



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YJW  
Title : Crystal Structure Of Quinupristin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui  
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2005-01-15  
Resolution : 2.90 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

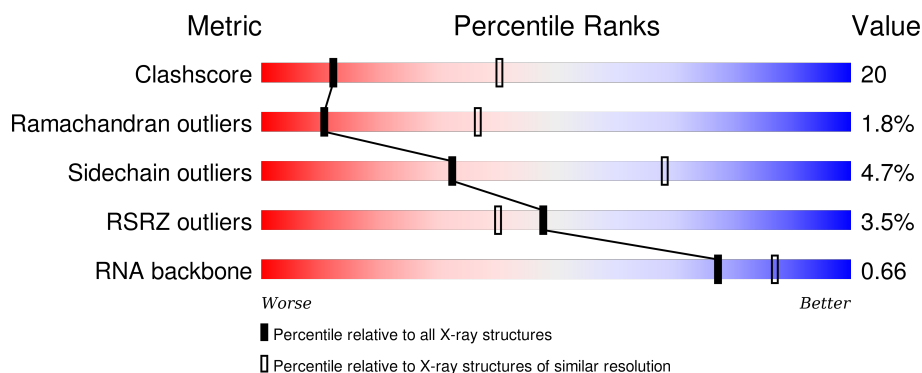
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div></div> <div>53% 35% 6% 6%</div> </div>
2	1	57	<div> <div></div> <div>65% 33%</div> </div>
3	2	50	<div> <div>4%</div> <div>46% 46% 8%</div> </div>
4	3	92	<div> <div></div> <div>55% 45%</div> </div>
5	4	8	<div> <div></div> <div>88% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
6	9	122	
7	A	240	
8	B	338	
9	C	246	
10	D	177	
11	E	178	
12	F	120	
13	G	348	
14	H	177	
15	I	162	
16	J	145	
17	K	132	
18	L	165	
19	M	195	
20	N	187	
21	O	116	
22	P	149	
23	Q	96	
24	R	155	
25	S	85	
26	T	120	
27	U	66	
28	V	71	
29	W	154	
30	X	92	

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Mol	Chain	Length	Quality of chain
31	Y	241	
32	Z	83	

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
33	MG	7	8064	-	-	-	X
34	K	7	8401	-	-	-	X
35	NA	8	8502	-	-	-	X
35	NA	8	8503	-	-	-	X
35	NA	8	8521	-	-	-	X
35	NA	8	8525	-	-	-	X
35	NA	8	8527	-	-	-	X
35	NA	8	8529	-	-	-	X
35	NA	8	8531	-	-	-	X
35	NA	8	8532	-	-	-	X
35	NA	8	8535	-	-	-	X
35	NA	8	8553	-	-	-	X
35	NA	8	8556	-	-	-	X
35	NA	8	8559	-	-	-	X
35	NA	8	8561	-	-	-	X
35	NA	8	8562	-	-	-	X
35	NA	8	8565	-	-	-	X
35	NA	8	8568	-	-	-	X
35	NA	8	8569	-	-	-	X
35	NA	8	8571	-	-	-	X
35	NA	8	8572	-	-	-	X
35	NA	8	8573	-	-	-	X
35	NA	8	8574	-	-	-	X
35	NA	8	8577	-	-	-	X
35	NA	8	8578	-	-	-	X
35	NA	8	8582	-	-	-	X
35	NA	9	8583	-	-	-	X
35	NA	L	8580	-	-	-	X
35	NA	R	8586	-	-	-	X
36	CL	8	8812	-	-	X	-
36	CL	8	8815	-	-	-	X
36	CL	N	8807	-	-	X	-

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99111 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 RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10873	19053	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	MODIFIED RESIDUE	GB 55229667
0	2099	A	G	ENGINEERED	GB 55229667
0	2587	OMU	U	MODIFIED RESIDUE	GB 55229667
0	2588	OMG	G	MODIFIED RESIDUE	GB 55229667
0	2619	UR3	U	MODIFIED RESIDUE	GB 55229667
0	2621	PSU	U	MODIFIED RESIDUE	GB 55229667

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 5 is a protein called QUINUPRISTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

- Molecule 6 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L2P.

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

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L3P.

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

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L5P.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L6P.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L7AE.

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

- Molecule 13 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L13P.

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

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L15P.

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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L18P.

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

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L18E.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L19E.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L21E.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L22P.



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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L23P.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24P.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L24E.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29P.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30P.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31E.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32E.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	7	110	Total	Mg	0	0
			110	110		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	3	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	7	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	A	1	Total Na 1 1	0	0
35	8	74	Total Na 74 74	0	0
35	R	2	Total Na 2 2	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	8	10	Total Cl 10 10	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0
37	3	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5874	Total 5874	O 5874	0	0
38	1	59	Total 59	O 59	0	0
38	2	46	Total 46	O 46	0	0
38	3	67	Total 67	O 67	0	0
38	4	2	Total 2	O 2	0	0
38	9	141	Total 141	O 141	0	0
38	A	119	Total 119	O 119	0	0
38	B	144	Total 144	O 144	0	0
38	C	176	Total 176	O 176	0	0
38	D	48	Total 48	O 48	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	E	42	Total 42	O 42	0	0
38	F	26	Total 26	O 26	0	0
38	G	20	Total 20	O 20	0	0
38	H	67	Total 67	O 67	0	0
38	I	9	Total 9	O 9	0	0
38	J	56	Total 56	O 56	0	0
38	K	60	Total 60	O 60	0	0
38	L	80	Total 80	O 80	0	0
38	M	125	Total 125	O 125	0	0
38	N	60	Total 60	O 60	0	0
38	O	44	Total 44	O 44	0	0
38	P	70	Total 70	O 70	0	0
38	Q	48	Total 48	O 48	0	0
38	R	82	Total 82	O 82	0	0
38	S	33	Total 33	O 33	0	0
38	T	39	Total 39	O 39	0	0
38	U	29	Total 29	O 29	0	0
38	V	13	Total 13	O 13	0	0
38	W	69	Total 69	O 69	0	0
38	X	27	Total 27	O 27	0	0
38	Y	100	Total 100	O 100	0	0

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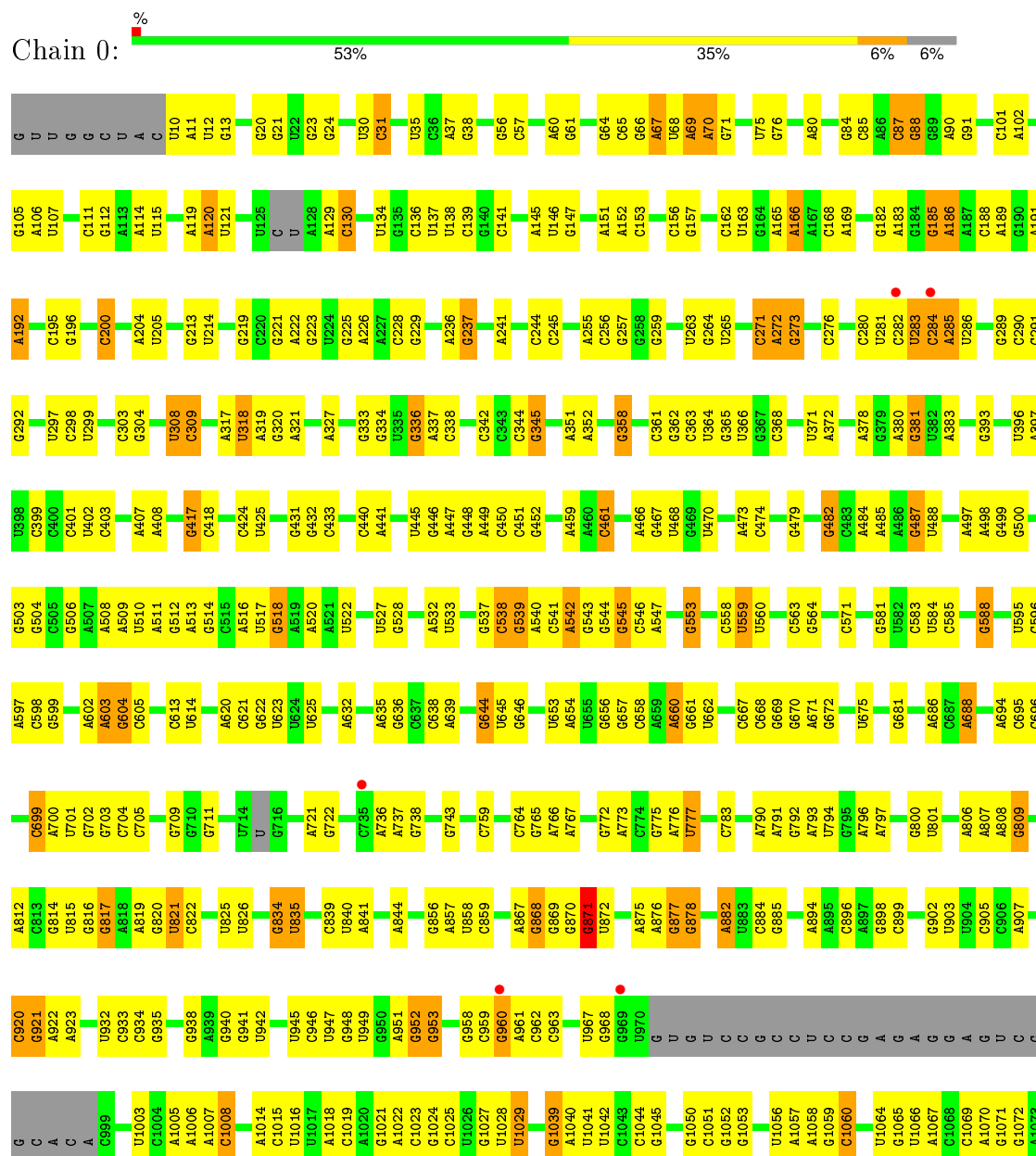
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	Z	35	Total	O	0	0
			35	35		

