



# wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 10:06 AM GMT

PDB ID : 3PIP  
Title : Crystal structure of the synergistic antibiotic pair lankamycin and lankacidin in complex with the large ribosomal subunit  
Authors : Belousoff, M.J.; Shapira, T.; Bashan, A.; Zimmerman, E.; Kinashi, H.; Rozenberg, H.; Yonath, A.  
Deposited on : 2010-11-07  
Resolution : 3.45 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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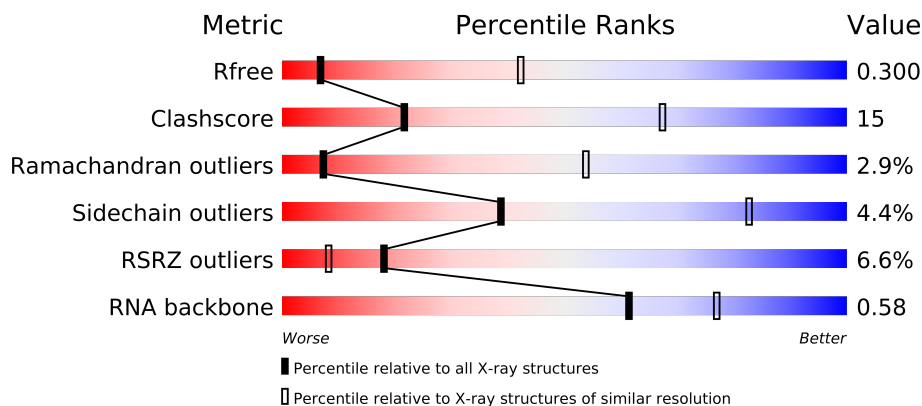
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	<b>FAILED</b>
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 3.45 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	1149 (3.62-3.30)
Clashscore	79885	1012 (3.60-3.32)
Ramachandran outliers	78287	1401 (3.62-3.30)
Sidechain outliers	78261	1401 (3.62-3.30)
RSRZ outliers	66119	1149 (3.62-3.30)
RNA backbone	1838	1004 (4.10-2.76)

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. 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	X	2880	
2	Y	123	
3	A	274	
4	B	211	
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	

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Mol	Chain	Length	Quality of chain
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	
30	4	37	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
31	LC2	X	2881	-	X
32	LMA	X	2882	-	X
33	MG	X	2883	-	X
33	MG	X	2884	-	X
33	MG	X	2885	-	X
33	MG	X	2886	-	X
33	MG	X	2887	-	X
33	MG	X	2888	-	X
33	MG	X	2890	-	X
33	MG	X	2891	-	X
33	MG	X	2892	-	X
33	MG	X	2893	-	X
33	MG	X	2894	-	X
33	MG	X	2895	-	X
33	MG	X	2898	-	X
33	MG	X	2899	-	X
33	MG	X	2900	-	X
33	MG	X	2901	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	MG	X	2903	-	X
33	MG	X	2904	-	X
33	MG	X	2905	-	X
33	MG	X	2906	-	X
33	MG	X	2907	-	X
33	MG	X	2908	-	X
33	MG	X	2910	-	X
33	MG	X	2911	-	X
33	MG	X	2913	-	X
33	MG	X	2914	-	X
33	MG	X	2915	-	X
33	MG	X	2917	-	X
33	MG	X	2918	-	X
33	MG	X	2919	-	X
33	MG	X	2920	-	X
33	MG	X	2922	-	X
33	MG	X	2925	-	X
33	MG	X	2926	-	X
33	MG	X	2927	-	X
33	MG	X	2929	-	X
33	MG	X	2931	-	X
33	MG	X	2932	-	X
33	MG	X	2933	-	X
33	MG	X	2934	-	X
33	MG	X	2935	-	X
33	MG	X	2937	-	X
33	MG	X	2938	-	X
33	MG	X	2939	-	X
33	MG	X	2942	-	X
33	MG	X	2948	-	X
33	MG	X	2949	-	X
33	MG	X	2950	-	X
33	MG	X	2951	-	X
33	MG	X	2952	-	X
33	MG	X	2953	-	X
34	K	X	2955	-	X
34	K	X	2956	-	X
34	K	X	2957	-	X
35	NA	X	2958	-	X
35	NA	X	2959	-	X
35	NA	X	2960	-	X
35	NA	X	2961	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	X	2962	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 83963 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 RIBOSOMAL 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2644	Total	C	N	O	P	0	0	0
			56750	25314	10473	18320	2643			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	253	Total	C	N	O	S	0	0	0
			1920	1196	382	340	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1394	889	244	254	7			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	63	Total	C	N	O	S	0	0	0
			451	280	82	86	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	134	Total	C	N	O	0	0	0
			1005	616	203	186			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	126	Total	C	N	O	S	0	0	0
			1004	633	197	172	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			714	452	130	130	2			

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

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

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



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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O		0	0	0
			537	334	110	93				

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

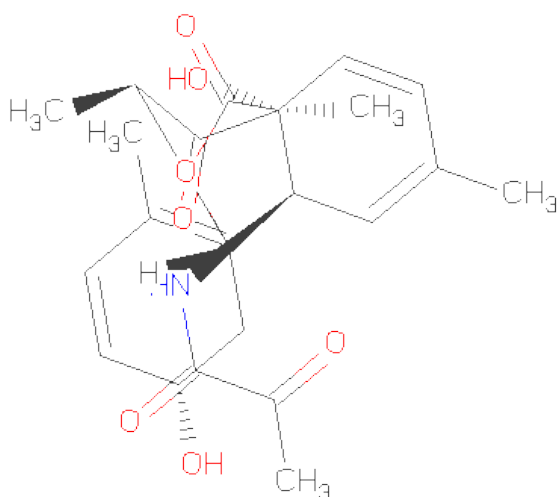
- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

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

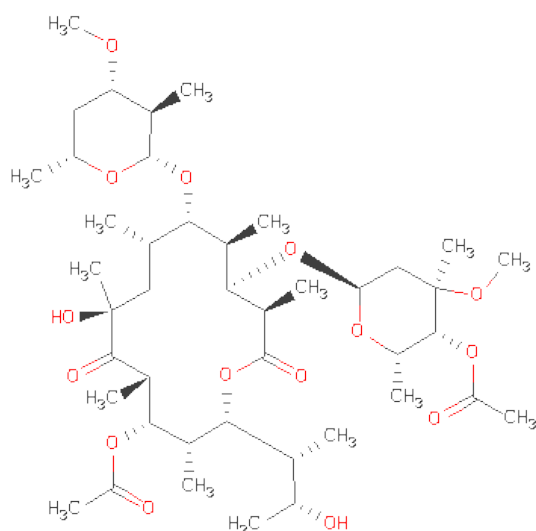
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	37	Total	C	N	O	S	0	0	0
			297	179	66	47	5			

