



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 05:54 AM GMT

PDB ID : 2I2T

Title : Crystal Structure of Ribosome with messenger RNA and the Anticodon stem-loop of P-site tRNA. This file contains the 50s subunit of one 70s ribosome. The entire crystal structure contains two 70s ribosomes and is described in remark 400.

Authors : Berk, V.; Zhang, W.; Pai, R.D.; Cate, J.H.D.

Deposited on : 2006-08-16

Resolution : 3.22 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

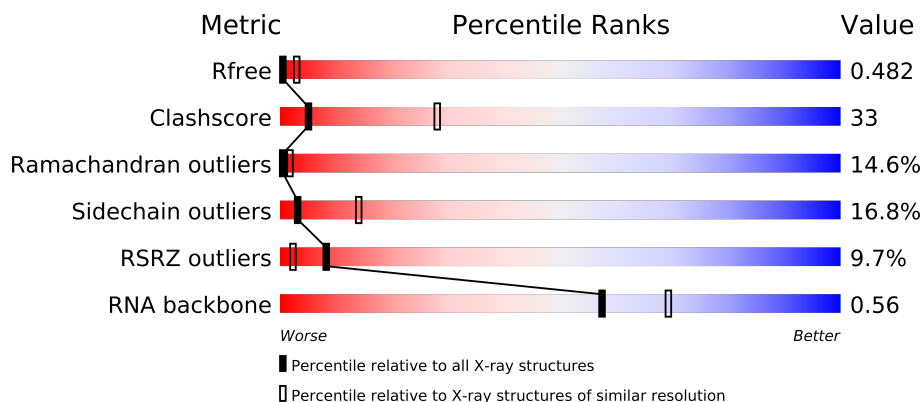
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.22 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	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)
RNA backbone	1838	1004 (3.74-2.70)

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. 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	C	272	
4	D	209	
5	E	201	
6	F	178	
7	G	176	
8	H	149	
9	I	141	
10	J	142	
11	K	123	
12	L	144	

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Mol	Chain	Length	Quality of chain
13	M	136	
14	N	127	
15	O	117	
16	P	114	
17	Q	117	
18	R	103	
19	S	110	
20	T	100	
21	U	103	
22	V	94	
23	W	84	
24	X	77	
25	Y	63	
26	Z	58	
27	0	56	
28	1	54	
29	2	46	
30	3	64	
31	4	38	

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	2918	-	X
33	MG	B	2929	-	X
33	MG	B	2935	-	X
33	MG	B	2949	-	X
33	MG	B	2955	-	X
33	MG	B	2961	-	X
33	MG	B	2962	-	X
33	MG	B	2983	-	X
33	MG	B	2991	-	X
33	MG	B	2997	-	X
33	MG	B	3006	-	X
33	MG	B	3019	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 90315 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 ribosomal RNA.

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 ribosomal RNA.

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 L2.

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

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

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

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	0	56	Total	C	N	O	S		
			444	269	94	80	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	118	Total	Mg	0	0
			118	118		
33	J	1	Total	Mg	0	0
			1	1		

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	2	1	Total	O	0	0
			1	1		
34	4	5	Total	O	0	0
			5	5		

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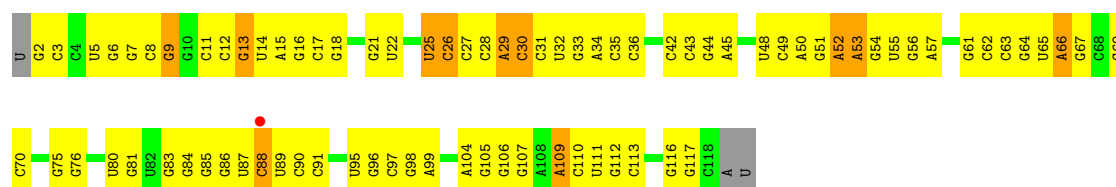
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	B	532	Total 532	O 532	0	0
34	C	8	Total 8	O 8	0	0
34	E	3	Total 3	O 3	0	0
34	J	3	Total 3	O 3	0	0
34	L	2	Total 2	O 2	0	0
34	N	2	Total 2	O 2	0	0

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 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.

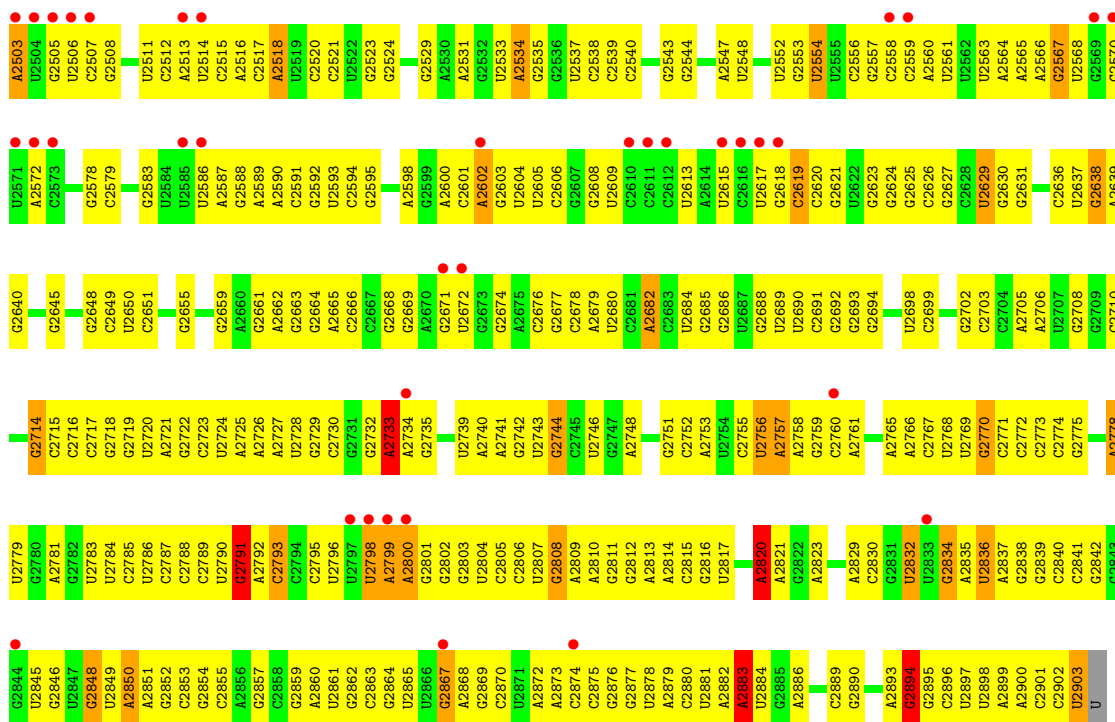
• Molecule 1: 5S ribosomal RNA

Chain A: 



