



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:14 AM UTC

PDB ID : 2ZJP / pdb_00002zjp
Title : Thiopeptide antibiotic Nosiheptide bound to the large ribosomal subunit of *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 : 2008-03-07
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

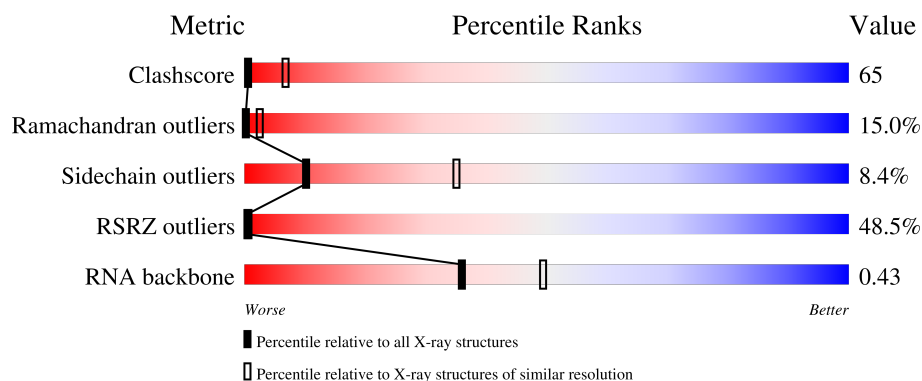
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)
RNA backbone	3983	1007 (4.30-3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1	55	96% 95%
2	2	47	98% 96%
3	3	66	95% 92% 5%
4	4	37	54% 22% 70% 8%
5	5	13	8% 23% 62% 15%

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Mol	Chain	Length	Quality of chain
6	A	274	
7	B	211	
8	C	205	
9	D	180	
10	E	185	
11	F	144	
12	G	174	
13	H	134	
14	I	156	
15	J	142	
16	K	116	
17	L	114	
18	M	166	
19	N	118	
20	O	100	
21	P	134	
22	Q	95	
23	R	115	
24	S	237	
25	T	91	
26	U	81	
27	V	67	
28	W	55	
29	X	2880	
30	Y	60	

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Mol	Chain	Length	Quality of chain
31	Z	123	

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
33	NO1	5	14	-	X	-	-
34	MG	X	2881	-	-	-	X
34	MG	X	2883	-	-	-	X
34	MG	X	2889	-	-	-	X
34	MG	X	2892	-	-	-	X
34	MG	X	2896	-	-	-	X
34	MG	X	2901	-	-	-	X
34	MG	X	2906	-	-	-	X
34	MG	Z	124	-	-	-	X
34	MG	Z	125	-	-	-	X
34	MG	Z	129	-	-	-	X
5	MH6	5	10	-	X	-	-
5	DHA	5	12	-	X	-	-
5	DBU	5	4	-	X	-	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 84444 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 5 is a protein called NOSIHEPTIDE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	5	13	Total C N O S 69 40 12 11 6	0	0	1

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	F	144	Total	C	N	O	S	0	0	0
			1044	663	179	197	5			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	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 16 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

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

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

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

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

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

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

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

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

- Molecule 29 is a RNA chain called RIBOSOMAL 23S RNA.

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

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

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

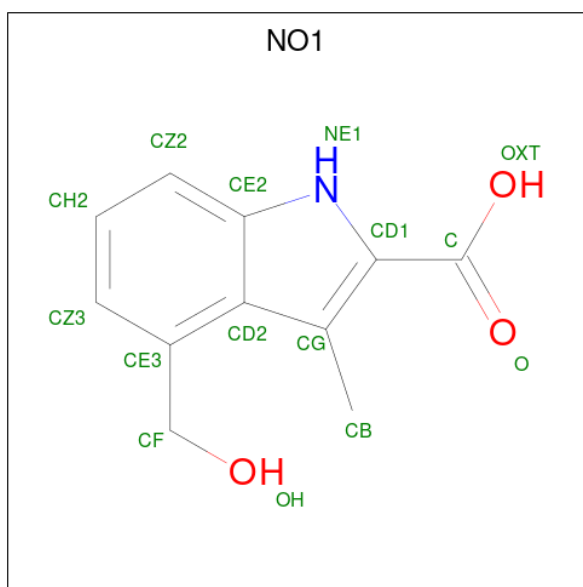
- Molecule 31 is a RNA chain called RIBOSOMAL 5S RNA.

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

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	4	1	Total	Zn	0	0
			1	1		
32	Y	1	Total	Zn	0	0
			1	1		

- Molecule 33 is 4-(hydroxymethyl)-3-methyl-1H-indole-2-carboxylic acid (CCD ID: NO1) (formula: C₁₁H₁₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	5	1	Total	C	N	O	0	0
			13	11	1	1		

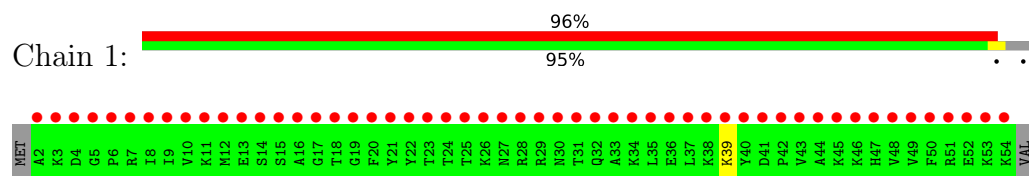
- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	M	1	Total	Mg	0	0
			1	1		
34	X	28	Total	Mg	0	0
			28	28		
34	Z	6	Total	Mg	0	0
			6	6		

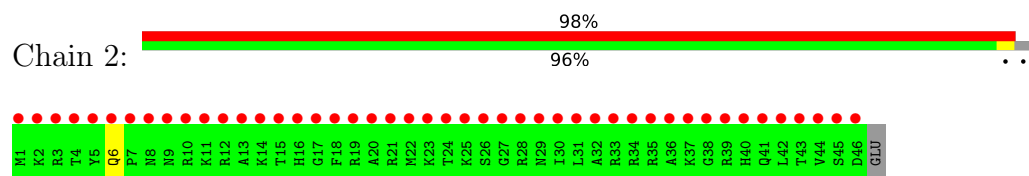
3 Residue-property plots [i](#)