- Molecule 31 is N-[(1S,2R,3E,5E,7S,9E,11E,13S,15R,19R)-7,13-DIHYDROXY-1,4,10,19-TE TRAMETHYL-17,18-DIOXO-16-OXABICYCLO[13.2.2]NONADECA-3,5,9,11-TETRAEN-2-YL]-2-OXOPROPANAMIDE (three-letter code: LC2) (formula: C<sub>25</sub>H<sub>33</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	X	1	Total	C	N	O	0	0
			33	25	1	7		

- Molecule 32 is LANKAMYCIN (three-letter code: LMA) (formula: C<sub>43</sub>H<sub>74</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	O	0	0
			58	43	15		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	71	Total	Mg	0	0
			71	71		
33	I	1	Total	Mg	0	0
			1	1		
33	U	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	X	4	Total	K	0	0
			4	4		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

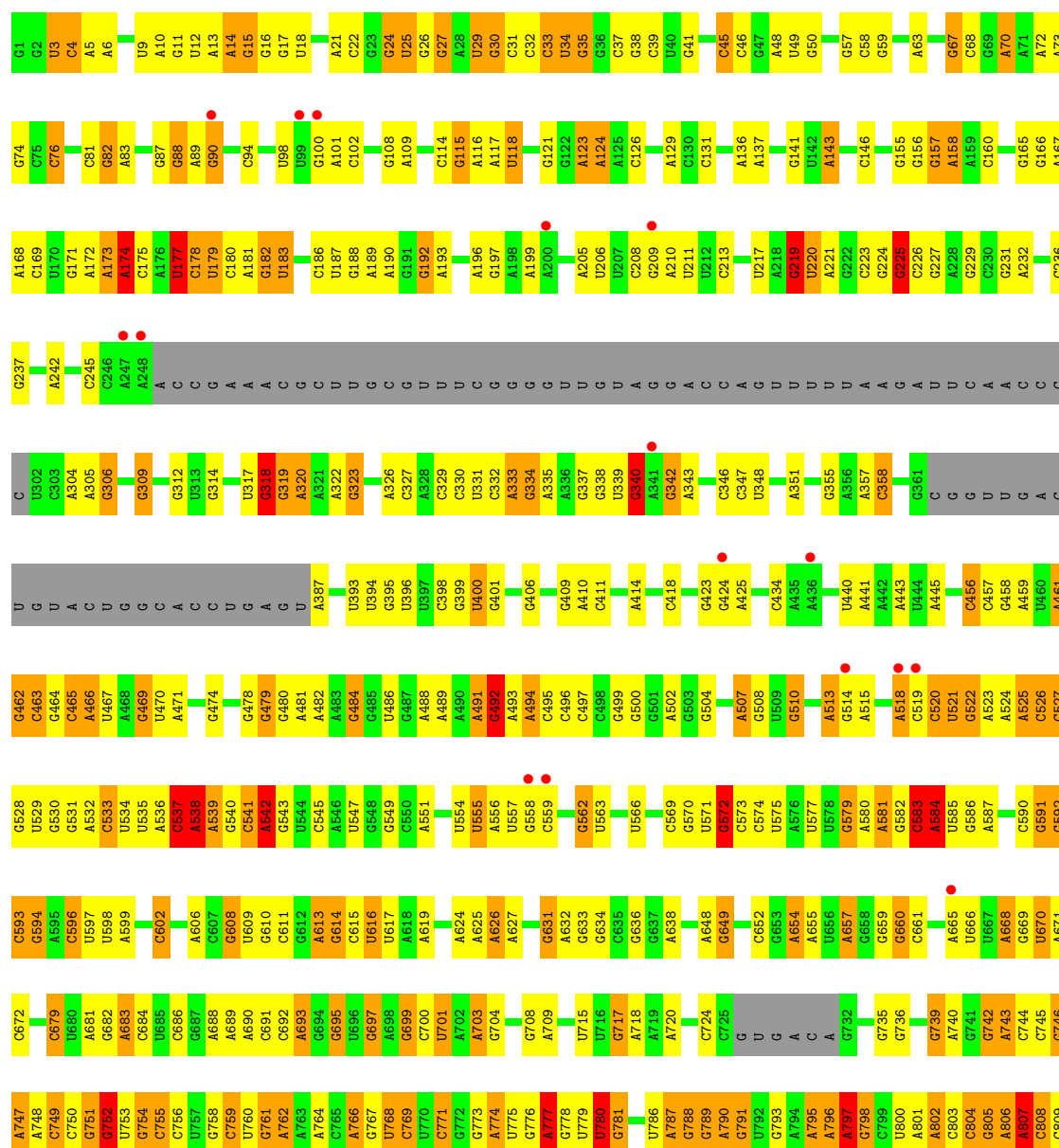
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	X	5	Total	Na	0	0
			5	5		

