



# wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 03:18 AM GMT

PDB ID : 2QBI  
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin and ribosome recycling factor (RRF). This file contains the 50S subunit of the first 70S ribosome, with gentamicin and RRF bound. The entire crystal structure contains two 70S ribosomes and is described in remark 400.  
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.  
Deposited on : 2007-06-17  
Resolution : 4.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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

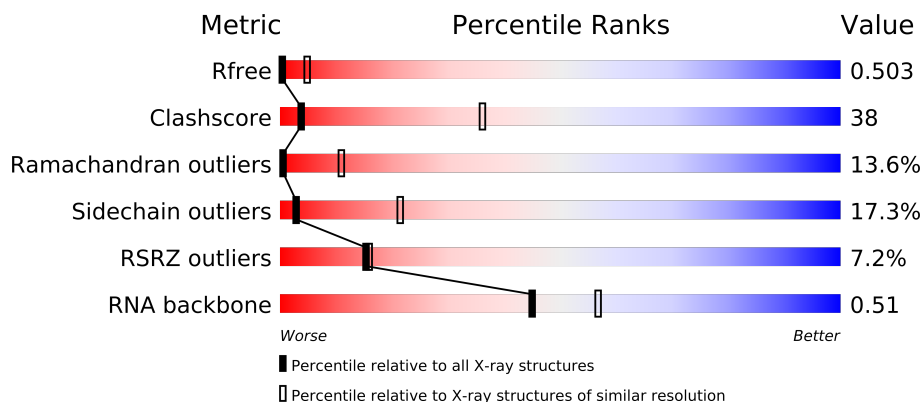
MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683



# 1 Overall quality at a glance

The reported resolution of this entry is 4.00 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))
$R_{free}$	66092	1035 (4.52-3.46)
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)
RNA backbone	1838	1018 (5.00-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	120	
2	B	2904	
3	I	141	
4	C	272	
5	D	209	
6	K	123	
7	P	114	
8	E	201	
9	Y	58	
10	0	56	
11	4	38	
12	1	54	

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Mol	Chain	Length	Quality of chain
13	3	64	
14	V	94	
15	2	46	
16	L	144	
17	M	136	
18	X	63	
19	H	149	
20	J	142	
21	N	127	
22	O	117	
23	Q	117	
24	S	110	
25	U	103	
26	F	178	
27	G	176	
28	R	103	
29	T	100	
30	Z	78	
31	W	84	
32	6	185	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
33	MG	B	2907	-	X
33	MG	B	2908	-	X
33	MG	B	2912	-	X
33	MG	B	2919	-	X
33	MG	B	2929	-	X
33	MG	B	2935	-	X
33	MG	B	2937	-	X
33	MG	B	2939	-	X
33	MG	B	2942	-	X
33	MG	B	2946	-	X
33	MG	B	2951	-	X
33	MG	B	2968	-	X
33	MG	B	2971	-	X
33	MG	B	2976	-	X
33	MG	B	2984	-	X
33	MG	B	2997	-	X
33	MG	B	3004	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	MG	B	3010	-	X
33	MG	B	3012	-	X
34	LLL	B	3015	-	X



## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 91765 atoms, of which 0 are hydrogen and 0 are deuterium.

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 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 3 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 6 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			



- Molecule 7 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	P	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 8 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 9 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Y	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 10 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 11 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 12 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 13 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 14 is a protein called 50S ribosomal protein L25.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	V	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 15 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	M	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 18 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 19 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	H	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 20 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	J	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 21 is a protein called 50S ribosomal protein L17.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	N	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	O	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 23 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Q	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	S	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	U	102	Total	C	N	O		0	0	0
			779	492	146	141				

- Molecule 26 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	F	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 27 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	G	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 28 is a protein called 50S ribosomal protein L21.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	T	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 30 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Z	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	W	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 32 is a protein called 50S ribosomal protein RRF.

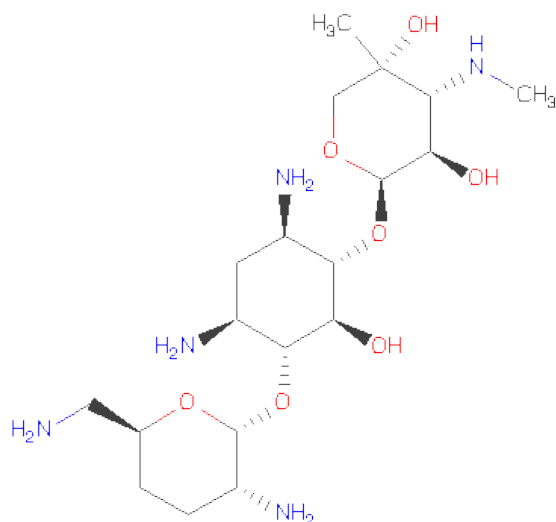
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	110	Total	Mg	0	0
			110	110		

- Molecule 34 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C<sub>19</sub>H<sub>39</sub>N<sub>5</sub>O<sub>7</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	N	O	0	0
			31	19	5	7		

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	4	1	Total	Zn	0	0
			1	1		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	B	493	Total	O	0	0
			493	493		
36	C	6	Total	O	0	0
			6	6		
36	D	1	Total	O	0	0
			1	1		
36	E	2	Total	O	0	0
			2	2		
36	L	3	Total	O	0	0
			3	3		
36	T	1	Total	O	0	0
			1	1		

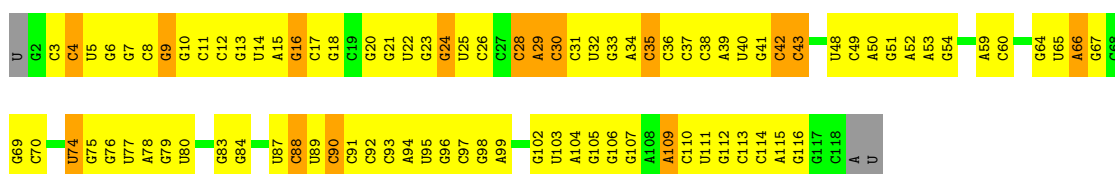


### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

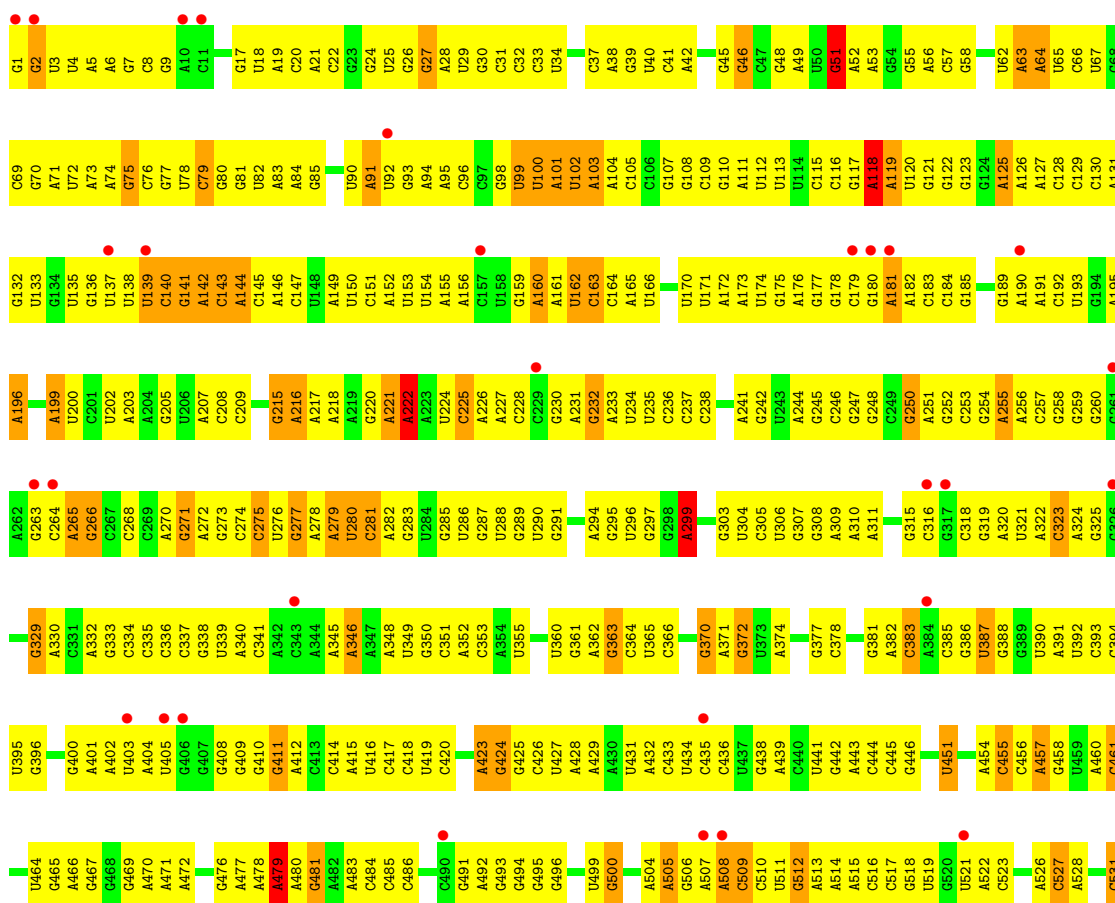
#### • Molecule 1: 5S rRNA

Chain A:



