



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:36 PM GMT

PDB ID : 3I20
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.
Deposited on : 2009-06-28
Resolution : 3.71 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>

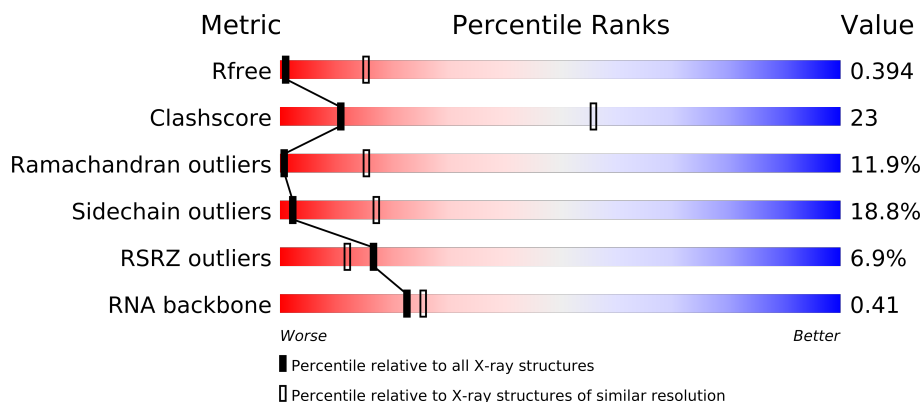
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.71 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	1103 (4.04-3.40)
Clashscore	79885	1026 (3.98-3.46)
Ramachandran outliers	78287	1082 (4.00-3.44)
Sidechain outliers	78261	1075 (4.00-3.44)
RSRZ outliers	66119	1104 (4.04-3.40)
RNA backbone	1838	1008 (4.52-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	2903	
2	B	118	
3	C	273	
4	D	209	
5	E	201	
6	F	179	
7	G	177	
8	H	149	
9	I	142	
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	115	
17	Q	118	
18	R	103	
19	S	110	
20	T	100	
21	U	104	
22	V	94	
23	W	85	
24	X	78	
25	Y	63	
26	Z	59	
27	0	57	
28	1	55	
29	2	46	
30	3	65	
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
32	MG	A	2909	-	X
32	MG	A	2912	-	X
32	MG	A	2914	-	X
32	MG	A	2918	-	X
32	MG	A	2923	-	X
32	MG	A	2924	-	X
32	MG	A	2929	-	X
32	MG	A	2933	-	X
32	MG	A	2934	-	X
32	MG	A	2937	-	X
32	MG	A	2938	-	X
32	MG	A	2961	-	X
32	MG	A	2964	-	X
32	MG	A	2971	-	X
32	MG	A	2974	-	X
32	MG	A	2975	-	X
32	MG	A	2984	-	X
32	MG	A	2988	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	A	3002	-	X
32	MG	A	3006	-	X
32	MG	A	3013	-	X
32	MG	A	3027	-	X
32	MG	A	3034	-	X
32	MG	A	3039	-	X
32	MG	B	120	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 90740 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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- 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	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	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	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	B	4	Total	Mg	0	0
			4	4		
32	A	136	Total	Mg	0	0
			136	136		
32	D	1	Total	Mg	0	0
			1	1		

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	4	1	Total	Zn	0	0
			1	1		

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	614	Total	O	0	0
			614	614		

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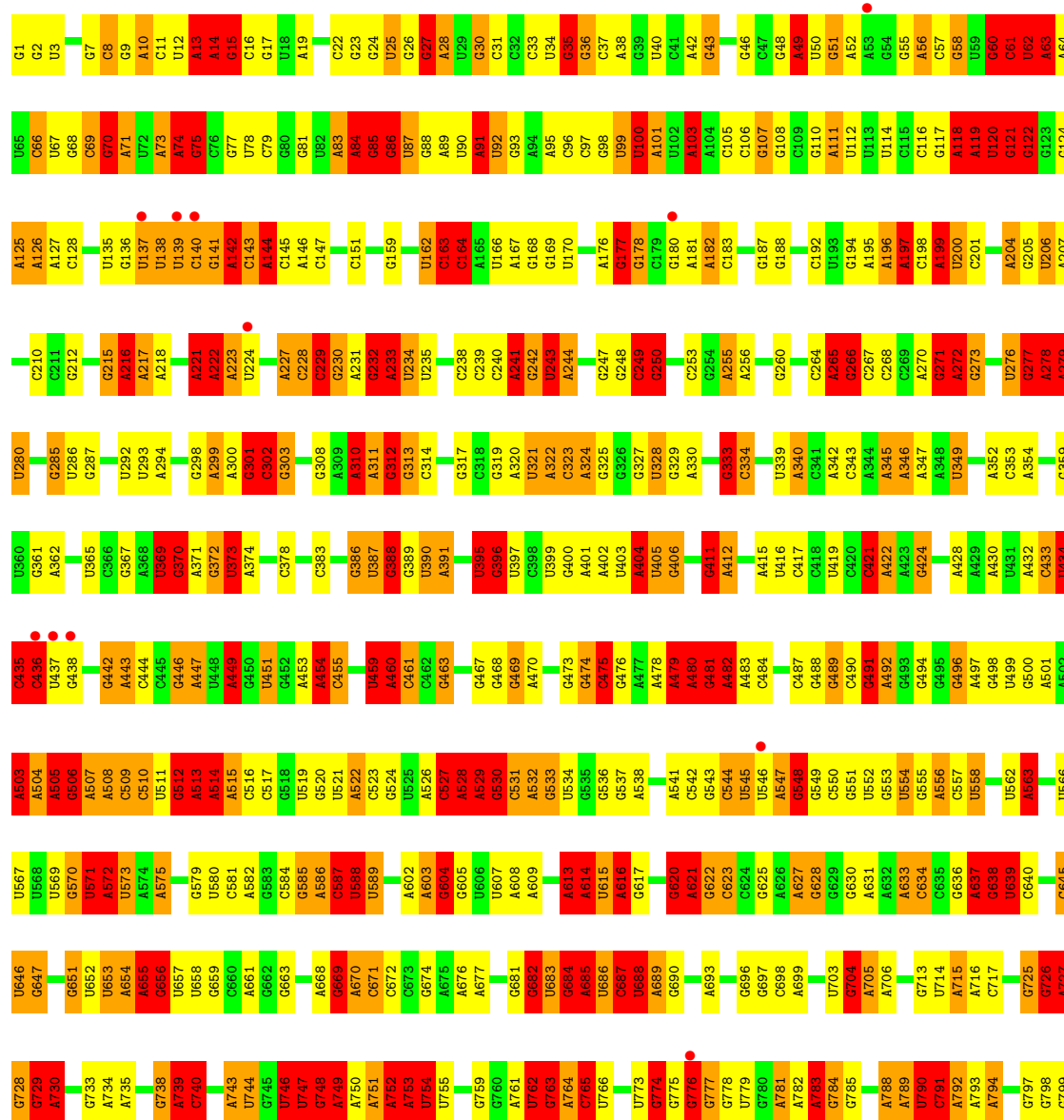
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	B	20	Total 20	O 20	0	0
34	C	8	Total 8	O 8	0	0
34	D	3	Total 3	O 3	0	0
34	E	1	Total 1	O 1	0	0
34	L	4	Total 4	O 4	0	0
34	N	3	Total 3	O 3	0	0
34	T	1	Total 1	O 1	0	0
34	2	1	Total 1	O 1	0	0
34	3	2	Total 2	O 2	0	0
34	4	3	Total 3	O 3	0	0

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.

