



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:30 am GMT

PDB ID : 2ZJR
Title : Refined native structure of the large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Harms, J.M.; Wilson, D.N.; Schlutzen, F.; Connell, S.R.; Stachelhaus, T.; Zaborowska, Z.; Spahn, C.M.T.; Fucini, P.
Deposited on : 2008-03-08
Resolution : 2.91 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

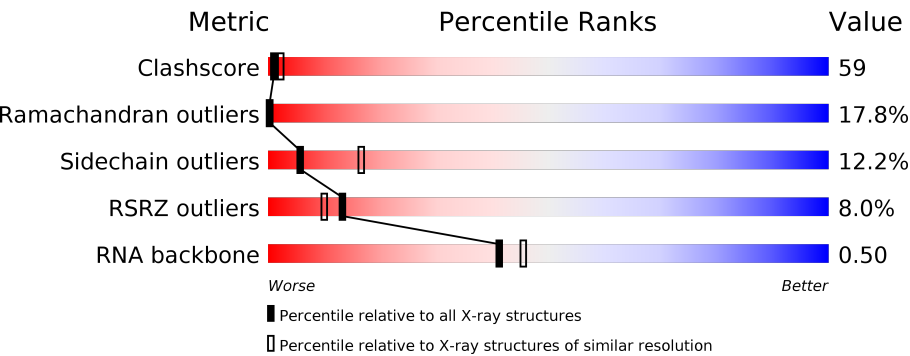
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2045 (2.94-2.90)
Ramachandran outliers	110173	1997 (2.94-2.90)
Sidechain outliers	110143	1999 (2.94-2.90)
RSRZ outliers	101464	1825 (2.94-2.90)
RNA backbone	2435	1023 (3.24-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2880	<div><div>4%</div><div>16%48%20%9%7%</div></div>
2	Y	123	<div><div>2%</div><div>23%59%15%</div></div>
3	A	274	<div><div>7%</div><div>16%54%16%12%</div></div>
4	B	211	<div><div></div><div>29%52%12%</div></div>
5	C	205	<div><div>5%</div><div>11%56%25%</div></div>
6	D	180	<div><div>7%</div><div>11%69%16%</div></div>

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Mol	Chain	Length	Quality of chain
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	142	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	
30	4	37	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	2882	-	-	-	X
31	MG	X	2888	-	-	-	X
31	MG	X	2899	-	-	-	X
31	MG	X	2906	-	-	-	X
31	MG	X	2908	-	-	-	X
31	MG	X	2910	-	-	-	X
31	MG	Y	124	-	-	-	X

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 83819 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 ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

- Molecule 2 is a RNA chain called ribosomal 5S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O		0	0	0
			1067	655	216	196				

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	INITIATING METHIONINE	UNP Q9RXJ5

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C 53 53	0	0	53

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

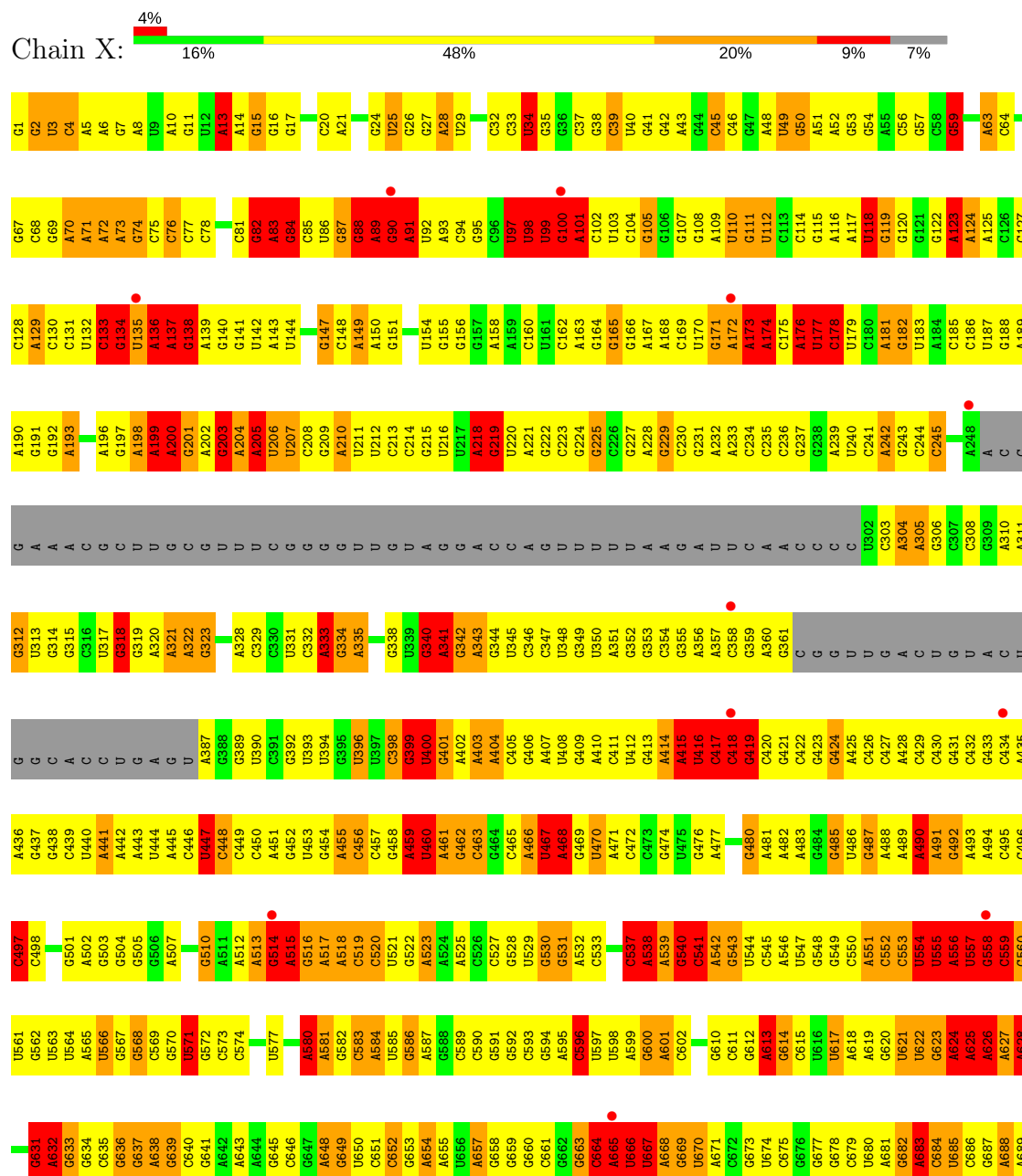
- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	30	Total Mg 30 30	0	0
31	Y	5	Total Mg 5 5	0	0

