



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:32 PM UTC

PDB ID : 3CCM / pdb_00003ccm
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2611U
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

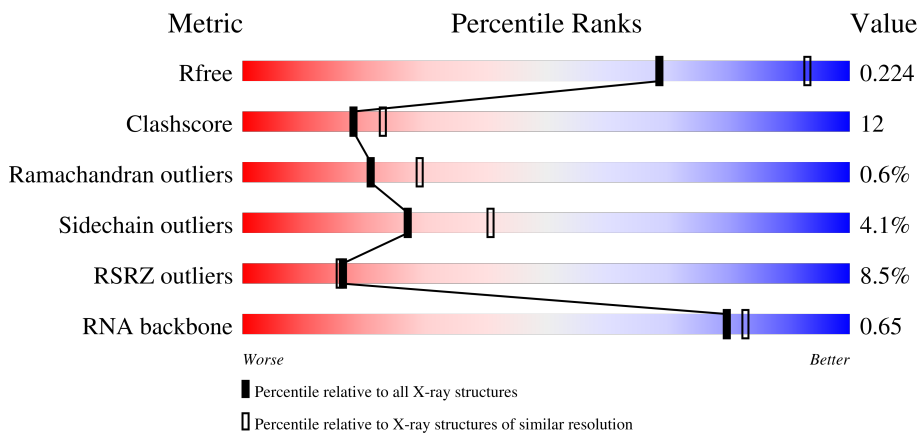
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

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

Mol	Chain	Length	Quality of chain
1	A	240	8% (Poor fit) 74% (0 outliers) 19% (1 outlier) 6% (2 outliers)
2	B	338	6% (Poor fit) 65% (0 outliers) 30% (1 outlier)
3	C	246	4% (Poor fit) 70% (0 outliers) 26% (1 outlier)
4	D	177	53% (Poor fit) 51% (0 outliers) 24% (1 outlier) 21% (Not modelled)

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Mol	Chain	Length	Quality of chain
5	E	178	11% 70% 25% ..
6	F	120	21% 72% 28% .
7	G	348	3% 6% 92% .
8	H	177	9% 69% 20% 10% .
9	I	162	39% 32% 10% 57% .
10	J	145	5% 74% 22% ..
11	K	132	% 73% 23% .
12	L	165	18% 62% 23% 12% .
13	M	196	12% 74% 23% ..
14	N	187	19% 65% 30% ..
15	O	116	4% 76% 19% ..
16	P	149	2% 80% 16% .
17	Q	96	3% 78% 17% ..
18	R	155	% 74% 20% ..
19	S	85	5% 80% 15% 5%
20	T	120	6% 69% 28% ..
21	U	67	3% 51% 27% 21% .
22	V	71	21% 65% 24% 8% .
23	W	154	% 68% 30% .
24	X	92	11% 62% 23% 11% .
25	Y	241	2% 42% 15% 41% .
26	Z	116	17% 42% 20% 37% .
27	1	57	68% 30% .
28	2	50	18% 58% 34% 8% .
29	3	92	4% 82% 16% .

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8518	-	-	-	X
35	NA	0	8562	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99119 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 L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	237	1753	1072	352	324	5	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	337	2625	1616	493	511	5	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	246	1860	1130	345	384	1	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	140	1094	685	195	210	4	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	172	1357	840	224	289	4	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	119	890	551	141	197	1	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	29	240	149	39	51	1	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	160	1282	798	240	238	6	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	70	519	323	81	114	1	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	142	1120	696	199	222	3	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	132	994	609	189	192	4	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	L	145	1118	670	222	226	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	194	1558	943	333	281	1	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	186	1445	895	262	286	2	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	O	115	865	529	161	175	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
16	P	143	1136	683	229	224	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	Q	95	735	450	141	144	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	R	150	1149	713	209	223	4	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	81	641	389	111	138	3	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
20	T	119	950	568	180	202	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O	0	0	0
			1130	686	228	216			

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59017	26348	10870	19054	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	0	87	Total	Mg	0	0
			87	87		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	J	3	Total Cl 3 3	0	0
33	L	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	0	10	Total Cl 10 10	0	0

- Molecule 34 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	3	Total Sr 3 3	0	0
34	B	1	Total Sr 1 1	0	0
34	F	1	Total Sr 1 1	0	0
34	R	1	Total Sr 1 1	0	0
34	S	1	Total Sr 1 1	0	0
34	1	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	0	94	Total Sr 94 94	0	0
34	9	3	Total Sr 3 3	0	0

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	T	1	Total Na 1 1	0	0
35	0	66	Total Na 66 66	0	0
35	9	2	Total Na 2 2	0	0

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Cd 1 1	0	0
36	U	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	3	1	Total Cd 1 1	0	0

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	117	Total O 117 117	0	0
38	B	139	Total O 139 139	0	0
38	C	165	Total O 165 165	0	0
38	D	48	Total O 48 48	0	0
38	E	49	Total O 49 49	0	0
38	F	25	Total O 25 25	0	0
38	G	18	Total O 18 18	0	0
38	H	71	Total O 71 71	0	0
38	I	8	Total O 8 8	0	0
38	J	55	Total O 55 55	0	0
38	K	55	Total O 55 55	0	0
38	L	79	Total O 79 79	0	0
38	M	138	Total O 138 138	0	0
38	N	58	Total O 58 58	0	0
38	O	40	Total O 40 40	0	0
38	P	61	Total O 61 61	0	0
38	Q	49	Total O 49 49	0	0
38	R	78	Total O 78 78	0	0
38	S	32	Total O 32 32	0	0
38	T	36	Total O 36 36	0	0
38	U	28	Total O 28 28	0	0
38	V	13	Total O 13 13	0	0

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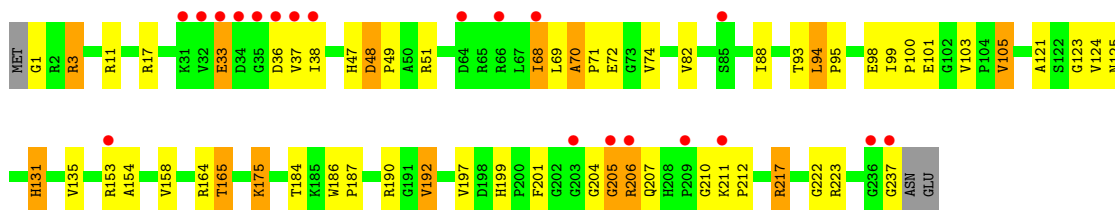
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	W	68	Total O 68 68	0	0
38	X	24	Total O 24 24	0	0
38	Y	97	Total O 97 97	0	0
38	Z	29	Total O 29 29	0	0
38	1	51	Total O 51 51	0	0
38	2	37	Total O 37 37	0	0
38	3	72	Total O 72 72	0	0
38	0	5938	Total O 5938 5938	0	0
38	9	145	Total O 145 145	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

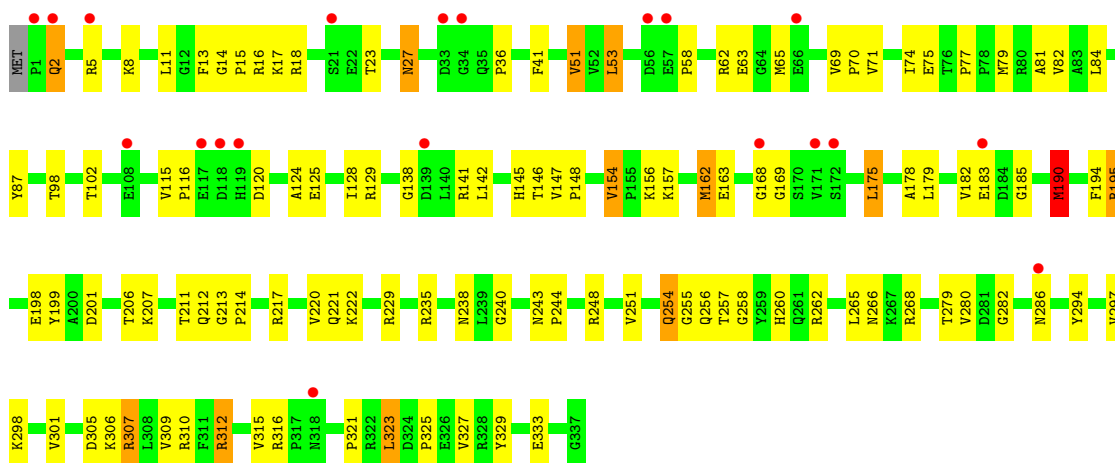
- Molecule 1: 50S ribosomal protein L2P

Chain A: 



