



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:18 PM GMT

PDB ID : 1NJI  
Title : Structure of chloramphenicol bound to the 50S ribosomal subunit  
Authors : Hansen, J.L.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2002-12-31  
Resolution : 3.00 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

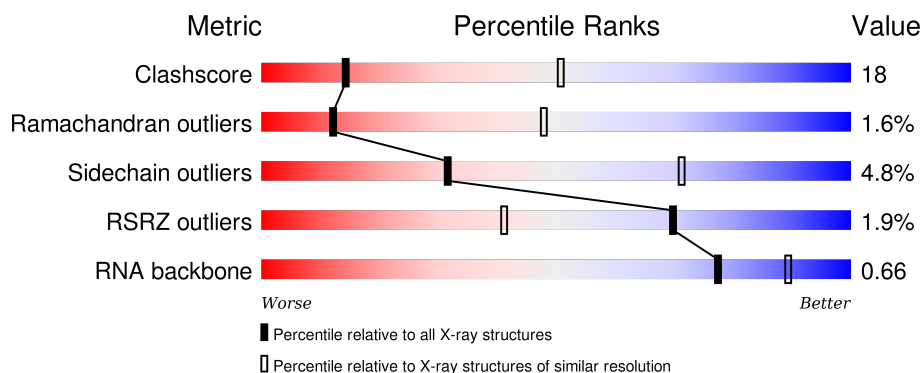
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



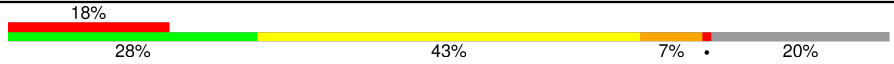

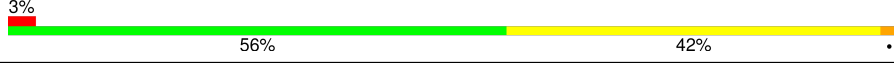
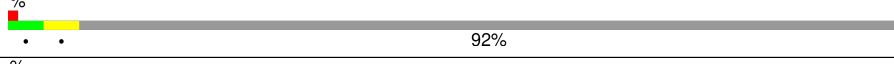
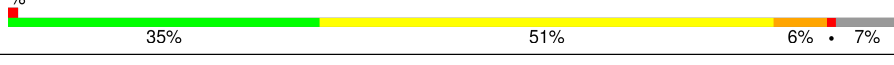
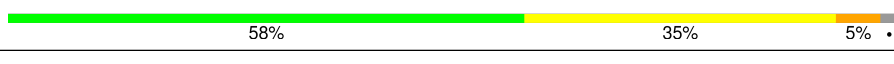
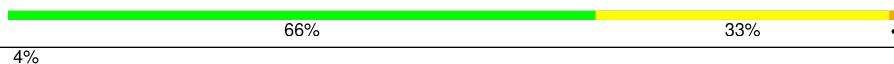
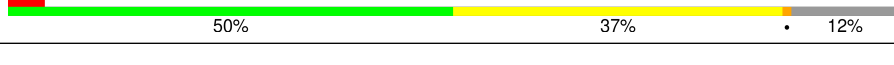
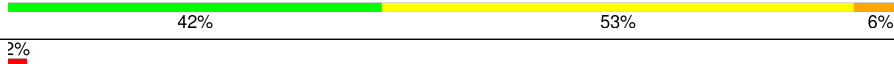
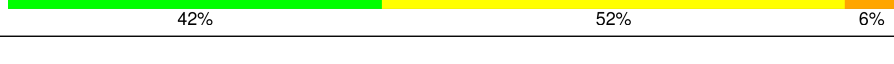

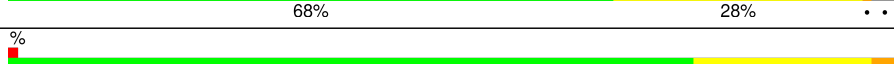
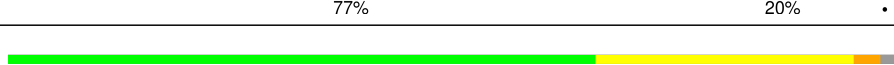
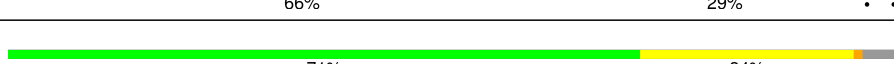




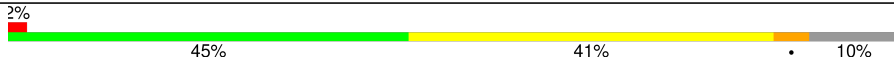
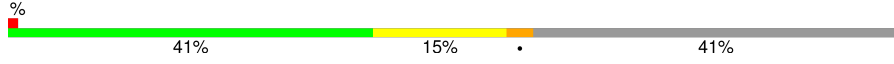

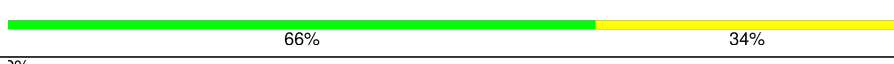



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	2922	<div> <div>57%</div> <div>31%</div> <div>6%</div> <div>6%</div> </div>
2	B	122	<div>5%</div> <div>56%</div> <div>30%</div> <div>11%</div> <div></div>
3	C	239	<div>2%</div> <div>54%</div> <div>39%</div> <div>6%</div> <div></div>
4	D	337	<div>51%</div> <div>44%</div> <div>5%</div>
5	E	246	<div>57%</div> <div>38%</div> <div>5%</div>

*Continued on next page...*

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Mol	Chain	Length	Quality of chain
6	F	176	
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

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
31	MG	A	8060	-	-	-	X
31	MG	A	8064	-	-	-	X
31	MG	A	8066	-	-	-	X
31	MG	A	8088	-	-	-	X
32	K	A	8202	-	-	-	X
33	NA	A	8303	-	-	-	X
33	NA	A	8308	-	-	-	X
33	NA	A	8310	-	-	-	X
33	NA	A	8321	-	-	-	X
33	NA	A	8325	-	-	-	X
33	NA	A	8326	-	-	-	X
33	NA	A	8327	-	-	-	X
33	NA	A	8332	-	-	-	X
33	NA	A	8335	-	-	-	X
33	NA	A	8339	-	-	-	X
33	NA	A	8350	-	-	-	X
33	NA	A	8356	-	-	-	X
33	NA	A	8359	-	-	-	X
33	NA	A	8361	-	-	-	X
33	NA	A	8362	-	-	-	X
33	NA	A	8364	-	-	-	X
33	NA	A	8368	-	-	-	X
33	NA	A	8371	-	-	-	X
33	NA	A	8372	-	-	-	X
33	NA	A	8373	-	-	-	X
33	NA	A	8374	-	-	-	X
33	NA	A	8376	-	-	-	X
33	NA	A	8378	-	-	-	X
33	NA	A	8379	-	-	-	X
33	NA	A	8381	-	-	-	X
33	NA	A	8382	-	-	-	X
33	NA	B	8383	-	-	-	X
33	NA	M	8380	-	-	-	X
33	NA	S	8386	-	-	-	X
34	CL	A	8515	-	-	-	X
34	CL	D	8519	-	-	-	X

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98536 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	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	SEE REMARK 999	UNP P20279
D	310	ARG	PHE	SEE REMARK 999	UNP P20279

- Molecule 5 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O	0	0	0
			1114	668	222	224			

- Molecule 14 is a protein called 50S ribosomal protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called 50S ribosomal protein L18E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O	0	0	0
			864	529	161	174			

- Molecule 17 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O	0	0	0
			1133	680	230	223			

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O	S	0	0	0
			949	568	180	201				

- Molecule 22 is a protein called 50S ribosomal protein L24E.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

- Molecule 25 is a protein called 50S ribosomal protein L31E.