3 Residue-property plots

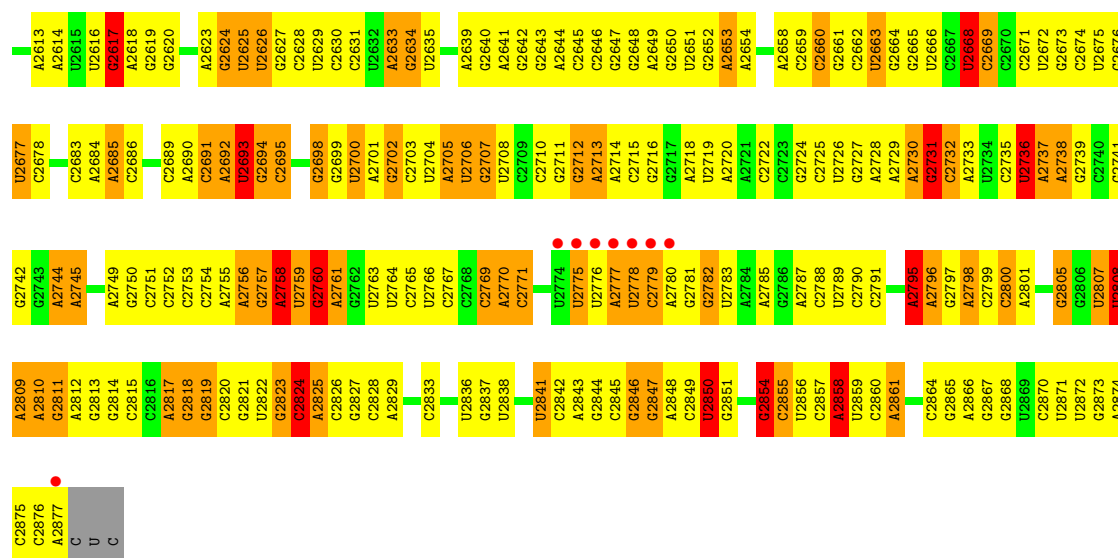
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ribosomal 23S RNA

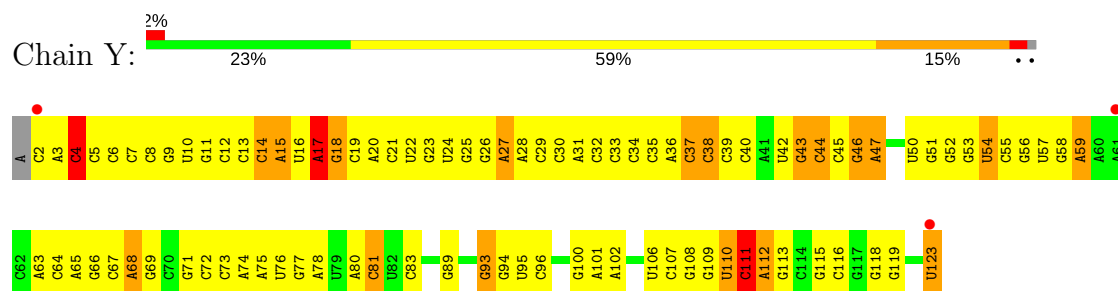


A1587	C1522	U1459	A1321	C1252	A1188	G1125	A1065	U1005	U942	U891	U816	G752	A1590
A1588	A1523	G1460	G1322	C1253	G1189	A1126	G1066	C1006	U943	C882	A817	U753	C891
A1589	A1524	C1461	G1323	G1254	G1190	C1127	G1067	A1007	A944	A883	C818	G754	C892
	A1525	C1462	G1324		G1191	G1128	A1068	G1008	C945	C884	C819	C755	A693
C1593	U1526	U1463	U1325	G1258	A1192	A1129	G1069	C1009	U946	A885	A821	C756	G694
U1594	G1527	A1464	U1326		G1193	U1130	G1070	U1010	C947	A886	A820	U757	G695
A1595	C1528	G1465	C1327	G1261	U1194	G1131	U1071	A1011	C948	C887	G822	G758	U696
A1596	C1529	C1466	C1328	U1262	U1195	C1132	U1072	A1012		C888	U823	C759	G897
A1597	U1530	U1467	U1329	G1263	U1196	G1133	G1073	G1013	G951	C889	U824	U760	A898
C1598	A1531	A1468	G1330	C1264	U1197	C1134	G1074	U1014	A952	U890	C825	G761	G699
G1599	A1532	U1469	G1331	G1265	C1198	C1135	C1075	U1015	G953	A891	U826	A762	C700
U1600	G1533	G1470	G1332	U1266	U1199	G1136	U1077	C1016	U954	G	C827	A763	U701
U1601		A1408	G1333	A1267	G1200	A1137	U1078	C1018	G955	G	C828	A764	A702
G1602		C1472	A1334	U1268	G1201	A1138	A1079	C1019	A956	G	C829	C765	A703
A1603		U1473	A1335	C1269	U1202	A1139	G1079	A1020	G957	G	C830	A766	G704
C1606	A1538	U1474	G1336	C1270	A1203	A1140	A1080	U1021	G958	G	G831	G767	C705
U1607	U1539	G1475	G1337		G1204	G1141	G1082	A1022	U960	C	A832	U768	A706
U1608	C1540	U1476	U1338	G1273	G1205	U1142	C1083	U1023		C	A833	U770	U707
G1609	G1541	C1477	U1339	C1274	G1206	A1143	A1084	G1024	G963	U	A834	U771	G708
			C1340	A1275	U1207	U1144	A1085	G1025		A	U835	C771	A709
U1610	U1542	U1482	G1341	U1276		C1145	G1086	A1026	A964	C	C836	G772	C710
U1611	G1543	G1483	U1342	G1277	G1211	G1146	C1087	U1027	G965	C	U837	G773	C711
U1612	A1544	C1417	C1343	A1278	U1212	G1147	A1088	C1027	A966	A	U838	A774	A712
G1613		G1418	G1344	G1279	U1213	G1148	C1089	G1028	G967	G	U839	U775	G713
C1614	U1547	U1486	G1345	U1280	U1214	G1149	C1090	C1029	C968	C	U840	G776	G714
C1615	C1548	C1487	C1346	A1281	A1215	C1150	C1091	U1030	U969	U	C841	A777	U715
U1618	U1550	G1488	C1347	A1282		U1151	C1092	C1031	A970	U	A842	U778	U716
U1619	U1551	C1489	C1348	C1283	C1218	C1152	U1093	A1032	A971	A	G843	U779	C717
A1620	C1552	G1490	A1349	A1284	C1219	A1153	C1094	U1033	C972	C	G844	U780	A718
G1621	U1553	U1491	G1350	A1285	G1220	A1154	C1095	U1034	U973	C	U845	A781	A719
C1622	G1554	A1492	G1351	U1286	C1221	G1155	A1096	G1035	U974	C	U846	U782	A720
A1623	A1555	A1493	C1352	A1287	G1222	U1156	C1097	G1036		A911	C847	U783	C721
G1624	C1557	G1494	A1353	U1288	G1223	U1157	A1098	U1037	G977	A912	A848		C722
A1625	G1558	G1496	A1354	A1289	A1224		C1099	U1038	U978	A913	U852	A787	C723
A1626	U1559	U1431	A1355		A1225	C1163	A1099	A1039	G980	C914		G788	C724
C1627	G1560	G1432	G1356	G1293	A1226	C1164	G1100	A1040	C981	A918	U857	G789	C725
A1628	U1561	A1433	C1358	U1295	G1228	G1165	G1101	G1041	C982	U919	G858	G791	G726
G1629	U1562	U1434	G1359	U1296	C1229	A1166	G1102	G1042	G983	A920	U859	U792	G727
A1630	U1563	G1435	G1360	A1297	C1230	A1167	G1103	U1043	G984	A921	U860	G793	G728
C1631	C1564	U1370		G1298	A1231	C1168	U1105	A1044	G985	A922	G861	A794	A729
A1632		U1371	G1370	U1299	U1232	C1169	A1106	U1046	A986	A923	A862	A795	C730
C1633		A1372	G1371	A1300	C1233	U1170	U1107	G1047	G987	C924	C863	A796	A731
A1634		G1373	A1372	U1301	A1234	A1171	U1108	U1048	G988	U925	C864	A797	G732
G1635		C1374	G1373	C1302	C1235	U1172	A1109	C1049	G989	C926	A865	G798	G733
G1636	C1572	C1375	G1374	U1303	C1236	G1173	G1110	U1050	A990	C927	U866		G735
U1637	G1573	G1376	C1375	U1304	G1237	G1174	C1111	G1051	A991	C928	G868	A801	G736
		G1377	G1377	G1309	A1238	A1175	U1112	C1052	A992	A929	U869	A802	C737
G1642		A1378	A1378	G1310	C1239	U1176	C1113	G1053	C993	A930	C869	C803	G738
A1643				C1311	G1240	U1177	U1114	C1054	A994	C931	C870	C804	G739
U1644				G1312	G1241	C1178	C1115	A1055	A995	G932	U871	C805	A740
U1645				G1313	A1242	A1179	U1116	U1056	C996	G933	G872	A806	G741
C1648				A1314	G1243	A1180	G1117	A1057	C997	C934	A873	A807	G742
				G1315		C1181	G1118	G1058	C998	C935	U874	A743	A743
U1651	C1581	U1452	A1386	G1316	G1246	U1182	U1119	A1059	A999	A936	G875	G744	C744
G1652	A1582	C1517	G1387	G1317	U1247	C1183	C1120	C1060	G1000	C937	A876	C745	C745
			G1388	G1317	G1248	G1184	G1121	A1061	A1001	G938	C877	G746	G746
C1655	U1585	G1519	C1389	G1318	G1249	C1185	A1122	G1062	C1002	C939	C878	A813	A747
U1656		U1521	A1390	A1319	G1250	G1186	G1123	G1063	C1003	C940	G879	G814	G751
			A1391	A1320	G1251	A1187	U1124	C1064	A1004	U941	C880	A815	