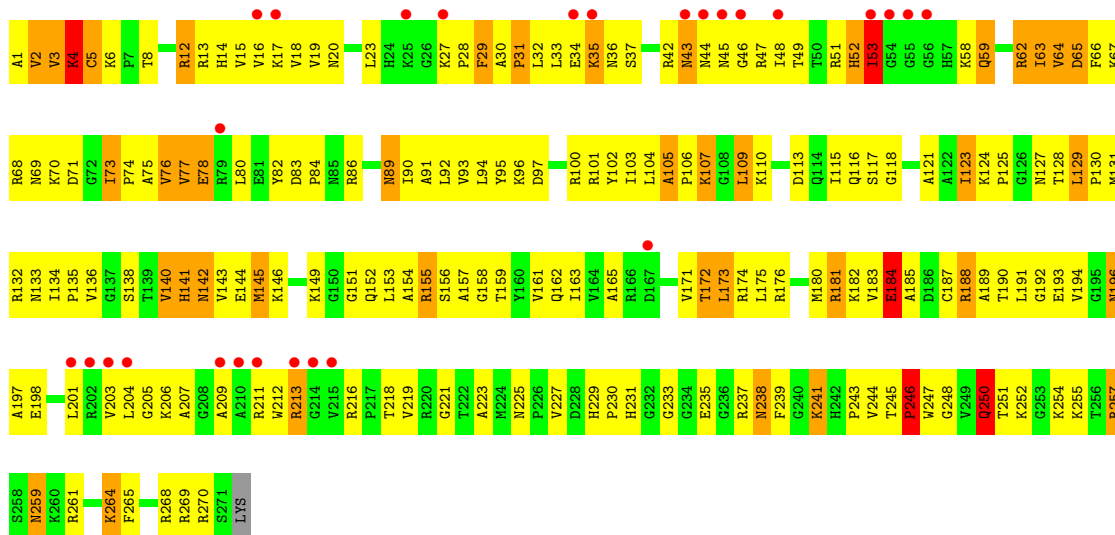
U1476	A1477	C1478	G1482	G1483	U1484	U1485	U1486	U1487	C1488	C1489	A1490	G1491	G1492	C1493	A1494	A1495	A1496	U1497	C1498	A1504	A1505	C1507	A1508	A1509	U1513	U1514	A1515	G1516	G1517	U1523	G1524	A1525	C1526	G1527	A1532	C1533	U1534	A1535	C1536	G1537	C1461	C1462	U1538	U1539	G1540	C1541	U1542	G1543	A1544	A1545	G1546	C1472	A1548	A1549	C1475	U1550	
C1349	C1350	U1352	A1353	A1354	C1355	C1356	C1357	G1358	A1359	G1360	G1361	C1362	C1363	G1364	A1365	A1366	C1367	G1368	G1369	C1370	G1371	U1372	A1373	G1374	U1375	C1376	G1377	U1378	U1379	G1380	G1381	C1382	A1383	A1384	A1385	C1386	A1387	U1390	U1391	A1392	A1393	U1394	C1395	U1396	U1397	C1398	C1399	G1400	G1401	U1402	A1403	A1404	U1405	A1406	G1407	G1408	U1409
G1283	A1284	A1285	A1286	A1287	G1288	C1289	C1290	C1291	C1292	C1293	G1296	C1297	C1300	A1301	A1302	C1306	A1307	A1308	G1309	G1310	G1311	G1312	U1313	C1314	C1315	U1316	G1317	U1318	C1319	C1320	U1321	A1322	C1323	G1324	U1325	U1326	A1327	A1328	U1329	G1332	G1333	G1334	C1335	A1336	G1337	G1338	G1339	G1401	U1402	A1403	A1404	U1405	C1345	G1346	A1347	C1348	
U1219	G1220	C1221	U1224	G1225	A1226	G1227	G1228	C1229	A1230	U1231	G1232	C1233	U1234	G1235	G1236	A1237	G1238	U1239	U1240	A1241	U1242	C1243	A1244	G1245	G1248	U1249	G1250	G1251	G1252	A1253	U1254	U1255	G1256	C1257	U1258	G1259	A1260	C1261	A1262	U1263	G1266	U1267	A1268	A1269	C1270	G1271	A1272	U1273	A1274	A1275	A1276	G1279	G1280	G1281	U1282		
U1148	G1149	C1150	A1151	C1152	C1153	A1156	G1157	C1158	U1159	G1160	G1163	C1164	A1165	G1166	A1169	C1170	G1171	U1172	U1173	U1174	A1175	U1176	G1177	C1178	U1179	U1180	G1181	U1182	U1183	U1184	G1187	U1188	A1189	G1190	G1191	G1192	U1193	C1196	G1197	U1198	U1199	C1200	U1203	A1204	U1205	G1206	G1210	C1211	G1212	A1213	G1218						
U1081	U1082	U1083	A1084	U1085	A1086	U1087	A1088	A1089	U1090	G1091	C1092	U1097	A1098	U1099	C1100	U1101	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	G1115	G1116	C1117	G1118	U1119	C1121	G1125	A1126	A1127	G1128	A1129	U1130	G1131	U1132	A1133	A1134	C1135	G1136	G1137	U1138	U1139	C1140	U1141	A1142	A1143	A1144	C1145	C1146	A1147			
A1014	U1015	G1016	G1017	U1018	U1019	A1020	A1021	G1022	U1023	G1024	G1025	A1028	A1029	C1030	G1031	A1032	U1033	G1036	G1037	G1038	A1039	A1040	G1041	G1042	C1045	A1046	G1047	A1048	C1049	G1051	C1052	C1053	A1054	G1055	G1056	A1057	U1058	G1059	U1060	U1061	G1062	C1063	C1064	U1065	G1068	A1069	A1070	G1071	C1072	C1076	A1077	A1080					
A933	U934	C935	A936	A941	G942	A943	A944	A945	C946	A947	G948	G949	G950	G956	C957	U958	A959	A960	C961	G962	U963	C964	U967	C968	G969	U970	A973	G974	A981	G982	A983	C986	C987	U988	A989	C990	C991	C992	C995	A996	G997	C998	U999	A1000	A1001	C1005	A1010	G1011	U1012	C1013							
G869	U870	U871	C872	G873	G874	G875	C876	A877	A878	G	G	G	G	U	C	A	U	C	C	G	A	C	U	A	C	A899	C902	C903	G904	A905	U906	G907	C908	A909	A910	A911	C912	U913	A918	U919	A920	C921	C922	G923	G924	A925	G926	A927	A928	U929	G930	U931	U932				
U803	A804	C805	U806	U807	G808	G809	U810	U811	C812	U813	C814	C815	C816	C817	G818	A819	A820	A821	G822	C823	A824	U825	U826	U827	U828	U832	A833	C834	C835	G836	C837	C838	U839	C840	G841	U842	A845	U846	U847	C848	A849	U850	C851	U852	C853	C854	C855	G856	C857	C858	U860	A863	G864	C865			
G600	C601	A602	A603	G604	G605	U606	U607	A608	A609	C610	G611	G612	A613	A614	U615	A616	G620	C623	G624	G625	A626	A627	G628	G629	G630	A631	A632	A633	C634	C635	G636	A637	G638	U639	C640	A643	A644	C645	U646	G647	G648	G649	C650	G651	U652	U653	A654	A655	C656	U657	U658	C660	A661	G664			
U665	A666	U667	C668	G669	A670	C671	C672	A673	A674	G675	A676	A677	C678	C679	C680	G681	U682	U683	G684	A685	U686	U688	A689	G690	C691	C692	A693	U694	G695	G696	C697	C698	U699	G700	G701	U702	U703	G704	A705	U709	U710	G711	G712	U713	U714	A715	U716	C717	A718	C719	U720	U721	A722	C723	U724	G725	G726
A727	G728	G729	A730	C740	U741	A742	A743	U744	G745	A746	U747	G748	A749	A750	A751	U752	U753	U754	U755	A756	G757	U762	G763	A764	U766	U767	G768	U769	G770	C771	C772	U773	G774	G775	G776	G777	U778	U779	G780	A781	A782	A783	G784	G785	A788	A789	A794	C795	G796	C797	G798	G799	A800				
U540	A541	C542	G543	C544	U545	U546	A547	A548	C549	G550	G551	U552	G553	U554	G555	A556	C557	U558	G559	C560	U562	A563	C564	C565	U566	U567	U568	U569	G570	U571	A572	U573	A574	A575	U576	G577	G578	G579	U580	C581	A582	G583	C584	G585	A586	C587	U588	U589	A590	U591	A592	U593	U594	C595	U596	U597	A599