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

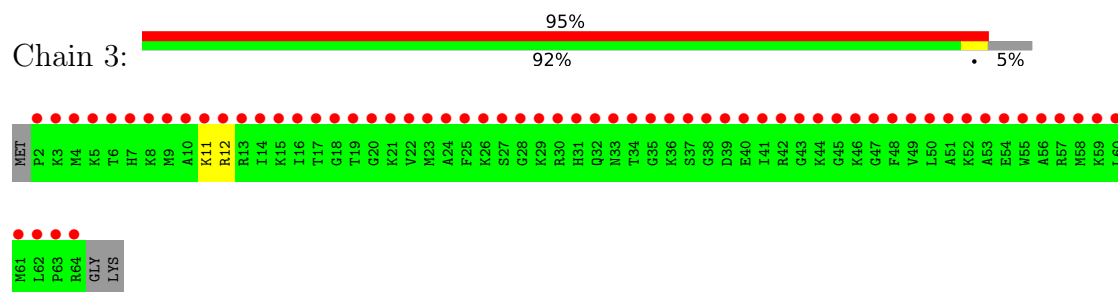
- Molecule 1: 50S RIBOSOMAL PROTEIN L33



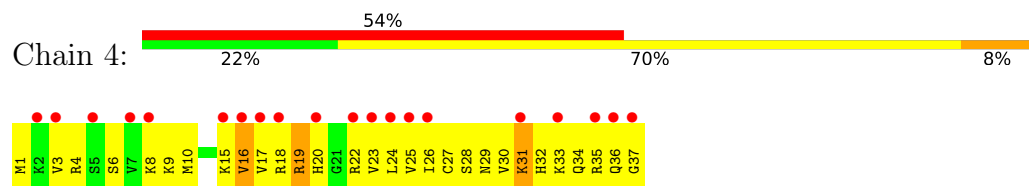
- Molecule 2: 50S RIBOSOMAL PROTEIN L34



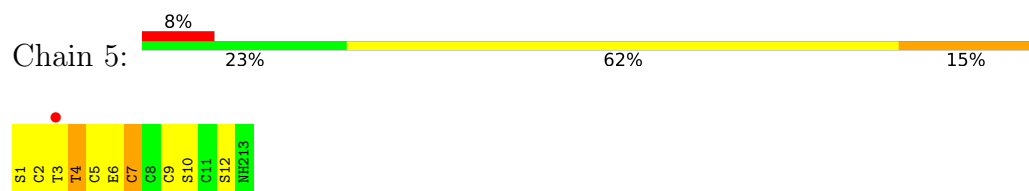
- Molecule 3: 50S RIBOSOMAL PROTEIN L35

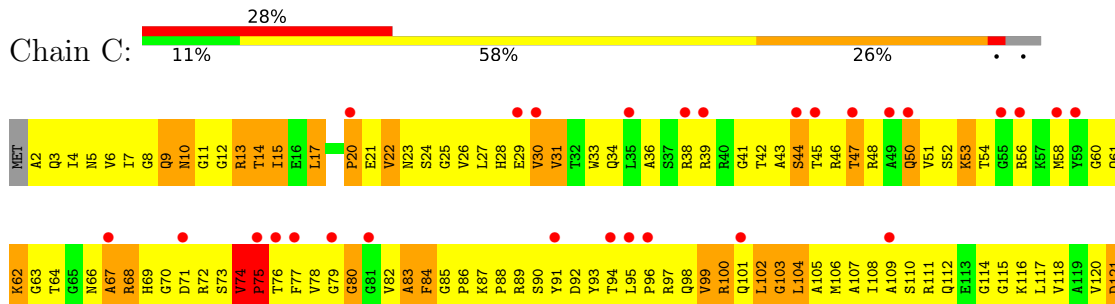


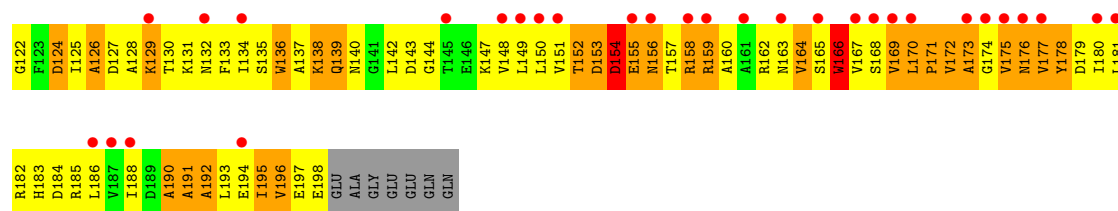
- Molecule 4: 50S RIBOSOMAL PROTEIN L36



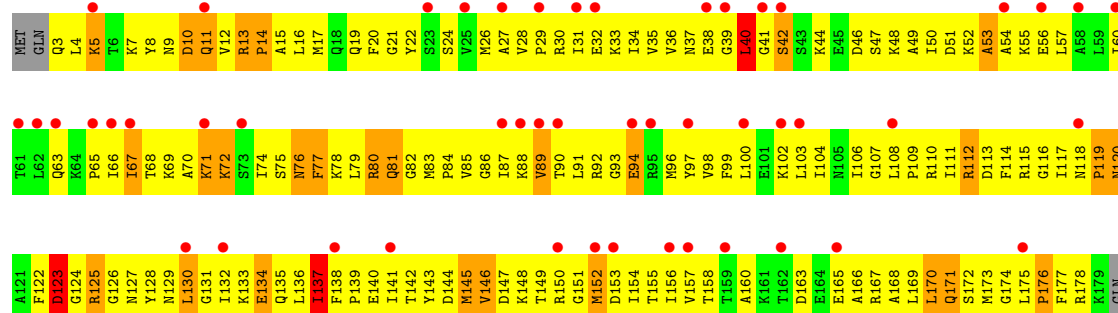
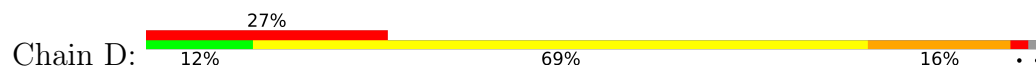
- Molecule 5: NOSIHEPTIDE



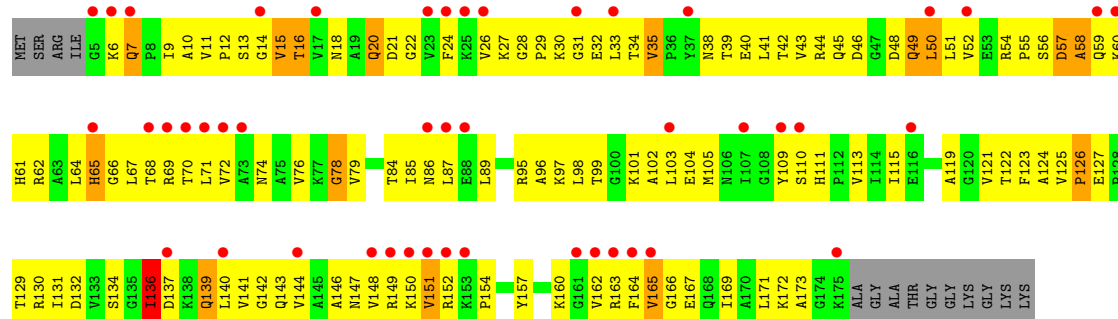




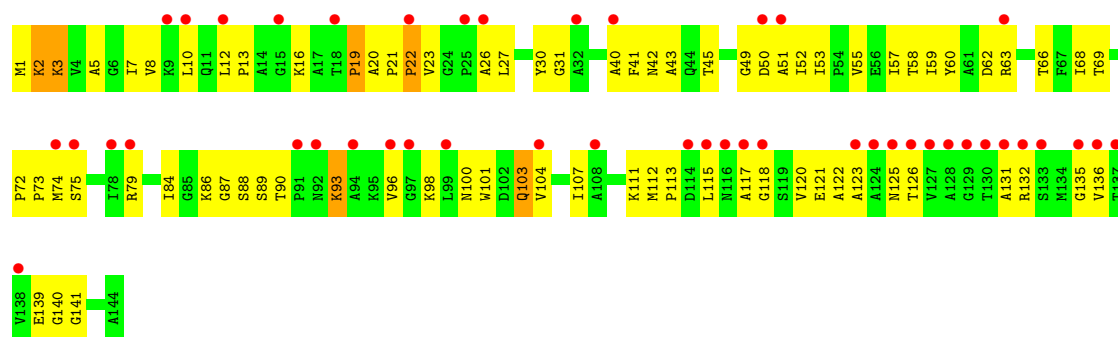
• Molecule 9: 50S RIBOSOMAL PROTEIN L5



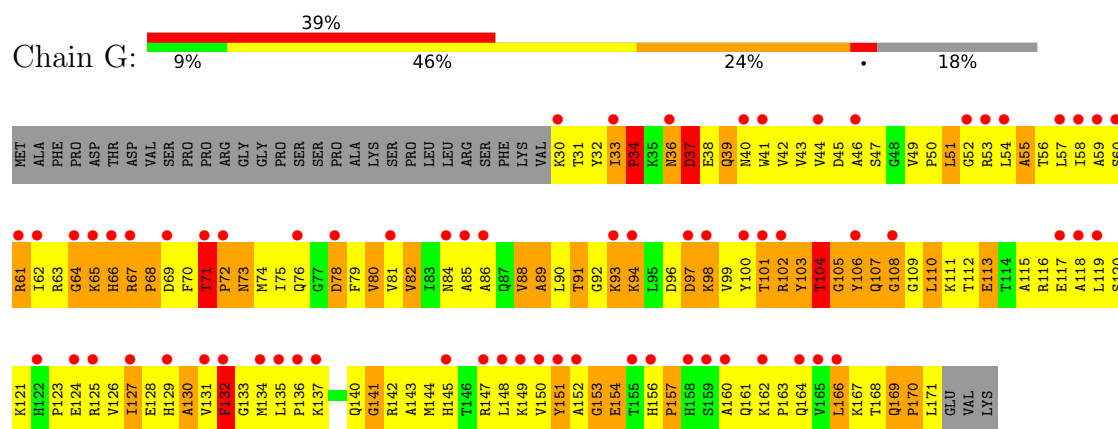
• Molecule 10: 50S RIBOSOMAL PROTEIN L6



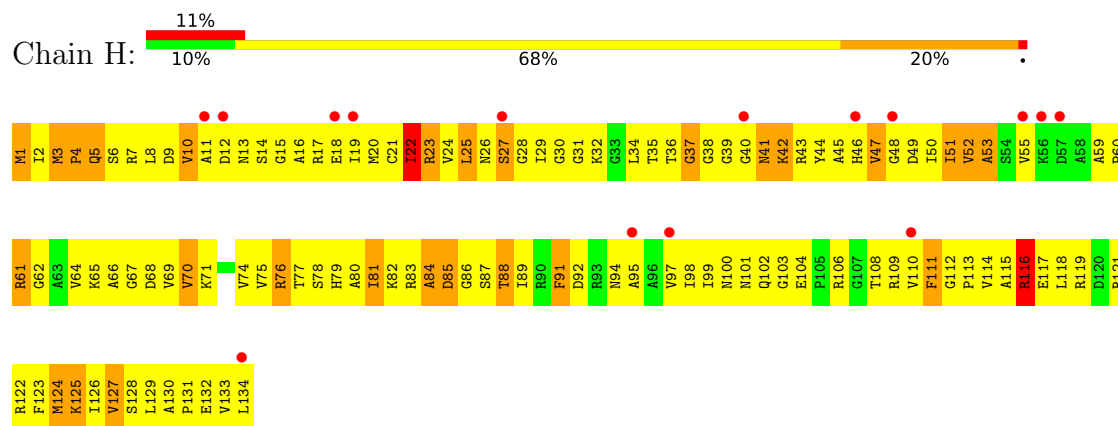
• Molecule 11: 50S RIBOSOMAL PROTEIN L11



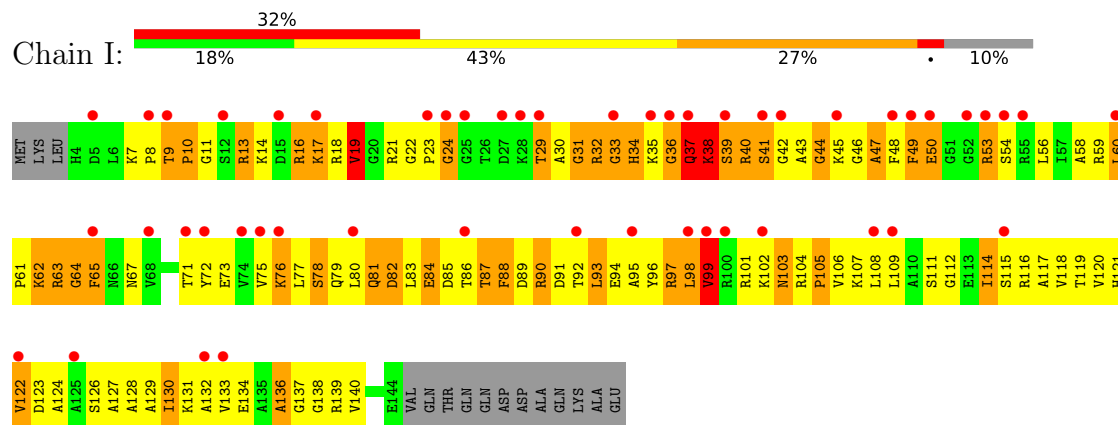
• Molecule 12: 50S RIBOSOMAL PROTEIN L13