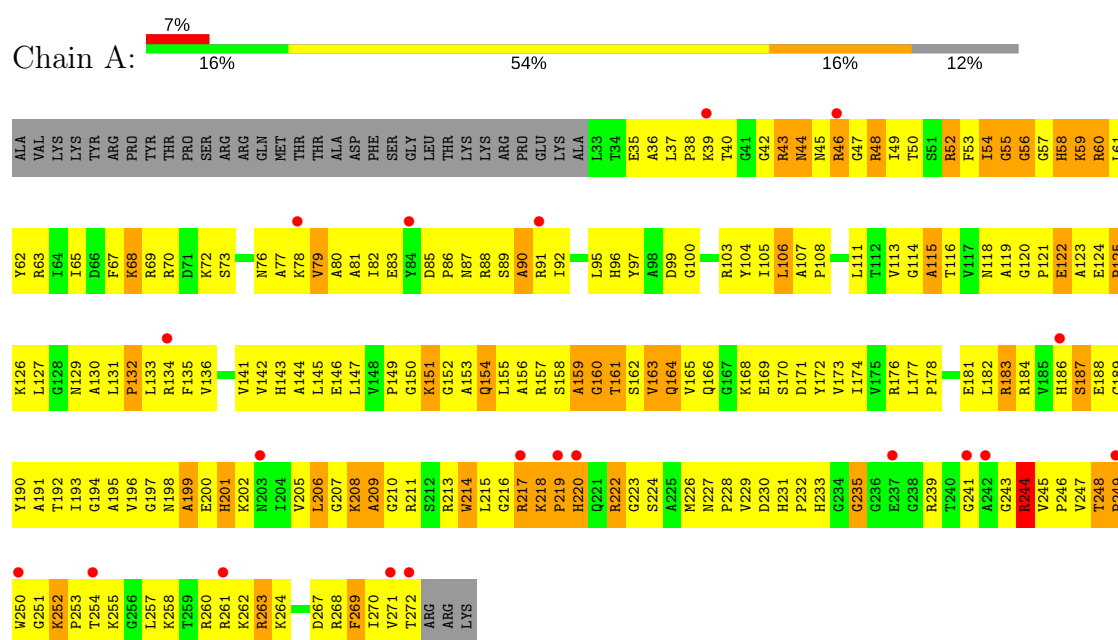




• Molecule 2: ribosomal 5S RNA

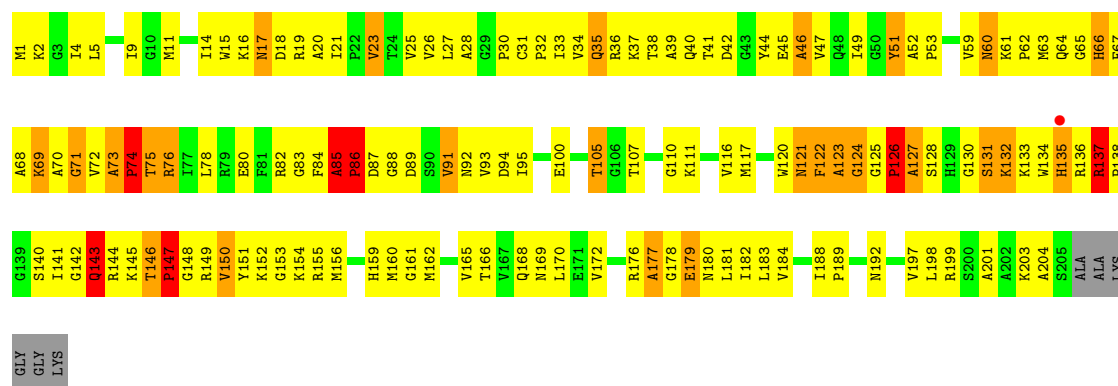


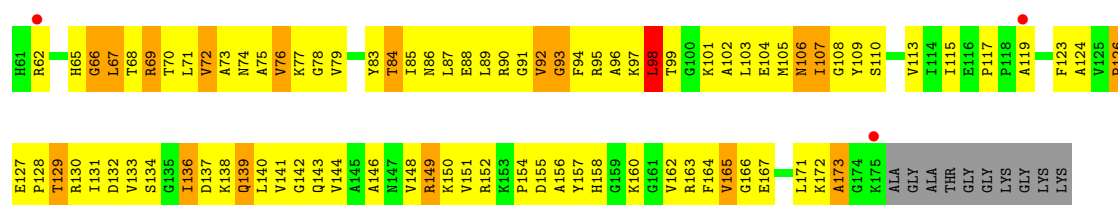
• Molecule 3: 50S ribosomal protein L2



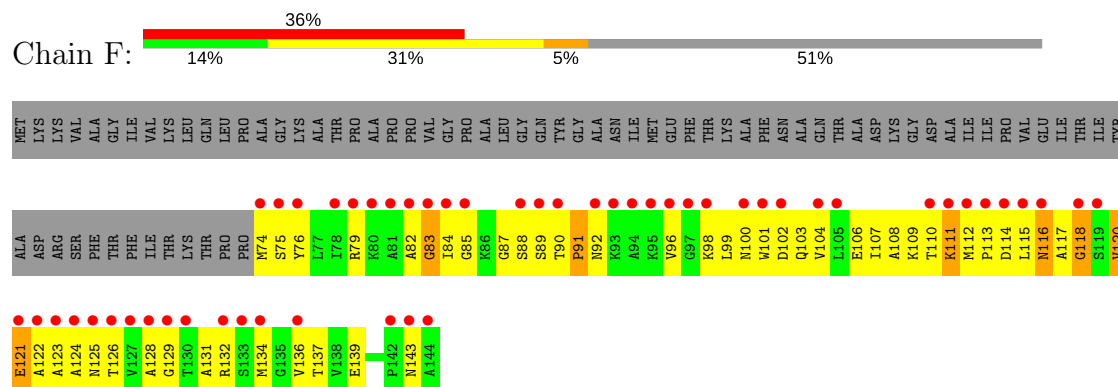
• Molecule 4: 50S ribosomal protein L3



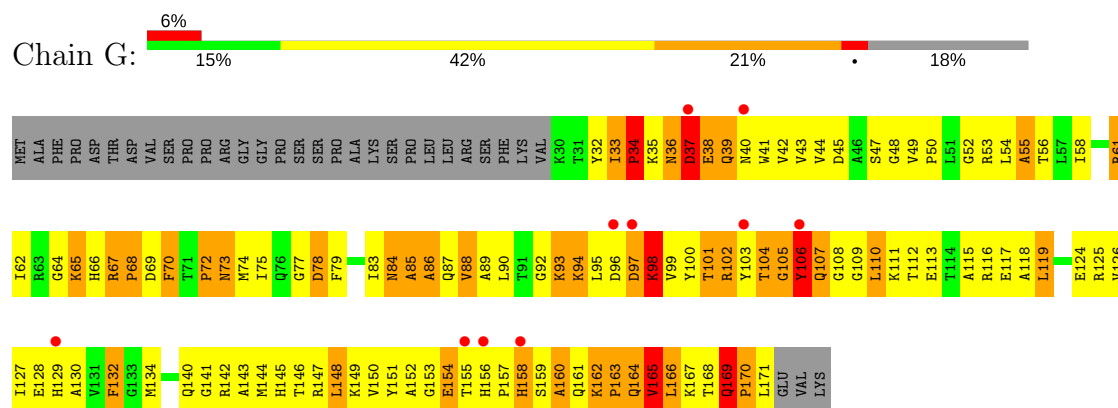




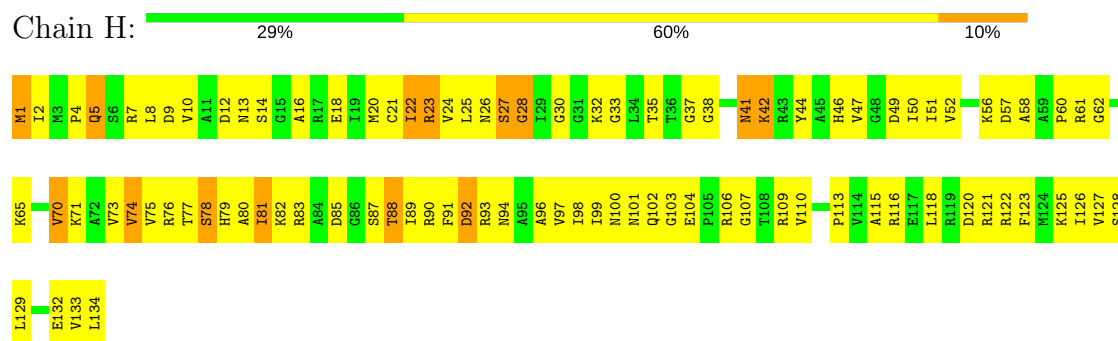
• Molecule 8: 50S ribosomal protein L11