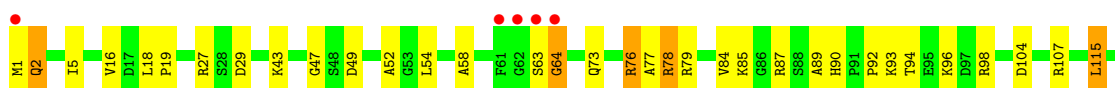
- Molecule 2: 50S ribosomal protein L3P

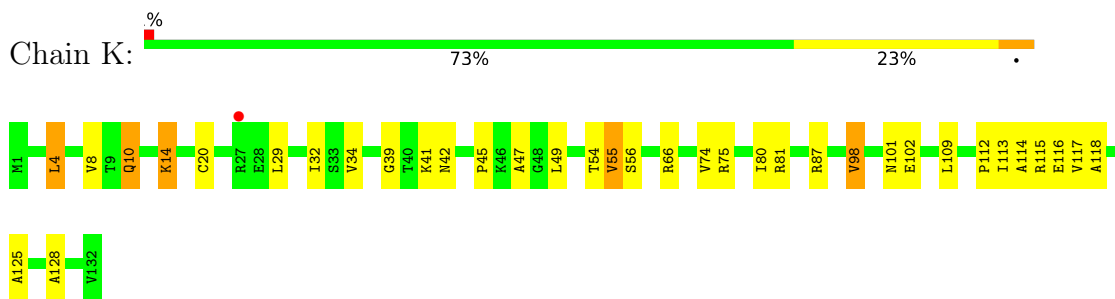
Chain B: 



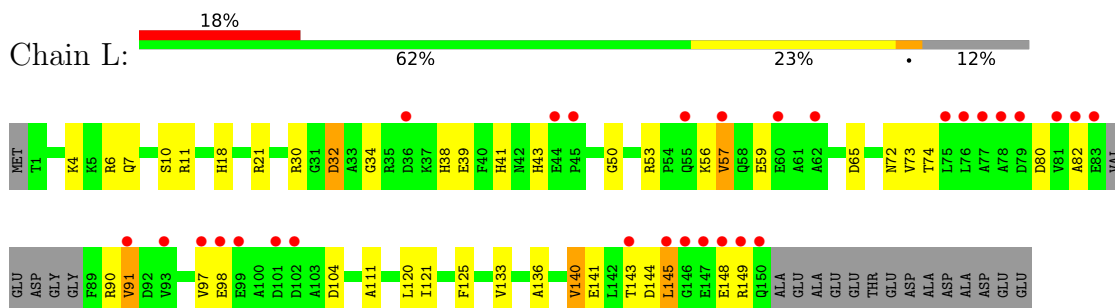
- Molecule 3: 50S ribosomal protein L4P

Chain C: 

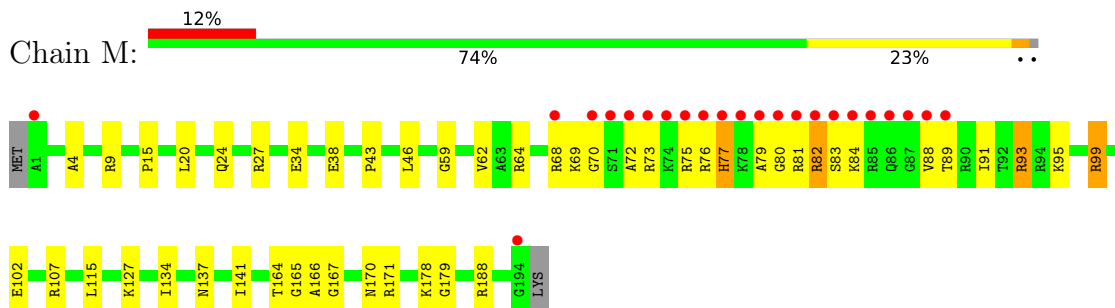




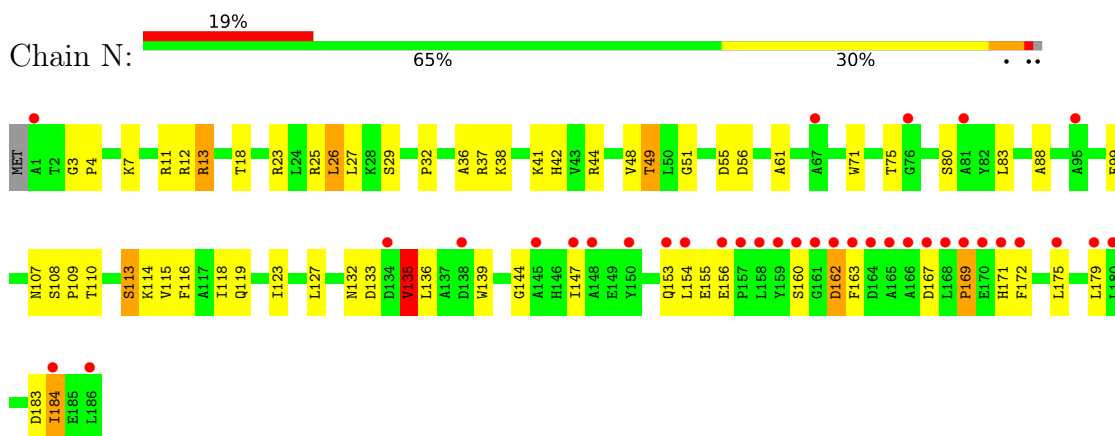
- Molecule 12: 50S ribosomal protein L15P



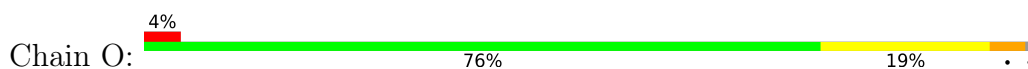
- Molecule 13: 50S ribosomal protein L15e



- Molecule 14: 50S ribosomal protein L18P

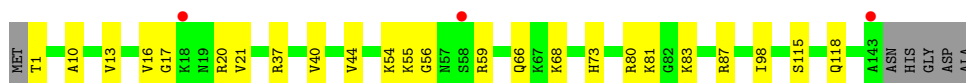
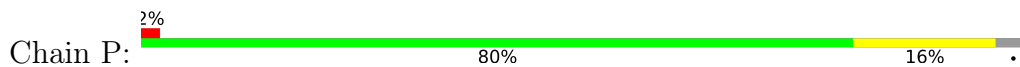


- Molecule 15: 50S ribosomal protein L18e

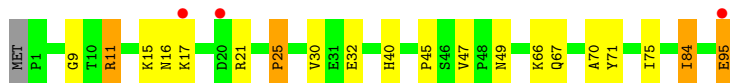
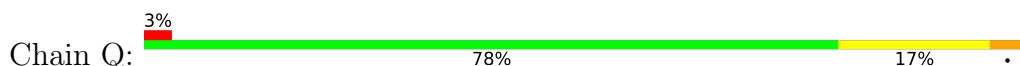




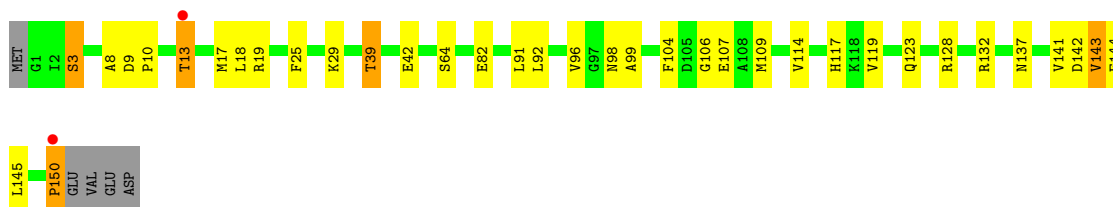
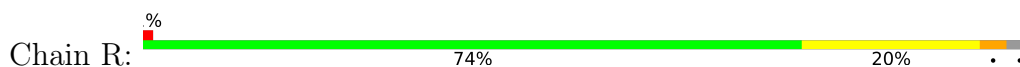
- Molecule 16: 50S ribosomal protein L19e



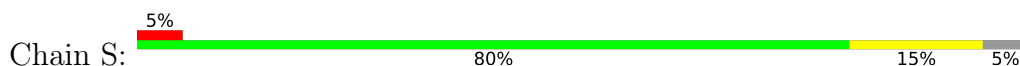
- Molecule 17: 50S ribosomal protein L21e