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

- Molecule 26 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	142	Total	C	N	O	S	0	0	0
			1130	686	228	216				

- Molecule 27 is a protein called 50S ribosomal protein L37AE.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	1	1	Total	Mg	0	0
			1	1		
31	D	1	Total	Mg	0	0
			1	1		
31	B	1	Total	Mg	0	0
			1	1		
31	C	1	Total	Mg	0	0
			1	1		
31	Z	1	Total	Mg	0	0
			1	1		
31	A	109	Total	Mg	0	0
			109	109		
31	4	1	Total	Mg	0	0
			1	1		
31	U	1	Total	Mg	0	0
			1	1		
31	L	1	Total	Mg	0	0
			1	1		

- Molecule 32 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	2	Total K 2 2	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	J	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	E	1	Total Na 1 1	0	0
33	B	2	Total Na 2 2	0	0
33	C	1	Total Na 1 1	0	0
33	A	71	Total Na 71 71	0	0
33	T	1	Total Na 1 1	0	0
33	N	1	Total Na 1 1	0	0
33	U	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0
33	S	2	Total Na 2 2	0	0
33	M	1	Total Na 1 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

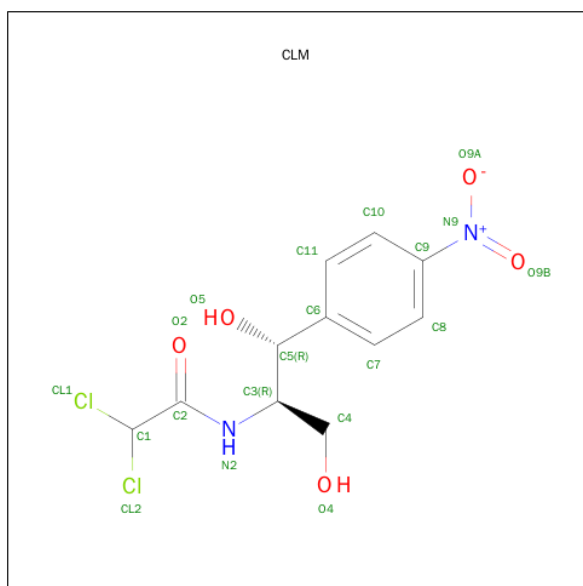
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	P	1	Total Cl 1 1	0	0
34	D	1	Total Cl 1 1	0	0
34	K	3	Total Cl 3 3	0	0
34	C	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	Z	1	Total	Cl	0	0
			1	1		
34	A	9	Total	Cl	0	0
			9	9		
34	4	1	Total	Cl	0	0
			1	1		
34	N	1	Total	Cl	0	0
			1	1		
34	O	1	Total	Cl	0	0
			1	1		
34	R	1	Total	Cl	0	0
			1	1		
34	S	1	Total	Cl	0	0
			1	1		
34	M	1	Total	Cl	0	0
			1	1		

- Molecule 35 is CHLORAMPHENICOL (three-letter code: CLM) (formula:  $C_{11}H_{12}Cl_2N_2O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	A	1	Total	C	Cl	N	O	
			20	11	2	2	5	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	P	1	Total Cd 1 1	0	0
36	2	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	4	1	Total Cd 1 1	0	0
36	V	1	Total Cd 1 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	5906	Total O 5906 5906	0	0
37	B	143	Total O 143 143	0	0
37	C	123	Total O 123 123	0	0
37	D	147	Total O 147 147	0	0
37	E	167	Total O 167 167	0	0
37	F	50	Total O 50 50	0	0
37	G	45	Total O 45 45	0	0
37	H	29	Total O 29 29	0	0
37	I	21	Total O 21 21	0	0
37	J	76	Total O 76 76	0	0
37	K	54	Total O 54 54	0	0
37	L	61	Total O 61 61	0	0
37	M	78	Total O 78 78	0	0
37	N	125	Total O 125 125	0	0
37	O	69	Total O 69 69	0	0

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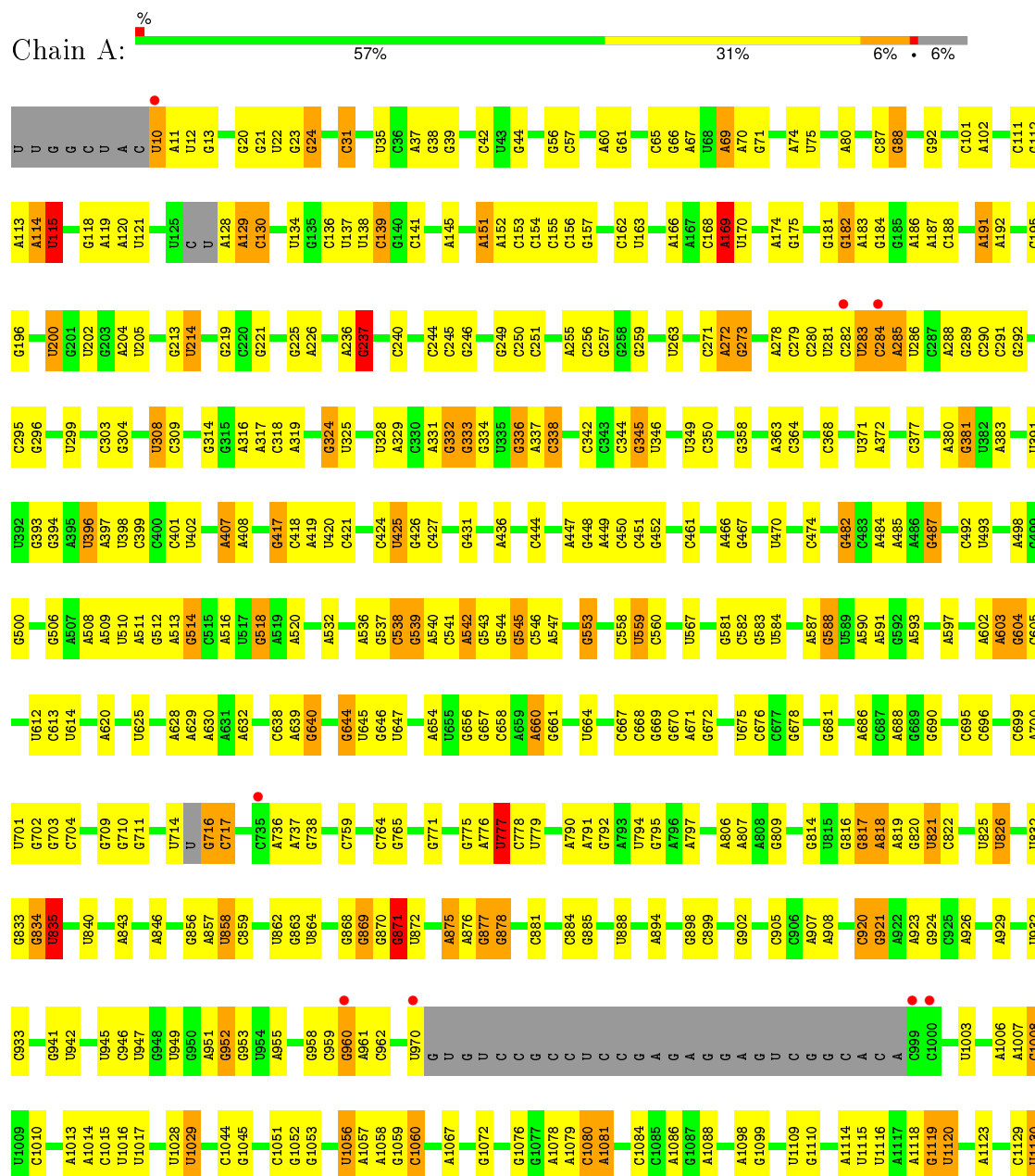
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	P	45	Total 45	O 45	0	0
37	Q	73	Total 73	O 73	0	0
37	R	53	Total 53	O 53	0	0
37	S	85	Total 85	O 85	0	0
37	T	35	Total 35	O 35	0	0
37	U	40	Total 40	O 40	0	0
37	V	28	Total 28	O 28	0	0
37	W	17	Total 17	O 17	0	0
37	X	69	Total 69	O 69	0	0
37	Y	28	Total 28	O 28	0	0
37	Z	98	Total 98	O 98	0	0
37	1	37	Total 37	O 37	0	0
37	2	54	Total 54	O 54	0	0
37	3	43	Total 43	O 43	0	0
37	4	68	Total 68	O 68	0	0