### 3 Residue-property plots

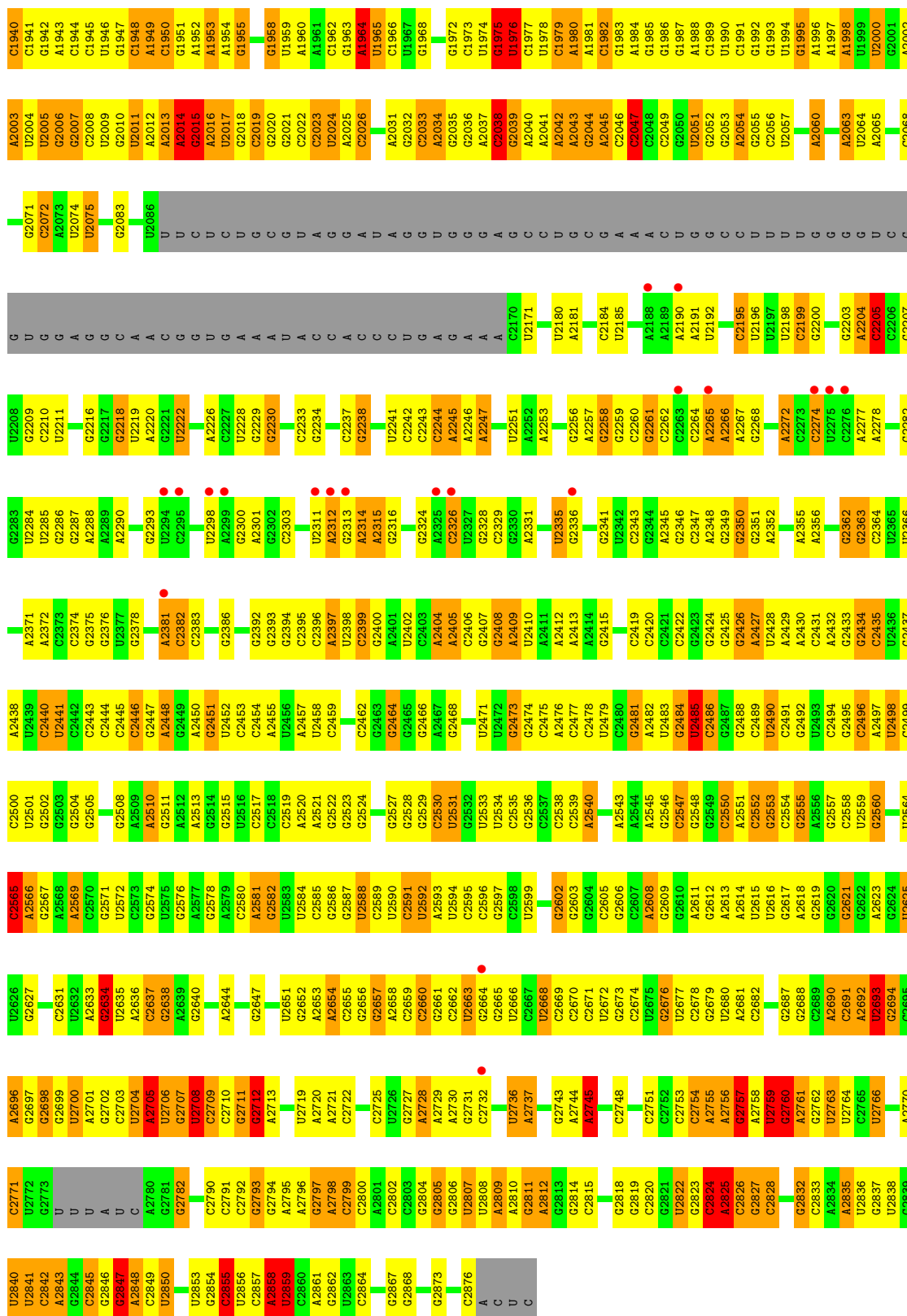
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

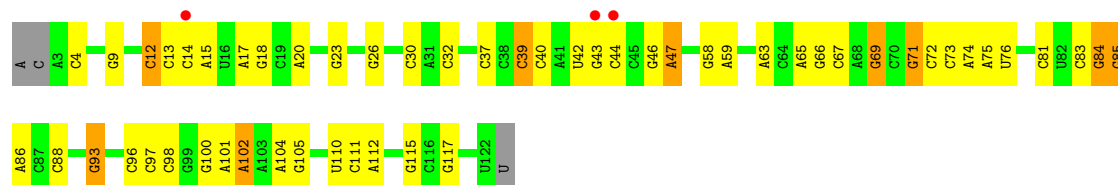
#### • Molecule 1: RIBOSOMAL 23S RNA

Chain X: 