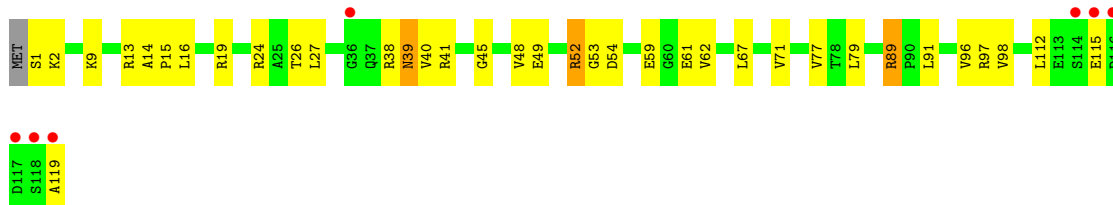
- Molecule 18: 50S ribosomal protein L22P



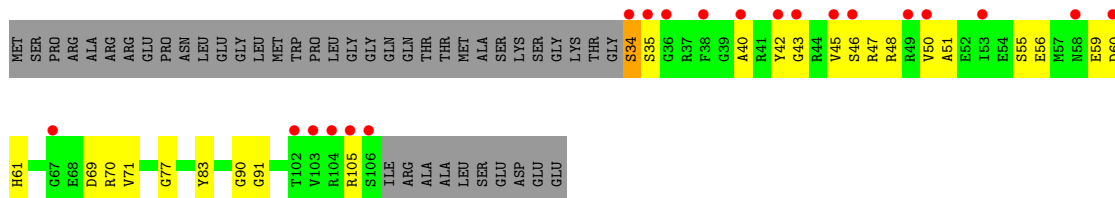
- Molecule 19: 50S ribosomal protein L23P



- Molecule 20: 50S ribosomal protein L24P



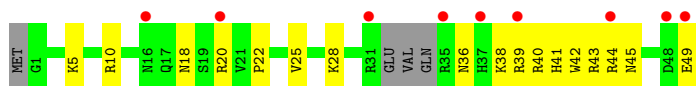
- Molecule 21: 50S ribosomal protein L24e



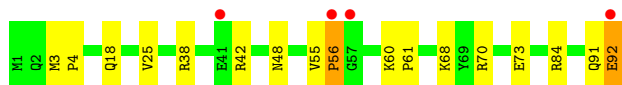
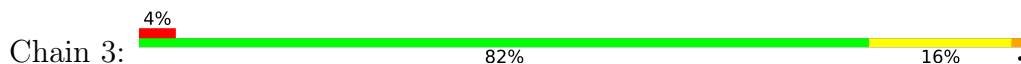
• Molecule 27: 50S ribosomal protein L37e



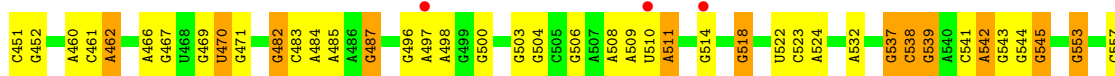
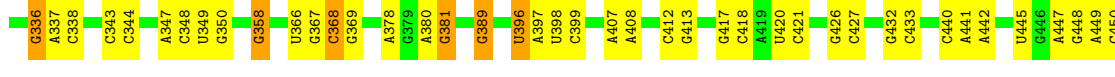
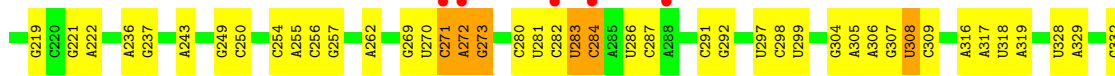
• Molecule 28: 50S ribosomal protein L39e



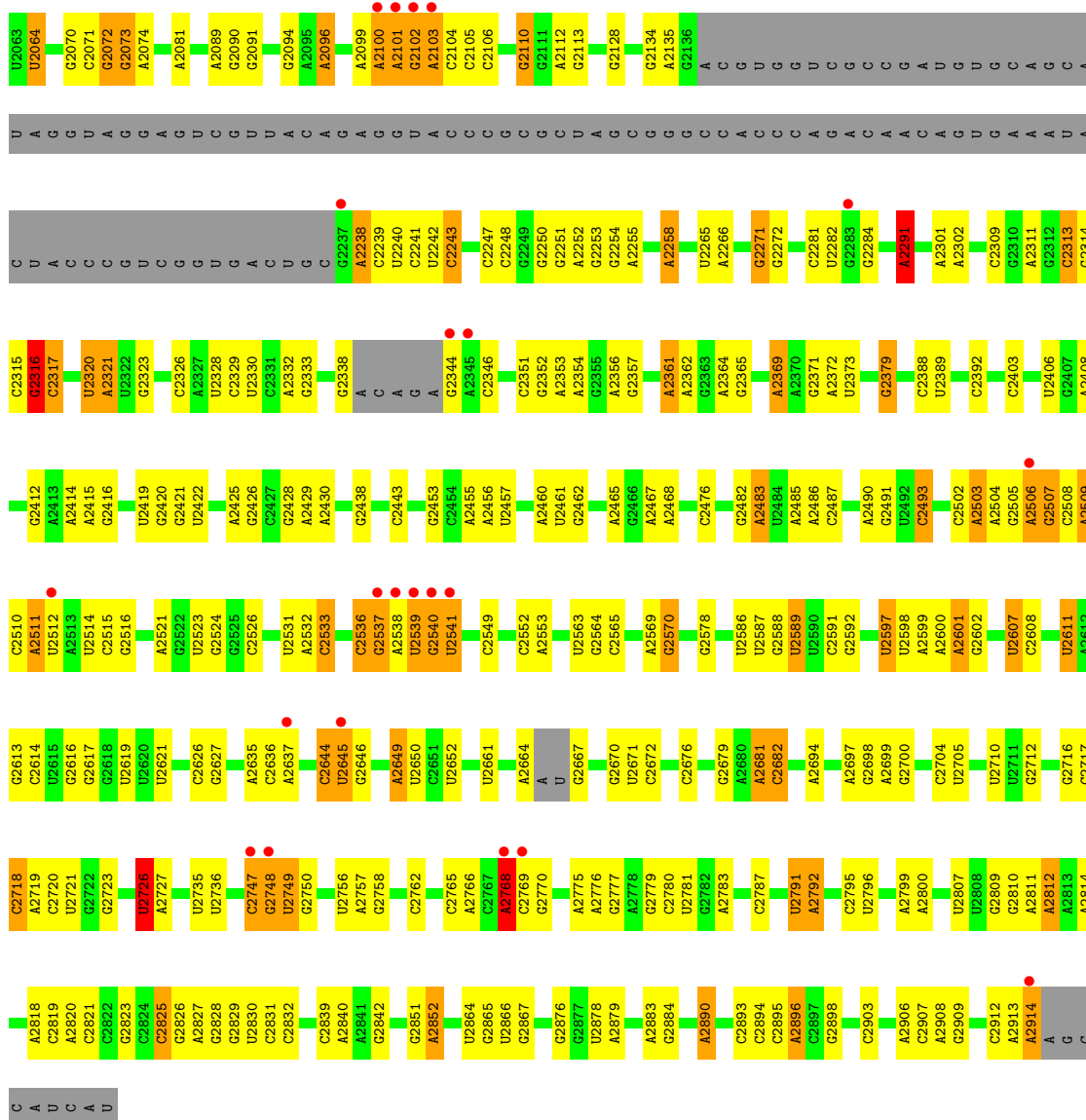
• Molecule 29: 50S ribosomal protein L44E