G2437	U2438	A2439	C2440	U2441	C2442	C2443	G2444	G2445	G2446	G2447	A2448	U2449	A2450	A2451	A2452	A2453	A2454	G2455	G2456	G2457	G2458	A2459	U2460	C2461	C2462	C2463	A2464	A2465	C2466	A2467	A2468	A2469	A2470	A2471	A2472	C2473	C2474	C2475	A2476	A2477	A2478	U2479	C2480	G2481	G2485	C2486	G2487	G2488	U2489	G2490	U2491	U2492	U2493	C2498	C2499	U2500	G2501	C2502												
G2370	G2373	C2374	A2377	A2378	G2379	C2380	A2381	G2382	G2383	A2384	G2385	A2386	U2387	G2391	A2392	U2393	C2394	C2395	G2396	G2400	U2401	U2402	G2403	G2404	U2405	A2406	A2407	U2408	C2399	A2410	A2411	A2412	G2413	G2414	G2415	C2416	C2417	A2418	U2419	C2420	G2421	C2422	U2423	U2424	A2425	C2426	G2427	G2428	G2429	A2430	U2431	A2434	C2435	G2436	C2437	A2438	G2439	U2501	G2502											
C2306	G2307	A2308	G2309	C2310	C2311	U2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	U2320	U2321	A2322	C2323	U2324	C2325	A2326	A2327	A2328	U2329	C2330	C2331	C2332	C2333	U2334	C2335	A2336	G2337	C2338	C2339	A2340	C2341	C2342	G2345	A2346	C2347	U2348	A2352	G2353	C2354	C2355	U2356	C2359	G2360	C2361	C2362	C2363	C2364	C2365	A2366	C2367	C2368	A2369														
G2242	U2243	U2244	U2245	A2246	A2247	C2248	U2249	G2250	G2253	G2256	U2257	C2258	U2259	U2260	C2261	C2262	C2263	C2264	U2265	A2266	A2267	C2268	C2269	A2270	C2271	U2272	U2273	A2274	G2275	A2278	C2279	C2280	C2281	C2282	C2283	A2284	C2285	C2286	A2287	A2288	G2289	G2290	U2291	U2292	C2293	C2294	C2295	U2296	A2297	C2298	U2299	C2300	C2301	G2304	U2305															
C	C2179	U2180	U2181	U2182	A2183	A2184	U2185	U2186	U2187	U2188	U2189	A2191	U2192	U2193	U2194	U2195	C2196	U2197	A2198	A2199	C2200	U2203	G2204	A2205	C2206	C2207	C2208	C2209	U2210	A2211	U2212	U2213	C2214	C2215	G2216	G2217	G2218	U2219	U2220	G2221	C2222	A2225	G2228	U2229	U2230	U2231	C2232	U2233	G2234	G2235	G2238	G2239	U2240	A2241																
A	U	A	G	G	U	G	G	A	G	C	U	U	U	U	U	A2134	A2135	G2136	U2139	G2140	G2141	A2142	C2143	G2144	C2145	C2146	A2147	G2148	U2149	C2150	U2151	U2152	C2153	A2154	U2155	G2156	G2157	A	G	C	U	C	G	A	C	C	U	U	U	U	C	A	A	C																
G1988	G1989	U1991	U1992	U1993	C1994	U1995	C1996	C1997	C2000	C2001	C2008	A2009	G2010	U2011	C2012	A2013	A2014	A2015	U2016	C2017	G2018	A2019	A2020	C2021	U2022	C2023	C2024	C2025	U2026	G2027	U2028	G2029	A2030	C2031	C2032	A2033	U2034	G2035	C2036	A2037	U2038	U2039	G2101	G2102	C2103	C2104	U2105	U2106	G2107	A2108	U2109	U2110	U	U	A	G	C	C2065												
G1906	G1907	C1908	C1909	A1913	C1914	U1915	G1921	G1922	U1923	C1924	C1925	U1926	A1927	U1928	G1929	G1930	U1931	G1935	A1936	A1937	A1938	U1939	U1940	U1943	C1944	G1945	U1946	C1947	G1948	U1949	U1955	U1956	C1957	C1958	G1959	A1960	C1961	C1962	U1963	G1964	C1965	A1966	C1967	G1968	A1969	U1970	U1971	U1972	G1973	C1974	C1985	G1986	A1987	U1988	U1989	C1992	G1903	U1904	C1995											
C1843	C1844	G1845	G1846	A1847	A1848	G1849	G1850	A1853	A1854	U1855	U1856	G1857	U1858	U1859	G1860	G1861	G1862	G1863	U1864	U1865	A1866	G1867	C1868	G1869	C1870	A1871	C1872	G1873	A1874	G1875	G1878	C1879	U1880	C1881	U1882	U1883	G1884	U1885	U1886	C1887	G1888	A1889	U1890	G1891	C1892	C1893	C1894	C1895	G1896	U1897	U1898	U1899	C1902	G1903	U1904	C1905														
U1779	A1780	U1781	U1782	A1783	A1784	U1785	A1786	C1788	U1789	C1790	A1791	U1794	C1795	U1796	G1797	U1798	G1799	C1800	A1801	A1802	C1803	C1804	A1805	C1806	A1807	A1808	A1809	A1810	G1811	U1812	G1813	G1814	A1815	C1816	G1817	U1818	A1819	U1820	A1821	C1822	G1823	G1824	U1825	C1826	U1827	A1828	A1829	C1830	C1833	U1834	C1837	C1838	G1839	G1842																
A1713	U1714	G1715	U1716	A1717	U1720	G1721	G1722	G1723	G1724	U1725	C1726	C1727	U1728	U1729	G1730	G1731	C1732	G1733	U1734	A1735	U1736	G1737	G1738	A1739	G1740	C1741	G1742	G1743	A1744	A1745	U1746	G1747	G1748	A1749	G1750	U1751	A1754	U1755	G1756	U1757	U1758	A1759	U1760	C1761	A1762	G1763	G1764	U1765	G1766	G1767	U1773	C1774	U1775	G1776	U1777	U1778														
C1825	A1834	U1835	A1836	U1837	G1838	C1839	A1840	G1842	G1843	G1844	G1845	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	U1901	U1902	U1903	U1904	U1905
A1551	A1552	A1553	C1554	C1555	C1556	C1557	C1558	U1559	C1560	C1561	U1562	U1563	C1564	C1565	A1566	G1567	A1568	A1569	A1570	A1571	A1572	C1573	C1574	C1575	C1576	C1577	U1578	A1579	G1580	A1581	C1582	U1583	C1584	C1585	A1586	A1590	A1591	C1592	A1593	U1594	C1595	U1599	C1600	U1601	U1602	A1603	A1608	A1609	A1610	A1616	C1617	C1618	G1622	U1624																



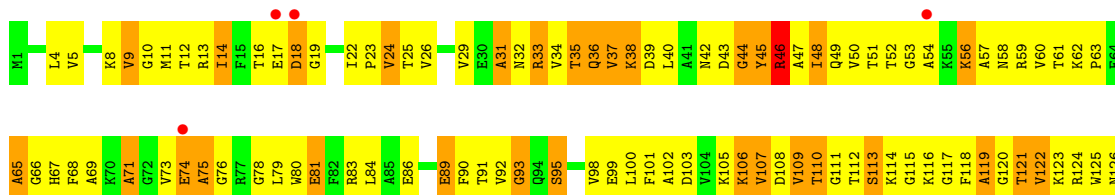
• Molecule 3: 50S ribosomal protein L2

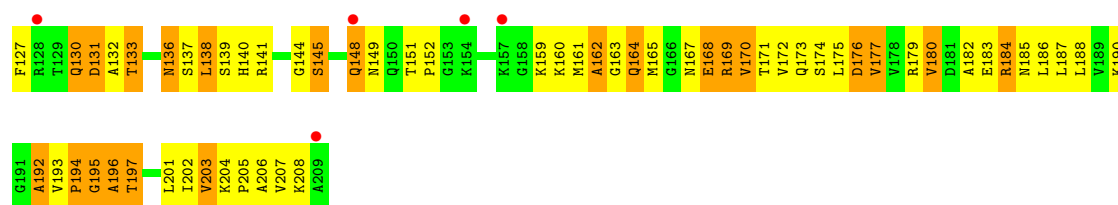
Chain C:

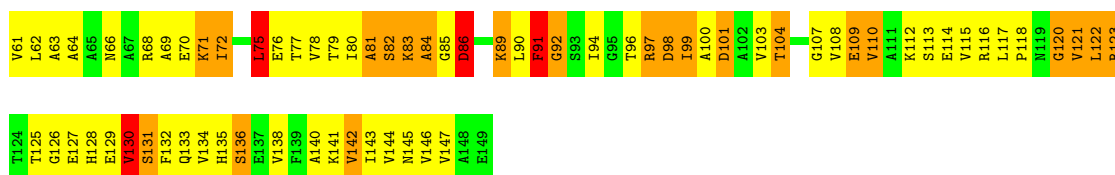


• Molecule 4: 50S ribosomal protein L3

Chain D:

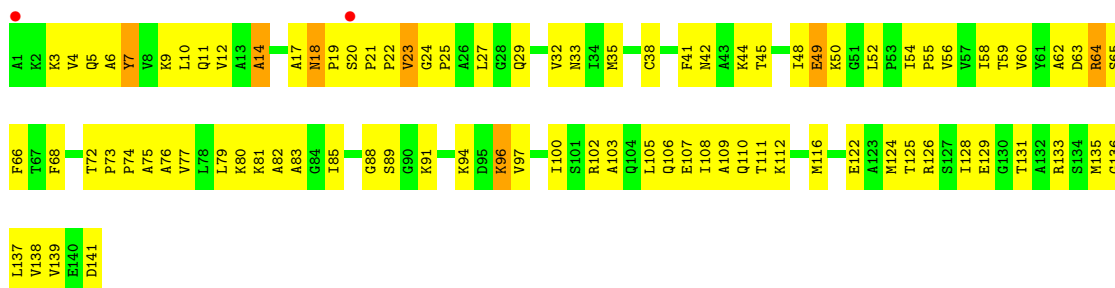






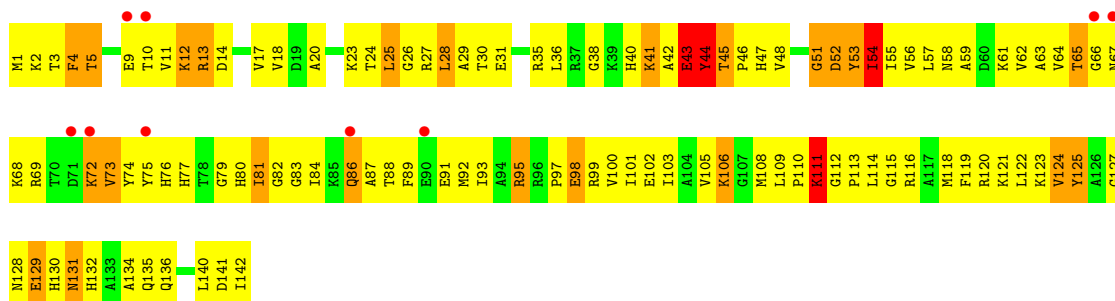
• Molecule 9: 50S ribosomal protein L11

Chain I:



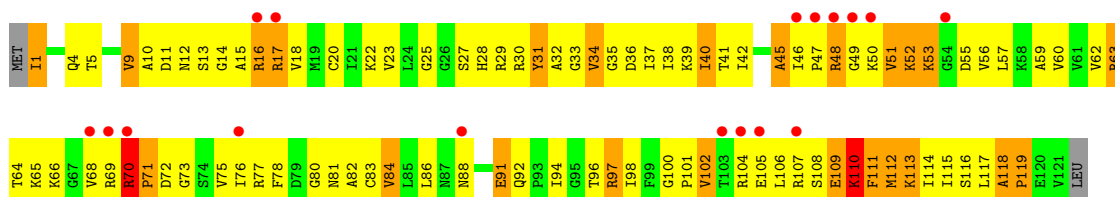
• Molecule 10: 50S ribosomal protein L13

Chain J:



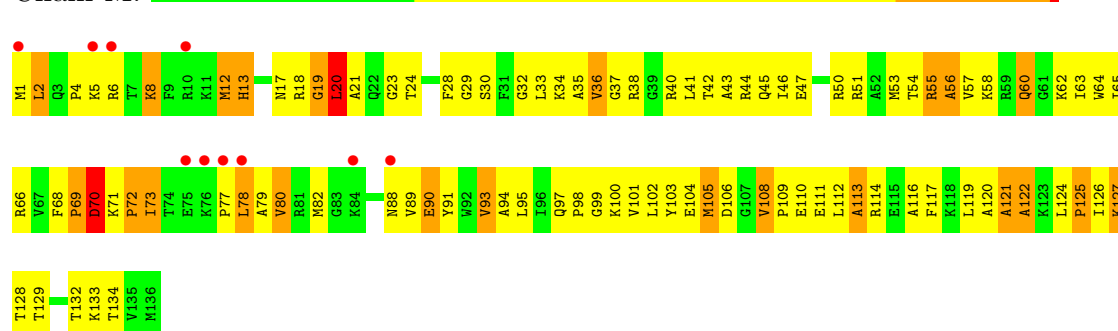
• Molecule 11: 50S ribosomal protein L14

Chain K:



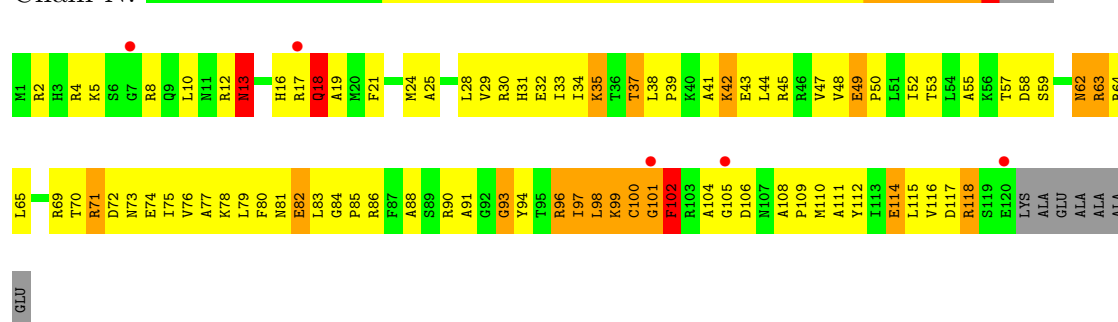
- Molecule 13: 50S ribosomal protein L16

Chain M:



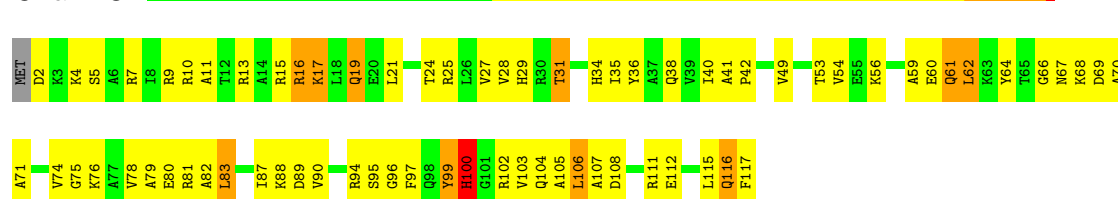
- Molecule 14: 50S ribosomal protein L17