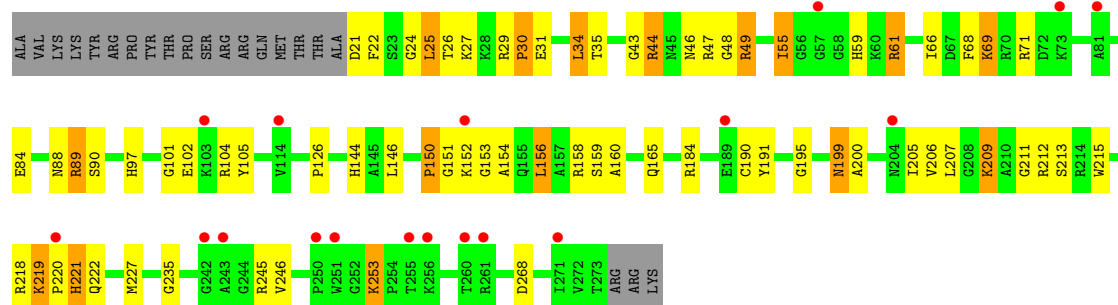
A1851	U1766	C1700	G1559	C1466	A1391	G1308	G1243	U1177	G1098	U1023	G953	A886	U810
G1852	G1767	C1701	G1562	U1467	U1392	G1309	G1246	C1178	A1099	G1028	U954	A886	G811
C1853	U1768	C1702	U1563	U1469	G1393	C1310	G1246	A1179	U1100	G1029	G955	G887	G812
A1867	U1769	C1703	U1564	U1470	G1394	C1311	G1249	A1180	U1101	U1030	A956	G888	A816
A1868	U1770	U1704	U1565	G1471	A1396	G1312	G1250	C1181	G1104	C1031	G957	C889	U816
	C1772	U1705	G1566	G1472	A1397	U1314	G1251	U1182		A1032	C959	U890	A817
G1874	U1773	U1706		U1473	A1398	A1315	C1252	C1183	U1108	G1033	U960	A	G818
	C1774	U1707	C1570	U1474	C1399	G1316	G1253	G		U1034	G961	G	C819
A1884	U1775	U1709	G1571	U1475	C1400	A1406	G1254	C		G1035	C962	G	
	A1776	U1710	C1572	G1476	A1407	G1317	G1255	G		G1036	C963	G	A821
G1888	U1777	C1711	U1573	U1477	A1408	A1318	U1256	A		U1037	A964	C	
G	U1778	G1713	A1574	U1478	U1409	G1324	C1257	C		U1038	G965	C	U824
G	C1779		C1575	G1479	G1407	U1325	G1258	C			A966	C	C825
C	A1780		G1576	U1480	U1408	U1326	A1259	G		G1041	G967	U	U826
C	A1781		G1577	U1481	U1409	C1327	A1260	A		U1044	C968	A	C827
C	C1781		U1578	U1482	U1410	C1328	U1261	G		U1045	U969	C	C828
U	A1782		U1579	U1488	C1411	G1329	G1262	U1194		U1046	C970	C	C829
U					C1412	U1330	G1263	U1195		U1047	A971	G	C830
A	U1789				U1413	G1331	C1264	G1196			C972	G	G831
A	C1790		A1582	G1488	G1419	G1332	G1265	U1197		U1051	U974	C	A832
A	C1791		A1583	U1490	G1420	G1333	G1266	C1198		G1052	U975	U	A833
C	C1792		G1584	G1494	U1421	A1334	A1267	U1199		G1053	U976	U	U834
U	A1793		A1585	G1496	U1426	A1335	U1268	G1200		C1054	C977	A	U835
U			A1586	C1497	U1426	G1336	G1269	G1201			C978	C	G836
A	C1801		U1592		U1426	G1337	C1270	U1202		A	C981	C	U837
A	A1802				U1426	G1338	C1271	U1203		U	C982		A838
C	G1806		U1601	C1506	G	G1341	G1272	G1204		G1058	A911		U839
C	A1807		G1602	C1514	G1428	U1342	G1273	G1205		A1059	C915		U840
U	A1808				U1429	U1343				G1060	U916		G841
U	G		A1605	U1521	G1430	C1343	U1276	G1209		A1061	U917		A842
C	U1733		C1606	C	U1431	G1344	G1277	C1210		G1062	A918		G843
U1909	G1735		A1607	A	G1432	G1345	G1278	G1211		G1063	U919		G844
A1910	C1736		C	C	A1433	C1346	G1279	U1212		C992	G920		U845
A1911	G1737		G1609	A	U1434		U1280	U1213		C993	A921		
G1912						G1351	A1281	C1214		G1064	A922		G849
	G1741		G1613	U1526	A1437		A1282	A1215		G1069	A923		U850
			C1614	G1527	G1438	A1355	C1283			G1070	C924		C851
G1916	G1744		C1615	C1528	G1439	G1356	G1284	G1220			U925		
C1917	C1745		C1616		U1440	U1357	A1285	C1152		G1074	C997		G858
G1918	U1746		G1617		A1441	C1358	U1286	A1154			C998		U859
A1919					C1442	G1359	A1287	G1222			A999		U860
A1920	G1747		G1536		C1442			G1223			G928		G861
A1921	U1748		G1621	U1539	G1443	C1364	A1288	A1224			A1001		A862
G1922	C1749		G1622	C1540	C1444	U1365	A1289	G1225			U1005		C863
U1923	A1750		C1623		A1445	A1366	A1290	A1226			C1006		C864
C1924	U1751		A1624	G1543	U1446		A1291	A1227			U1007		
	U1752		A1625	G1544	U1447	G1371	A1292	C1229			C937		
	A1753		A1626	U1545	A1448		A1293				C938		
G1928	G1754		C1627	G1546	G1449	A1378	U1294	C1229			C939		C870
U1929	U1755		C1628		U1450	A1379	U1295				U1010		U871
C1930	C1756		G1629	U1546	C1451	U1379	G1296	U1232			A1011		G872
			A1630	C1549	U1452	C1380	G1297	A1233			A1012		U873
G1931	C1758		C1631	C1550	U1453	G1381	U1298	C1234			U943		A874
G1932	U1759		A1632	U1551	C1456	G1382	A1299	C1235			A944		G875
G1933	G1760		C1633	C1552	A1457	C1383	A1300	C1236			C1016		G876
U1934	U1761		A1634	G1553	U1458	G1384		G1237			C1017		G877
A1935	C1762		G1635	U1554	U1459			U1238			C1018		C878
A1936	U1763		G1636	A1555	U1460	U1304	U1304	A1239			U1019		A879
G1937	C1841		U1637	A1556	G1460	C1387	U1305	G1240			A1020		G899
U1938	U1843		G1638		U1465	G1388	U1306	G1241			A1096		G950
U1939	C1765						U1307	A1242			A1097		A884





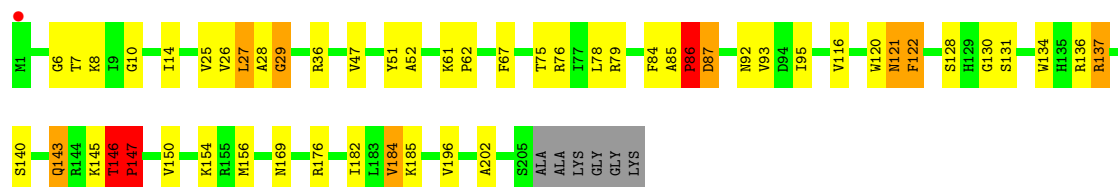
• Molecule 3: 50S ribosomal protein L2

Chain A:



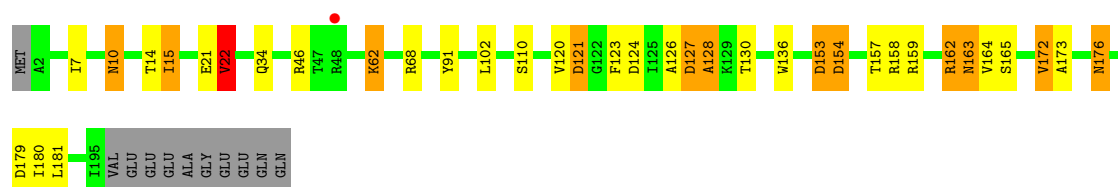
• Molecule 4: 50S ribosomal protein L3

Chain B:



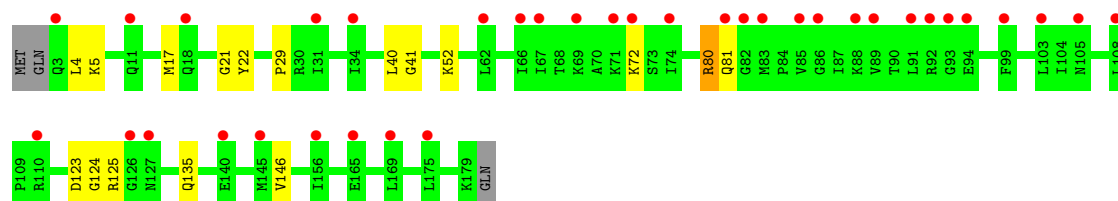
• Molecule 5: 50S ribosomal protein L4

Chain C:



• Molecule 6: 50S ribosomal protein L5

Chain D:



• Molecule 7: 50S ribosomal protein L6

Chain E:







- Molecule 14: 50S ribosomal protein L18

Chain L:



- Molecule 15: 50S ribosomal protein L19

Chain M:



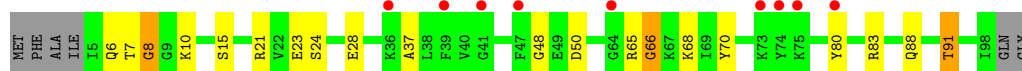
- Molecule 16: 50S ribosomal protein L20

Chain N:



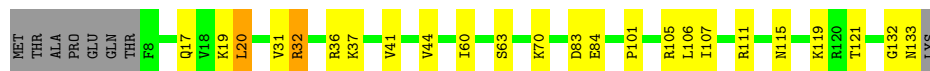
- Molecule 17: 50S ribosomal protein L21

Chain O:



- Molecule 18: 50S ribosomal protein L22

Chain P:



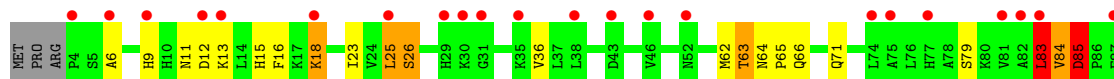
- Molecule 19: 50S ribosomal protein L23

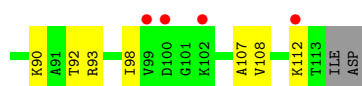
Chain Q:



- Molecule 20: 50S ribosomal protein L24

Chain R:





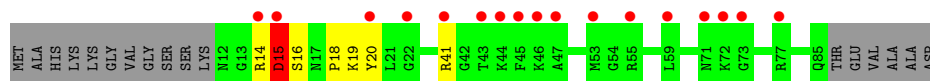
- Molecule 21: 50S ribosomal protein L25

Chain S:



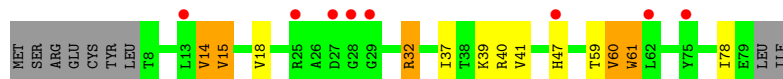
- Molecule 22: 50S ribosomal protein L27

Chain T:



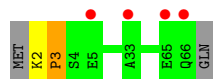
- Molecule 23: 50S ribosomal protein L28

Chain U:



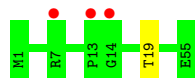
- Molecule 24: 50S ribosomal protein L29

Chain V:



- Molecule 25: 50S ribosomal protein L30

Chain W:



- Molecule 26: 50S ribosomal protein L32

Chain Z:

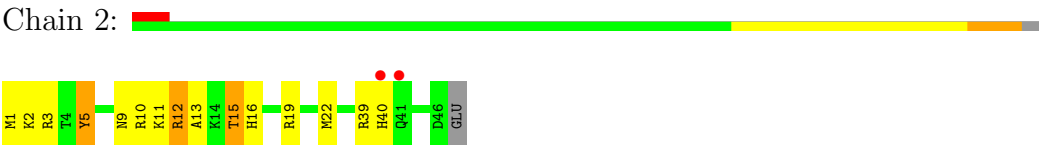


- Molecule 27: 50S ribosomal protein L33

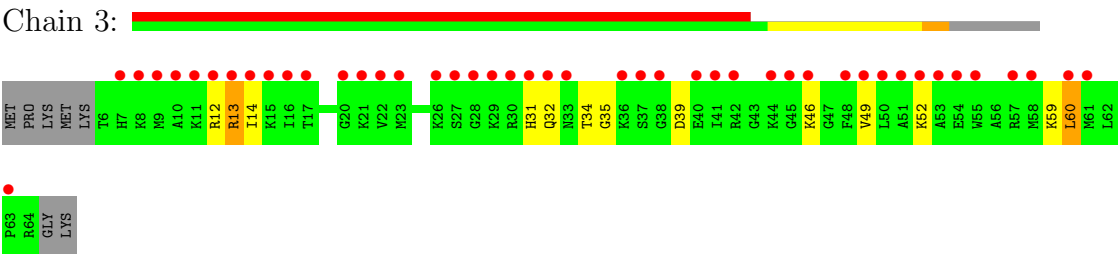
Chain 1:



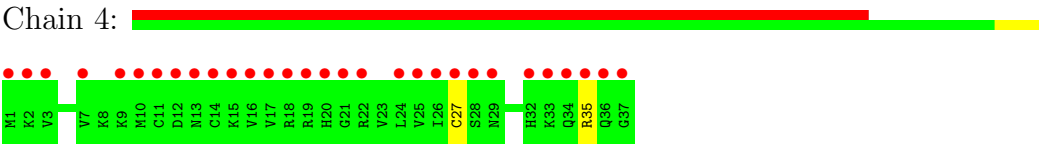
● Molecule 28: 50S ribosomal protein L34



● Molecule 29: 50S ribosomal protein L35



● Molecule 30: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.72Å 408.56Å 693.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.45 93.01 – 3.44	Depositor EDS
% Data completeness (in resolution range)	83.3 (20.00-3.45) 82.4 (93.01-3.44)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.41Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4.486)	Depositor
R, $R_{free}$	0.257 , 0.301 0.261 , 0.300	Depositor DCC
$R_{free}$ test set	2645 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.0	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 262327 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	83963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: NA, K, LC2, MG, LMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	X	1.17	260/63542 (0.4%)	1.58	1813/99100 (1.8%)
2	Y	0.80	1/2863 (0.0%)	1.13	21/4461 (0.5%)
3	A	0.65	0/1958	0.83	2/2638 (0.1%)
4	B	0.85	0/1567	0.93	2/2105 (0.1%)
5	C	0.84	0/1504	0.84	1/2036 (0.0%)
6	D	0.46	0/1413	0.56	0/1896
7	E	0.57	0/1308	0.60	0/1771
8	F	0.37	0/455	0.45	0/611
9	G	0.75	0/1138	0.82	0/1539
10	H	0.94	0/1007	0.99	0/1352
11	I	0.62	0/1016	0.71	0/1359
12	J	0.80	0/1113	0.80	0/1486
13	K	0.93	1/886 (0.1%)	1.01	0/1188
14	L	0.72	0/785	0.93	1/1048 (0.1%)
15	M	0.99	0/884	1.07	1/1186 (0.1%)
16	N	0.93	0/994	0.85	0/1323
17	O	0.77	0/750	0.81	0/1000
18	P	1.01	2/1017 (0.2%)	0.97	1/1362 (0.1%)
19	Q	0.66	0/725	0.69	0/974
20	R	0.66	0/835	0.72	1/1121 (0.1%)
21	S	0.51	0/1370	0.60	1/1862 (0.1%)
22	T	0.74	0/563	0.77	0/747
23	U	0.57	0/541	0.70	1/723 (0.1%)
24	V	0.67	0/529	0.63	0/704
25	W	0.60	0/426	0.71	0/568
26	Z	0.89	0/464	0.94	1/622 (0.2%)
27	1	0.32	0/438	0.60	0/583
28	2	0.57	0/387	0.54	0/509
29	3	0.22	0/468	0.38	0/614
30	4	0.69	1/298 (0.3%)	0.58	0/390
All	All	1.06	265/91244 (0.3%)	1.42	1846/136878 (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
7	E	0	4
8	F	0	3
9	G	0	8
10	H	0	2
11	I	0	1
12	J	0	1
All	All	0	19