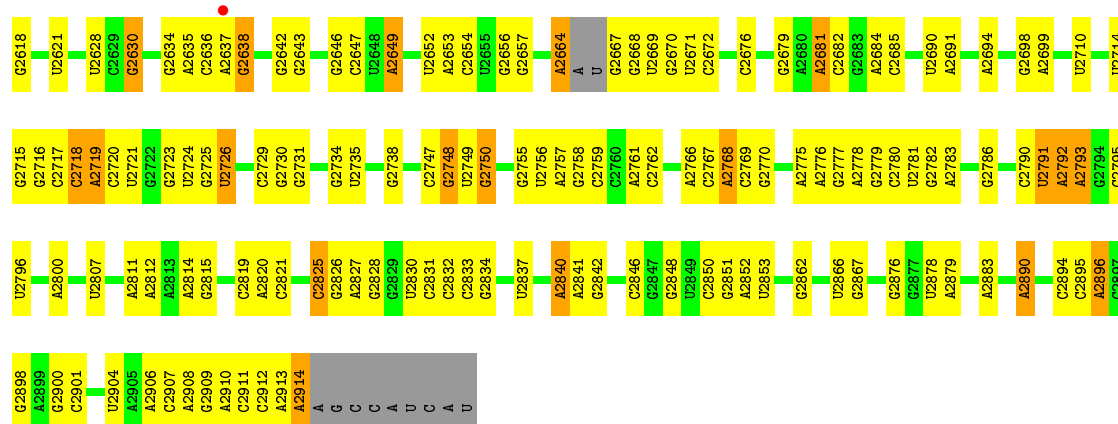
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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



U2593	A2493	U2330	G2287	C	A2101	C1982	A1759	G1855	G1535	G1430	A1328	U1206	G1131
C2596	U2494	G2338	A2238	A	G2102	C1993	C1762	A1656	C1536	A1434	A1329	A1207	A1132
U2527	U2495	A	C2241	G	C2104	U1996	C1777	A1657	G1543	U1435	A1329	C1208	A1133
C2583	C2443	A	U2242	U	G2110	A1997	U1878	A1658	U1544	C1436	U1333	C1209	G1134
C2594	C2446	G	C2247	C	G2114	U2001	U1879	C1666	C1545	G1437	C1334	G1211	U1136
U2595	U2457	A	G2251	C	C2114	C2002	U1883	A1667	G1546	G1438	C1335	C1212	G1137
C2536	C2344	C	A2252	C	C2119	C2003	G1884	U1668	G1555	C1439	G1340	C1213	U1138
C2537	A2345	C	U2257	G	U2120	U2004	C1887	U1669	U1559	U1440	A1341	G1214	U1139
U2541	C2346	C	G2256	C	G2121	G2005	U1771	G1670	U	A1441	C1342	C1216	C1140
U2544	A2353	G	G2257	G	G2122	U2008	G1772	C1679	G1561	A1442	C1343	G1217	G1151
U2545	A2354	U	A2258	U	G2128	U2009	G1773	C1680	C1562	G1445	G1351	U1218	G1159
U2468	A2355	A	U2265	G	A2103	A2010	A1778	G1681	G1563	U1446	A1352	U1219	A1160
U2546	A2357	C	A2266	C	U2133	A2011	U1779	A1682	C1564	U1447	C1353	C1229	A1161
C2547	C2357	C	G2267	C	G2134	U2012	C1787	A1684	A1573	C1450	G1354	U1234	G1162
C2548	A2361	G	C2268	G	A2135	G2013	U1788	A1685	U1573	C1451	A1355	G1235	U1163
C2552	A2362	G	C2269	G	G2136	C2020	G1789	G1688	A1580	U1457	C1360	A1236	U1164
A2553	G2270	C	G2271	C	A	C2021	C1798	C1692	C1584	A1458	G1361	A1237	G1165
U2557	C2366	C	G2272	C	C	G2022	U1921	C1692	C1585	C1462	U1362	G1238	G1167
U2558	A2369	C	C2273	C	U	A2030	G1926	G1706	G1588	A1463	A1372	U1242	U1169
C2559	U2377	G	G2274	G	G	G2033	A1927	G1707	G1589	A1470	A1375	G1243	A1170
U2563	U2276	A	U2277	A	U	U2034	G1933	A1717	G1592	C1474	C1377	U1244	A1171
C2564	U2277	G	U2278	C	C	G	C1940	G1706	C1593	C1477	C1376	U1245	A1172
C2565	C2281	U	C2282	U	C	G2044	A1941	G1707	C1594	C1478	C1377	G1246	A1173
U2570	U2282	C	U2283	A	C	A2054	G1819	A1717	G1595	U1478	U1383	U1249	A1174
C2578	G2283	A	C2284	C	G	U2064	G1820	U1722	U1596	C1483	C1384	C1250	G1175
U2586	U2291	C	U2292	C	A	C2065	C1826	G1723	U1599	G1484	G1391	C1251	C1176
U2587	A2291	G	U2293	G	U	G2070	G1827	U1724	U1599	A1485	A1392	U1266	U1180
C2588	U2297	U	U2298	U	U	C2071	G1828	C1725	A1603	A1494	C1394	C1267	A1181
U2589	A2300	A	A2301	A	C	G2072	C1834	G1730	G1604	C1495	G1398	C1268	C1182
C2591	A2302	A	A2303	A	A	A2074	U1835	A1732	G1605	G1496	A1399	G1269	C1183
U2592	A2408	U	A2409	U	C	U2078	A1840	C1734	C1613	A1406	A1406	U1270	U1185
U2595	C2412	C	U2413	C	U	A2081	A1842	C1735	A1615	U1500	A1407	C1273	C1186
A2596	A2414	A	G2415	A	G	G2082	U1845	A1737	U1625	U1503	U1408	U1279	A1188
A2601	C2418	C	C2419	C	C	A2083	U1846	C1738	A1626	A1504	G1409	C1289	A1189
C2602	U2419	C	G2420	C	G	G2090	C1851	G1739	G1627	U1505	A1413	G1290	G1190
C2603	C2421	U	C2422	U	G	G2091	U1850	U1741	A1630	U1506	A1414	A1191	A1192
A2604	U2422	C	C2423	C	A	C2092	G1851	A1742	A1630	A1515	G1415	U1298	A1193
U2607	C2424	G	U2425	G	C	G2093	U1964	G1743	C1633	C1516	G1416	G1299	A1194
C2608	A2426	C	C2427	C	G	G2094	C1971	A1742	G1634	U1517	U1418	U1304	G1195
G2611	C2428	A	C2429	A	C	U2095	G1974	G1743	U1635	G1523	U1419	C1305	C1196
A2612	U2326	U	U2327	U	C	A2096	C1975	G1751	G1636	U1524	C1421	U1306	U1197
C2613	C2327	G	C2328	G	A	G2097	C1861	A1754	A1637	G1525	U1422	G1311	A1198
C2614	U2328	C	U2329	C	U	C2098	C1864	A1755	A1641	A1526	C1423	G1312	A1200
U2615	C2329	C	C2330	C	A	C2099	G1979	A1756	A1642	A1527	U1424	A1313	A1201
						A2100	A1981	U1757	U1654	G1529	G1426	U1314	A1202
								U1758				G1325	G1203
													U1205