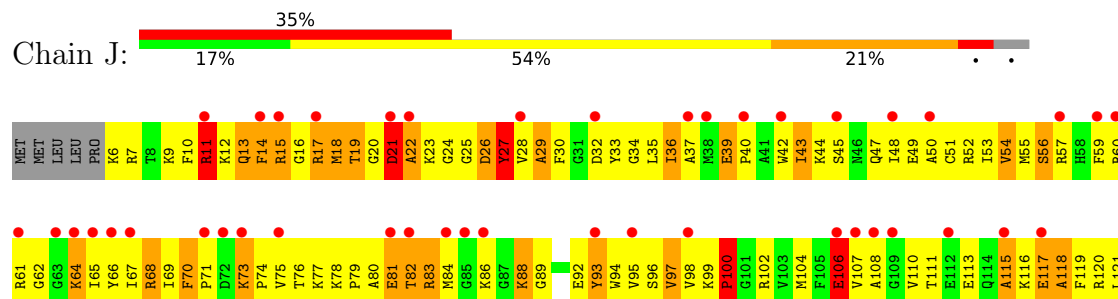
• Molecule 13: 50S RIBOSOMAL PROTEIN L14

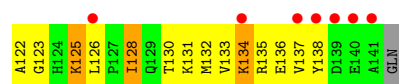


• Molecule 14: 50S RIBOSOMAL PROTEIN L15

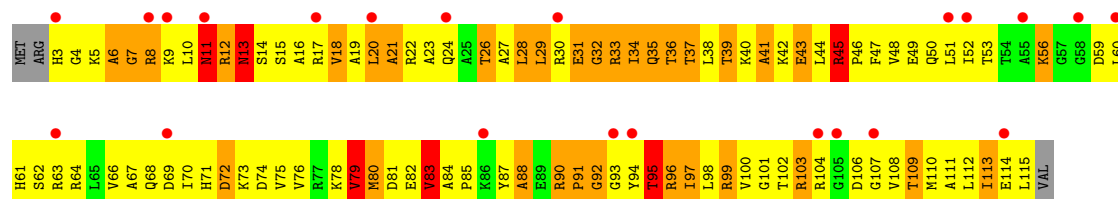
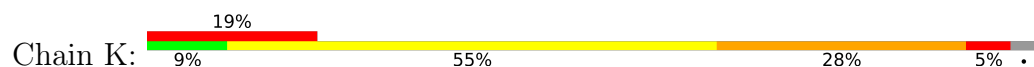


• Molecule 15: 50S RIBOSOMAL PROTEIN L16

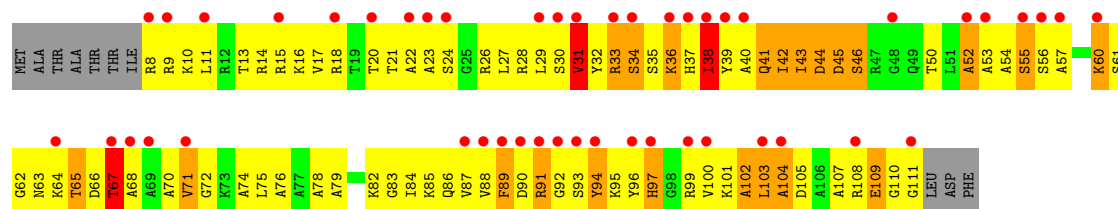
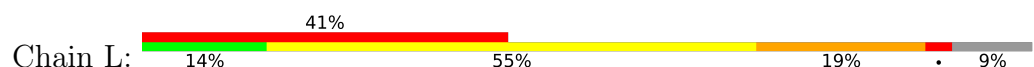




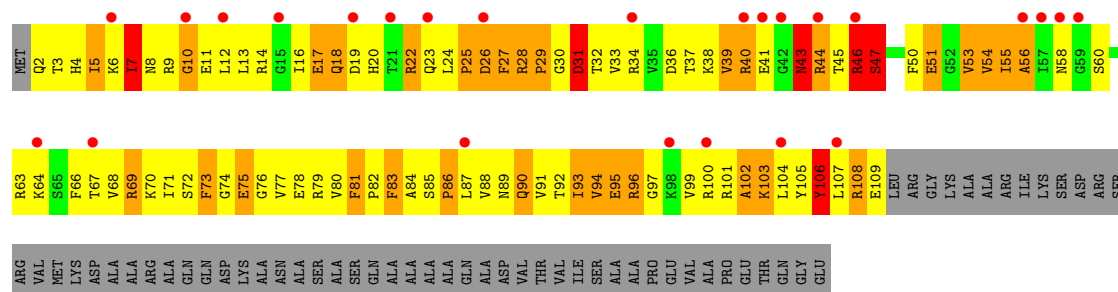
• Molecule 16: 50S RIBOSOMAL PROTEIN L17



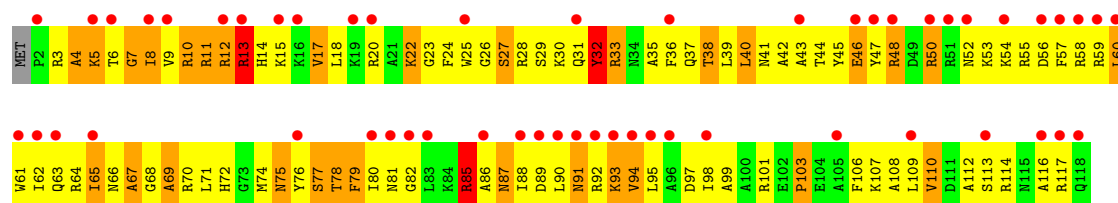
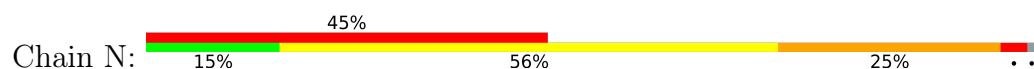
• Molecule 17: 50S RIBOSOMAL PROTEIN L18



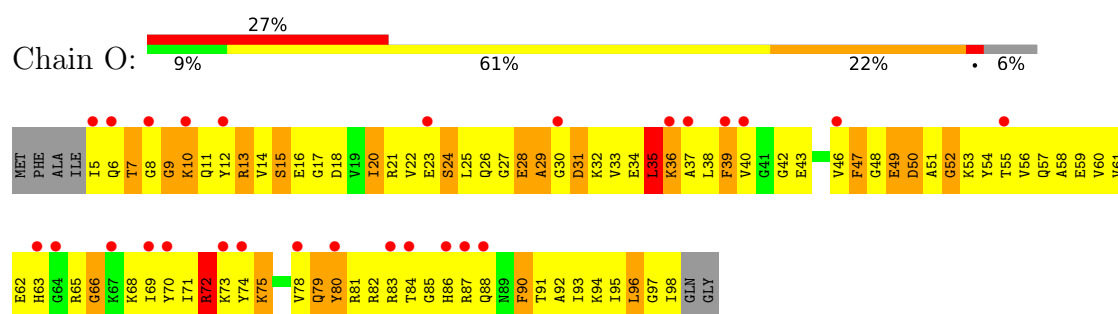
• Molecule 18: 50S RIBOSOMAL PROTEIN L19



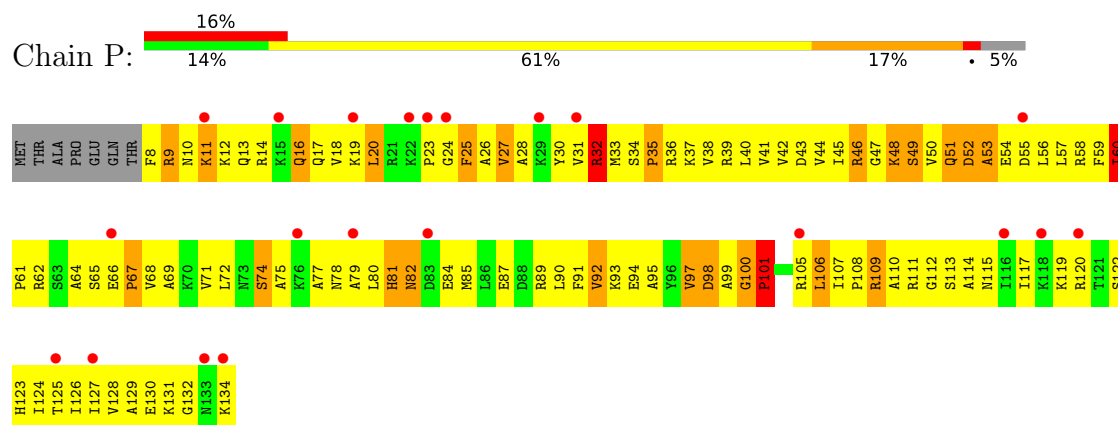
• Molecule 19: 50S RIBOSOMAL PROTEIN L20



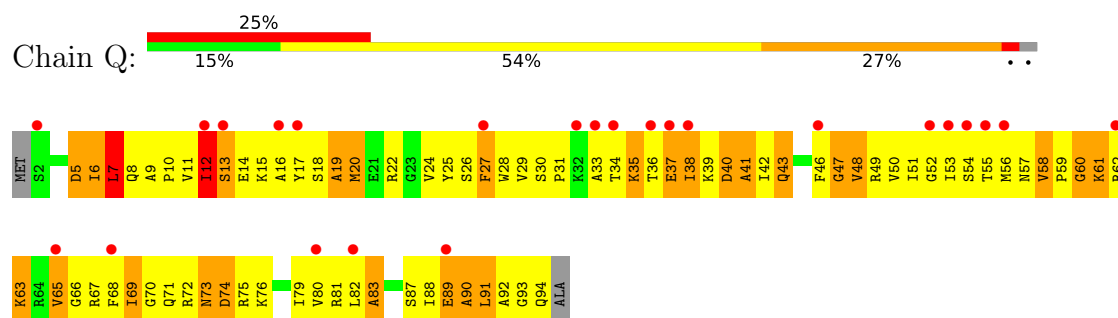
• Molecule 20: 50S RIBOSOMAL PROTEIN L21