### 3 Residue-property plots

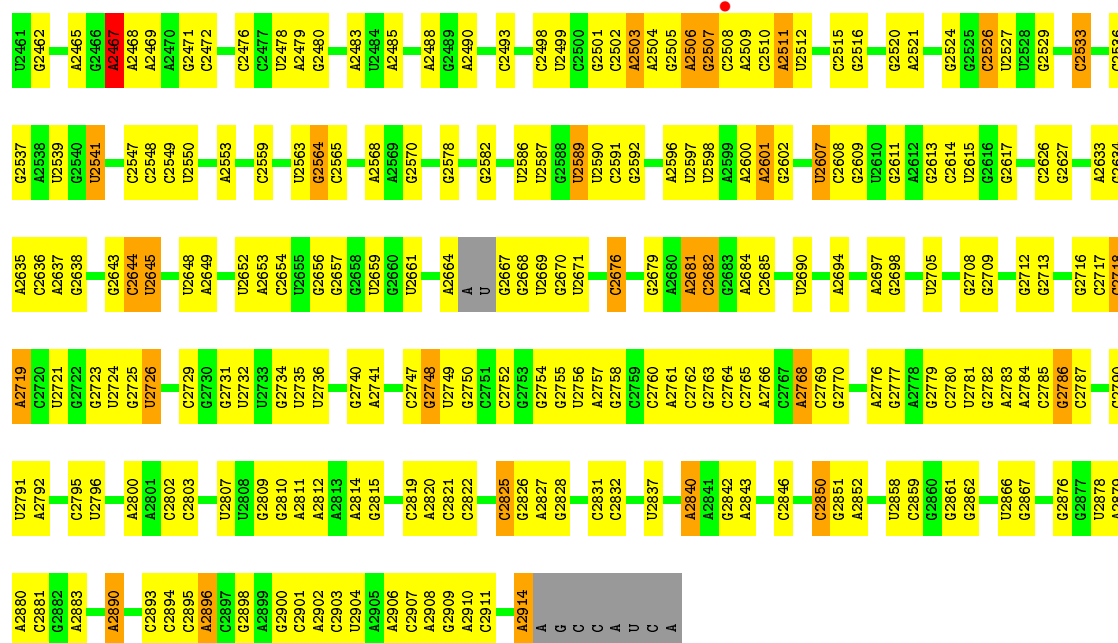
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 23S RIBOSOMAL RNA



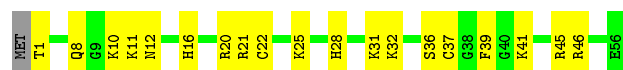
A2369	G2272	C	G	C2035	C1940	U1825	C1735	G1636	G1535	C1439	A1348	A1242	A1173	G1074
A2370	C2273	A	U	C2036	A1941	C1826	A1736	A1637	C1536	U1440	A1352	C1243	A1174	A1081
G2371	G2274	G	C	C2037	C1942	A1829	U1741	U1638	C1537	A1441	C1352	U1244	G1175	
A2372	G2275	A	C	A2038	C1943	C1830	G1742	A1641	G1543	A1442	G1353	U1245	C1176	A1086
U2373	U2276	C	C	C2039	G1946	C1834	G1743	A1642	U1544	U1446	G1354	A1246	A1177	G1087
	U2277	A	G	C2040	G1947	U1835	G1744	C1643	C1545		C1355	C1250	G1178	A1088
U2377	C2281	C	G	G2044	G1948	G1834					C1360	C1251	U1180	
U2378	U2282	A	U	G2045	G1949	U1835	U1748	A1653	A1559	C1451	C1363	C1261	A1181	A1097
A2380	A2291	G	U	G2050	G1950	U1838	C1750	U1654	U		G1366	G1260	A1098	
C2381		G	G	G2051	A1840	A1839	G1751	G1655	U1561	U1461	C1366	A1261	C1182	G1099
A2382	U2297	G	C	A2054	C1841	G1841	G1752	A1656	C1562	C1462			C1184	
G2383	U2298	A	A	A2055	A1845		C1753	A1657	G1563		U1266	U1266	U1185	C1102
U2384	C2299	A	G	A2056	C		A1754	A1658	C1564		G1267	G1267	C1186	
G2385	A2300	U	G	U2064	U		A1755	A1659	G1571	A1471	G1268	G1268	U1187	U1109
U2386	A2301	C	A	C2065	A		U1761	C1666	A1572	C1474	A1278	G1269	C1188	G1110
U2387	A2302	C	U	G2072	U		C1762	A1667	A1573		U1279	G1273	G1190	U1111
C2388	A2303	U	A	A2074	G		C1763	U1668	C1574		C1277	C1277	G1191	G1112
U2389		C	G	C1854	A		U1766	G1669	U1580	A1477	G1376		A1189	
	C2309	C	U	C1856	C		A1767	A1670	A1581	G1479	G1386		G1196	U1120
	G2312	C	A		C		C1768	C1674	C1584	C1483	G1387	A1287	C1197	U1121
A2401	C2313	G	G	U1964	U		C1769	U1677	C1585	G1484		C1289	U1198	U1122
A2402	C2314	U	G	C1965	U		U1770	A1678	C1586		G1391	G1290	A1199	A1123
	C2315	C	A	U1966			C1771	A1679	U1587	U1488	A1392	G1291	A1194	G1118
C2411	G2316	G	U	U1967			C1772	C1679	G1588	G1489	A1393	G1292	G1195	G1119
G2412	C2317	G	C	A1968			G1773	C1682	G1589	G1490	C1394	U1293	A1202	C1129
A2413	U2320	U	G	U1969			G1774	A1683	G1592	A1493		A1294	A1203	U1130
A2414	A2321	C	U	G1970			A1778	G1684	C1593	A1494	G1398	G1295	G1204	G1131
A2415		U	U	U1971			A1779	A1685	C1594	U1496	A1399	G1299	U1205	A1132
U2419	G2324	U	U	U1972			C1783	A1686	C1595	G1497	A1406	G1299	U1206	G1137
G2420	U2325	C	A	C1973			U1784	A1687	C1596	U1500	A1408	U1304	A1207	G1138
G2421	C2326	C	C	C1975			G1785	U1702	G1597	A1501	G1409	C1305	C1208	U1139
U2422		G	G	G1976			C1786	U1702	U1599	U1502		U1306	G1210	C1140
U2424	C2329	A	G	U1977			U1788		G1600	U1503	A1413	A1307	G1211	A1150
A2425	U2330	G	U	A1978			G1789	A1710	A1603	U1504	A1414	A1308	C1212	G1151
U2426		U	U	U1980			U1791	A1711	G1604	U1505	G1415	U1314	C1213	A1154
	C2335	C	A	U1996			C1790	A1712	G1605	U1506	G1416	G1315	A1214	A1155
C2431	G2336	C	C	A1997			G1791	G1713	G1605		G1417	G1316	G1215	C1156
A2432	C2337	C	G				C1798	C1715	G1614	C1513	U1418	G1325	C1217	C1157
A2433	G2338	A	G	G2000			G1799	A1716	A1615	C1514	U1419	G1326		G1158
A2434		C	C	G2001				A1717	A1616	U1515	C1420	A1328	G1226	G1159
U2435	A	G	G	C2002			G1804	G1718	C1617	U1516	U1422	G1227	G1160	A1161
	G2344	A	U	U2003			G1805	G1719	G1618	C1517	C1423	G1331	G1162	
G2442		C	A	G2004			G1806		G1619	A1518		G1332	U1163	
C2443	A2353	G	G	G2005			C1810	U1722	C1620	U1524	A1427	U1333	U1164	
U2444	A2354	C	C	U2008			A1811	G1724	A1624	G1525	A1232	U1334	G1165	
U2445		G	G	A2011			G1819	C1725	U1625	A1526	U1234	C1335	A1166	
G2446	C2359	G	G	U2012			A1821	G1730	A1626	A1527	G1430		G1167	
	A2361	C	C	G2013			A1822	C1731	G1627	G1529	A1434	G1340	G1168	
G2453		C	C	A			A1823	C1732	C1633		U1435	A1341	U1169	
C2454	A2362	U	U	U2032			G1823	A1733	G1634	A1533	C1436	C1342	U1170	
A2455	G2363	C	C	C1935			C1936	C1734	U1635	C1534	G1438	C1343	A1171	
A2456		C	C	C1936									G1172	
A2460	G2365	G	G	U2034										