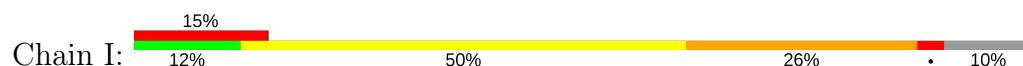
• Molecule 9: 50S ribosomal protein L13

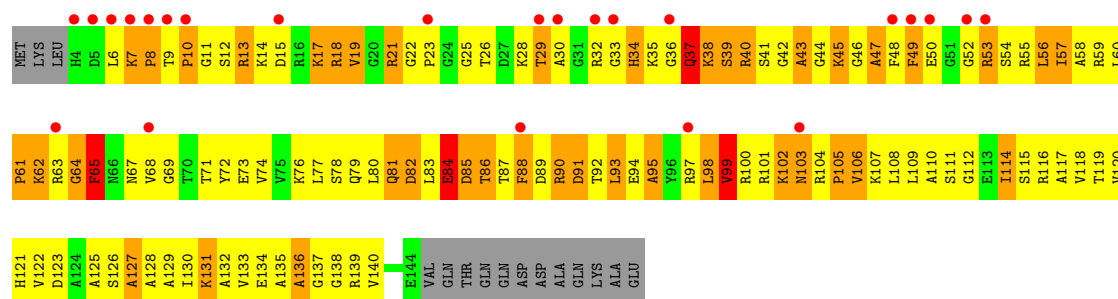


• Molecule 10: 50S ribosomal protein L14

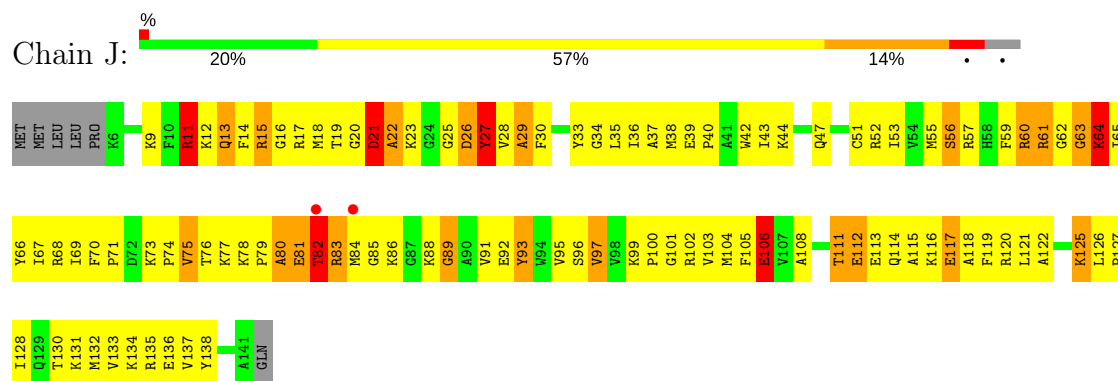


• Molecule 11: 50S ribosomal protein L15

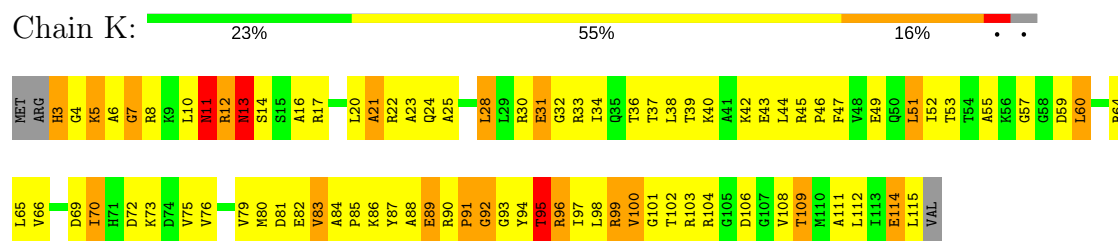




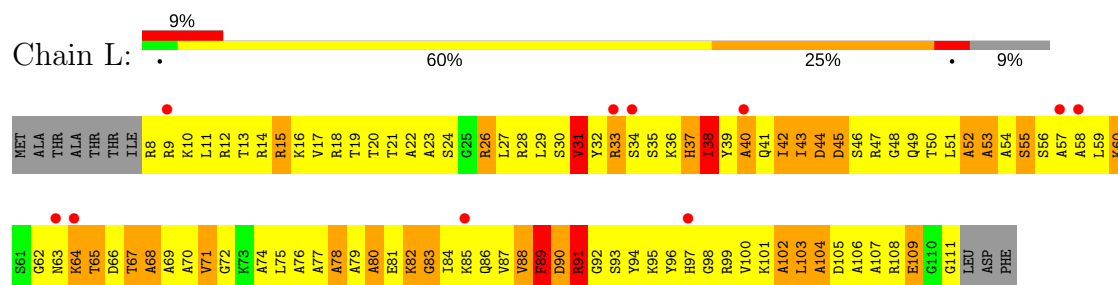
• Molecule 12: 50S ribosomal protein L16