• Molecule 2: 5S ribosomal RNA



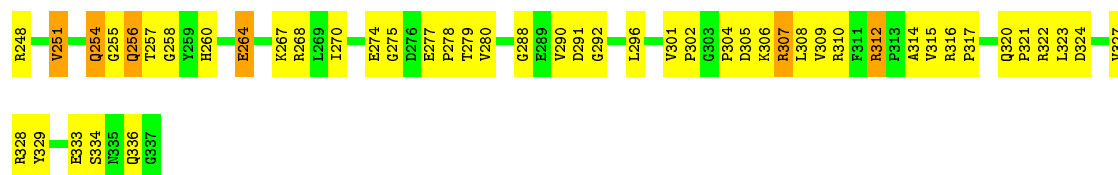
• Molecule 3: 50S ribosomal protein L2P



• Molecule 4: 50S ribosomal protein L3P

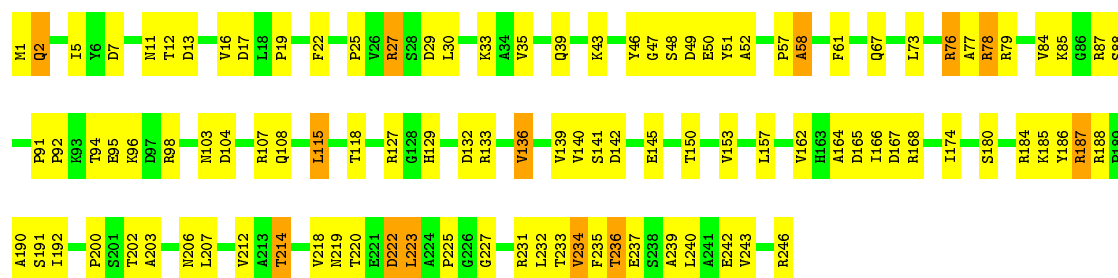






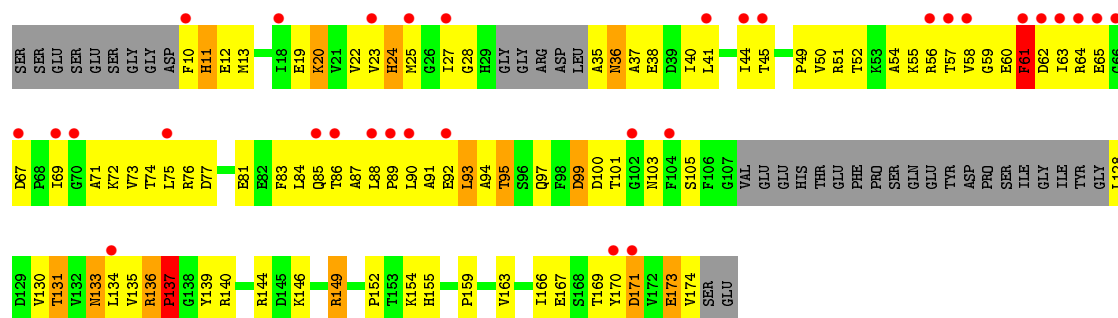
• Molecule 5: 50S ribosomal protein L4E

Chain E: 57% 38% 5%



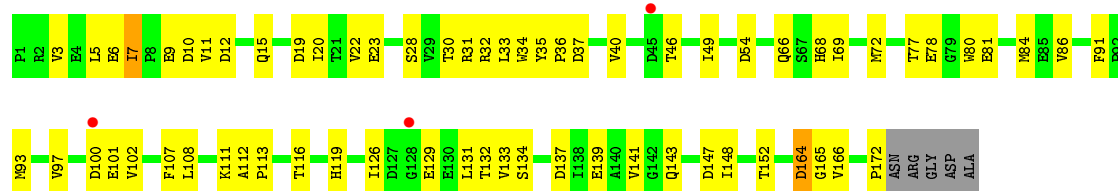
• Molecule 6: 50S ribosomal protein L5P

Chain F: 18% 28% 43% 7% 20%



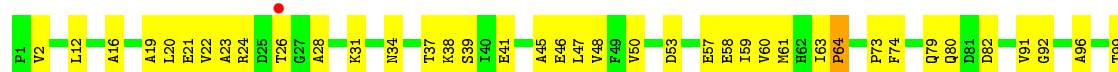
• Molecule 7: 50S ribosomal protein L6P

Chain G: 2% 60% 36%



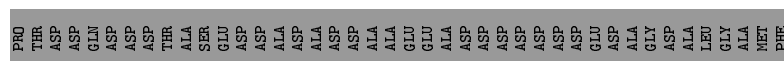
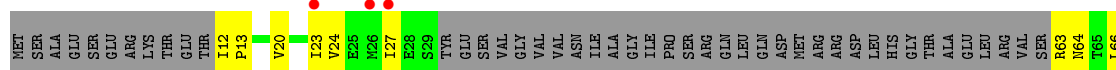
• Molecule 8: 50S ribosomal protein L7Ae

Chain H: 3% 56% 42%

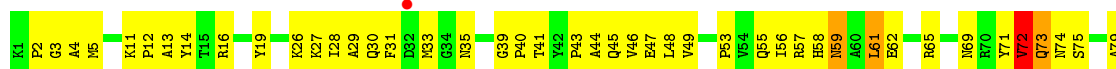




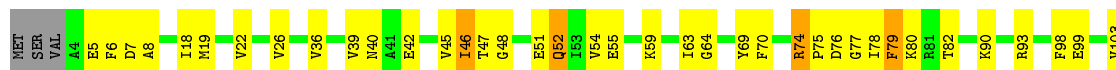
- Molecule 9: Acidic ribosomal protein P0 homolog



- Molecule 10: 50S ribosomal protein L10e

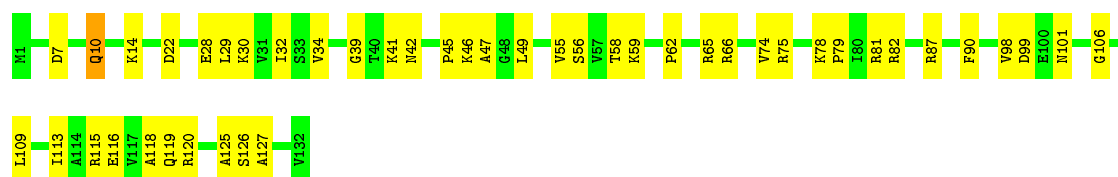


- Molecule 11: 50S ribosomal protein L13P

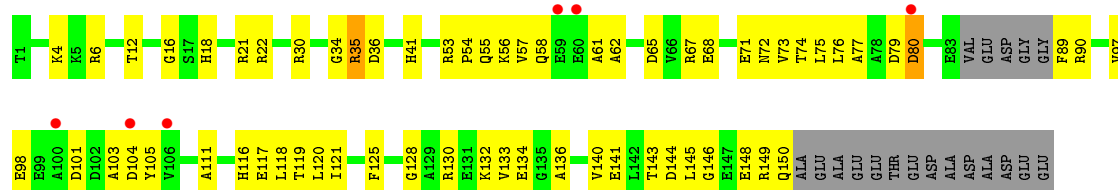


- Molecule 12: 50S ribosomal protein L14P

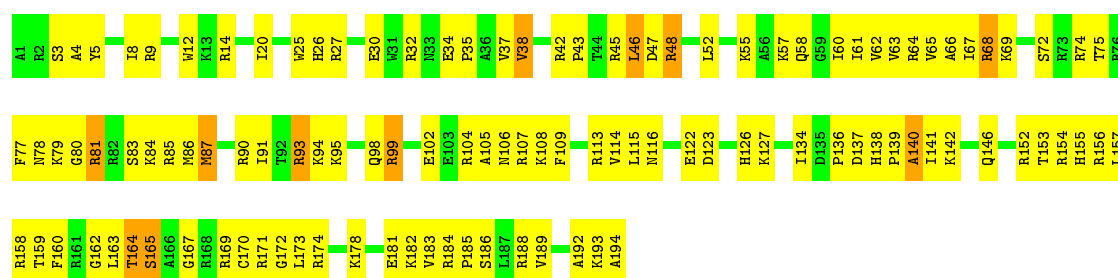




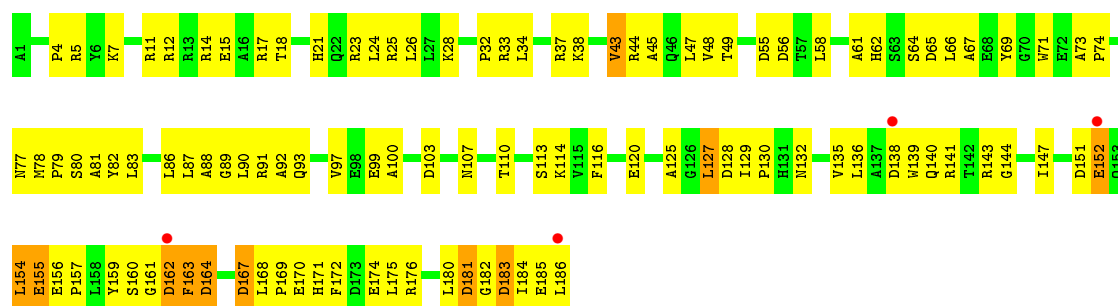
- Molecule 13: 50S ribosomal protein L15P