• Molecule 2: 50S RIBOSOMAL PROTEIN L37E

Chain 1: 65% 33%



• Molecule 3: 50S RIBOSOMAL PROTEIN L39E

Chain 2: 4% 46% 46% 8%



• Molecule 4: 50S RIBOSOMAL PROTEIN L44E

Chain 3: 55% 45%

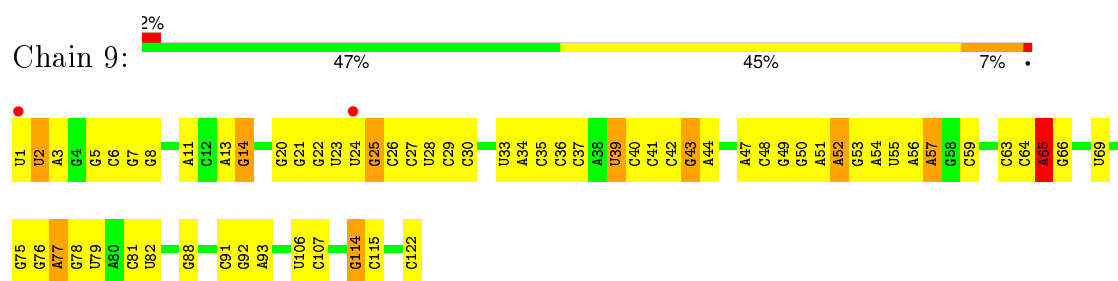


• Molecule 5: QUINUPRISTIN

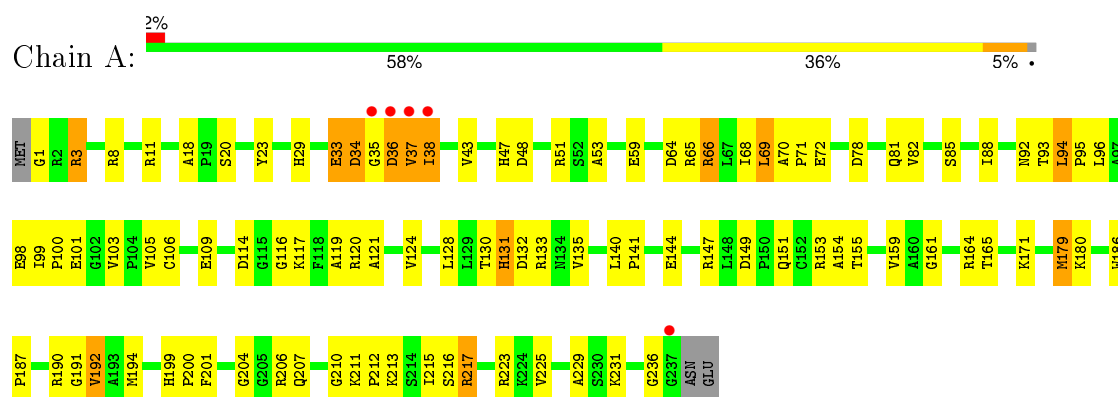
Chain 4: 88% 13%



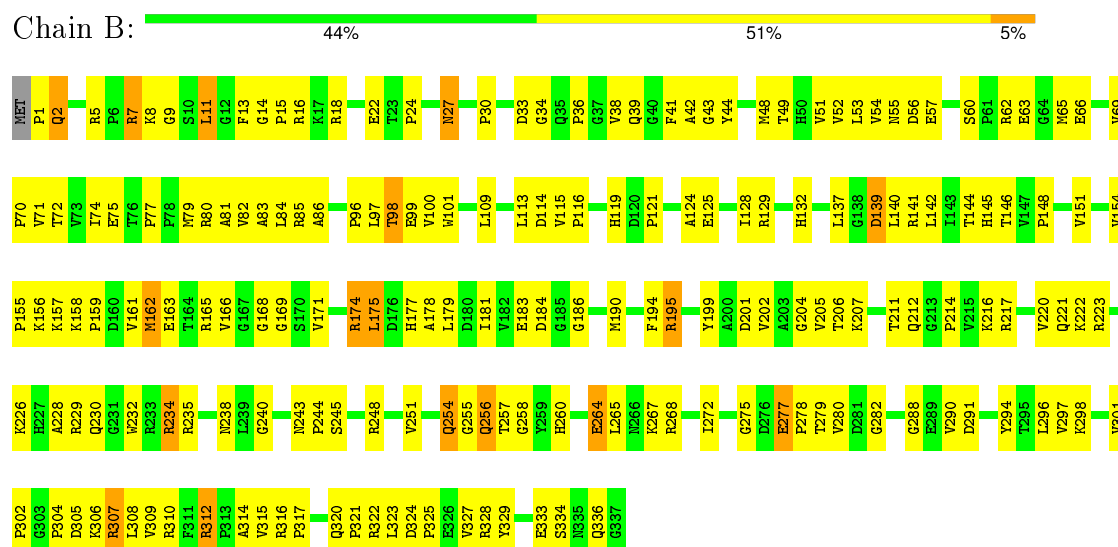
• Molecule 6: 5S RIBOSOMAL RNA



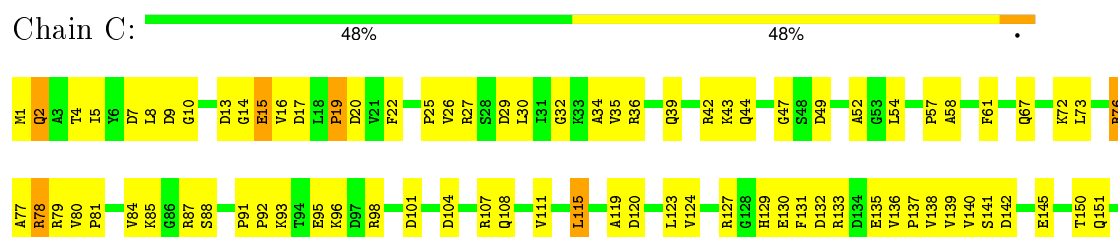
• Molecule 7: 50S RIBOSOMAL PROTEIN L2P

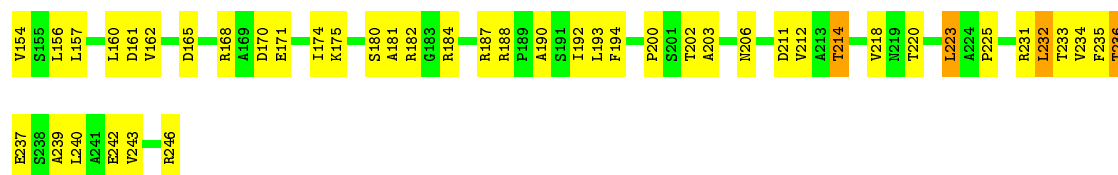


• Molecule 8: 50S RIBOSOMAL PROTEIN L3P

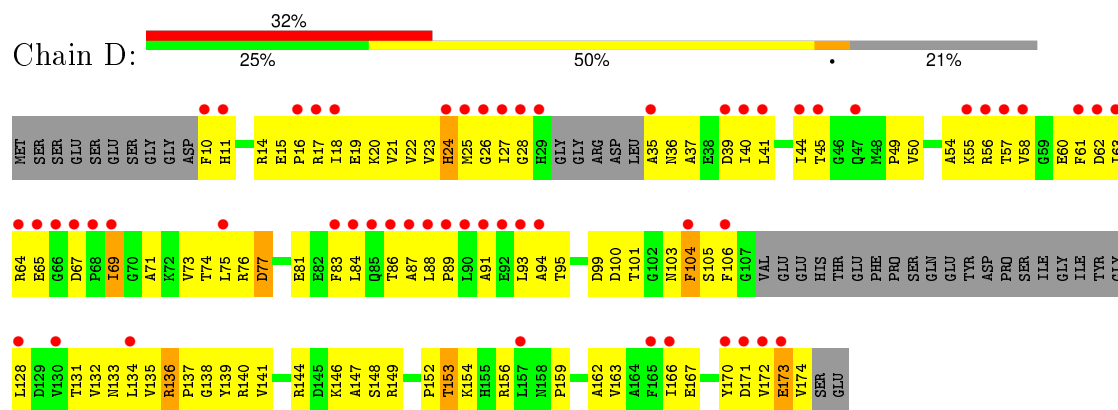


• Molecule 9: 50S RIBOSOMAL PROTEIN L4E

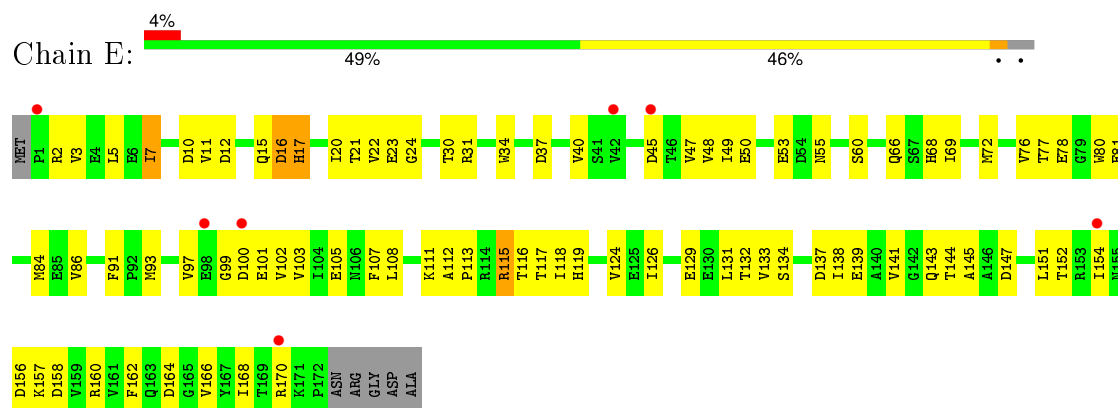




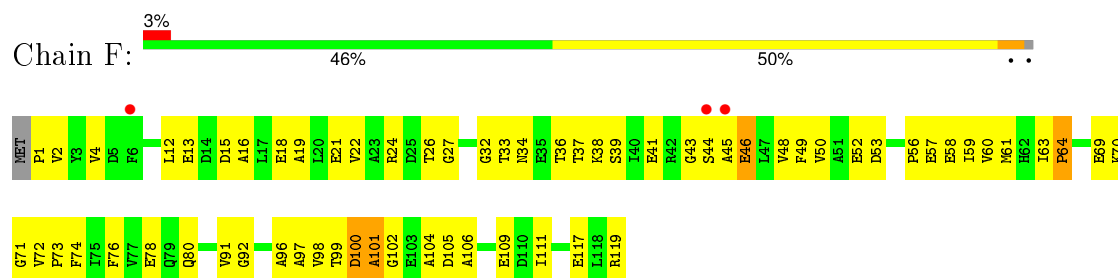
• Molecule 10: 50S RIBOSOMAL PROTEIN L5P



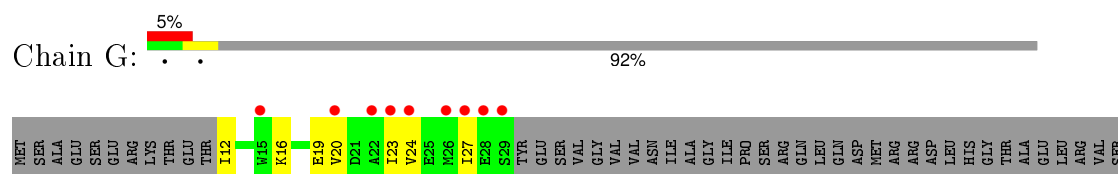
• Molecule 11: 50S RIBOSOMAL PROTEIN L6P

