	C	1	5
4	D	0	5
5	E	1	2
6	F	0	3
7	G	0	1
8	H	0	10
9	I	0	8
10	J	1	11
11	K	0	11
12	L	0	7
13	M	0	1
14	N	0	4
15	O	0	1
16	P	0	10
17	Q	0	4
18	R	1	5
19	S	1	10
20	T	1	6
21	U	0	8
22	V	0	9
23	W	0	2
24	X	0	4
25	Y	1	6
26	Z	0	6
27	a	0	2
28	b	0	3
31	e	0	5
32	f	0	6
33	g	0	13

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	i	6	0
All	All	13	183

The worst 5 of 2021 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	k	22	C	C1'-N1	28.08	1.90	1.48
34	i	1322	U	C2'-C1'	-25.56	1.25	1.53
34	i	66	G	C2'-C1'	-24.65	1.26	1.53
34	i	652	G	C2'-C1'	-23.81	1.27	1.53
34	i	858	A	C2'-C1'	-23.76	1.27	1.53

The worst 5 of 3231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	109	ARG	NE-CZ-NH2	-53.45	93.58	120.30
8	H	109	ARG	NE-CZ-NH1	42.58	141.59	120.30
34	i	1774	G	P-O3'-C3'	38.31	165.68	119.70
34	i	1114	C	O4'-C1'-N1	35.28	136.42	108.20
34	i	582	C	O4'-C1'-N1	32.53	134.22	108.20

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	157	ASN	CA
5	E	171	ASP	CA
10	J	138	ARG	CA
18	R	3	ARG	CA
19	S	92	ASP	CA

5 of 183 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ALA	Mainchain
1	A	23	THR	Mainchain
1	A	4	ALA	Peptide
1	A	63	ARG	Sidechain
1	A	97	THR	Mainchain

5.2 Too-close contacts

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	1642	0	1638	603	0
2	B	1741	0	1808	523	0
3	C	1742	0	1829	582	0
4	D	1764	0	1855	595	0
5	E	2083	0	2189	523	0
6	F	1509	0	1556	476	0
7	G	1923	0	2086	499	3
8	H	1530	0	1624	476	0
9	I	1679	0	1762	431	3
10	J	1498	0	1598	537	0
11	K	827	0	853	351	18
12	L	1296	0	1370	397	0
13	M	950	0	969	245	0
14	N	1208	0	1294	261	0
15	O	1016	0	1037	293	0
16	P	1060	0	1120	483	0
17	Q	1124	0	1189	439	0
18	R	1019	0	1067	349	0
19	S	1139	0	1188	427	1
20	T	1112	0	1149	393	0
21	U	822	0	886	208	0
22	V	619	0	620	278	0
23	W	1034	0	1079	262	0
24	X	1106	0	1177	310	0
25	Y	1021	0	1083	490	0
26	Z	598	0	652	210	0
27	a	844	0	895	0	0
28	b	659	0	680	0	0
29	c	506	0	534	0	0
30	d	445	0	441	0	0
31	e	473	0	519	0	31
32	f	581	0	598	0	0
33	g	2436	0	2388	0	0
34	i	37514	0	18808	0	78
35	j	1607	0	811	0	0
36	k	273	0	139	0	0
37	n	648	0	642	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	79048	0	61133	9794	81

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 94.

The worst 5 of 9794 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)
3:C:197:LYS:HA	3:C:200:LEU:CD2	1.22	1.68
9:I:141:ARG:CB	9:I:144:LYS:HB2	1.24	1.68
17:Q:135:PRO:HD3	17:Q:141:TYR:CE1	1.15	1.66
11:K:16:PHE:CE2	11:K:79:LEU:HB2	1.24	1.65
16:P:41:GLN:CG	16:P:84:ILE:HG21	1.18	1.64

The worst 5 of 81 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)
31:e:123:PHE:CD1	34:i:1759:C:C4'[3_564]	0.62	1.58
31:e:123:PHE:CE1	34:i:1759:C:C5'[3_564]	0.70	1.50
34:i:531:U:O2'	34:i:1767:C:O4'[3_564]	0.72	1.48
31:e:125:LYS:CE	34:i:1761:C:OP1[3_564]	0.73	1.47
11:K:97:SER:O	34:i:76:U:OP1[3_564]	0.95	1.25