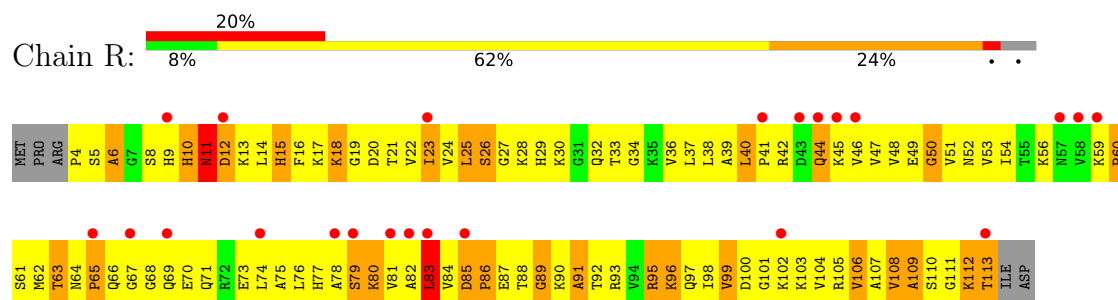
• Molecule 21: 50S RIBOSOMAL PROTEIN L22



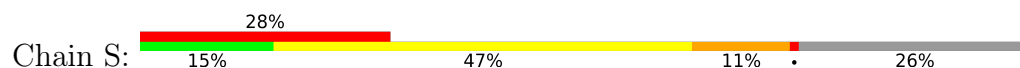
• Molecule 22: 50S RIBOSOMAL PROTEIN L23

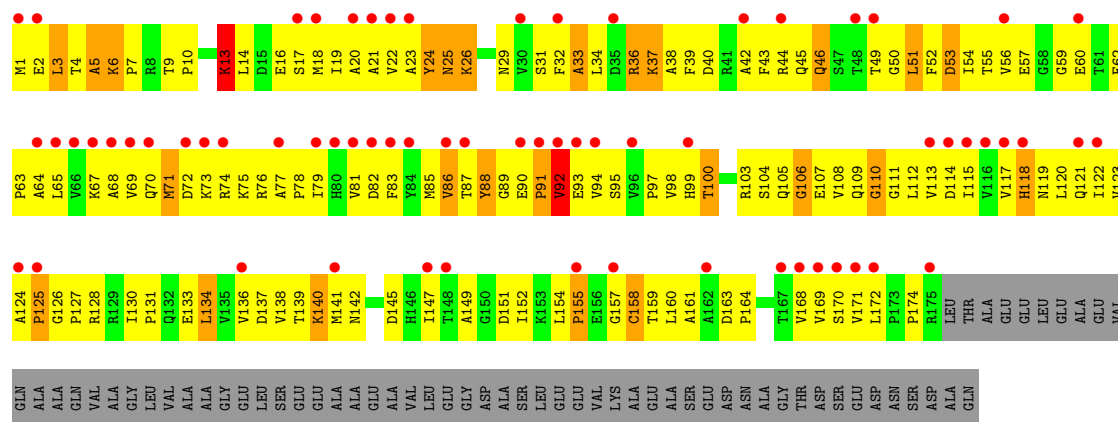


• Molecule 23: 50S RIBOSOMAL PROTEIN L24

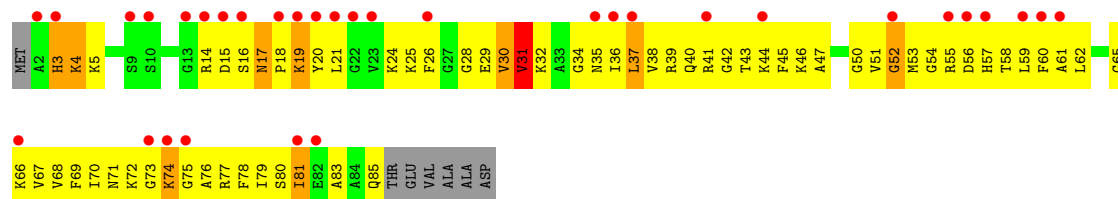


• Molecule 24: 50S RIBOSOMAL PROTEIN L25

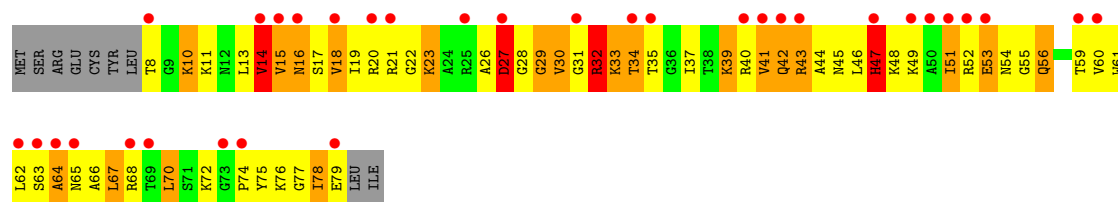
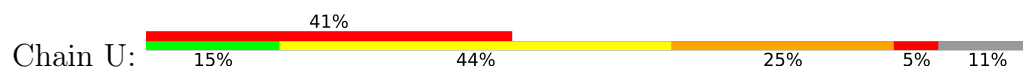




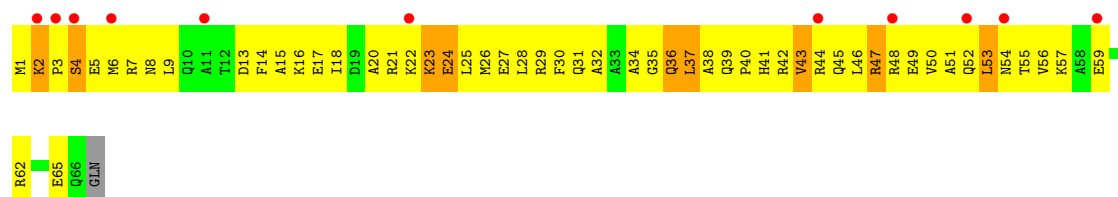
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



• Molecule 26: 50S RIBOSOMAL PROTEIN L28



• Molecule 27: 50S RIBOSOMAL PROTEIN L29

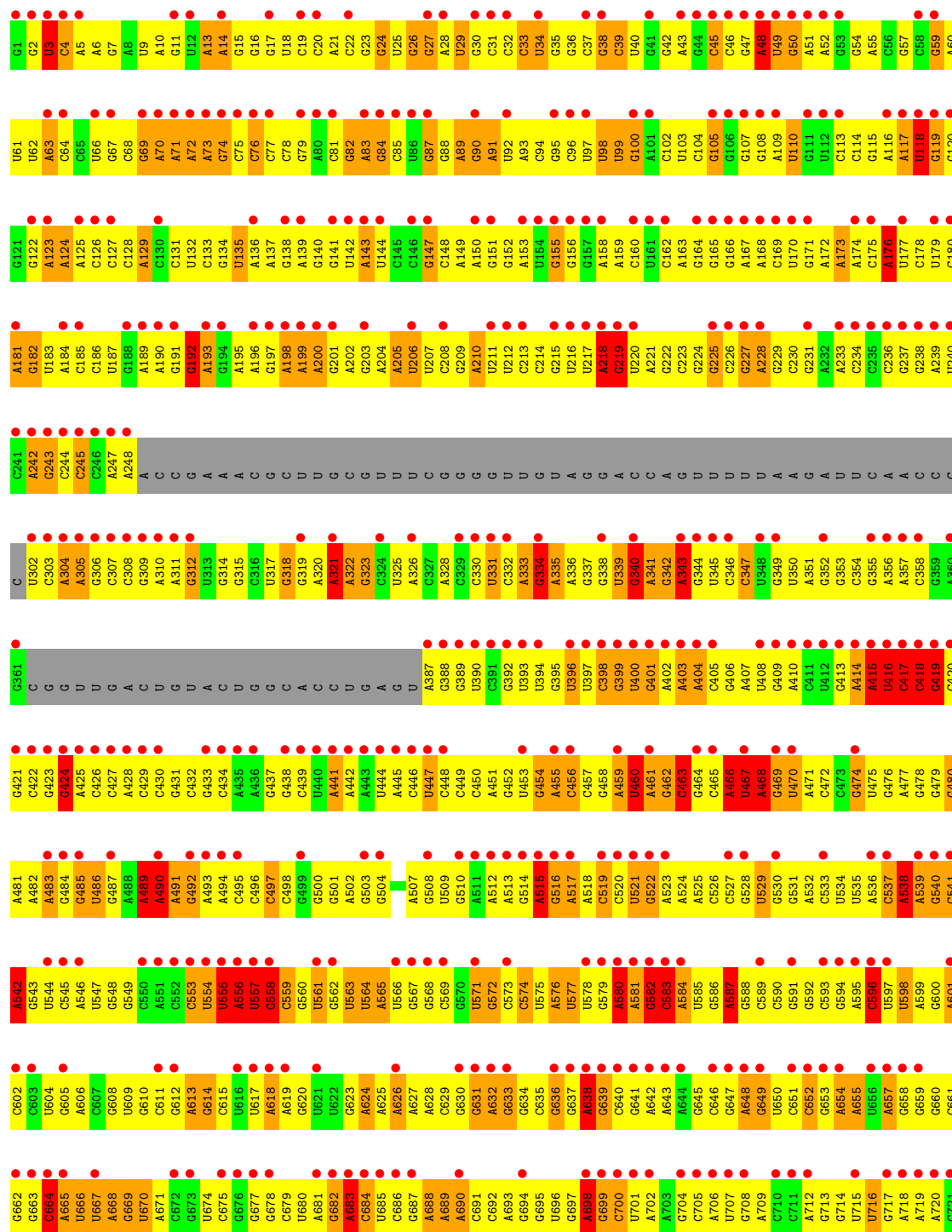
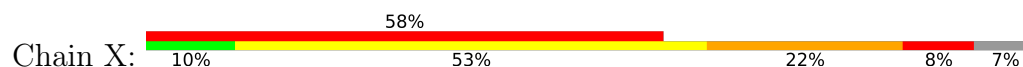


