



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 08:31 PM GMT

PDB ID : 4WFN  
Title : Crystal structure of the large ribosomal subunit (50S) of *Deinococcus radiodurans* containing a three residue insertion in L22 in complex with erythromycin  
Authors : Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.  
Deposited on : 2014-09-16  
Resolution : 3.54 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

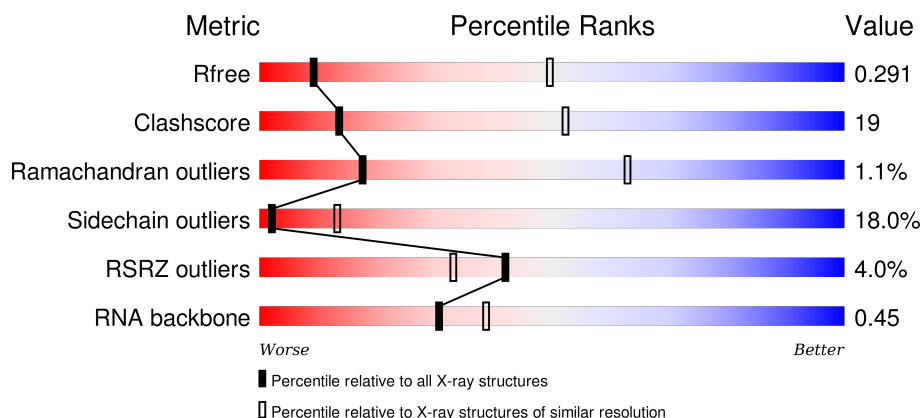
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.54 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))
$R_{free}$	91344	1136 (3.68-3.40)
Clashscore	102246	1248 (3.68-3.40)
Ramachandran outliers	100387	1208 (3.68-3.40)
Sidechain outliers	100360	1208 (3.68-3.40)
RSRZ outliers	91569	1143 (3.68-3.40)
RNA backbone	2183	1052 (4.26-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div>3%</div> <div>40%</div> <div>45%</div> <div>10%</div> <div>5%</div> </div>
2	B	211	<div> <div>2%</div> <div>45%</div> <div>43%</div> <div>10%</div> <div>•</div> </div>
3	C	205	<div> <div>7%</div> <div>42%</div> <div>44%</div> <div>8%</div> <div>5%</div> </div>
4	D	180	<div> <div>8%</div> <div>48%</div> <div>46%</div> <div>5%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	185	
6	G	174	
7	H	134	
8	I	156	
9	J	141	
10	K	116	
11	L	114	
12	M	165	
13	N	118	
14	O	100	
15	P	137	
16	Q	95	
17	R	115	
18	S	237	
19	T	91	
20	U	81	
21	V	67	
22	W	55	
23	Z	60	
24	1	55	
25	2	47	
26	3	65	
27	X	2880	
28	Y	124	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MG	K	201	-	-	-	X
29	MG	K	202	-	-	-	X
29	MG	X	2903	-	-	-	X
29	MG	X	2909	-	-	-	X
29	MG	X	2910	-	-	-	X
29	MG	X	2913	-	-	-	X
29	MG	X	2914	-	-	-	X
29	MG	X	2916	-	-	-	X
29	MG	X	2922	-	-	-	X
29	MG	X	2923	-	-	-	X
29	MG	X	2926	-	-	-	X
29	MG	X	2939	-	-	-	X
29	MG	X	2942	-	-	-	X
29	MG	X	2944	-	-	-	X
29	MG	X	2947	-	-	-	X
29	MG	X	2948	-	-	-	X
29	MG	X	2954	-	-	-	X
29	MG	X	2957	-	-	-	X
29	MG	X	2959	-	-	-	X
29	MG	X	2961	-	-	-	X
29	MG	X	2965	-	-	-	X

## 2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 84118 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1987	1235	399	350	3			

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			

- Molecule 4 is a protein called 50S ribosomal protein L5.

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

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L13.

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

- Molecule 7 is a protein called 50S ribosomal protein L14.

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

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	134	Total	C	N	O		0	0	0
			1011	619	206	186				

- Molecule 9 is a protein called 50S ribosomal protein L16.

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

- Molecule 10 is a protein called 50S ribosomal protein L17.

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

- Molecule 11 is a protein called 50S ribosomal protein L18.

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

- Molecule 12 is a protein called 50S ribosomal protein L19.

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

- Molecule 13 is a protein called 50S ribosomal protein L20.

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

- Molecule 14 is a protein called 50S ribosomal protein L21.

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

- Molecule 15 is a protein called 50S ribosomal protein L22,50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	P	130	Total	C	N	O	S		
			1038	655	205	176	2	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	110	VAL	-	linker	UNP Q9RXJ7
P	111	PRO	-	linker	UNP Q9RXJ7
P	112	ARG	-	linker	UNP Q9RXJ7

- Molecule 16 is a protein called 50S ribosomal protein L23.

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

- Molecule 17 is a protein called 50S ribosomal protein L24.

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

- Molecule 18 is a protein called 50S ribosomal protein L25.

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

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	T	74	Total	C	N	O	S		
			556	351	107	97	1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L28.

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

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- Molecule 22 is a protein called 50S ribosomal protein L30.