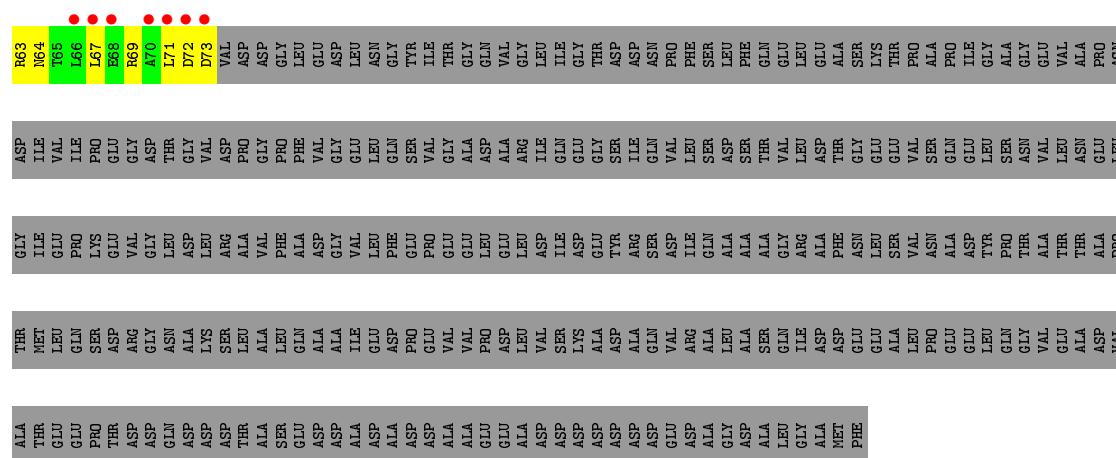


• Molecule 12: 50S RIBOSOMAL PROTEIN L7AE

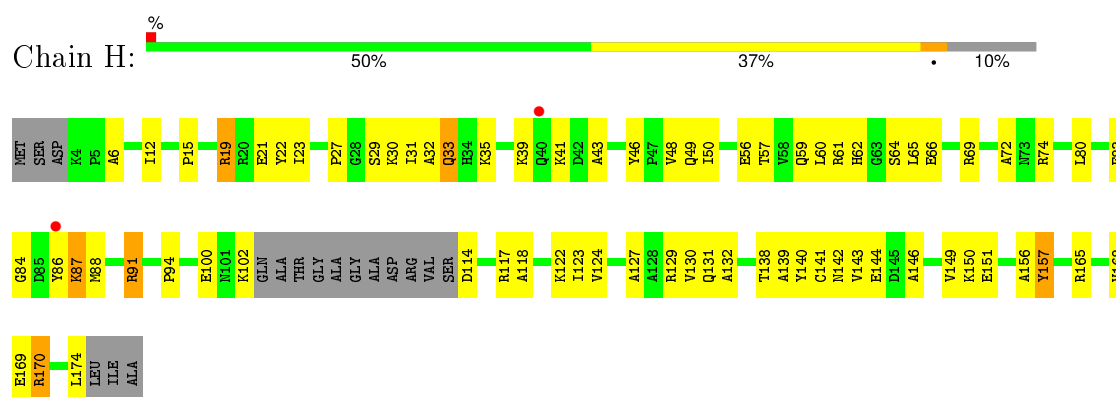


• Molecule 13: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

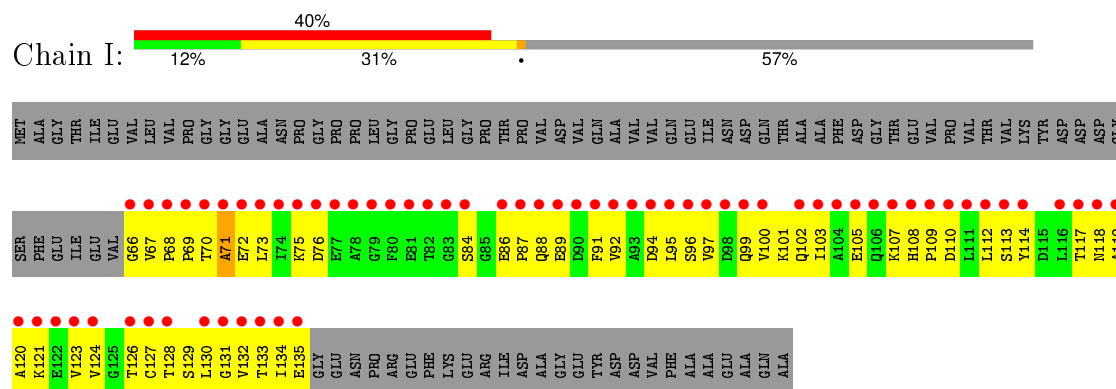




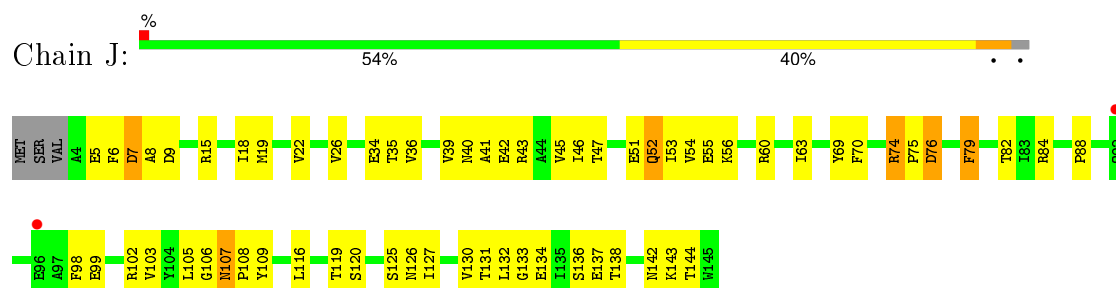
• Molecule 14: 50S RIBOSOMAL PROTEIN L10E



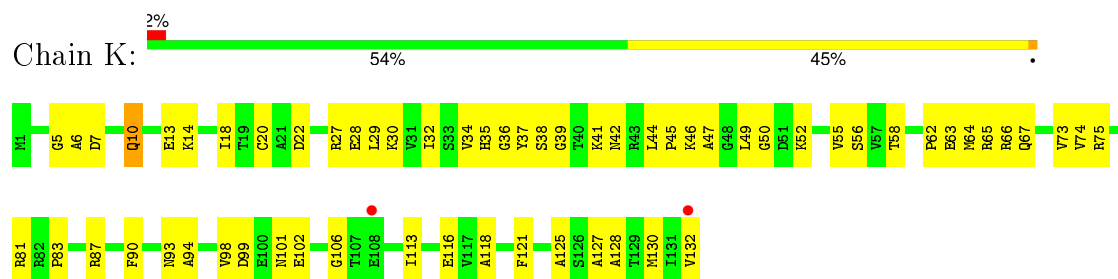
• Molecule 15: 50S RIBOSOMAL PROTEIN L11P



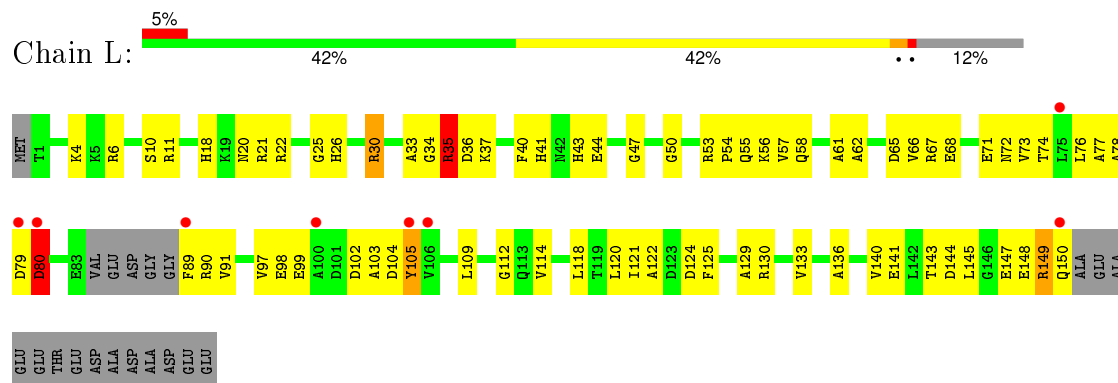
• Molecule 16: 50S RIBOSOMAL PROTEIN L13P



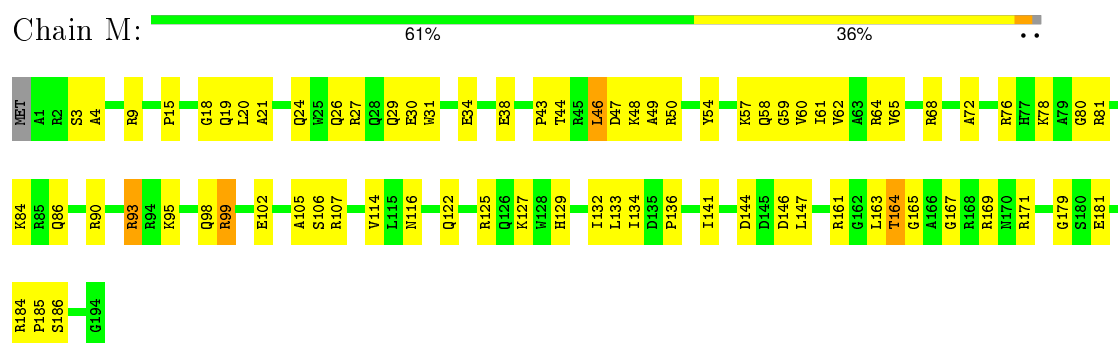
- Molecule 17: 50S RIBOSOMAL PROTEIN L14P



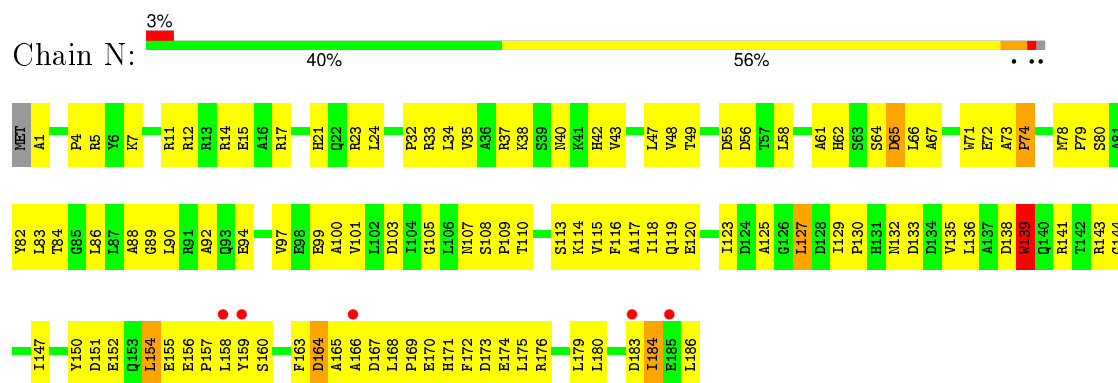
- Molecule 18: 50S RIBOSOMAL PROTEIN L15P



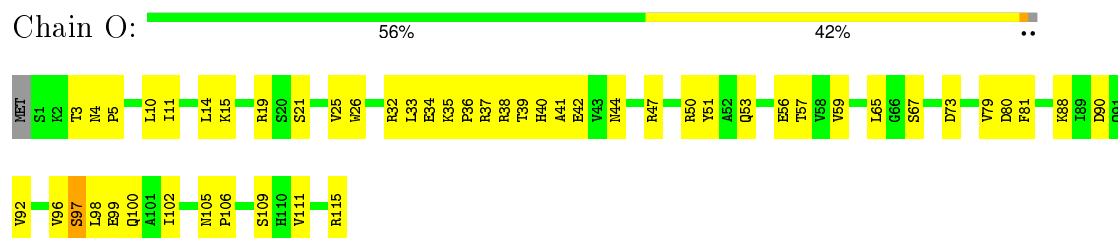
- Molecule 19: 50S RIBOSOMAL PROTEIN L15E



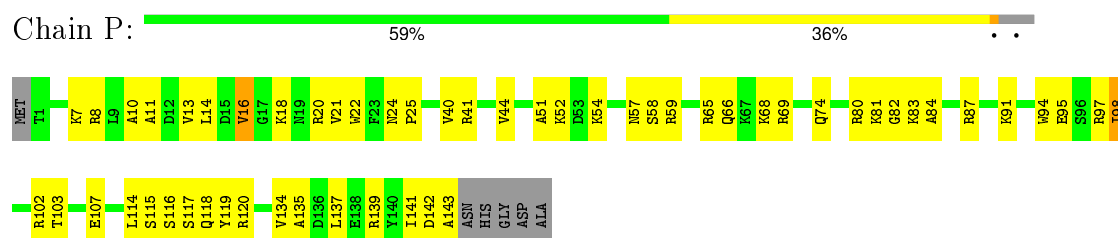
- Molecule 20: 50S RIBOSOMAL PROTEIN L18P



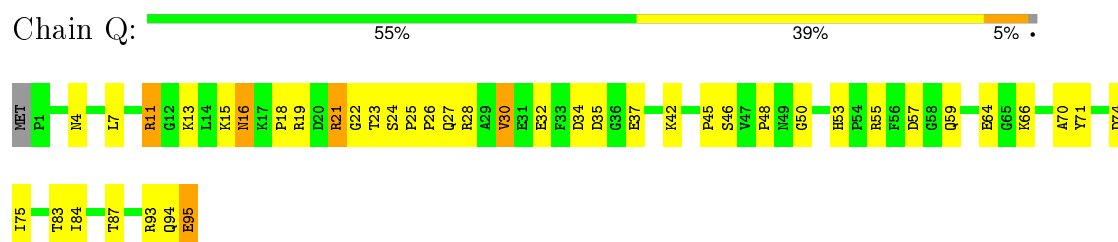
- Molecule 21: 50S RIBOSOMAL PROTEIN L18E