• Molecule 28: 50S RIBOSOMAL PROTEIN L30



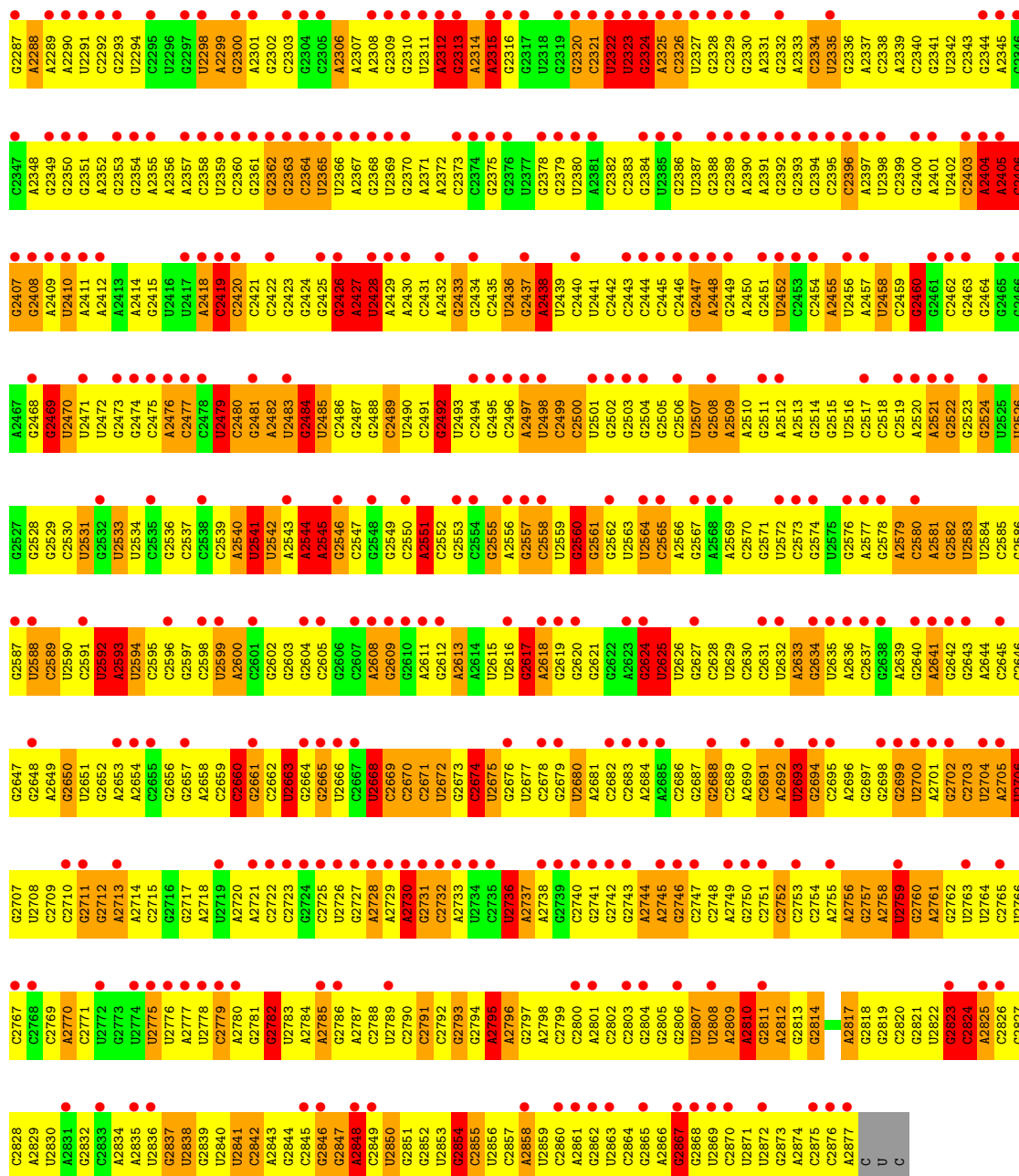


● Molecule 29: RIBOSOMAL 23S RNA

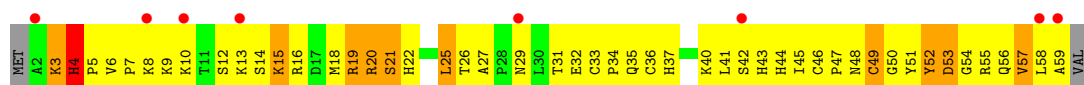


G1442	G1443	G1444	A1445	A1446	U1447	A1448	G1449	G1450	C1451	G1452	A1453	G1454	C1455	A1456	A1457	A1458	U1459	G1460	C1461	C1462	A1463	A1464	G1465	G1466	U1467	A1468	U1469	G1470	G1471	C1472	U1473	A1474	U1475	G1476	C1477	U1478	G1479	G1480	U1481	G1482	G1483	G1484	U1485	A1486	G1487	C1488	U1489	C1490	C1491	A1492	A1493	G1494	G1495	G1496	G1497	G1498	A1499	G1500	C1501						
G1382	C1383	G1384	C1385	G1386	A1387	C1388	C1389	G1390	G1391	U1392	G1393	G1394	A1395	C1396	G1397	G1398	C1399	A1400	G1401	G1402	C1403	A1404	A1405	A1406	G1407	A1408	U1409	C1410	C1411	C1412	U1413	G1414	C1415	G1416	C1417	U1418	G1419	A1420	U1421	C1422	A1423	U1424	G1425	U1426	G1427	G1428	U1429	G1430	U1431	G1432	A1433	U1434	G1435	G1436	A1437	G1438	U1439	G1440	A1441						
G1322	G1323	G1324	U1325	U1326	C1327	C1328	C1329	G1330	G1331	G1332	G1333	A1334	A1335	G1336	G1337	G1338	U1339	C1340	G1341	U1342	C1343	C1344	G1345	G1346	C1347	C1348	A1349	C1350	G1351	C1352	A1353	A1354	A1355	G1356	U1357	G1358	G1359	G1360	G1361	U1362	G1363	C1364	U1365	U1366	A1367	G1368	C1369	G1370	U1371	A1372	G1373	C1374	C1375	G1376	G1377	A1378	C1379	A1380	G1381						
U1262	G1263	G1264	G1265	G1266	A1267	U1268	G1269	C1270	C1271	G1272	G1273	C1274	A1275	U1276	G1277	A1278	G1279	U1280	A1281	A1282	C1283	G1284	A1285	U1286	A1287	A1288	A1289	A1290	G1291	C1292	A1293	G1294	U1295	G1296	A1297	G1298	A1299	A1300	U1301	C1302	U1303	U1304	C1305	U1306	U1307	G1308	G1309	G1310	C1311	G1312	U1313	A1314	A1315	G1316	G1317	A1318	C1319	A1320	A1321						
U1202	A1203	G1204	G1205	G1206	G1207	A1208	G1209	C1210	U1211	U1212	U1213	U1214	A1215	G1216	U1217	A1218	C1219	G1220	C1221	G1222	C1223	A1224	G1225	A1226	A1227	G1228	C1229	C1230	A1231	U1232	A1233	C1234	C1235	G1236	G1237	A1238	A1239	G1240	G1241	A1242	G1243	U1244	G1245	G1246	U1247	G1248	G1249	A1250	G1251	C1252	C1253	A1254	A1255	G1256	U1257	G1258	A1259	U1260	G1261						
G1182	C1183	A1184	G1185	G1186	C1187	A1188	C1189	C1190	U1191	C1192	U1193	C1194	A1195	A1196	A1197	U1198	A1199	G1200	U1101	G1102	C1103	G1104	U1105	A1106	A1107	U1108	A1109	G1110	C1111	U1112	C1113	A1114	C1115	U1116	A1117	G1118	U1119	C1120	G1121	A1122	C1123	U1124	G1125	A1126	G1127	G1128	A1129	U1130	G1131	C1132	G1133	C1134	C1135	G1136	U1137	A1138	A1139	A1140	U1141						
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C962	G963	A964	G965	A966	G967	C968	A969	U970	A971	C972	U973	U974	C975	C976	G977	U978	A979	G980	C981	C982	G983	A984	G985	A986	G987	G988	A989	G990	C991	C992	C993	A994	A995	C996	C997	C998	A999	G1000	A1001	C1002	C1003	U1004	U1005	C1006	A1007	G1008	G1009	U1010	A1011	A1012	G1013	G1014	U1015	A1016	C1017	C1018	U1019	A1020	A1021						
G862	C863	G864	U865	C866	C867	A868	G869	C890	C891	U892	C893	U894	G895	G896	U897	G898	U899	G900	A901	C902	C903	C904	A865	U866	C867	U868	C869	U890	A891	G	A892	A873	G874	G875	A876	G877	C878	A879	C880	U881	C882	A883	C884	A885	A886	G887	C888	C889	C890	A891	G	A892	G	A893	G	A894	G	A895	C	A896	C	A897	U	A898	C
U782	G783	U784	U785	U786	A787	G788	G789	A790	C791	U792	G793	U794	A795	G796	A797	G798	C799	U800	A801	A802	C803	C804	C805	A806	A807	C808	C809	U810	C811	C812	U813	A814	A815	C816	U817	C818	C819	U820	A821	C822	U823	U824	A825	U826	C827	C828	C829	C830	C831	A832	A833	G	A834	U835	G	U836	C	U837	A838	U839	U840	C841			
G722	C723	G724	C725	U726	U727	G728	A729	C730	A731	U732	G733	U734	G735	G736	C737	G738	C739	U740	A741	G742	A743	C744	C745	G746	A747	C748	C749	U750	C751	C752	U753	G754	C755	C756	U757	G758	C759	U760	G761	C762	A763	A764	C765	A766	U767	U768	C769	U770	C771	G772	G773	A774	U775	G	U776	C	A777	G778	U779	U780	G781				