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

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	56	Total	C	N	O	S	0	0	0
			443	272	91	75	5			

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 27 is a RNA chain called 23S ribosomal RNA.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	2680	Total	C	N	O	P	0	0	0
			57533	25663	10626	18564	2680			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

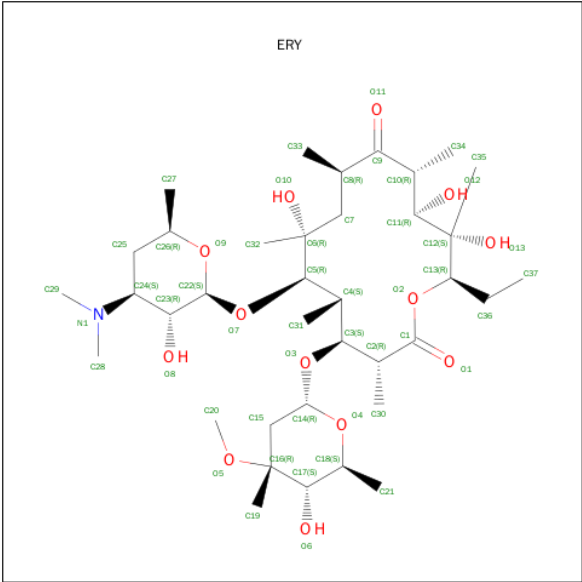
- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	122	Total	C	N	O	P	0	0	0
			2602	1161	476	843	122			

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	X	64	Total	Mg	0	0
			64	64		
29	B	1	Total	Mg	0	0
			1	1		
29	A	1	Total	Mg	0	0
			1	1		
29	K	2	Total	Mg	0	0
			2	2		
29	M	2	Total	Mg	0	0
			2	2		

- Molecule 30 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C<sub>37</sub>H<sub>67</sub>NO<sub>13</sub>).

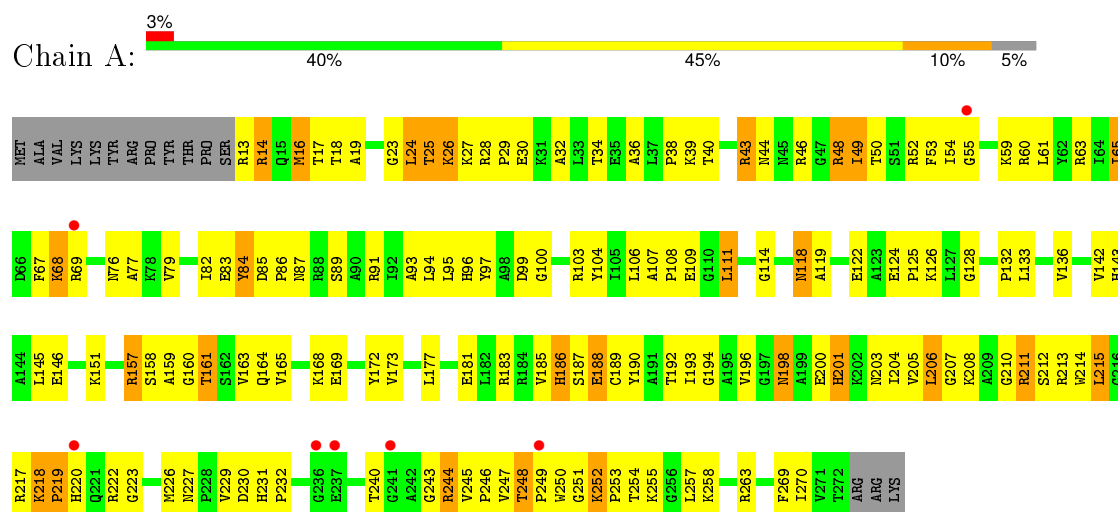


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	X	1	Total	C	N	O	0	0
			51	37	1	13		

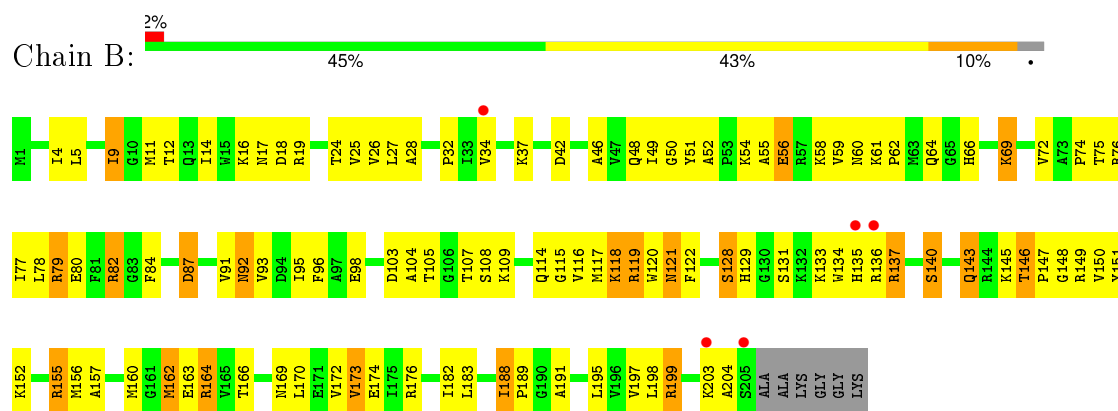
### 3 Residue-property plots

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.

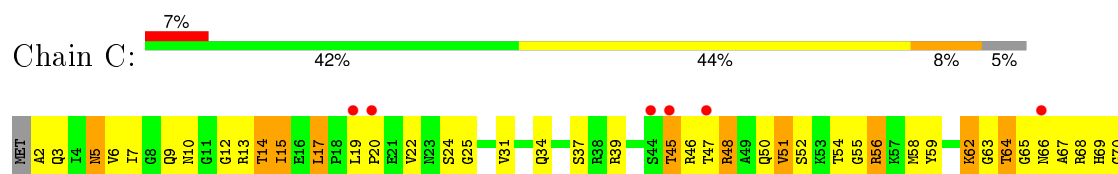
#### • Molecule 1: 50S ribosomal protein L2