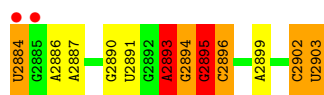
• Molecule 1: 23S rRNA

Chain A: 



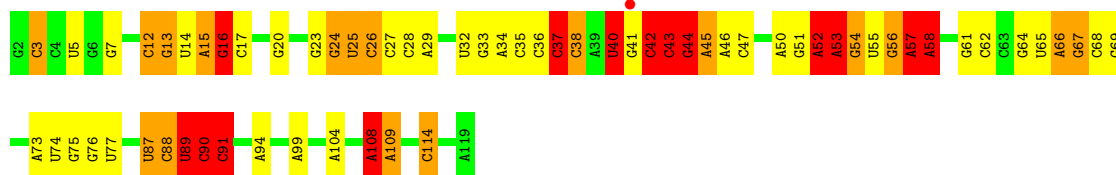
A1763	A1713		C1558	A1490	G1408	A1342	C1208	G1139	G1075	A1008	A947	U858	A800
A1764	U1714	A1641	U1559	G1491	G1411	G1343	U1209	C1140	C1076	A1009	C945	G869	G801
A1765	G1715	G1492	G1560	G1492	U1411	U1344	G1210	A1141	A1077	A1010	G949	U870	A802
A1766	G1716	C1493	C1561	C1493	U1411	C1345	C1211	A1142	U1078	G1011	G950	U871	U803
A1767	A1717	A1494	A1565	A1494	U1415	G1346	G1212	A1143	C1079	U1012	C951		A804
A1768		G1415	C1565	A1495	G1416	A1347	G1213	A1144	A1060	C1013	G954		G805
A1769	G1721	A1496	A1566	A1496	C1417	C1348	G1214	C1145	U1081	A1014	U955		G806
G1790	G1722	A1497	G1567	A1497	G1418	C1349	G1215	C1146	U1082	U1015	U956		U807
A1791	A1723	C1498	G1568	C1498	A1419	C1350	G1216	A1147	U1083	G1016	U957		G809
G1792	U1724	C1499	C1569	C1499	A1420	C1351	U1217	U1148	A1084	G1017	U958	A	G810
	U1725	A1570	A1570		G1421	U1352		G1149	A1085	U1018	A959	U	U810
U1796		A1571	A1571	A1503	G1422	G1356	G1223	C1150	A1066	U1019	G960	C	U811
G1797	G1728	A1572	A1572	A1504	G1423	C1357	U1224	A1151	G1087	A1020	A960	C	C812
U1798	U1729				G1424	C1357	G1225	C1152	A1088	A1021	C961	C	U813
G1799	G1730	U1578		A1508	G1425	G1358	G1226	C1153	A1089	U1022	G962	C	C814
C1800	G1731	C1566		A1509	G1426	A1359	G1227	G1154	A1090	G1023	U963	G	
A1801	C1732	G1581	G1581	G1510	U1427	G1360	G1228	A1155	C1091	G1024	C964	A892	C817
A1802	G1733	C1582	C1582	G1511	A1428	G1361	G1229	C1156	C1092	G1025	C965	C893	C818
A1803	G1734	A1583	A1583	C1512	G1429	C1362	C1230	G1157	G1093	G1026	U966	U894	A819
A1804	U1735	U1584	U1584	U1513	G1430	C1363		C1158		A1027	U967	U895	A820
A1805	A1736	G1661	C1585	G1514	A1431	G1364	G1232	U1159	A1096	A1028	C968	U896	A821
C1806	G1737	A1515		G1516	A1435	A1365	U1234	G1160	U1097	A1029	G969	C897	A822
G1807	G1738	G1517	U1588	G1517	G1436	G1368	G1235	C1161	A1098		U970		C823
A1808	A1739	C1518	U1589	C1518	G1437	A1369	G1236	G1162		U1033	G971	A900	U824
A1809		G1519		G1519	U1438	C1370	G1237		C1102	G1034	A972	C901	A825
A1810	G1743		C1595			C1371	G1238	A1165	A1103	U1035	A973		U826
U1811	A1744	U1520		G1521	U1442	U1372	U1239	C1167	C1104	G1036	G974	G907	U827
U1812	A1745	G1521	C1600	G1521	U1443	A1373	U1240	U1175	C1105	U1037	A975	C908	U828
G1813	A1746	U1522	G1601	A1522	U1444	G1374	A1241	U1176	A1111	G1047	A981	C915	A833
G1814	U1747	U1602	U1602	U1523	G1444	G1374		U1177	G1112	A1048	C982	C915	C835
A1815		A1603	A1603	G1524	G1445	U1375	G1245	G1171	G1107	C1049	A983	G916	C836
C1816	G1753	C1604	C1604	A1525			A1246	U1172	U1108	A1050	A984	A917	C837
A1817	A1754	C1605	C1605	G1526	C1451	A1378	G1247	U1173	C1109	G1045	A979	C912	U832
U1818	G1755	G1673	C1606		G1452	U1379	A1248	U1174	G1110	A1046	A980	U913	A833
A1819	G1756	C1675	A1530	G1530	A1453	G1380	U1249	A1175	C1117	G1047	A981	C914	C834
U1820	A1757	A1608	C1531	C1531	G1454	G1381	G1250	U1176	G1112	A1048	C982	C915	C835
A1821	U1758	A1532	A1532	G1532	G1455	G1382	G1251	G1177	U1113	C1049	A983	G916	C836
U1759		C1533	C1533	C1533	G1456	A1383	G1252	G1179	C1114	A1050	A984	A917	C837
G1822	A1759	A1610	A1610	G1538	U1457	A1384	A1253	U1180	G1115	G1051	C985	A918	C838
G1823	G1760	C1611	C1611	U1534	U1457	A1384	U1254	U1181	C1116		C986	U919	C839
U1824	C1761	G1535	A1535	U1458	G1459	A1385	A1255	U1181	C1117	A1054	C987	A920	C840
U1825	A1762	C1536	C1536	G1537	C1461	C1386	U1256	G1182	C1118	G1055	A988	C921	C841
	G1763	U1537	U1537	U1460		A1387	G1257	U1183	U1119	G1056	G989	C922	U842
	U1765	C1461		C1461		G1388	C1258	U1184	G1120	A1057	A990	G923	
		U1468				G1389	G1259	G1185	C1121	U1058	C991	G924	
		U1468				G1392	A1260	G1187	G1122	G1059	C992		A845
		G1471	A1392	A1327		A1392	C1261	U1188	G1125	U1060	G993	A927	U847
		C1472	U1394	A1328		U1394	C1261	U1188	C1126	U1061	C994		C854
		G1476	U1396	A1330		U1396	A1264	A1190	A1127	G1062	C995	U931	C855
		U1476	U1397	C1330		U1397	A1265	G1194	G1128	G1063	A996	U932	C856
		A1477	C1398	G1332		C1398	G1266	A1194	U1065	C1064	G997	U934	C857
		G1478	U1400	G1333		U1400	U1267	G1195	U1066	A1000	C998	U934	C858
		G1482	U1403	C1334		U1403	A1268	C1196	U1067	G1068	A1001	G938	C859
		U1483	A1404	C1335		A1404	A1269	U1199	G1131	G1069	A1001		U860
		U1484	C1404	U1400		C1404	G1270	U1203	U1065	A1069	G1002	A941	A861
		U1487	U1405	U1403		U1405	G1271	U1202	U1066	A1070	G1003	G942	
			U1406	C1336		C1336	A1272	A1284	G1130	G1071	U1004	A943	C864
			U1407	G1337		U1407	U1273	U1206	U1067	C1072	C1005	C944	C865
				U1487			A1275	G1206	G1137	A1073	C1006	C946	A866
								C1207	G1138	G1074	C1007		C867