Chain N:



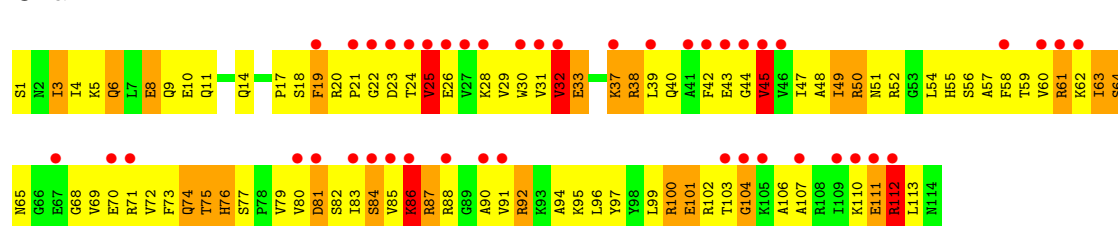
- Molecule 15: 50S ribosomal protein L18

Chain O:



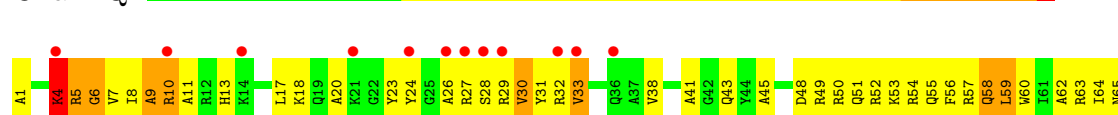
- Molecule 16: 50S ribosomal protein L19

Chain P:



- Molecule 17: 50S ribosomal protein L20

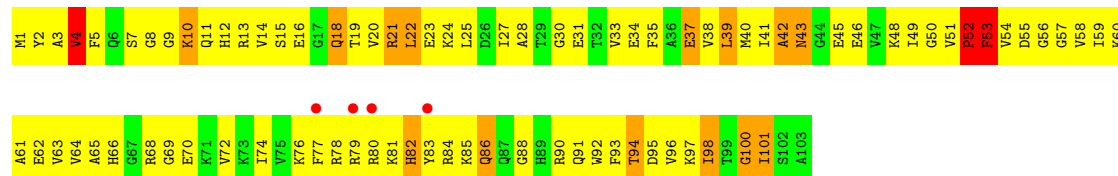
Chain Q:





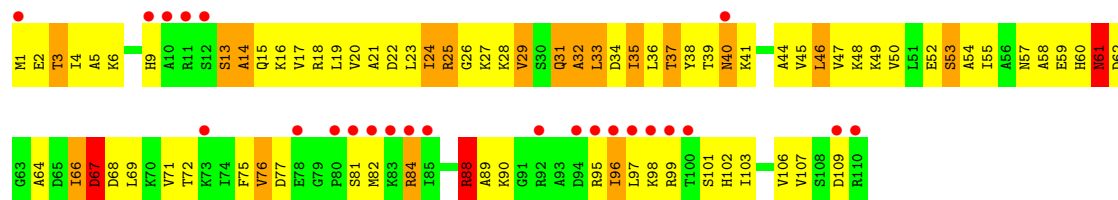
• Molecule 18: 50S ribosomal protein L21

Chain R:



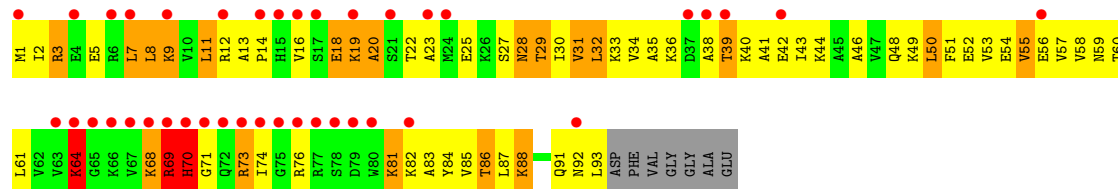
• Molecule 19: 50S ribosomal protein L22

Chain S:



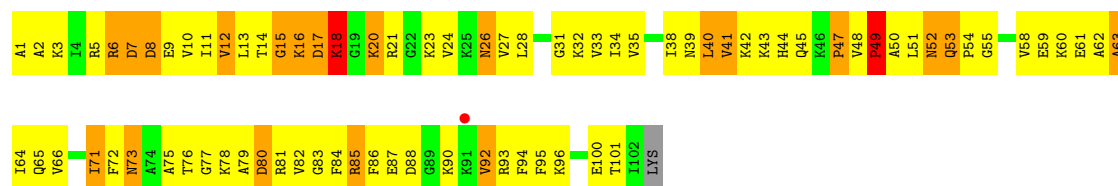
• Molecule 20: 50S ribosomal protein L23

Chain T:



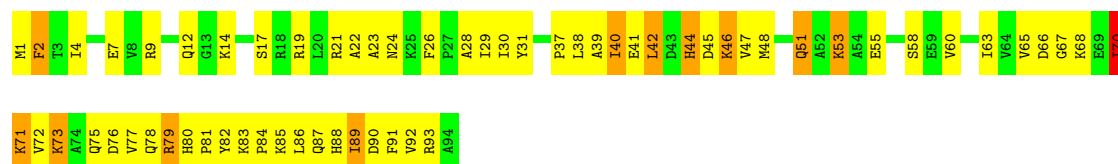
• Molecule 21: 50S ribosomal protein L24

Chain U:



• Molecule 22: 50S ribosomal protein L25

Chain V:



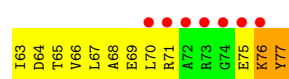
• Molecule 23: 50S ribosomal protein L27

Chain W: 



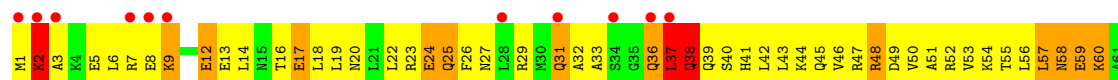
- Molecule 24: 50S ribosomal protein L28

Chain X: 



- Molecule 25: 50S ribosomal protein L29

Chain Y: 



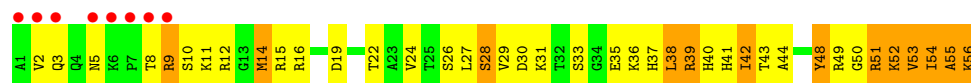
- Molecule 26: 50S ribosomal protein L30

Chain Z: 



- Molecule 27: 50S ribosomal protein L32

Chain 0: 



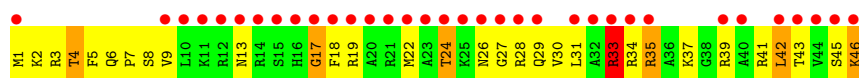
- Molecule 28: 50S ribosomal protein L33

Chain 1: 



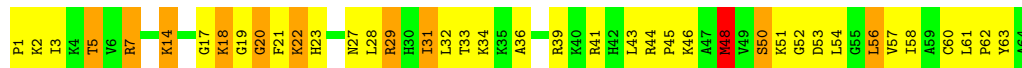
- Molecule 29: 50S ribosomal protein L34

Chain 2: 



- Molecule 30: 50S ribosomal protein L35

Chain 3:



- Molecule 31: 50S ribosomal protein L36

Chain 4:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.78Å 395.22Å 744.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.22 184.07 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.22) 75.7 (184.07-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.287 , 0.320 0.482 , 0.482	Depositor DCC
R_{free} test set	37268 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 12.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 753156 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.62	EDS
Total number of atoms	90315	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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