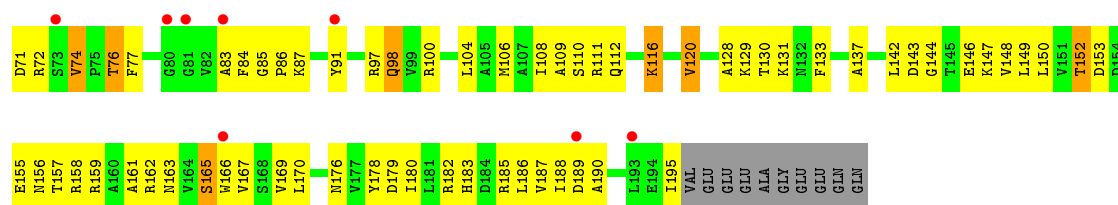


#### • Molecule 2: 50S ribosomal protein L3

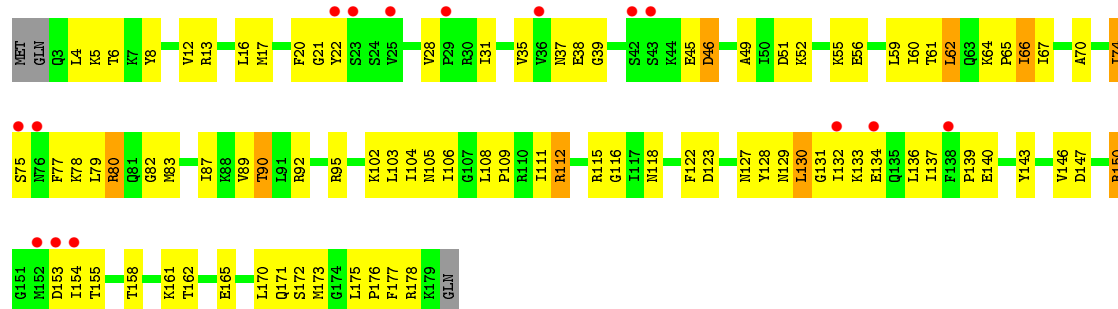


#### • Molecule 3: 50S ribosomal protein L4

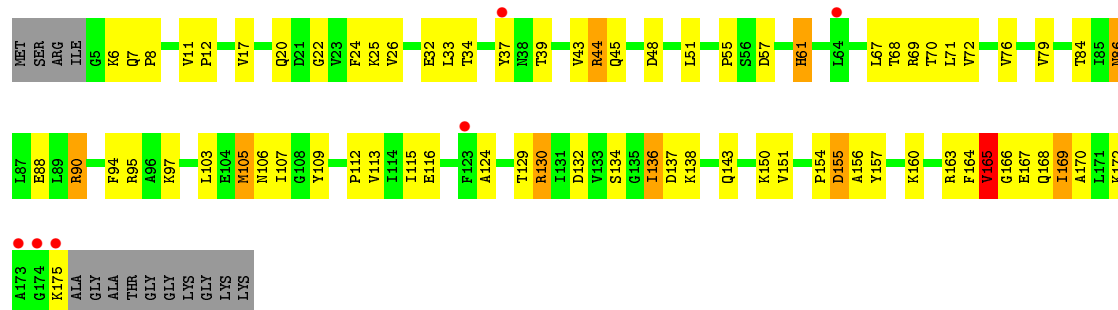




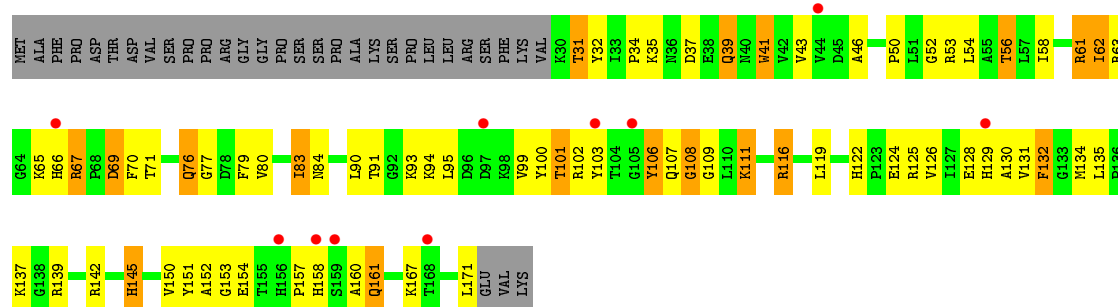
• Molecule 4: 50S ribosomal protein L5



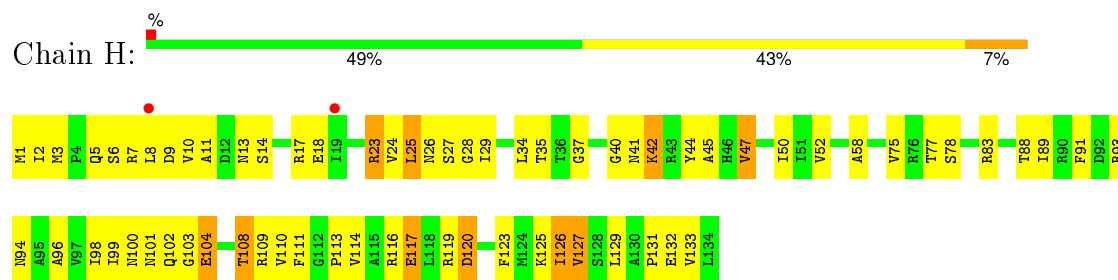
• Molecule 5: 50S ribosomal protein L6



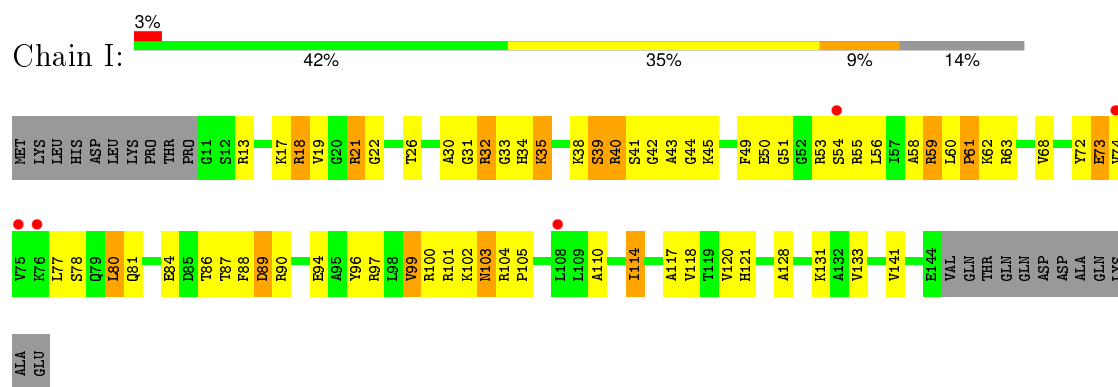
• Molecule 6: 50S ribosomal protein L13



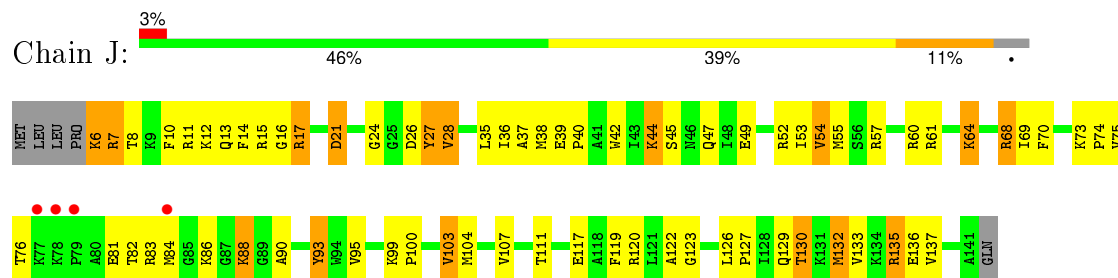
• Molecule 7: 50S ribosomal protein L14



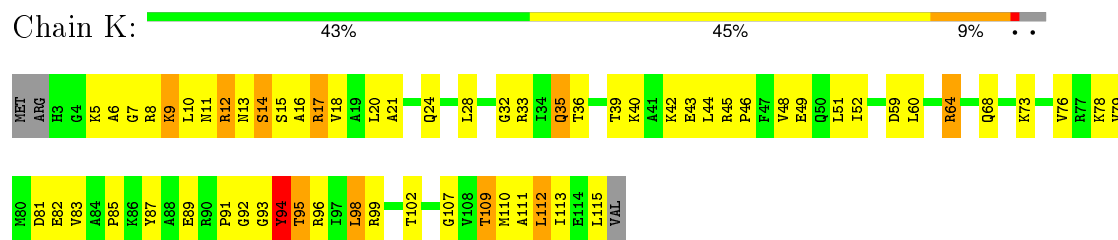
• Molecule 8: 50S ribosomal protein L15



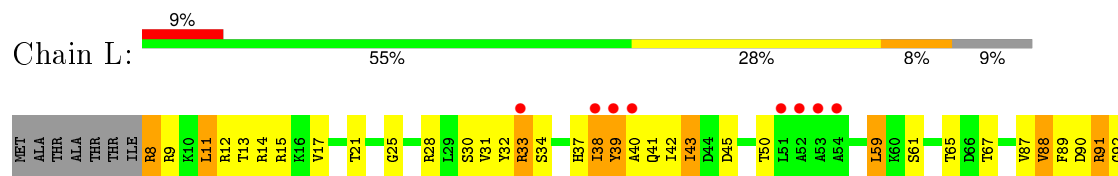