#### • Molecule 2: 23S rRNA

Chain B:



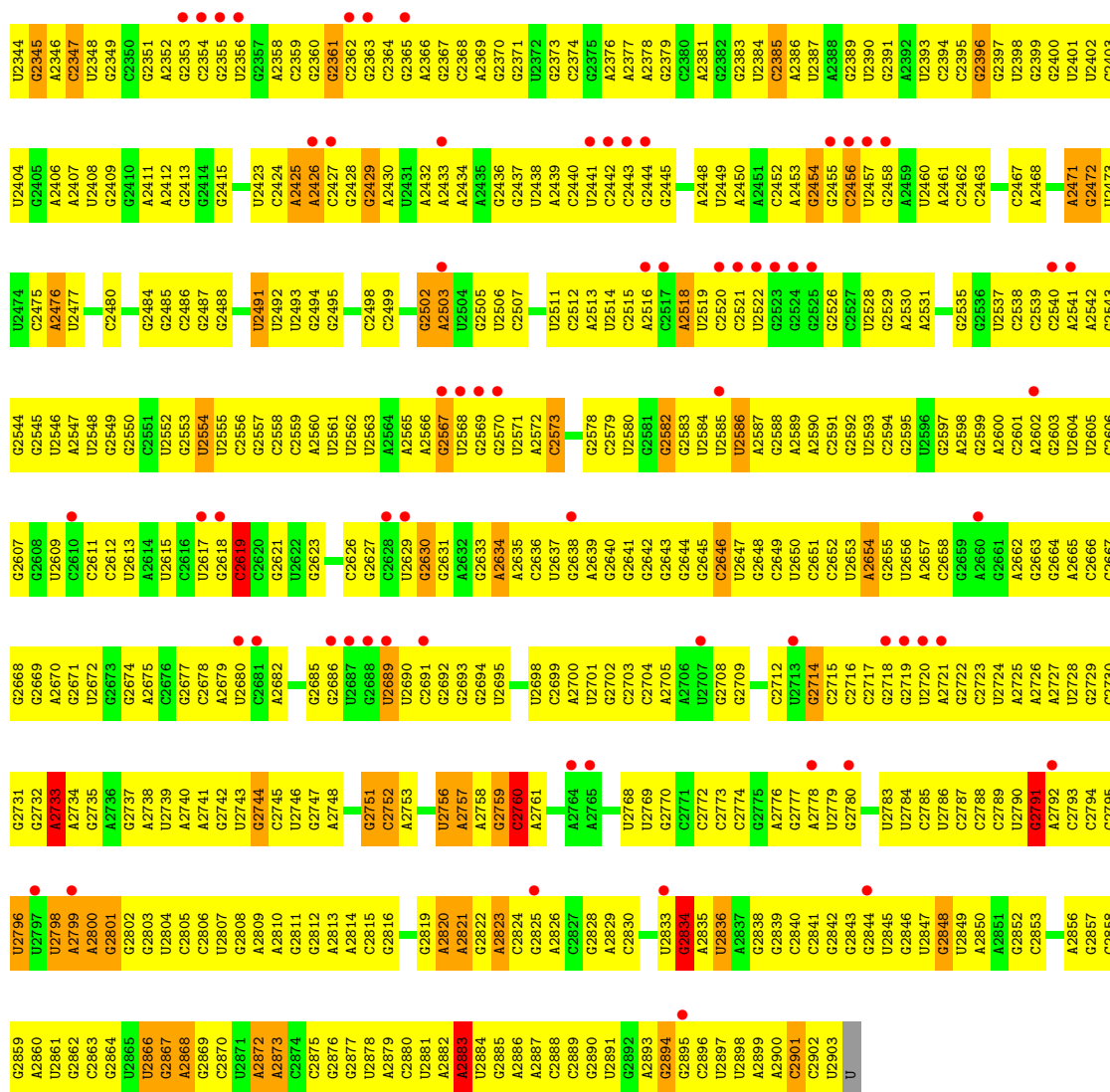


A1385	C1319	G1252	G1186	G1051	A980	A917	U850	G784	C719	U657	U596	A532
C1386	C1320	A1253	G1187	A981	A982	A918	C851	G785	U720	U658	G597	G533
A1387	A1321	U1254	U1119	C982	C983	U919	U852	U786	U721	U659	G598	A534
G1388	A1322	U1255	C1120	A1054	A983	U919	U853	C787	A722	G660	U599	G535
G1389	G1256	G1257	G1123	A1057	A984	A920	C854			A661	G601	A538
G1390	G1257	G1258	G1124	A1058	C985	C921	G855	C791	G725	G664	A602	G539
U1391	U1258	U1259	G1125	U1058	C986	C922	G856	A794	G726	U665	A603	C540
A1392	U1325	G1260	G1126	U1059	C987	C923	G857	C795	A727	U666	G604	A541
A1393	U1327	A1194	A1126	U1060	A987		U858	C796	G728	A667		
U1394	A1328	C1195	U1130	U1061	A988	A927	U859	C797	G729	A668	U607	C544
A1395	U1329	G1196	G1131	G1062	A989	U928	U860	C798	A730	A669	A608	U545
U1396	U1330	U1197	U1132	G1063	C991	U929	G861	C799	C731	A670	A609	U546
U1397	G1331	U1198	A1133	G1064	C992	U930	G862	G798	C732	C671	C610	A547
C1398	G1332	U1199	A1134	U1065	C993	U931	A863	G799	G733	C672	C611	G548
C1399	G1333	U1200	A1135	G1068	C994	U932	G864		A734	C673	G612	G549
U1400	G1334	U1201	C1136	C995	A996	U933	C865	U803	A735	C674	A613	C550
G1401	C1335	U1202	G1137	A1069		U934	A866	G805	C736	G675	A614	
U1402	A1336	U1203	G1138	A1070		C935	C867	C806	C737	A675		
A1403	G1337	A1204	G1139	A1071	A1000	A936	U868	U807	G738	A676	U615	G553
A1404	G1338	A1205	G1140	C1072	A1001	C937	G869	G808	A739	A677	A616	U554
U1405	G1339	U1273	C1141	C1076	G1002	G938	U870	G809	C740	C678	G617	G555
U1406	U1274	A1275	U1142	A1077		G939	U871	U810	A741	C679	U618	A556
G1407	G1341	A1276	A1143	U1078	C1007	G940	U872	U811	A742	C680	G619	C557
G1408		A1277	A1144	U1079		A941	C873	C812	A743	G681	G620	U558
	G1345	G1277	C1145	A1080	A1010	A942	G874	U813	U744	G682	A621	G559
U1411	G1346	C1278	C1146	A1081	G1011	A943	C875	C814	G745	U683	G622	C560
U1412	A1347	G1279	U1147	U1082	U1012	A944	C876	C815	U746	G684	C623	G561
A1413	C1348	G1280	A1148	U1083	C1013	A945	C877	C816	A747	G685	C624	U562
	C1349	U1281	G1149	U1084	A1014	A946	C878	C817	G748	U686	G625	A563
G1416	C1350	U1282	G1150	U1085	U1015	A947	G	C818		C687	A626	C564
C1417	C1351	G1283	C1151	A1086	G1016	C948	G	A819	U753	U688	A627	C565
U1418	U1352	U1284	A1152	A1087	G949		G	A820	U754	A689	G628	U566
A1419	A1353	A1285	C1153	A1088	G950	G949	G	A821	U755	G690	G629	U567
A1420	A1354	U1286	C1154	A1089	C951	C951	U	G822	U756	C691	G630	U568
G1421	G1355	A1287	C1155	U1090	A1020	G952	G	U823	G757	C692	A631	G570
G1422	G1356	U1288		A1091	C953	G954	A	U824	C758	A693	A632	U571
G1423	C1357	G1289	G1157	G1092	G955	U955	U	A825	G759	U694	A633	G572
G1424	G1358	C1291	C1161	C1092	U1023		C	U826	G760	G695	C634	U573
G1425	A1359	G1292	G1162	U1097	G1024	G956	C	U827	A761	G696	C635	A574
G1426		C1293	G1163	U1098	G1025	C957	C	U828	U762	G697	G636	A575
A1427	A1365	U1294	A1164	A1099	U1026	U958	C	A829	G763	C698	A637	U576
C1428	A1366	U1295	A1165	G1099	A1027	A959	G	G830	A764	A699	C638	U577
G1429	G1367	G1296	G1166	U1100	A1028	A960	A	U831	C765	G700	U639	G577
G1430	G1368	C1297	C1167	U1101	A1029	C961	C	U832	U766	G701	C640	
A1431	G1369	C1298		G1102		G962	U	A833	U767	U702	U641	U580
G1432	C1370	G1299	G1171	A1103	U1032	U963	U	G834	G768	U703	U642	C581
A1433	G1371	U1300	C1172	C1104	U1033	C964	A	C835		G704	A643	A582
A1434	U1372	A1301	U1173	U1105	C965	C965	C	G836	G771	A705	A644	G583
G1435	A1373	A1302	U1174	G1106	G1038	U967	C898	C837	C772	A706	C645	C584
G1436	G1374		A1175	G1107	A1039	U967	A899	C838	U773	G707	U646	G585
C1437	U1375	U1240	U1176	U1108	U1039	C968		U839	G774	G708	G647	A586
U1438	G1376	U1241	U1177	C1109	G1041	G969	G904	C840	G775	U709	C587	C587
A1439	G1377	A1244	C1178	G1110	G1042	U970	A905	C841	G776	U710	G649	U588
U1440	U1312	G1245	G1179	A1111	C1043	G971		U842	G777	G711	C650	U589
G1441	U1313	A1246	U1180	G1112	C1044	A972	A909		G778	G712	G651	A590
U1442	G1314	A1247	U1181	U1113	U1045	A973	A910	A845	U779	G713	U652	U591
U1443	C1315	G1248	G1182	C1114	A1046	G974	A911	U846	G780	A716	U653	A592
G1444	U1316	U1249	U1183	G1115	G1047	G975	C912	U847	A781	C717	A654	U593
G1445	G1317	G1250	U1184	G1116	G1047	A976	U913	C848	A782	U718	A655	U594
C1446	A1384	U1318	G1185	C1117	A1050	A979	G914	A849	A783	A718	G656	C595