The worst 5 of 265 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	616	U	C3'-C2'	-13.53	1.37	1.52
1	X	1775	A	O3'-P	-11.52	1.47	1.61
1	X	1299	A	N9-C4	-11.34	1.31	1.37
1	X	1260	A	N9-C4	-11.21	1.31	1.37
1	X	2669	C	N1-C6	-10.57	1.30	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	29	ARG	C-N-CD	-19.10	78.58	120.60
1	X	1678	G	N1-C6-O6	-18.90	108.56	119.90
1	X	2486	C	C5-C6-N1	17.23	129.62	121.00
1	X	2815	C	C6-N1-C2	17.04	127.12	120.30
14	L	54	ALA	CB-CA-C	16.51	134.87	110.10

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	E	125	VAL	Peptide
7	E	130	ARG	Sidechain
7	E	165	VAL	Peptide
7	E	174	GLY	Peptide
8	F	116	ASN	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	X	56750	0	0	826	3
2	Y	2561	0	0	25	0
3	A	1920	0	0	70	0
4	B	1539	0	0	54	0
5	C	1481	0	0	34	0
6	D	1394	0	0	11	0
7	E	1286	0	0	5	0
8	F	451	0	0	6	0
9	G	1114	0	0	32	0
10	H	997	0	0	25	0
11	I	1005	0	0	23	0
12	J	1090	0	0	26	0
13	K	878	0	0	25	0
14	L	779	0	0	23	0
15	M	871	0	0	15	3
16	N	978	0	0	24	0
17	O	741	0	0	16	0
18	P	1004	0	0	17	0
19	Q	714	0	0	8	0
20	R	825	0	0	24	0
21	S	1345	0	0	8	0
22	T	556	0	0	10	0
23	U	537	0	0	7	0
24	V	525	0	0	2	0
25	W	424	0	0	1	0
26	Z	452	0	0	10	0
27	1	431	0	0	28	0
28	2	383	0	0	15	0
29	3	462	0	0	10	0
30	4	297	0	0	1	0
31	X	33	0	0	7	0
32	X	58	0	69	37	0
33	I	1	0	0	0	0
33	U	1	0	0	0	0
33	X	71	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	X	4	0	0	0	0
35	X	5	0	0	0	0
All	All	83963	0	69	1250	3

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 15.

The worst 5 of 1250 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:699:G:N2	28:2:5:TYR:CE1	1.89	1.39
3:A:66:ILE:CG2	3:A:68:PHE:CZ	2.19	1.24
1:X:2662:C:O2	10:H:82:LYS:NZ	1.71	1.22
1:X:2045:A:C6	32:X:2882:LMA:H27A	1.75	1.21
1:X:1391:A:N7	1:X:1393:G:C6	2.10	1.20

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1552:C:O2	15:M:43:ASN:ND2[8_455]	0.99	1.21
1:X:1552:C:O2	15:M:43:ASN:CG[8_455]	1.93	0.27
1:X:1552:C:C2	15:M:43:ASN:ND2[8_455]	2.03	0.17

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	251/274 (92%)	207 (82%)	36 (14%)	8 (3%)	6	51
4	B	203/211 (96%)	174 (86%)	22 (11%)	7 (3%)	6	49
5	C	192/205 (94%)	153 (80%)	30 (16%)	9 (5%)	4	37
6	D	175/180 (97%)	146 (83%)	27 (15%)	2 (1%)	21	76
7	E	169/185 (91%)	147 (87%)	18 (11%)	4 (2%)	9	58
8	F	61/144 (42%)	51 (84%)	9 (15%)	1 (2%)	14	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	G	140/174 (80%)	118 (84%)	18 (13%)	4 (3%)	7	54
10	H	132/134 (98%)	115 (87%)	17 (13%)	0	100	100
11	I	132/156 (85%)	96 (73%)	29 (22%)	7 (5%)	3	33
12	J	134/141 (95%)	107 (80%)	25 (19%)	2 (2%)	15	68
13	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	25	79
14	L	102/114 (90%)	81 (79%)	20 (20%)	1 (1%)	22	78
15	M	106/166 (64%)	94 (89%)	9 (8%)	3 (3%)	8	54
16	N	115/118 (98%)	106 (92%)	7 (6%)	2 (2%)	14	66
17	O	92/100 (92%)	77 (84%)	12 (13%)	3 (3%)	6	50
18	P	124/134 (92%)	109 (88%)	13 (10%)	2 (2%)	14	67
19	Q	91/95 (96%)	66 (72%)	20 (22%)	5 (6%)	3	32
20	R	108/115 (94%)	82 (76%)	20 (18%)	6 (6%)	3	31
21	S	173/237 (73%)	140 (81%)	28 (16%)	5 (3%)	7	54
22	T	72/91 (79%)	57 (79%)	12 (17%)	3 (4%)	4	41
23	U	70/81 (86%)	44 (63%)	21 (30%)	5 (7%)	2	24
24	V	63/67 (94%)	58 (92%)	4 (6%)	1 (2%)	14	67
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
26	Z	55/60 (92%)	42 (76%)	12 (22%)	1 (2%)	13	65
27	1	51/55 (93%)	31 (61%)	15 (29%)	5 (10%)	1	14
28	2	44/47 (94%)	37 (84%)	7 (16%)	0	100	100
29	3	57/66 (86%)	37 (65%)	18 (32%)	2 (4%)	6	49
30	4	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3111/3558 (87%)	2556 (82%)	466 (15%)	89 (3%)	7	54