• Molecule 9: 50S ribosomal protein L16

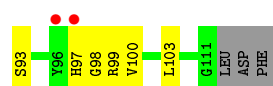


• Molecule 10: 50S ribosomal protein L17



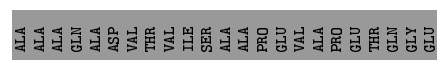
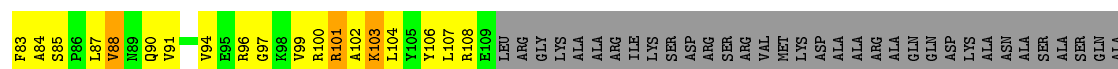
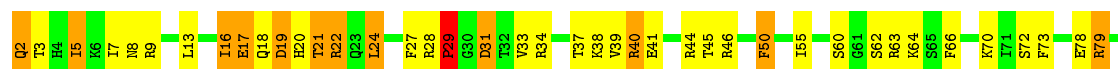
• Molecule 11: 50S ribosomal protein L18





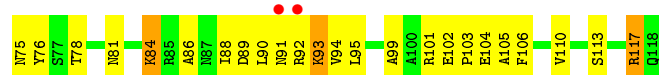
- Molecule 12: 50S ribosomal protein L19

Chain M: 29% 27% 9% 35%



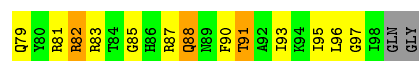
- Molecule 13: 50S ribosomal protein L20

Chain N: 2% 47% 44% 7%



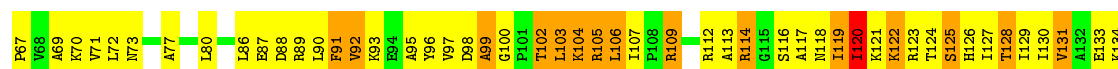
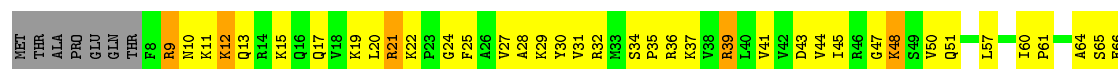
- Molecule 14: 50S ribosomal protein L21