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	206/295 (70%)	156 (76%)	23 (11%)	27 (13%)	0 6
2	B	213/264 (81%)	174 (82%)	24 (11%)	15 (7%)	1 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	224/278 (81%)	199 (89%)	14 (6%)	11 (5%)	2	27
4	D	225/243 (93%)	180 (80%)	23 (10%)	22 (10%)	1	12
5	E	261/263 (99%)	210 (80%)	27 (10%)	24 (9%)	1	14
6	F	189/204 (93%)	162 (86%)	15 (8%)	12 (6%)	1	22
7	G	235/249 (94%)	201 (86%)	19 (8%)	15 (6%)	1	22
8	H	188/194 (97%)	146 (78%)	11 (6%)	31 (16%)	0	4
9	I	204/208 (98%)	169 (83%)	13 (6%)	22 (11%)	0	10
10	J	180/194 (93%)	138 (77%)	18 (10%)	24 (13%)	0	6
11	K	96/165 (58%)	67 (70%)	11 (12%)	18 (19%)	0	3
12	L	156/158 (99%)	132 (85%)	10 (6%)	14 (9%)	1	15
13	M	122/132 (92%)	85 (70%)	16 (13%)	21 (17%)	0	4
14	N	148/151 (98%)	123 (83%)	19 (13%)	6 (4%)	3	30
15	O	134/151 (89%)	101 (75%)	14 (10%)	19 (14%)	0	5
16	P	125/145 (86%)	92 (74%)	16 (13%)	17 (14%)	0	6
17	Q	139/146 (95%)	110 (79%)	19 (14%)	10 (7%)	1	19
18	R	124/135 (92%)	97 (78%)	13 (10%)	14 (11%)	0	8
19	S	135/152 (89%)	106 (78%)	20 (15%)	9 (7%)	1	21
20	T	139/145 (96%)	119 (86%)	10 (7%)	10 (7%)	1	19
21	U	102/119 (86%)	76 (74%)	10 (10%)	16 (16%)	0	4
22	V	80/83 (96%)	55 (69%)	11 (14%)	14 (18%)	0	3
23	W	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	11	51
24	X	140/143 (98%)	121 (86%)	11 (8%)	8 (6%)	2	24
25	Y	124/133 (93%)	91 (73%)	15 (12%)	18 (14%)	0	5
26	Z	73/125 (58%)	52 (71%)	12 (16%)	9 (12%)	0	7
27	a	105/115 (91%)	72 (69%)	14 (13%)	19 (18%)	0	3
28	b	82/84 (98%)	57 (70%)	14 (17%)	11 (13%)	0	6
29	c	62/69 (90%)	44 (71%)	13 (21%)	5 (8%)	1	16
30	d	51/56 (91%)	46 (90%)	3 (6%)	2 (4%)	3	31
31	e	57/133 (43%)	37 (65%)	7 (12%)	13 (23%)	0	2
32	f	69/156 (44%)	38 (55%)	13 (19%)	18 (26%)	0	1
33	g	311/317 (98%)	271 (87%)	23 (7%)	17 (6%)	2	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	n	80/144 (56%)	61 (76%)	15 (19%)	4 (5%)	2	27
All	All	4906/5679 (86%)	3899 (80%)	510 (10%)	497 (10%)	1	12

5 of 497 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	31	ASP
1	A	45	GLY
1	A	103	PHE
1	A	164	ASN

5.3.2 Protein sidechains ⓘ

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	174/244 (71%)	139 (80%)	35 (20%)	1	9
2	B	196/231 (85%)	155 (79%)	41 (21%)	1	8
3	C	187/215 (87%)	147 (79%)	40 (21%)	1	8
4	D	190/202 (94%)	144 (76%)	46 (24%)	1	5
5	E	225/225 (100%)	173 (77%)	52 (23%)	1	6
6	F	161/170 (95%)	116 (72%)	45 (28%)	0	3
7	G	207/218 (95%)	157 (76%)	50 (24%)	1	5
8	H	170/174 (98%)	124 (73%)	46 (27%)	0	4
9	I	177/179 (99%)	142 (80%)	35 (20%)	1	10
10	J	157/168 (94%)	128 (82%)	29 (18%)	2	12
11	K	89/136 (65%)	61 (68%)	28 (32%)	0	2
12	L	142/142 (100%)	105 (74%)	37 (26%)	0	4
13	M	101/108 (94%)	78 (77%)	23 (23%)	1	6
14	N	130/131 (99%)	103 (79%)	27 (21%)	1	8
15	O	106/119 (89%)	87 (82%)	19 (18%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	116/130 (89%)	84 (72%)	32 (28%)	0	3
17	Q	117/121 (97%)	89 (76%)	28 (24%)	1	5
18	R	114/121 (94%)	90 (79%)	24 (21%)	1	8
19	S	119/132 (90%)	95 (80%)	24 (20%)	1	9
20	T	113/116 (97%)	87 (77%)	26 (23%)	1	6
21	U	94/107 (88%)	74 (79%)	20 (21%)	1	8
22	V	67/68 (98%)	50 (75%)	17 (25%)	0	5
23	W	112/113 (99%)	98 (88%)	14 (12%)	5	26
24	X	114/115 (99%)	91 (80%)	23 (20%)	1	9
25	Y	108/115 (94%)	85 (79%)	23 (21%)	1	8
26	Z	66/103 (64%)	53 (80%)	13 (20%)	1	10
27	a	91/99 (92%)	76 (84%)	15 (16%)	2	16
28	b	76/76 (100%)	63 (83%)	13 (17%)	2	15
29	c	57/62 (92%)	46 (81%)	11 (19%)	1	10
30	d	47/49 (96%)	35 (74%)	12 (26%)	0	5
31	e	49/106 (46%)	26 (53%)	23 (47%)	0	0
32	f	64/140 (46%)	43 (67%)	21 (33%)	0	2
33	g	272/275 (99%)	224 (82%)	48 (18%)	2	14
37	n	66/123 (54%)	48 (73%)	18 (27%)	0	4
All	All	4274/4833 (88%)	3316 (78%)	958 (22%)	1	7