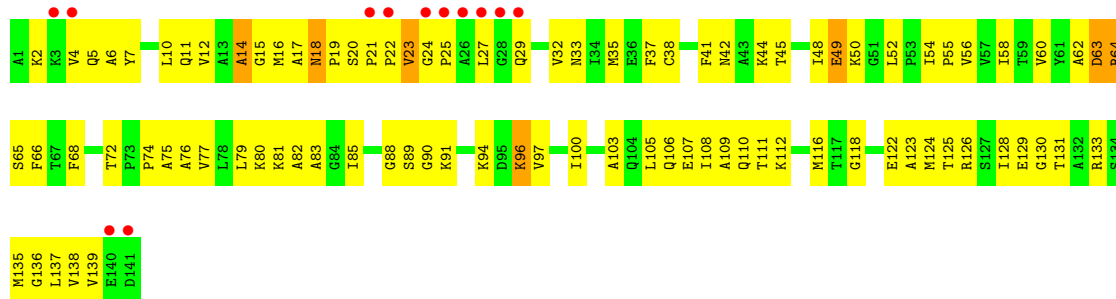
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• Molecule 3: 50S ribosomal protein L11

Chain I:

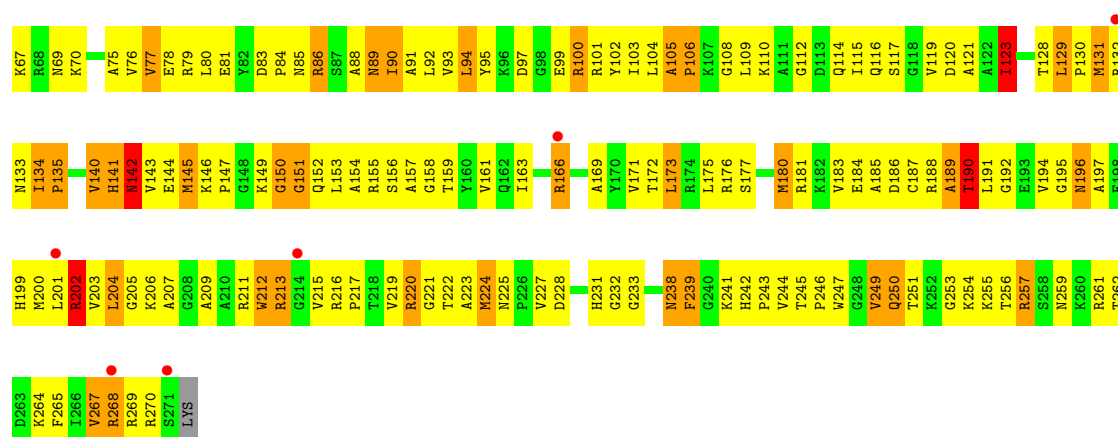


• Molecule 4: 50S ribosomal protein L2

Chain C:

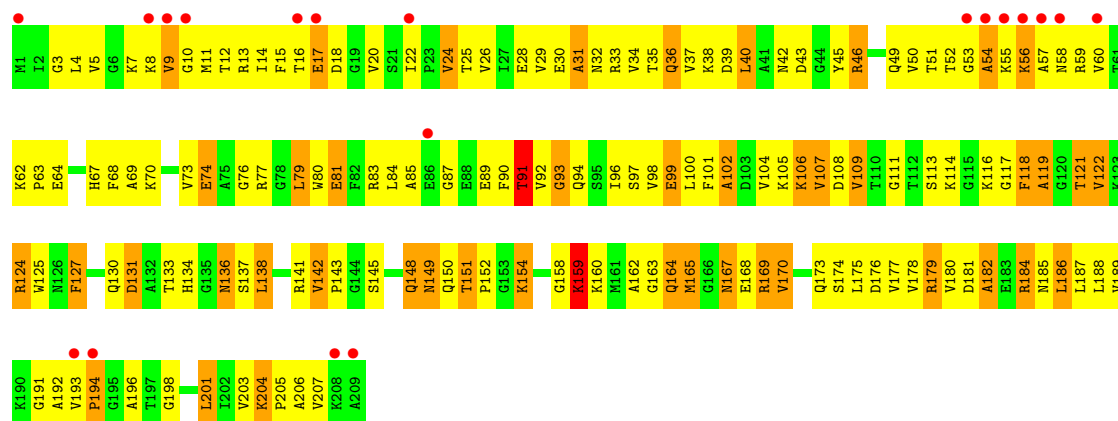






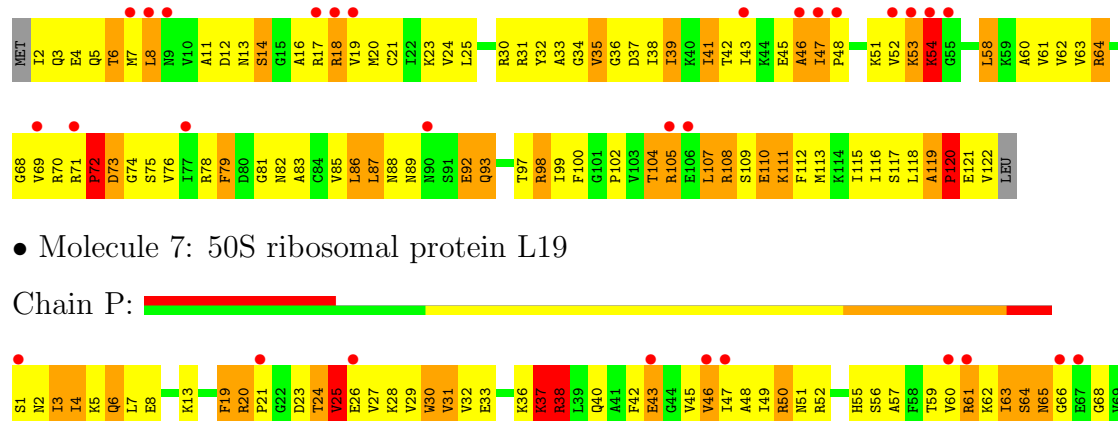
• Molecule 5: 50S ribosomal protein L3

Chain D:



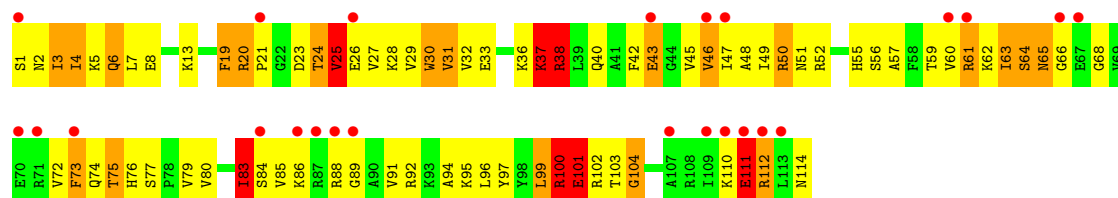
• Molecule 6: 50S ribosomal protein L14

Chain K:



