



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:46 PM GMT

PDB ID : 4V8O  
Title : Crystal structure of the hybrid state of ribosome in complex with the guanosine triphosphatase release factor 3  
Authors : Jin, H.; Kelley, A.C.; Ramakrishnan, V.  
Deposited on : 2011-07-26  
Resolution : 3.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



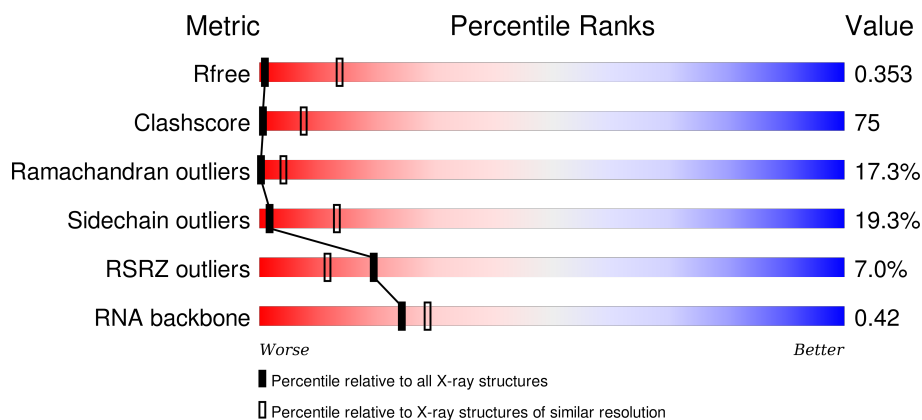
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

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  $\geq 3$ , 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	AA	1522	<div> <div>2%</div> <div>11% 64% 20% . .</div> </div>
2	AB	256	<div> <div>%</div> <div>9% 46% 31% 5% 8%</div> </div>
3	AC	239	<div> <div>%</div> <div>18% 46% 21% . 13%</div> </div>
4	AD	209	<div> <div>6%</div> <div>20% 60% 19%</div> </div>

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Mol	Chain	Length	Quality of chain
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	135	
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	77	
23	AX	9	
24	AY	529	
25	B0	85	
26	B1	98	
27	B2	72	
28	B3	60	
29	B4	71	

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Mol	Chain	Length	Quality of chain
30	B5	60	
31	B6	54	
32	B7	49	
33	B8	65	
34	B9	37	
35	BA	2915	
36	BB	122	
37	BC	229	
38	BD	276	
39	BE	206	
40	BF	210	
41	BG	182	
42	BH	180	
43	BJ	173	
44	BK	147	
45	BN	140	
46	BO	122	
47	BP	150	
48	BQ	141	
49	BR	118	
50	BS	112	
51	BT	146	
52	BU	118	
53	BV	101	
54	BW	113	

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Mol	Chain	Length	Quality of chain
55	BX	96	
56	BY	110	
57	BZ	206	

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
58	GCP	AY	1000	-	-	X	-



## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 151017 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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



- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 4 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
AL	1	MET	-	EXPRESSION TAG	UNP P17293
AL	2	VAL	-	EXPRESSION TAG	UNP P17293
AL	3	ALA	-	EXPRESSION TAG	UNP P17293
AL	4	LEU	-	EXPRESSION TAG	UNP P17293

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.



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

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 22 is a RNA chain called PE HYBRID STATE TRNA FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called MRNA 5'-R(\*AP\*AP\*AP\*AP\*AP\*AP\*UP\*GP\*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	9	Total	C	N	O	P	0	0	0
			192	88	39	57	8			

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	496	Total	C	N	O	S	0	0	0
			3934	2492	677	744	21			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	45	Total	C	N	O	S	0	0	1
			341	218	58	61	4			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	318	319	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	19	ILE	VAL	CONFLICT	UNP Q5SLP7
BC	27	HIS	ARG	CONFLICT	UNP Q5SLP7
BC	127	MET	LEU	CONFLICT	UNP Q5SLP7

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	156	Total	C	N	O	S	0	0	1
			1189	752	222	214	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BJ	131	Total	C	N	O	S	0	0	1
			654	393	131	130				

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BK	141	Total	C	N	O	S	0	0	1
			701	420	141	140				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BR	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BS	99	Total	C	N	O	S	0	0	1
			771	486	155	130				

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BX	93	Total	C	N	O	S	0	0	1
			726	471	132	123				

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

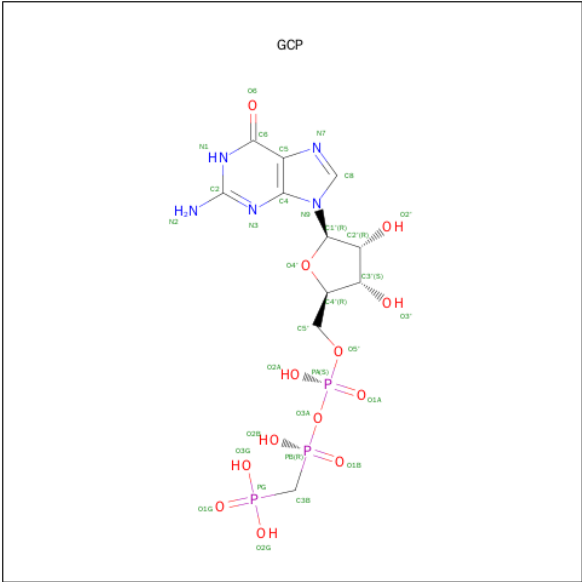
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			

- Molecule 58 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).





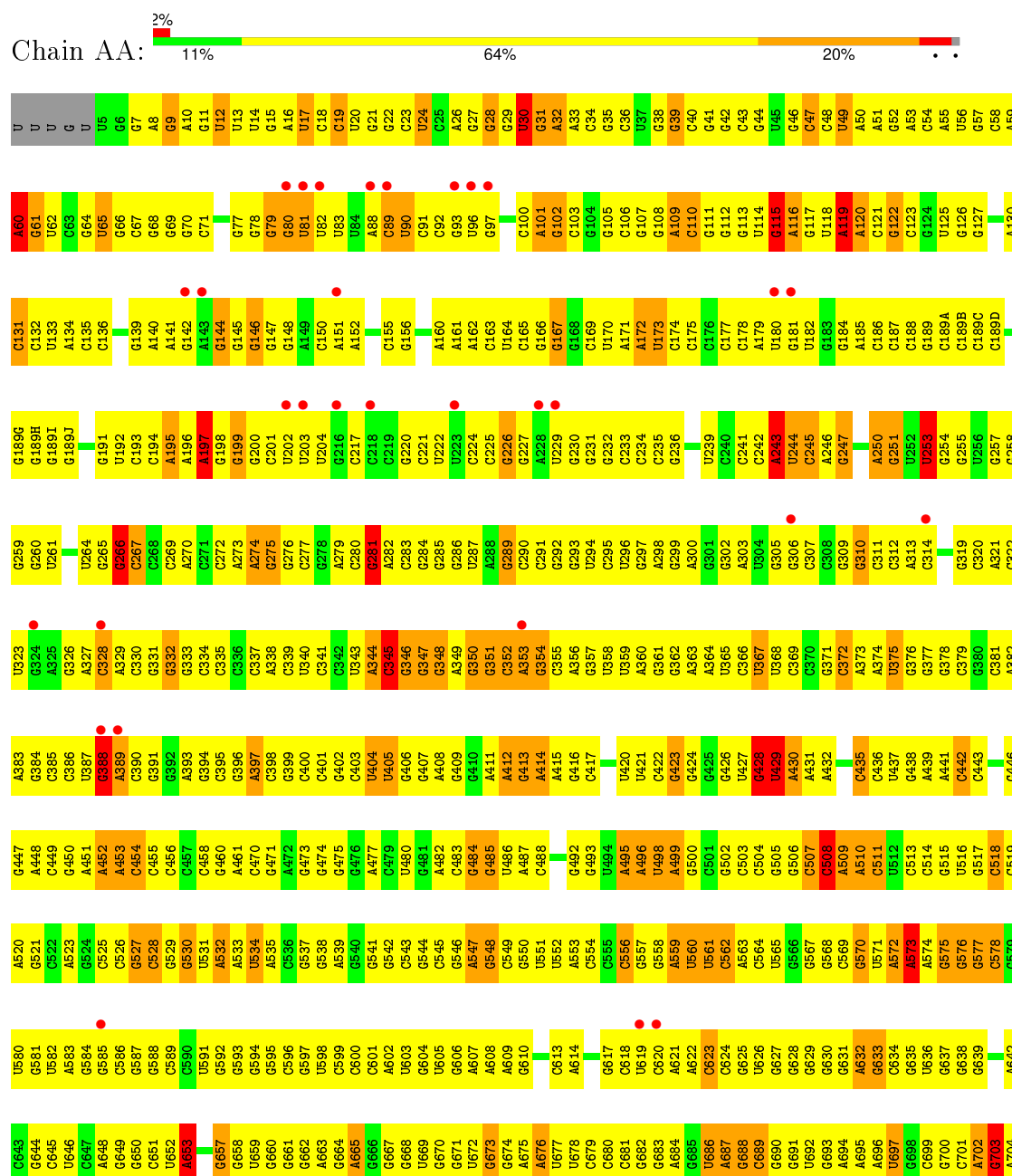
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	AY	1	Total	C	N	O	P	0	0
			32	11	5	13	3		



### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S rRNA



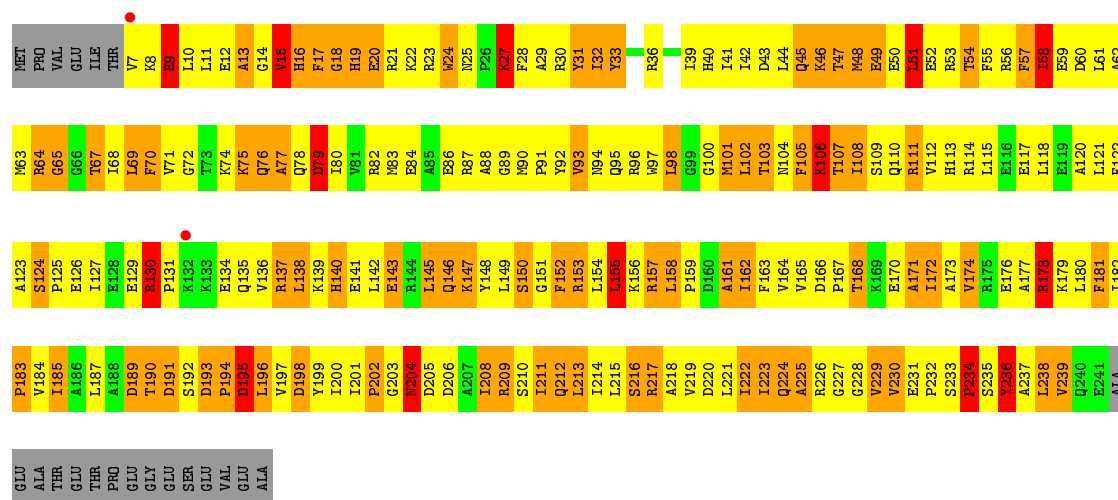


A1503	G1438	A1375	G1316	U1194	C1132	G1072	U1012	U952	A892	C826	A766	U705
G1504	C1439	U1376	C1317	C1195	G1133	U1073	G1013	G953	C893	U827	A767	A706
G1505	C1440	A1377	A1318	U1196	U1134	C1074	A1014	G954	C894	A828	A768	C707
U1506	A1441	C1378	A1319	C1259	U1135	C1075	A1015	U955	G895	G829	G769	C708
A1507	G1442	G1379	C1320	C1260	U1136	G1076	A1016	U956	C896	G830	G770	G709
G1508	G1442A	U1380	C1321	U1199	G1137	C1077	G1017	U957	C897	U831	G771	G710
C1509	A1442B	U1381	C1322	C1262	G1138	U1078	C1018	A958	C898	C832	U772	G711
U1510	G1443	C1382	G1323	C1263	U1139	G1079	C1019	A959	C899	U833	G773	G712
G1511	C1444	C1383	A1324	G1202	C1140	A1080	U1020	U960	A900	C834	G774	A713
U1512	U1445	C1384	C1325	C1203	C1141	G1081	G1021	U961	U835	G836	G775	G714
A1513	G1446	G1385	C1326	C1204	G1142	G1082	G1022	C962	G902	G837	G776	A715
C1514	A1447	G1386	C1327	U1205	G1143	U1083	U1025	G963	G903	G838	A777	A716
U1515	C1452	G1387	G1328	C1206	G1144	G1084	G1026	A964	C904	G839	C778	C717
G1516	G1456	C1388	A1329	G1207	U1145	U1085	C1027	A965	U905	U839	C779	G718
U1517	G1457	C1389	G1330	C1208	A1146	U1086	G1028	G966	G906	C840	A780	C719
A1518	G1458	U1390	G1331	G1209	C1147	G1087	C1029	C967	A907	U841	C781	C720
G1519	C1459	U1391	A1332	C1210	U1148	G1088	G1030	A968	A908	C848	A782	G721
U1520	A1460	G1392	A1333	U1211	C1149	G1089	G1030A	A969	A909	C849	C783	A722
G1521	G1461	U1393	G1334	U1212	U1150	U1090	G1030B	C970	C910	U850	C784	U723
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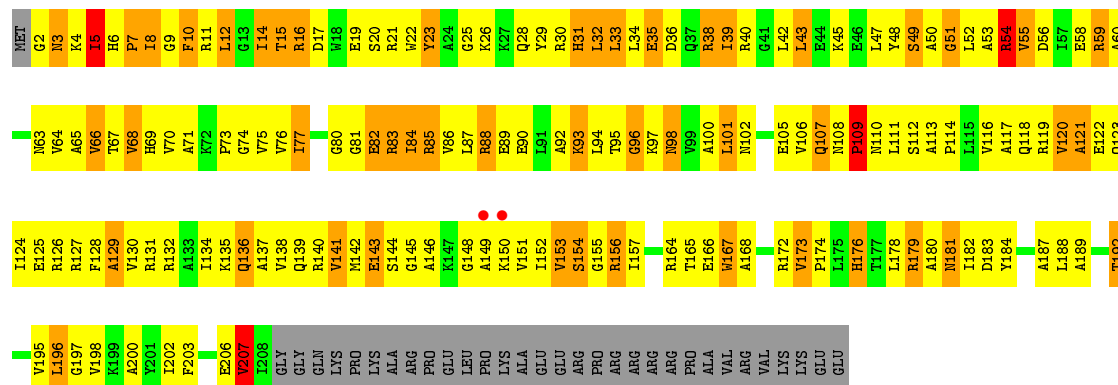
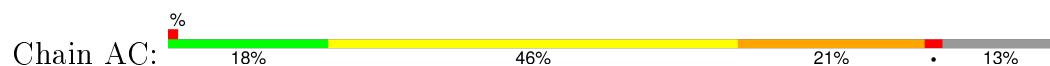
● Molecule 2: 30S RIBOSOMAL PROTEIN S2



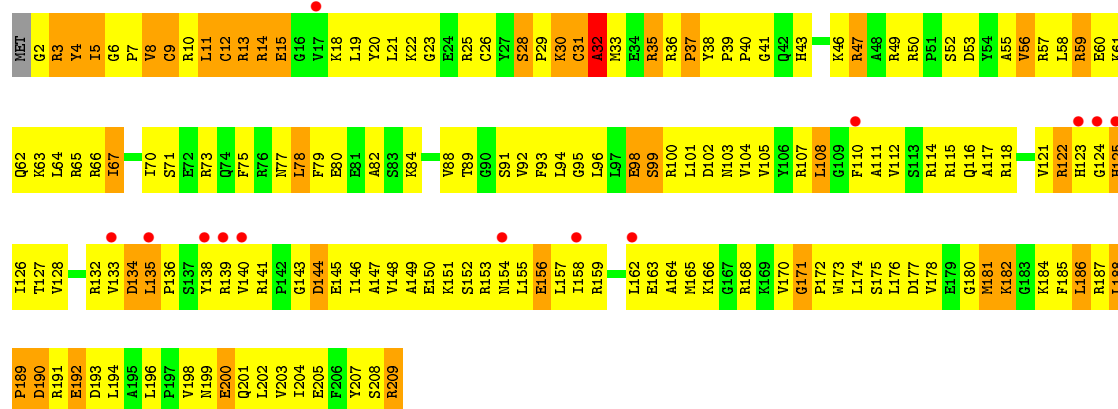




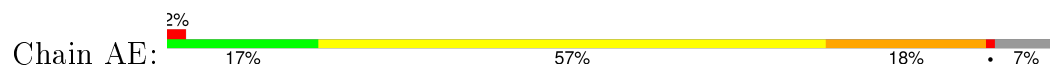
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



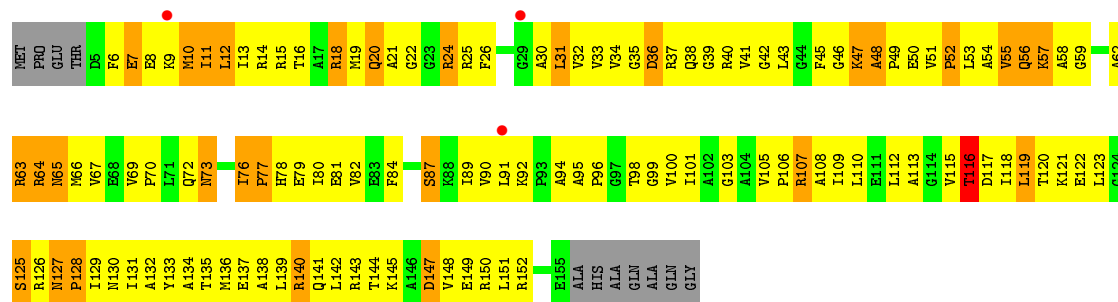
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



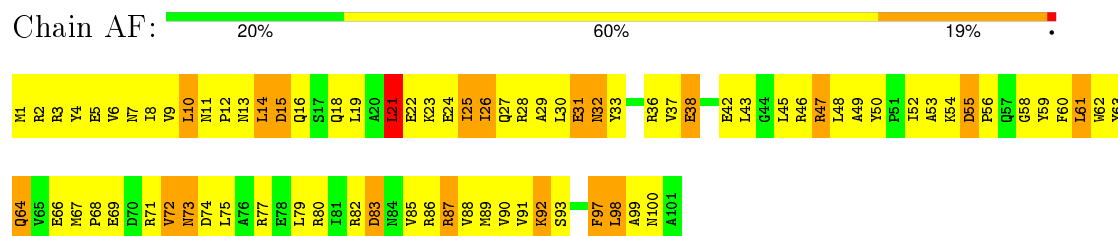
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



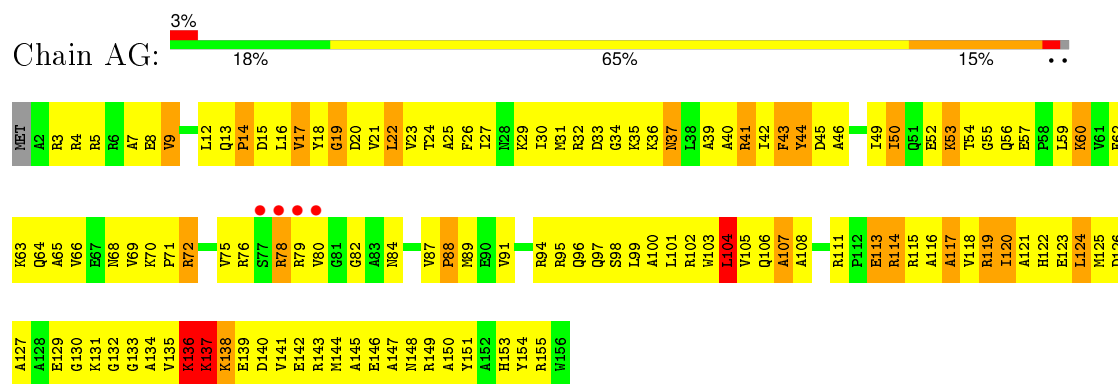




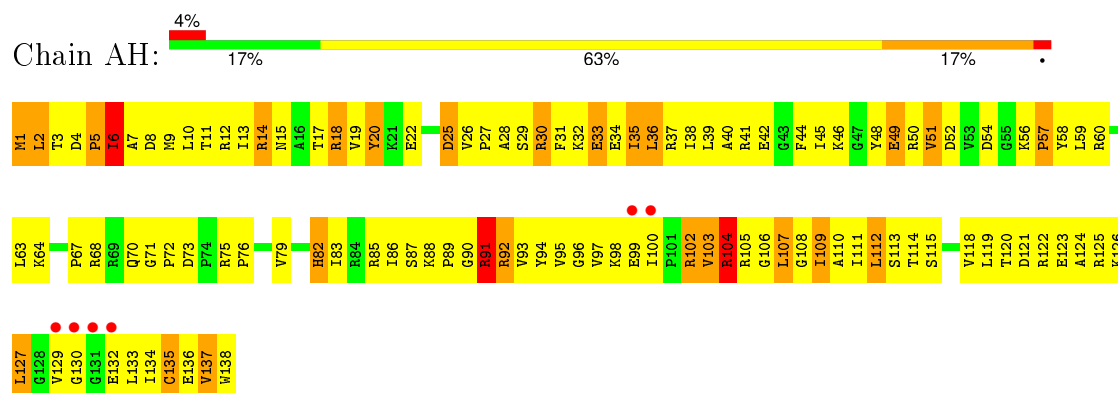
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



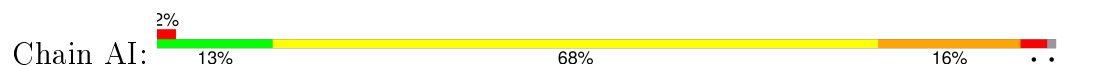
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



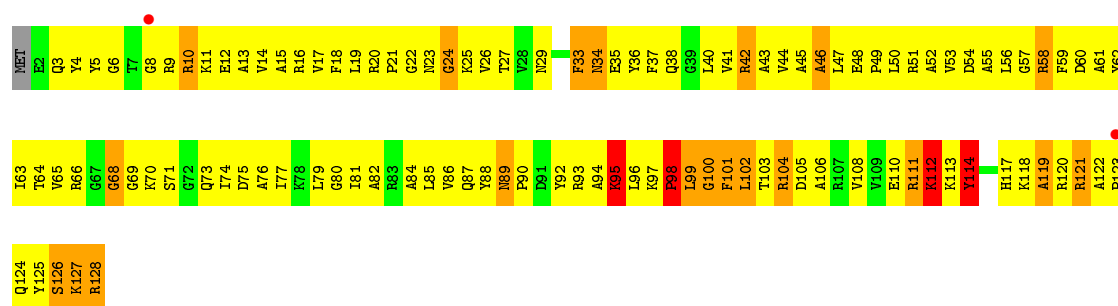
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



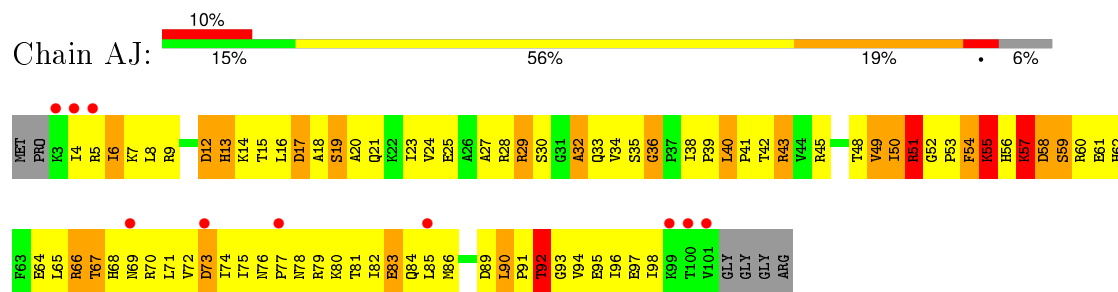
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