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	0.24	0/2803	0.72	0/4371
2	B	0.27	7/68314 (0.0%)	0.77	53/106569 (0.0%)
3	C	0.22	0/2121	0.52	0/2852
4	D	0.25	0/1586	0.60	0/2134
5	E	0.24	0/1571	0.61	2/2113 (0.1%)
6	F	0.26	0/1444	0.59	0/1937
7	G	0.23	0/1343	0.52	0/1816
8	H	0.28	0/1122	0.56	1/1515 (0.1%)
9	I	0.24	0/1046	0.46	0/1410
10	J	0.24	0/1152	0.59	0/1551
11	K	0.25	0/939	0.81	2/1258 (0.2%)
12	L	0.23	0/1054	0.58	0/1403
13	M	0.26	0/1093	0.56	0/1460
14	N	0.25	0/973	0.62	0/1301
15	O	0.24	0/902	0.55	0/1209
16	P	0.25	0/929	0.60	0/1242
17	Q	0.26	0/960	0.65	0/1278
18	R	0.26	0/829	0.58	0/1107
19	S	0.23	0/864	0.61	1/1156 (0.1%)
20	T	0.23	0/744	0.73	2/994 (0.2%)
21	U	0.26	0/787	0.56	0/1051
22	V	0.25	0/766	0.46	0/1025
23	W	0.31	0/603	0.65	0/797
24	X	0.25	0/635	0.58	0/848
25	Y	0.24	0/510	0.64	0/677
26	Z	0.24	0/453	0.55	0/605
27	0	0.23	0/450	0.65	0/599
28	1	0.27	0/416	0.55	0/554
29	2	0.26	0/380	0.58	0/498
30	3	0.26	0/513	0.66	2/676 (0.3%)
31	4	0.24	0/303	0.54	0/397
All	All	0.26	7/97605 (0.0%)	0.73	63/146403 (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	37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1086	A	C5-C6	-16.31	1.26	1.41
2	B	1088	A	C6-N1	-10.43	1.28	1.35
2	B	1060	U	C2-N3	7.75	1.43	1.37
2	B	1086	A	N3-C4	-6.90	1.30	1.34
2	B	1086	A	N7-C5	-6.28	1.35	1.39

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2791	G	O5'-P-OP1	-28.43	76.59	110.70
2	B	2204	G	O5'-P-OP2	-27.54	77.65	110.70
2	B	2204	G	O5'-P-OP1	18.07	132.38	110.70
2	B	2791	G	O5'-P-OP2	17.30	131.46	110.70
2	B	2203	U	OP2-P-O3'	14.24	136.52	105.20

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	221	A	Sidechain
2	B	222	A	Sidechain
2	B	299	A	Sidechain
2	B	361	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	87	0
2	B	60995	0	30678	2077	0
3	C	2082	0	2157	217	0
4	D	1565	0	1616	219	0
5	E	1552	0	1619	163	0
6	F	1420	0	1460	254	0
7	G	1323	0	1374	181	0
8	H	1111	0	1148	196	0
9	I	1032	0	1088	108	0
10	J	1129	0	1162	155	0
11	K	930	0	1003	98	0
12	L	1045	0	1117	123	0
13	M	1074	0	1157	109	0
14	N	960	0	1000	103	0
15	O	892	0	923	77	0
16	P	917	0	965	115	0
17	Q	947	0	1022	133	0
18	R	816	0	839	111	0
19	S	857	0	922	95	0
20	T	738	0	807	109	0
21	U	779	0	834	111	0
22	V	753	0	780	75	0
23	W	596	0	610	149	0
24	X	625	0	655	79	0
25	Y	509	0	543	84	0
26	Z	449	0	491	47	0
27	0	444	0	461	45	0
28	1	409	0	440	31	0
29	2	377	0	418	32	0
30	3	504	0	574	49	0
31	4	302	0	340	27	0
32	4	1	0	0	0	0
33	B	118	0	0	0	0
33	J	1	0	0	0	0
34	2	1	0	0	0	0
34	4	5	0	0	0	0
34	B	532	0	0	7	0
34	C	8	0	0	0	0
34	E	3	0	0	0	0
34	J	3	0	0	0	0
34	L	2	0	0	1	0
34	N	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	90315	0	59473	4978	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 33.

The worst 5 of 4978 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:148:GLN:HG3	4:D:152:PRO:HG2	1.29	1.15
11:K:70:ARG:HB3	11:K:71:PRO:CD	1.76	1.14
14:N:101:GLY:HA2	14:N:110:MET:H	1.06	1.13
2:B:855:G:H21	23:W:23:LYS:HG2	1.05	1.09
15:O:49:VAL:HG21	15:O:82:ALA:HB2	1.35	1.06

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	C	269/272 (99%)	166 (62%)	68 (25%)	35 (13%)	0	3
4	D	207/209 (99%)	113 (55%)	56 (27%)	38 (18%)	0	1
5	E	199/201 (99%)	126 (63%)	43 (22%)	30 (15%)	0	1
6	F	176/178 (99%)	97 (55%)	40 (23%)	39 (22%)	0	0
7	G	174/176 (99%)	94 (54%)	54 (31%)	26 (15%)	0	1
8	H	147/149 (99%)	69 (47%)	50 (34%)	28 (19%)	0	0
9	I	139/141 (99%)	118 (85%)	16 (12%)	5 (4%)	5	36
10	J	140/142 (99%)	88 (63%)	30 (21%)	22 (16%)	0	1
11	K	119/123 (97%)	75 (63%)	26 (22%)	18 (15%)	0	1
12	L	141/144 (98%)	81 (57%)	37 (26%)	23 (16%)	0	1
13	M	134/136 (98%)	77 (58%)	32 (24%)	25 (19%)	0	0
14	N	118/127 (93%)	75 (64%)	27 (23%)	16 (14%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	114/117 (97%)	85 (75%)	24 (21%)	5 (4%)	4	29
16	P	112/114 (98%)	71 (63%)	20 (18%)	21 (19%)	0	0
17	Q	115/117 (98%)	74 (64%)	28 (24%)	13 (11%)	1	4
18	R	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	3
19	S	108/110 (98%)	66 (61%)	26 (24%)	16 (15%)	0	1
20	T	91/100 (91%)	54 (59%)	23 (25%)	14 (15%)	0	1
21	U	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	1
22	V	92/94 (98%)	74 (80%)	11 (12%)	7 (8%)	2	12
23	W	77/84 (92%)	29 (38%)	23 (30%)	25 (32%)	0	0
24	X	75/77 (97%)	43 (57%)	26 (35%)	6 (8%)	1	11
25	Y	61/63 (97%)	37 (61%)	18 (30%)	6 (10%)	1	7
26	Z	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	3	24
27	0	54/56 (96%)	35 (65%)	8 (15%)	11 (20%)	0	0
28	1	48/54 (89%)	33 (69%)	7 (15%)	8 (17%)	0	1
29	2	44/46 (96%)	26 (59%)	13 (30%)	5 (11%)	1	4
30	3	62/64 (97%)	42 (68%)	15 (24%)	5 (8%)	1	10
31	4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	1	5
All	All	3309/3396 (97%)	2033 (61%)	794 (24%)	482 (15%)	0	2