Chain O: 4% 42% 45% 7% 6%

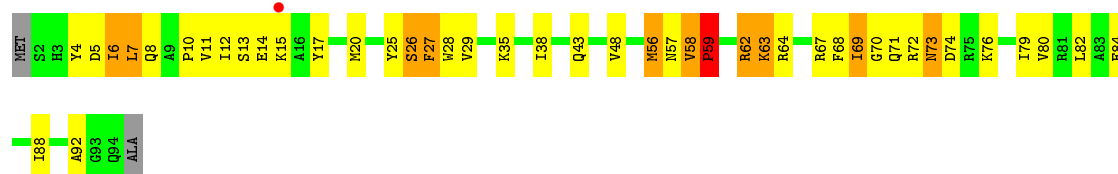


- Molecule 15: 50S ribosomal protein L22, 50S ribosomal protein L22

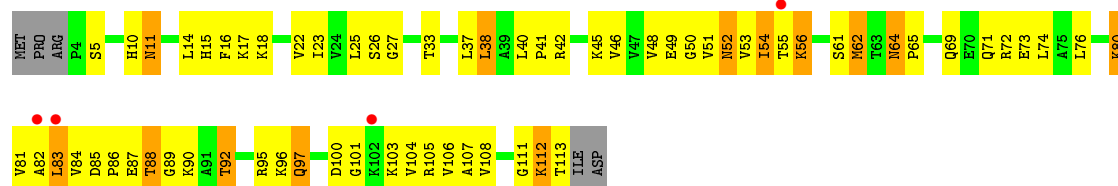
Chain P: 30% 50% 15% 5%



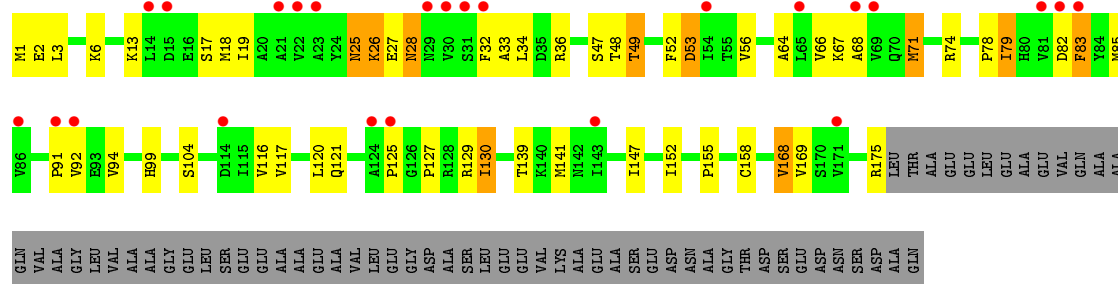
- Molecule 16: 50S ribosomal protein L23



• Molecule 17: 50S ribosomal protein L24



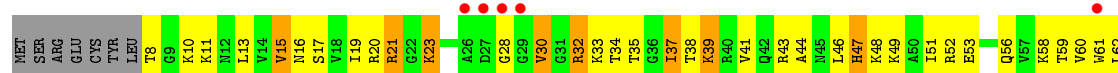
• Molecule 18: 50S ribosomal protein L25



• Molecule 19: 50S ribosomal protein L27



• Molecule 20: 50S ribosomal protein L28

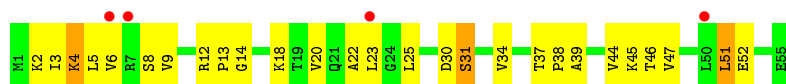




- Molecule 21: 50S ribosomal protein L29



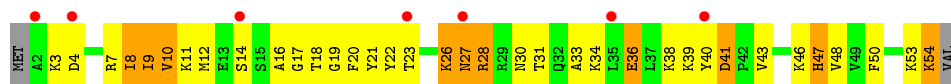
- Molecule 22: 50S ribosomal protein L30



- Molecule 23: 50S ribosomal protein L32



- Molecule 24: 50S ribosomal protein L33



- Molecule 25: 50S ribosomal protein L34



- Molecule 26: 50S ribosomal protein L35



- Molecule 27: 23S ribosomal RNA





G1058	G1059	G1060	G1061	G1062	A1065	G1066	G1067	G1068	G1069	G1070	U1071	U1072	G1073	G1074	U1080	A1081	G1082	G1083	G1084	G1085	C1086	C1087	A1088	C1089	C1090	C1091	A1096	A1097	A1098	A1099	U1101	G1102	C1103	G1104	U1105	A1106	A1107	U1108	A1109	G1110	C1113	G1121	A1122	G1123	U1124	C1120	G1127	G1128	A1057																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
C	A911	C914	C914	C914	A921	A922	C923	A924	C924	A928	A929	A930	A931	U1005	U1006	U1007	U1010	A1011	C1016	C1017	C1018	U1019	A1021	A1022	U1023	G1024	A1025	U1026	U1027	U1030	C1031	A1032	U1033	U1034	U1035	U1036	U1037	A1040	G1041	G1042	G1043	U1044	G1045	U1046	U1051	C1052	G1053	C1054	A1055	U1056	A1057																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
A833	A834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U852	U853	U854	U857	U858	U859	U860	C863	C864	A865	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134	U1135	U1136	U1137	U1138	U1139	U1140	U1141	U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	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	U1906	U1907	U1908	U1909	U1910	U1911	U1912	U1913	U1914	U1915	U1916	U1917	U1918	U1919	U1920	U1921	U1922	U1923	U1924	U1925	U1926	U1927	U1928	U1929	U1930	U1931	U1932	U1933	U1934	U1935	U1936	U1937	U1938	U1939	U1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.09Å 411.59Å 695.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.54 49.53 – 3.52	Depositor EDS
% Data completeness (in resolution range)	90.4 (19.99-3.54) 89.6 (49.53-3.52)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.234 , 0.282 0.243 , 0.291	Depositor DCC
$R_{free}$ test set	13480 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	100.0	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 13.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 268448 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	84118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.43	0/2025	0.70	0/2726
2	B	0.55	0/1567	0.76	0/2105
3	C	0.47	0/1504	0.72	1/2036 (0.0%)
4	D	0.29	0/1419	0.52	0/1903
5	E	0.29	0/1308	0.51	0/1771
6	G	0.47	0/1138	0.78	1/1539 (0.1%)
7	H	0.61	0/1007	0.80	0/1352
8	I	0.46	0/1022	0.76	0/1366
9	J	0.52	0/1113	0.75	0/1486
10	K	0.67	0/886	0.90	1/1188 (0.1%)
11	L	0.32	0/785	0.60	0/1048
12	M	0.61	0/884	0.87	1/1186 (0.1%)
13	N	0.45	0/994	0.68	0/1323
14	O	0.44	0/750	0.74	1/1000 (0.1%)
15	P	0.58	0/1052	0.79	1/1409 (0.1%)
16	Q	0.42	0/737	0.67	1/988 (0.1%)
17	R	0.45	0/835	0.72	0/1121
18	S	0.30	0/1370	0.53	0/1862
19	T	0.44	0/563	0.70	0/747
20	U	0.41	0/556	0.69	0/741
21	V	0.31	0/529	0.51	0/704
22	W	0.36	0/426	0.61	0/568
23	Z	0.52	0/455	0.87	0/611
24	1	0.47	0/438	0.74	0/583
25	2	0.46	0/387	0.79	1/509 (0.2%)
26	3	0.53	0/468	0.85	0/614
27	X	0.63	3/64429 (0.0%)	1.22	424/100499 (0.4%)
28	Y	0.44	1/2908 (0.0%)	0.96	1/4529 (0.0%)
All	All	0.58	4/91555 (0.0%)	1.11	433/137514 (0.3%)