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	221	HIS
4	B	86	PRO
4	B	122	PHE
4	B	137	ARG
4	B	147	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	194/215 (90%)	180 (93%)	14 (7%)	21	66
4	B	155/157 (99%)	147 (95%)	8 (5%)	32	78
5	C	154/163 (94%)	146 (95%)	8 (5%)	32	78
6	D	152/156 (97%)	151 (99%)	1 (1%)	91	97
7	E	136/144 (94%)	135 (99%)	1 (1%)	91	97
8	F	46/107 (43%)	46 (100%)	0	100	100
9	G	118/146 (81%)	111 (94%)	7 (6%)	28	74
10	H	103/103 (100%)	100 (97%)	3 (3%)	55	90
11	I	100/121 (83%)	93 (93%)	7 (7%)	21	67
12	J	110/115 (96%)	106 (96%)	4 (4%)	47	86
13	K	90/93 (97%)	85 (94%)	5 (6%)	30	76
14	L	74/82 (90%)	70 (95%)	4 (5%)	31	77
15	M	94/134 (70%)	90 (96%)	4 (4%)	40	83
16	N	96/97 (99%)	94 (98%)	2 (2%)	66	93
17	O	75/79 (95%)	73 (97%)	2 (3%)	57	90
18	P	108/115 (94%)	107 (99%)	1 (1%)	87	97
19	Q	73/76 (96%)	69 (94%)	4 (6%)	30	76
20	R	91/96 (95%)	83 (91%)	8 (9%)	14	55
21	S	149/192 (78%)	146 (98%)	3 (2%)	68	93
22	T	55/67 (82%)	54 (98%)	1 (2%)	71	93
23	U	54/66 (82%)	51 (94%)	3 (6%)	30	76
24	V	53/55 (96%)	53 (100%)	0	100	100
25	W	48/48 (100%)	48 (100%)	0	100	100
26	Z	51/53 (96%)	50 (98%)	1 (2%)	68	93
27	1	46/48 (96%)	36 (78%)	10 (22%)	1	8
28	2	39/40 (98%)	34 (87%)	5 (13%)	6	32
29	3	46/52 (88%)	41 (89%)	5 (11%)	9	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	4	35/35 (100%)	35 (100%)	0	100	100
All	All	2545/2855 (89%)	2434 (96%)	111 (4%)	39	83

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	103	VAL
15	M	5	ILE
28	2	9	ASN
12	J	135	ARG
13	K	54	THR

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	X	2630/2880 (91%)	470 (17%)	73 (2%)
2	Y	119/123 (96%)	22 (18%)	0
All	All	2749/3003 (91%)	492 (17%)	73 (2%)

5 of 492 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	14	A
1	X	34	U
1	X	35	G
1	X	39	C

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1324	G
1	X	1496	G
1	X	2736	U
1	X	1441	A
1	X	1607	A

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

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 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, 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	X	2644/2880 (91%)	-0.05	74 (2%) 50 22	44, 115, 240, 575	0
2	Y	120/123 (97%)	-0.28	3 (2%) 54 24	108, 183, 252, 342	0
3	A	253/274 (92%)	0.53	18 (7%) 16 7	66, 158, 225, 423	0
4	B	205/211 (97%)	0.08	1 (0%) 88 63	35, 85, 159, 249	0
5	C	194/205 (94%)	-0.16	1 (0%) 88 63	61, 142, 250, 381	0
6	D	177/180 (98%)	1.17	36 (20%) 1 2	174, 255, 358, 427	0
7	E	171/185 (92%)	0.07	4 (2%) 57 26	87, 183, 269, 354	0
8	F	63/144 (43%)	3.20	46 (73%) 0 0	208, 334, 476, 516	0
9	G	142/174 (81%)	0.38	8 (5%) 24 10	73, 126, 257, 421	0
10	H	134/134 (100%)	-0.21	0 100 100	39, 71, 135, 248	0
11	I	134/156 (85%)	0.39	5 (3%) 39 16	75, 168, 261, 375	0
12	J	136/141 (96%)	0.50	8 (5%) 22 9	76, 135, 223, 388	0
13	K	113/116 (97%)	-0.03	0 100 100	32, 61, 101, 128	0
14	L	104/114 (91%)	0.01	4 (3%) 38 16	134, 193, 300, 325	0
15	M	108/166 (65%)	-0.15	0 100 100	32, 73, 138, 298	0
16	N	117/118 (99%)	0.21	1 (0%) 81 49	57, 116, 177, 328	0
17	O	94/100 (94%)	0.53	9 (9%) 8 5	82, 145, 271, 322	0
18	P	126/134 (94%)	-0.13	0 100 100	33, 84, 149, 226	0
19	Q	93/95 (97%)	0.81	13 (13%) 3 3	86, 134, 245, 329	0
20	R	110/115 (95%)	1.20	26 (23%) 1 2	93, 166, 332, 423	0
21	S	175/237 (73%)	0.19	9 (5%) 27 11	130, 202, 285, 326	0
22	T	74/91 (81%)	1.19	17 (22%) 1 2	112, 141, 201, 284	0
23	U	72/81 (88%)	0.81	8 (11%) 6 4	119, 188, 304, 349	0
24	V	65/67 (97%)	0.21	4 (6%) 20 9	116, 175, 235, 292	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	55/55 (100%)	0.54	3 (5%) 24 10	97, 126, 181, 194	0
26	Z	57/60 (95%)	-0.23	0 100 100	44, 79, 182, 234	0
27	1	53/55 (96%)	1.79	21 (39%) 1 1	126, 192, 295, 403	0
28	2	46/47 (97%)	0.35	2 (4%) 34 14	72, 123, 258, 308	0
29	3	59/66 (89%)	2.93	45 (76%) 0 0	139, 213, 356, 435	0
30	4	37/37 (100%)	3.71	30 (81%) 0 0	152, 219, 307, 382	0
All	All	5931/6561 (90%)	0.23	396 (6%) 18 8	32, 131, 276, 575	0

The worst 5 of 396 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	28	GLY	12.7
8	F	94	ALA	8.5
30	4	24	LEU	8.4
30	4	15	LYS	8.3
8	F	99	LEU	8.1