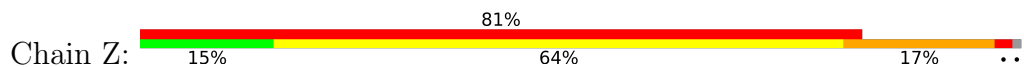
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U2228	A2168	C2048	G	G	G	U1926	G1806	A1746	A1685	A1624	U1564	G1503
G2229	A2169	C2049	A	A	A	U1927	A1867	A1747	A1686	A1625	G1565	G1504
G2230	C2170	G2050	G	G	G	G1928	A1868	U1748	A1687	A1626	G1566	U1505
G2231	U2171	U2051	C	C	C	U1929	A1869	G1749	U1688	C1627	A1567	C1506
G2232	U2172	G2052	C	C	C	C1930	U1870	A1750	U1689	C1628	A1568	G1507
G2233	G2173	G2053	U	U	U	G1931	A1811	A1751	U1690	G1629	A1569	G1508
G2234	A2174	A2054	G	G	G	G1932	U1812	U1752	G1691	A1630	C1570	A1509
G2235	A2175	G2055	C	C	C	G1933	U1813	U1753	C1692	G1631	G1571	A1510
G2236	U2176	C2056	G	G	G	U1934	G1814	G1754	A1693	A1632	C1572	A1511
G2237	U2177	U2057	A	A	A	A1935	G1815	G1755	A1694	C1633	G1573	A1512
G2238	U2178	A1998	A	A	A	A1936	G1816	C1756	U1695	A1634	A1574	U1513
G2239	C2179	U2058	A	A	A	G1937	U1817	C1757	U1696	G1635	C1575	C1514
C2240	U2180	U2059	C	C	C	U1938	G1818	C1758	U1697	G1636	G1576	U1515
U2241	A2181	A2060	U	U	U	U1939	C1878	A1759	C1698	U1637	G1577	A1516
C2242	A2182	C2061	G	G	G	C1940	G1879	A1760	A1699	G1638	U1578	C1517
C2243	C2183	U2062	U	U	U	U1941	G1880	G1761	C1700	U1639	G1579	G
C2244	G2184	A2063	G	G	G	C1942	U1881	G1762	C1701	C1640	C1580	G1520
A2245	U2185	U2064	C	C	C	G1943	C1882	G1763	C1702	C1641	C1581	U1521
A2246	G2186	G2065	U	U	U	C1945	A1883	A1764	C1703	G1642	A1582	C1522
A2247	A2187	U2067	U	U	U	U1946	C1885	G1765	G1704	A1643	A1523	A1523
A2248	A2188	C2068	U	U	U	G1947	C1886	U1766	U1705	G1644	C1524	A1524
U2249	A2189	U2069	U	U	U	C1948	G1887	G1767	A1706	U1645	A1525	A1525
G2250	A2190	G2070	G	G	G	A1949	U1827	U1768	A1707	G1646	U1526	U1526
A2191	A2191	U2071	G	G	G	C1950	C1828	U1769	C1708	U1647	G1527	U1527
A2192	U2192	C2072	G	G	G	G1951	C1829	U1770	U1709	C1643	C1528	C1528
C2193	C2193	A2073	G	G	G	A1952	C1830	A1771	U1710	A1649	C1529	C1529
C2194	A2194	C2073	U	U	U	C1953	G1831	C1772	C1711	U1530	C1530	C1530
G2195	U2195	U2074	C	C	C	A1954	U1833	C1773	G1712	A1583	C1531	C1531
G2196	U2196	G2075	C	C	C	G1955	G1834	A1774	U1591	G1652	U1591	A1532
A2197	U2197	C2076	G	G	G	A1956	U1835	A1775	G1713	C1653	G1533	G1533
U2198	G2198	G2077	U	U	U	C1957	A1836	A1776	A1714	A1654	A1534	A1534
U2199	C2199	C2078	U	U	U	C1958	C1837	A1777	G1715	C1655	A1535	A1535
G2200	G2200	U2080	G	G	G	U1959	G1838	U1778	G1716	U1656	U1536	U1536
C2201	A2201	G2081	A	A	A	A1960	A1839	C1779	A1597	A1657	U1537	U1537
C2202	G2202	C2082	G	G	G	A1961	C1840	C1780	C1598	A1538	U1539	U1539
G2203	G2203	G2083	G	G	G	C1962	G1841	C1781	G1599	C1540	C1540	C1540
A2204	A2204	G2084	C	C	C	G1963	U1842	A1782	U1721	G1661	U1601	G1541
C2205	C2205	G2085	A	A	A	U1965	U1843	G1783	G1722	G1662	G1602	G1542
C2206	C2206	U2086	A	A	A	C1966	C1844	C1784	C1723	G1663	A1603	G1543
G2207	U2087	U2087	C	C	C	G1968	A1845	A1785	C1725	G1664	A1604	A1544
U2208	U2088	C2088	G	G	G	G1969	U1846	C1786	C1726	A1544	G1545	G1545
G2209	C2089	C2089	G	G	G	U1970	G1847	U1787	C1727	C1665	C1546	C1546
U2210	U2090	U2090	U	U	U	C1971	U1848	U1788	A1728	G1666	A1605	G1547
C2211	C	C	G	G	G	G1972	C1849	U1789	C1729	A1667	A1606	U1547
U2212	U2111	A2031	A	A	A	C1973	A1850	G1790	G1730	G1668	A1607	U1548
G2213	G2213	C2032	A	A	A	U1974	A1851	C1791	C1731	U1608	U1608	U1548
G2214	G2214	C2033	A	A	A	G1975	G1852	C1792	A1669	G1609	C1549	C1549
C2215	A	A2034	U	U	U	U1976	G1853	A1793	G1670	A1610	C1550	C1550
G2216	U	G2035	A	A	A	C1977	G1854	A1794	U1733	A1671	U1551	U1551
G2217	C	G2036	C	C	C	U1978	G1855	C1795	C1734	A1672	G1552	G1552
G2218	C	A2037	C	C	C	U1979	G1856	A1796	G1735	G1673	G1553	G1553
U2219	A	C2038	A	A	A	U1980	U1857	A1797	C1736	C1674	G1554	G1554
A2220	A	G2039	A	A	A	A1981	G1858	G1798	U1737	C1675	A1555	A1555
G2221	C	A2040	C	C	C	C1982	C1859	G1799	U1738	G1676	A1556	A1556
G2222	U	U2041	C	C	C	A1983	A1859	A1799	G1739	U1677	G1557	G1557
G2223	A	A2042	U	U	U	C1984	A1860	A1800	G1740	U1678	C1558	C1558
G2224	G	A2043	G	G	G	U1985	G1861	C1801	G1741	U1679	A1559	A1559
U2225	U	G2044	U	U	U	U1986	C1862	A1802	G1742	U1680	A1560	A1560
G2226	G	A2045	G	G	G	C1987	U1863	G1803	C1743	C1621	A1561	A1561
A2165	A2165	U	G	G	G	G1988	G1864	U1804	G1744	G1683	G1622	G1622

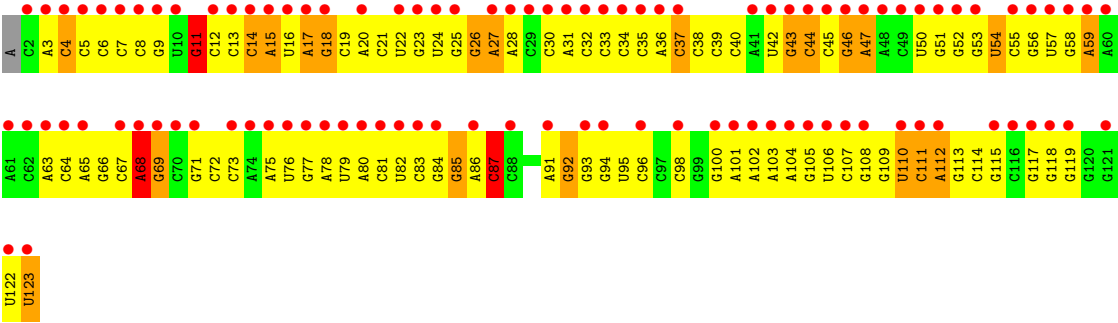


• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 31: RIBOSOMAL 5S RNA





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)	30.00 – 3.70 30.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	85.6 (30.00-3.70) 88.8 (30.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.300 , 0.340 0.323 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	109.2	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 118.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	84444	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: DBU, MH6, MG, DHA, NO1, 3GL, BB9, NH2, ZN

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$
4	4	0.58	0/298	0.94	2/390 (0.5%)
5	5	3.52	1/12 (8.3%)	2.72	1/12 (8.3%)
6	A	0.58	0/1862	1.03	9/2510 (0.4%)
7	B	0.97	2/1567 (0.1%)	1.38	22/2105 (1.0%)
8	C	0.68	0/1529	1.16	12/2070 (0.6%)
9	D	0.49	0/1419	0.94	2/1903 (0.1%)
10	E	0.55	0/1308	0.97	1/1771 (0.1%)
11	F	0.52	0/1063	0.93	2/1440 (0.1%)
12	G	0.70	0/1138	1.23	11/1539 (0.7%)
13	H	1.05	2/1007 (0.2%)	1.51	18/1352 (1.3%)
14	I	0.66	0/1081	1.13	8/1448 (0.6%)
15	J	0.73	0/1113	1.34	20/1486 (1.3%)
16	K	1.12	1/886 (0.1%)	1.54	17/1188 (1.4%)
17	L	0.65	0/785	1.09	5/1048 (0.5%)
18	M	1.02	3/884 (0.3%)	1.41	16/1186 (1.3%)
19	N	0.76	0/994	1.20	9/1323 (0.7%)
20	O	0.64	0/750	1.09	4/1000 (0.4%)
21	P	0.97	1/1027 (0.1%)	1.47	11/1373 (0.8%)
22	Q	0.62	0/737	1.06	5/988 (0.5%)
23	R	0.61	0/835	1.11	6/1121 (0.5%)
24	S	0.60	0/1370	0.99	3/1862 (0.2%)
25	T	0.60	0/633	1.02	4/838 (0.5%)
26	U	0.60	0/556	1.18	6/741 (0.8%)
27	V	0.55	0/537	1.01	2/714 (0.3%)
28	W	0.75	0/426	1.23	5/568 (0.9%)
29	X	0.58	3/64561 (0.0%)	0.99	371/100708 (0.4%)
30	Y	0.94	0/469	1.43	6/629 (1.0%)
31	Z	0.43	0/2904	0.74	1/4525 (0.0%)
All	All	0.63	13/91751 (0.0%)	1.04	579/137838 (0.4%)