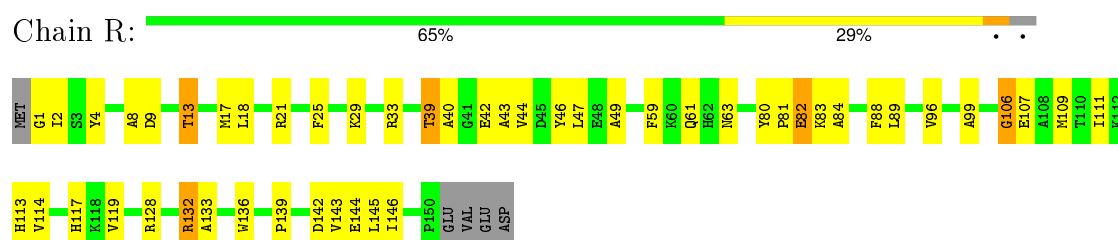
• Molecule 22: 50S RIBOSOMAL PROTEIN L19E



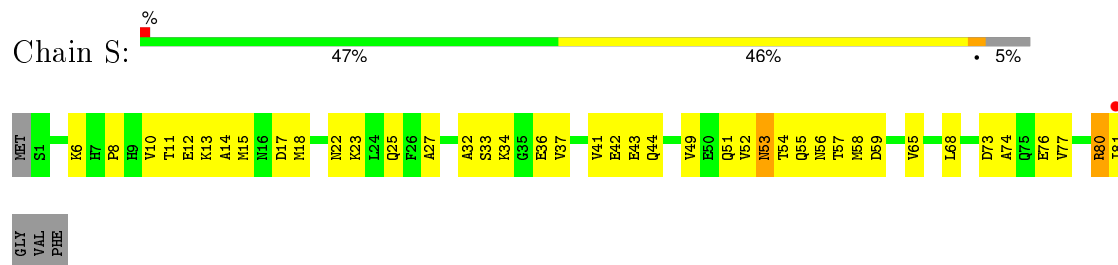
• Molecule 23: 50S RIBOSOMAL PROTEIN L21E



• Molecule 24: 50S RIBOSOMAL PROTEIN L22P

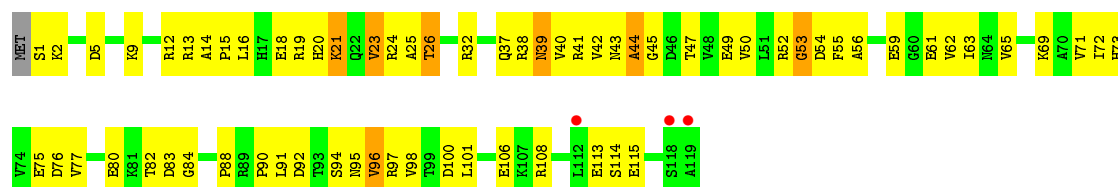


• Molecule 25: 50S RIBOSOMAL PROTEIN L23P

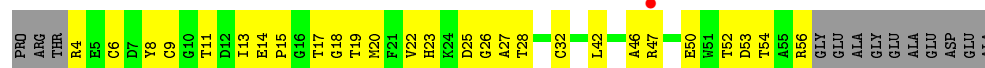


• Molecule 26: 50S RIBOSOMAL PROTEIN L24P

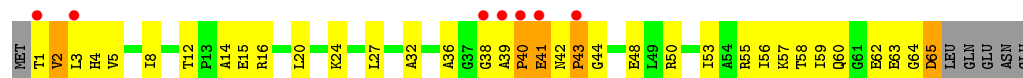




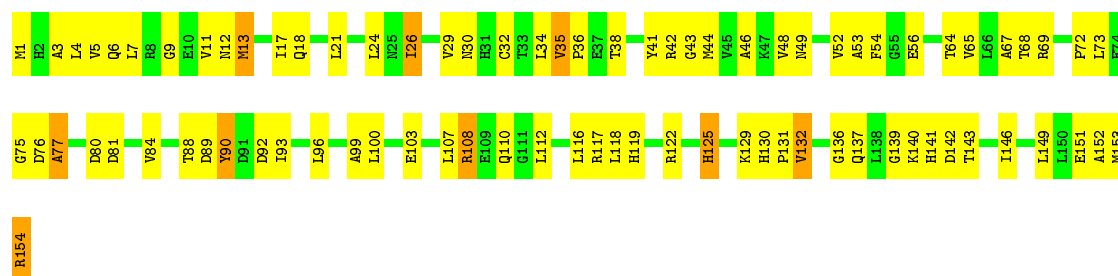
• Molecule 27: 50S RIBOSOMAL PROTEIN L24E



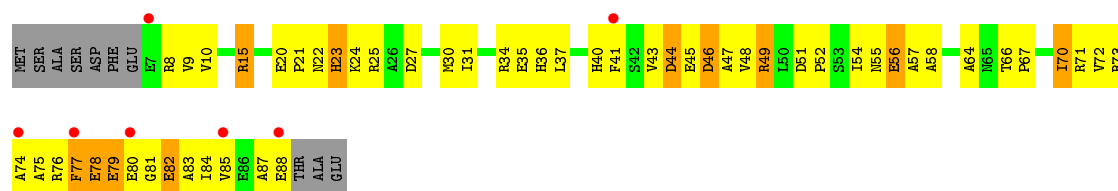
• Molecule 28: 50S RIBOSOMAL PROTEIN L29P



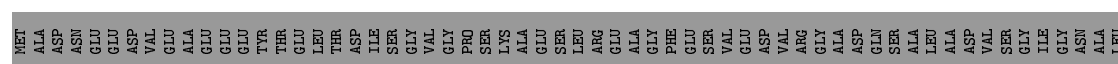
• Molecule 29: 50S RIBOSOMAL PROTEIN L30P

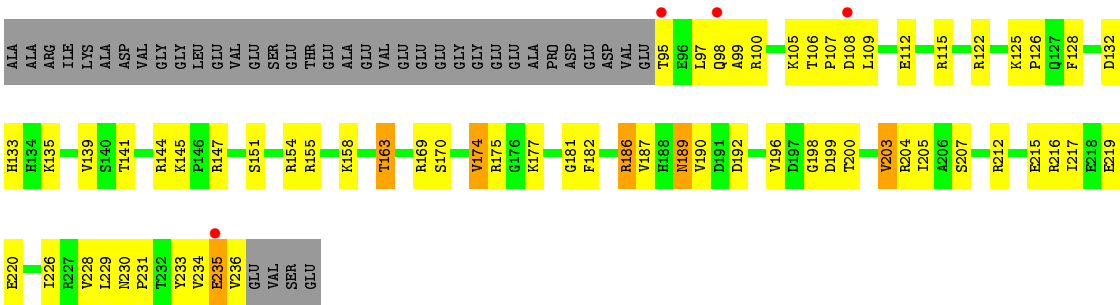


• Molecule 30: 50S RIBOSOMAL PROTEIN L31E

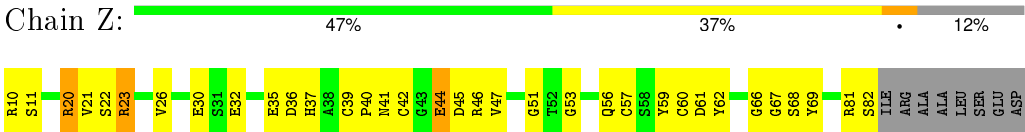


• Molecule 31: 50S RIBOSOMAL PROTEIN L32E





• Molecule 32: 50S RIBOSOMAL PROTEIN L37AE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.69 Å   299.78 Å   573.88 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.98 – 2.90 49.95 – 2.89	Depositor EDS
% Data completeness (in resolution range)	83.8 (29.98-2.90) 83.4 (49.95-2.89)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.91 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.171   ,   0.223 (Not available)   ,   (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 335760 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99111	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, DBB, CD, 1MA, UR3, OMU, 004, MHV, MHW, MHT, MHU, PSU

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	0	0.37	0/65957	0.69	13/102867 (0.0%)
2	1	0.38	0/438	0.61	0/578
3	2	0.34	0/401	0.56	0/529
4	3	0.37	0/771	0.57	0/1024
5	4	1.63	0/13	1.38	0/15
6	9	0.35	0/2904	0.69	1/4526 (0.0%)
7	A	0.33	0/1786	0.65	0/2408
8	B	0.33	0/2690	0.63	0/3652
9	C	0.36	0/1884	0.63	0/2551
10	D	0.32	0/1111	0.56	0/1498
11	E	0.33	0/1382	0.58	0/1880
12	F	0.33	0/901	0.57	0/1224
13	G	0.30	0/241	0.48	0/324
14	H	0.34	0/1302	0.64	0/1743
15	I	0.31	0/526	0.55	0/716
16	J	0.35	0/1136	0.59	0/1530
17	K	0.35	0/1001	0.67	0/1347
18	L	0.32	0/1130	0.63	0/1509
19	M	0.34	0/1582	0.60	0/2117
20	N	0.30	0/1474	0.64	0/1999
21	O	0.34	0/874	0.60	0/1181
22	P	0.33	0/1147	0.54	0/1528
23	Q	0.35	0/749	0.66	0/1005
24	R	0.34	0/1172	0.63	0/1578
25	S	0.34	0/648	0.59	0/875
26	T	0.32	0/958	0.61	0/1289
27	U	0.32	0/417	0.58	0/562
28	V	0.29	0/502	0.55	0/675
29	W	0.36	0/1219	0.62	0/1655
30	X	0.33	0/664	0.61	0/895
31	Y	0.35	0/1146	0.62	0/1536
32	Z	0.35	0/589	0.67	0/787

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.36	0/98715	0.67	14/147603 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	20
6	9	0	1
29	W	0	1
All	All	0	22

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	C1'-O4'-C4'	-6.45	104.74	109.90
1	0	1942	A	C5'-C4'-C3'	6.01	125.61	116.00
1	0	871	G	C5'-C4'-O4'	-5.83	102.10	109.10
1	0	2291	A	N9-C1'-C2'	5.68	121.39	114.00
1	0	2726	U	N1-C1'-C2'	5.63	121.33	114.00

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	792	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59020	0	29811	1125	0
2	1	431	0	426	27	0
3	2	396	0	413	30	0
4	3	755	0	728	38	0
5	4	73	0	64	1	0
6	9	2599	0	1325	72	0
7	A	1753	0	1766	116	0
8	B	2625	0	2533	203	0
9	C	1859	0	1816	140	0
10	D	1094	0	1085	111	0
11	E	1357	0	1266	79	0
12	F	890	0	843	56	0
13	G	240	0	231	19	0
14	H	1282	0	1292	88	0
15	I	519	0	500	62	0
16	J	1120	0	1098	75	0
17	K	992	0	1031	72	0
18	L	1118	0	1076	82	0
19	M	1558	0	1566	82	0
20	N	1445	0	1401	145	0
21	O	865	0	873	48	0
22	P	1136	0	1123	57	0
23	Q	735	0	729	45	0
24	R	1149	0	1122	59	0
25	S	641	0	605	39	0
26	T	950	0	923	71	0
27	U	410	0	364	35	0
28	V	499	0	511	43	0
29	W	1196	0	1137	116	0
30	X	654	0	653	59	0
31	Y	1130	0	1133	69	0
32	Z	578	0	539	24	0
33	3	1	0	0	0	0
33	7	110	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	7	2	0	0	0	0
35	8	74	0	0	0	0
35	9	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	3	1	0	0	0	0
36	8	10	0	0	2	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	2	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5874	0	0	198	0
38	1	59	0	0	8	0
38	2	46	0	0	5	0
38	3	67	0	0	11	0
38	4	2	0	0	0	0
38	9	141	0	0	9	0
38	A	119	0	0	19	0
38	B	144	0	0	20	0
38	C	176	0	0	37	0
38	D	48	0	0	22	0
38	E	42	0	0	11	0
38	F	26	0	0	5	0
38	G	20	0	0	2	0
38	H	67	0	0	15	0
38	I	9	0	0	3	0
38	J	56	0	0	4	0
38	K	60	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	L	80	0	0	20	0
38	M	125	0	0	12	0
38	N	60	0	0	11	0
38	O	44	0	0	7	0
38	P	70	0	0	5	0
38	Q	48	0	0	7	0
38	R	82	0	0	6	0
38	S	33	0	0	5	0
38	T	39	0	0	8	0
38	U	29	0	0	3	0
38	V	13	0	0	3	0
38	W	69	0	0	12	0
38	X	27	0	0	6	0
38	Y	100	0	0	15	0
38	Z	35	0	0	2	0
All	All	99111	0	59983	2986	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 20.