5 of 482 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	53	ILE
3	C	78	GLU
3	C	140	VAL
3	C	184	GLU
3	C	246	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	
3	C	216/217 (100%)	182 (84%)	34 (16%)	4	17
4	D	164/164 (100%)	136 (83%)	28 (17%)	3	14
5	E	165/165 (100%)	130 (79%)	35 (21%)	1	8
6	F	149/149 (100%)	116 (78%)	33 (22%)	1	6
7	G	137/137 (100%)	110 (80%)	27 (20%)	2	9
8	H	114/114 (100%)	85 (75%)	29 (25%)	1	2
9	I	109/109 (100%)	107 (98%)	2 (2%)	71	93
10	J	116/116 (100%)	100 (86%)	16 (14%)	5	24
11	K	102/104 (98%)	84 (82%)	18 (18%)	3	13
12	L	102/103 (99%)	87 (85%)	15 (15%)	4	21
13	M	109/109 (100%)	93 (85%)	16 (15%)	4	21
14	N	100/103 (97%)	85 (85%)	15 (15%)	4	20
15	O	86/87 (99%)	76 (88%)	10 (12%)	8	35
16	P	99/99 (100%)	76 (77%)	23 (23%)	1	5
17	Q	89/89 (100%)	73 (82%)	16 (18%)	2	12
18	R	84/84 (100%)	67 (80%)	17 (20%)	2	9
19	S	93/93 (100%)	79 (85%)	14 (15%)	4	19
20	T	80/84 (95%)	65 (81%)	15 (19%)	2	11
21	U	83/84 (99%)	69 (83%)	14 (17%)	3	14
22	V	78/78 (100%)	67 (86%)	11 (14%)	5	23
23	W	59/62 (95%)	49 (83%)	10 (17%)	3	14
24	X	67/67 (100%)	56 (84%)	11 (16%)	3	15
25	Y	55/55 (100%)	43 (78%)	12 (22%)	1	7
26	Z	48/48 (100%)	43 (90%)	5 (10%)	10	39
27	0	47/47 (100%)	40 (85%)	7 (15%)	4	20
28	1	45/48 (94%)	38 (84%)	7 (16%)	4	17
29	2	38/38 (100%)	33 (87%)	5 (13%)	6	27
30	3	51/51 (100%)	44 (86%)	7 (14%)	5	25
31	4	34/34 (100%)	29 (85%)	5 (15%)	4	21
All	All	2719/2738 (99%)	2262 (83%)	457 (17%)	3	14

5 of 457 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	20	CYS
14	N	21	PHE
26	Z	19	HIS
11	K	63	ARG
12	L	117	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	138	GLN
15	O	19	GLN
25	Y	38	GLN
11	K	4	GLN
12	L	54	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	116/120 (96%)	19 (16%)	2 (1%)
2	B	2837/2904 (97%)	416 (14%)	13 (0%)
All	All	2953/3024 (97%)	435 (14%)	15 (0%)

5 of 435 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	13	G
1	A	15	A
1	A	16	G
1	A	25	U

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1608	A
2	B	1930	G
2	B	2430	A
2	B	1210	G
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 120 ligands modelled in this entry, 120 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.

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	A	117/120 (97%)	0.18	1 (0%) 81 35	44, 75, 109, 180	0
2	B	2841/2904 (97%)	0.20	302 (10%) 7 2	13, 70, 147, 180	0
3	C	271/272 (99%)	0.34	27 (9%) 8 2	16, 66, 111, 151	0
4	D	209/209 (100%)	0.01	9 (4%) 34 7	25, 83, 146, 180	0
5	E	201/201 (100%)	0.43	31 (15%) 3 1	22, 78, 139, 172	0
6	F	178/178 (100%)	-0.22	0 100 100	49, 111, 174, 180	0
7	G	176/176 (100%)	-0.27	6 (3%) 43 9	47, 112, 165, 176	0
8	H	149/149 (100%)	0.07	7 (4%) 30 6	52, 131, 180, 180	0
9	I	141/141 (100%)	-0.25	2 (1%) 72 24	110, 167, 180, 180	0
10	J	142/142 (100%)	-0.03	9 (6%) 19 4	32, 86, 133, 180	0
11	K	121/123 (98%)	0.69	17 (14%) 3 1	32, 74, 148, 180	0
12	L	143/144 (99%)	-0.16	1 (0%) 84 40	27, 69, 121, 180	0
13	M	136/136 (100%)	0.09	10 (7%) 14 4	33, 65, 132, 168	0
14	N	120/127 (94%)	0.14	5 (4%) 35 7	43, 88, 131, 169	0
15	O	116/117 (99%)	-0.33	0 100 100	34, 77, 118, 138	0
16	P	114/114 (100%)	1.82	44 (38%) 1 0	43, 84, 145, 164	0
17	Q	117/117 (100%)	0.33	12 (10%) 7 2	34, 73, 135, 149	0
18	R	103/103 (100%)	-0.09	4 (3%) 37 8	44, 95, 146, 177	0
19	S	110/110 (100%)	1.17	24 (21%) 1 1	47, 84, 138, 180	0
20	T	93/100 (93%)	2.05	39 (41%) 1 0	44, 93, 163, 180	0
21	U	102/103 (99%)	-0.22	1 (0%) 79 31	48, 106, 162, 175	0
22	V	94/94 (100%)	0.04	0 100 100	37, 84, 140, 180	0
23	W	79/84 (94%)	-0.06	4 (5%) 27 5	6, 53, 116, 154	0
24	X	77/77 (100%)	0.73	10 (12%) 4 1	24, 63, 107, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	63/63 (100%)	0.96	13 (20%) 1 1	47, 108, 165, 180	0
26	Z	58/58 (100%)	-0.14	0 100 100	40, 74, 124, 150	0
27	0	56/56 (100%)	0.29	8 (14%) 3 1	35, 87, 152, 180	0
28	1	50/54 (92%)	0.03	4 (8%) 12 3	43, 72, 122, 140	0
29	2	46/46 (100%)	3.01	34 (73%) 0 0	42, 61, 97, 162	0
30	3	64/64 (100%)	-0.27	0 100 100	21, 56, 99, 136	0
31	4	38/38 (100%)	-0.18	0 100 100	36, 86, 126, 146	0
All	All	6325/6420 (98%)	0.23	624 (9%) 8 2	6, 77, 159, 180	0

The worst 5 of 624 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2799	A	13.3
2	B	508	A	11.6
2	B	504	A	11.5
24	X	75	GLU	10.0
20	T	70	HIS	9.5