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
5	5	1	0
19	N	0	1
29	X	1	199
30	Y	0	1
31	Z	0	4
All	All	2	205

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	1	SER	CA-CB	-7.80	1.37	1.53
18	M	103	LYS	CA-C	7.38	1.58	1.52
7	B	113	THR	CA-CB	6.91	1.63	1.52
13	H	10	VAL	CA-CB	-6.29	1.46	1.53
29	X	557	U	C1'-N1	6.25	1.56	1.47

The worst 5 of 579 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1055	A	N9-C1'-C2'	-22.98	77.53	112.00
29	X	557	U	N1-C1'-C2'	17.00	139.50	114.00
21	P	60	ILE	CA-C-N	16.79	136.43	118.97
21	P	60	ILE	C-N-CA	16.79	136.43	118.97
29	X	417	C	N1-C1'-C2'	15.49	137.23	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	5	1	SER	CA
29	X	2592	U	C1'

5 of 205 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	N	32	TYR	Sidechain
29	X	228	A	Sidechain
29	X	24	G	Sidechain
29	X	26	G	Sidechain
29	X	321	A	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	1	53	0	0	2	0
2	2	46	0	0	1	0
3	3	63	0	0	2	0
4	4	297	0	328	68	0
5	5	69	0	34	3	0
6	A	1826	0	1885	319	0
7	B	1539	0	1600	311	0
8	C	1506	0	1525	353	0
9	D	1400	0	1481	317	0
10	E	1286	0	1336	211	0
11	F	1044	0	1088	102	0
12	G	1114	0	1144	291	0
13	H	997	0	1046	212	0
14	I	1067	0	1103	252	0
15	J	1090	0	1125	269	0
16	K	878	0	930	211	0
17	L	779	0	820	189	0
18	M	871	0	894	225	0
19	N	978	0	1020	210	0
20	O	741	0	756	195	0
21	P	1014	0	1096	208	0
22	Q	726	0	753	151	0
23	R	825	0	881	220	0
24	S	1345	0	1372	231	0
25	T	625	0	655	121	0
26	U	552	0	604	153	0
27	V	533	0	558	97	0
28	W	424	0	470	71	0
29	X	57651	0	29048	4652	0
30	Y	457	0	460	110	0
31	Z	2598	0	1328	177	0
32	4	1	0	0	0	0
32	Y	1	0	0	0	0
33	5	13	0	7	0	0
34	M	1	0	0	0	0
34	X	28	0	0	0	0
34	Z	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	84444	0	55347	9100	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 65.

The worst 5 of 9100 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)
18:M:108:ARG:O	18:M:109:GLU:HG3	1.25	1.33
29:X:1854:G:O2'	29:X:1855:G:H5'	1.31	1.28
29:X:1053:G:H2'	29:X:1054:C:C6	1.71	1.25
29:X:1386:A:H5''	29:X:2191:A:N6	1.48	1.25
29:X:2196:U:H2'	29:X:2197:U:O4'	1.31	1.23

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	35/37 (95%)	20 (57%)	12 (34%)	3 (9%)	0	8
5	5	2/13 (15%)	1 (50%)	1 (50%)	0	100	100
6	A	238/274 (87%)	166 (70%)	51 (21%)	21 (9%)	0	8
7	B	203/211 (96%)	143 (70%)	33 (16%)	27 (13%)	0	3
8	C	195/205 (95%)	94 (48%)	55 (28%)	46 (24%)	0	0
9	D	175/180 (97%)	99 (57%)	50 (29%)	26 (15%)	0	2
10	E	169/185 (91%)	110 (65%)	40 (24%)	19 (11%)	0	4
11	F	142/144 (99%)	101 (71%)	33 (23%)	8 (6%)	1	16
12	G	140/174 (80%)	76 (54%)	34 (24%)	30 (21%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	H	132/134 (98%)	106 (80%)	18 (14%)	8 (6%)	1	14
14	I	139/156 (89%)	60 (43%)	41 (30%)	38 (27%)	0	0
15	J	134/142 (94%)	76 (57%)	41 (31%)	17 (13%)	0	4
16	K	111/116 (96%)	70 (63%)	23 (21%)	18 (16%)	0	2
17	L	102/114 (90%)	65 (64%)	23 (22%)	14 (14%)	0	3
18	M	106/166 (64%)	64 (60%)	22 (21%)	20 (19%)	0	1
19	N	115/118 (98%)	65 (56%)	30 (26%)	20 (17%)	0	2
20	O	92/100 (92%)	52 (56%)	23 (25%)	17 (18%)	0	1
21	P	125/134 (93%)	84 (67%)	26 (21%)	15 (12%)	0	4
22	Q	91/95 (96%)	45 (50%)	25 (28%)	21 (23%)	0	0
23	R	108/115 (94%)	61 (56%)	28 (26%)	19 (18%)	0	1
24	S	173/237 (73%)	96 (56%)	50 (29%)	27 (16%)	0	2
25	T	82/91 (90%)	56 (68%)	16 (20%)	10 (12%)	0	4
26	U	70/81 (86%)	34 (49%)	19 (27%)	17 (24%)	0	0
27	V	64/67 (96%)	44 (69%)	12 (19%)	8 (12%)	0	4
28	W	53/55 (96%)	36 (68%)	13 (24%)	4 (8%)	1	11
30	Y	56/60 (93%)	35 (62%)	15 (27%)	6 (11%)	0	5
All	All	3052/3404 (90%)	1859 (61%)	734 (24%)	459 (15%)	0	2

5 of 459 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	54	ILE
6	A	59	LYS
7	B	76	ARG
7	B	85	ALA
7	B	86	PRO

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	
4	4	35/35 (100%)	35 (100%)	0	100	100
5	5	2/3 (67%)	2 (100%)	0	100	100
6	A	185/215 (86%)	173 (94%)	12 (6%)	15	43
7	B	155/157 (99%)	143 (92%)	12 (8%)	12	38
8	C	157/163 (96%)	147 (94%)	10 (6%)	16	43
9	D	153/156 (98%)	144 (94%)	9 (6%)	18	44
10	E	136/144 (94%)	130 (96%)	6 (4%)	25	50
11	F	107/107 (100%)	104 (97%)	3 (3%)	38	58
12	G	118/146 (81%)	102 (86%)	16 (14%)	3	19
13	H	103/103 (100%)	92 (89%)	11 (11%)	6	27
14	I	108/121 (89%)	98 (91%)	10 (9%)	8	32
15	J	110/116 (95%)	98 (89%)	12 (11%)	6	26
16	K	90/93 (97%)	72 (80%)	18 (20%)	1	9
17	L	74/82 (90%)	62 (84%)	12 (16%)	2	14
18	M	94/134 (70%)	80 (85%)	14 (15%)	3	16
19	N	96/97 (99%)	90 (94%)	6 (6%)	16	43
20	O	75/79 (95%)	69 (92%)	6 (8%)	11	37
21	P	109/115 (95%)	101 (93%)	8 (7%)	13	40
22	Q	75/76 (99%)	69 (92%)	6 (8%)	11	37
23	R	91/96 (95%)	80 (88%)	11 (12%)	5	22
24	S	149/192 (78%)	140 (94%)	9 (6%)	17	44
25	T	62/67 (92%)	60 (97%)	2 (3%)	34	56
26	U	57/66 (86%)	49 (86%)	8 (14%)	3	18
27	V	54/55 (98%)	54 (100%)	0	100	100
28	W	48/48 (100%)	45 (94%)	3 (6%)	16	43
30	Y	51/53 (96%)	46 (90%)	5 (10%)	7	30
All	All	2494/2719 (92%)	2285 (92%)	209 (8%)	10	35

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	K	97	ILE
18	M	90	GLN
26	U	70	LEU

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Mol	Chain	Res	Type
17	L	31	VAL
17	L	94	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
21	P	115	ASN
25	T	71	ASN
22	Q	73	ASN
24	S	70	GLN
27	V	45	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2680/2880 (93%)	655 (24%)	239 (8%)
31	Z	121/123 (98%)	24 (19%)	1 (0%)
All	All	2801/3003 (93%)	679 (24%)	240 (8%)

5 of 679 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	4	C
29	X	13	A
29	X	14	A
29	X	27	G
29	X	29	U

5 of 240 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	1299	A
29	X	2660	C
29	X	1632	A
29	X	2593	A
29	X	2848	A

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

Of 10 non-standard protein/DNA/RNA residues modelled in this entry, 1 is modelled with single atom - leaving 9 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
5	3GL	5	6	33,5	8,8,10	4.42	6 (75%)	9,10,13	1.46	1 (11%)
5	BB9	5	11	5	2,5,6	0.87	0	1,5,7	1.88	0
5	BB9	5	7	5	2,5,6	3.84	2 (100%)	1,5,7	4.78	1 (100%)
5	MH6	5	10	5	3,4,6	3.51	1 (33%)	2,4,7	3.46	2 (100%)
5	DHA	5	12	5	3,4,5	5.58	2 (66%)	2,4,6	2.84	2 (100%)
5	BB9	5	5	5	2,5,6	4.83	1 (50%)	1,5,7	0.14	0
5	BB9	5	2	5	2,5,6	7.48	1 (50%)	1,5,7	6.06	1 (100%)
5	BB9	5	9	5	2,4,6	1.59	1 (50%)	3,4,7	2.18	2 (66%)
5	DBU	5	4	5	3,4,6	4.98	3 (100%)	3,4,7	2.50	2 (66%)