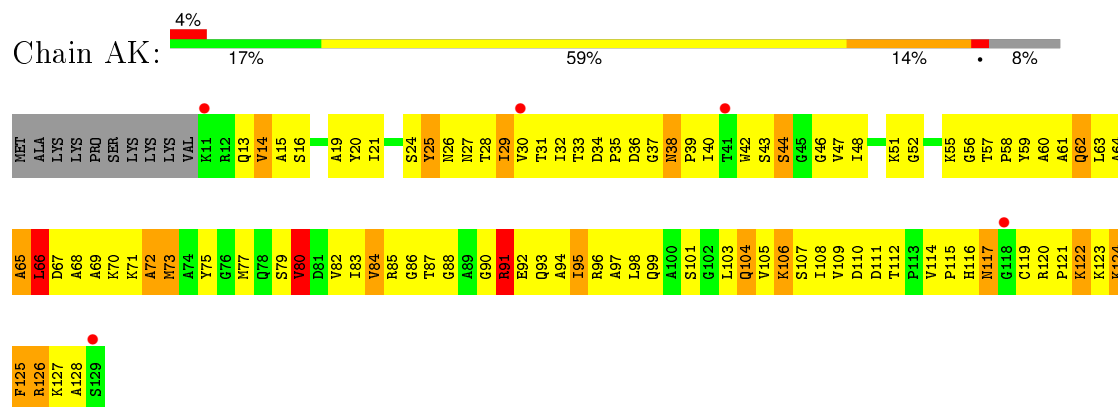




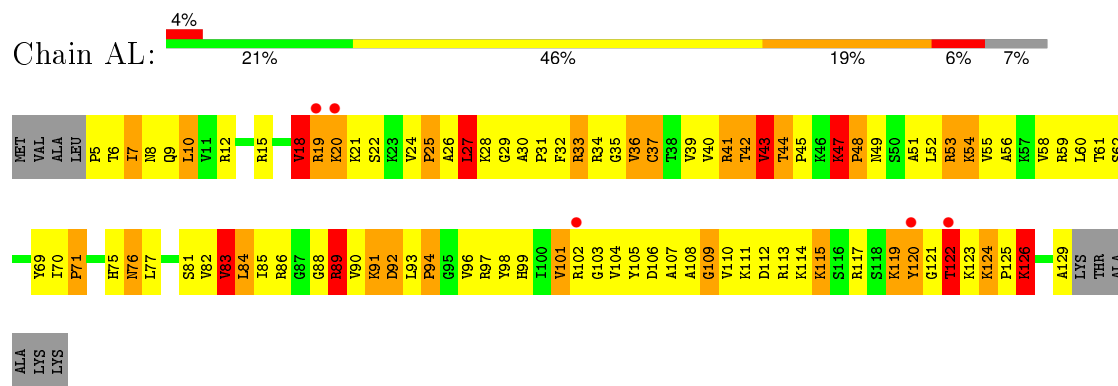
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

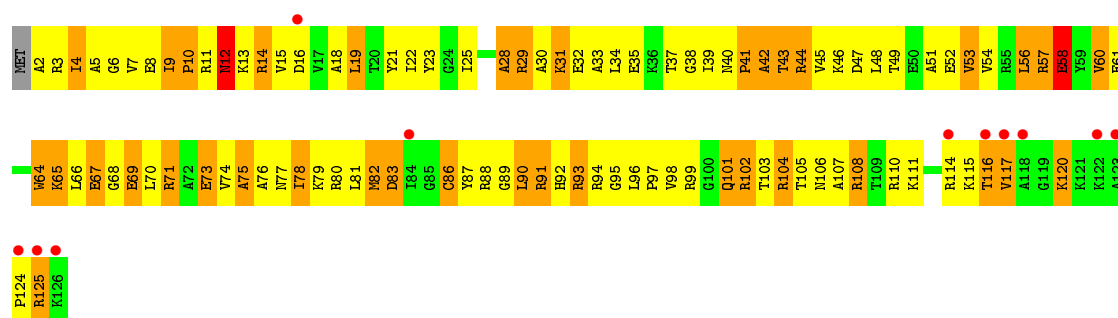


• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13





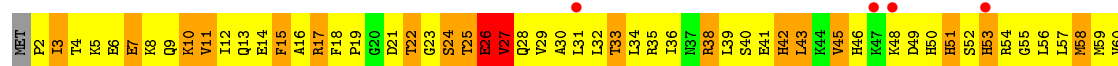
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN: 8% 57% 25% 8%



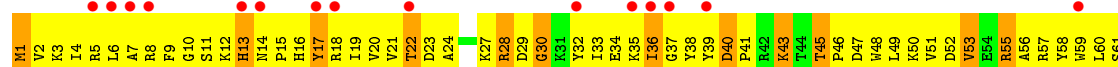
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 4% 10% 56% 30% ..



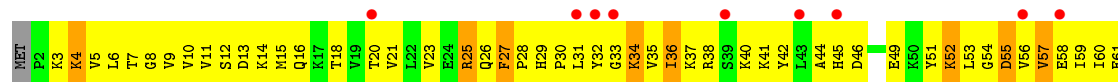
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP: 20% 11% 65% 19% 5%



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

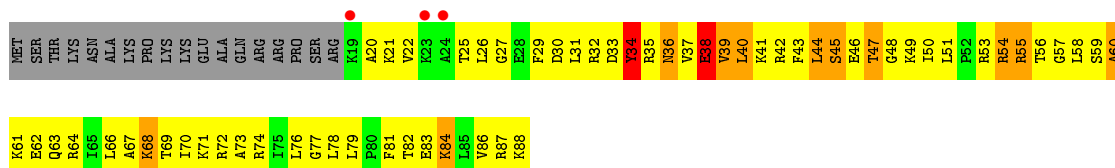
Chain AQ: 12% 18% 64% 13% 5%



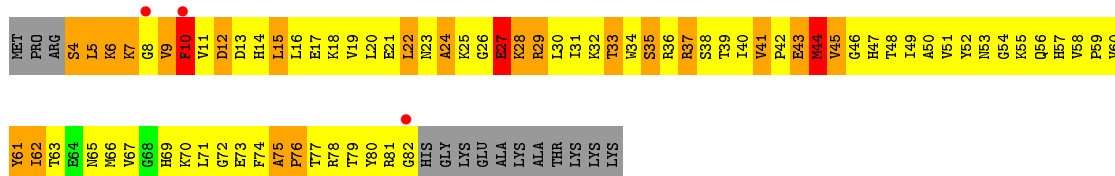
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR: 3% 10% 55% 13% 20%

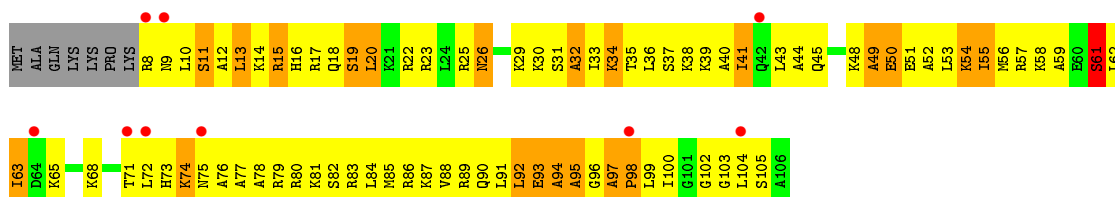
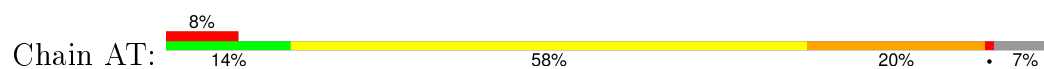




• Molecule 19: 30S RIBOSOMAL PROTEIN S19



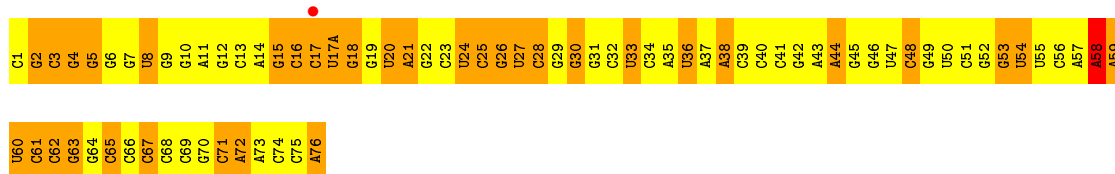
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 22: PE HYBRID STATE TRNA FMET



• Molecule 23: MRNA 5'-R(\*AP\*AP\*AP\*AP\*AP\*AP\*UP\*GP\*UP)-3'

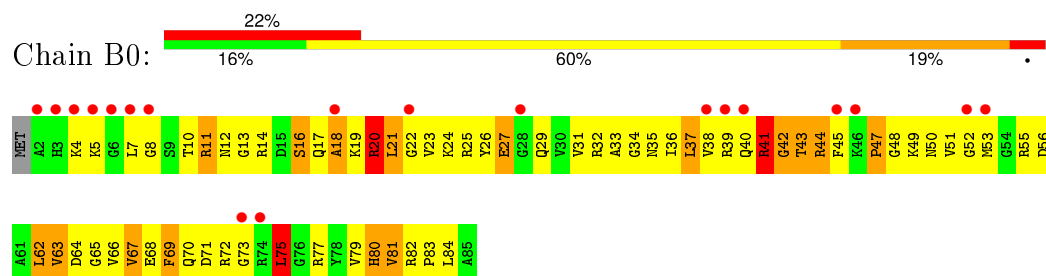


• Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 3

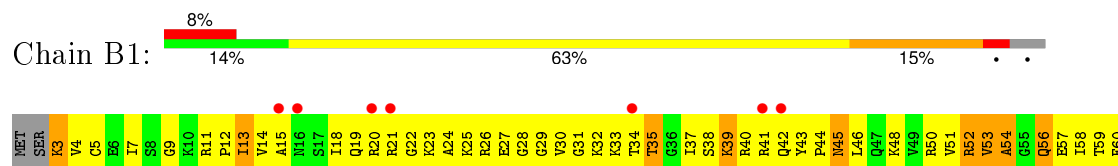




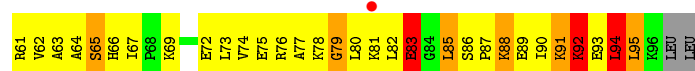
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



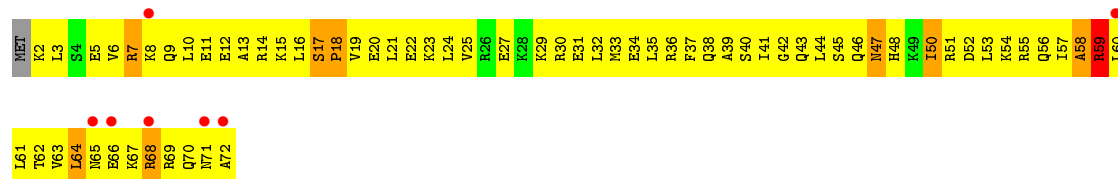
• Molecule 26: 50S RIBOSOMAL PROTEIN L28







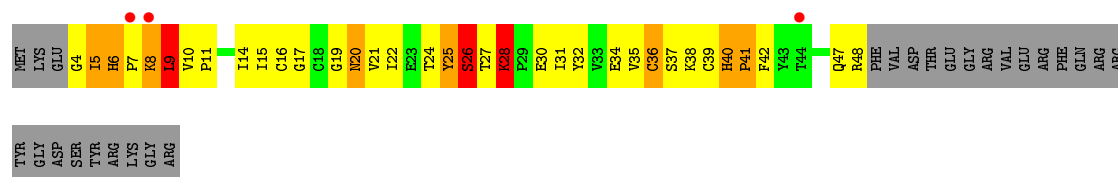
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



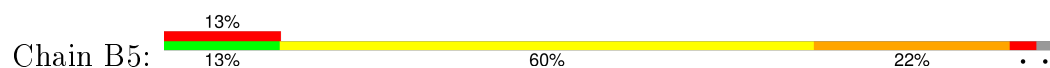
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



• Molecule 29: 50S RIBOSOMAL PROTEIN L31



• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 31: 50S RIBOSOMAL PROTEIN L33