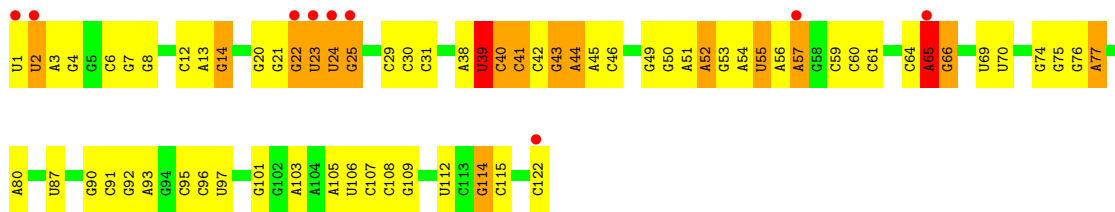
• Molecule 30: 23S RIBOSOMAL RNA



U	G1848	G1735	A1630	A1501	A1369	G1290	G1197	C1103	U888	G787	A666	C558
A	G1849	A1736	A1631	A1502	A1372	A1294	U1198	C1104	A894	A788	A667	U589
C	U1850	A1737	A1632	U1503	A1373	A1298	A1199	U1109	C992	A790	C668	U560
U	A1852	G1738	G1633	U1504	C1377	U1299	C1201	G1110	G902	G799	G670	G561
A	C1856	U1740	G1634	U1506	G1378	G1300	A1202	C1000	C905	A793	C563	A562
U	U1741	U1741	U1634	U1511	U1380	U1300	G1203	U1001	C906	U794	G564	G544
G	C1862	G1744	A1641	G1512	U1384	C1304	C1204	A1006	A907	A795	A565	A566
A	G1863	G1745	A1642	G1518	C1384	C1305	U1205	A1007	A907	A796	U567	U567
C	G1864	U1519	U1654	U1518	G1391	U1309	U1206	A1008	A912	A797	A686	A687
C	A1865	U1520	G1655	U1519	A1392	U1310	A1207	C1008	A912	A806	G581	G581
C	A1866	G1751	A1657	G1522	A1392	G1311	C1208	U1009	A922	A807	C687	C687
C	G1867	G1752	A1657	A1522	C1396	G1311	C1209	U1014	C923	A808	U582	U582
U	G1868	A1755	A1658	A1523	G1397	G1312	G1210	C1015	A923	G809	C696	C696
U	U1871	G1756	A1659	U1524	G1398	A1313	C1211	U1016	A923	A809	C697	C697
U	G1872	G1757	G1660	U1525	G1399	G1314	C1212	C1018	A926	A810	A698	A698
U	G1873	A1759	C1666	A1526	A1400	G1315	C1214	G1021	A926	A811	C699	C699
U	G1877	G1760	A1667	A1527	C1400	G1316	A1215	A1022	A943	G816	A700	A700
U	U1878	U1761	A1668	A1528	A1406	A1321	G1216	C1025	A944	G817	A701	A603
U	U1879	C1762	G1675	G1529	A1407	G1322	U1217	C1025	A944	G818	A702	A603
U	U1883	U1766	C1675	G1535	A1414	G1325	U1218	U1029	A949	A819	G702	G604
U	A1886	U1767	C1679	G1536	G1415	G1328	U1219	U1042	A950	A819	G703	C605
U	G1902	C1768	C1680	G1552	G1417	A1328	U1220	C1043	A951	A821	C704	C606
U	U1903	C1769	C1681	C1553	U1418	G1331	G1229	C1044	A951	C822	A708	A608
U	U1909	G1773	G1683	C1554	U1419	A1231	A1230	G1045	A951	G830	G709	U612
U	U1985	G1777	A1685	G1555	U1422	G1333	A1231	G1046	A951	U831	G710	C613
U	U1997	A1778	C1686	U1559	C1423	G1334	U1234	G1053	A961	A834	U714	U619
G	A1910	A1779	C1687	U	C1426	G1336	U1235	G1055	A961	U835	G716	A620
G	A1919	C1787	C1692	C1562	C1426	G1339	U1237	G1059	A968	U840	G730	G622
G	A1920	U1788	A1693	C1562	G1441	G1340	C1238	A1058	A969	U840	G730	G622
G	A1921	G1789	A1693	A1573	A1441	A1341	A1171	A1059	A969	C848	U734	U625
G	A1922	C1790	G1697	C1574	A1442	G1240	G1173	C1060	A970	C848	U734	U625
G	G1925	U1791	C1700	G1588	U1446	G1241	A1174	U1066	U	G856	A737	G627
G	G1926	C1798	A1701	G1589	C1451	A1242	G1175	A1067	U	A857	A741	A628
G	A1927	U1798	U1702	G1592	C1451	U1244	A1177	C	U	U858	C741	A629
G	G1928	C1816	U1710	C1593	C1452	G1245	A1178	G1072	C	A861	G744	A630
G	G1929	U1817	A1710	C1594	A1471	A1246	U1179	C	C	A867	A632	A632
G	A1934	C1818	C1714	G1595	C1474	U1249	U1180	C	C	A867	A750	A635
G	C1935	G1820	C1715	U1596	G1475	A1352	U1181	U	U	G868	U751	A636
G	U1939	A1829	A1716	A1597	A1476	C1353	C1183	A1081	C	G869	C757	G637
G	A1941	A1829	A1717	A1598	C1477	G1354	U1185	A1082	C	G870	C757	G637
G	A1942	C1834	U1722	A1603	U1478	A1355	C1186	C1083	C	A872	A758	C638
G	C1943	U1835	G1723	G1604	A1482	A1357	U1187	C1084	A	U872	C759	A639
G	U1946	U1838	U1724	G1605	C1483	A1359	U1188	C1085	A	A875	A767	G644
G	U1947	U1839	C1725	A1615	G1484	C1360	U1189	A1086	A	A876	A767	U645
G	G1948	A1840	G1730	A1615	U1488	G1363	U1190	G1087	A	G877	C770	U645
G	G1949	G1841	C1731	A1624	U1496	C1366	A1191	A1088	G	G878	G775	G656
G	U1950	A1842	A1733	U1625	G1497	A1367	U1192	A1088	G	G879	A776	G657
G	U1951	A1847	C1734	U1627	G1497	U1368	A1193	A1098	U	C880	A776	G657
G	U2001	U1951	A1847	U1627	G1497	U1368	U1194	G1099	C	U883	U777	A660
G	A2062	U2062	U1951	U1627	G1497	U1368	U1196	G1109	C	C887	U779	U664



● Molecule 31: 5S RIBOSOMAL RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.53Å 298.18Å 573.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.55 49.70 – 2.55	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.70-2.55) 94.5 (49.70-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.40Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.240 0.189 , 0.224	Depositor DCC
R_{free} test set	6547 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtrriage
Anisotropy	0.109	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99119	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 1MA, OMU, CL, NA, UR3, K, MG, SR, CD, OMG

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	0/1786	0.96	7/2408 (0.3%)
2	B	0.44	1/2690 (0.0%)	1.01	15/3652 (0.4%)
3	C	0.45	0/1885	0.99	10/2552 (0.4%)
4	D	0.38	0/1111	0.95	8/1498 (0.5%)
5	E	0.38	0/1382	0.87	5/1880 (0.3%)
6	F	0.40	0/901	0.91	2/1224 (0.2%)
7	G	0.35	0/241	0.80	0/324
8	H	0.38	0/1302	0.93	6/1743 (0.3%)
9	I	0.40	0/526	0.91	2/716 (0.3%)
10	J	0.42	0/1136	0.89	2/1530 (0.1%)
11	K	0.40	0/1004	0.96	3/1351 (0.2%)
12	L	0.40	0/1130	0.93	4/1509 (0.3%)
13	M	0.44	0/1582	0.88	3/2116 (0.1%)
14	N	0.37	0/1474	1.04	13/1999 (0.7%)
15	O	0.42	0/874	0.95	6/1181 (0.5%)
16	P	0.40	0/1147	0.84	0/1528
17	Q	0.41	0/749	1.06	6/1005 (0.6%)
18	R	1.28	7/1172 (0.6%)	1.39	11/1578 (0.7%)
19	S	0.38	0/648	0.87	1/875 (0.1%)
20	T	0.38	0/958	0.95	2/1289 (0.2%)
21	U	0.37	0/417	0.80	1/562 (0.2%)
22	V	0.38	0/502	0.94	2/675 (0.3%)
23	W	0.44	0/1219	0.94	2/1655 (0.1%)
24	X	0.44	0/664	0.96	4/895 (0.4%)
25	Y	0.43	0/1146	0.95	2/1536 (0.1%)
26	Z	0.38	0/584	0.99	2/781 (0.3%)
27	1	0.46	0/438	0.86	1/578 (0.2%)
28	2	0.43	0/401	0.79	0/529
29	3	0.41	0/771	0.85	2/1024 (0.2%)
30	0	0.37	0/65953	0.61	26/102860 (0.0%)
31	9	0.36	0/2904	0.59	2/4526 (0.0%)
All	All	0.41	8/98697 (0.0%)	0.72	150/147579 (0.1%)

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
18	R	1	0
30	0	0	46
31	9	0	3
All	All	1	49

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	26.63	2.82	1.49
18	R	150	PRO	CA-C	-18.15	1.14	1.52
18	R	150	PRO	CG-CD	13.66	1.97	1.50
18	R	150	PRO	N-CA	13.28	1.67	1.47
18	R	150	PRO	C-O	11.79	1.47	1.23

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-28.38	56.17	110.10
18	R	150	PRO	N-CA-C	-20.39	61.12	112.10
18	R	150	PRO	N-CA-CB	12.19	116.40	103.00
18	R	150	PRO	CA-N-CD	11.97	128.76	112.00
4	D	170	TYR	N-CA-C	9.94	125.35	113.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 49 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	182	G	Sidechain
30	0	26	U	Sidechain
30	0	270	U	Sidechain
30	0	332	G	Sidechain
30	0	396	U	Sidechain