## 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
33	MG	X	2942	1/1	0.62	178.20	77,77,77,77	0
35	NA	X	2962	1/1	1.08	88.65	98,98,98,98	0
33	MG	X	2886	1/1	1.10	88.06	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	X	2927	1/1	0.70	35.50	65,65,65,65	0
33	MG	X	2914	1/1	0.46	34.82	74,74,74,74	0
33	MG	X	2905	1/1	0.67	34.00	50,50,50,50	0
33	MG	X	2949	1/1	0.48	32.29	83,83,83,83	0
33	MG	X	2948	1/1	0.75	29.49	110,110,110,110	0
33	MG	X	2884	1/1	0.97	28.38	72,72,72,72	0
33	MG	X	2903	1/1	0.54	22.45	65,65,65,65	0
33	MG	X	2899	1/1	0.53	21.55	41,41,41,41	0
33	MG	X	2893	1/1	0.42	19.64	66,66,66,66	0
33	MG	X	2951	1/1	0.47	17.88	142,142,142,142	0
33	MG	X	2938	1/1	0.58	17.35	62,62,62,62	0
34	K	X	2957	1/1	0.56	16.64	82,82,82,82	0
33	MG	X	2925	1/1	0.58	16.19	80,80,80,80	0
33	MG	X	2898	1/1	0.37	15.98	19,19,19,19	0
33	MG	X	2931	1/1	0.66	15.22	72,72,72,72	0
33	MG	X	2883	1/1	0.53	15.16	23,23,23,23	0
33	MG	X	2937	1/1	0.45	13.91	109,109,109,109	0
33	MG	X	2913	1/1	0.39	13.89	63,63,63,63	0
33	MG	X	2933	1/1	0.34	13.58	83,83,83,83	0
33	MG	X	2908	1/1	0.65	13.54	80,80,80,80	0
33	MG	X	2885	1/1	0.49	12.47	68,68,68,68	0
33	MG	X	2934	1/1	0.38	12.15	56,56,56,56	0
35	NA	X	2958	1/1	0.53	11.95	48,48,48,48	0
33	MG	X	2888	1/1	0.53	11.24	51,51,51,51	0
34	K	X	2956	1/1	0.38	9.73	146,146,146,146	0
33	MG	X	2929	1/1	0.69	9.35	61,61,61,61	0
33	MG	X	2904	1/1	0.43	8.48	64,64,64,64	0
35	NA	X	2961	1/1	0.39	8.36	75,75,75,75	0
33	MG	X	2918	1/1	0.49	8.23	84,84,84,84	0
33	MG	X	2906	1/1	0.37	7.65	52,52,52,52	0
34	K	X	2955	1/1	0.19	7.56	113,113,113,113	0
33	MG	X	2939	1/1	0.52	7.22	54,54,54,54	0
33	MG	X	2920	1/1	0.37	7.07	100,100,100,100	0
33	MG	X	2917	1/1	0.26	6.74	104,104,104,104	0
33	MG	X	2895	1/1	0.28	6.58	26,26,26,26	0
32	LMA	X	2882	58/58	0.39	6.10	120,120,120,120	0
33	MG	X	2910	1/1	0.30	5.89	44,44,44,44	0
33	MG	X	2894	1/1	0.45	5.85	65,65,65,65	0
35	NA	X	2960	1/1	0.44	5.73	86,86,86,86	0
33	MG	X	2950	1/1	0.31	5.55	36,36,36,36	0
35	NA	X	2959	1/1	0.35	5.42	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	X	2891	1/1	0.31	5.25	50,50,50,50	0
33	MG	X	2911	1/1	0.63	5.02	124,124,124,124	0
33	MG	X	2919	1/1	0.37	4.80	65,65,65,65	0
33	MG	X	2922	1/1	0.33	4.69	53,53,53,53	0
33	MG	X	2887	1/1	0.39	4.58	35,35,35,35	0
33	MG	X	2932	1/1	0.35	4.51	62,62,62,62	0
33	MG	X	2900	1/1	0.61	4.35	42,42,42,42	0
33	MG	X	2953	1/1	0.41	4.04	53,53,53,53	0
33	MG	X	2907	1/1	0.26	3.92	46,46,46,46	0
33	MG	X	2901	1/1	0.34	3.22	19,19,19,19	0
33	MG	X	2915	1/1	0.46	3.08	67,67,67,67	0
31	LC2	X	2881	33/33	0.32	3.05	49,106,118,122	0
33	MG	X	2935	1/1	0.24	2.73	36,36,36,36	0
33	MG	X	2926	1/1	0.41	2.57	67,67,67,67	0
33	MG	X	2892	1/1	0.28	2.54	71,71,71,71	0
33	MG	X	2890	1/1	0.36	2.17	59,59,59,59	0
33	MG	X	2952	1/1	0.30	2.02	59,59,59,59	0
33	MG	X	2940	1/1	0.30	1.90	71,71,71,71	0
33	MG	U	82	1/1	0.38	1.49	72,72,72,72	0
33	MG	X	2928	1/1	0.31	1.30	29,29,29,29	0
33	MG	X	2941	1/1	0.20	0.92	71,71,71,71	0
33	MG	X	2902	1/1	0.17	0.75	89,89,89,89	0
33	MG	X	2944	1/1	0.24	0.68	77,77,77,77	0
33	MG	X	2896	1/1	0.26	0.49	24,24,24,24	0
33	MG	X	2889	1/1	0.25	0.47	61,61,61,61	0
33	MG	X	2924	1/1	0.14	0.34	51,51,51,51	0
33	MG	X	2936	1/1	0.23	0.27	55,55,55,55	0
34	K	X	2954	1/1	0.23	0.27	70,70,70,70	0
33	MG	I	157	1/1	0.46	0.19	67,67,67,67	0
33	MG	X	2921	1/1	0.18	-0.01	61,61,61,61	0
33	MG	X	2916	1/1	0.19	-0.28	44,44,44,44	0
33	MG	X	2923	1/1	0.17	-0.48	97,97,97,97	0
33	MG	X	2912	1/1	0.18	-0.49	62,62,62,62	0
33	MG	X	2930	1/1	0.20	-0.59	77,77,77,77	0
33	MG	X	2943	1/1	0.19	-0.83	43,43,43,43	0
33	MG	X	2897	1/1	0.16	-0.93	79,79,79,79	0
33	MG	X	2945	1/1	0.12	-1.35	67,67,67,67	0
33	MG	X	2946	1/1	0.15	-1.45	123,123,123,123	0
33	MG	X	2947	1/1	0.11	-2.26	56,56,56,56	0
33	MG	X	2909	1/1	0.15	-2.74	58,58,58,58	0



## 6.5 Other polymers ⓘ

There are no such residues in this entry.