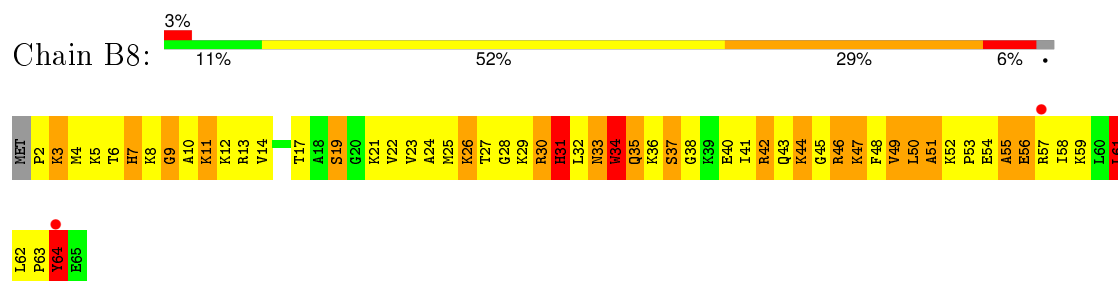


• Molecule 32: 50S RIBOSOMAL PROTEIN L34

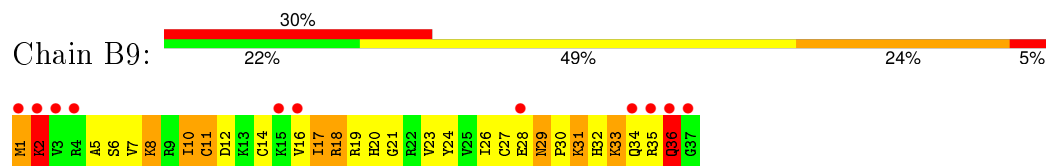




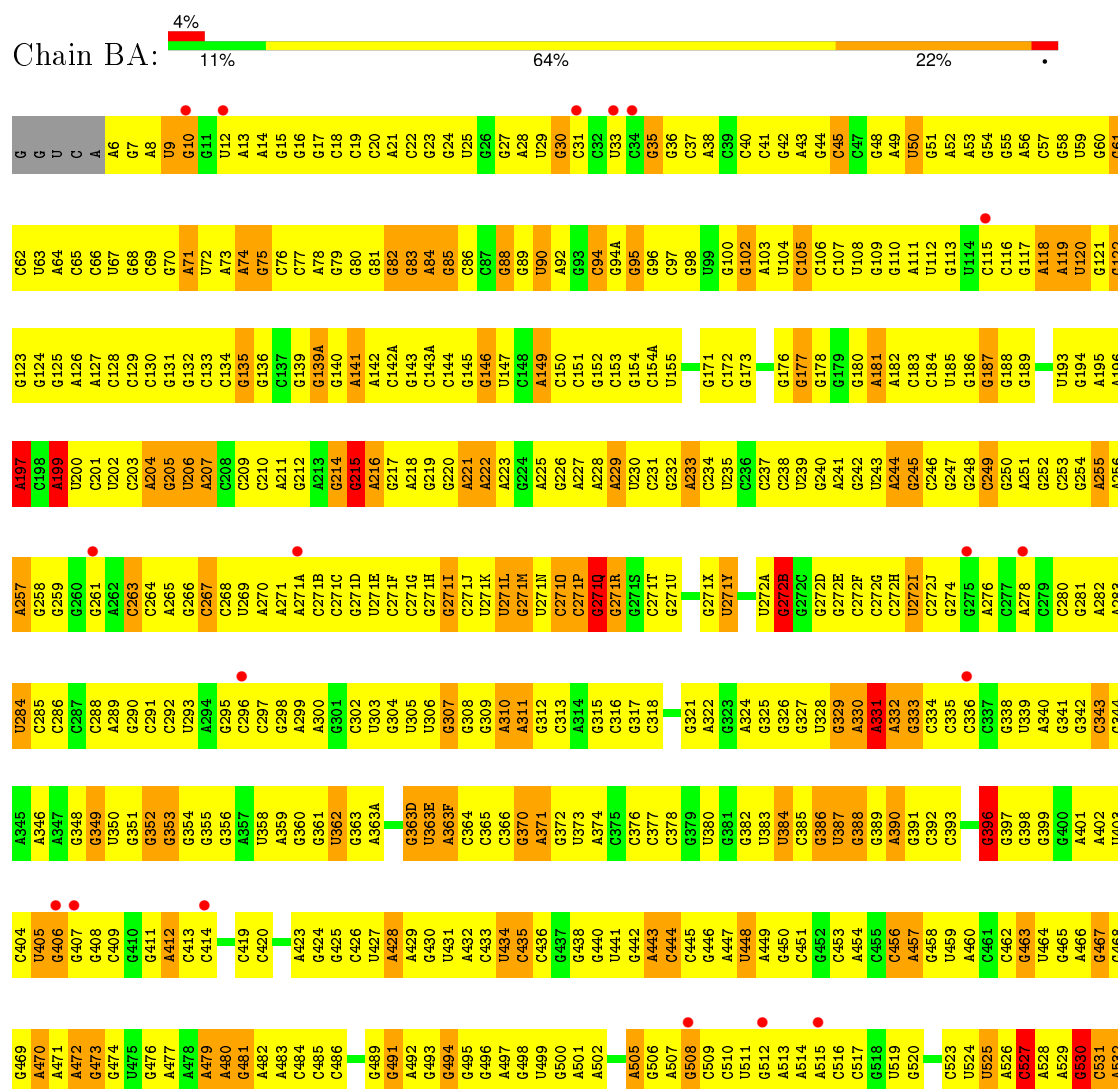
- Molecule 33: 50S RIBOSOMAL PROTEIN L35



- Molecule 34: 50S RIBOSOMAL PROTEIN L36



- Molecule 35: 23S RIBOSOMAL RNA



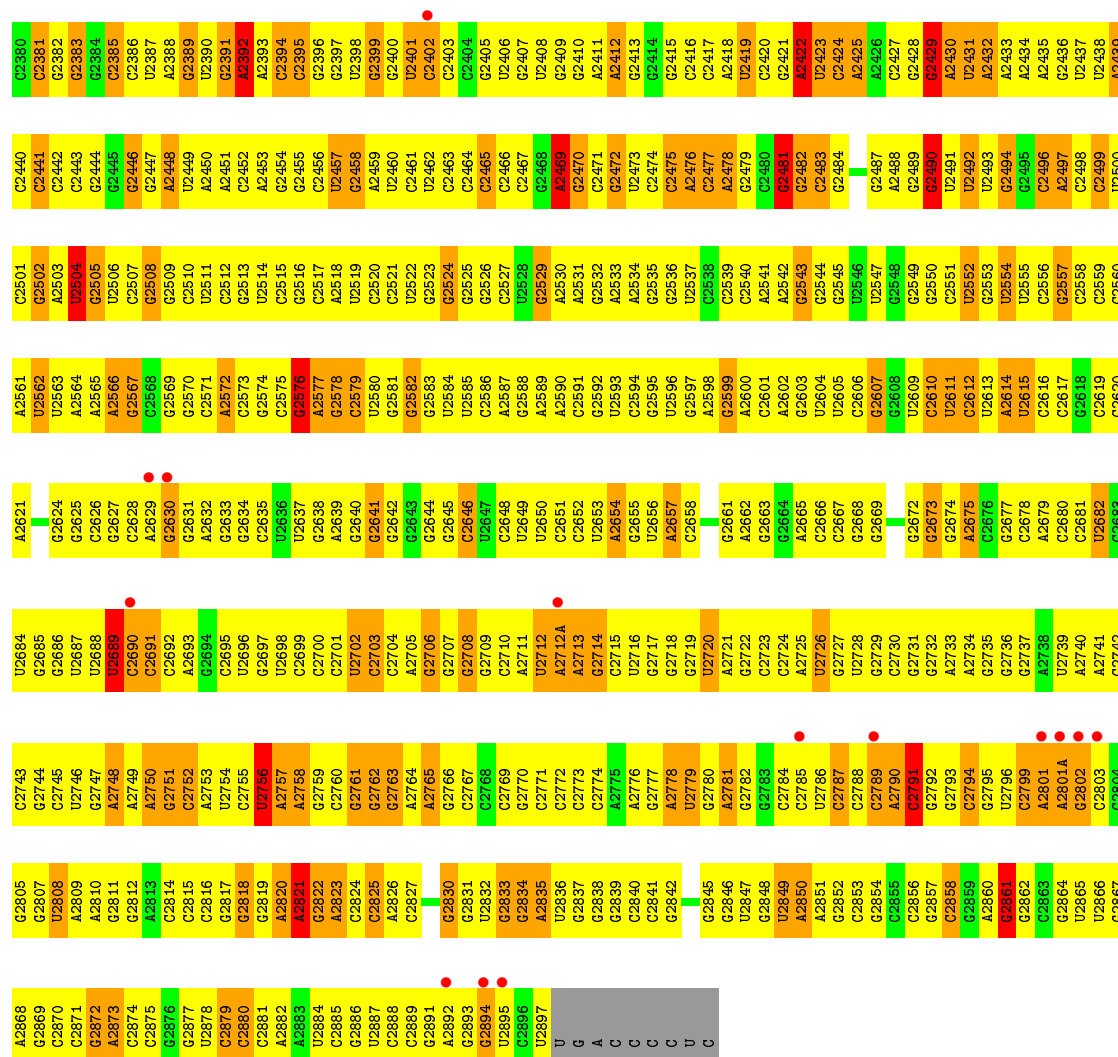


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G1422	C1363	U1300	G1239	C1179	G1117	A1057	G997	G938	G875	C814	G749	U689	
G1423	G1364	A1301	U1240	C1180	G1118	G1058	C998	G939	C876	C815	A750	G690	
G1424		A1302	A1241	C1181	C1119	U1059	U999	G940	U877	C816	A751	C691	
G1425		G1303	A1242	G1182	G1120	U1060	A1000	A941	A878	C917	A752	C692	
G1426	A1366	C1304	G1243	G1183	C1121	U1061	A1001	G942	G879	G618	C753	C693	



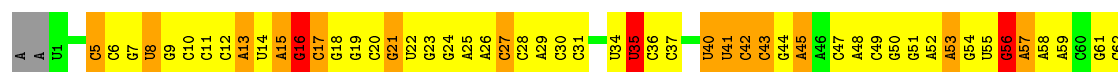
A2320	C2260	G2124	C2064	G2002	C1941	G1881	G1811	C1751	U1671	C1611	C1549	A1427
A2321	C2261	G2125	C2065	C2006	C1942	C1882	A1812	C1752	C1672	C1612	G1550	C1428
A2322	C2262	A2126	C2066	C2007	U1943	G1883	G1813	G1753	U1673	A1614	G1490	C1429
A2323	C2263	G2127	G2067	C2008	U1944	A1884	G1814	C1754	G1674	A1615	G1491	C1430
A2324	C2264	C2128	U2068	C2009	C1947	A1885	A1815	A1755	C1675	A1616	C1493	C1431
A2325	C2265	C2129	G2069	G2010	G1948	C1886	G1816	G1756	A1676	A1617	A1554	C1432
A2326	A2266	U2130	G2070	C2011	G1949	C1887	G1817	U1757	A1677	C1618	A1494	C1433
A2327	A2267	G2131	A2071	U2011	G1950	G1888	U1818	G1758	G1678	A1619	A1495	U1433
A2328	A2268	U2132	C2072	C2012	G1951	A1889	A1819	A1759	U1679	G1620	U1496	A1434
A2329	A2269	C2133	C2073	A2013	U1951	G1890	A1820	A1760	U1680	U1621	A1558	C1436
A2330	G2270	A2134	C2074	A2014	A1952	G1891	A1821	C1761	G1681	G1622	C1437	G1437
A2331	G2271	C2137	U2075	A2015	A1953	C1892	G1822	A1763	G1682	G1623	U1438	U1438
A2332	G2272	U2135	U2076	U2016	G1954	C1893	G1823	G1763	G1683	G1624	A1439	A1439
A2333	A2273	C2138	A2077	U2017	U1955	C1894	G1824	G1764	C1684	C1625	G1501	G1440
A2334	A2274	C2139	C2078	G2018	U1956	G1895	A1825	C1765	G1685	G1626	C1502	G1441
A2335	G2275	C2140	U2079	A2019	U1957	G1896	A1826	U1766	C1686	C1627	U1503	G1442
A2336	G2276	C2141	G2080	C2020	C1958	U1897	C1827	C1767	A1689	G1628	C1504	G1443
A2337	G2277	C2142	C2081	C2021	G1959	U1898	G1828	U1768	A1690	U1629	C1505	G1444
A2338	G2278	C2143	A2082	U2022	A1960	G1899	A1829	G1769	C1691		A1507	A1445
A2339	G2279	U2144	G2083	G2023	C1961	A1900	C1830	G1770	U1692	A1631A	A1508	C1445A
A2340	G2280	C2145	C2084	G2024	C1962	A1901	G1831	C1771	U1693	A1632	A1509	C1446
A2341	G2281	C2146	C2085	C2025	U1963	C1902	C1832	G1772	C1694	G1633	A1509A	G1447
A2342	G2282	C2147	U2086	C2026	G1964	G1903	U1833	A1773	C1695	G1634	A1572	G1448
A2343	C2283	G2148	G2087	G2027	C1965	G1904	U1834	G1774	G1696	G1635	G1510	A1449
A2344	C2284	C2149	G2088	U2028	A1966	C1905	G1835	U1775	G1697	G1636	C1511	G1450
G2345	C2285	U2150	U2089	G2029	C1967	G1906	C1836	G1776	A1698	A1637	G1512	C1450A
A2346	A2286	G2151	G2090	A2030	G1968	G1907	C1837	U1777	G1699	A1638	C1513	C1451
A2347	G2287	C2152	U2091	A2031	A1969	C1908	C1838	U1778	A1700	G1639	U1514	A1452
U2348	A2288	G2153	U2092	G2032	A1970	G1909	G1839	U1779	A1701	U1640	G1515	A1453
A2349	G2289	C2154	G2093	A2033	A1971	G1910	G1840	A1780	G1702	A1641	C1516	G1455
A2350	G2290	G2155	C2094	U2034	A1972	U1911	U1841	C1781	G1705	G1642	G1517	A1456
G2351	C2291	C2156	C2095	C2035	G1973	A1912	G1842	C1782	G1706	G1643	A1581	A1457
A2352	C2292	G2157	U2096	C2036	C1974	A1913	C1843	C1783	G1707	G1644	C1582	C1458
A2353	U2293	A2158	C2097	G2037	G1975	C1914	C1844	A1784	C1708	C1645	A1583	G1459
G2354	C2294	G2159	U2098	G2038	U1976	U1915	G1845	A1785	G1709	G1646	U1523	A1460
C2355	C2295	G2160	U2099	C2039	A1977	A1916	U1846	C1786	U1709	C1647	G1524	G1461
C2356	U2296	C2161	G2100	C2040	A1978	U1917	A1847	A1787	G1710	C1648	G1525	C1462
U2357	C2297	G2162	G2101	U2041	C1979	A1918	A1848	C1788	G1711	C1649	C1526	C1463
G2358	A2298	C2163	U2102	A2042	U1980	A1919	G1849	A1789	G1712	G1650	G1527	C1464
C2359	G2299	C2164	C2103	C2043	A1981	C1920	G1850	C1790	U1713	G1651	A1528	G1465
A2360	G2300		G2104	C2044	C1982	G1921	A1851	A1791	G1714	C1652	A1529	C1466
A2361	C2301	U2167	C2105	C2045	C1983	G1922	C1852	G1792	G1717	A1653	C1530	C1468
G2362	G2302	G2168	G2106	G2046	G1984	U1923	A1853	C1793	G1718	G1654	G1531	A1469
C2363	G2303	A2169	C2107	U2047	G1985	C1924	A1854	U1794	G1719	A1655		G1470
C2364	G2304	A2170	C2108	G2048	A1986	C1925	G1855	C1795	U1720	A1656	U1534	A1471
A2365	A2305	A2171	U2109	G2049	G1987	U1926	G1856	U1796	G1721	C1657	A1535	A1472
A2366	C2306	U2172	C2110	C2050	C1988	A1927	G1857	C1797	A1722	C1658	C1536	G1473
G2367	G2307	A2173	C2111	A2051	G1989	A1928	G1858	U1798	U1739	C1659	G1537	G1474
C2368	G2308	C2174	G2112	G2052	U1990	G1929	A1859	G1799	G1740	C1660	G1538	G1475
A2369	A2309		U2113	G2053	U1991	G1930	G1860	C1800	A1741	G1661	G1539	C1476
G2370	A2310	C2177	A2114	A2054	C1992	U1931	G1861	G1801	G1742	A1662	U1540	A1477
G2371	A2311	C2178	C2115	C2055	U1993	A1932	G1862	A1802	C1743	A1663	G1541	G1478
G2372	U2312	C2179	G2116	G2056	C1994	G1933	G1863	A1803	C1744	A1664	A1542	G1479
G2373	C2313	U2180	A2117	A2057	U1995	C1934	U1864	C1804		C1665	C1543	G1480
G2374	C2314	G2181	U2118	A2058	G1996	G1935	G1865	U1805	G1746	G1666	A1544	U1481
G2375	G2315	G2182	A2119	A2059	G1997	U1936	C1866	C1806	G1747	G1667	A1545	G1482
A2376	C2316	C2183	G2120	A2060	G1998	A1937		G1807	G1747A	A1668	C1546	G1484
A2377	G2317	G2184	U2121	G2061	C1999	U1938	G1878	U1808	G1748	A1669	C1547	G1485
A2378	G2318	C2185	U2122	A2062	G1999	A1939	C1879	U1809	A1749	G1670		A1486
G2379	G2319	G2186	G2123	C2063	A2001	U1940	C1880	A1810	G1750			