5.2 Too-close contacts [i](#)

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	1753	0	1766	52	0
2	B	2625	0	2533	89	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	40	0
5	E	1357	0	1266	37	0
6	F	890	0	843	24	0
7	G	240	0	231	6	0
8	H	1282	0	1292	32	0
9	I	519	0	500	19	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	36	0
13	M	1558	0	1572	48	0
14	N	1445	0	1401	50	0
15	O	865	0	873	24	0
16	P	1136	0	1123	23	0
17	Q	735	0	729	16	0
18	R	1149	0	1122	33	0
19	S	641	0	605	9	0
20	T	950	0	924	25	0
21	U	410	0	364	14	0
22	V	499	0	511	15	0
23	W	1196	0	1137	54	0
24	X	654	0	653	16	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	15	0
27	1	431	0	426	23	0
28	2	396	0	413	19	0
29	3	755	0	728	13	0
30	0	59017	0	29811	1046	0
31	9	2599	0	1325	79	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	1	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	94	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	1	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5938	0	0	160	0
38	1	51	0	0	1	0
38	2	37	0	0	1	0
38	3	72	0	0	4	0
38	9	145	0	0	9	0
38	A	117	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	B	139	0	0	16	0
38	C	165	0	0	10	0
38	D	48	0	0	5	0
38	E	49	0	0	1	0
38	F	25	0	0	1	0
38	G	18	0	0	1	0
38	H	71	0	0	5	0
38	I	8	0	0	0	0
38	J	55	0	0	1	0
38	K	55	0	0	1	0
38	L	79	0	0	8	0
38	M	138	0	0	3	0
38	N	58	0	0	6	0
38	O	40	0	0	0	0
38	P	61	0	0	1	0
38	Q	49	0	0	2	0
38	R	78	0	0	2	0
38	S	32	0	0	3	0
38	T	36	0	0	3	0
38	U	28	0	0	2	0
38	V	13	0	0	2	0
38	W	68	0	0	5	0
38	X	24	0	0	3	0
38	Y	97	0	0	8	0
38	Z	29	0	0	3	0
All	All	99119	0	59911	1813	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 12.

The worst 5 of 1813 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.97	1.41
30:0:2537:G:H5''	30:0:2538:A:H5''	1.17	1.14
30:0:871:G:C8	30:0:871:G:H5'	1.83	1.14
30:0:1205:U:H2'	30:0:1206:U:H5''	1.27	1.12
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	209 (89%)	24 (10%)	2 (1%)	14	20
2	B	335/338 (99%)	315 (94%)	18 (5%)	2 (1%)	21	29
3	C	244/246 (99%)	233 (96%)	11 (4%)	0	100	100
4	D	134/177 (76%)	111 (83%)	20 (15%)	3 (2%)	5	5
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	14	20
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	149 (96%)	7 (4%)	0	100	100
9	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	8	10
10	J	140/145 (97%)	133 (95%)	5 (4%)	2 (1%)	9	11
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	5	5
13	M	192/196 (98%)	183 (95%)	9 (5%)	0	100	100
14	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	4	3
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
20	T	117/120 (98%)	113 (97%)	3 (3%)	1 (1%)	14	20
21	U	51/67 (76%)	49 (96%)	2 (4%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	4	4
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	9	11
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	11	15
All	All	3705/4472 (83%)	3486 (94%)	195 (5%)	24 (1%)	21	29

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
10	J	5	GLU
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE

5.3.2 Protein sidechains [i](#)

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	179/182 (98%)	166 (93%)	13 (7%)	13	18
2	B	282/283 (100%)	262 (93%)	20 (7%)	13	19
3	C	193/193 (100%)	180 (93%)	13 (7%)	15	21
4	D	117/148 (79%)	113 (97%)	4 (3%)	32	48
5	E	152/156 (97%)	147 (97%)	5 (3%)	33	50
6	F	93/94 (99%)	92 (99%)	1 (1%)	65	79
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	129 (96%)	5 (4%)	30	45
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	114 (97%)	4 (3%)	32	48
11	K	106/106 (100%)	102 (96%)	4 (4%)	29	44
12	L	113/127 (89%)	110 (97%)	3 (3%)	39	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	153 (97%)	5 (3%)	34	51
14	N	149/150 (99%)	145 (97%)	4 (3%)	39	58
15	O	93/94 (99%)	88 (95%)	5 (5%)	20	30
16	P	113/117 (97%)	111 (98%)	2 (2%)	51	70
17	Q	79/80 (99%)	76 (96%)	3 (4%)	29	44
18	R	117/122 (96%)	114 (97%)	3 (3%)	40	59
19	S	71/74 (96%)	70 (99%)	1 (1%)	59	75
20	T	105/106 (99%)	99 (94%)	6 (6%)	18	28
21	U	44/53 (83%)	43 (98%)	1 (2%)	44	62
22	V	51/57 (90%)	50 (98%)	1 (2%)	48	67
23	W	130/130 (100%)	124 (95%)	6 (5%)	24	36
24	X	66/74 (89%)	62 (94%)	4 (6%)	17	25
25	Y	120/196 (61%)	111 (92%)	9 (8%)	12	17
26	Z	60/94 (64%)	59 (98%)	1 (2%)	53	72
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	42 (100%)	0	100	100
29	3	79/79 (100%)	76 (96%)	3 (4%)	29	44
All	All	3095/3646 (85%)	2969 (96%)	126 (4%)	27	41

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	87	LYS
24	X	79	GLU
12	L	140	VAL
24	X	72	VAL
25	Y	189	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
18	R	94	ASN
23	W	119	HIS
18	R	113	HIS
19	S	55	GLN

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Mol	Chain	Res	Type
24	X	23	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	251 (9%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	3 (2%)
All	All	2866/3045 (94%)	268 (9%)	31 (1%)

5 of 268 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1684	A
30	0	2791	U
30	0	1856	C
31	9	55	U
30	0	2718	C

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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	OMG	0	2588	30	23,26,27	0.28	0	32,38,41	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	1MA	0	628	30,35	21,25,26	0.72	1 (4%)	30,37,40	0.74	1 (3%)
30	PSU	0	2621	30	18,21,22	1.49	2 (11%)	21,30,33	1.38	3 (14%)
30	OMU	0	2587	30	19,22,23	0.33	0	25,31,34	0.45	0
30	UR3	0	2619	30	19,22,23	0.36	0	26,32,35	0.71	1 (3%)

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	OMG	0	2588	30	-	0/9/27/28	0/3/3/3
30	1MA	0	628	30,35	-	2/7/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	4.99	1.43	1.36
30	0	628	1MA	C6-N6	2.45	1.33	1.28
30	0	2621	PSU	C6-C5	2.15	1.37	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C6-C5-C4	4.00	120.87	118.17
30	0	2619	UR3	C4-N3-C2	2.83	126.86	124.58
30	0	2621	PSU	C6-N1-C2	-2.83	120.06	122.69
30	0	628	1MA	N1-C2-N3	2.79	129.31	126.00
30	0	2621	PSU	O2-C2-N1	2.74	125.61	122.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8
30	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2588	OMG	3	0
30	0	2587	OMU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 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.

No monomer is involved in short contacts.

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, 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	237/240 (98%)	0.40	20 (8%) 17 16	20, 40, 77, 100	0
2	B	337/338 (99%)	0.45	20 (5%) 28 27	21, 44, 73, 83	0
3	C	246/246 (100%)	0.16	9 (3%) 45 46	17, 36, 60, 73	0
4	D	140/177 (79%)	2.77	94 (67%) 0 0	48, 89, 116, 126	0
5	E	172/178 (96%)	0.97	19 (11%) 10 10	34, 59, 79, 85	0
6	F	119/120 (99%)	1.15	25 (21%) 2 2	34, 61, 91, 105	0
7	G	29/348 (8%)	1.96	10 (34%) 1 0	70, 87, 96, 98	0
8	H	160/177 (90%)	0.69	16 (10%) 12 12	32, 50, 85, 91	0
9	I	70/162 (43%)	4.06	63 (90%) 0 0	124, 138, 156, 156	0
10	J	142/145 (97%)	0.34	7 (4%) 35 34	27, 41, 63, 89	0
11	K	132/132 (100%)	0.14	1 (0%) 82 84	23, 39, 63, 72	0
12	L	145/165 (87%)	0.99	29 (20%) 3 2	18, 55, 103, 118	0
13	M	194/196 (98%)	0.35	23 (11%) 9 8	23, 34, 54, 59	0
14	N	186/187 (99%)	1.16	35 (18%) 3 2	34, 52, 104, 112	0
15	O	115/116 (99%)	0.49	5 (4%) 40 40	31, 45, 61, 69	0
16	P	143/149 (95%)	0.39	3 (2%) 63 64	28, 43, 56, 68	0
17	Q	95/96 (98%)	0.11	3 (3%) 50 51	29, 37, 55, 66	0
18	R	150/155 (96%)	-0.06	2 (1%) 75 75	23, 36, 57, 71	0
19	S	81/85 (95%)	0.39	4 (4%) 35 34	33, 48, 70, 81	0
20	T	119/120 (99%)	0.62	7 (5%) 28 27	29, 46, 74, 101	0
21	U	53/67 (79%)	0.43	2 (3%) 44 45	33, 46, 65, 74	0
22	V	65/71 (91%)	1.47	15 (23%) 2 1	41, 63, 106, 113	0
23	W	154/154 (100%)	0.21	2 (1%) 75 75	26, 42, 59, 71	0
24	X	82/92 (89%)	0.75	10 (12%) 8 7	34, 49, 77, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.09	4 (2%) 55 56	19, 34, 58, 80	0
26	Z	73/116 (62%)	1.35	20 (27%) 1 1	36, 55, 72, 89	0
27	1	56/57 (98%)	-0.38	0 100 100	18, 24, 34, 41	0
28	2	46/50 (92%)	0.95	9 (19%) 3 2	25, 49, 74, 86	0
29	3	92/92 (100%)	0.36	4 (4%) 40 40	27, 45, 60, 74	0
30	0	2749/2923 (94%)	-0.49	92 (3%) 49 50	14, 35, 77, 154	0
31	9	122/122 (100%)	0.22	9 (7%) 20 19	29, 54, 76, 138	0
All	All	6646/7517 (88%)	0.18	562 (8%) 16 16	14, 41, 89, 156	0