• Molecule 7: 50S ribosomal protein L19

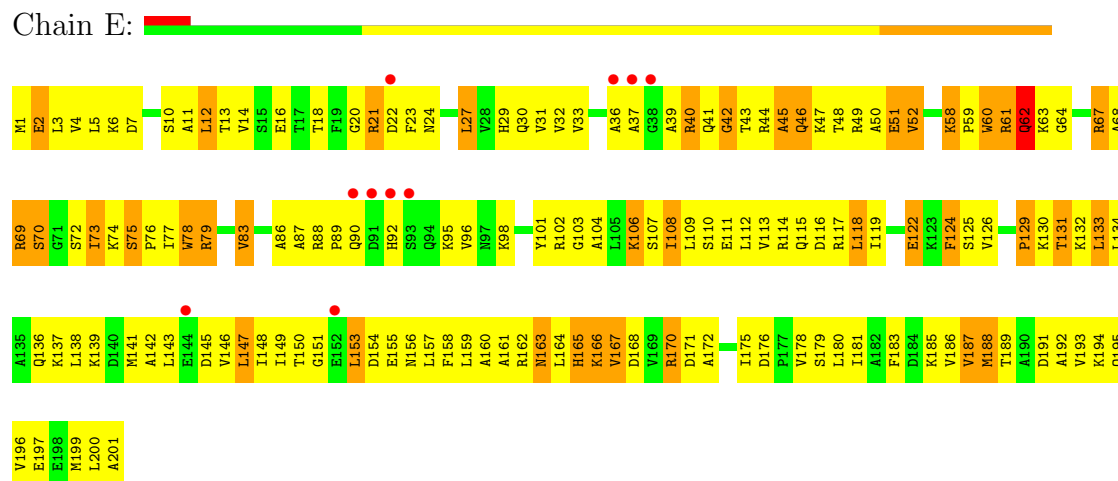
Chain P:



• Molecule 8: 50S ribosomal protein L4

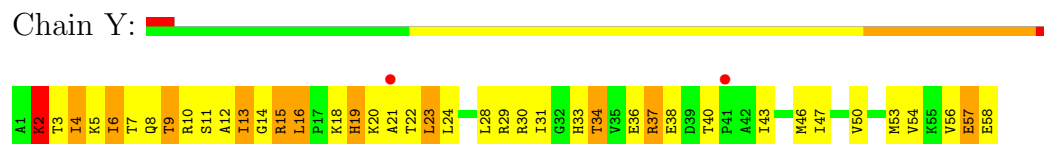


## Chain E:



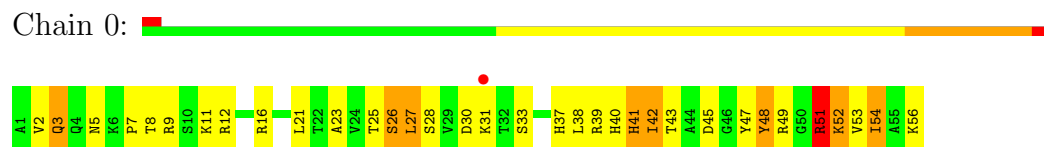
- Molecule 9: 50S ribosomal protein L30

Chain Y:



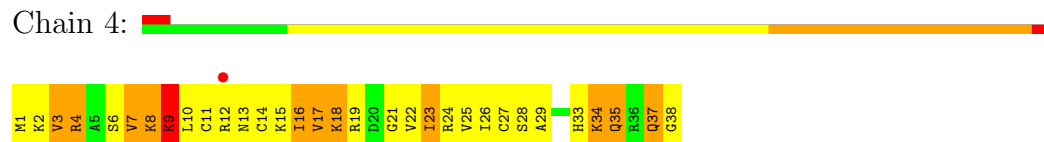
- Molecule 10: 50S ribosomal protein L32

## Chain 0:



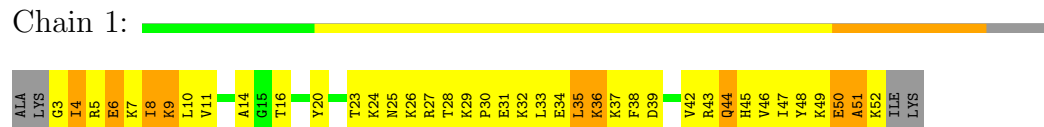
- Molecule 11: 50S ribosomal protein L36

Chain 4:



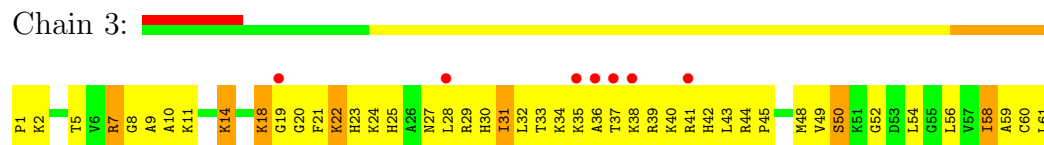
- Molecule 12: 50S ribosomal protein L33

Chain 1:



- Molecule 13: 50S ribosomal protein L35

Chain 3:

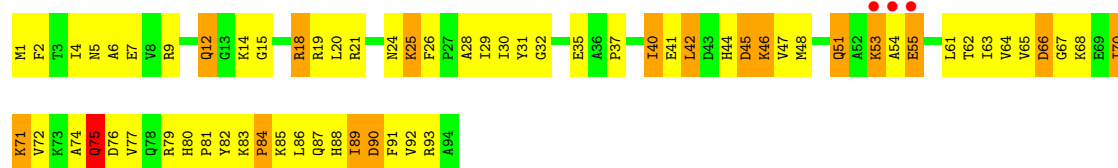


- Molecule 14: 50S ribosomal protein L25

Chain V:

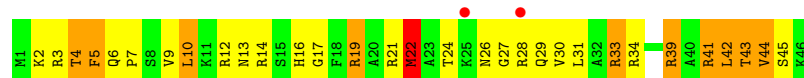






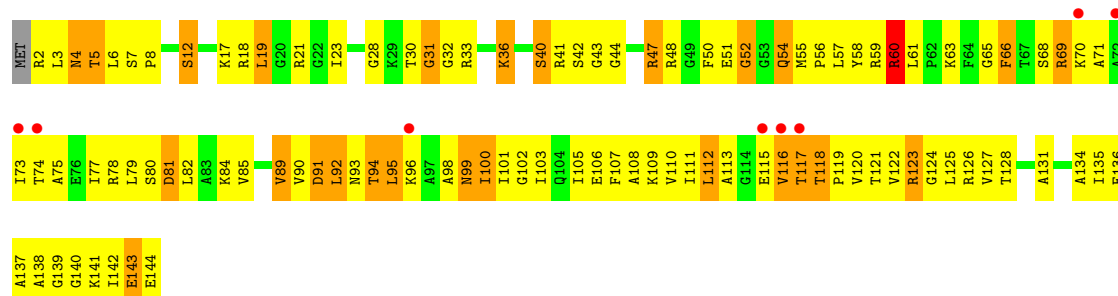
• Molecule 15: 50S ribosomal protein L34

Chain 2:



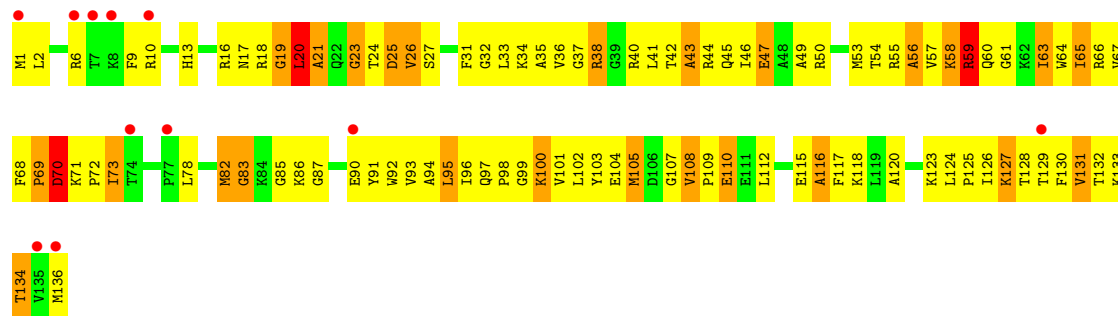
• Molecule 16: 50S ribosomal protein L15

Chain L:



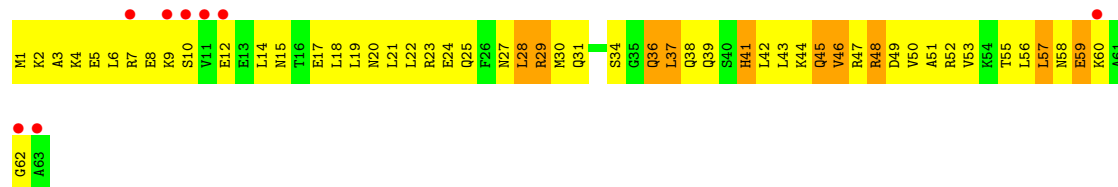
• Molecule 17: 50S ribosomal protein L16

Chain M:



• Molecule 18: 50S ribosomal protein L29

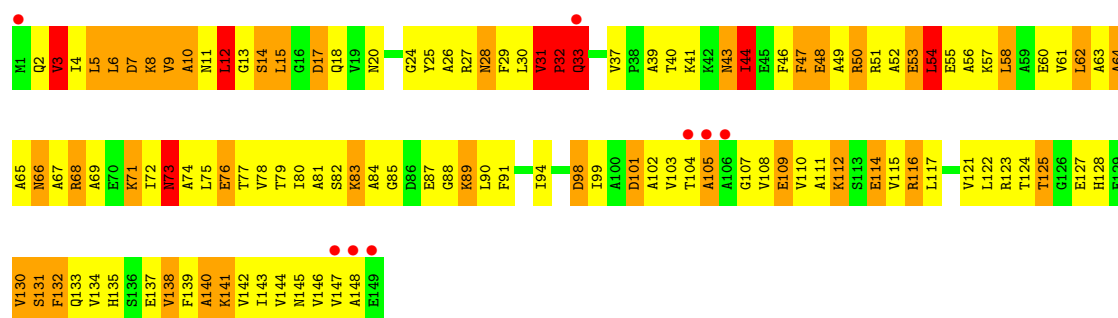
Chain X:



• Molecule 19: 50S ribosomal protein L9

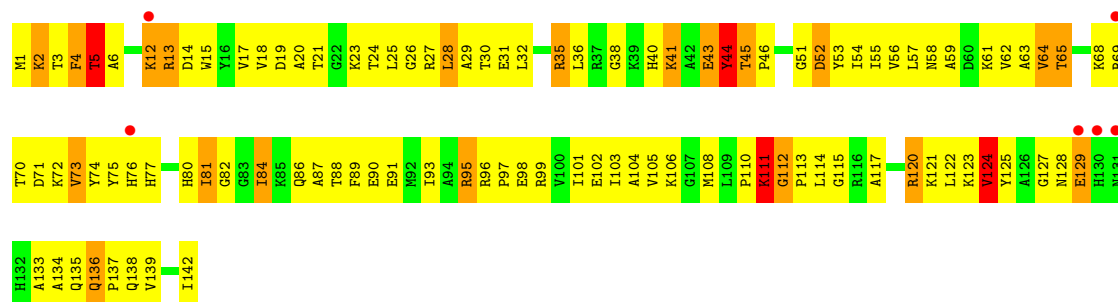
Chain H:





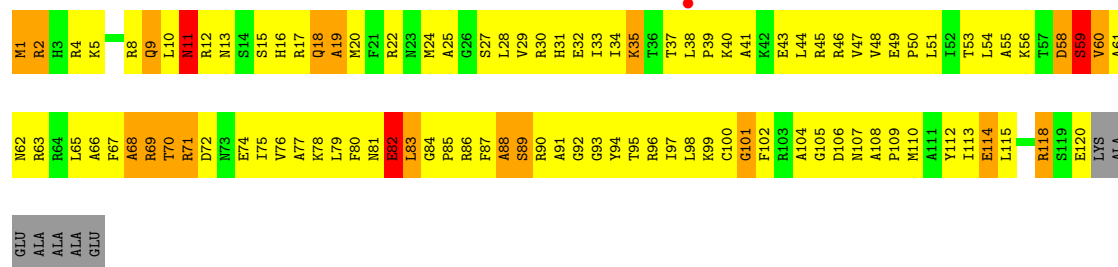
- Molecule 20: 50S ribosomal protein L13

Chain J:



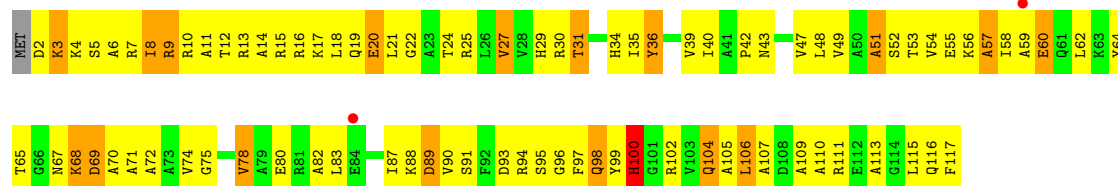
- Molecule 21: 50S ribosomal protein L17

Chain N:



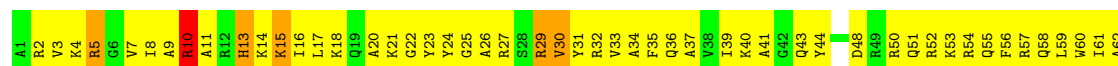
- Molecule 22: 50S ribosomal protein L18

Chain O:



- Molecule 23: 50S ribosomal protein L20

Chain Q:







• Molecule 24: 50S ribosomal protein L22

Chain S:



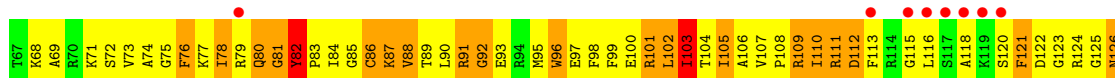
• Molecule 25: 50S ribosomal protein L24

Chain U:



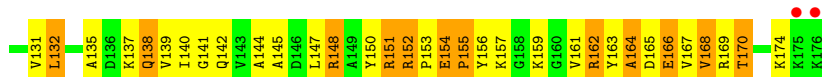
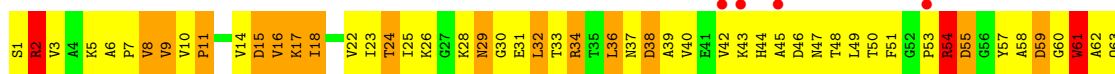
• Molecule 26: 50S ribosomal protein L5

Chain F:



• Molecule 27: 50S ribosomal protein L6

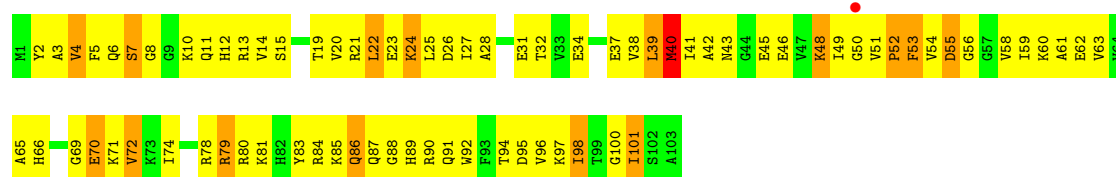
Chain G:



• Molecule 28: 50S ribosomal protein L21

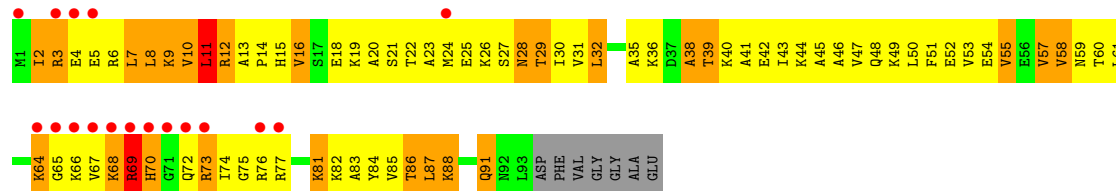


Chain R:



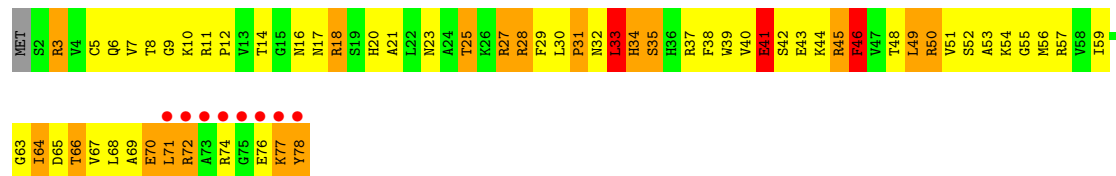
- Molecule 29: 50S ribosomal protein L23

Chain T:



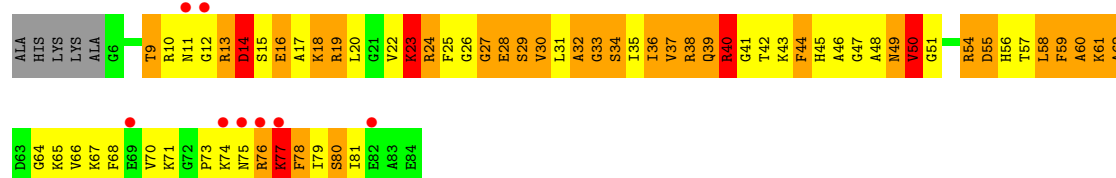
- Molecule 30: 50S ribosomal protein L28

Chain Z:



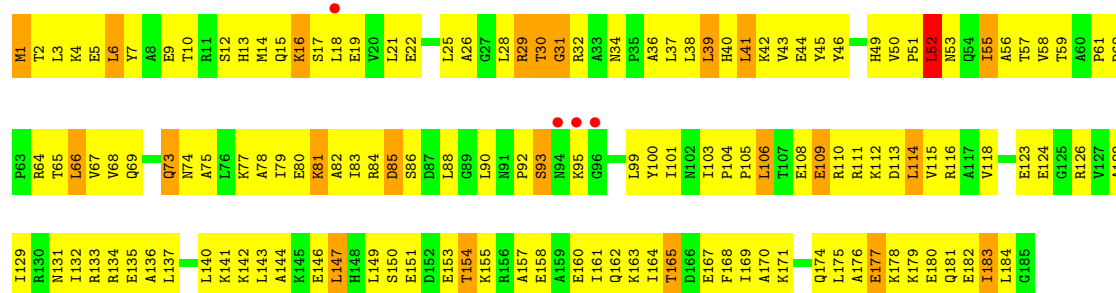
- Molecule 31: 50S ribosomal protein L27

Chain W:



- Molecule 32: 50S ribosomal protein RRF

Chain 6:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.54Å 378.89Å 736.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 138.07 – 4.15	Depositor EDS
% Data completeness (in resolution range)	87.4 (40.00-4.00) 87.4 (138.07-4.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 4.15Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.261 , 0.305 0.494 , 0.503	Depositor DCC
$R_{free}$ test set	16745 reflections (4.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	133.1	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 20.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 382905 reflections	Xtriage
$F_o, F_c$ correlation	0.61	EDS
Total number of atoms	91765	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.28	0/2803	0.76	1/4371 (0.0%)
2	B	0.28	6/68314 (0.0%)	0.78	48/106569 (0.0%)
3	I	0.24	0/1046	0.47	0/1410
4	C	0.22	0/2121	0.48	0/2852
5	D	0.24	0/1586	0.49	0/2134
6	K	0.24	0/939	0.55	0/1258
7	P	0.24	0/929	0.51	0/1242
8	E	0.24	0/1571	0.51	0/2113
9	Y	0.23	0/453	0.49	0/605
10	O	0.22	0/450	0.55	0/599
11	4	0.23	0/303	0.47	0/397
12	1	0.27	0/416	0.49	0/554
13	3	0.24	0/513	0.48	0/676
14	V	0.25	0/766	0.43	0/1025
15	2	0.25	0/380	0.48	0/498
16	L	0.23	0/1054	0.48	0/1403
17	M	0.25	0/1093	0.48	0/1460
18	X	0.24	0/510	0.53	0/677
19	H	0.25	0/1122	0.48	0/1515
20	J	0.24	0/1152	0.48	0/1551
21	N	0.24	0/973	0.51	0/1301
22	O	0.23	0/902	0.49	0/1209
23	Q	0.25	0/960	0.49	0/1278
24	S	0.22	0/864	0.52	0/1156
25	U	0.25	0/787	0.47	0/1051
26	F	0.26	0/1444	0.52	0/1937
27	G	0.23	0/1343	0.47	0/1816
28	R	0.25	0/829	0.50	0/1107
29	T	0.23	0/744	0.55	0/994
30	Z	0.25	0/635	0.51	0/848
31	W	0.28	0/603	0.51	0/797
32	6	0.23	0/1497	0.52	1/2017 (0.0%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.27	6/99102 (0.0%)	0.72	50/148420 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1086	A	C5-C6	-16.56	1.26	1.41
2	B	1088	A	C6-N1	-10.52	1.28	1.35
2	B	1060	U	C2-N3	7.84	1.43	1.37
2	B	1086	A	N7-C5	-6.61	1.35	1.39
2	B	1086	A	N3-C4	-6.44	1.30	1.34

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2204	G	O5'-P-OP2	-28.90	76.02	110.70
2	B	2791	G	O5'-P-OP1	-28.07	77.02	110.70
2	B	2204	G	O5'-P-OP1	18.05	132.37	110.70
2	B	2791	G	O5'-P-OP2	17.97	132.26	110.70
2	B	2790	U	OP1-P-O3'	14.57	137.26	105.20

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	118	A	Sidechain
2	B	221	A	Sidechain
2	B	222	A	Sidechain
2	B	232	G	Sidechain
2	B	51	G	Sidechain



## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2507	0	1270	106	0
2	B	60995	0	30678	2530	0
3	I	1032	0	1088	119	0
4	C	2082	0	2157	237	0
5	D	1565	0	1616	206	0
6	K	930	0	1000	122	0
7	P	917	0	965	98	0
8	E	1552	0	1619	194	0
9	Y	449	0	491	49	0
10	O	444	0	461	49	0
11	4	302	0	340	38	0
12	1	409	0	440	58	0
13	3	504	0	574	51	0
14	V	753	0	780	97	0
15	2	377	0	418	38	0
16	L	1045	0	1117	148	0
17	M	1074	0	1157	129	0
18	X	509	0	543	55	0
19	H	1111	0	1148	186	0
20	J	1129	0	1162	136	0
21	N	960	0	1000	130	0
22	O	892	0	923	94	0
23	Q	947	0	1022	171	0
24	S	857	0	922	101	0
25	U	779	0	834	114	0
26	F	1420	0	1460	220	0
27	G	1323	0	1374	218	0
28	R	816	0	839	113	0
29	T	738	0	807	125	0
30	Z	625	0	652	82	0
31	W	596	0	610	120	0
32	6	1478	0	1526	192	0
33	B	110	0	0	0	0
34	B	31	0	39	2	0
35	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	B	493	0	0	8	0
36	C	6	0	0	0	0
36	D	1	0	0	0	0
36	E	2	0	0	0	0
36	L	3	0	0	0	0
36	T	1	0	0	0	0
All	All	91765	0	61032	5804	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

The worst 5 of 5804 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:H:31:VAL:HB	19:H:32:PRO:HD2	1.23	1.17
16:L:143:GLU:HG2	16:L:144:GLU:H	1.09	1.10
2:B:322:A:H2'	8:E:163:ASN:HD21	1.02	1.10
2:B:855:G:H21	31:W:23:LYS:HG2	1.17	1.08
2:B:1203:U:H1'	16:L:4:ASN:HD21	1.12	1.07

There are no symmetry-related clashes.

## 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	
3	I	139/141 (99%)	120 (86%)	14 (10%)	5 (4%)	5	54
4	C	269/272 (99%)	155 (58%)	66 (24%)	48 (18%)	0	5
5	D	207/209 (99%)	122 (59%)	54 (26%)	31 (15%)	0	8
6	K	119/123 (97%)	78 (66%)	24 (20%)	17 (14%)	0	10
7	P	112/114 (98%)	61 (54%)	32 (29%)	19 (17%)	0	6
8	E	199/201 (99%)	125 (63%)	50 (25%)	24 (12%)	1	14
9	Y	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	0	54/56 (96%)	39 (72%)	8 (15%)	7 (13%)	0	12
11	4	36/38 (95%)	16 (44%)	10 (28%)	10 (28%)	0	1
12	1	48/54 (89%)	37 (77%)	7 (15%)	4 (8%)	1	27
13	3	62/64 (97%)	35 (56%)	21 (34%)	6 (10%)	1	21
14	V	92/94 (98%)	64 (70%)	22 (24%)	6 (6%)	2	36
15	2	44/46 (96%)	30 (68%)	10 (23%)	4 (9%)	1	24
16	L	141/144 (98%)	89 (63%)	31 (22%)	21 (15%)	0	8
17	M	134/136 (98%)	84 (63%)	29 (22%)	21 (16%)	0	7
18	X	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	12
19	H	147/149 (99%)	76 (52%)	46 (31%)	25 (17%)	0	6
20	J	140/142 (99%)	85 (61%)	37 (26%)	18 (13%)	0	12
21	N	118/127 (93%)	76 (64%)	29 (25%)	13 (11%)	1	16
22	O	114/117 (97%)	74 (65%)	29 (25%)	11 (10%)	1	21
23	Q	115/117 (98%)	75 (65%)	31 (27%)	9 (8%)	1	28
24	S	108/110 (98%)	68 (63%)	29 (27%)	11 (10%)	1	19
25	U	100/103 (97%)	58 (58%)	23 (23%)	19 (19%)	0	4
26	F	176/178 (99%)	103 (58%)	44 (25%)	29 (16%)	0	7
27	G	174/176 (99%)	99 (57%)	42 (24%)	33 (19%)	0	4
28	R	101/103 (98%)	72 (71%)	20 (20%)	9 (9%)	1	25
29	T	91/100 (91%)	48 (53%)	23 (25%)	20 (22%)	0	2
30	Z	75/78 (96%)	50 (67%)	13 (17%)	12 (16%)	0	7
31	W	77/84 (92%)	28 (36%)	23 (30%)	26 (34%)	0	0
32	6	183/185 (99%)	162 (88%)	16 (9%)	5 (3%)	8	61
All	All	3492/3582 (98%)	2204 (63%)	812 (23%)	476 (14%)	0	11