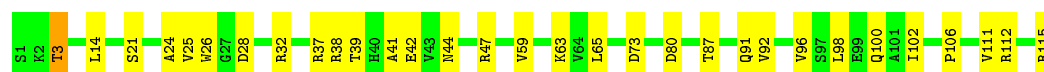
- Molecule 14: 50S ribosomal protein L15E



- Molecule 15: 50S ribosomal protein L18P

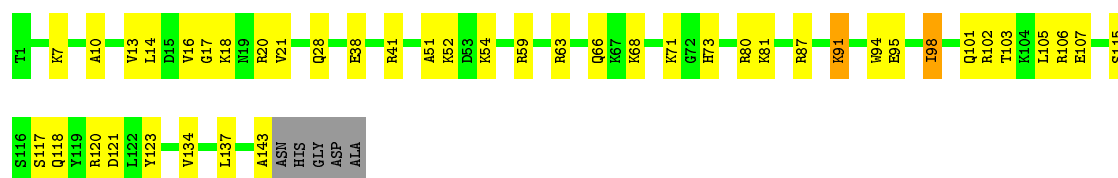


- Molecule 16: 50S ribosomal protein L18E




- Molecule 17: 50S ribosomal protein L19E

Chain Q: 



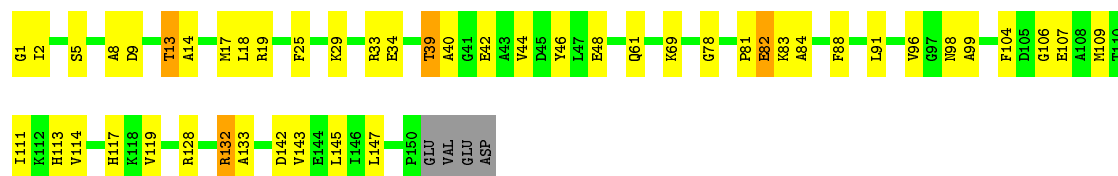
- Molecule 18: 50S ribosomal protein L21e

Chain R: 



- Molecule 19: 50S ribosomal protein L22P

Chain S: 



- Molecule 20: 50S ribosomal protein L23P

Chain T: 



- Molecule 21: 50S ribosomal protein L24P

Chain U: 



- Molecule 22: 50S ribosomal protein L24E

Chain V: 



- Molecule 23: 50S ribosomal protein L29P



Chain 2:  66% 34%



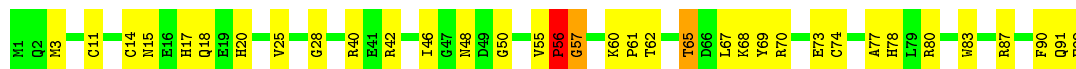
- Molecule 29: 50S ribosomal protein L39e

Chain 3:  2% 48% 46% . .



- Molecule 30: 50S ribosomal protein L44E

Chain 4:  62% 35% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.72Å 299.75Å 573.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.96 – 2.87	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-3.00) 92.7 (49.96-2.87)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	0.25	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.68 (at 2.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.176 , 0.209 0.175 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 61.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 399416 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	98536	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLM, MG, CL, NA, K, CD

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	0.47	5/66076 (0.0%)	0.73	32/103052 (0.0%)
2	B	0.49	0/2905	0.77	4/4528 (0.1%)
3	C	0.44	0/1787	0.73	0/2409
4	D	0.41	0/2689	0.69	0/3652
5	E	0.46	0/1883	0.69	0/2551
6	F	0.35	0/1111	0.62	0/1498
7	G	0.40	0/1382	0.62	0/1880
8	H	0.37	0/896	0.59	0/1219
9	I	0.34	0/241	0.51	0/324
10	J	0.44	0/1246	0.77	1/1686 (0.1%)
11	K	0.44	0/1135	0.64	0/1530
12	L	0.42	0/1003	0.70	0/1351
13	M	0.40	0/1126	0.70	0/1504
14	N	0.47	0/1633	0.74	0/2180
15	O	0.35	0/1473	0.67	0/1999
16	P	0.40	0/873	0.67	0/1181
17	Q	0.41	0/1143	0.58	0/1521
18	R	0.46	0/748	0.73	0/1005
19	S	0.44	0/1172	0.71	0/1578
20	T	0.39	0/648	0.63	1/875 (0.1%)
21	U	0.39	0/957	0.68	0/1289
22	V	0.38	0/417	0.62	0/562
23	W	0.34	0/502	0.58	0/675
24	X	0.42	0/1218	0.69	0/1655
25	Y	0.41	0/664	0.64	0/895
26	Z	0.45	0/1146	0.68	0/1536
27	1	0.46	0/575	0.76	0/763
28	2	0.49	0/437	0.75	0/578
29	3	0.39	0/398	0.57	0/527
30	4	0.47	0/771	0.66	0/1024
All	All	0.46	5/98255 (0.0%)	0.71	38/147027 (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	A	1	90
2	B	1	3
All	All	2	93

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2097	G	O3'-P	8.81	1.71	1.61
1	A	2097	G	C3'-O3'	-7.93	1.31	1.42
1	A	2098	C	P-O5'	-7.79	1.51	1.59
1	A	1206	U	P-OP2	6.71	1.60	1.49
1	A	2098	C	P-OP1	-5.46	1.39	1.49

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-18.95	63.51	105.20
1	A	1164	U	OP2-P-O3'	-17.97	65.67	105.20
1	A	1165	G	O5'-P-OP1	-14.27	92.85	105.70
2	B	3024	U	C2'-C3'-O3'	9.63	130.69	109.50
1	A	1563	G	C2'-C3'-O3'	9.41	130.20	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