The worst 5 of 562 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	10.7
22	V	39	ALA	9.8
14	N	166	ALA	9.2
9	I	113	SER	9.2
4	D	10	PHE	8.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	UR3	0	2619	21/22	0.95	0.09	43,48,52,56	0
30	PSU	0	2621	20/21	0.97	0.07	29,31,42,42	0
30	OMG	0	2588	24/25	0.98	0.06	23,29,30,31	0
30	1MA	0	628	23/24	0.98	0.05	20,23,25,25	0
30	OMU	0	2587	21/22	0.98	0.06	23,27,29,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	SR	0	9006	1/1	0.48	0.20	199,199,199,199	0
32	MG	0	8010	1/1	0.65	0.19	69,69,69,69	0
32	MG	0	8038	1/1	0.67	0.13	80,80,80,80	0
32	MG	0	8037	1/1	0.67	0.39	77,77,77,77	0
37	K	0	8401	1/1	0.67	0.30	97,97,97,97	0
35	NA	0	8562	1/1	0.72	0.40	61,61,61,61	0
32	MG	0	8085	1/1	0.74	0.34	90,90,90,90	0
32	MG	0	8082	1/1	0.74	0.15	63,63,63,63	0
34	SR	0	8983	1/1	0.75	0.20	151,151,151,151	0
32	MG	0	8079	1/1	0.75	0.18	52,52,52,52	0
34	SR	0	8979	1/1	0.76	0.20	193,193,193,193	0
32	MG	0	8056	1/1	0.77	0.23	66,66,66,66	0
34	SR	0	8971	1/1	0.78	0.17	153,153,153,153	0
35	NA	0	8518	1/1	0.78	0.50	81,81,81,81	0
35	NA	0	8569	1/1	0.79	0.27	61,61,61,61	0
32	MG	B	8042	1/1	0.79	0.30	75,75,75,75	0
35	NA	0	8517	1/1	0.80	0.29	68,68,68,68	0
35	NA	0	8556	1/1	0.81	0.21	38,38,38,38	0
32	MG	0	8040	1/1	0.81	0.38	81,81,81,81	0
34	SR	0	8919	1/1	0.81	0.17	167,167,167,167	0
35	NA	0	8575	1/1	0.81	0.48	78,78,78,78	0
35	NA	0	8520	1/1	0.81	0.33	49,49,49,49	0
35	NA	0	8525	1/1	0.82	0.22	57,57,57,57	0
35	NA	0	8573	1/1	0.82	0.26	69,69,69,69	0
35	NA	0	8509	1/1	0.82	0.25	60,60,60,60	0
34	SR	0	9001	1/1	0.82	0.15	142,142,142,142	0
35	NA	0	8533	1/1	0.83	0.16	57,57,57,57	0
35	NA	0	8554	1/1	0.83	0.17	55,55,55,55	0
32	MG	0	8063	1/1	0.83	0.43	74,74,74,74	0
32	MG	0	8067	1/1	0.83	0.22	55,55,55,55	0
35	NA	0	8514	1/1	0.84	0.21	34,34,34,34	0
35	NA	0	8571	1/1	0.84	0.19	83,83,83,83	0
34	SR	0	8991	1/1	0.84	0.28	171,171,171,171	0
35	NA	0	8559	1/1	0.84	0.31	67,67,67,67	0
35	NA	0	8536	1/1	0.84	0.29	62,62,62,62	0
34	SR	0	9004	1/1	0.85	0.15	182,182,182,182	0
32	MG	0	8049	1/1	0.85	0.25	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8996	1/1	0.85	0.26	173,173,173,173	0
35	NA	0	8511	1/1	0.85	0.14	61,61,61,61	0
35	NA	9	8543	1/1	0.85	0.30	60,60,60,60	0
34	SR	0	8987	1/1	0.85	0.47	199,199,199,199	0
34	SR	0	8922	1/1	0.86	0.45	164,164,164,164	0
34	SR	0	8959	1/1	0.86	0.11	129,129,129,129	0
32	MG	0	8071	1/1	0.87	0.26	73,73,73,73	0
35	NA	0	8542	1/1	0.87	0.13	44,44,44,44	0
32	MG	0	8081	1/1	0.87	0.24	65,65,65,65	0
32	MG	0	8035	1/1	0.88	0.22	63,63,63,63	0
32	MG	0	8065	1/1	0.88	0.39	68,68,68,68	0
35	NA	0	8516	1/1	0.88	0.21	50,50,50,50	0
35	NA	0	8555	1/1	0.88	0.34	59,59,59,59	0
35	NA	0	8528	1/1	0.88	0.19	67,67,67,67	0
35	NA	0	8558	1/1	0.88	0.14	39,39,39,39	0
32	MG	0	8048	1/1	0.88	0.11	55,55,55,55	0
32	MG	0	8017	1/1	0.89	0.31	67,67,67,67	0
35	NA	0	8561	1/1	0.89	0.32	67,67,67,67	0
35	NA	0	8534	1/1	0.89	0.12	56,56,56,56	0
34	SR	0	8976	1/1	0.89	0.17	122,122,122,122	0
34	SR	9	8980	1/1	0.89	0.14	144,144,144,144	0
34	SR	9	9003	1/1	0.89	0.12	122,122,122,122	0
34	SR	0	8955	1/1	0.89	0.21	140,140,140,140	0
32	MG	0	8064	1/1	0.89	0.12	54,54,54,54	0
35	NA	9	8572	1/1	0.89	0.19	66,66,66,66	0
35	NA	0	8512	1/1	0.89	0.25	63,63,63,63	0
37	K	0	8402	1/1	0.89	0.15	77,77,77,77	0
35	NA	0	8504	1/1	0.90	0.10	34,34,34,34	0
32	MG	0	8076	1/1	0.90	0.11	52,52,52,52	0
34	SR	0	8949	1/1	0.90	0.35	184,184,184,184	0
35	NA	0	8564	1/1	0.90	0.10	49,49,49,49	0
35	NA	0	8565	1/1	0.90	0.12	39,39,39,39	0
32	MG	0	8089	1/1	0.90	0.09	48,48,48,48	0
35	NA	0	8535	1/1	0.90	0.19	55,55,55,55	0
34	SR	0	9002	1/1	0.90	0.19	141,141,141,141	0
32	MG	0	8045	1/1	0.90	0.18	40,40,40,40	0
34	SR	0	8986	1/1	0.90	0.22	136,136,136,136	0
34	SR	0	8962	1/1	0.90	0.38	165,165,165,165	0
34	SR	0	8989	1/1	0.90	0.18	149,149,149,149	0
35	NA	0	8522	1/1	0.90	0.15	52,52,52,52	0
34	SR	0	8993	1/1	0.91	0.14	154,154,154,154	0
35	NA	0	8526	1/1	0.91	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	SR	0	9007	1/1	0.91	0.45	178,178,178,178	0
35	NA	0	8557	1/1	0.91	0.26	63,63,63,63	0
32	MG	0	8069	1/1	0.91	0.13	75,75,75,75	0
34	SR	0	9000	1/1	0.91	0.12	125,125,125,125	0
32	MG	9	8074	1/1	0.91	0.28	42,42,42,42	0
32	MG	0	8044	1/1	0.91	0.17	62,62,62,62	0
32	MG	0	8080	1/1	0.91	0.10	54,54,54,54	0
35	NA	M	8539	1/1	0.92	0.10	34,34,34,34	0
35	NA	0	8546	1/1	0.92	0.13	51,51,51,51	0
32	MG	0	8066	1/1	0.92	0.29	67,67,67,67	0
35	NA	0	8570	1/1	0.92	0.08	35,35,35,35	0
32	MG	0	8016	1/1	0.92	0.12	75,75,75,75	0
34	SR	0	8969	1/1	0.92	0.32	115,115,115,115	0
32	MG	0	8092	1/1	0.92	0.08	53,53,53,53	0
34	SR	0	8990	1/1	0.92	0.11	132,132,132,132	0