5 of 476 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	18	ASN
4	C	17	LYS
4	C	51	ARG
4	C	59	GLN
4	C	77	VAL



### 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	
3	I	109/109 (100%)	107 (98%)	2 (2%)	71	93
4	C	216/217 (100%)	179 (83%)	37 (17%)	3	22
5	D	164/164 (100%)	135 (82%)	29 (18%)	3	20
6	K	102/104 (98%)	80 (78%)	22 (22%)	1	11
7	P	99/99 (100%)	80 (81%)	19 (19%)	2	16
8	E	165/165 (100%)	143 (87%)	22 (13%)	6	37
9	Y	48/48 (100%)	38 (79%)	10 (21%)	2	13
10	0	47/47 (100%)	38 (81%)	9 (19%)	2	16
11	4	34/34 (100%)	28 (82%)	6 (18%)	3	20
12	1	45/48 (94%)	40 (89%)	5 (11%)	9	46
13	3	51/51 (100%)	45 (88%)	6 (12%)	8	42
14	V	78/78 (100%)	64 (82%)	14 (18%)	2	19
15	2	38/38 (100%)	28 (74%)	10 (26%)	1	7
16	L	102/103 (99%)	91 (89%)	11 (11%)	9	48
17	M	109/109 (100%)	87 (80%)	22 (20%)	2	14
18	X	55/55 (100%)	46 (84%)	9 (16%)	3	25
19	H	114/114 (100%)	79 (69%)	35 (31%)	0	5
20	J	116/116 (100%)	100 (86%)	16 (14%)	5	34
21	N	100/103 (97%)	84 (84%)	16 (16%)	3	27
22	O	86/87 (99%)	71 (83%)	15 (17%)	3	21
23	Q	89/89 (100%)	79 (89%)	10 (11%)	9	45
24	S	93/93 (100%)	77 (83%)	16 (17%)	3	22
25	U	83/84 (99%)	65 (78%)	18 (22%)	1	11
26	F	149/149 (100%)	117 (78%)	32 (22%)	1	11
27	G	137/137 (100%)	110 (80%)	27 (20%)	2	15
28	R	84/84 (100%)	71 (84%)	13 (16%)	4	28
29	T	80/84 (95%)	64 (80%)	16 (20%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Z	67/68 (98%)	53 (79%)	14 (21%)	1	12
31	W	59/62 (95%)	42 (71%)	17 (29%)	0	5
32	6	157/157 (100%)	137 (87%)	20 (13%)	6	39
All	All	2876/2896 (99%)	2378 (83%)	498 (17%)	3	21

5 of 498 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	X	18	LEU
20	J	111	LYS
30	Z	78	TYR
18	X	57	LEU
19	H	68	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
17	M	13	HIS
19	H	28	ASN
29	T	92	ASN
17	M	17	ASN
18	X	27	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	116/120 (96%)	17 (14%)	0
2	B	2837/2904 (97%)	457 (16%)	17 (0%)
All	All	2953/3024 (97%)	474 (16%)	17 (0%)

5 of 474 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	C
1	A	9	G
1	A	16	G
1	A	24	G
1	A	26	C



5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1210	G
2	B	1301	A
2	B	2336	A
2	B	1205	A
2	B	2425	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 112 ligands modelled in this entry, 111 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
34	LLL	B	3015	-	33,33,33	3.08	13 (39%)	49,49,49	1.54	5 (10%)

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
34	LLL	B	3015	-	-	0/12/65/65	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	3015	LLL	C22-C32	8.45	1.58	1.52
34	B	3015	LLL	C22-C12	6.82	1.57	1.52
34	B	3015	LLL	O53-C53	6.00	1.52	1.43
34	B	3015	LLL	C43-C33	4.98	1.63	1.54
34	B	3015	LLL	C42-C32	4.52	1.59	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	3015	LLL	C93-N33-C33	6.50	117.55	113.85
34	B	3015	LLL	C53-O53-C13	4.37	117.45	111.22
34	B	3015	LLL	C83-C43-C33	2.61	116.49	112.15
34	B	3015	LLL	C11-O51-C51	2.56	115.79	113.19
34	B	3015	LLL	O43-C43-C83	-2.46	102.66	108.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	A	117/120 (97%)	-0.26	0 100 100	49, 85, 136, 180	0
2	B	2841/2904 (97%)	0.41	253 (8%) 10 12	6, 60, 150, 180	0
3	I	141/141 (100%)	-0.02	12 (8%) 11 13	72, 166, 180, 180	0
4	C	271/272 (99%)	0.29	15 (5%) 24 21	5, 47, 107, 156	0
5	D	209/209 (100%)	0.43	19 (9%) 9 12	8, 72, 145, 180	0
6	K	121/123 (98%)	0.70	20 (16%) 2 4	16, 62, 142, 180	0
7	P	114/114 (100%)	0.98	24 (21%) 1 3	28, 86, 155, 173	0
8	E	201/201 (100%)	0.14	10 (4%) 28 24	5, 76, 143, 180	0
9	Y	58/58 (100%)	0.11	2 (3%) 43 35	22, 84, 137, 180	0
10	0	56/56 (100%)	0.42	1 (1%) 65 52	5, 81, 149, 180	0
11	4	38/38 (100%)	0.29	1 (2%) 53 42	5, 71, 153, 168	0
12	1	50/54 (92%)	-0.25	0 100 100	32, 87, 132, 174	0
13	3	64/64 (100%)	0.71	7 (10%) 6 9	19, 64, 105, 133	0
14	V	94/94 (100%)	0.00	3 (3%) 45 36	37, 92, 143, 180	0
15	2	46/46 (100%)	0.55	2 (4%) 34 28	5, 50, 123, 143	0
16	L	143/144 (99%)	0.39	8 (5%) 24 21	7, 72, 131, 180	0
17	M	136/136 (100%)	0.36	11 (8%) 12 14	16, 68, 144, 165	0
18	X	63/63 (100%)	0.38	8 (12%) 4 6	24, 92, 169, 180	0
19	H	149/149 (100%)	0.21	8 (5%) 25 22	13, 125, 180, 180	0
20	J	142/142 (100%)	0.20	6 (4%) 35 29	13, 77, 132, 166	0
21	N	120/127 (94%)	0.02	1 (0%) 83 70	5, 68, 136, 180	0
22	O	116/117 (99%)	-0.28	2 (1%) 67 53	29, 94, 144, 180	0
23	Q	117/117 (100%)	-0.07	1 (0%) 81 68	5, 72, 134, 171	0
24	S	110/110 (100%)	0.08	1 (0%) 81 68	5, 67, 129, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	U	102/103 (99%)	-0.06	5 (4%) 28 25	13, 88, 148, 177	0
26	F	178/178 (100%)	0.02	14 (7%) 13 14	39, 115, 174, 180	0
27	G	176/176 (100%)	0.08	6 (3%) 43 35	8, 102, 172, 180	0
28	R	103/103 (100%)	-0.09	1 (0%) 79 65	18, 99, 151, 173	0
29	T	93/100 (93%)	0.76	17 (18%) 2 4	13, 83, 160, 180	0
30	Z	77/78 (98%)	0.70	8 (10%) 7 9	12, 57, 112, 152	0
31	W	79/84 (94%)	0.54	8 (10%) 7 10	19, 88, 139, 180	0
32	6	185/185 (100%)	0.15	4 (2%) 59 46	23, 123, 180, 180	0
All	All	6510/6606 (98%)	0.30	478 (7%) 15 15	5, 71, 163, 180	0

The worst 5 of 478 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	X	63	ALA	8.3
2	B	1293	C	8.1
2	B	2523	G	7.6
2	B	1537	G	7.2
30	Z	76	GLU	7.2