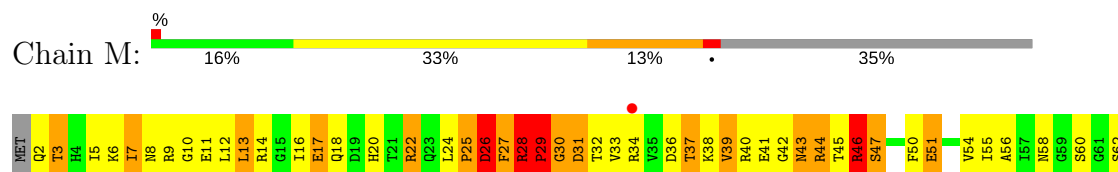
• Molecule 13: 50S ribosomal protein L17

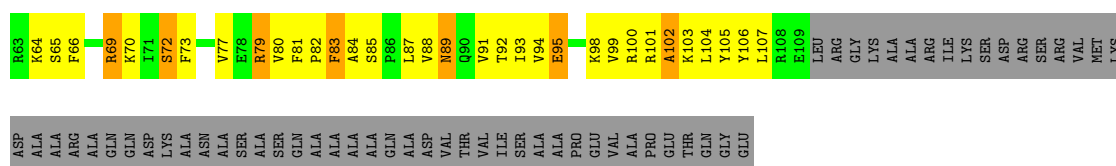


• Molecule 14: 50S ribosomal protein L18

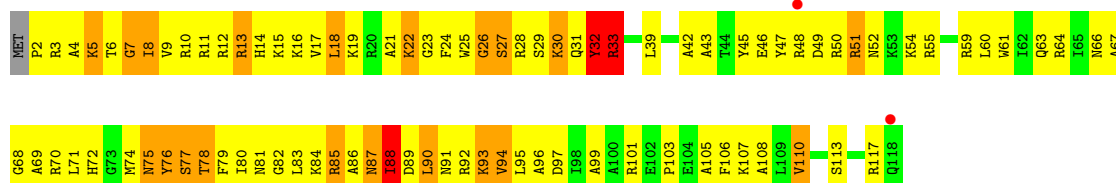


• Molecule 15: 50S ribosomal protein L19

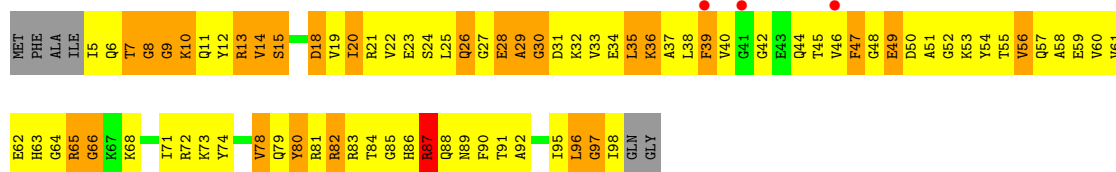
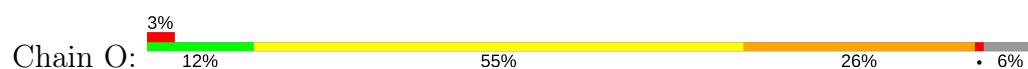




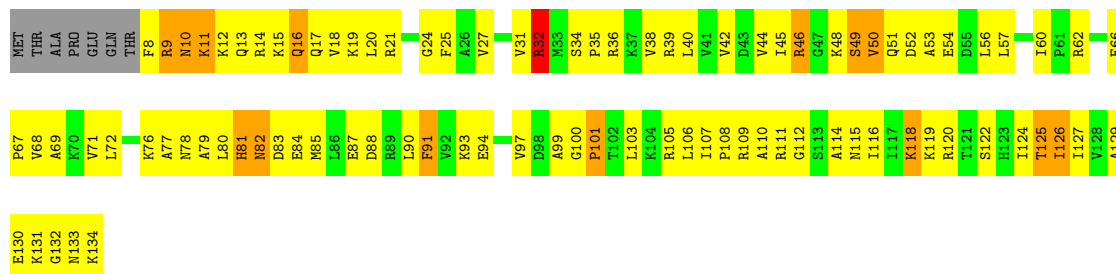
• Molecule 16: 50S ribosomal protein L20



• Molecule 17: 50S ribosomal protein L21



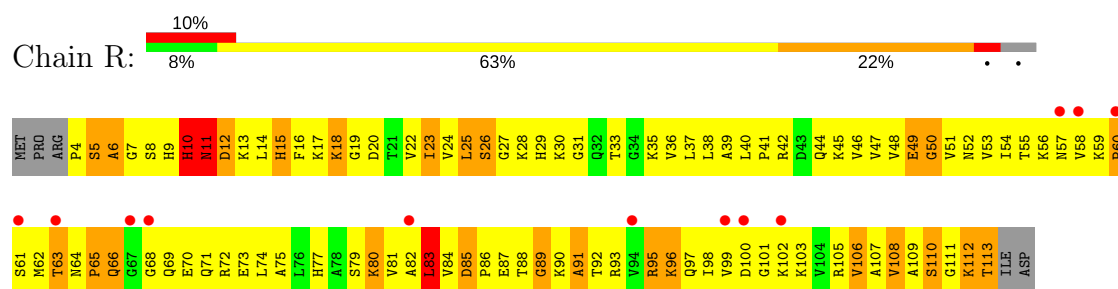
• Molecule 18: 50S ribosomal protein L22



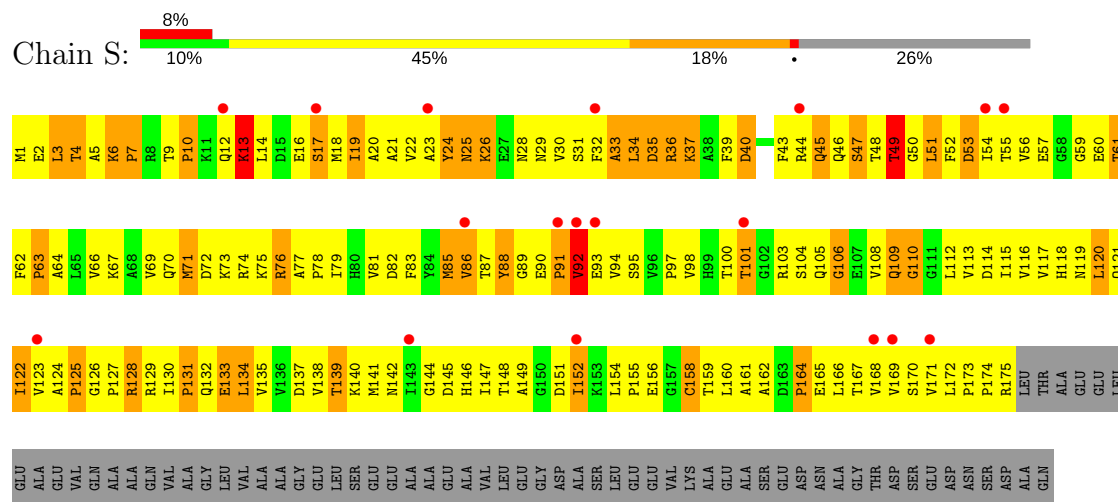
• Molecule 19: 50S ribosomal protein L23