G2816	G2747	G2864	G2527	G2465	U2402	C2332	A2199	G2136	C2066	C1997	A1848
U2817	A2748	A2665	U2528	A2468	C2403	A2383	C2200	U2137	G2067	A1998	G1849
U2818	A2749	G2666	G2529	A2469	U2404	U2334	G2201	G2140	U2068	A1932	U1850
U2819	A2750	C2667	A2530	G2470	G2405	A2335	G2202	G2141	G2069	A1936	U1851
A2820	G2751	G2668	A2531	A2471	A2406	G2336	G2203	A2142	A2070	A1938	U1852
G2821	C2752	U2592	G2532	G2472	U2407	G2337	A2204	G2143	A2071	A1941	A1853
G2822	A2753	G2593	U2533	G2473	U2408	C2338	C2205	C2144	G2072	C1942	A1854
A2823	G2754	G2594	A2534	U2474	G2409	C2339	C2206	G2145	C2073	U1943	U1855
G2824	A2755	G2595	G2535	C2475	A2410	A2340	G2207	C2146	U2074	U1944	U1856
G2825	C2756	A2600	G2536	A2476	A2411	G2341	G2208	C2147	U2075	G1857	A1858
	A2757	A2601	C2537	U2477	G2412	C2342	U2210	G2148	U2076	U1945	U1859
A2828	A2679	G2602	C2538	A2478	G2413	U2343	A2211	U2149	A2077	U1946	G1860
G2829	C2680	G2603	G2539	A2479	G2414	U2344	A2212	C2150	C2078	C1947	G1861
G2830	C2681	G2604	C2540	U2480	G2415	G2345	U2213	U2151	U2079	A2013	
U2831	A2764	A2604	A2541	G2481	C2416	A2346	C2214	U2152	U2080	U1950	U1865
U2832	A2765	G2605	A2542	G2482	C2417	C2347	C2215	G2157	U2081	U1951	A1866
G2833	U2769	G2606	G2543	A2483	U2418	U2348	G2216	U2155	C2091	A1952	G1867
U2834	G2770	U2609	G2544	G2484	U2419	G2349	G2217	G2156	A2019	A1953	G1868
U2835	G2771	G2610	G2545	G2485	U2420	C2350	G2218	G2157	A2020	G1954	G1869
U2836	C2772	G2611	U2546	C2486	G2421	C2351	U2219	A	C2021	U1955	C1870
A2837		G2612	A2547	G2487	C2422	G2352	U2220	C	U2022	U1956	A1871
	A2776	G2613	U2548	U2488	U2423	C2353	G2221	G	G2023	C1957	A1872
G2842	G2777	G2614	G2549	A2489	C2424	G2354	G2222	C	G2024	G1958	G1873
G2843	A2778	U2615	G2550	U2490	A2425	G2355	G2223	A	G2025	G1959	C1874
	U2779	G2616	U2551	G2491	A2426	G2356	G2224	G	U2026	C1961	G1875
G2846	G2780	G2617	G2552	C2492	C2427	G2357	C2225	C	G2027	U1962	A1876
U2847	A2781	G2618	G2553	U2493	U2428	G2358	A2226	C	A2030	U1963	C1881
U2848	U2782	G2619	U2554	G2494	G2429	G2359	A2227	C	A2031	G1964	U1882
A2849	G2783	G2620	U2555	G2495	U2430	C2360	U2228	C	G2032	C1965	U1883
A2851	U2701		G2556	G2496	A2431	G2361	G2229	U	A2033	U1966	G1884
	U2707		G2557	A2497	U2432	C2362	U2230	G	U2034	G1967	A1885
G2852	G2787	G2625	G2558	A2498	A2433	G2363	C2232	A	G2035	G1968	
G2853	C2788	U2629	C2559	G2499	A2435	G2364	U2233	A	A2036	A1969	A1889
G2854	G2789	G2630	A2560	C2500	G2436	G2365	G2234	U	A2037	U1970	A1900
G2855	U2790	U2631	U2561	C2501	A2439	G2366	G2235	A	G2038	U1971	A1901
A2856	G2791	G2632	U2562	G2502	U2440	G2367	G2236	C	G2039	G1972	
G2857	A2792	A2632	U2563	A2503	U2441	U2372	G2237	C	G2043	C1973	C1905
	C2793	G2715	A2564	U2504	C2442	G2373	G2238	A	C2044	C1974	G1906
A2860	C2794	G2636	A2565	U2505	U2443	A2381	U2240	C	G2045	G1975	G1907
U2861	C2795	U2637	U2566	G2506	G2443	G2382	A2241	C	G2046	U1976	C1908
G2862	U2796	G2638	G2567	G2507	G2444	A2383	U2242	C	G2047	A1977	
G2863	U2797	A2639	U2568	C2508	G2445	G2384	U2243	G	G2048	A1978	
G2864	U2798	G2640	G2569	G2509	G2446	U2384	A2311	U2180	A	U1979	U1911
U2865	G2799	G2641	G2570	C2510	G2447	C2385	G2246	U2181	G	G1980	A1912
U2866	A2800		U2571	U2511	A2448	A2386	A2247	U2182	G	A1981	A1913
G2867	G2801	G2645	A2572	G2512	U2449	U2387	U2248	A2183	G	U1982	C1914
A2868	A2725	C2646	C2573	A2451	A2450	A2388	G2249	U2184	U2051	G1983	U1915
G2869	A2726		G2574	C2452	A2451	G2389	G2250	U2185	G	A2054	A1916
	A2727	U2650	G2575	G2513	A2452	U2390	G2251	U2186	G	C2055	U1917
A2872	U2728	C2651	G2576	G2514	A2453	U2391	G2252	U2187	A	G2056	A1918
G2873	G2729	U2652	A2577	G2515	G2454	A2392	G2253	U2188	G	A1987	A1919
U2874	C2807	C2653	G2578	A2516	G2455	U2392	G2254	U2189	G	G1988	C1925
G2875	G2731	A2654	C2579	A2517	G2456	A2393	G2255	G2190	G	U1991	U1926
C2876	A2809	G2655	U2580	U2519	U2457	C2394	G2256	G2191	C	U1992	A1928
A2877	A2810	G2656	G2581	G2520	G2458	G2395	U2257	U2193	U	U1993	G1929
	A2734	A2657	C2521	A2459	U2459	A2396	G2258	U2194	U	C2063	U1930
A2879	G2812	G2658	G2582	C2522	U2460	U2397	U2259	U2195	U	U1995	
G2880	A2813	U2584	U2583	A2461	C2462	U2398	C2260	G2196	G	C1996	
U2881	A2741	G2662	G2525	C2462		G2399	G2261	U2197	U		
A2882		G2663	G2526	G2526		U2401	U2262	A2198			



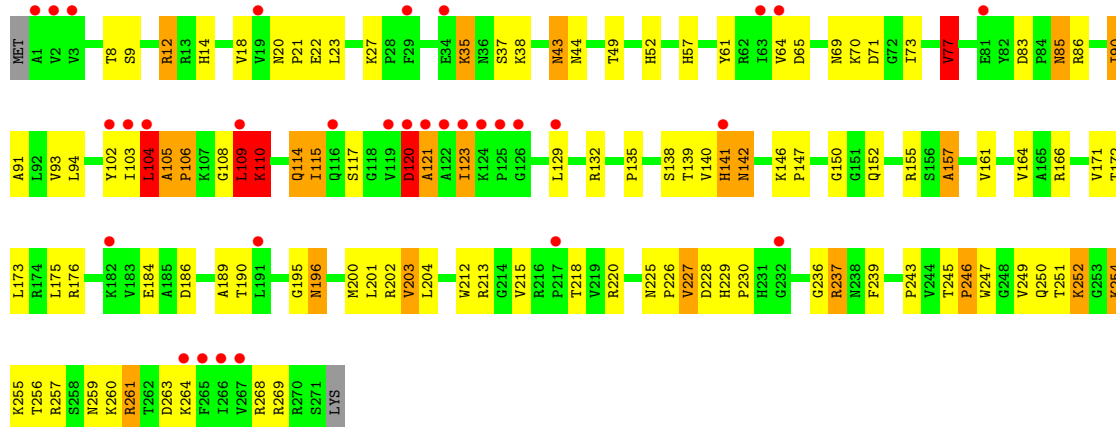
• Molecule 2: 5S rRNA

Chain B:



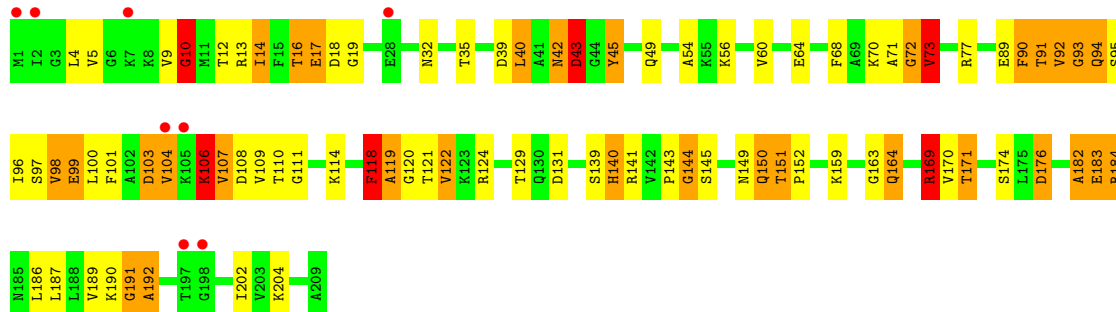
• Molecule 3: 50S ribosomal protein L2

Chain C:



• Molecule 4: 50S ribosomal protein L3

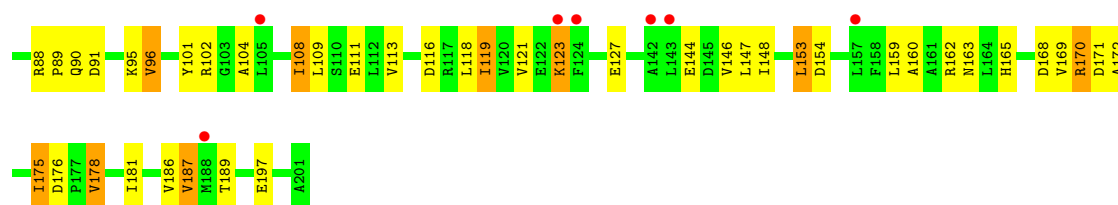
Chain D:



• Molecule 5: 50S ribosomal protein L4

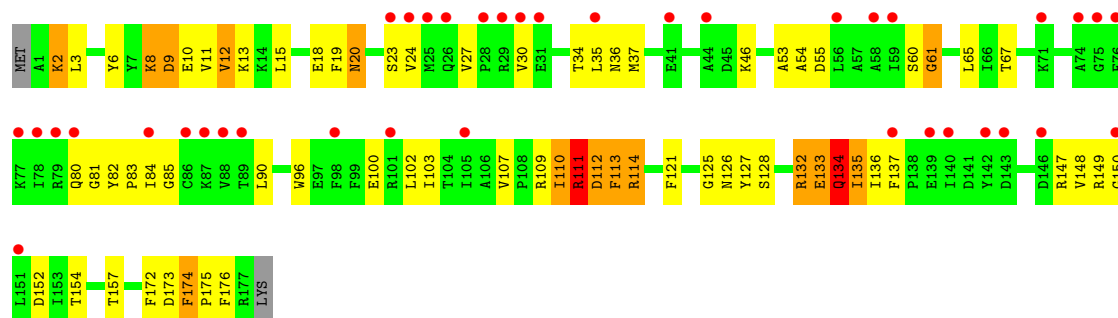
Chain E:





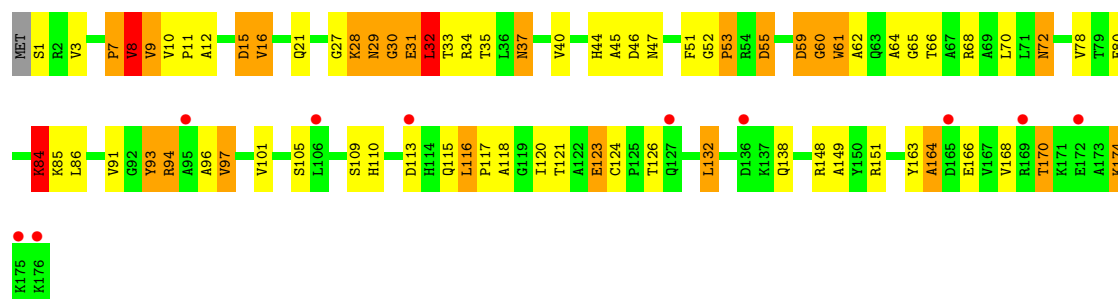
• Molecule 6: 50S ribosomal protein L5

Chain F:



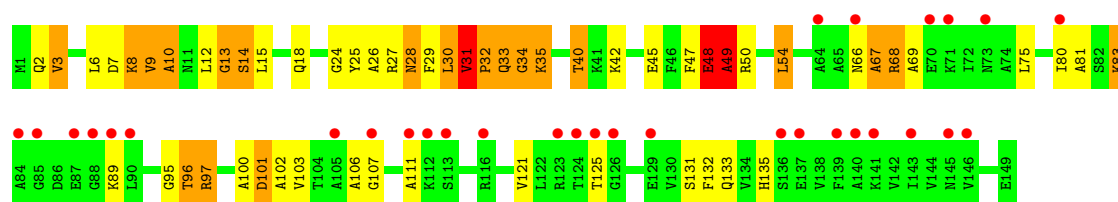
• Molecule 7: 50S ribosomal protein L6

Chain G:



• Molecule 8: 50S ribosomal protein L9

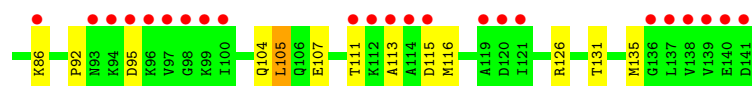
Chain H:



• Molecule 9: 50S ribosomal protein L11

Chain I:





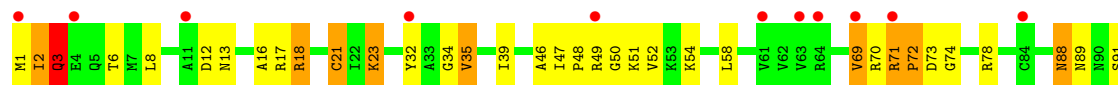
• Molecule 10: 50S ribosomal protein L13

Chain J:



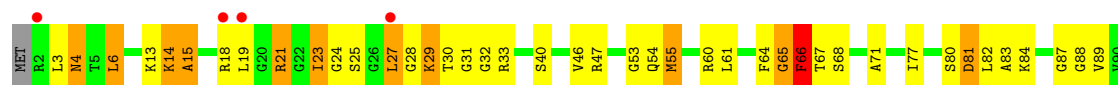
• Molecule 11: 50S ribosomal protein L14

Chain K:



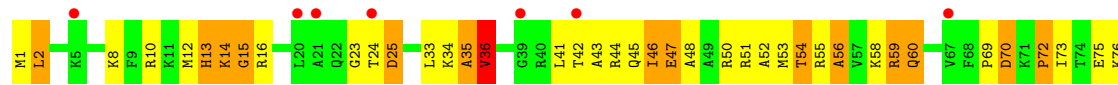
• Molecule 12: 50S ribosomal protein L15

Chain L:



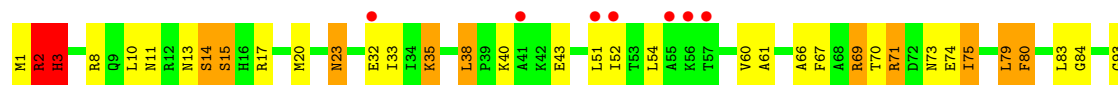
• Molecule 13: 50S ribosomal protein L16

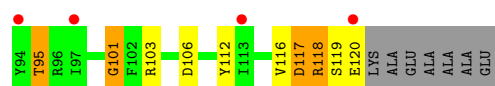
Chain M:



• Molecule 14: 50S ribosomal protein L17

Chain N:





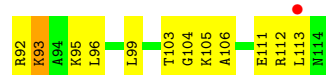
- Molecule 15: 50S ribosomal protein L18

Chain O:



- Molecule 16: 50S ribosomal protein L19

Chain P:



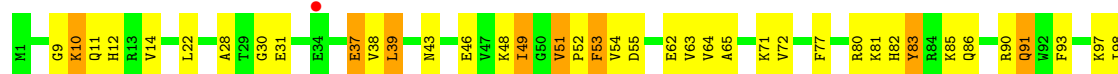
- Molecule 17: 50S ribosomal protein L20

Chain Q:



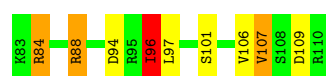
- Molecule 18: 50S ribosomal protein L21

Chain R:

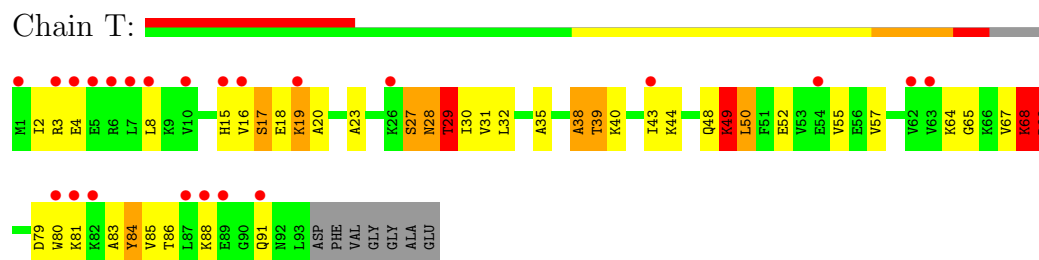


- Molecule 19: 50S ribosomal protein L22

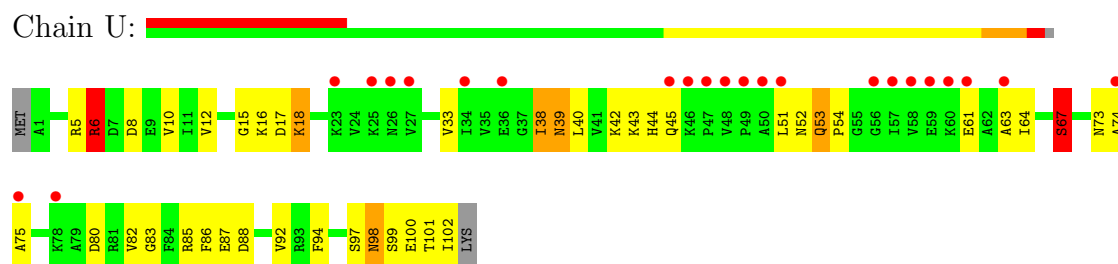
Chain S:



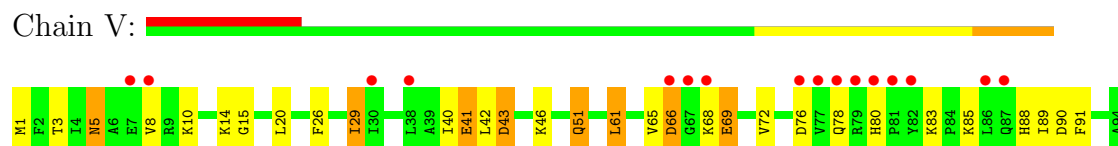
- Molecule 20: 50S ribosomal protein L23



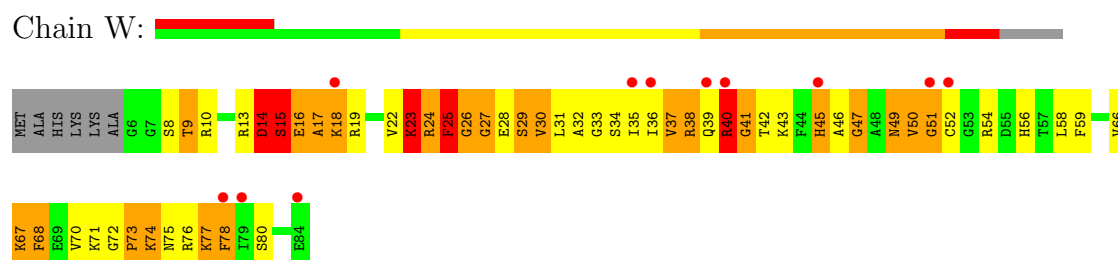
- Molecule 21: 50S ribosomal protein L24



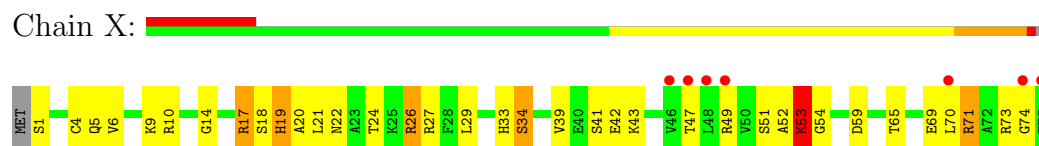
- Molecule 22: 50S ribosomal protein L25



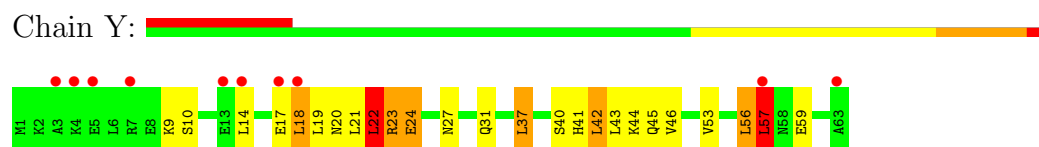
- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L30

Chain Z: 



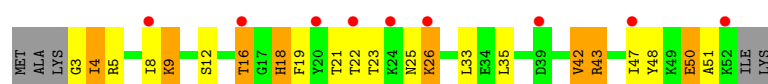
- Molecule 27: 50S ribosomal protein L32

Chain 0: 



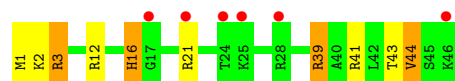
- Molecule 28: 50S ribosomal protein L33

Chain 1: 



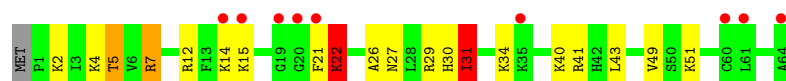
- Molecule 29: 50S ribosomal protein L34

Chain 2: 



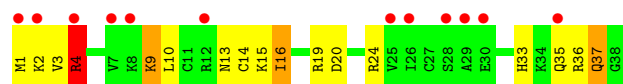
- Molecule 30: 50S ribosomal protein L35

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	210.95Å 433.08Å 624.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.44 – 3.71 73.44 – 3.71	Depositor EDS
% Data completeness (in resolution range)	75.7 (73.44-3.71) 75.7 (73.44-3.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.227 , 0.268 0.387 , 0.394	Depositor DCC
R_{free} test set	9145 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	109.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 27.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 452802 reflections	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	90740	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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	0.76	12/68626 (0.0%)	1.69	1758/107056 (1.6%)
2	B	0.66	0/2828	1.67	74/4410 (1.7%)
3	C	0.45	0/2121	0.72	1/2852 (0.0%)
4	D	0.50	0/1586	0.75	1/2134 (0.0%)
5	E	0.44	0/1571	0.67	0/2113
6	F	0.41	0/1434	0.68	3/1926 (0.2%)
7	G	0.43	0/1343	0.65	0/1816
8	H	0.70	6/1122 (0.5%)	0.83	6/1515 (0.4%)
9	I	0.24	0/1046	0.50	0/1410
10	J	0.55	0/1152	0.75	0/1551
11	K	0.55	0/947	0.83	0/1268
12	L	0.42	0/1054	0.77	1/1403 (0.1%)
13	M	0.51	0/1093	0.77	1/1460 (0.1%)
14	N	0.55	0/973	0.79	0/1301
15	O	0.42	0/902	0.63	0/1209
16	P	0.51	0/929	0.77	0/1242
17	Q	0.60	0/960	0.71	0/1278
18	R	0.56	0/829	0.85	1/1107 (0.1%)
19	S	0.50	0/864	0.75	0/1156
20	T	0.48	0/744	0.70	0/994
21	U	0.41	0/787	0.70	0/1051
22	V	0.48	0/766	0.66	0/1025
23	W	0.51	0/603	0.76	0/797
24	X	0.42	0/635	0.67	0/848
25	Y	0.40	0/510	0.66	0/677
26	Z	0.52	0/453	0.77	0/605
27	0	0.45	0/450	0.79	0/599
28	1	0.40	0/416	0.63	0/554
29	2	0.47	0/380	0.73	0/498
30	3	0.51	0/513	0.76	0/676
31	4	0.47	0/303	0.76	0/397
All	All	0.70	18/97940 (0.0%)	1.52	1846/146928 (1.3%)