32	MG	0	8050	1/1	0.92	0.15	63,63,63,63	0
34	SR	0	8957	1/1	0.92	0.19	149,149,149,149	0
34	SR	0	8981	1/1	0.92	0.14	115,115,115,115	0
32	MG	0	8030	1/1	0.93	0.19	51,51,51,51	0
34	SR	0	8994	1/1	0.93	0.36	173,173,173,173	0
32	MG	0	8078	1/1	0.93	0.10	52,52,52,52	0
35	NA	0	8552	1/1	0.93	0.19	51,51,51,51	0
35	NA	0	8553	1/1	0.93	0.20	61,61,61,61	0
35	NA	S	8510	1/1	0.93	0.08	32,32,32,32	0
34	SR	0	8902	1/1	0.93	0.38	112,112,112,112	0
35	NA	0	8574	1/1	0.93	0.27	47,47,47,47	0
32	MG	0	8041	1/1	0.93	0.11	52,52,52,52	0
32	MG	0	8007	1/1	0.93	0.14	53,53,53,53	0
34	SR	0	8944	1/1	0.93	0.14	117,117,117,117	0
34	SR	0	8975	1/1	0.93	0.11	114,114,114,114	0
32	MG	0	8090	1/1	0.93	0.07	51,51,51,51	0
35	NA	0	8560	1/1	0.94	0.17	67,67,67,67	0
34	SR	0	8982	1/1	0.94	0.22	116,116,116,116	0
32	MG	0	8068	1/1	0.94	0.09	50,50,50,50	0
35	NA	0	8563	1/1	0.94	0.30	64,64,64,64	0
32	MG	0	8047	1/1	0.94	0.22	66,66,66,66	0
33	CL	B	8819	1/1	0.94	0.14	57,57,57,57	0
35	NA	0	8545	1/1	0.94	0.16	40,40,40,40	0
32	MG	A	8051	1/1	0.94	0.12	51,51,51,51	0
32	MG	0	8073	1/1	0.94	0.14	72,72,72,72	0
34	SR	0	8974	1/1	0.94	0.14	119,119,119,119	0
32	MG	0	8084	1/1	0.94	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	NA	0	8523	1/1	0.94	0.10	48,48,48,48	0
32	MG	0	8062	1/1	0.94	0.17	46,46,46,46	0
32	MG	0	8077	1/1	0.94	0.06	34,34,34,34	0
35	NA	0	8506	1/1	0.94	0.06	44,44,44,44	0
32	MG	0	8002	1/1	0.94	0.08	33,33,33,33	0
35	NA	R	8532	1/1	0.95	0.05	32,32,32,32	0
32	MG	0	8070	1/1	0.95	0.06	50,50,50,50	0
35	NA	T	8537	1/1	0.95	0.05	26,26,26,26	0
34	SR	0	8963	1/1	0.95	0.09	135,135,135,135	0
35	NA	0	8505	1/1	0.95	0.18	37,37,37,37	0
34	SR	0	8997	1/1	0.95	0.14	115,115,115,115	0
34	SR	0	8951	1/1	0.95	0.07	99,99,99,99	0
34	SR	0	8985	1/1	0.95	0.23	98,98,98,98	0
35	NA	0	8544	1/1	0.95	0.22	53,53,53,53	0
34	SR	0	8970	1/1	0.95	0.08	73,73,73,73	0
33	CL	0	8816	1/1	0.95	0.19	49,49,49,49	0
35	NA	0	8548	1/1	0.95	0.26	41,41,41,41	0
34	SR	0	8988	1/1	0.95	0.12	110,110,110,110	0
34	SR	0	8956	1/1	0.95	0.11	111,111,111,111	0
34	SR	0	8938	1/1	0.95	0.14	102,102,102,102	0
32	MG	T	8057	1/1	0.95	0.18	32,32,32,32	0
35	NA	J	8538	1/1	0.95	0.05	47,47,47,47	0
34	SR	0	8960	1/1	0.95	0.09	100,100,100,100	0
34	SR	S	8961	1/1	0.96	0.08	98,98,98,98	0
32	MG	0	8087	1/1	0.96	0.05	33,33,33,33	0
35	NA	0	8521	1/1	0.96	0.16	70,70,70,70	0
32	MG	0	8043	1/1	0.96	0.07	51,51,51,51	0
32	MG	0	8027	1/1	0.96	0.03	36,36,36,36	0
32	MG	0	8091	1/1	0.96	0.10	50,50,50,50	0
34	SR	0	8992	1/1	0.96	0.25	108,108,108,108	0
32	MG	0	8029	1/1	0.96	0.10	35,35,35,35	0
32	MG	0	8059	1/1	0.96	0.04	31,31,31,31	0
33	CL	A	8809	1/1	0.96	0.14	51,51,51,51	0
32	MG	0	8025	1/1	0.96	0.09	40,40,40,40	0
35	NA	0	8508	1/1	0.96	0.06	36,36,36,36	0
35	NA	0	8541	1/1	0.96	0.10	33,33,33,33	0
35	NA	0	8566	1/1	0.96	0.08	37,37,37,37	0
35	NA	0	8567	1/1	0.96	0.33	59,59,59,59	0
32	MG	0	8026	1/1	0.96	0.06	44,44,44,44	0
34	SR	A	8929	1/1	0.96	0.12	78,78,78,78	0
34	SR	0	8958	1/1	0.96	0.04	57,57,57,57	0
34	SR	0	8984	1/1	0.96	0.06	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	NA	0	8547	1/1	0.96	0.14	49,49,49,49	0
34	SR	A	8977	1/1	0.96	0.09	88,88,88,88	0
35	NA	0	8549	1/1	0.96	0.16	73,73,73,73	0
35	NA	0	8550	1/1	0.96	0.20	37,37,37,37	0
35	NA	0	8551	1/1	0.96	0.08	40,40,40,40	0
34	SR	B	8950	1/1	0.96	0.08	83,83,83,83	0
34	SR	0	8998	1/1	0.97	0.07	99,99,99,99	0
34	SR	0	8939	1/1	0.97	0.04	62,62,62,62	0
32	MG	0	8039	1/1	0.97	0.16	42,42,42,42	0
34	SR	0	8946	1/1	0.97	0.05	75,75,75,75	0
33	CL	J	8802	1/1	0.97	0.06	49,49,49,49	0
33	CL	J	8821	1/1	0.97	0.07	52,52,52,52	0
33	CL	3	8804	1/1	0.97	0.05	48,48,48,48	0
33	CL	0	8803	1/1	0.97	0.09	38,38,38,38	0
32	MG	0	8075	1/1	0.97	0.05	37,37,37,37	0
35	NA	C	8503	1/1	0.97	0.09	19,19,19,19	0
32	MG	0	8031	1/1	0.97	0.07	39,39,39,39	0
35	NA	0	8530	1/1	0.97	0.15	41,41,41,41	0
32	MG	0	8088	1/1	0.97	0.05	25,25,25,25	0
35	NA	Q	8540	1/1	0.97	0.05	39,39,39,39	0
32	MG	0	8032	1/1	0.97	0.04	42,42,42,42	0
32	MG	0	8023	1/1	0.97	0.04	30,30,30,30	0
32	MG	0	8036	1/1	0.97	0.12	37,37,37,37	0
34	SR	0	8965	1/1	0.97	0.07	80,80,80,80	0
32	MG	0	8060	1/1	0.97	0.11	41,41,41,41	0
32	MG	Y	8086	1/1	0.97	0.04	30,30,30,30	0
35	NA	0	8507	1/1	0.97	0.07	19,19,19,19	0
34	SR	0	8926	1/1	0.97	0.10	69,69,69,69	0
34	SR	0	8995	1/1	0.97	0.09	94,94,94,94	0
34	SR	0	8972	1/1	0.97	0.21	121,121,121,121	0
36	CD	O	8705	1/1	0.97	0.07	88,88,88,88	0
32	MG	0	8015	1/1	0.97	0.09	50,50,50,50	0
35	NA	0	8513	1/1	0.97	0.07	32,32,32,32	0
35	NA	0	8527	1/1	0.98	0.05	35,35,35,35	0
32	MG	0	8083	1/1	0.98	0.03	35,35,35,35	0
35	NA	0	8529	1/1	0.98	0.07	29,29,29,29	0