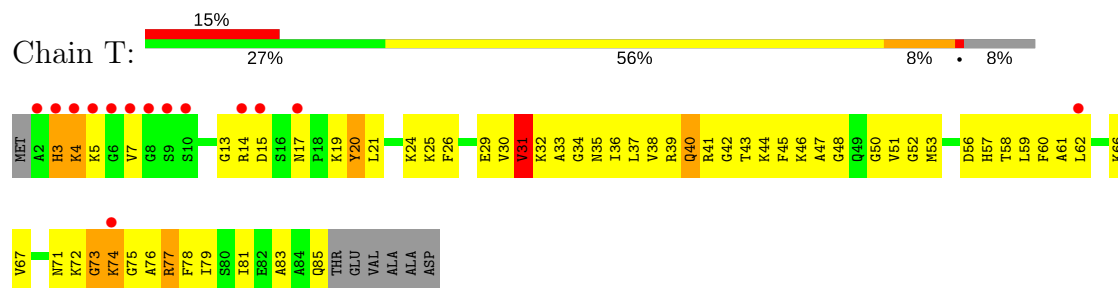
• Molecule 20: 50S ribosomal protein L24



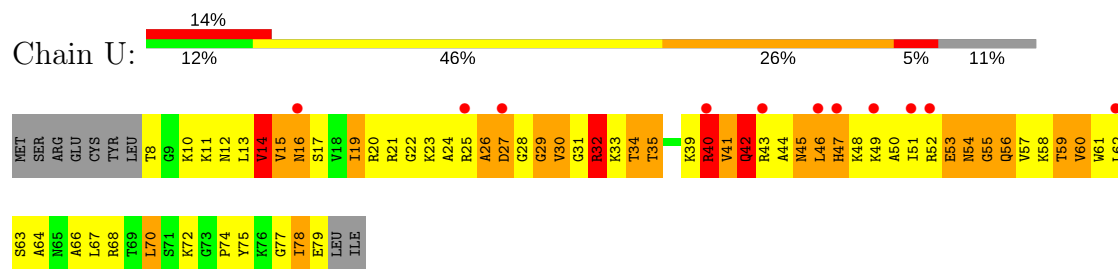
• Molecule 21: 50S ribosomal protein L25



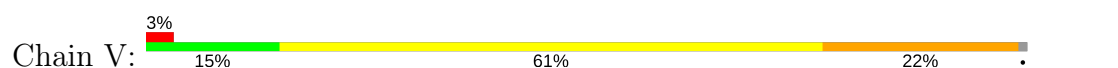
• Molecule 22: 50S ribosomal protein L27

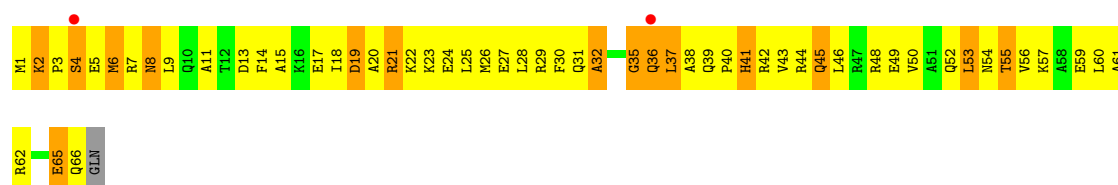


• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29





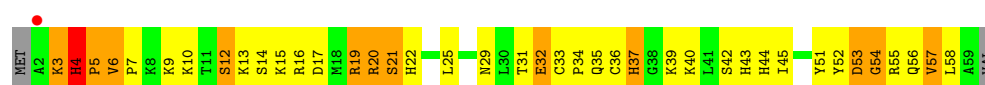
- Molecule 25: 50S ribosomal protein L30

Chain W: 25% 62% 13%



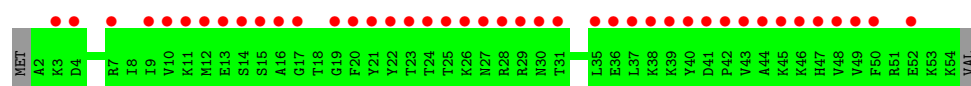
- Molecule 26: 50S ribosomal protein L32

Chain Z: 2% 30% 45% 20%



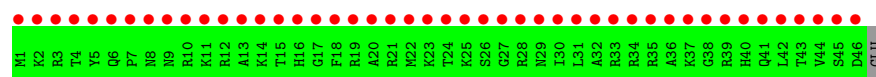
- Molecule 27: 50S ribosomal protein L33

Chain 1: 76% 96%



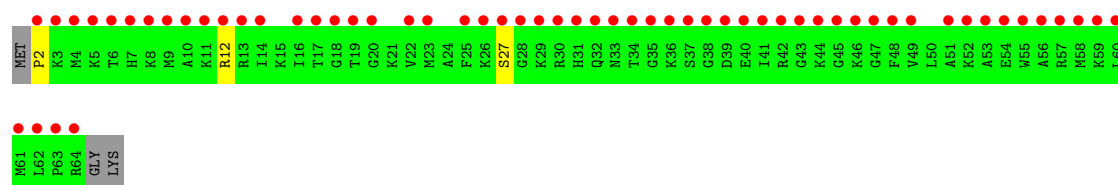
- Molecule 28: 50S ribosomal protein L34

Chain 2: 98% 98%



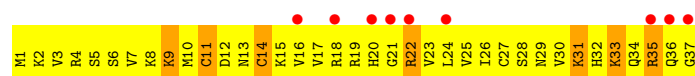
- Molecule 29: 50S ribosomal protein L35

Chain 3: 89% 91% 5% 5%



- Molecule 30: 50S ribosomal protein L36

Chain 4: 24% 81% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 408.90Å 694.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.91 29.92 – 2.91	Depositor EDS
% Data completeness (in resolution range)	94.1 (29.90-2.91) 94.1 (29.92-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.277 , 0.311 0.267 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	83819	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	X	0.90	156/64561 (0.2%)	1.15	809/100708 (0.8%)
2	Y	0.50	0/2904	0.73	0/4525
3	A	0.50	0/1862	0.82	0/2510
4	B	0.70	0/1567	0.99	6/2105 (0.3%)
5	C	0.60	0/1529	0.87	0/2070
6	D	0.47	0/1419	0.70	0/1903
7	E	0.46	0/1308	0.76	0/1771
8	F	0.65	0/508	1.11	2/683 (0.3%)
9	G	0.59	0/1138	0.92	2/1539 (0.1%)
10	H	0.72	0/1007	0.93	1/1352 (0.1%)
11	I	0.60	0/1081	0.89	0/1448
12	J	0.59	0/1113	0.86	1/1486 (0.1%)
13	K	0.83	0/886	1.04	1/1188 (0.1%)
14	L	0.48	0/785	0.82	1/1048 (0.1%)
15	M	0.72	0/884	1.15	6/1186 (0.5%)
16	N	0.54	0/994	0.80	0/1323
17	O	0.54	0/750	0.83	0/1000
18	P	0.73	0/1027	0.90	0/1373
19	Q	0.58	0/737	0.88	3/988 (0.3%)
20	R	0.48	0/835	0.84	0/1121
21	S	0.48	0/1370	0.71	0/1862
22	T	0.52	0/633	0.77	0/838
23	U	0.51	0/556	0.87	0/741
24	V	0.44	0/537	0.67	0/714
25	W	0.51	0/426	0.83	0/568
26	Z	0.68	0/469	0.95	1/629 (0.2%)
30	4	0.45	0/298	0.65	0/390
All	All	0.82	156/91184 (0.2%)	1.08	833/137069 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	225
2	Y	0	4
9	G	0	1
16	N	0	1
19	Q	0	1
All	All	0	232