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
4	D	0	1
8	H	0	2
14	N	0	1
All	All	0	4

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1142	A	N9-C4	-13.92	1.29	1.37
8	H	48	GLU	C-O	9.51	1.41	1.23
1	A	2451	A	C8-N7	9.03	1.37	1.31
8	H	48	GLU	CA-CB	6.93	1.69	1.53
8	H	48	GLU	CA-C	-6.56	1.35	1.52

The worst 5 of 1846 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2447	G	C6-N1-C2	-22.51	111.59	125.10
1	A	2451	A	C5-N7-C8	-17.23	95.28	103.90
1	A	2347	C	N1-C1'-C2'	-16.79	92.17	114.00
1	A	790	U	P-O3'-C3'	-16.12	100.36	119.70
2	B	88	C	O4'-C1'-N1	-15.24	96.01	108.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	10	GLY	Peptide
8	H	48	GLU	Mainchain
8	H	49	ALA	Mainchain
14	N	101	GLY	Peptide

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	61274	0	0	1337	0
2	B	2529	0	0	36	0
3	C	2082	0	0	61	0
4	D	1565	0	0	66	0
5	E	1552	0	0	40	0
6	F	1410	0	0	36	0
7	G	1323	0	0	36	0
8	H	1111	0	0	21	0
9	I	1032	0	0	6	0
10	J	1129	0	0	49	0
11	K	938	0	0	26	0
12	L	1045	0	0	36	0
13	M	1074	0	0	37	0
14	N	960	0	0	25	0
15	O	892	0	0	28	0
16	P	917	0	0	31	0
17	Q	947	0	0	45	0
18	R	816	0	0	18	0
19	S	857	0	0	25	0
20	T	738	0	0	21	0
21	U	779	0	0	18	0
22	V	753	0	0	19	0
23	W	596	0	0	52	0
24	X	625	0	0	22	0
25	Y	509	0	0	14	0
26	Z	449	0	0	6	0
27	0	444	0	0	10	0
28	1	409	0	0	10	0
29	2	377	0	0	6	0
30	3	504	0	0	12	0
31	4	302	0	0	11	0
32	A	136	0	0	0	0
32	B	4	0	0	0	0
32	D	1	0	0	0	0
33	4	1	0	0	0	0
34	2	1	0	0	0	0
34	3	2	0	0	0	0
34	4	3	0	0	0	0
34	A	614	0	0	11	0
34	B	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	8	0	0	1	0
34	D	3	0	0	3	0
34	E	1	0	0	0	0
34	L	4	0	0	0	0
34	N	3	0	0	0	0
34	T	1	0	0	0	0
All	All	90740	0	0	2029	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 23.

The worst 5 of 2029 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:118:A:C8	1:A:119:A:C8	2.61	0.89
1:A:1509:A:O2'	1:A:1510:G:O5'	1.92	0.88
1:A:954:G:C5	1:A:955:U:C5	2.61	0.87
1:A:370:G:O2'	1:A:424:G:OP1	1.92	0.87
1:A:13:A:O2'	1:A:15:G:N7	2.10	0.85

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	269/273 (98%)	192 (71%)	48 (18%)	29 (11%)	1	18
4	D	207/209 (99%)	141 (68%)	35 (17%)	31 (15%)	0	9
5	E	199/201 (99%)	138 (69%)	41 (21%)	20 (10%)	1	21
6	F	175/179 (98%)	133 (76%)	26 (15%)	16 (9%)	1	25
7	G	174/177 (98%)	114 (66%)	34 (20%)	26 (15%)	0	9
8	H	147/149 (99%)	63 (43%)	53 (36%)	31 (21%)	0	3
9	I	139/142 (98%)	84 (60%)	42 (30%)	13 (9%)	1	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	140/142 (99%)	100 (71%)	22 (16%)	18 (13%)	0	13
11	K	120/123 (98%)	86 (72%)	17 (14%)	17 (14%)	0	11
12	L	141/144 (98%)	106 (75%)	23 (16%)	12 (8%)	1	27
13	M	134/136 (98%)	95 (71%)	16 (12%)	23 (17%)	0	7
14	N	118/127 (93%)	85 (72%)	23 (20%)	10 (8%)	1	27
15	O	114/117 (97%)	84 (74%)	20 (18%)	10 (9%)	1	26
16	P	112/115 (97%)	74 (66%)	23 (20%)	15 (13%)	0	12
17	Q	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	2	39
18	R	101/103 (98%)	75 (74%)	14 (14%)	12 (12%)	1	15
19	S	108/110 (98%)	81 (75%)	20 (18%)	7 (6%)	2	37
20	T	91/100 (91%)	55 (60%)	20 (22%)	16 (18%)	0	6
21	U	100/104 (96%)	68 (68%)	16 (16%)	16 (16%)	0	8
22	V	92/94 (98%)	76 (83%)	15 (16%)	1 (1%)	21	79
23	W	77/85 (91%)	32 (42%)	18 (23%)	27 (35%)	0	0
24	X	75/78 (96%)	58 (77%)	12 (16%)	5 (7%)	2	36
25	Y	61/63 (97%)	39 (64%)	15 (25%)	7 (12%)	1	16
26	Z	56/59 (95%)	43 (77%)	10 (18%)	3 (5%)	3	43
27	0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	13
28	1	48/55 (87%)	32 (67%)	9 (19%)	7 (15%)	0	10
29	2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	4	48
30	3	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	6	58
31	4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	1	28
All	All	3309/3409 (97%)	2291 (69%)	625 (19%)	393 (12%)	1	15

5 of 393 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	35	LYS
3	C	77	VAL
3	C	104	LEU
3	C	106	PRO
3	C	110	LYS

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	216/218 (99%)	173 (80%)	43 (20%)	2	14
4	D	164/164 (100%)	136 (83%)	28 (17%)	3	23
5	E	165/165 (100%)	130 (79%)	35 (21%)	1	12
6	F	148/150 (99%)	130 (88%)	18 (12%)	7	41
7	G	137/138 (99%)	107 (78%)	30 (22%)	1	11
8	H	114/114 (100%)	97 (85%)	17 (15%)	4	31
9	I	109/110 (99%)	94 (86%)	15 (14%)	5	35
10	J	116/116 (100%)	90 (78%)	26 (22%)	1	10
11	K	103/104 (99%)	84 (82%)	19 (18%)	2	18
12	L	102/103 (99%)	81 (79%)	21 (21%)	2	13
13	M	109/109 (100%)	90 (83%)	19 (17%)	3	21
14	N	100/103 (97%)	81 (81%)	19 (19%)	2	16
15	O	86/87 (99%)	69 (80%)	17 (20%)	2	15
16	P	99/100 (99%)	79 (80%)	20 (20%)	2	14
17	Q	89/90 (99%)	73 (82%)	16 (18%)	2	19
18	R	84/84 (100%)	69 (82%)	15 (18%)	2	20
19	S	93/93 (100%)	73 (78%)	20 (22%)	1	11
20	T	80/84 (95%)	61 (76%)	19 (24%)	1	8
21	U	83/85 (98%)	69 (83%)	14 (17%)	3	24
22	V	78/78 (100%)	64 (82%)	14 (18%)	2	20
23	W	59/63 (94%)	43 (73%)	16 (27%)	1	6
24	X	67/68 (98%)	53 (79%)	14 (21%)	1	12
25	Y	55/55 (100%)	44 (80%)	11 (20%)	2	14
26	Z	48/49 (98%)	34 (71%)	14 (29%)	0	5
27	0	47/48 (98%)	42 (89%)	5 (11%)	10	49
28	1	45/49 (92%)	37 (82%)	8 (18%)	2	20
29	2	38/38 (100%)	32 (84%)	6 (16%)	4	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	3	51/52 (98%)	44 (86%)	7 (14%)	5	35
31	4	34/34 (100%)	30 (88%)	4 (12%)	8	43
All	All	2719/2751 (99%)	2209 (81%)	510 (19%)	2	17