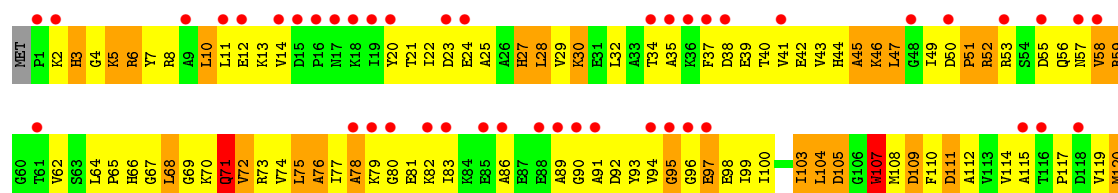
## • Molecule 36: 5S RIBOSOMAL RNA

Chain BB: 11% 60% 23% . .

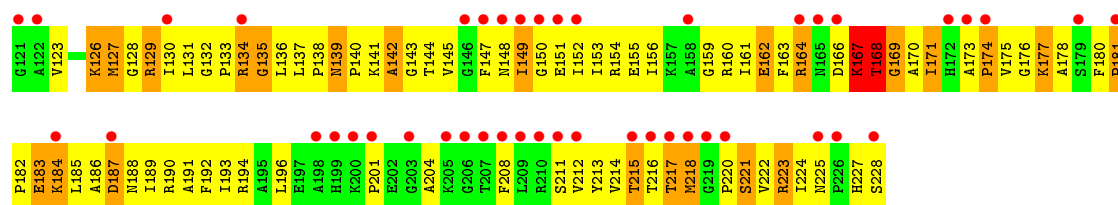


## • Molecule 37: 50S RIBOSOMAL PROTEIN L1

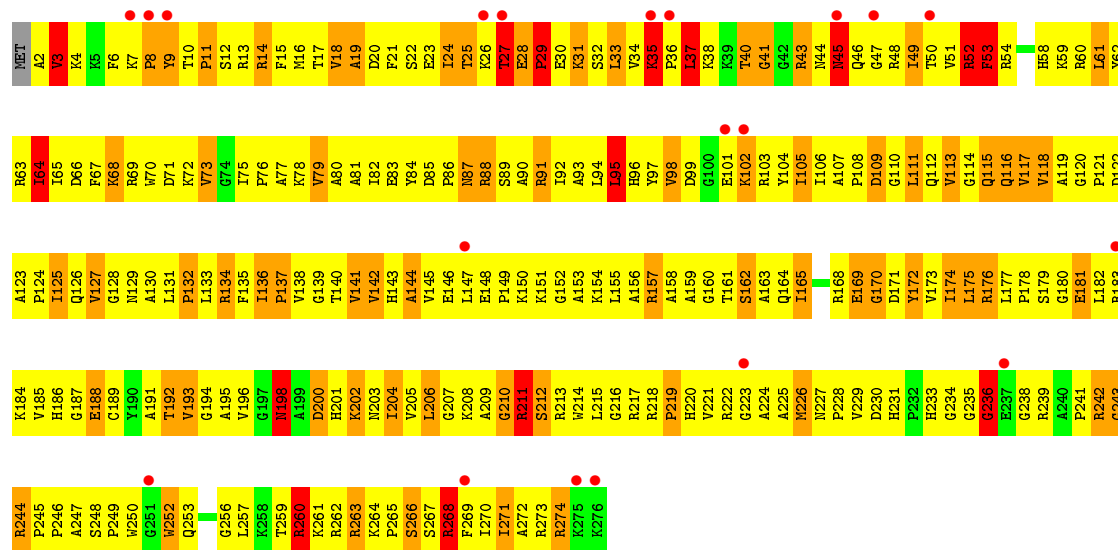
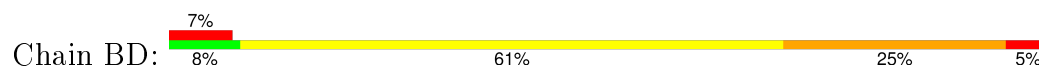
Chain BC: 22% 39% 54% 22% .



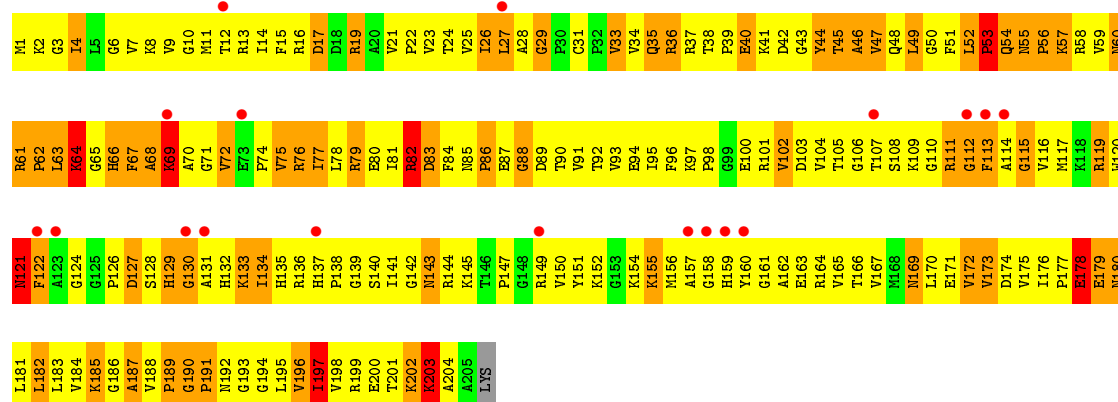
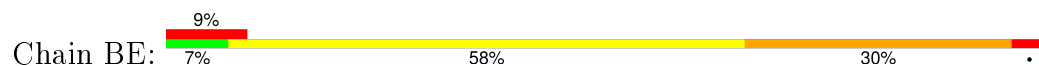




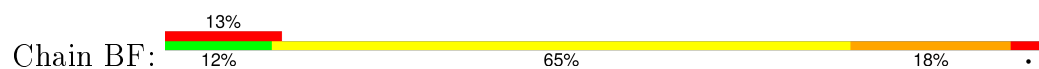
• Molecule 38: 50S RIBOSOMAL PROTEIN L2



• Molecule 39: 50S RIBOSOMAL PROTEIN L3

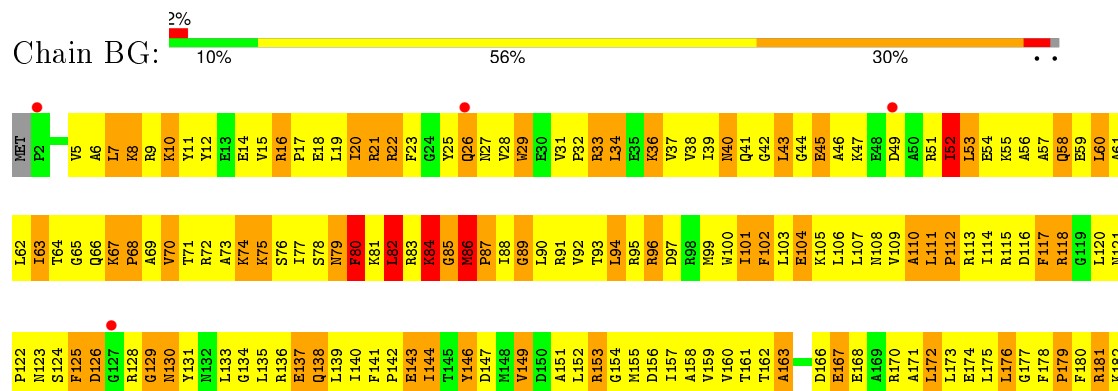


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

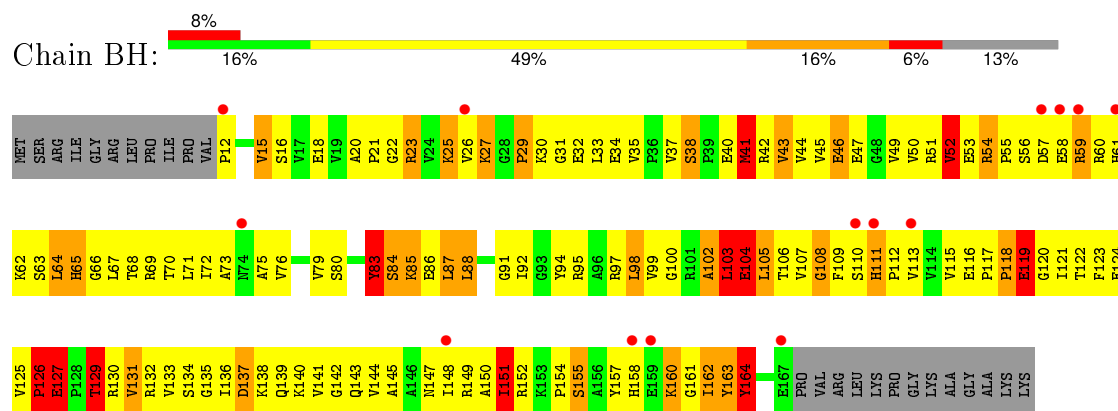




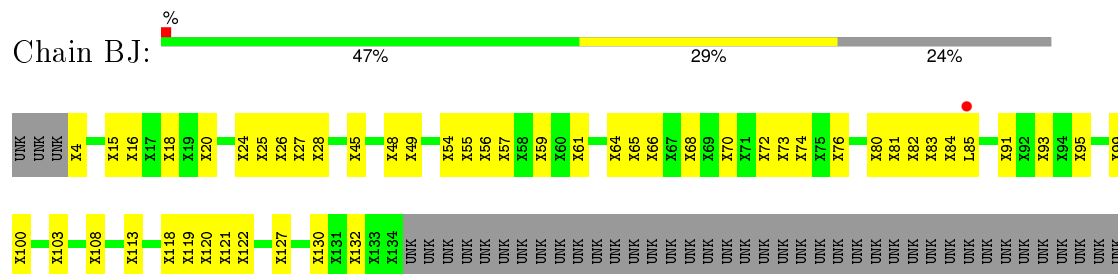
- Molecule 41: 50S RIBOSOMAL PROTEIN L5



- Molecule 42: 50S RIBOSOMAL PROTEIN L6



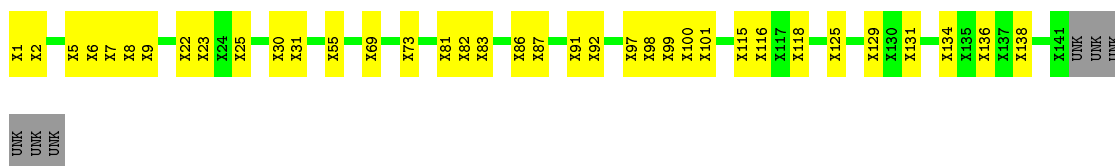
• Molecule 43: 50S RIBOSOMAL PROTEIN L10