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
2	B	0	1
6	G	0	1
7	H	0	1
8	I	0	3
10	K	0	2
16	Q	0	1
17	R	0	1
19	T	0	1
20	U	0	1
23	Z	0	1
25	2	0	1
26	3	0	1
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	2	C	OP3-P	-10.49	1.48	1.61
27	X	1	G	OP3-P	-10.37	1.48	1.61
27	X	1981	A	N3-C4	-5.23	1.31	1.34
27	X	774	A	N3-C4	5.08	1.37	1.34

The worst 5 of 433 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	1468	A	C8-N9-C4	-12.74	100.70	105.80
27	X	1746	A	O5'-P-OP1	-12.19	94.73	105.70
27	X	1670	G	C8-N9-C4	11.14	110.86	106.40
27	X	537	C	C6-N1-C2	-10.97	115.91	120.30
27	X	774	A	N7-C8-N9	10.55	119.08	113.80

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	146	THR	Peptide
6	G	108	GLY	Peptide
7	H	26	ASN	Peptide
8	I	35	LYS	Peptide

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Mol	Chain	Res	Type	Group
8	I	40	ARG	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1987	0	2056	145	0
2	B	1539	0	1600	109	0
3	C	1481	0	1504	99	0
4	D	1400	0	1481	55	0
5	E	1286	0	1336	54	0
6	G	1114	0	1144	73	0
7	H	997	0	1046	56	0
8	I	1011	0	1047	72	0
9	J	1090	0	1125	64	0
10	K	878	0	930	45	0
11	L	779	0	820	36	0
12	M	871	0	894	61	0
13	N	978	0	1020	52	0
14	O	741	0	756	51	0
15	P	1038	0	1125	85	0
16	Q	726	0	753	32	0
17	R	825	0	881	52	0
18	S	1345	0	1372	37	0
19	T	556	0	579	30	0
20	U	552	0	604	35	0
21	V	525	0	546	19	0
22	W	424	0	470	16	0
23	Z	443	0	444	26	0
24	1	431	0	456	29	0
25	2	383	0	414	26	0
26	3	462	0	506	53	0
27	X	57533	0	28987	1351	0
28	Y	2602	0	1327	61	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	K	2	0	0	0	0
29	M	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	X	64	0	0	0	0
30	X	51	0	67	9	0
All	All	84118	0	55290	2473	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 2473 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:VAL:HG22	2:B:136:ARG:HG3	1.32	1.11
23:Z:19:ARG:NH2	27:X:1277:G:OP1	1.90	1.04
13:N:66:ASN:HB3	13:N:76:TYR:HB2	1.46	0.97
27:X:854:G:H1	27:X:948:C:H42	1.04	0.96
7:H:40:GLY:HA3	27:X:2545:A:H61	1.29	0.95

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	
1	A	258/275 (94%)	221 (86%)	34 (13%)	3 (1%)	16	61
2	B	203/211 (96%)	178 (88%)	24 (12%)	1 (0%)	34	77
3	C	192/205 (94%)	164 (85%)	26 (14%)	2 (1%)	19	65
4	D	175/180 (97%)	155 (89%)	19 (11%)	1 (1%)	30	74
5	E	169/185 (91%)	157 (93%)	11 (6%)	1 (1%)	30	74
6	G	140/174 (80%)	127 (91%)	13 (9%)	0	100	100
7	H	132/134 (98%)	120 (91%)	11 (8%)	1 (1%)	24	69
8	I	132/156 (85%)	102 (77%)	26 (20%)	4 (3%)	5	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	134/141 (95%)	113 (84%)	21 (16%)	0	100	100
10	K	111/116 (96%)	102 (92%)	8 (7%)	1 (1%)	21	67
11	L	102/114 (90%)	86 (84%)	16 (16%)	0	100	100
12	M	106/165 (64%)	99 (93%)	6 (6%)	1 (1%)	21	67
13	N	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	11	53
14	O	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
15	P	128/137 (93%)	109 (85%)	15 (12%)	4 (3%)	5	41
16	Q	91/95 (96%)	76 (84%)	12 (13%)	3 (3%)	5	39
17	R	108/115 (94%)	91 (84%)	16 (15%)	1 (1%)	21	67
18	S	173/237 (73%)	154 (89%)	19 (11%)	0	100	100
19	T	72/91 (79%)	62 (86%)	9 (12%)	1 (1%)	14	57
20	U	70/81 (86%)	52 (74%)	14 (20%)	4 (6%)	2	24
21	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
22	W	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
23	Z	54/60 (90%)	48 (89%)	6 (11%)	0	100	100
24	1	51/55 (93%)	38 (74%)	10 (20%)	3 (6%)	2	23
25	2	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
26	3	57/65 (88%)	46 (81%)	10 (18%)	1 (2%)	11	52
All	All	3025/3379 (90%)	2632 (87%)	359 (12%)	34 (1%)	17	63

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	P	120	ILE
16	Q	6	ILE
16	Q	69	ILE
1	A	24	LEU
1	A	25	THR