32	MG	0	8014	1/1	0.98	0.09	23,23,23,23	0
33	CL	0	8811	1/1	0.98	0.05	54,54,54,54	0
33	CL	0	8812	1/1	0.98	0.06	43,43,43,43	0
33	CL	0	8813	1/1	0.98	0.05	34,34,34,34	0
32	MG	0	8053	1/1	0.98	0.17	45,45,45,45	0
33	CL	0	8822	1/1	0.98	0.21	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8964	1/1	0.98	0.05	76,76,76,76	0
34	SR	0	9008	1/1	0.98	0.03	59,59,59,59	0
34	SR	9	8968	1/1	0.98	0.07	96,96,96,96	0
32	MG	0	8001	1/1	0.98	0.03	9,9,9,9	0
34	SR	0	8966	1/1	0.98	0.05	68,68,68,68	0
34	SR	0	8967	1/1	0.98	0.06	86,86,86,86	0
32	MG	0	8072	1/1	0.98	0.04	36,36,36,36	0
32	MG	0	8008	1/1	0.98	0.10	27,27,27,27	0
34	SR	F	9005	1/1	0.98	0.07	77,77,77,77	0
32	MG	K	8054	1/1	0.98	0.03	20,20,20,20	0
34	SR	0	8973	1/1	0.98	0.05	79,79,79,79	0
34	SR	3	8999	1/1	0.98	0.05	63,63,63,63	0
35	NA	0	8501	1/1	0.98	0.05	30,30,30,30	0
35	NA	0	8502	1/1	0.98	0.26	52,52,52,52	0
32	MG	0	8018	1/1	0.98	0.11	13,13,13,13	0
34	SR	0	8910	1/1	0.98	0.13	60,60,60,60	0
34	SR	0	8915	1/1	0.98	0.04	58,58,58,58	0
32	MG	0	8020	1/1	0.98	0.10	22,22,22,22	0
32	MG	0	8093	1/1	0.98	0.06	29,29,29,29	0
34	SR	0	8925	1/1	0.98	0.06	55,55,55,55	0
32	MG	0	8022	1/1	0.98	0.04	7,7,7,7	0
34	SR	0	8928	1/1	0.98	0.04	67,67,67,67	0
34	SR	0	8931	1/1	0.98	0.04	61,61,61,61	0
34	SR	0	8933	1/1	0.98	0.04	54,54,54,54	0
35	NA	0	8515	1/1	0.98	0.06	28,28,28,28	0
35	NA	0	8568	1/1	0.98	0.17	33,33,33,33	0
32	MG	0	8033	1/1	0.98	0.05	45,45,45,45	0
32	MG	0	8034	1/1	0.98	0.04	25,25,25,25	0
34	SR	0	8941	1/1	0.98	0.03	60,60,60,60	0
35	NA	0	8519	1/1	0.98	0.11	29,29,29,29	0
32	MG	0	8013	1/1	0.98	0.04	41,41,41,41	0
32	MG	0	8024	1/1	0.98	0.06	45,45,45,45	0
33	CL	L	8810	1/1	0.98	0.10	43,43,43,43	0
33	CL	N	8807	1/1	0.98	0.08	43,43,43,43	0
35	NA	0	8524	1/1	0.98	0.07	27,27,27,27	0
34	SR	0	8953	1/1	0.98	0.06	76,76,76,76	0
33	CL	R	8806	1/1	0.98	0.07	28,28,28,28	0
34	SR	0	8942	1/1	0.99	0.03	55,55,55,55	0
34	SR	0	8943	1/1	0.99	0.03	49,49,49,49	0
32	MG	0	8021	1/1	0.99	0.06	24,24,24,24	0
34	SR	0	8945	1/1	0.99	0.03	71,71,71,71	0
35	NA	0	8531	1/1	0.99	0.04	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	A	8930	1/1	0.99	0.04	57,57,57,57	0
34	SR	0	8947	1/1	0.99	0.06	73,73,73,73	0
34	SR	0	8948	1/1	0.99	0.03	57,57,57,57	0
32	MG	0	8012	1/1	0.99	0.06	4,4,4,4	0
32	MG	0	8005	1/1	0.99	0.03	29,29,29,29	0
33	CL	M	8818	1/1	0.99	0.04	22,22,22,22	0
34	SR	0	8954	1/1	0.99	0.05	60,60,60,60	0
34	SR	R	8912	1/1	0.99	0.03	55,55,55,55	0
32	MG	0	8052	1/1	0.99	0.03	29,29,29,29	0
34	SR	1	8952	1/1	0.99	0.02	47,47,47,47	0
33	CL	O	8808	1/1	0.99	0.07	52,52,52,52	0
32	MG	0	8003	1/1	0.99	0.04	24,24,24,24	0
34	SR	0	8904	1/1	0.99	0.07	20,20,20,20	0
34	SR	0	8906	1/1	0.99	0.04	50,50,50,50	0
34	SR	0	8907	1/1	0.99	0.08	50,50,50,50	0
34	SR	0	8908	1/1	0.99	0.03	46,46,46,46	0
33	CL	Y	8820	1/1	0.99	0.05	27,27,27,27	0
34	SR	0	8911	1/1	0.99	0.03	48,48,48,48	0
34	SR	0	8914	1/1	0.99	0.08	67,67,67,67	0
32	MG	0	8055	1/1	0.99	0.07	12,12,12,12	0
34	SR	0	8916	1/1	0.99	0.02	45,45,45,45	0
34	SR	0	8917	1/1	0.99	0.03	46,46,46,46	0
32	MG	0	8019	1/1	0.99	0.09	18,18,18,18	0
34	SR	0	8920	1/1	0.99	0.04	63,63,63,63	0
34	SR	0	8921	1/1	0.99	0.03	46,46,46,46	0
33	CL	0	8805	1/1	0.99	0.05	39,39,39,39	0
34	SR	0	8923	1/1	0.99	0.02	54,54,54,54	0
34	SR	0	8978	1/1	0.99	0.02	47,47,47,47	0
34	SR	0	8924	1/1	0.99	0.03	50,50,50,50	0
32	MG	0	8058	1/1	0.99	0.09	3,3,3,3	0
32	MG	0	8046	1/1	0.99	0.02	1,1,1,1	0
34	SR	0	8927	1/1	0.99	0.06	58,58,58,58	0
32	MG	0	8011	1/1	0.99	0.05	26,26,26,26	0
33	CL	0	8814	1/1	0.99	0.11	35,35,35,35	0
33	CL	0	8815	1/1	0.99	0.06	38,38,38,38	0
34	SR	0	8934	1/1	0.99	0.03	52,52,52,52	0
34	SR	0	8935	1/1	0.99	0.02	54,54,54,54	0
34	SR	0	8936	1/1	0.99	0.02	44,44,44,44	0
32	MG	0	8061	1/1	0.99	0.07	17,17,17,17	0
33	CL	0	8817	1/1	0.99	0.09	33,33,33,33	0
36	CD	3	8704	1/1	0.99	0.06	63,63,63,63	0
34	SR	0	8940	1/1	0.99	0.03	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	CL	J	8801	1/1	0.99	0.07	42,42,42,42	0
32	MG	0	8009	1/1	1.00	0.16	1,1,1,1	0
34	SR	0	8901	1/1	1.00	0.04	35,35,35,35	0
32	MG	0	8028	1/1	1.00	0.11	1,1,1,1	0
34	SR	0	8903	1/1	1.00	0.07	36,36,36,36	0
32	MG	0	8004	1/1	1.00	0.04	13,13,13,13	0
34	SR	0	8905	1/1	1.00	0.11	43,43,43,43	0
34	SR	0	8918	1/1	1.00	0.10	45,45,45,45	0
34	SR	1	8913	1/1	1.00	0.02	32,32,32,32	0
32	MG	0	8006	1/1	1.00	0.14	1,1,1,1	0
36	CD	U	8701	1/1	1.00	0.08	62,62,62,62	0
36	CD	Z	8703	1/1	1.00	0.10	67,67,67,67	0
36	CD	1	8702	1/1	1.00	0.04	54,54,54,54	0
34	SR	3	8932	1/1	1.00	0.03	65,65,65,65	0
34	SR	0	8909	1/1	1.00	0.02	44,44,44,44	0
34	SR	0	8937	1/1	1.00	0.01	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.