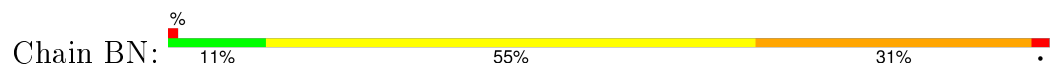
- Molecule 44: 50S RIBOSOMAL PROTEIN L11



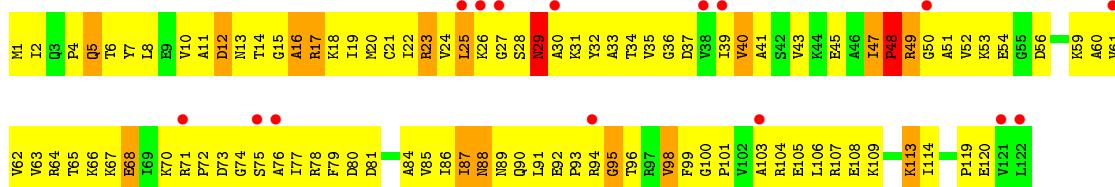




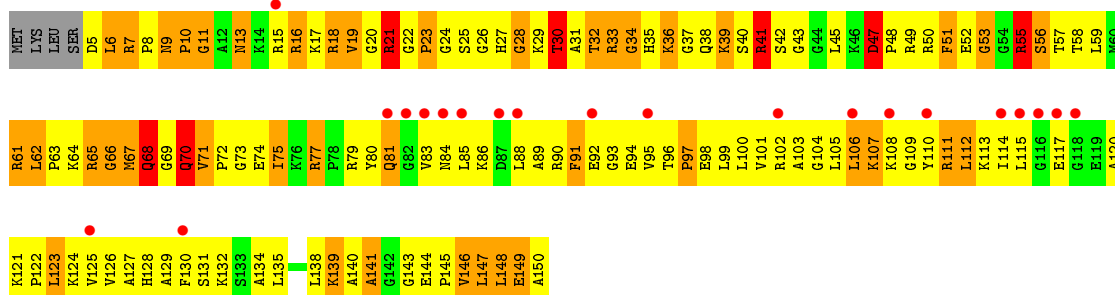
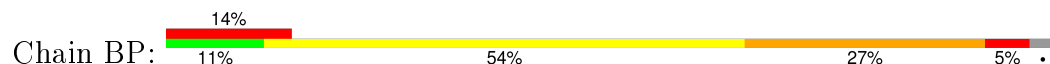
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



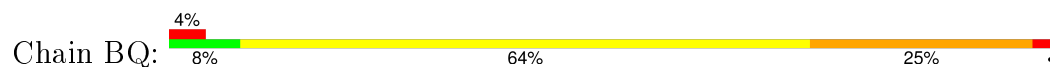
• Molecule 46: 50S RIBOSOMAL PROTEIN L14



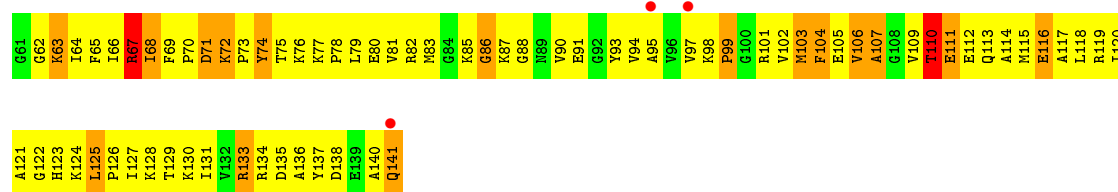
• Molecule 47: 50S RIBOSOMAL PROTEIN L15



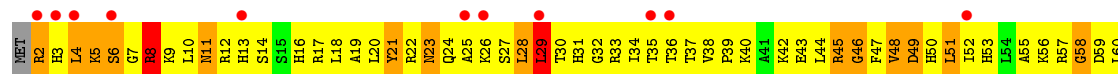
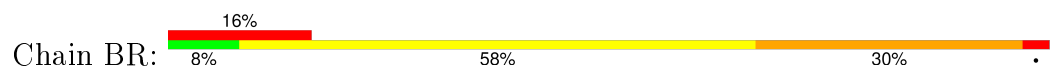
• Molecule 48: 50S RIBOSOMAL PROTEIN L16







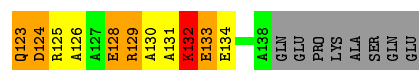
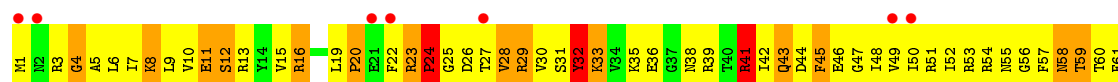
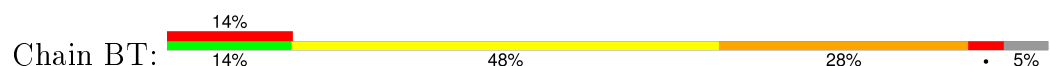
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



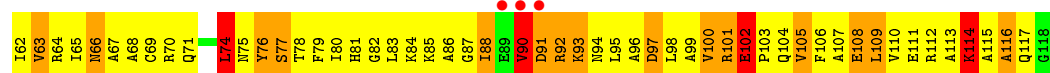
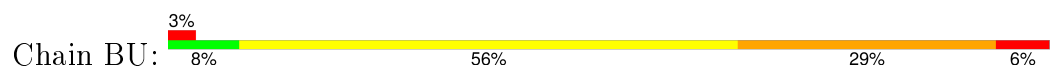
• Molecule 50: 50S RIBOSOMAL PROTEIN L18



• Molecule 51: 50S RIBOSOMAL PROTEIN L19

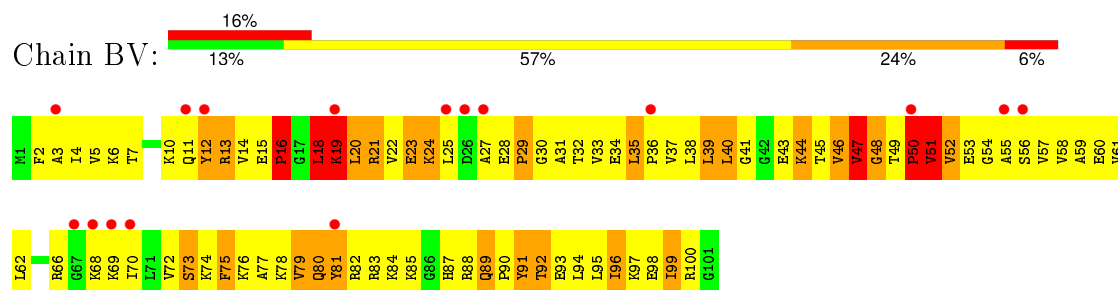


• Molecule 52: 50S RIBOSOMAL PROTEIN L20

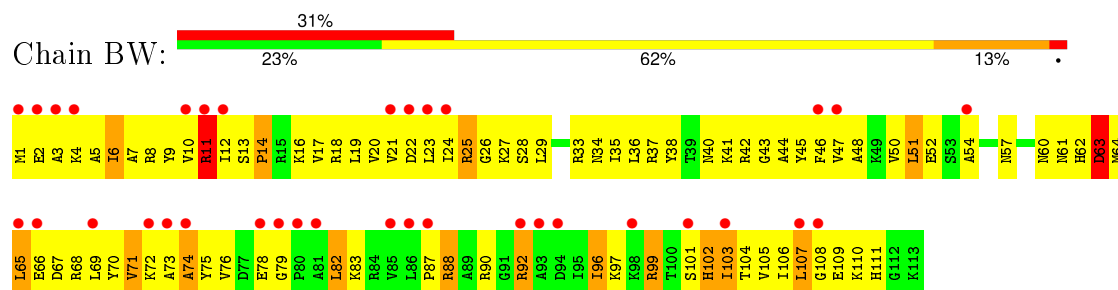




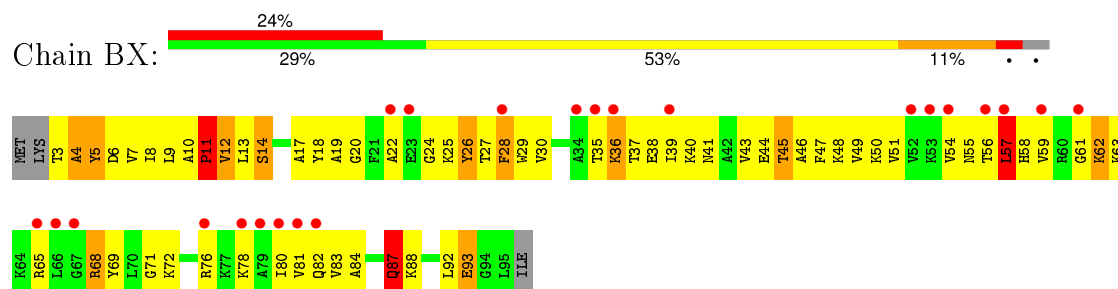
- Molecule 53: 50S RIBOSOMAL PROTEIN L21



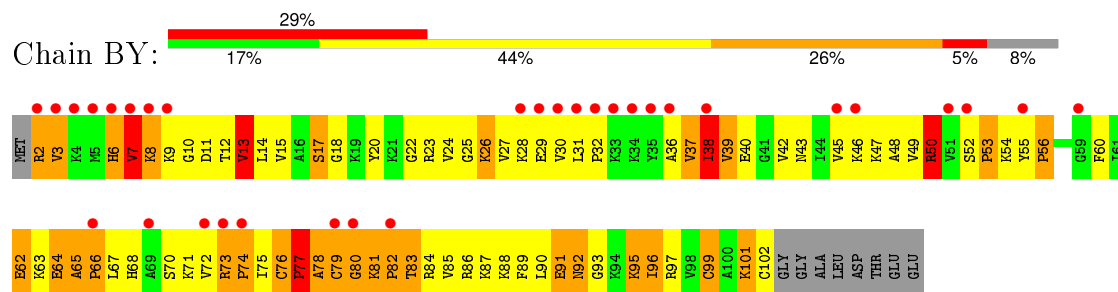
- Molecule 54: 50S RIBOSOMAL PROTEIN L22



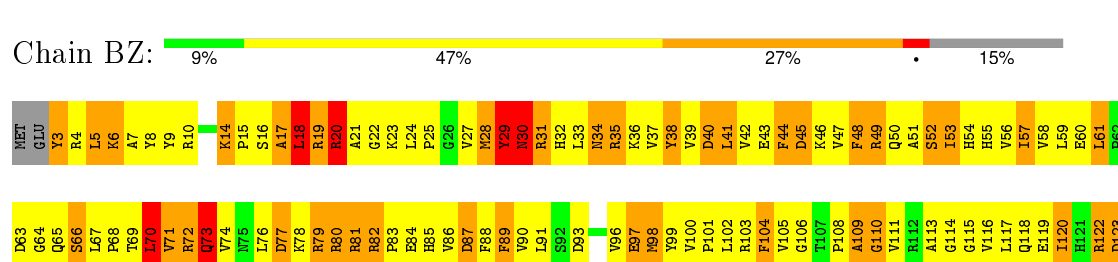
- Molecule 55: 50S RIBOSOMAL PROTEIN L23