### 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	
1	A	202/216 (94%)	163 (81%)	39 (19%)	2	11
2	B	155/157 (99%)	127 (82%)	28 (18%)	2	13
3	C	154/163 (94%)	131 (85%)	23 (15%)	4	22
4	D	153/156 (98%)	140 (92%)	13 (8%)	13	50
5	E	136/144 (94%)	115 (85%)	21 (15%)	3	21
6	G	118/146 (81%)	93 (79%)	25 (21%)	1	8
7	H	103/103 (100%)	88 (85%)	15 (15%)	4	23
8	I	101/121 (84%)	82 (81%)	19 (19%)	2	11
9	J	110/115 (96%)	87 (79%)	23 (21%)	1	9
10	K	90/93 (97%)	70 (78%)	20 (22%)	1	7
11	L	74/82 (90%)	57 (77%)	17 (23%)	1	6
12	M	94/133 (71%)	71 (76%)	23 (24%)	1	5
13	N	96/97 (99%)	81 (84%)	15 (16%)	3	20
14	O	75/79 (95%)	61 (81%)	14 (19%)	2	11
15	P	112/118 (95%)	87 (78%)	25 (22%)	1	7
16	Q	75/76 (99%)	61 (81%)	14 (19%)	2	11
17	R	91/96 (95%)	72 (79%)	19 (21%)	1	9
18	S	149/192 (78%)	135 (91%)	14 (9%)	11	45
19	T	55/67 (82%)	44 (80%)	11 (20%)	1	10
20	U	57/66 (86%)	45 (79%)	12 (21%)	1	9
21	V	53/55 (96%)	46 (87%)	7 (13%)	5	27
22	W	48/48 (100%)	39 (81%)	9 (19%)	2	11
23	Z	50/53 (94%)	44 (88%)	6 (12%)	6	31
24	1	46/48 (96%)	32 (70%)	14 (30%)	0	3
25	2	39/40 (98%)	28 (72%)	11 (28%)	0	3
26	3	46/51 (90%)	36 (78%)	10 (22%)	1	8
All	All	2482/2715 (91%)	2035 (82%)	447 (18%)	2	13

5 of 447 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	130	THR

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Mol	Chain	Res	Type
12	M	29	PRO
24	1	8	ILE
10	K	9	LYS
11	L	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	3	HIS
13	N	41	ASN
19	T	85	GLN
10	K	11	ASN
12	M	2	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	2673/2880 (92%)	638 (23%)	40 (1%)
28	Y	121/124 (97%)	29 (23%)	1 (0%)
All	All	2794/3004 (93%)	667 (23%)	41 (1%)

5 of 667 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	X	3	U
27	X	4	C
27	X	13	A
27	X	14	A
27	X	17	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	X	1391	A
27	X	1625	A
27	X	2756	A
27	X	1441	A
27	X	1496	G

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 71 ligands modelled in this entry, 70 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
30	ERY	X	2902	-	53,53,53	0.85	1 (1%)	82,82,82	1.29	10 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	ERY	X	2902	-	-	0/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	X	2902	ERY	C4-C3	-2.20	1.49	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	X	2902	ERY	O8-C23-C22	-2.72	103.96	110.01
30	X	2902	ERY	C2-C3-C4	-2.41	105.94	112.77
30	X	2902	ERY	C30-C2-C1	-2.26	103.83	109.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	X	2902	ERY	C13-O2-C1	-2.23	114.36	118.10
30	X	2902	ERY	C16-C15-C14	-2.17	111.25	115.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	X	2902	ERY	9	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	260/275 (94%)	0.07	7 (2%) 58 48	48, 104, 163, 221	0
2	B	205/211 (97%)	-0.28	5 (2%) 62 52	27, 50, 107, 233	0
3	C	194/205 (94%)	0.12	14 (7%) 18 14	39, 102, 180, 292	0
4	D	177/180 (98%)	0.28	15 (8%) 13 11	114, 175, 232, 282	0
5	E	171/185 (92%)	-0.18	6 (3%) 48 37	57, 131, 192, 243	0
6	G	142/174 (81%)	0.03	10 (7%) 19 15	38, 77, 160, 339	0
7	H	134/134 (100%)	-0.35	2 (1%) 76 68	33, 45, 87, 135	0
8	I	134/156 (85%)	0.27	5 (3%) 45 36	55, 126, 192, 315	0
9	J	136/141 (96%)	0.05	4 (2%) 55 45	56, 94, 163, 214	0
10	K	113/116 (97%)	-0.46	0 100 100	27, 32, 67, 100	0
11	L	104/114 (91%)	0.15	10 (9%) 10 9	130, 161, 200, 243	0
12	M	108/165 (65%)	-0.43	0 100 100	30, 43, 95, 242	0
13	N	117/118 (99%)	-0.15	2 (1%) 73 64	41, 76, 133, 232	0
14	O	94/100 (94%)	-0.21	4 (4%) 39 30	52, 94, 178, 204	0
15	P	130/137 (94%)	-0.37	0 100 100	33, 51, 147, 188	0
16	Q	93/95 (97%)	-0.35	1 (1%) 82 74	49, 94, 162, 192	0
17	R	110/115 (95%)	0.06	4 (3%) 46 37	65, 100, 189, 259	0
18	S	175/237 (73%)	0.55	24 (13%) 4 4	93, 144, 224, 285	0
19	T	74/91 (81%)	0.21	7 (9%) 10 9	72, 112, 158, 228	0
20	U	72/81 (88%)	0.49	5 (6%) 20 15	75, 119, 185, 238	0
21	V	65/67 (97%)	-0.19	2 (3%) 52 43	76, 115, 164, 208	0
22	W	55/55 (100%)	0.32	4 (7%) 18 14	72, 91, 128, 190	0
23	Z	56/60 (93%)	-0.39	0 100 100	32, 40, 80, 152	0
24	1	53/55 (96%)	0.59	7 (13%) 4 5	102, 129, 217, 266	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	2	46/47 (97%)	0.18	1 (2%) 65 55	38, 67, 122, 169	0
26	3	59/65 (90%)	0.45	5 (8%) 13 11	81, 100, 172, 278	0
27	X	2680/2880 (93%)	-0.14	88 (3%) 50 40	26, 76, 186, 299	0
28	Y	122/124 (98%)	-0.10	4 (3%) 50 40	74, 153, 190, 332	0
All	All	5879/6383 (92%)	-0.06	236 (4%) 42 33	26, 89, 188, 339	0

The worst 5 of 236 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	S	23	ALA	8.1
18	S	22	VAL	8.0
18	S	15	ASP	7.6
27	X	1072	U	7.4
27	X	731	A	6.9