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1123	G	C3'-O3'	14.43	1.62	1.42
1	X	1123	G	C4'-C3'	13.55	1.68	1.53
1	X	2322	U	C3'-O3'	12.22	1.59	1.42
1	X	1187	A	C2'-C1'	11.44	1.66	1.53
1	X	100	G	C3'-O3'	10.61	1.57	1.42

The worst 5 of 833 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1055	A	N9-C1'-C2'	-29.46	75.70	114.00
1	X	513	A	N9-C1'-C2'	24.54	145.90	114.00
1	X	2297	G	N9-C1'-C2'	21.75	142.27	114.00
1	X	557	U	N1-C1'-C2'	19.63	139.52	114.00
1	X	2298	U	N1-C1'-C2'	19.50	139.35	114.00

There are no chirality outliers.

5 of 232 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	13	A	Sidechain
1	X	15	G	Sidechain
1	X	32	C	Sidechain
1	X	34	U	Sidechain
1	X	59	G	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	X	57651	0	29047	3656	0
2	Y	2598	0	1328	160	0
3	A	1826	0	1885	387	0
4	B	1539	0	1600	265	0
5	C	1506	0	1525	369	0
6	D	1400	0	1481	377	0
7	E	1286	0	1336	242	0
8	F	503	0	520	94	0
9	G	1114	0	1144	264	0
10	H	997	0	1046	152	0
11	I	1067	0	1103	273	0
12	J	1090	0	1125	254	0
13	K	878	0	930	120	0
14	L	779	0	820	236	0
15	M	871	0	894	198	0
16	N	978	0	1020	216	0
17	O	741	0	756	192	0
18	P	1014	0	1096	152	0
19	Q	726	0	753	183	0
20	R	825	0	881	263	0
21	S	1345	0	1372	294	0
22	T	625	0	655	97	0
23	U	552	0	604	201	0
24	V	533	0	558	107	0
25	W	424	0	470	67	0
26	Z	457	0	464	67	0
27	1	53	0	0	0	0
28	2	46	0	0	0	0
29	3	63	0	0	3	0
30	4	297	0	330	68	0
31	X	30	0	0	0	0
31	Y	5	0	0	0	0
All	All	83819	0	54743	8176	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

The worst 5 of 8176 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:135:U:H2'	1:X:136:A:C8	1.59	1.37
1:X:2195:C:C5	1:X:2196:U:C5	2.22	1.28
1:X:623:G:N2	1:X:626:A:C2	2.01	1.26
1:X:1053:G:H2'	1:X:1054:C:C6	1.71	1.25
1:X:333:A:H3'	5:C:162:ARG:NH2	1.49	1.24

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	A	238/274 (87%)	147 (62%)	53 (22%)	38 (16%)	0	0
4	B	203/211 (96%)	147 (72%)	31 (15%)	25 (12%)	0	1
5	C	195/205 (95%)	99 (51%)	48 (25%)	48 (25%)	0	0
6	D	175/180 (97%)	91 (52%)	59 (34%)	25 (14%)	0	0
7	E	169/185 (91%)	100 (59%)	39 (23%)	30 (18%)	0	0
8	F	69/144 (48%)	45 (65%)	19 (28%)	5 (7%)	1	3
9	G	140/174 (80%)	80 (57%)	28 (20%)	32 (23%)	0	0
10	H	132/134 (98%)	114 (86%)	11 (8%)	7 (5%)	2	7
11	I	139/156 (89%)	62 (45%)	33 (24%)	44 (32%)	0	0
12	J	134/142 (94%)	74 (55%)	36 (27%)	24 (18%)	0	0
13	K	111/116 (96%)	85 (77%)	12 (11%)	14 (13%)	0	1
14	L	102/114 (90%)	55 (54%)	22 (22%)	25 (24%)	0	0
15	M	106/166 (64%)	71 (67%)	21 (20%)	14 (13%)	0	0
16	N	115/118 (98%)	72 (63%)	25 (22%)	18 (16%)	0	0
17	O	92/100 (92%)	57 (62%)	16 (17%)	19 (21%)	0	0
18	P	125/134 (93%)	94 (75%)	20 (16%)	11 (9%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	91/95 (96%)	44 (48%)	23 (25%)	24 (26%)	0	0
20	R	108/115 (94%)	60 (56%)	24 (22%)	24 (22%)	0	0
21	S	173/237 (73%)	94 (54%)	40 (23%)	39 (22%)	0	0
22	T	82/91 (90%)	48 (58%)	20 (24%)	14 (17%)	0	0
23	U	70/81 (86%)	35 (50%)	18 (26%)	17 (24%)	0	0
24	V	64/67 (96%)	32 (50%)	20 (31%)	12 (19%)	0	0
25	W	53/55 (96%)	42 (79%)	6 (11%)	5 (9%)	1	1
26	Z	56/60 (93%)	41 (73%)	7 (12%)	8 (14%)	0	0
30	4	35/37 (95%)	17 (49%)	9 (26%)	9 (26%)	0	0
All	All	2977/3391 (88%)	1806 (61%)	640 (22%)	531 (18%)	0	0

5 of 531 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	60	ARG
3	A	187	SER
3	A	209	ALA
3	A	217	ARG
3	A	220	HIS

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	A	185/215 (86%)	167 (90%)	18 (10%)	9	28
4	B	155/157 (99%)	139 (90%)	16 (10%)	8	25
5	C	157/163 (96%)	132 (84%)	25 (16%)	3	8
6	D	153/156 (98%)	136 (89%)	17 (11%)	7	21
7	E	136/144 (94%)	124 (91%)	12 (9%)	12	33
8	F	51/107 (48%)	49 (96%)	2 (4%)	37	71
9	G	118/146 (81%)	101 (86%)	17 (14%)	4	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	103/103 (100%)	93 (90%)	10 (10%)	9	28
11	I	108/121 (89%)	91 (84%)	17 (16%)	3	8
12	J	110/116 (95%)	97 (88%)	13 (12%)	6	18
13	K	90/93 (97%)	73 (81%)	17 (19%)	2	5
14	L	74/82 (90%)	57 (77%)	17 (23%)	1	2
15	M	94/134 (70%)	81 (86%)	13 (14%)	4	12
16	N	96/97 (99%)	85 (88%)	11 (12%)	6	19
17	O	75/79 (95%)	66 (88%)	9 (12%)	6	17
18	P	109/115 (95%)	100 (92%)	9 (8%)	13	36
19	Q	75/76 (99%)	67 (89%)	8 (11%)	8	23
20	R	91/96 (95%)	79 (87%)	12 (13%)	5	13
21	S	149/192 (78%)	133 (89%)	16 (11%)	8	23
22	T	62/67 (92%)	58 (94%)	4 (6%)	20	49
23	U	57/66 (86%)	44 (77%)	13 (23%)	1	2
24	V	54/55 (98%)	48 (89%)	6 (11%)	7	21
25	W	48/48 (100%)	43 (90%)	5 (10%)	8	24
26	Z	51/53 (96%)	43 (84%)	8 (16%)	3	8
30	4	35/35 (100%)	33 (94%)	2 (6%)	24	55
All	All	2436/2716 (90%)	2139 (88%)	297 (12%)	6	16