- Molecule 56: 50S RIBOSOMAL PROTEIN L24



- Molecule 57: 50S RIBOSOMAL PROTEIN L25









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.70Å 229.30Å 307.00Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	44.90 – 3.80 44.91 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.90-3.80) 96.6 (44.91-3.60)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.293 , 0.351 0.306 , 0.353	Depositor DCC
$R_{free}$ test set	5623 reflections (2.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	110.2	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 41.0	EDS
Estimated twinning fraction	0.166 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.15$	Xtriage
Outliers	6 of 2273458 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	151017	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: GCP

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	AA	0.79	12/36190 (0.0%)	0.89	56/56486 (0.1%)
2	AB	0.62	0/1936	0.96	1/2611 (0.0%)
3	AC	0.60	0/1637	0.93	3/2207 (0.1%)
4	AD	0.50	0/1733	0.86	2/2318 (0.1%)
5	AE	0.63	0/1163	0.94	1/1566 (0.1%)
6	AF	0.56	0/856	0.88	0/1154
7	AG	0.59	0/1276	0.85	0/1709
8	AH	0.56	0/1136	0.91	1/1527 (0.1%)
9	AI	0.56	0/1029	0.83	0/1378
10	AJ	0.59	0/808	0.88	0/1087
11	AK	0.57	0/900	0.89	0/1213
12	AL	0.59	0/987	1.01	2/1322 (0.2%)
13	AM	0.59	0/999	0.95	0/1338
14	AN	0.71	0/501	1.03	1/664 (0.2%)
15	AO	0.65	0/745	0.86	0/992
16	AP	0.53	0/717	0.88	0/965
17	AQ	0.61	0/837	0.92	1/1119 (0.1%)
18	AR	0.60	0/579	0.89	1/768 (0.1%)
19	AS	0.68	0/643	0.91	1/867 (0.1%)
20	AT	0.54	0/765	0.80	0/1007
21	AU	0.70	0/213	0.95	1/279 (0.4%)
22	AV	0.65	0/1832	0.82	0/2855
23	AX	0.66	0/216	0.77	0/335
24	AY	1.05	19/4005 (0.5%)	1.16	32/5407 (0.6%)
25	B0	0.61	0/671	0.98	2/892 (0.2%)
26	B1	0.49	0/739	0.85	0/983
27	B2	0.51	0/600	0.82	0/793
28	B3	0.57	0/473	0.93	0/636
29	B4	0.69	0/350	0.80	0/476
30	B5	0.64	0/473	0.89	0/639
31	B6	0.79	0/440	1.09	2/586 (0.3%)
32	B7	0.53	0/427	0.79	0/563



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	B8	0.68	0/516	0.92	0/681
34	B9	0.53	0/310	0.85	0/407
35	BA	0.76	16/69976 (0.0%)	0.86	82/109244 (0.1%)
36	BB	0.76	1/2853 (0.0%)	0.89	5/4451 (0.1%)
37	BC	0.81	4/1775 (0.2%)	0.94	4/2392 (0.2%)
38	BD	0.69	0/2195	1.07	9/2955 (0.3%)
39	BE	0.59	0/1597	0.95	1/2155 (0.0%)
40	BF	0.61	0/1659	0.88	0/2246
41	BG	0.58	0/1499	0.92	3/2016 (0.1%)
42	BH	0.66	0/1211	0.88	0/1636
43	BJ	0.53	0/7	0.70	0/8
45	BN	0.57	0/1132	0.91	1/1527 (0.1%)
46	BO	0.60	0/943	0.90	0/1269
47	BP	0.57	0/1131	1.08	6/1504 (0.4%)
48	BQ	0.63	0/1143	1.00	3/1527 (0.2%)
49	BR	0.49	0/974	0.92	1/1302 (0.1%)
50	BS	0.66	0/779	1.12	6/1038 (0.6%)
51	BT	0.60	0/1156	0.92	3/1544 (0.2%)
52	BU	0.63	0/975	0.91	1/1297 (0.1%)
53	BV	0.54	0/790	0.97	2/1057 (0.2%)
54	BW	0.59	0/907	0.82	0/1216
55	BX	0.63	0/740	0.83	1/995 (0.1%)
56	BY	0.61	0/789	0.90	0/1053
57	BZ	0.62	0/1435	0.95	0/1949
All	All	0.73	52/162368 (0.0%)	0.89	235/242211 (0.1%)

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	AA	3	125
9	AI	0	1
11	AK	0	1
17	AQ	0	1
21	AU	0	1
22	AV	0	5
24	AY	0	5
30	B5	0	1
35	BA	3	160
36	BB	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	BH	0	1
45	BN	0	1
48	BQ	0	1
53	BV	0	1
All	All	6	316

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	191	TYR	CE2-CZ	11.85	1.53	1.38
24	AY	189	GLU	CG-CD	-10.57	1.36	1.51
24	AY	191	TYR	CD1-CE1	10.46	1.55	1.39
24	AY	504	ILE	C-N	-9.62	1.11	1.34
24	AY	444	LEU	C-N	-9.54	1.12	1.34

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	191	TYR	CB-CG-CD1	-18.01	110.19	121.00
24	AY	307	MET	CG-SD-CE	13.35	121.55	100.20
24	AY	319	ARG	NE-CZ-NH1	12.45	126.52	120.30
24	AY	504	ILE	C-N-CA	-12.18	91.26	121.70
1	AA	1498	U	C2'-C3'-O3'	11.78	135.42	109.50

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1049	U	C3'
1	AA	1399	C	C3'
1	AA	1498	U	C3'
35	BA	1300	U	C3'
35	BA	1799	G	C3'

5 of 316 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	19	C	Sidechain
1	AA	28	G	Sidechain
1	AA	96	U	Sidechain



## 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	AA	32329	0	16318	2581	0
2	AB	1901	0	1951	513	1
3	AC	1613	0	1677	306	0
4	AD	1703	0	1767	335	0
5	AE	1147	0	1207	231	0
6	AF	843	0	857	144	0
7	AG	1257	0	1296	177	0
8	AH	1116	0	1177	205	0
9	AI	1011	0	1043	205	0
10	AJ	795	0	840	196	0
11	AK	885	0	904	152	0
12	AL	971	0	1057	217	0
13	AM	988	0	1059	192	0
14	AN	492	0	533	153	0
15	AO	734	0	771	229	0
16	AP	701	0	720	131	0
17	AQ	824	0	891	158	0
18	AR	574	0	644	122	0
19	AS	630	0	652	209	0
20	AT	763	0	861	150	0
21	AU	209	0	221	48	0
22	AV	1640	0	837	194	0
23	AX	192	0	99	22	0
24	AY	3934	0	3922	1256	0
25	B0	662	0	688	138	0
26	B1	732	0	808	131	0
27	B2	598	0	653	126	0
28	B3	468	0	523	108	0
29	B4	341	0	339	89	0
30	B5	459	0	480	131	0
31	B6	433	0	461	109	0
32	B7	419	0	467	110	0
33	B8	508	0	576	154	0
34	B9	307	0	338	70	0
35	BA	62477	0	31497	5291	0
36	BB	2551	0	1295	230	0
37	BC	1742	0	1794	377	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	2145	0	2234	780	0
39	BE	1564	0	1629	448	0
40	BF	1624	0	1677	415	0
41	BG	1474	0	1535	340	0
42	BH	1189	0	1247	282	0
43	BJ	654	0	157	36	0
44	BK	701	0	168	41	0
45	BN	1105	0	1180	270	0
46	BO	933	0	996	182	0
47	BP	1114	0	1187	361	0
48	BQ	1122	0	1179	291	0
49	BR	960	0	1021	236	0
50	BS	771	0	832	206	0
51	BT	1142	0	1202	332	0
52	BU	958	0	1015	317	0
53	BV	779	0	852	219	0
54	BW	896	0	953	173	0
55	BX	726	0	778	114	0
56	BY	776	0	870	193	0
57	BZ	1403	0	1432	371	0
58	AY	32	0	14	11	0
All	All	151017	0	103381	18980	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 75.

The worst 5 of 18980 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)
24:AY:111:MET:CE	24:AY:139:THR:HG23	1.18	1.62
24:AY:331:LEU:CD2	24:AY:379:PHE:HD2	1.19	1.51
24:AY:331:LEU:HD22	24:AY:379:PHE:CD2	1.46	1.47
37:BC:127:MET:SD	37:BC:127:MET:CG	2.03	1.45
24:AY:135:THR:CG2	24:AY:136:PRO:HD2	1.44	1.45

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:62:ALA:O	37:BC:30:LYS:O[2_656]	2.18	0.02



## 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	
2	AB	233/256 (91%)	110 (47%)	62 (27%)	61 (26%)	0	1
3	AC	205/239 (86%)	134 (65%)	39 (19%)	32 (16%)	0	5
4	AD	206/209 (99%)	131 (64%)	51 (25%)	24 (12%)	0	9
5	AE	149/162 (92%)	108 (72%)	31 (21%)	10 (7%)	1	25
6	AF	99/101 (98%)	67 (68%)	24 (24%)	8 (8%)	1	18
7	AG	153/156 (98%)	85 (56%)	44 (29%)	24 (16%)	0	5
8	AH	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	0	9
9	AI	125/128 (98%)	78 (62%)	28 (22%)	19 (15%)	0	5
10	AJ	97/105 (92%)	60 (62%)	23 (24%)	14 (14%)	0	6
11	AK	117/129 (91%)	72 (62%)	32 (27%)	13 (11%)	0	10
12	AL	123/135 (91%)	66 (54%)	33 (27%)	24 (20%)	0	3
13	AM	123/126 (98%)	63 (51%)	31 (25%)	29 (24%)	0	1
14	AN	58/61 (95%)	33 (57%)	12 (21%)	13 (22%)	0	1
15	AO	86/89 (97%)	59 (69%)	21 (24%)	6 (7%)	1	23
16	AP	82/88 (93%)	55 (67%)	17 (21%)	10 (12%)	0	8
17	AQ	98/105 (93%)	82 (84%)	10 (10%)	6 (6%)	2	27
18	AR	68/88 (77%)	37 (54%)	18 (26%)	13 (19%)	0	3
19	AS	77/93 (83%)	42 (54%)	18 (23%)	17 (22%)	0	1
20	AT	97/106 (92%)	46 (47%)	32 (33%)	19 (20%)	0	3
21	AU	23/27 (85%)	11 (48%)	8 (35%)	4 (17%)	0	4
24	AY	488/529 (92%)	314 (64%)	88 (18%)	86 (18%)	0	3
25	B0	82/85 (96%)	64 (78%)	9 (11%)	9 (11%)	0	10
26	B1	92/98 (94%)	63 (68%)	16 (17%)	13 (14%)	0	6
27	B2	69/72 (96%)	38 (55%)	22 (32%)	9 (13%)	0	7
28	B3	58/60 (97%)	38 (66%)	15 (26%)	5 (9%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	B4	43/71 (61%)	26 (60%)	9 (21%)	8 (19%)	0	3
30	B5	57/60 (95%)	34 (60%)	11 (19%)	12 (21%)	0	2
31	B6	48/54 (89%)	18 (38%)	16 (33%)	14 (29%)	0	0
32	B7	47/49 (96%)	29 (62%)	10 (21%)	8 (17%)	0	4
33	B8	62/65 (95%)	30 (48%)	16 (26%)	16 (26%)	0	1
34	B9	35/37 (95%)	19 (54%)	10 (29%)	6 (17%)	0	4
37	BC	226/229 (99%)	158 (70%)	39 (17%)	29 (13%)	0	7
38	BD	273/276 (99%)	195 (71%)	46 (17%)	32 (12%)	0	9
39	BE	203/206 (98%)	99 (49%)	48 (24%)	56 (28%)	0	0
40	BF	206/210 (98%)	134 (65%)	35 (17%)	37 (18%)	0	3
41	BG	179/182 (98%)	95 (53%)	47 (26%)	37 (21%)	0	2
42	BH	154/180 (86%)	111 (72%)	23 (15%)	20 (13%)	0	7
43	BJ	1/173 (1%)	1 (100%)	0	0	100	100
45	BN	137/140 (98%)	78 (57%)	28 (20%)	31 (23%)	0	1
46	BO	120/122 (98%)	84 (70%)	23 (19%)	13 (11%)	0	11
47	BP	144/150 (96%)	70 (49%)	37 (26%)	37 (26%)	0	1
48	BQ	139/141 (99%)	79 (57%)	40 (29%)	20 (14%)	0	6
49	BR	115/118 (98%)	69 (60%)	27 (24%)	19 (16%)	0	4
50	BS	97/112 (87%)	41 (42%)	23 (24%)	33 (34%)	0	0
51	BT	136/146 (93%)	75 (55%)	31 (23%)	30 (22%)	0	1
52	BU	115/118 (98%)	59 (51%)	27 (24%)	29 (25%)	0	1
53	BV	99/101 (98%)	56 (57%)	21 (21%)	22 (22%)	0	1
54	BW	111/113 (98%)	72 (65%)	25 (22%)	14 (13%)	0	8
55	BX	91/96 (95%)	55 (60%)	27 (30%)	9 (10%)	1	13
56	BY	99/110 (90%)	33 (33%)	36 (36%)	30 (30%)	0	0
57	BZ	174/206 (84%)	88 (51%)	48 (28%)	38 (22%)	0	1
All	All	6255/6850 (91%)	3758 (60%)	1413 (23%)	1084 (17%)	0	4