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
29	MG	X	2957	1/1	0.94	0.82	88.73	52,52,52,52	0
29	MG	X	2903	1/1	0.95	0.67	34.47	30,30,30,30	0
29	MG	X	2961	1/1	0.93	1.06	30.91	56,56,56,56	0
29	MG	X	2916	1/1	0.93	0.88	29.58	41,41,41,41	0
29	MG	X	2965	1/1	0.91	0.91	24.90	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MG	X	2926	1/1	0.93	0.91	20.54	44,44,44,44	0
29	MG	X	2914	1/1	0.99	0.57	18.26	27,27,27,27	0
29	MG	X	2909	1/1	0.97	0.46	16.41	28,28,28,28	0
29	MG	X	2942	1/1	0.97	0.67	15.69	46,46,46,46	0
29	MG	K	202	1/1	0.76	0.82	10.86	27,27,27,27	0
29	MG	X	2910	1/1	0.96	0.62	10.67	56,56,56,56	0
29	MG	X	2922	1/1	0.97	0.35	10.03	29,29,29,29	0
29	MG	X	2944	1/1	0.97	0.40	8.85	35,35,35,35	0
29	MG	X	2939	1/1	0.93	0.62	8.75	50,50,50,50	0
29	MG	X	2959	1/1	0.97	0.66	8.48	41,41,41,41	0
29	MG	X	2954	1/1	0.97	0.45	8.37	45,45,45,45	0
29	MG	X	2913	1/1	0.96	0.47	6.57	43,43,43,43	0
29	MG	X	2923	1/1	0.94	0.39	6.22	40,40,40,40	0
29	MG	X	2947	1/1	0.96	0.26	2.58	34,34,34,34	0
29	MG	X	2948	1/1	0.96	0.29	2.26	34,34,34,34	0
29	MG	K	201	1/1	0.86	0.46	2.24	27,27,27,27	0
30	ERY	X	2902	51/51	0.94	0.24	0.92	31,34,36,36	0
29	MG	A	301	1/1	0.93	0.39	0.54	54,54,54,54	0
29	MG	X	2915	1/1	0.83	0.18	-0.69	63,63,63,63	0
29	MG	X	2929	1/1	0.98	0.13	-1.42	30,30,30,30	0
29	MG	X	2931	1/1	0.87	0.56	-	46,46,46,46	0
29	MG	X	2937	1/1	0.95	0.70	-	44,44,44,44	0
29	MG	X	2952	1/1	0.91	0.43	-	29,29,29,29	0
29	MG	X	2956	1/1	0.93	0.52	-	27,27,27,27	0
29	MG	X	2921	1/1	0.95	0.33	-	28,28,28,28	0
29	MG	B	301	1/1	0.80	0.77	-	34,34,34,34	0
29	MG	X	2960	1/1	0.92	0.32	-	61,61,61,61	0
29	MG	X	2949	1/1	0.98	0.44	-	42,42,42,42	0
29	MG	X	2924	1/1	0.99	0.23	-	38,38,38,38	0
29	MG	X	2936	1/1	0.96	0.65	-	45,45,45,45	0
29	MG	X	2911	1/1	0.91	0.53	-	56,56,56,56	0
29	MG	X	2938	1/1	0.98	0.79	-	31,31,31,31	0
29	MG	X	2927	1/1	0.95	0.35	-	29,29,29,29	0
29	MG	X	2904	1/1	0.95	0.55	-	32,32,32,32	0
29	MG	X	2920	1/1	0.96	0.45	-	52,52,52,52	0
29	MG	X	2932	1/1	0.98	0.40	-	37,37,37,37	0
29	MG	X	2901	1/1	0.94	0.39	-	69,69,69,69	0
29	MG	X	2946	1/1	0.91	0.19	-	46,46,46,46	0
29	MG	X	2943	1/1	0.93	0.97	-	42,42,42,42	0
29	MG	X	2906	1/1	0.85	0.85	-	28,28,28,28	0
29	MG	X	2962	1/1	0.94	0.13	-	69,69,69,69	0
29	MG	X	2945	1/1	0.97	0.14	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MG	X	2958	1/1	0.82	0.49	-	44,44,44,44	0
29	MG	X	2917	1/1	0.91	0.86	-	40,40,40,40	0
29	MG	X	2930	1/1	0.80	1.01	-	29,29,29,29	0
29	MG	X	2919	1/1	0.82	0.10	-	62,62,62,62	0
29	MG	X	2925	1/1	0.91	1.08	-	31,31,31,31	0
29	MG	X	2953	1/1	0.99	0.38	-	56,56,56,56	0
29	MG	M	201	1/1	0.97	0.36	-	35,35,35,35	0
29	MG	X	2912	1/1	0.96	0.14	-	27,27,27,27	0
29	MG	X	2940	1/1	0.98	0.37	-	36,36,36,36	0
29	MG	X	2934	1/1	0.95	0.26	-	29,29,29,29	0
29	MG	X	2907	1/1	0.90	0.78	-	28,28,28,28	0
29	MG	M	202	1/1	0.97	0.36	-	35,35,35,35	0
29	MG	X	2955	1/1	0.97	0.47	-	30,30,30,30	0
29	MG	X	2935	1/1	0.97	0.49	-	34,34,34,34	0
29	MG	X	2950	1/1	0.95	0.40	-	32,32,32,32	0
29	MG	X	2905	1/1	0.95	0.50	-	31,31,31,31	0
29	MG	X	2941	1/1	0.97	0.46	-	38,38,38,38	0
29	MG	X	2908	1/1	0.94	0.60	-	32,32,32,32	0
29	MG	X	2918	1/1	0.98	0.82	-	43,43,43,43	0
29	MG	X	2951	1/1	0.92	0.75	-	32,32,32,32	0
29	MG	X	2964	1/1	0.93	0.88	-	28,28,28,28	0
29	MG	X	2933	1/1	0.86	0.65	-	36,36,36,36	0
29	MG	X	2963	1/1	0.90	0.31	-	56,56,56,56	0
29	MG	X	2928	1/1	0.98	0.39	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.