5 of 297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	11	ARG
14	L	37	HIS
23	U	70	LEU
12	J	64	LYS
13	K	13	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
13	K	13	ASN
16	N	34	ASN
25	W	49	HIS

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Mol	Chain	Res	Type
14	L	37	HIS
14	L	97	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	695 (25%)	0
2	Y	121/123 (98%)	25 (20%)	0
All	All	2801/3003 (93%)	720 (25%)	0

5 of 720 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	4	C
1	X	13	A
1	X	14	A
1	X	25	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 35 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2686/2880 (93%)	-0.21	110 (4%) 38 33	3, 38, 98, 118	0
2	Y	122/123 (99%)	-0.03	3 (2%) 58 54	24, 67, 89, 101	0
3	A	240/274 (87%)	0.27	20 (8%) 12 9	17, 53, 65, 71	0
4	B	205/211 (97%)	-0.45	1 (0%) 90 90	2, 21, 43, 56	0
5	C	197/205 (96%)	0.02	10 (5%) 29 25	14, 43, 58, 66	0
6	D	177/180 (98%)	0.45	12 (6%) 18 14	50, 60, 67, 69	0
7	E	171/185 (92%)	-0.09	5 (2%) 52 47	38, 53, 64, 68	0
8	F	71/144 (49%)	2.85	52 (73%) 0 0	0, 77, 83, 85	0
9	G	142/174 (81%)	0.10	10 (7%) 17 13	24, 39, 53, 63	0
10	H	134/134 (100%)	-0.52	0 100 100	3, 17, 33, 42	0
11	I	141/156 (90%)	0.77	24 (17%) 2 1	21, 53, 62, 71	0
12	J	136/142 (95%)	-0.03	2 (1%) 74 72	28, 43, 60, 65	0
13	K	113/116 (97%)	-0.47	0 100 100	2, 10, 24, 34	0
14	L	104/114 (91%)	0.27	10 (9%) 9 6	38, 51, 58, 63	0
15	M	108/166 (65%)	-0.54	1 (0%) 84 83	3, 18, 43, 55	0
16	N	117/118 (99%)	-0.19	2 (1%) 70 68	5, 37, 54, 61	0
17	O	94/100 (94%)	-0.16	3 (3%) 48 42	22, 47, 59, 64	0
18	P	127/134 (94%)	-0.50	0 100 100	4, 18, 47, 59	0
19	Q	93/95 (97%)	-0.00	2 (2%) 62 59	29, 42, 57, 68	0
20	R	110/115 (95%)	0.35	12 (10%) 6 4	35, 46, 61, 65	0
21	S	175/237 (73%)	0.64	18 (10%) 7 5	49, 58, 64, 68	0
22	T	84/91 (92%)	0.62	14 (16%) 2 1	26, 44, 59, 70	0
23	U	72/81 (88%)	0.73	11 (15%) 2 1	41, 53, 63, 67	0
24	V	66/67 (98%)	-0.11	2 (3%) 51 45	38, 52, 65, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.39	0 100 100	21, 37, 49, 64	0
26	Z	58/60 (96%)	-0.42	1 (1%) 70 68	4, 16, 38, 44	0
27	1	53/55 (96%)	3.45	42 (79%) 0 0	37, 47, 56, 60	0
28	2	46/47 (97%)	6.25	46 (100%) 0 0	11, 27, 34, 37	0
29	3	63/66 (95%)	5.67	59 (93%) 0 0	21, 36, 46, 48	0
30	4	37/37 (100%)	1.01	9 (24%) 1 0	44, 52, 58, 59	0
All	All	5997/6562 (91%)	0.10	481 (8%) 13 10	0, 43, 85, 118	0

The worst 5 of 481 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	37	SER	16.5
29	3	38	GLY	16.4
29	3	39	ASP	11.5
29	3	33	ASN	11.4
29	3	43	GLY	11.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	MG	X	2910	1/1	0.62	0.37	21.14	19,19,19,19	0
31	MG	X	2908	1/1	0.72	0.50	18.84	17,17,17,17	0
31	MG	Y	124	1/1	0.80	0.43	12.62	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	2882	1/1	0.66	0.29	9.39	12,12,12,12	0
31	MG	X	2906	1/1	0.91	0.44	7.52	13,13,13,13	0
31	MG	X	2899	1/1	0.88	0.22	4.59	19,19,19,19	0
31	MG	X	2888	1/1	0.83	0.23	4.54	3,3,3,3	0
31	MG	X	2895	1/1	0.97	0.35	1.84	3,3,3,3	0
31	MG	X	2904	1/1	0.96	0.14	-0.57	3,3,3,3	0
31	MG	Y	128	1/1	0.82	0.16	-	41,41,41,41	0
31	MG	X	2897	1/1	0.93	0.51	-	3,3,3,3	0
31	MG	X	2909	1/1	0.86	0.12	-	3,3,3,3	0
31	MG	X	2907	1/1	0.96	0.17	-	58,58,58,58	0
31	MG	X	2894	1/1	0.95	0.38	-	15,15,15,15	0
31	MG	X	2886	1/1	0.51	0.33	-	41,41,41,41	0
31	MG	X	2891	1/1	0.99	0.51	-	12,12,12,12	0
31	MG	X	2883	1/1	0.76	0.19	-	49,49,49,49	0
31	MG	X	2881	1/1	0.83	0.24	-	59,59,59,59	0
31	MG	X	2901	1/1	0.93	0.28	-	3,3,3,3	0
31	MG	X	2892	1/1	0.87	0.19	-	22,22,22,22	0
31	MG	X	2898	1/1	0.92	0.42	-	3,3,3,3	0
31	MG	X	2889	1/1	0.98	0.36	-	3,3,3,3	0
31	MG	X	2902	1/1	0.97	0.11	-	60,60,60,60	0
31	MG	X	2885	1/1	0.84	0.52	-	56,56,56,56	0
31	MG	X	2905	1/1	0.92	0.28	-	6,6,6,6	0
31	MG	Y	125	1/1	0.97	0.20	-	9,9,9,9	0
31	MG	X	2900	1/1	0.83	0.40	-	3,3,3,3	0
31	MG	Y	127	1/1	0.90	0.18	-	12,12,12,12	0
31	MG	X	2896	1/1	0.92	0.25	-	3,3,3,3	0
31	MG	X	2893	1/1	0.84	0.21	-	13,13,13,13	0
31	MG	X	2890	1/1	0.84	0.20	-	49,49,49,49	0
31	MG	X	2903	1/1	0.93	0.24	-	24,24,24,24	0
31	MG	X	2884	1/1	0.53	0.42	-	55,55,55,55	0
31	MG	Y	126	1/1	0.74	0.29	-	25,25,25,25	0
31	MG	X	2887	1/1	0.94	0.15	-	3,3,3,3	0

6.5 Other polymers [i](#)

There are no such residues in this entry.