5 of 93 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	U	Sidechain
1	A	118	G	Sidechain
1	A	22	U	Sidechain
1	A	24	G	Sidechain
1	A	44	G	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	A	59017	0	29806	952	0
2	B	2600	0	1326	73	0
3	C	1754	0	1763	128	0
4	D	2624	0	2533	176	0
5	E	1858	0	1816	125	0
6	F	1094	0	1085	127	0
7	G	1357	0	1266	70	0
8	H	885	0	854	64	0
9	I	240	0	231	15	0
10	J	1215	0	1215	152	0
11	K	1119	0	1098	68	0
12	L	993	0	1027	50	0
13	M	1114	0	1072	61	0
14	N	1605	0	1676	160	0
15	O	1444	0	1401	117	0
16	P	864	0	873	32	0
17	Q	1133	0	1127	46	0
18	R	734	0	728	18	0
19	S	1149	0	1122	55	0
20	T	641	0	605	20	0
21	U	949	0	923	55	0
22	V	410	0	365	30	0
23	W	499	0	511	30	0
24	X	1195	0	1137	96	0
25	Y	654	0	653	49	0
26	Z	1130	0	1133	62	0
27	1	563	0	598	59	0
28	2	430	0	426	24	0
29	3	393	0	406	25	0
30	4	755	0	728	35	0
31	1	1	0	0	0	0
31	4	1	0	0	0	0
31	A	109	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	D	1	0	0	0	0
31	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	U	1	0	0	0	0
31	Z	1	0	0	0	0
32	A	2	0	0	0	0
33	A	71	0	0	0	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	T	1	0	0	0	0
33	U	1	0	0	0	0
34	4	1	0	0	0	0
34	A	9	0	0	0	0
34	C	1	0	0	0	0
34	D	1	0	0	1	0
34	K	3	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0
34	O	1	0	0	0	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Z	1	0	0	0	0
35	A	20	0	11	0	0
36	1	1	0	0	1	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	37	0	0	9	0
37	2	54	0	0	2	0
37	3	43	0	0	4	0
37	4	68	0	0	11	0
37	A	5906	0	0	192	0
37	B	143	0	0	14	0
37	C	123	0	0	19	0
37	D	147	0	0	32	0
37	E	167	0	0	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	F	50	0	0	19	0
37	G	45	0	0	8	0
37	H	29	0	0	7	0
37	I	21	0	0	1	0
37	J	76	0	0	24	0
37	K	54	0	0	3	0
37	L	61	0	0	8	0
37	M	78	0	0	16	0
37	N	125	0	0	19	0
37	O	69	0	0	13	0
37	P	45	0	0	7	0
37	Q	73	0	0	6	0
37	R	53	0	0	3	0
37	S	85	0	0	7	0
37	T	35	0	0	4	0
37	U	40	0	0	7	0
37	V	28	0	0	6	0
37	W	17	0	0	2	0
37	X	69	0	0	17	0
37	Y	28	0	0	6	0
37	Z	98	0	0	18	0
All	All	98536	0	59515	2717	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 18.

The worst 5 of 2717 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)
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.57	1.18
5:E:236:THR:HG22	5:E:239:ALA:H	1.03	1.15
1:A:156:C:H5''	14:N:171:ARG:HD3	1.29	1.15
27:1:38:LYS:HE2	27:1:45:LYS:HE2	1.33	1.07
1:A:1160:G:H5'	1:A:1161:A:H5'	1.32	1.06

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	235/239 (98%)	210 (89%)	20 (8%)	5 (2%)	9	40
4	D	335/337 (99%)	304 (91%)	24 (7%)	7 (2%)	9	40
5	E	244/246 (99%)	219 (90%)	24 (10%)	1 (0%)	39	80
6	F	134/176 (76%)	96 (72%)	29 (22%)	9 (7%)	1	8
7	G	170/177 (96%)	162 (95%)	8 (5%)	0	100	100
8	H	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	11	46
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	135 (89%)	12 (8%)	5 (3%)	5	26
11	K	140/145 (97%)	129 (92%)	8 (6%)	3 (2%)	9	40
12	L	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	13	50
13	M	141/164 (86%)	122 (86%)	16 (11%)	3 (2%)	9	40
14	N	192/194 (99%)	170 (88%)	20 (10%)	2 (1%)	19	61
15	O	184/186 (99%)	167 (91%)	10 (5%)	7 (4%)	4	22
16	P	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
17	Q	141/148 (95%)	137 (97%)	4 (3%)	0	100	100
18	R	93/95 (98%)	87 (94%)	6 (6%)	0	100	100
19	S	148/154 (96%)	138 (93%)	9 (6%)	1 (1%)	26	70
20	T	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
21	U	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	21	64
22	V	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	5	27
24	X	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	15	53
25	Y	80/91 (88%)	70 (88%)	9 (11%)	1 (1%)	15	53
26	Z	140/240 (58%)	136 (97%)	4 (3%)	0	100	100
27	1	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	85 (94%)	3 (3%)	2 (2%)	8	38
All	All	3633/4235 (86%)	3317 (91%)	259 (7%)	57 (2%)	12	48

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	20	LYS
6	F	93	LEU
6	F	95	THR
6	F	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	
3	C	179/181 (99%)	165 (92%)	14 (8%)	16	49
4	D	282/282 (100%)	266 (94%)	16 (6%)	25	64
5	E	193/193 (100%)	178 (92%)	15 (8%)	16	49
6	F	117/147 (80%)	108 (92%)	9 (8%)	16	50
7	G	152/155 (98%)	148 (97%)	4 (3%)	54	85
8	H	92/92 (100%)	92 (100%)	0	100	100
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	112 (92%)	10 (8%)	14	46
11	K	118/121 (98%)	109 (92%)	9 (8%)	16	51
12	L	106/106 (100%)	103 (97%)	3 (3%)	51	84
13	M	112/126 (89%)	108 (96%)	4 (4%)	42	79
14	N	166/166 (100%)	157 (95%)	9 (5%)	27	66
15	O	149/149 (100%)	143 (96%)	6 (4%)	38	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	91 (98%)	2 (2%)	60	88
17	Q	113/116 (97%)	110 (97%)	3 (3%)	52	85
18	R	79/79 (100%)	75 (95%)	4 (5%)	29	69
19	S	117/121 (97%)	113 (97%)	4 (3%)	44	81
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	102 (97%)	3 (3%)	50	84
22	V	44/52 (85%)	44 (100%)	0	100	100
23	W	51/56 (91%)	50 (98%)	1 (2%)	63	89
24	X	130/130 (100%)	122 (94%)	8 (6%)	23	60
25	Y	66/73 (90%)	62 (94%)	4 (6%)	23	61
26	Z	120/195 (62%)	110 (92%)	10 (8%)	14	46
27	1	56/56 (100%)	53 (95%)	3 (5%)	27	66
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	57	87
30	4	79/79 (100%)	77 (98%)	2 (2%)	55	86
All	All	3027/3441 (88%)	2883 (95%)	144 (5%)	31	71

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	142	VAL
13	M	30	ARG
26	Z	189	ASN
10	J	166	ASN
11	K	112	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	116	HIS
17	Q	66	GLN
29	3	16	ASN
14	N	26	HIS
15	O	107	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	239 (8%)	38 (1%)
2	B	121/122 (99%)	18 (14%)	6 (4%)
All	All	2868/3044 (94%)	257 (8%)	44 (1%)

5 of 257 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1352	A
1	A	1856	C
2	B	3024	U
1	A	1377	C
1	A	1563	G

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 232 ligands modelled in this entry, 231 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected



value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
35	CLM	A	9001	-	18,20,20	1.46	1 (5%)	22,27,27	1.13	3 (13%)

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
35	CLM	A	9001	-	-	0/22/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	9001	CLM	C5-C3	-4.55	1.47	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
35	A	9001	CLM	C11-C10-C9	-2.34	116.87	120.15
35	A	9001	CLM	C8-C9-N9	-2.09	117.80	119.48
35	A	9001	CLM	O4-C4-C3	2.18	116.97	111.12