5 of 958 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	53	LYS
15	O	28	PHE
32	f	118	ARG
11	K	98	ARG
13	M	18	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	19	ASN

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Mol	Chain	Res	Type
16	P	41	GLN
33	g	20	GLN
12	L	121	GLN
13	M	82	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	i	1720/1863 (92%)	496 (28%)	0
35	j	74/75 (98%)	17 (22%)	0
36	k	12/24 (50%)	3 (25%)	0
All	All	1806/1962 (92%)	516 (28%)	0

5 of 516 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	i	2	A
34	i	3	C
34	i	4	C
34	i	8	U
34	i	16	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	208/295 (70%)	0.76	40 (19%) 1 8	188, 273, 325, 347	0
2	B	215/264 (81%)	1.43	74 (34%) 0 6	140, 249, 309, 321	0
3	C	226/278 (81%)	2.77	109 (48%) 0 4	76, 163, 267, 285	0
4	D	227/243 (93%)	4.76	165 (72%) 0 3	110, 175, 253, 280	0
5	E	263/263 (100%)	2.65	133 (50%) 0 4	38, 138, 196, 225	0
6	F	191/204 (93%)	5.05	154 (80%) 0 2	133, 175, 212, 224	0
7	G	237/249 (95%)	1.41	72 (30%) 0 6	68, 198, 289, 311	0
8	H	190/194 (97%)	0.09	22 (11%) 5 13	129, 278, 329, 340	0
9	I	206/208 (99%)	3.71	118 (57%) 0 3	17, 164, 268, 289	0
10	J	182/194 (93%)	0.70	33 (18%) 1 9	73, 158, 221, 259	0
11	K	98/165 (59%)	1.83	29 (29%) 1 6	167, 238, 289, 308	0
12	L	158/158 (100%)	1.68	63 (39%) 0 5	22, 90, 224, 255	0
13	M	124/132 (93%)	-0.17	5 (4%) 39 38	280, 347, 384, 417	0
14	N	150/151 (99%)	0.73	23 (15%) 2 10	46, 118, 251, 261	0
15	O	136/151 (90%)	2.01	52 (38%) 0 5	45, 205, 320, 353	0
16	P	127/145 (87%)	3.25	70 (55%) 0 4	163, 254, 297, 310	0
17	Q	141/146 (96%)	1.88	49 (34%) 0 5	108, 200, 225, 231	0
18	R	126/135 (93%)	0.07	14 (11%) 6 13	130, 194, 302, 306	0
19	S	137/152 (90%)	0.93	24 (17%) 2 9	151, 218, 239, 249	0
20	T	141/145 (97%)	0.10	7 (4%) 30 32	161, 214, 230, 234	0
21	U	104/119 (87%)	3.98	64 (61%) 0 3	116, 213, 258, 269	0
22	V	82/83 (98%)	0.65	12 (14%) 3 10	175, 237, 316, 328	0
23	W	129/130 (99%)	1.71	47 (36%) 0 5	75, 141, 196, 216	0
24	X	142/143 (99%)	2.42	62 (43%) 0 5	22, 54, 84, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	126/133 (94%)	0.27	9 (7%) 17 21	85, 153, 198, 218	0
26	Z	75/125 (60%)	0.82	13 (17%) 2 9	197, 207, 217, 225	0
27	a	107/115 (93%)	1.56	27 (25%) 1 7	55, 111, 285, 317	0
28	b	84/84 (100%)	0.05	6 (7%) 17 21	156, 236, 276, 286	0
29	c	64/69 (92%)	2.45	36 (56%) 0 4	125, 173, 216, 221	0
30	d	53/56 (94%)	1.75	21 (39%) 0 5	136, 159, 235, 256	0
31	e	59/133 (44%)	0.72	12 (20%) 1 8	63, 136, 177, 192	0
32	f	71/156 (45%)	-0.55	0 100 100	145, 320, 392, 408	0
33	g	313/317 (98%)	0.38	37 (11%) 5 13	190, 248, 277, 291	0
34	i	1797/1863 (96%)	1.40	474 (26%) 1 7	13, 142, 348, 527	0
35	j	75/75 (100%)	1.25	21 (28%) 1 7	308, 379, 421, 436	0
36	k	13/24 (54%)	3.59	12 (92%) 0 1	186, 317, 324, 325	0
37	n	82/144 (56%)	1.70	31 (37%) 0 5	212, 216, 222, 224	0
All	All	6859/7641 (89%)	1.63	2140 (31%) 0 6	13, 190, 328, 527	0

The worst 5 of 2140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	i	697	G	34.6
34	i	698	G	32.3
4	D	95	GLY	23.9
34	i	695	C	22.6
34	i	696	G	22.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.