The worst 5 of 2986 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)
6:9:6:C:H5''	20:N:37:ARG:NH1	1.59	1.16
1:0:156:C:H5''	19:M:171:ARG:HD3	1.25	1.15
6:9:6:C:H5''	20:N:37:ARG:HH12	0.97	1.14
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.07
1:0:871:G:H8	1:0:871:G:H5'	1.10	1.06

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	
2	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
3	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
4	3	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	17	51
5	4	2/8 (25%)	2 (100%)	0	0	100	100
7	A	235/240 (98%)	203 (86%)	28 (12%)	4 (2%)	11	38
8	B	335/338 (99%)	294 (88%)	36 (11%)	5 (2%)	13	42
9	C	244/246 (99%)	218 (89%)	21 (9%)	5 (2%)	9	33
10	D	134/177 (76%)	92 (69%)	39 (29%)	3 (2%)	8	31
11	E	170/178 (96%)	158 (93%)	11 (6%)	1 (1%)	30	67
12	F	117/120 (98%)	100 (86%)	12 (10%)	5 (4%)	3	13
13	G	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	4	15
14	H	156/177 (88%)	139 (89%)	14 (9%)	3 (2%)	10	35
15	I	68/162 (42%)	50 (74%)	16 (24%)	2 (3%)	6	23
16	J	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	9	32
17	K	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
18	L	141/165 (86%)	113 (80%)	24 (17%)	4 (3%)	6	24
19	M	192/195 (98%)	175 (91%)	17 (9%)	0	100	100
20	N	184/187 (98%)	154 (84%)	21 (11%)	9 (5%)	3	10
21	O	113/116 (97%)	100 (88%)	12 (11%)	1 (1%)	21	57
22	P	141/149 (95%)	127 (90%)	14 (10%)	0	100	100
23	Q	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	17	51
24	R	148/155 (96%)	133 (90%)	14 (10%)	1 (1%)	26	63
25	S	79/85 (93%)	68 (86%)	11 (14%)	0	100	100
26	T	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	7	26
27	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
28	V	63/71 (89%)	53 (84%)	6 (10%)	4 (6%)	2	5
29	W	152/154 (99%)	138 (91%)	13 (9%)	1 (1%)	26	63
30	X	80/92 (87%)	66 (82%)	9 (11%)	5 (6%)	2	5
31	Y	140/241 (58%)	133 (95%)	7 (5%)	0	100	100
32	Z	71/83 (86%)	54 (76%)	14 (20%)	3 (4%)	3	13
All	All	3707/4445 (83%)	3245 (88%)	397 (11%)	65 (2%)	11	37

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	34	ASP
7	A	37	VAL
8	B	184	ASP
9	C	8	LEU
10	D	173	GLU

### 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	
2	1	46/47 (98%)	46 (100%)	0	100	100
3	2	42/46 (91%)	41 (98%)	1 (2%)	57	86
4	3	79/79 (100%)	79 (100%)	0	100	100
5	4	2/2 (100%)	2 (100%)	0	100	100
7	A	179/182 (98%)	168 (94%)	11 (6%)	23	56
8	B	282/283 (100%)	264 (94%)	18 (6%)	22	53
9	C	193/193 (100%)	181 (94%)	12 (6%)	23	55
10	D	117/148 (79%)	109 (93%)	8 (7%)	20	49
11	E	152/156 (97%)	146 (96%)	6 (4%)	39	75
12	F	93/94 (99%)	90 (97%)	3 (3%)	46	81
13	G	27/283 (10%)	27 (100%)	0	100	100
14	H	134/145 (92%)	128 (96%)	6 (4%)	34	70
15	I	58/130 (45%)	58 (100%)	0	100	100
16	J	118/121 (98%)	110 (93%)	8 (7%)	20	49
17	K	106/106 (100%)	105 (99%)	1 (1%)	84	96
18	L	113/127 (89%)	107 (95%)	6 (5%)	28	63
19	M	158/159 (99%)	151 (96%)	7 (4%)	35	70
20	N	149/150 (99%)	144 (97%)	5 (3%)	44	79
21	O	93/94 (99%)	90 (97%)	3 (3%)	46	81
22	P	113/117 (97%)	109 (96%)	4 (4%)	43	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	Q	79/80 (99%)	74 (94%)	5 (6%)	22	54
24	R	117/122 (96%)	113 (97%)	4 (3%)	44	79
25	S	71/74 (96%)	68 (96%)	3 (4%)	36	73
26	T	105/106 (99%)	98 (93%)	7 (7%)	20	50
27	U	44/52 (85%)	44 (100%)	0	100	100
28	V	51/57 (90%)	50 (98%)	1 (2%)	63	88
29	W	130/130 (100%)	122 (94%)	8 (6%)	23	55
30	X	66/74 (89%)	58 (88%)	8 (12%)	6	18
31	Y	120/196 (61%)	114 (95%)	6 (5%)	30	65
32	Z	60/68 (88%)	56 (93%)	4 (7%)	20	50
All	All	3097/3621 (86%)	2952 (95%)	145 (5%)	32	68

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	J	7	ASP
19	M	68	ARG
30	X	82	GLU
16	J	52	GLN
17	K	10	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
16	J	52	GLN
19	M	24	GLN
30	X	23	HIS
16	J	107	ASN
18	L	18	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	245 (8%)	23 (0%)
6	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	261 (9%)	24 (0%)

5 of 261 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1474	C
1	0	2791	U
1	0	1377	C
1	0	1450	C

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

10 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	$\# Z  > 2$
1	OMU	0	2587	1,35	12,22,23	1.07	1 (8%)	19,31,34	3.16	2 (10%)
1	OMG	0	2588	1	17,26,27	1.05	1 (5%)	21,38,41	2.53	3 (14%)
1	UR3	0	2619	1	12,22,23	0.84	0	16,32,35	0.76	0
1	PSU	0	2621	1	13,21,22	1.67	2 (15%)	18,30,33	6.07	4 (22%)
1	1MA	0	628	1,35	14,25,26	1.02	1 (7%)	15,37,40	1.13	1 (6%)
5	MHW	4	1	33,5	9,9,10	2.52	4 (44%)	8,11,13	1.21	1 (12%)
5	DBB	4	3	5	4,5,6	0.97	0	3,5,7	1.56	1 (33%)
5	MHU	4	5	5	13,15,16	2.77	6 (46%)	15,19,21	1.28	1 (6%)
5	MHV	4	6	5	7,9,10	1.96	2 (28%)	8,11,13	1.58	2 (25%)
5	004	4	7	5	9,10,11	3.13	3 (33%)	10,12,14	2.79	3 (30%)

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
1	OMU	0	2587	1,35	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3
5	MHW	4	1	33,5	-	0/2/2/4	0/1/1/1
5	DBB	4	3	5	-	0/2/4/6	0/0/0/0
5	MHU	4	5	5	-	0/8/12/14	0/1/1/1
5	MHV	4	6	5	-	0/1/12/14	0/1/1/1
5	004	4	7	5	-	0/4/6/8	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.12	1.47	1.52
5	4	6	MHV	CD2-CG	2.27	1.55	1.50
5	4	7	004	CG1-CB	2.39	1.42	1.39
5	4	1	MHW	CA-C	2.46	1.51	1.48
5	4	5	MHU	CE1-CD1	2.53	1.43	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.18	114.82	128.33
1	0	2588	OMG	C5-C6-N1	-8.70	111.69	123.59
1	0	628	1MA	C2-N3-C4	-3.72	110.64	116.40
5	4	7	004	CB-CA-N	-3.53	104.21	112.54
5	4	5	MHU	O-C-CA	-3.41	116.43	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 232 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 ⓘ

### 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	0	2749/2922 (94%)	-0.18	33 (1%) 81 78	18, 42, 85, 147	0
2	1	56/57 (98%)	-0.55	0 100 100	23, 28, 34, 41	0
3	2	46/50 (92%)	0.11	2 (4%) 39 32	24, 56, 82, 96	0
4	3	92/92 (100%)	0.03	1 (1%) 82 80	30, 48, 61, 79	0
5	4	2/8 (25%)	-0.10	0 100 100	49, 49, 49, 54	0
6	9	122/122 (100%)	-0.12	2 (1%) 74 72	36, 57, 84, 148	0
7	A	237/240 (98%)	-0.10	5 (2%) 67 62	21, 44, 80, 100	0
8	B	337/338 (99%)	-0.11	0 100 100	23, 50, 76, 86	0
9	C	246/246 (100%)	-0.31	0 100 100	19, 39, 62, 72	0
10	D	140/177 (79%)	1.76	56 (40%) 0 0	47, 94, 117, 125	0
11	E	172/178 (96%)	0.49	7 (4%) 41 34	41, 61, 83, 88	0
12	F	119/120 (99%)	0.37	3 (2%) 61 55	41, 63, 88, 104	0
13	G	29/348 (8%)	2.38	16 (55%) 0 0	71, 87, 95, 96	0
14	H	160/177 (90%)	0.11	2 (1%) 79 78	36, 52, 88, 105	0
15	I	70/162 (43%)	4.12	65 (92%) 0 0	108, 118, 136, 138	0
16	J	142/145 (97%)	-0.06	2 (1%) 78 76	34, 46, 66, 86	0
17	K	132/132 (100%)	-0.21	2 (1%) 76 74	26, 46, 65, 75	0
18	L	145/165 (87%)	0.40	8 (5%) 29 22	22, 60, 100, 114	0
19	M	194/195 (99%)	-0.47	0 100 100	25, 36, 52, 59	0
20	N	186/187 (99%)	0.06	5 (2%) 58 52	34, 58, 100, 110	0
21	O	115/116 (99%)	-0.12	0 100 100	33, 47, 66, 71	0
22	P	143/149 (95%)	-0.02	0 100 100	33, 49, 61, 73	0
23	Q	95/96 (98%)	-0.13	0 100 100	28, 39, 54, 66	0
24	R	150/155 (96%)	-0.19	0 100 100	28, 40, 58, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	S	81/85 (95%)	0.02	1 (1%) 81 78	37, 52, 71, 79	0
26	T	119/120 (99%)	0.23	3 (2%) 61 55	35, 51, 80, 94	0
27	U	53/66 (80%)	0.09	1 (1%) 70 66	39, 51, 67, 78	0
28	V	65/71 (91%)	0.71	7 (10%) 8 4	46, 66, 105, 112	0
29	W	154/154 (100%)	-0.16	0 100 100	27, 42, 59, 71	0
30	X	82/92 (89%)	0.37	7 (8%) 13 8	38, 55, 76, 96	0
31	Y	142/241 (58%)	-0.08	4 (2%) 56 50	24, 40, 62, 81	0
32	Z	73/83 (87%)	-0.18	0 100 100	39, 53, 69, 87	0
All	All	6648/7489 (88%)	0.00	232 (3%) 48 40	18, 46, 91, 148	0