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	A	2754/2922 (94%)	-0.33	41 (1%) 76 49	14, 38, 82, 130	0
2	B	122/122 (100%)	-0.07	6 (4%) 33 13	31, 55, 80, 139	0
3	C	237/239 (99%)	-0.15	4 (1%) 73 45	21, 42, 74, 95	0
4	D	337/337 (100%)	-0.29	1 (0%) 94 84	20, 49, 73, 84	0
5	E	246/246 (100%)	-0.41	0 100 100	16, 39, 62, 72	0
6	F	140/176 (79%)	1.28	32 (22%) 1 1	46, 89, 107, 111	0
7	G	172/177 (97%)	0.32	3 (1%) 73 45	39, 61, 80, 85	0
8	H	119/119 (100%)	0.09	3 (2%) 61 30	39, 61, 86, 93	0
9	I	29/348 (8%)	1.56	5 (17%) 2 1	65, 82, 89, 92	0
10	J	156/167 (93%)	-0.05	2 (1%) 79 53	31, 51, 77, 81	0
11	K	142/145 (97%)	-0.23	0 100 100	29, 43, 64, 83	0
12	L	132/132 (100%)	-0.44	0 100 100	28, 45, 63, 70	0
13	M	145/164 (88%)	0.17	6 (4%) 41 16	17, 57, 93, 107	0
14	N	194/194 (100%)	-0.44	0 100 100	22, 36, 55, 65	0
15	O	186/186 (100%)	0.09	4 (2%) 65 35	31, 54, 93, 107	0
16	P	115/115 (100%)	-0.27	0 100 100	31, 47, 63, 67	0
17	Q	143/148 (96%)	-0.10	0 100 100	30, 47, 59, 68	0
18	R	95/95 (100%)	-0.39	1 (1%) 82 58	27, 37, 53, 66	0
19	S	150/154 (97%)	-0.30	0 100 100	24, 39, 58, 66	0
20	T	81/84 (96%)	-0.30	0 100 100	37, 51, 70, 72	0
21	U	119/119 (100%)	0.02	4 (3%) 49 21	33, 49, 73, 86	0
22	V	53/66 (80%)	-0.03	0 100 100	33, 49, 65, 73	0
23	W	65/70 (92%)	0.72	5 (7%) 16 6	43, 64, 99, 103	0
24	X	154/154 (100%)	-0.40	0 100 100	28, 41, 58, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	82/91 (90%)	0.22	2 (2%) 62 32	36, 51, 74, 93	0
26	Z	142/240 (59%)	-0.26	3 (2%) 67 36	18, 38, 59, 78	0
27	1	73/73 (100%)	-0.30	0 100 100	36, 52, 68, 75	0
28	2	56/56 (100%)	-0.63	0 100 100	18, 27, 32, 41	0
29	3	46/48 (95%)	0.07	1 (2%) 65 35	28, 52, 78, 91	0
30	4	92/92 (100%)	-0.04	0 100 100	26, 47, 61, 73	0
All	All	6577/7279 (90%)	-0.19	123 (1%) 70 41	14, 44, 83, 139	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	W	1	THR	8.6
2	B	3001	U	6.0
2	B	3025	G	5.8
6	F	57	THR	4.7
25	Y	88	GLU	4.7