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
5	3GL	5	6	33,5	-	0/8/8/12	-
5	BB9	5	11	5	-	0/0/4/6	-
5	BB9	5	7	5	-	0/0/4/6	-
5	MH6	5	10	5	-	1/1/2/6	-
5	DHA	5	12	5	-	0/0/2/4	-
5	BB9	5	5	5	-	0/0/4/6	-
5	BB9	5	2	5	-	0/0/4/6	-
5	BB9	5	9	5	-	0/0/2/6	-
5	DBU	5	4	5	-	1/1/2/6	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	2	BB9	C-CA	10.55	1.62	1.45
5	5	6	3GL	CG-CD	9.34	1.65	1.52
5	5	12	DHA	C-CA	8.95	1.60	1.45
5	5	5	BB9	C-CA	6.83	1.56	1.45
5	5	4	DBU	CA-N	6.65	1.49	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	2	BB9	O-C-CA	-6.06	117.79	125.39
5	5	7	BB9	O-C-CA	-4.78	119.39	125.39
5	5	10	MH6	C-CA-CB	3.83	126.14	118.21
5	5	4	DBU	C-CA-N	-3.68	112.42	116.44
5	5	12	DHA	O-C-CA	-3.37	119.22	125.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	5	10	MH6	C-CA-CB-OG
5	5	4	DBU	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	5	7	BB9	2	0
5	5	4	DBU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 37 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	$\# Z > 2$
33	NO1	5	14	5	14,14,16	5.62	7 (50%)	19,20,23	3.57	14 (73%)

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
33	NO1	5	14	5	-	0/2/2/6	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	14	NO1	CD2-CE3	15.11	1.61	1.40
33	5	14	NO1	CF-CE3	-8.01	1.36	1.51
33	5	14	NO1	CH2-CZ3	7.56	1.51	1.38
33	5	14	NO1	CD1-NE1	6.39	1.47	1.38
33	5	14	NO1	CZ3-CE3	-5.27	1.29	1.39

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	5	14	NO1	CZ2-CE2-CD2	6.35	135.30	121.75
33	5	14	NO1	CE2-CD2-CE3	-5.77	106.80	120.88
33	5	14	NO1	CF-CE3-CD2	-5.44	114.51	121.67
33	5	14	NO1	CZ2-CE2-NE1	-4.40	121.93	130.83
33	5	14	NO1	CE2-CD2-CG	4.11	115.81	107.50

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	53/55 (96%)	9.08	53 (100%) 0 0	91, 120, 138, 158	0
2	2	46/47 (97%)	12.01	46 (100%) 0 0	42, 90, 116, 151	0
3	3	63/66 (95%)	10.03	63 (100%) 0 0	52, 106, 135, 145	0
4	4	37/37 (100%)	2.24	20 (54%) 0 0	73, 124, 148, 152	0
5	5	3/13 (23%)	1.55	1 (33%) 1 1	84, 84, 84, 84	0
6	A	240/274 (87%)	2.50	139 (57%) 0 0	36, 129, 160, 198	0
7	B	205/211 (97%)	1.19	46 (22%) 2 3	13, 85, 130, 161	0
8	C	197/205 (96%)	1.53	58 (29%) 1 2	24, 110, 147, 170	0
9	D	177/180 (98%)	1.49	49 (27%) 1 2	101, 136, 160, 179	0
10	E	171/185 (92%)	1.52	46 (26%) 1 2	79, 131, 158, 176	0
11	F	144/144 (100%)	1.91	45 (31%) 1 1	117, 148, 172, 188	0
12	G	142/174 (81%)	2.05	68 (47%) 0 1	30, 112, 143, 169	0
13	H	134/134 (100%)	0.85	15 (11%) 10 11	13, 67, 106, 127	0
14	I	141/156 (90%)	1.81	50 (35%) 1 1	13, 128, 156, 181	0
15	J	136/142 (95%)	1.97	50 (36%) 1 1	25, 112, 155, 202	0
16	K	113/116 (97%)	0.92	22 (19%) 3 4	13, 57, 111, 148	0
17	L	104/114 (91%)	2.12	47 (45%) 0 1	73, 125, 149, 167	0
18	M	108/166 (65%)	1.23	25 (23%) 2 2	13, 76, 121, 150	0
19	N	117/118 (99%)	2.07	53 (45%) 0 1	16, 104, 144, 182	0
20	O	94/100 (94%)	1.61	27 (28%) 1 2	28, 117, 151, 160	0
21	P	127/134 (94%)	0.96	21 (16%) 4 6	13, 76, 126, 155	0
22	Q	93/95 (97%)	1.54	24 (25%) 1 2	35, 114, 152, 159	0
23	R	110/115 (95%)	1.24	23 (20%) 2 3	53, 118, 145, 161	0
24	S	175/237 (73%)	1.97	67 (38%) 1 1	78, 136, 159, 184	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)		Q<0.9	
25	T	84/91 (92%)	1.89	33 (39%)	1	1	75, 117, 145, 181	0
26	U	72/81 (88%)	2.23	33 (45%)	0	1	60, 130, 160, 180	0
27	V	66/67 (98%)	1.11	11 (16%)	4	6	83, 126, 158, 168	0
28	W	55/55 (100%)	1.84	21 (38%)	1	1	35, 105, 140, 169	0
29	X	2686/2880 (93%)	2.79	1680 (62%)	0	0	13, 114, 186, 250	0
30	Y	58/60 (96%)	1.07	8 (13%)	6	8	13, 70, 119, 132	0
31	Z	122/123 (99%)	3.26	100 (81%)	0	0	38, 143, 188, 205	0
All	All	6073/6575 (92%)	2.41	2944 (48%)	0	1	13, 116, 174, 250	0

The worst 5 of 2944 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	35	LEU	25.0
3	3	32	GLN	21.4
2	2	33	ARG	20.9
1	1	23	THR	20.3
3	3	61	MET	20.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
5	DHA	5	12	5/6	0.27	0.18	83,83,83,83	0
5	NH2	5	13	1/1	0.45	0.13	83,83,83,83	0
5	BB9	5	7	6/7	0.54	0.18	83,83,83,83	0
5	BB9	5	9	5/7	0.61	0.16	83,83,83,83	0
5	MH6	5	10	5/7	0.65	0.12	83,83,83,83	0
5	DBU	5	4	5/7	0.66	0.22	83,83,83,83	0
5	3GL	5	6	9/11	0.67	0.13	83,83,83,83	0
5	BB9	5	2	6/7	0.67	0.17	83,83,83,83	0
5	BB9	5	5	6/7	0.74	0.13	83,83,83,83	0
5	BB9	5	11	6/7	0.89	0.10	83,83,83,83	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
34	MG	Z	128	1/1	0.45	0.19	110,110,110,110	0
34	MG	X	2889	1/1	0.53	0.43	131,131,131,131	0
34	MG	X	2883	1/1	0.61	0.59	104,104,104,104	0
34	MG	X	2901	1/1	0.62	0.66	100,100,100,100	0
34	MG	Z	124	1/1	0.65	0.67	113,113,113,113	0
34	MG	X	2882	1/1	0.67	0.19	112,112,112,112	0
34	MG	X	2896	1/1	0.68	0.77	86,86,86,86	0
34	MG	X	2892	1/1	0.69	0.61	109,109,109,109	0
34	MG	Z	129	1/1	0.69	0.44	101,101,101,101	0
33	NO1	5	14	13/15	0.72	0.20	83,83,83,83	0
34	MG	Z	127	1/1	0.73	0.30	98,98,98,98	0
34	MG	X	2891	1/1	0.76	0.20	84,84,84,84	0
34	MG	X	2881	1/1	0.76	0.94	77,77,77,77	0
34	MG	Z	126	1/1	0.77	0.33	122,122,122,122	0
34	MG	Z	125	1/1	0.78	0.49	83,83,83,83	0
34	MG	X	2906	1/1	0.79	0.72	82,82,82,82	0
34	MG	X	2902	1/1	0.81	0.86	76,76,76,76	0
34	MG	X	2885	1/1	0.81	0.28	98,98,98,98	0
34	MG	X	2897	1/1	0.83	0.71	100,100,100,100	0
34	MG	X	2893	1/1	0.83	0.84	85,85,85,85	0
34	MG	X	2903	1/1	0.84	0.54	82,82,82,82	0
34	MG	X	2904	1/1	0.85	0.33	81,81,81,81	0
34	MG	X	2908	1/1	0.85	0.99	83,83,83,83	0
34	MG	M	167	1/1	0.87	0.39	68,68,68,68	0
34	MG	X	2888	1/1	0.87	0.74	73,73,73,73	0
34	MG	X	2886	1/1	0.88	0.32	80,80,80,80	0
34	MG	X	2887	1/1	0.90	0.95	98,98,98,98	0
34	MG	X	2894	1/1	0.91	0.87	57,57,57,57	0
34	MG	X	2907	1/1	0.91	0.21	66,66,66,66	0
34	MG	X	2900	1/1	0.91	0.24	104,104,104,104	0
32	ZN	Y	61	1/1	0.92	0.09	118,118,118,118	0
34	MG	X	2884	1/1	0.93	0.28	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	MG	X	2898	1/1	0.93	0.36	57,57,57,57	0
34	MG	X	2899	1/1	0.94	0.38	57,57,57,57	0
34	MG	X	2895	1/1	0.95	0.20	81,81,81,81	0
34	MG	X	2905	1/1	0.96	0.38	123,123,123,123	0
34	MG	X	2890	1/1	0.96	0.19	58,58,58,58	0
32	ZN	4	38	1/1	0.99	0.05	125,125,125,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.