5 of 510 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	114	LYS
14	N	75	ILE
26	Z	9	THR
12	L	21	ARG
13	M	58	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2850/2903 (98%)	925 (32%)	497 (17%)
2	B	117/118 (99%)	32 (27%)	22 (18%)
All	All	2967/3021 (98%)	957 (32%)	519 (17%)

5 of 957 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	13	A
1	A	14	A
1	A	15	G
1	A	28	A

5 of 519 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1326	U
1	A	1682	G
1	A	2799	A
1	A	1378	A
1	A	1510	G

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 142 ligands modelled in this entry, 142 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	2854/2903 (98%)	-0.26	53 (1%) 64 41	52, 81, 194, 355	0
2	B	118/118 (100%)	-0.27	1 (0%) 83 63	66, 101, 133, 171	0
3	C	271/273 (99%)	0.67	32 (11%) 5 6	60, 99, 129, 161	0
4	D	209/209 (100%)	0.30	8 (3%) 38 25	55, 75, 114, 129	0
5	E	201/201 (100%)	0.43	7 (3%) 42 26	56, 96, 129, 157	0
6	F	177/179 (98%)	1.04	38 (21%) 1 2	120, 166, 201, 215	0
7	G	176/177 (99%)	0.51	10 (5%) 23 15	83, 108, 134, 152	0
8	H	149/149 (100%)	1.18	31 (20%) 1 2	110, 239, 259, 264	0
9	I	141/142 (99%)	2.54	60 (42%) 1 1	243, 307, 359, 366	0
10	J	142/142 (100%)	0.27	6 (4%) 35 22	59, 76, 102, 132	0
11	K	122/123 (99%)	0.83	20 (16%) 2 3	55, 73, 113, 169	0
12	L	143/144 (99%)	0.54	10 (6%) 16 11	55, 93, 124, 136	0
13	M	136/136 (100%)	0.59	10 (7%) 14 11	58, 81, 111, 138	0
14	N	120/127 (94%)	0.67	11 (9%) 9 8	61, 76, 96, 141	0
15	O	116/117 (99%)	0.52	7 (6%) 21 15	96, 105, 123, 147	0
16	P	114/115 (99%)	0.33	4 (3%) 42 26	64, 81, 119, 134	0
17	Q	117/118 (99%)	0.24	2 (1%) 67 44	56, 77, 99, 120	0
18	R	103/103 (100%)	0.16	1 (0%) 79 57	55, 87, 114, 131	0
19	S	110/110 (100%)	0.20	2 (1%) 65 43	55, 70, 105, 159	0
20	T	93/100 (93%)	1.20	23 (24%) 1 2	65, 105, 142, 151	0
21	U	102/104 (98%)	1.22	23 (22%) 1 2	89, 114, 136, 158	0
22	V	94/94 (100%)	0.74	16 (17%) 2 3	71, 90, 116, 126	0
23	W	79/85 (92%)	0.99	11 (13%) 4 4	68, 86, 136, 156	0
24	X	77/78 (98%)	0.99	9 (11%) 5 6	65, 101, 124, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	63/63 (100%)	0.73	10 (15%) 3 3	101, 123, 149, 159	0
26	Z	58/59 (98%)	0.78	4 (6%) 17 12	64, 74, 111, 141	0
27	0	56/57 (98%)	-0.21	0 100 100	54, 77, 113, 132	0
28	1	50/55 (90%)	1.19	9 (18%) 2 3	76, 100, 118, 132	0
29	2	46/46 (100%)	0.87	6 (13%) 4 5	62, 75, 103, 137	0
30	3	64/65 (98%)	0.91	9 (14%) 3 4	58, 73, 96, 120	0
31	4	38/38 (100%)	1.54	12 (31%) 1 2	69, 84, 110, 120	0
All	All	6339/6430 (98%)	0.26	445 (7%) 17 11	52, 89, 233, 366	0

The worst 5 of 445 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	10	LEU	27.7
8	H	112	LYS	13.0
9	I	13	ALA	11.0
9	I	7	TYR	10.0
9	I	11	GLN	9.4