The worst 5 of 232 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	I	88	GLN	8.7
15	I	132	VAL	8.5
15	I	128	THR	7.9
15	I	70	THR	7.5
15	I	66	GLY	7.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	OMG	0	2588	24/25	0.98	0.14	-	28,31,34,35	0
5	MHW	4	1	9/10	0.96	0.20	-	46,47,49,50	0
1	PSU	0	2621	20/21	0.98	0.14	-	33,35,37,38	0
5	MHV	4	6	9/10	0.94	0.18	-	53,55,59,59	0
1	UR3	0	2619	21/22	0.98	0.13	-	30,35,39,42	0
1	OMU	0	2587	21/22	0.98	0.15	-	29,32,37,38	0
5	DBB	4	3	6/7	0.94	0.18	-	51,51,52,53	0
5	MHU	4	5	15/16	0.95	0.17	-	56,59,62,63	0
1	1MA	0	628	23/24	0.98	0.15	-	25,28,31,32	0
5	004	4	7	10/11	0.95	0.20	-	45,48,49,51	0

## 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	8	8574	1/1	0.93	0.64	47.17	60,60,60,60	0
36	CL	8	8815	1/1	0.87	0.43	38.62	88,88,88,88	0
35	NA	8	8521	1/1	0.94	0.42	36.34	61,61,61,61	0
35	NA	8	8582	1/1	0.08	0.93	35.68	81,81,81,81	0
35	NA	9	8583	1/1	0.73	0.71	28.85	85,85,85,85	0
35	NA	8	8556	1/1	0.97	0.53	28.41	43,43,43,43	0
35	NA	8	8562	1/1	0.89	0.34	26.48	75,75,75,75	0
35	NA	8	8527	1/1	0.94	0.31	24.60	60,60,60,60	0
35	NA	L	8580	1/1	0.94	0.71	23.86	61,61,61,61	0
35	NA	8	8559	1/1	0.89	0.49	23.55	54,54,54,54	0
35	NA	8	8502	1/1	0.98	0.26	21.86	44,44,44,44	0
35	NA	8	8573	1/1	0.71	0.45	19.98	54,54,54,54	0
35	NA	8	8568	1/1	0.83	0.35	19.33	72,72,72,72	0
33	MG	7	8064	1/1	0.85	0.39	18.80	37,37,37,37	0
35	NA	8	8578	1/1	0.97	0.38	18.17	45,45,45,45	0
35	NA	8	8572	1/1	0.53	0.47	17.36	75,75,75,75	0
35	NA	R	8586	1/1	0.60	0.59	17.05	75,75,75,75	0
35	NA	8	8561	1/1	0.96	0.21	16.92	44,44,44,44	0
35	NA	8	8535	1/1	0.93	0.26	15.24	47,47,47,47	0
35	NA	8	8529	1/1	0.76	0.31	14.98	81,81,81,81	0
35	NA	8	8532	1/1	0.74	0.35	14.43	47,47,47,47	0
35	NA	8	8569	1/1	0.91	0.37	13.90	65,65,65,65	0
35	NA	8	8565	1/1	0.92	0.51	11.86	43,43,43,43	0
35	NA	8	8571	1/1	0.88	0.23	11.50	53,53,53,53	0
35	NA	8	8577	1/1	0.92	0.23	5.43	64,64,64,64	0
35	NA	8	8531	1/1	0.95	0.17	4.76	62,62,62,62	0
35	NA	8	8503	1/1	0.93	0.20	4.70	50,50,50,50	0
34	K	7	8401	1/1	0.96	0.20	4.22	86,86,86,86	0
35	NA	8	8525	1/1	0.97	0.16	3.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	8	8553	1/1	0.98	0.20	2.89	39,39,39,39	0
35	NA	8	8550	1/1	0.97	0.14	1.22	43,43,43,43	0
35	NA	8	8566	1/1	0.94	0.20	0.94	40,40,40,40	0
35	NA	C	8504	1/1	0.82	0.25	0.92	32,32,32,32	0
33	MG	7	8102	1/1	0.96	0.16	0.77	49,49,49,49	0
33	MG	7	8053	1/1	0.98	0.13	0.37	48,48,48,48	0
35	NA	A	8545	1/1	0.96	0.16	0.09	38,38,38,38	0
33	MG	7	8060	1/1	0.97	0.14	-0.23	44,44,44,44	0
36	CL	O	8808	1/1	0.94	0.18	-0.26	74,74,74,74	0
35	NA	8	8564	1/1	0.90	0.14	-0.62	35,35,35,35	0
35	NA	8	8533	1/1	0.81	0.12	-0.81	37,37,37,37	0
36	CL	8	8813	1/1	0.99	0.12	-0.83	46,46,46,46	0
35	NA	8	8514	1/1	0.95	0.12	-0.94	27,27,27,27	0
36	CL	8	8816	1/1	0.97	0.13	-0.99	56,56,56,56	0
37	CD	Z	8703	1/1	1.00	0.11	-1.29	59,59,59,59	0
37	CD	U	8701	1/1	1.00	0.08	-1.41	60,60,60,60	0
36	CL	J	8821	1/1	0.96	0.11	-1.47	57,57,57,57	0
36	CL	B	8819	1/1	0.98	0.12	-1.50	40,40,40,40	0
35	NA	M	8547	1/1	0.97	0.12	-1.64	30,30,30,30	0
35	NA	Q	8548	1/1	0.94	0.09	-1.72	33,33,33,33	0
35	NA	8	8517	1/1	0.95	0.10	-1.94	28,28,28,28	0
37	CD	3	8704	1/1	0.98	0.05	-1.98	55,55,55,55	0
36	CL	L	8810	1/1	0.95	0.11	-2.10	46,46,46,46	0
35	NA	R	8537	1/1	0.92	0.09	-2.15	33,33,33,33	0
35	NA	8	8539	1/1	0.97	0.13	-2.29	26,26,26,26	0
34	K	7	8402	1/1	0.93	0.12	-2.34	62,62,62,62	0
35	NA	J	8546	1/1	0.95	0.09	-2.39	61,61,61,61	0
33	MG	Y	8108	1/1	0.98	0.12	-2.47	34,34,34,34	0
35	NA	8	8509	1/1	0.97	0.09	-2.61	40,40,40,40	0
33	MG	7	8074	1/1	0.99	0.06	-2.70	25,25,25,25	0
33	MG	T	8073	1/1	0.91	0.11	-2.77	45,45,45,45	0
36	CL	8	8812	1/1	0.98	0.07	-3.19	39,39,39,39	0
37	CD	1	8702	1/1	0.99	0.08	-3.30	56,56,56,56	0
35	NA	8	8543	1/1	0.95	0.09	-3.37	42,42,42,42	0
33	MG	B	8055	1/1	0.97	0.09	-3.48	32,32,32,32	0
33	MG	7	8017	1/1	0.98	0.05	-3.53	26,26,26,26	0
33	MG	7	8044	1/1	0.98	0.06	-3.58	37,37,37,37	0
33	MG	A	8065	1/1	0.98	0.08	-3.62	44,44,44,44	0
33	MG	3	8078	1/1	0.95	0.04	-3.65	40,40,40,40	0
35	NA	8	8538	1/1	0.94	0.06	-3.66	55,55,55,55	0
35	NA	8	8576	1/1	0.99	0.10	-3.67	29,29,29,29	0
36	CL	M	8818	1/1	0.99	0.08	-3.77	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	7	8056	1/1	0.98	0.12	-3.90	40,40,40,40	0
33	MG	7	8067	1/1	0.97	0.10	-4.10	38,38,38,38	0
35	NA	8	8544	1/1	0.97	0.05	-4.12	30,30,30,30	0
33	MG	7	8004	1/1	0.99	0.07	-4.19	27,27,27,27	0
33	MG	7	8058	1/1	0.98	0.08	-4.36	32,32,32,32	0
33	MG	7	8003	1/1	0.99	0.12	-4.46	31,31,31,31	0
33	MG	7	8077	1/1	0.95	0.07	-4.69	28,28,28,28	0
33	MG	7	8012	1/1	0.98	0.07	-4.71	25,25,25,25	0
35	NA	8	8505	1/1	0.94	0.11	-4.83	29,29,29,29	0
33	MG	7	8032	1/1	0.98	0.07	-4.90	40,40,40,40	0
33	MG	7	8057	1/1	0.97	0.10	-5.02	42,42,42,42	0
35	NA	8	8523	1/1	0.98	0.12	-5.03	39,39,39,39	0
33	MG	7	8013	1/1	0.98	0.10	-5.08	37,37,37,37	0
33	MG	7	8111	1/1	0.98	0.06	-5.22	40,40,40,40	0
33	MG	7	8015	1/1	0.96	0.06	-5.33	38,38,38,38	0
33	MG	7	8096	1/1	0.94	0.08	-5.35	41,41,41,41	0
33	MG	7	8018	1/1	0.98	0.09	-5.69	34,34,34,34	0
33	MG	7	8020	1/1	0.99	0.08	-5.73	22,22,22,22	0
33	MG	7	8080	1/1	0.98	0.07	-5.79	38,38,38,38	0
33	MG	7	8001	1/1	0.95	0.07	-5.87	30,30,30,30	0
33	MG	7	8033	1/1	0.96	0.09	-6.06	31,31,31,31	0
35	NA	8	8520	1/1	0.99	0.10	-6.32	25,25,25,25	0
33	MG	7	8109	1/1	0.99	0.08	-6.39	23,23,23,23	0
33	MG	7	8038	1/1	0.98	0.08	-6.88	28,28,28,28	0
33	MG	7	8101	1/1	0.97	0.11	-7.12	49,49,49,49	0
36	CL	3	8804	1/1	0.98	0.08	-7.27	53,53,53,53	0
33	MG	7	8084	1/1	0.99	0.03	-7.62	42,42,42,42	0
33	MG	7	8052	1/1	0.96	0.05	-7.85	35,35,35,35	0
33	MG	7	8010	1/1	0.97	0.07	-7.93	24,24,24,24	0
33	MG	7	8014	1/1	0.98	0.07	-8.08	31,31,31,31	0
33	MG	7	8008	1/1	0.96	0.04	-8.22	33,33,33,33	0
33	MG	7	8035	1/1	0.96	0.05	-8.25	50,50,50,50	0
33	MG	7	8107	1/1	0.92	0.08	-8.28	73,73,73,73	0
33	MG	7	8002	1/1	0.96	0.04	-8.42	26,26,26,26	0