5 of 1084 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL

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Mol	Chain	Res	Type
2	AB	18	GLY
2	AB	19	HIS
2	AB	24	TRP

### 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	
2	AB	202/220 (92%)	152 (75%)	50 (25%)	1	7
3	AC	160/188 (85%)	133 (83%)	27 (17%)	2	19
4	AD	180/181 (99%)	154 (86%)	26 (14%)	4	28
5	AE	115/123 (94%)	94 (82%)	21 (18%)	2	15
6	AF	90/90 (100%)	76 (84%)	14 (16%)	3	24
7	AG	126/127 (99%)	114 (90%)	12 (10%)	11	46
8	AH	119/119 (100%)	101 (85%)	18 (15%)	3	25
9	AI	98/99 (99%)	82 (84%)	16 (16%)	3	21
10	AJ	88/92 (96%)	71 (81%)	17 (19%)	2	13
11	AK	90/99 (91%)	73 (81%)	17 (19%)	2	14
12	AL	104/111 (94%)	86 (83%)	18 (17%)	2	18
13	AM	99/101 (98%)	79 (80%)	20 (20%)	1	12
14	AN	49/50 (98%)	36 (74%)	13 (26%)	0	5
15	AO	79/80 (99%)	52 (66%)	27 (34%)	0	2
16	AP	72/74 (97%)	64 (89%)	8 (11%)	8	39
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	10	46
18	AR	61/77 (79%)	54 (88%)	7 (12%)	7	37
19	AS	69/80 (86%)	58 (84%)	11 (16%)	3	23
20	AT	76/82 (93%)	69 (91%)	7 (9%)	11	48
21	AU	19/22 (86%)	17 (90%)	2 (10%)	8	41
24	AY	427/453 (94%)	308 (72%)	119 (28%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	B0	66/67 (98%)	49 (74%)	17 (26%)	0	6
26	B1	78/83 (94%)	65 (83%)	13 (17%)	3	20
27	B2	66/67 (98%)	61 (92%)	5 (8%)	16	56
28	B3	51/52 (98%)	42 (82%)	9 (18%)	2	17
29	B4	39/63 (62%)	29 (74%)	10 (26%)	0	6
30	B5	51/52 (98%)	47 (92%)	4 (8%)	16	55
31	B6	49/52 (94%)	37 (76%)	12 (24%)	1	7
32	B7	41/42 (98%)	36 (88%)	5 (12%)	6	34
33	B8	53/55 (96%)	42 (79%)	11 (21%)	1	11
34	B9	34/34 (100%)	26 (76%)	8 (24%)	1	7
37	BC	180/181 (99%)	150 (83%)	30 (17%)	3	20
38	BD	217/218 (100%)	150 (69%)	67 (31%)	0	3
39	BE	165/166 (99%)	134 (81%)	31 (19%)	2	14
40	BF	165/166 (99%)	142 (86%)	23 (14%)	4	30
41	BG	155/156 (99%)	127 (82%)	28 (18%)	2	16
42	BH	128/148 (86%)	90 (70%)	38 (30%)	0	4
43	BJ	1/1 (100%)	1 (100%)	0	100	100
45	BN	117/119 (98%)	99 (85%)	18 (15%)	3	24
46	BO	100/100 (100%)	89 (89%)	11 (11%)	8	39
47	BP	112/116 (97%)	91 (81%)	21 (19%)	2	14
48	BQ	111/111 (100%)	87 (78%)	24 (22%)	1	9
49	BR	100/101 (99%)	78 (78%)	22 (22%)	1	9
50	BS	77/88 (88%)	60 (78%)	17 (22%)	1	9
51	BT	120/127 (94%)	96 (80%)	24 (20%)	1	12
52	BU	92/94 (98%)	74 (80%)	18 (20%)	1	13
53	BV	82/82 (100%)	65 (79%)	17 (21%)	1	11
54	BW	91/92 (99%)	81 (89%)	10 (11%)	8	39
55	BX	74/78 (95%)	63 (85%)	11 (15%)	4	26
56	BY	84/91 (92%)	69 (82%)	15 (18%)	2	16
57	BZ	155/179 (87%)	117 (76%)	38 (24%)	1	7
All	All	5271/5546 (95%)	4255 (81%)	1016 (19%)	2	13



5 of 1016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	B0	5	LYS
37	BC	108	MET
53	BV	91	TYR
25	B0	80	HIS
30	B5	25	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
25	B0	70	GLN
33	B8	35	GLN
53	BV	89	GLN
26	B1	45	ASN
28	B3	52	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	273 (18%)	58 (3%)
22	AV	76/77 (98%)	36 (47%)	3 (3%)
23	AX	8/9 (88%)	5 (62%)	0
35	BA	2900/2915 (99%)	654 (22%)	73 (2%)
36	BB	118/122 (96%)	24 (20%)	1 (0%)
All	All	4605/4645 (99%)	992 (21%)	135 (2%)

5 of 992 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 135 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	50	U
35	BA	603	A

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Mol	Chain	Res	Type
35	BA	2282	G
35	BA	71	A
35	BA	331	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	$\# Z  > 2$
58	GCP	AY	1000	-	26,34,34	2.52	6 (23%)	34,54,54	2.09	10 (29%)

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
58	GCP	AY	1000	-	-	0/15/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	PG-O2G	-2.64	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	PG-O1G	2.04	1.54	1.50
58	AY	1000	GCP	C4-N3	4.53	1.42	1.35
58	AY	1000	GCP	C2-N1	4.89	1.44	1.35
58	AY	1000	GCP	PB-O3A	5.74	1.64	1.58

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AY	1000	GCP	C5-C6-N1	-6.33	114.93	123.59
58	AY	1000	GCP	N3-C2-N1	-3.96	121.42	127.44
58	AY	1000	GCP	PA-O3A-PB	-2.84	124.74	132.73
58	AY	1000	GCP	O3G-PG-O1G	-2.77	105.32	112.40
58	AY	1000	GCP	C1'-N9-C4	-2.54	123.10	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AY	1000	GCP	11	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1504/1522 (98%)	-0.09	34 (2%) 64 48	52, 140, 199, 200	0
2	AB	235/256 (91%)	-0.41	2 (0%) 85 74	40, 110, 177, 200	0
3	AC	207/239 (86%)	-0.47	2 (0%) 84 72	37, 117, 174, 200	0
4	AD	208/209 (99%)	0.24	13 (6%) 23 14	48, 158, 200, 200	0
5	AE	151/162 (93%)	-0.16	3 (1%) 68 53	38, 112, 171, 200	0
6	AF	101/101 (100%)	-0.57	0 100 100	59, 135, 188, 200	0
7	AG	155/156 (99%)	-0.34	4 (2%) 59 43	46, 128, 189, 200	0
8	AH	138/138 (100%)	-0.08	6 (4%) 39 25	36, 114, 180, 200	0
9	AI	127/128 (99%)	-0.09	2 (1%) 74 60	32, 121, 172, 200	0
10	AJ	99/105 (94%)	0.41	10 (10%) 9 6	32, 125, 191, 200	0
11	AK	119/129 (92%)	-0.09	5 (4%) 40 26	40, 116, 179, 200	0
12	AL	125/135 (92%)	0.27	5 (4%) 42 28	45, 119, 192, 200	0
13	AM	125/126 (99%)	0.30	11 (8%) 12 8	64, 127, 200, 200	0
14	AN	60/61 (98%)	-0.26	0 100 100	28, 104, 172, 200	0
15	AO	88/89 (98%)	0.06	4 (4%) 37 24	59, 130, 188, 200	0
16	AP	84/88 (95%)	1.05	18 (21%) 1 1	79, 156, 200, 200	0
17	AQ	100/105 (95%)	0.71	13 (13%) 5 4	66, 141, 200, 200	0
18	AR	70/88 (79%)	0.01	3 (4%) 39 25	59, 124, 176, 200	0
19	AS	79/93 (84%)	0.14	3 (3%) 44 30	57, 118, 197, 200	0
20	AT	99/106 (93%)	0.56	9 (9%) 11 7	87, 153, 200, 200	0
21	AU	25/27 (92%)	0.72	4 (16%) 3 2	46, 117, 175, 185	0
22	AV	77/77 (100%)	-0.62	1 (1%) 79 65	77, 151, 189, 199	0
23	AX	9/9 (100%)	0.20	0 100 100	79, 156, 192, 199	0
24	AY	496/529 (93%)	0.45	53 (10%) 8 5	71, 170, 202, 202	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	B0	84/85 (98%)	1.14	19 (22%) 1 1	37, 118, 194, 200	0
26	B1	94/98 (95%)	0.58	8 (8%) 13 9	65, 143, 197, 200	0
27	B2	71/72 (98%)	0.14	7 (9%) 9 6	101, 153, 200, 200	0
28	B3	60/60 (100%)	0.67	5 (8%) 14 9	54, 126, 198, 200	0
29	B4	45/71 (63%)	-0.03	3 (6%) 21 12	108, 174, 200, 200	0
30	B5	59/60 (98%)	0.40	8 (13%) 4 3	62, 150, 200, 200	0
31	B6	50/54 (92%)	0.80	10 (20%) 1 1	62, 139, 186, 200	0
32	B7	49/49 (100%)	0.58	5 (10%) 9 6	78, 153, 197, 200	0
33	B8	64/65 (98%)	0.16	2 (3%) 52 36	66, 129, 179, 200	0
34	B9	37/37 (100%)	1.41	11 (29%) 1 1	71, 142, 178, 194	0
35	BA	2901/2915 (99%)	0.13	108 (3%) 45 30	51, 159, 201, 202	0
36	BB	119/122 (97%)	-0.42	0 100 100	66, 123, 172, 190	0
37	BC	228/229 (99%)	2.02	89 (39%) 0 1	87, 182, 200, 200	0
38	BD	275/276 (99%)	0.17	20 (7%) 18 11	40, 117, 175, 200	0
39	BE	205/206 (99%)	0.22	18 (8%) 12 8	51, 143, 199, 200	0
40	BF	208/210 (99%)	0.52	27 (12%) 5 4	51, 156, 200, 200	0
41	BG	181/182 (99%)	-0.06	4 (2%) 65 50	47, 134, 194, 200	0
42	BH	156/180 (86%)	0.33	14 (8%) 12 7	78, 165, 200, 200	0
43	BJ	1/173 (0%)	3.28	1 (100%) 0 0	174, 174, 174, 174	0
44	BK	0/147	-	-	-	-
45	BN	139/140 (99%)	0.03	2 (1%) 78 63	69, 131, 190, 200	0
46	BO	122/122 (100%)	0.48	15 (12%) 5 5	59, 133, 198, 200	0
47	BP	146/150 (97%)	0.86	21 (14%) 3 3	65, 147, 200, 200	0
48	BQ	141/141 (100%)	0.06	6 (4%) 39 25	20, 107, 171, 200	0
49	BR	117/118 (99%)	0.80	19 (16%) 3 2	81, 169, 200, 200	0
50	BS	99/112 (88%)	0.08	7 (7%) 19 11	49, 123, 194, 200	0
51	BT	138/146 (94%)	0.52	21 (15%) 3 2	89, 162, 200, 200	0
52	BU	117/118 (99%)	-0.02	3 (2%) 59 43	47, 121, 179, 200	0
53	BV	101/101 (100%)	0.83	16 (15%) 3 2	42, 146, 200, 200	0
54	BW	113/113 (100%)	1.32	35 (30%) 1 1	78, 165, 200, 200	0
55	BX	93/96 (96%)	1.12	23 (24%) 1 1	38, 167, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
56	BY	101/110 (91%)	1.53	32 (31%) 1 1	86, 169, 200, 200	0
57	BZ	176/206 (85%)	-0.26	1 (0%) 90 82	43, 122, 195, 200	0
All	All	10971/11642 (94%)	0.21	765 (6%) 19 11	20, 146, 200, 202	0

The worst 5 of 765 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BC	165	ASN	14.4
37	BC	173	ALA	12.1
37	BC	216	THR	11.8
28	B3	1	MET	10.8
24	AY	349	MET	10.7

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
58	GCP	AY	1000	32/32	0.82	0.23	-0.50	95,109,121,122	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.