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
32	MG	A	2914	1/1	0.79	31.90	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2929	1/1	0.39	29.98	59,59,59,59	0
32	MG	A	2933	1/1	0.30	13.22	58,58,58,58	0
32	MG	A	3002	1/1	0.41	11.92	58,58,58,58	0
32	MG	A	2988	1/1	0.30	9.09	59,59,59,59	0
32	MG	A	2937	1/1	0.28	8.96	57,57,57,57	0
32	MG	A	3013	1/1	0.31	8.92	61,61,61,61	0
32	MG	B	120	1/1	0.26	7.74	118,118,118,118	0
32	MG	A	3027	1/1	0.73	7.53	59,59,59,59	0
32	MG	A	3034	1/1	1.06	6.91	68,68,68,68	0
32	MG	A	3039	1/1	0.37	6.62	64,64,64,64	0
32	MG	A	2974	1/1	0.37	6.32	55,55,55,55	0
32	MG	A	2912	1/1	0.26	5.61	61,61,61,61	0
32	MG	A	2918	1/1	0.32	5.60	55,55,55,55	0
32	MG	A	2964	1/1	0.67	4.97	56,56,56,56	0
32	MG	A	2975	1/1	0.54	3.80	55,55,55,55	0
32	MG	A	2938	1/1	0.20	3.62	72,72,72,72	0
32	MG	A	2934	1/1	0.26	3.60	59,59,59,59	0
32	MG	A	2961	1/1	0.39	3.50	63,63,63,63	0
32	MG	A	3006	1/1	0.23	2.87	81,81,81,81	0
32	MG	A	2909	1/1	0.25	2.87	101,101,101,101	0
32	MG	A	2984	1/1	0.23	2.62	56,56,56,56	0
32	MG	A	2971	1/1	0.22	2.58	65,65,65,65	0
32	MG	A	2923	1/1	0.29	2.57	63,63,63,63	0
32	MG	A	2924	1/1	0.30	2.44	59,59,59,59	0
32	MG	A	2968	1/1	0.35	1.99	55,55,55,55	0
32	MG	A	2940	1/1	0.20	1.96	58,58,58,58	0
32	MG	A	2936	1/1	0.24	1.76	56,56,56,56	0
32	MG	A	3038	1/1	0.21	1.64	60,60,60,60	0
32	MG	A	2960	1/1	0.31	1.62	61,61,61,61	0
32	MG	A	2948	1/1	0.32	1.37	80,80,80,80	0
32	MG	A	2919	1/1	0.18	1.26	56,56,56,56	0
32	MG	A	2999	1/1	0.18	1.21	61,61,61,61	0
32	MG	A	2972	1/1	0.17	1.08	65,65,65,65	0
32	MG	A	3028	1/1	0.20	1.07	58,58,58,58	0
32	MG	A	3023	1/1	0.17	0.99	59,59,59,59	0
32	MG	A	3036	1/1	0.28	0.67	73,73,73,73	0
32	MG	A	3004	1/1	0.27	0.61	54,54,54,54	0
32	MG	A	2963	1/1	0.25	0.59	56,56,56,56	0
32	MG	A	3025	1/1	0.23	0.56	57,57,57,57	0
32	MG	D	210	1/1	0.18	0.55	55,55,55,55	0
32	MG	A	2916	1/1	0.22	0.53	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2925	1/1	0.16	0.40	55,55,55,55	0
32	MG	A	3022	1/1	0.18	0.33	68,68,68,68	0
32	MG	A	2955	1/1	0.16	0.29	54,54,54,54	0
32	MG	A	3012	1/1	0.18	0.17	60,60,60,60	0
32	MG	A	3008	1/1	0.24	0.11	55,55,55,55	0
32	MG	A	2962	1/1	0.13	0.03	69,69,69,69	0
32	MG	A	2973	1/1	0.20	-0.15	158,158,158,158	0
32	MG	B	122	1/1	0.17	-0.27	69,69,69,69	0
32	MG	A	3035	1/1	0.21	-0.30	61,61,61,61	0
32	MG	A	2920	1/1	0.16	-0.30	56,56,56,56	0
32	MG	A	3019	1/1	0.14	-0.41	55,55,55,55	0
32	MG	A	3003	1/1	0.18	-0.54	74,74,74,74	0
32	MG	A	2995	1/1	0.10	-0.64	127,127,127,127	0
32	MG	A	2907	1/1	0.13	-0.66	86,86,86,86	0
32	MG	A	2954	1/1	0.13	-0.79	57,57,57,57	0
32	MG	A	2991	1/1	0.10	-0.82	77,77,77,77	0
32	MG	A	3018	1/1	0.21	-0.83	65,65,65,65	0
32	MG	A	3024	1/1	0.16	-0.84	64,64,64,64	0
32	MG	A	2998	1/1	0.10	-0.89	92,92,92,92	0
32	MG	A	2950	1/1	0.15	-0.91	78,78,78,78	0
32	MG	A	2932	1/1	0.13	-0.92	54,54,54,54	0
32	MG	A	2943	1/1	0.12	-0.95	58,58,58,58	0
32	MG	A	2910	1/1	0.14	-0.97	111,111,111,111	0
32	MG	A	2942	1/1	0.14	-0.99	57,57,57,57	0
32	MG	A	2922	1/1	0.08	-1.06	86,86,86,86	0
32	MG	A	3017	1/1	0.11	-1.06	88,88,88,88	0
32	MG	A	2917	1/1	0.15	-1.18	55,55,55,55	0
32	MG	A	2966	1/1	0.15	-1.19	54,54,54,54	0
32	MG	A	2994	1/1	0.14	-1.21	88,88,88,88	0
32	MG	A	2915	1/1	0.12	-1.29	54,54,54,54	0
32	MG	A	2986	1/1	0.13	-1.29	59,59,59,59	0
32	MG	A	2982	1/1	0.08	-1.30	110,110,110,110	0
32	MG	A	2987	1/1	0.12	-1.32	61,61,61,61	0
32	MG	A	3032	1/1	0.12	-1.34	55,55,55,55	0
32	MG	A	3015	1/1	0.15	-1.35	64,64,64,64	0
32	MG	A	3029	1/1	0.08	-1.35	70,70,70,70	0
32	MG	A	2951	1/1	0.09	-1.38	91,91,91,91	0
32	MG	A	2945	1/1	0.12	-1.39	68,68,68,68	0
32	MG	A	2927	1/1	0.12	-1.55	60,60,60,60	0
32	MG	A	2946	1/1	0.06	-1.58	68,68,68,68	0
32	MG	A	2913	1/1	0.09	-1.64	64,64,64,64	0
32	MG	A	2931	1/1	0.11	-1.68	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2996	1/1	0.09	-1.74	104,104,104,104	0
32	MG	A	2957	1/1	0.12	-1.75	62,62,62,62	0
32	MG	A	2949	1/1	0.12	-1.78	77,77,77,77	0
32	MG	A	2997	1/1	0.13	-1.81	92,92,92,92	0
32	MG	A	2941	1/1	0.07	-1.86	59,59,59,59	0
32	MG	A	3037	1/1	0.12	-1.88	55,55,55,55	0
32	MG	A	2935	1/1	0.09	-1.88	57,57,57,57	0
32	MG	A	2908	1/1	0.07	-1.89	91,91,91,91	0
32	MG	A	3014	1/1	0.08	-1.92	55,55,55,55	0
32	MG	A	3026	1/1	0.12	-1.92	79,79,79,79	0
32	MG	A	2939	1/1	0.08	-1.92	65,65,65,65	0
32	MG	A	2959	1/1	0.09	-2.08	64,64,64,64	0
33	ZN	4	802	1/1	0.04	-2.08	99,99,99,99	0
32	MG	A	3021	1/1	0.11	-2.10	60,60,60,60	0
32	MG	A	3007	1/1	0.13	-2.15	55,55,55,55	0
32	MG	A	2983	1/1	0.06	-2.25	93,93,93,93	0
32	MG	A	2977	1/1	0.09	-2.28	54,54,54,54	0
32	MG	A	2989	1/1	0.14	-2.31	60,60,60,60	0
32	MG	A	2979	1/1	0.12	-2.32	62,62,62,62	0
32	MG	A	2978	1/1	0.09	-2.35	58,58,58,58	0
32	MG	A	2905	1/1	0.08	-2.38	61,61,61,61	0
32	MG	A	2976	1/1	0.05	-2.40	61,61,61,61	0
32	MG	A	3033	1/1	0.12	-2.55	68,68,68,68	0
32	MG	A	2958	1/1	0.10	-2.61	62,62,62,62	0
32	MG	A	3030	1/1	0.10	-2.62	57,57,57,57	0
32	MG	B	121	1/1	0.07	-2.63	127,127,127,127	0
32	MG	A	2965	1/1	0.20	-2.66	55,55,55,55	0
32	MG	A	3010	1/1	0.09	-2.70	67,67,67,67	0
32	MG	A	2981	1/1	0.10	-2.73	100,100,100,100	0
32	MG	A	2928	1/1	0.10	-2.75	59,59,59,59	0
32	MG	A	3000	1/1	0.06	-2.76	65,65,65,65	0
32	MG	A	2993	1/1	0.07	-2.95	63,63,63,63	0
32	MG	A	3005	1/1	0.08	-3.01	57,57,57,57	0
32	MG	A	2944	1/1	0.12	-3.03	60,60,60,60	0
32	MG	A	2969	1/1	0.07	-3.23	61,61,61,61	0
32	MG	A	3011	1/1	0.09	-3.25	58,58,58,58	0
32	MG	A	2985	1/1	0.08	-3.26	55,55,55,55	0
32	MG	A	2926	1/1	0.06	-3.41	59,59,59,59	0
32	MG	A	2930	1/1	0.04	-3.50	59,59,59,59	0
32	MG	A	2967	1/1	0.08	-3.55	55,55,55,55	0
32	MG	A	2970	1/1	0.07	-3.70	57,57,57,57	0
32	MG	A	3009	1/1	0.09	-3.73	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3016	1/1	0.10	-3.79	54,54,54,54	0
32	MG	A	2990	1/1	0.08	-3.88	61,61,61,61	0
32	MG	A	2911	1/1	0.07	-4.02	59,59,59,59	0
32	MG	A	2953	1/1	0.11	-4.21	56,56,56,56	0
32	MG	A	2906	1/1	0.04	-4.29	90,90,90,90	0
32	MG	A	2921	1/1	0.05	-4.37	80,80,80,80	0
32	MG	A	3001	1/1	0.12	-4.52	72,72,72,72	0
32	MG	A	2947	1/1	0.12	-4.84	88,88,88,88	0
32	MG	A	2952	1/1	0.06	-5.25	61,61,61,61	0
32	MG	B	123	1/1	0.05	-5.93	74,74,74,74	0
32	MG	A	3031	1/1	0.06	-6.43	64,64,64,64	0
32	MG	A	3020	1/1	0.07	-7.52	67,67,67,67	0
32	MG	A	2956	1/1	0.06	-7.76	57,57,57,57	0
32	MG	A	2980	1/1	0.10	-7.84	63,63,63,63	0
32	MG	A	2904	1/1	0.08	-10.66	61,61,61,61	0
32	MG	A	2992	1/1	0.07	-13.78	66,66,66,66	0

6.5 Other polymers ⓘ

There are no such residues in this entry.