33	MG	7	8091	1/1	0.94	0.05	-8.51	41,41,41,41	0
33	MG	7	8007	1/1	1.00	0.07	-9.67	12,12,12,12	0
33	MG	7	8019	1/1	0.99	0.05	-10.31	23,23,23,23	0
33	MG	7	8006	1/1	0.98	0.04	-10.69	46,46,46,46	0
33	MG	7	8054	1/1	0.98	0.09	-11.46	24,24,24,24	0
33	MG	7	8088	1/1	0.95	0.07	-20.34	25,25,25,25	0
36	CL	J	8801	1/1	0.96	0.18	-	55,55,55,55	0
35	NA	8	8570	1/1	0.98	0.13	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	7	8094	1/1	0.93	0.13	-	47,47,47,47	0
36	CL	R	8806	1/1	0.97	0.15	-	43,43,43,43	0
33	MG	7	8030	1/1	0.99	0.08	-	31,31,31,31	0
33	MG	7	8029	1/1	0.99	0.08	-	33,33,33,33	0
35	NA	8	8518	1/1	0.95	0.17	-	26,26,26,26	0
33	MG	K	8069	1/1	0.94	0.07	-	46,46,46,46	0
33	MG	7	8093	1/1	0.96	0.21	-	48,48,48,48	0
35	NA	8	8542	1/1	0.97	0.12	-	35,35,35,35	0
33	MG	7	8105	1/1	0.97	0.22	-	53,53,53,53	0
33	MG	7	8042	1/1	0.99	0.10	-	31,31,31,31	0
33	MG	7	8114	1/1	0.97	0.09	-	49,49,49,49	0
36	CL	8	8822	1/1	0.94	0.27	-	88,88,88,88	0
33	MG	7	8090	1/1	0.96	0.18	-	41,41,41,41	0
33	MG	7	8112	1/1	0.77	0.26	-	47,47,47,47	0
35	NA	8	8575	1/1	0.94	0.30	-	58,58,58,58	0
35	NA	8	8506	1/1	0.94	0.41	-	33,33,33,33	0
35	NA	8	8563	1/1	0.85	0.33	-	60,60,60,60	0
33	MG	7	8025	1/1	0.98	0.03	-	42,42,42,42	0
37	CD	O	8705	1/1	0.98	0.08	-	70,70,70,70	0
35	NA	8	8579	1/1	0.92	0.31	-	46,46,46,46	0
33	MG	9	8095	1/1	0.94	0.09	-	53,53,53,53	0
35	NA	8	8519	1/1	0.98	0.13	-	22,22,22,22	0
33	MG	7	8117	1/1	0.98	0.09	-	46,46,46,46	0
35	NA	8	8510	1/1	0.80	0.51	-	36,36,36,36	0
36	CL	J	8802	1/1	0.95	0.14	-	63,63,63,63	0
33	MG	7	8097	1/1	0.97	0.06	-	26,26,26,26	0
33	MG	7	8009	1/1	0.99	0.07	-	22,22,22,22	0
33	MG	7	8099	1/1	0.89	0.16	-	45,45,45,45	0
33	MG	7	8049	1/1	0.90	0.25	-	58,58,58,58	0
35	NA	8	8515	1/1	0.98	0.12	-	48,48,48,48	0
33	MG	7	8087	1/1	0.86	0.18	-	46,46,46,46	0
36	CL	N	8807	1/1	0.97	0.13	-	57,57,57,57	0
33	MG	7	8051	1/1	0.91	0.12	-	58,58,58,58	0
33	MG	7	8040	1/1	0.98	0.13	-	70,70,70,70	0
35	NA	8	8567	1/1	0.97	0.14	-	35,35,35,35	0
33	MG	7	8027	1/1	0.97	0.11	-	40,40,40,40	0
36	CL	8	8811	1/1	0.97	0.14	-	57,57,57,57	0
33	MG	7	8047	1/1	0.90	0.20	-	62,62,62,62	0
33	MG	7	8063	1/1	0.98	0.07	-	51,51,51,51	0
36	CL	A	8809	1/1	0.91	0.19	-	58,58,58,58	0
33	MG	7	8100	1/1	0.95	0.10	-	73,73,73,73	0
33	MG	7	8024	1/1	0.99	0.06	-	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	7	8081	1/1	0.94	0.10	-	50,50,50,50	0
35	NA	8	8541	1/1	0.93	0.13	-	29,29,29,29	0
33	MG	7	8116	1/1	0.97	0.11	-	20,20,20,20	0
35	NA	8	8540	1/1	0.84	0.25	-	44,44,44,44	0
33	MG	7	8043	1/1	0.98	0.06	-	35,35,35,35	0
33	MG	7	8104	1/1	0.95	0.20	-	48,48,48,48	0
33	MG	7	8115	1/1	0.88	0.11	-	46,46,46,46	0
33	MG	7	8110	1/1	0.95	0.08	-	60,60,60,60	0
35	NA	8	8534	1/1	0.96	0.07	-	26,26,26,26	0
33	MG	7	8066	1/1	0.98	0.18	-	96,96,96,96	0
33	MG	7	8023	1/1	0.99	0.06	-	34,34,34,34	0
35	NA	8	8584	1/1	0.86	0.15	-	45,45,45,45	0
33	MG	7	8076	1/1	0.99	0.08	-	47,47,47,47	0
35	NA	8	8560	1/1	0.98	0.40	-	49,49,49,49	0
35	NA	9	8551	1/1	0.84	0.13	-	31,31,31,31	0
33	MG	7	8083	1/1	0.99	0.04	-	22,22,22,22	0
35	NA	S	8512	1/1	0.98	0.13	-	10,10,10,10	0
33	MG	7	8089	1/1	0.93	0.11	-	49,49,49,49	0
33	MG	7	8046	1/1	0.92	0.11	-	52,52,52,52	0
33	MG	7	8113	1/1	0.95	0.24	-	42,42,42,42	0
35	NA	8	8581	1/1	0.93	0.16	-	40,40,40,40	0
33	MG	7	8070	1/1	0.97	0.11	-	41,41,41,41	0
35	NA	8	8530	1/1	0.89	0.31	-	41,41,41,41	0
35	NA	8	8508	1/1	0.88	0.15	-	39,39,39,39	0
33	MG	7	8011	1/1	0.95	0.08	-	21,21,21,21	0
35	NA	8	8513	1/1	0.88	0.17	-	47,47,47,47	0
33	MG	7	8041	1/1	0.95	0.20	-	38,38,38,38	0
35	NA	8	8552	1/1	0.91	0.36	-	40,40,40,40	0
35	NA	8	8524	1/1	0.91	0.21	-	39,39,39,39	0
33	MG	7	8050	1/1	0.88	0.19	-	72,72,72,72	0
35	NA	8	8549	1/1	0.98	0.11	-	34,34,34,34	0
35	NA	8	8585	1/1	0.92	0.32	-	38,38,38,38	0
36	CL	Y	8820	1/1	0.98	0.11	-	30,30,30,30	0
33	MG	7	8062	1/1	0.92	0.06	-	52,52,52,52	0
33	MG	7	8072	1/1	0.93	0.08	-	56,56,56,56	0
33	MG	7	8037	1/1	0.99	0.07	-	44,44,44,44	0
33	MG	7	8021	1/1	0.98	0.10	-	32,32,32,32	0
33	MG	7	8036	1/1	0.99	0.05	-	32,32,32,32	0
33	MG	7	8034	1/1	0.91	0.09	-	29,29,29,29	0
35	NA	8	8528	1/1	0.97	0.32	-	50,50,50,50	0
35	NA	8	8526	1/1	0.61	0.61	-	72,72,72,72	0
35	NA	8	8507	1/1	0.83	0.43	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	8	8558	1/1	0.90	0.46	-	48,48,48,48	0
33	MG	7	8016	1/1	0.98	0.11	-	23,23,23,23	0
33	MG	7	8061	1/1	0.94	0.08	-	27,27,27,27	0
35	NA	H	8522	1/1	0.90	0.15	-	38,38,38,38	0
33	MG	7	8079	1/1	0.99	0.10	-	20,20,20,20	0
35	NA	8	8516	1/1	0.92	0.25	-	39,39,39,39	0
33	MG	7	8071	1/1	0.97	0.09	-	59,59,59,59	0
33	MG	7	8031	1/1	0.99	0.08	-	28,28,28,28	0
36	CL	8	8817	1/1	0.88	0.17	-	58,58,58,58	0
33	MG	7	8082	1/1	0.92	0.17	-	58,58,58,58	0
33	MG	7	8045	1/1	0.97	0.08	-	58,58,58,58	0
35	NA	8	8511	1/1	0.80	0.30	-	50,50,50,50	0
36	CL	8	8814	1/1	0.96	0.12	-	51,51,51,51	0
33	MG	7	8103	1/1	0.87	0.44	-	79,79,79,79	0
33	MG	7	8098	1/1	0.90	0.16	-	42,42,42,42	0
33	MG	7	8039	1/1	0.98	0.10	-	33,33,33,33	0
35	NA	8	8555	1/1	0.93	0.55	-	71,71,71,71	0
33	MG	7	8026	1/1	0.99	0.07	-	19,19,19,19	0
33	MG	7	8048	1/1	0.98	0.07	-	48,48,48,48	0
33	MG	7	8022	1/1	0.99	0.08	-	36,36,36,36	0
33	MG	7	8106	1/1	0.98	0.05	-	35,35,35,35	0
33	MG	7	8086	1/1	0.98	0.16	-	41,41,41,41	0
35	NA	8	8557	1/1	0.91	0.07	-	49,49,49,49	0
35	NA	8	8536	1/1	0.94	0.13	-	44,44,44,44	0
33	MG	7	8005	1/1	0.99	0.10	-	27,27,27,27	0
33	MG	7	8075	1/1	0.87	0.08	-	55,55,55,55	0
33	MG	7	8085	1/1	0.99	0.09	-	65,65,65,65	0
36	CL	8	8803	1/1	0.98	0.16	-	43,43,43,43	0
33	MG	7	8028	1/1	0.99	0.09	-	39,39,39,39	0
36	CL	8	8805	1/1	0.95	0.19	-	57,57,57,57	0
35	NA	8	8501	1/1	0.96	0.14	-	21,21,21,21	0
33	MG	7	8059	1/1	0.97	0.06	-	27,27,27,27	0
35	NA	8	8554	1/1	0.86	0.29	-	55,55,55,55	0
33	MG	7	8092	1/1	0.93	0.29	-	75,75,75,75	0
33	MG	7	8068	1/1	0.93	0.07	-	34,34,34,34	0

## 6.5 Other polymers

There are no such residues in this entry.