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	MG	B	2935	1/1	0.57	5.99	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	B	2961	1/1	2.21	4.87	100,100,100,100	0
33	MG	B	2929	1/1	0.71	4.83	63,63,63,63	0
33	MG	B	3006	1/1	0.46	3.93	71,71,71,71	0
33	MG	B	2955	1/1	0.63	2.54	94,94,94,94	0
33	MG	B	2991	1/1	0.27	2.25	63,63,63,63	0
33	MG	B	2983	1/1	0.62	2.18	46,46,46,46	0
33	MG	B	2918	1/1	0.35	2.15	76,76,76,76	0
33	MG	B	2997	1/1	0.71	1.87	120,120,120,120	0
33	MG	B	2924	1/1	0.27	1.72	45,45,45,45	0
33	MG	B	2996	1/1	0.29	1.66	62,62,62,62	0
33	MG	B	3019	1/1	0.51	1.56	106,106,106,106	0
33	MG	B	2951	1/1	0.16	1.12	131,131,131,131	0
33	MG	B	2962	1/1	0.55	1.02	62,62,62,62	0
33	MG	B	2907	1/1	0.50	0.82	20,20,20,20	0
33	MG	B	2964	1/1	0.14	0.40	33,33,33,33	0
33	MG	B	2970	1/1	0.19	0.35	51,51,51,51	0
33	MG	B	2954	1/1	0.45	0.33	54,54,54,54	0
33	MG	B	2949	1/1	0.65	0.31	60,60,60,60	0
33	MG	B	2985	1/1	0.37	0.24	85,85,85,85	0
33	MG	B	3004	1/1	0.17	0.14	128,128,128,128	0
33	MG	B	2930	1/1	0.26	0.05	26,26,26,26	0
33	MG	B	3010	1/1	0.16	-0.01	53,53,53,53	0
33	MG	B	2992	1/1	0.32	-0.01	76,76,76,76	0
33	MG	B	2909	1/1	0.17	-0.02	52,52,52,52	0
33	MG	B	2917	1/1	0.43	-0.03	52,52,52,52	0
33	MG	B	2928	1/1	0.20	-0.05	47,47,47,47	0
33	MG	B	3011	1/1	0.33	-0.06	86,86,86,86	0
33	MG	B	3012	1/1	0.23	-0.08	30,30,30,30	0
33	MG	B	2995	1/1	0.33	-0.33	44,44,44,44	0
33	MG	B	2975	1/1	0.32	-0.35	41,41,41,41	0
33	MG	B	2953	1/1	0.24	-0.37	40,40,40,40	0
33	MG	B	2994	1/1	0.16	-0.43	71,71,71,71	0
33	MG	B	2945	1/1	0.17	-0.44	28,28,28,28	0
33	MG	B	2925	1/1	0.13	-0.49	45,45,45,45	0
33	MG	B	2936	1/1	0.24	-0.52	53,53,53,53	0
33	MG	B	2979	1/1	0.45	-0.53	44,44,44,44	0
33	MG	B	2933	1/1	0.29	-0.54	81,81,81,81	0
33	MG	B	2932	1/1	0.45	-0.55	54,54,54,54	0
33	MG	B	2998	1/1	0.13	-0.58	81,81,81,81	0
33	MG	B	2969	1/1	0.14	-0.65	46,46,46,46	0
33	MG	B	2940	1/1	0.13	-0.65	52,52,52,52	0
33	MG	B	2923	1/1	0.20	-0.71	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	B	3000	1/1	0.12	-0.76	49,49,49,49	0
33	MG	B	2937	1/1	0.12	-0.80	86,86,86,86	0
33	MG	B	2920	1/1	0.12	-0.80	91,91,91,91	0
33	MG	B	2963	1/1	0.31	-0.87	37,37,37,37	0
33	MG	B	3022	1/1	0.11	-0.90	113,113,113,113	0
33	MG	B	3018	1/1	0.11	-0.92	57,57,57,57	0
33	MG	B	2919	1/1	0.30	-0.93	69,69,69,69	0
32	ZN	4	101	1/1	0.11	-1.03	72,72,72,72	0
33	MG	B	2965	1/1	0.23	-1.03	57,57,57,57	0
33	MG	B	2960	1/1	0.17	-1.03	49,49,49,49	0
33	MG	B	2921	1/1	0.12	-1.06	35,35,35,35	0
33	MG	B	2938	1/1	0.11	-1.07	70,70,70,70	0
33	MG	B	3014	1/1	0.17	-1.21	56,56,56,56	0
33	MG	B	2926	1/1	0.09	-1.25	56,56,56,56	0
33	MG	B	2947	1/1	0.15	-1.28	107,107,107,107	0
33	MG	B	3015	1/1	0.18	-1.30	43,43,43,43	0
33	MG	B	3005	1/1	0.20	-1.32	50,50,50,50	0
33	MG	B	2977	1/1	0.32	-1.32	30,30,30,30	0
33	MG	B	2916	1/1	0.07	-1.42	32,32,32,32	0
33	MG	B	3007	1/1	0.08	-1.44	38,38,38,38	0
33	MG	B	2946	1/1	0.10	-1.45	90,90,90,90	0
33	MG	B	2944	1/1	0.05	-1.45	64,64,64,64	0
33	MG	B	2959	1/1	0.10	-1.47	72,72,72,72	0
33	MG	B	2948	1/1	0.18	-1.60	62,62,62,62	0
33	MG	B	2939	1/1	0.14	-1.60	40,40,40,40	0
33	MG	B	2988	1/1	0.10	-1.63	61,61,61,61	0
33	MG	B	2968	1/1	0.15	-1.70	63,63,63,63	0
33	MG	B	2987	1/1	0.15	-1.74	47,47,47,47	0
33	MG	B	2922	1/1	0.10	-1.75	42,42,42,42	0
33	MG	B	2912	1/1	0.06	-1.75	63,63,63,63	0
33	MG	B	3017	1/1	0.06	-1.78	41,41,41,41	0
33	MG	B	3002	1/1	0.08	-1.80	73,73,73,73	0
33	MG	B	3003	1/1	0.06	-1.85	41,41,41,41	0
33	MG	B	2958	1/1	0.07	-1.85	56,56,56,56	0
33	MG	B	2993	1/1	0.15	-1.87	51,51,51,51	0
33	MG	B	2989	1/1	0.05	-1.87	57,57,57,57	0
33	MG	B	2976	1/1	0.20	-2.03	58,58,58,58	0
33	MG	B	2972	1/1	0.11	-2.07	40,40,40,40	0
33	MG	B	2911	1/1	0.07	-2.12	115,115,115,115	0
33	MG	B	2915	1/1	0.08	-2.13	45,45,45,45	0
33	MG	B	2942	1/1	0.08	-2.15	125,125,125,125	0
33	MG	B	2967	1/1	0.09	-2.19	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	MG	B	2984	1/1	0.05	-2.20	65,65,65,65	0
33	MG	B	2913	1/1	0.05	-2.21	92,92,92,92	0
33	MG	B	2957	1/1	0.11	-2.22	43,43,43,43	0
33	MG	B	3016	1/1	0.08	-2.23	27,27,27,27	0
33	MG	B	2978	1/1	0.14	-2.28	25,25,25,25	0
33	MG	B	2966	1/1	0.05	-2.30	42,42,42,42	0
33	MG	B	2982	1/1	0.07	-2.31	71,71,71,71	0
33	MG	B	3020	1/1	0.02	-2.42	24,24,24,24	0
33	MG	B	2971	1/1	0.09	-2.44	39,39,39,39	0
33	MG	B	3001	1/1	0.11	-2.44	112,112,112,112	0
33	MG	B	2990	1/1	0.04	-2.51	50,50,50,50	0
33	MG	B	2956	1/1	0.07	-2.67	33,33,33,33	0
33	MG	B	2986	1/1	0.06	-2.70	80,80,80,80	0
33	MG	B	2943	1/1	0.05	-2.74	55,55,55,55	0
33	MG	B	2905	1/1	0.16	-2.76	57,57,57,57	0
33	MG	B	2973	1/1	0.04	-2.79	28,28,28,28	0
33	MG	B	2910	1/1	0.04	-2.90	35,35,35,35	0
33	MG	B	2952	1/1	0.10	-2.90	38,38,38,38	0
33	MG	B	2927	1/1	0.06	-2.98	15,15,15,15	0
33	MG	B	2931	1/1	0.04	-3.25	40,40,40,40	0
33	MG	B	3021	1/1	0.04	-3.49	82,82,82,82	0
33	MG	B	2941	1/1	0.03	-3.51	56,56,56,56	0
33	MG	B	3008	1/1	0.05	-3.56	38,38,38,38	0
33	MG	B	2934	1/1	0.12	-3.66	111,111,111,111	0
33	MG	B	2980	1/1	0.08	-3.70	56,56,56,56	0
33	MG	B	2906	1/1	0.04	-4.33	31,31,31,31	0
33	MG	B	3009	1/1	0.06	-4.33	64,64,64,64	0
33	MG	B	2999	1/1	0.06	-4.53	48,48,48,48	0
33	MG	B	2981	1/1	0.08	-4.68	50,50,50,50	0
33	MG	B	2950	1/1	0.10	-4.89	90,90,90,90	0
33	MG	B	2974	1/1	0.10	-5.10	52,52,52,52	0
33	MG	B	3013	1/1	0.07	-5.70	52,52,52,52	0
33	MG	B	2914	1/1	0.14	-10.36	95,95,95,95	0
33	MG	B	2908	1/1	0.04	-36.66	65,65,65,65	0
33	MG	J	216	1/1	1.18	-	160,160,160,160	0

6.5 Other polymers ⓘ

There are no such residues in this entry.