## 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	B	2937	1/1	0.81	103.73	141,141,141,141	0
33	MG	B	2908	1/1	0.45	23.12	73,73,73,73	0
33	MG	B	2935	1/1	0.71	15.66	63,63,63,63	0
33	MG	B	2912	1/1	1.37	12.19	75,75,75,75	0
33	MG	B	3010	1/1	0.67	7.13	39,39,39,39	0
33	MG	B	2946	1/1	0.23	7.10	135,135,135,135	0
33	MG	B	2968	1/1	0.61	6.84	37,37,37,37	0
33	MG	B	2939	1/1	0.59	5.38	82,82,82,82	0
33	MG	B	2951	1/1	0.32	5.07	116,116,116,116	0
33	MG	B	2976	1/1	0.45	4.96	79,79,79,79	0
33	MG	B	3004	1/1	0.54	3.64	151,151,151,151	0
33	MG	B	2907	1/1	0.32	3.26	51,51,51,51	0
33	MG	B	2971	1/1	0.29	3.05	24,24,24,24	0
33	MG	B	3012	1/1	0.43	2.99	44,44,44,44	0
33	MG	B	2997	1/1	0.23	2.96	131,131,131,131	0
33	MG	B	2929	1/1	0.53	2.50	42,42,42,42	0
34	LLL	B	3015	31/31	0.27	2.36	107,107,107,107	0
33	MG	B	2984	1/1	0.22	2.28	77,77,77,77	0
33	MG	B	2942	1/1	0.31	2.20	152,152,152,152	0
33	MG	B	2950	1/1	0.27	1.87	64,64,64,64	0
33	MG	B	2920	1/1	0.33	1.81	91,91,91,91	0
33	MG	B	2998	1/1	0.24	1.79	47,47,47,47	0
33	MG	B	2982	1/1	0.23	1.48	101,101,101,101	0
33	MG	B	3002	1/1	0.34	1.36	16,16,16,16	0
33	MG	B	2991	1/1	0.45	1.31	114,114,114,114	0
33	MG	B	2919	1/1	0.56	1.16	42,42,42,42	0
33	MG	B	2973	1/1	0.37	1.08	10,10,10,10	0
33	MG	B	2933	1/1	0.25	0.90	17,17,17,17	0
33	MG	B	2955	1/1	0.21	0.78	65,65,65,65	0
33	MG	B	2931	1/1	0.21	0.53	42,42,42,42	0
33	MG	B	2934	1/1	0.27	0.51	70,70,70,70	0
33	MG	B	2964	1/1	0.28	0.39	22,22,22,22	0
33	MG	B	2960	1/1	0.23	0.38	31,31,31,31	0
33	MG	B	2961	1/1	0.28	0.24	65,65,65,65	0
33	MG	B	2996	1/1	0.29	0.19	45,45,45,45	0
33	MG	B	2977	1/1	0.32	0.07	38,38,38,38	0
33	MG	B	2923	1/1	0.18	0.06	40,40,40,40	0
33	MG	B	2924	1/1	0.43	0.06	36,36,36,36	0
33	MG	B	2922	1/1	0.25	0.05	50,50,50,50	0
33	MG	B	2915	1/1	0.23	-0.01	29,29,29,29	0
33	MG	B	2947	1/1	0.21	-0.03	122,122,122,122	0
33	MG	B	3000	1/1	0.19	-0.06	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	B	2921	1/1	0.29	-0.07	73,73,73,73	0
33	MG	B	3003	1/1	0.21	-0.07	56,56,56,56	0
33	MG	B	3013	1/1	0.26	-0.07	59,59,59,59	0
33	MG	B	2954	1/1	0.24	-0.17	33,33,33,33	0
33	MG	B	2983	1/1	0.27	-0.20	63,63,63,63	0
33	MG	B	2918	1/1	0.20	-0.26	58,58,58,58	0
33	MG	B	3009	1/1	0.27	-0.30	60,60,60,60	0
33	MG	B	2994	1/1	0.27	-0.34	91,91,91,91	0
33	MG	B	2956	1/1	0.21	-0.38	36,36,36,36	0
33	MG	B	2999	1/1	0.17	-0.43	81,81,81,81	0
33	MG	B	2967	1/1	0.23	-0.64	28,28,28,28	0
33	MG	B	2913	1/1	0.10	-0.83	96,96,96,96	0
33	MG	B	3008	1/1	0.18	-0.90	28,28,28,28	0
33	MG	B	2979	1/1	0.31	-0.95	29,29,29,29	0
33	MG	B	2958	1/1	0.10	-0.99	46,46,46,46	0
33	MG	B	2952	1/1	0.12	-1.11	7,7,7,7	0
33	MG	B	2948	1/1	0.15	-1.15	52,52,52,52	0
33	MG	B	2936	1/1	0.20	-1.17	49,49,49,49	0
33	MG	B	2969	1/1	0.09	-1.19	5,5,5,5	0
33	MG	B	2985	1/1	0.13	-1.22	16,16,16,16	0
33	MG	B	2928	1/1	0.15	-1.24	44,44,44,44	0
33	MG	B	2978	1/1	0.21	-1.28	13,13,13,13	0
33	MG	B	2938	1/1	0.07	-1.33	59,59,59,59	0
33	MG	B	2906	1/1	0.10	-1.36	30,30,30,30	0
33	MG	B	2993	1/1	0.22	-1.36	25,25,25,25	0
35	ZN	4	617	1/1	0.05	-1.38	64,64,64,64	0
33	MG	B	2989	1/1	0.15	-1.39	43,43,43,43	0
33	MG	B	2974	1/1	0.23	-1.40	59,59,59,59	0
33	MG	B	2953	1/1	0.13	-1.57	35,35,35,35	0
33	MG	B	2916	1/1	0.12	-1.63	53,53,53,53	0
33	MG	B	2909	1/1	0.20	-1.65	20,20,20,20	0
33	MG	B	2944	1/1	0.04	-1.69	27,27,27,27	0
33	MG	B	3001	1/1	0.16	-1.69	88,88,88,88	0
33	MG	B	2957	1/1	0.10	-1.84	79,79,79,79	0
33	MG	B	2995	1/1	0.21	-1.87	37,37,37,37	0
33	MG	B	2932	1/1	0.08	-1.89	61,61,61,61	0
33	MG	B	2927	1/1	0.12	-1.89	11,11,11,11	0
33	MG	B	3005	1/1	0.13	-1.90	5,5,5,5	0
33	MG	B	2980	1/1	0.10	-1.90	20,20,20,20	0
33	MG	B	2981	1/1	0.12	-1.92	83,83,83,83	0
33	MG	B	2986	1/1	0.21	-1.95	5,5,5,5	0
33	MG	B	2917	1/1	0.27	-1.97	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	B	3007	1/1	0.12	-2.12	20,20,20,20	0
33	MG	B	2975	1/1	0.15	-2.17	89,89,89,89	0
33	MG	B	2940	1/1	0.08	-2.24	62,62,62,62	0
33	MG	B	2925	1/1	0.13	-2.24	51,51,51,51	0
33	MG	B	3006	1/1	0.04	-2.26	31,31,31,31	0
33	MG	B	2987	1/1	0.13	-2.34	28,28,28,28	0
33	MG	B	2992	1/1	0.09	-2.38	36,36,36,36	0
33	MG	B	2949	1/1	0.14	-2.40	38,38,38,38	0
33	MG	B	2911	1/1	0.06	-2.42	53,53,53,53	0
33	MG	B	2941	1/1	0.04	-2.42	44,44,44,44	0
33	MG	B	2914	1/1	0.12	-2.59	40,40,40,40	0
33	MG	B	2963	1/1	0.11	-2.63	60,60,60,60	0
33	MG	B	2930	1/1	0.14	-2.71	43,43,43,43	0
33	MG	B	2910	1/1	0.11	-2.78	20,20,20,20	0
33	MG	B	2965	1/1	0.12	-2.83	56,56,56,56	0
33	MG	B	2943	1/1	0.10	-2.87	5,5,5,5	0
33	MG	B	2990	1/1	0.08	-3.00	18,18,18,18	0
33	MG	B	2972	1/1	0.17	-3.16	61,61,61,61	0
33	MG	B	2962	1/1	0.12	-3.26	11,11,11,11	0
33	MG	B	2959	1/1	0.14	-3.89	53,53,53,53	0
33	MG	B	3011	1/1	0.03	-4.13	30,30,30,30	0
33	MG	B	2905	1/1	0.07	-4.19	29,29,29,29	0
33	MG	B	2970	1/1	0.07	-4.32	25,25,25,25	0
33	MG	B	2988	1/1	0.09	-4.49	77,77,77,77	0
33	MG	B	2926	1/1	0.06	-4.76	37,37,37,37	0
33	MG	B	3014	1/1	0.06	-4.79	40,40,40,40	0
33	MG	B	2966	1/1	0.06	-7.34	27,27,27,27	0
33	MG	B	2945	1/1	0.07	-9.90	8,8,8,8	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.