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
31	MG	A	8066	1/1	0.89	0.47	55.12	38,38,38,38	0
33	NA	A	8378	1/1	0.89	0.86	36.93	47,47,47,47	0
33	NA	A	8371	1/1	0.39	0.49	34.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	A	8325	1/1	0.96	0.38	30.66	58,58,58,58	0
33	NA	A	8374	1/1	0.91	0.63	27.14	56,56,56,56	0
33	NA	A	8376	1/1	0.78	0.46	23.38	53,53,53,53	0
33	NA	A	8382	1/1	0.68	0.53	20.20	74,74,74,74	0
33	NA	A	8362	1/1	0.89	0.28	18.65	65,65,65,65	0
33	NA	A	8359	1/1	0.79	0.38	16.42	49,49,49,49	0
33	NA	A	8335	1/1	0.92	0.25	13.83	53,53,53,53	0
33	NA	M	8380	1/1	0.92	0.56	12.86	57,57,57,57	0
33	NA	A	8350	1/1	0.92	0.28	12.56	44,44,44,44	0
33	NA	A	8372	1/1	0.88	0.31	11.74	62,62,62,62	0
33	NA	S	8386	1/1	0.81	0.49	11.43	83,83,83,83	0
33	NA	A	8310	1/1	0.84	0.29	11.42	21,21,21,21	0
33	NA	A	8364	1/1	0.63	0.27	10.30	33,33,33,33	0
34	CL	D	8519	1/1	0.90	0.30	9.99	53,53,53,53	0
34	CL	A	8515	1/1	0.94	0.26	9.36	67,67,67,67	0
33	NA	A	8368	1/1	0.83	0.27	9.27	63,63,63,63	0
31	MG	A	8088	1/1	0.74	0.24	9.22	44,44,44,44	0
33	NA	A	8332	1/1	0.91	0.24	8.31	28,28,28,28	0
33	NA	A	8321	1/1	0.97	0.24	8.28	45,45,45,45	0
33	NA	A	8373	1/1	0.78	0.30	8.22	49,49,49,49	0
33	NA	A	8356	1/1	0.96	0.22	7.80	40,40,40,40	0
33	NA	A	8361	1/1	0.95	0.21	6.87	58,58,58,58	0
33	NA	A	8326	1/1	0.81	0.27	6.59	42,42,42,42	0
32	K	A	8202	1/1	0.92	0.20	5.72	56,56,56,56	0
33	NA	A	8381	1/1	0.90	0.20	5.57	45,45,45,45	0
33	NA	B	8383	1/1	0.81	0.25	3.94	45,45,45,45	0
33	NA	A	8339	1/1	0.92	0.18	3.71	17,17,17,17	0
31	MG	A	8060	1/1	0.99	0.18	3.69	36,36,36,36	0
33	NA	A	8303	1/1	0.97	0.17	3.66	41,41,41,41	0
31	MG	A	8064	1/1	0.96	0.17	3.03	20,20,20,20	0
33	NA	A	8308	1/1	0.91	0.16	2.69	49,49,49,49	0
33	NA	A	8379	1/1	0.93	0.16	2.30	51,51,51,51	0
33	NA	A	8327	1/1	0.91	0.17	2.21	47,47,47,47	0
31	MG	A	8101	1/1	0.92	0.15	1.79	55,55,55,55	0
31	MG	A	8044	1/1	0.94	0.15	1.46	42,42,42,42	0
31	MG	A	8052	1/1	0.97	0.17	1.29	52,52,52,52	0
33	NA	A	8365	1/1	0.96	0.21	1.04	33,33,33,33	0
31	MG	A	8112	1/1	0.94	0.16	0.79	49,49,49,49	0
34	CL	N	8518	1/1	0.93	0.21	0.76	41,41,41,41	0
33	NA	A	8324	1/1	0.82	0.20	0.33	46,46,46,46	0
34	CL	4	8504	1/1	0.83	0.23	0.19	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	A	8331	1/1	0.98	0.14	0.17	38,38,38,38	0
34	CL	K	8521	1/1	0.94	0.16	-0.22	50,50,50,50	0
33	NA	A	8338	1/1	0.96	0.14	-0.51	43,43,43,43	0
33	NA	A	8366	1/1	0.96	0.15	-0.55	53,53,53,53	0
32	K	A	8201	1/1	0.97	0.14	-0.83	55,55,55,55	0
31	MG	4	8078	1/1	0.91	0.12	-0.87	35,35,35,35	0
33	NA	E	8304	1/1	0.83	0.16	-1.01	30,30,30,30	0
33	NA	A	8323	1/1	0.97	0.14	-1.03	37,37,37,37	0
33	NA	K	8346	1/1	0.89	0.14	-1.08	43,43,43,43	0
33	NA	C	8345	1/1	0.90	0.15	-1.11	49,49,49,49	0
31	MG	A	8100	1/1	0.94	0.12	-1.19	80,80,80,80	0
33	NA	A	8333	1/1	0.76	0.11	-1.20	24,24,24,24	0
33	NA	A	8317	1/1	0.95	0.12	-1.43	29,29,29,29	0
33	NA	S	8337	1/1	0.91	0.11	-1.49	35,35,35,35	0
34	CL	P	8508	1/1	0.96	0.14	-1.55	71,71,71,71	0
33	NA	A	8353	1/1	0.95	0.11	-1.56	27,27,27,27	0
31	MG	A	8059	1/1	0.95	0.12	-1.67	37,37,37,37	0
36	CD	1	8403	1/1	0.96	0.10	-1.75	56,56,56,56	0
36	CD	V	8401	1/1	0.93	0.08	-1.82	63,63,63,63	0
31	MG	A	8057	1/1	0.94	0.12	-1.87	38,38,38,38	0
31	MG	A	8018	1/1	0.95	0.11	-1.95	50,50,50,50	0
31	MG	C	8065	1/1	0.96	0.11	-1.99	50,50,50,50	0
31	MG	A	8070	1/1	0.97	0.09	-2.01	47,47,47,47	0
31	MG	A	8012	1/1	0.99	0.11	-2.05	37,37,37,37	0
33	NA	J	8309	1/1	0.97	0.07	-2.12	24,24,24,24	0
31	MG	A	8013	1/1	0.97	0.12	-2.15	48,48,48,48	0
31	MG	A	8053	1/1	0.95	0.12	-2.16	49,49,49,49	0
36	CD	4	8404	1/1	0.96	0.07	-2.26	59,59,59,59	0
33	NA	U	8343	1/1	0.95	0.10	-2.35	34,34,34,34	0
36	CD	2	8402	1/1	0.98	0.07	-2.42	57,57,57,57	0
31	MG	D	8055	1/1	0.95	0.07	-2.48	48,48,48,48	0
34	CL	A	8505	1/1	0.93	0.14	-2.49	53,53,53,53	0
31	MG	A	8058	1/1	0.97	0.12	-2.51	43,43,43,43	0
31	MG	A	8074	1/1	0.98	0.06	-2.59	28,28,28,28	0
33	NA	N	8347	1/1	0.97	0.08	-2.74	17,17,17,17	0
31	MG	A	8004	1/1	0.96	0.09	-2.74	33,33,33,33	0
31	MG	U	8073	1/1	0.88	0.09	-2.75	52,52,52,52	0
31	MG	A	8107	1/1	0.96	0.04	-2.83	34,34,34,34	0
34	CL	A	8512	1/1	0.99	0.07	-2.83	41,41,41,41	0
34	CL	M	8510	1/1	0.97	0.12	-2.97	60,60,60,60	0
31	MG	A	8067	1/1	0.97	0.13	-3.02	49,49,49,49	0
31	MG	A	8054	1/1	0.97	0.11	-3.04	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	R	8348	1/1	0.96	0.08	-3.14	27,27,27,27	0
33	NA	A	8305	1/1	0.93	0.12	-3.14	32,32,32,32	0
31	MG	A	8022	1/1	0.77	0.11	-3.24	26,26,26,26	0
31	MG	A	8056	1/1	0.98	0.07	-3.38	44,44,44,44	0
31	MG	A	8027	1/1	0.98	0.04	-3.46	30,30,30,30	0
31	MG	Z	8109	1/1	0.94	0.11	-3.48	33,33,33,33	0
31	MG	A	8038	1/1	0.96	0.10	-3.66	31,31,31,31	0
33	NA	A	8344	1/1	0.95	0.05	-4.01	15,15,15,15	0
31	MG	A	8084	1/1	0.99	0.10	-4.15	60,60,60,60	0
31	MG	A	8020	1/1	0.97	0.08	-4.31	36,36,36,36	0
31	MG	A	8077	1/1	0.97	0.09	-5.30	40,40,40,40	0
31	MG	A	8015	1/1	0.95	0.05	-5.46	41,41,41,41	0
31	MG	A	8006	1/1	0.98	0.04	-5.47	28,28,28,28	0
31	MG	A	8008	1/1	0.98	0.06	-5.49	43,43,43,43	0
31	MG	A	8039	1/1	0.99	0.05	-5.50	52,52,52,52	0
31	MG	A	8007	1/1	0.98	0.08	-5.71	26,26,26,26	0
31	MG	A	8017	1/1	0.97	0.04	-5.74	22,22,22,22	0
31	MG	A	8002	1/1	0.99	0.06	-5.86	38,38,38,38	0
31	MG	A	8032	1/1	0.98	0.05	-6.32	26,26,26,26	0
31	MG	A	8091	1/1	0.94	0.05	-6.80	37,37,37,37	0
31	MG	A	8108	1/1	0.92	0.07	-7.23	77,77,77,77	0
31	MG	A	8096	1/1	0.96	0.06	-7.43	42,42,42,42	0
31	MG	A	8014	1/1	0.98	0.06	-7.54	30,30,30,30	0
31	MG	A	8003	1/1	0.99	0.06	-8.05	18,18,18,18	0
31	MG	A	8019	1/1	0.98	0.05	-8.35	27,27,27,27	0
33	NA	A	8320	1/1	0.98	0.07	-9.22	20,20,20,20	0
31	MG	A	8033	1/1	0.96	0.05	-9.35	31,31,31,31	0
31	MG	A	8010	1/1	0.98	0.05	-9.83	29,29,29,29	0
31	MG	A	8035	1/1	0.97	0.04	-10.74	39,39,39,39	0
31	MG	A	8080	1/1	0.97	0.08	-11.87	42,42,42,42	0
31	MG	A	8021	1/1	0.97	0.09	-11.87	36,36,36,36	0
31	MG	A	8001	1/1	0.97	0.04	-11.91	22,22,22,22	0
31	MG	A	8009	1/1	0.97	0.06	-	32,32,32,32	0
31	MG	A	8072	1/1	0.87	0.18	-	56,56,56,56	0
31	MG	A	8110	1/1	0.96	0.05	-	34,34,34,34	0
33	NA	A	8315	1/1	0.89	0.22	-	34,34,34,34	0
31	MG	A	8024	1/1	0.94	0.10	-	18,18,18,18	0
33	NA	A	8311	1/1	0.95	0.18	-	51,51,51,51	0
31	MG	A	8071	1/1	0.98	0.08	-	72,72,72,72	0
33	NA	A	8352	1/1	0.83	0.30	-	51,51,51,51	0
34	CL	A	8517	1/1	0.90	0.14	-	51,51,51,51	0
31	MG	A	8041	1/1	0.96	0.20	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	A	8360	1/1	0.95	0.42	-	42,42,42,42	0
31	MG	A	8047	1/1	0.94	0.10	-	65,65,65,65	0
31	MG	A	8045	1/1	0.92	0.12	-	63,63,63,63	0
31	MG	A	8034	1/1	0.98	0.04	-	26,26,26,26	0
33	NA	A	8341	1/1	0.93	0.15	-	25,25,25,25	0
31	MG	A	8068	1/1	0.81	0.11	-	61,61,61,61	0
33	NA	A	8301	1/1	0.96	0.17	-	24,24,24,24	0
31	MG	A	8093	1/1	0.95	0.08	-	40,40,40,40	0
31	MG	A	8113	1/1	0.85	0.19	-	35,35,35,35	0
33	NA	A	8336	1/1	0.98	0.04	-	34,34,34,34	0
34	CL	A	8516	1/1	0.96	0.19	-	69,69,69,69	0
31	MG	A	8049	1/1	0.62	0.51	-	69,69,69,69	0
31	MG	A	8040	1/1	0.97	0.11	-	54,54,54,54	0
31	MG	A	8085	1/1	0.87	0.17	-	59,59,59,59	0
31	MG	A	8029	1/1	0.98	0.07	-	40,40,40,40	0
31	MG	A	8099	1/1	0.95	0.22	-	48,48,48,48	0
31	MG	A	8075	1/1	0.94	0.08	-	52,52,52,52	0
35	CLM	A	9001	20/20	0.78	0.32	-	57,61,68,69	0
31	MG	A	8104	1/1	0.96	0.14	-	42,42,42,42	0
33	NA	A	8307	1/1	0.66	0.25	-	51,51,51,51	0
34	CL	A	8522	1/1	0.97	0.18	-	66,66,66,66	0
31	MG	A	8043	1/1	0.95	0.11	-	41,41,41,41	0
36	CD	P	8405	1/1	0.97	0.05	-	90,90,90,90	0
33	NA	A	8328	1/1	0.94	0.28	-	30,30,30,30	0
31	MG	A	8083	1/1	0.98	0.07	-	42,42,42,42	0
34	CL	A	8514	1/1	0.95	0.12	-	47,47,47,47	0
33	NA	A	8302	1/1	0.89	0.28	-	34,34,34,34	0
31	MG	A	8030	1/1	0.98	0.06	-	30,30,30,30	0
31	MG	A	8042	1/1	0.90	0.22	-	41,41,41,41	0
31	MG	A	8005	1/1	0.97	0.09	-	36,36,36,36	0
33	NA	A	8330	1/1	0.90	0.31	-	27,27,27,27	0
31	MG	A	8115	1/1	0.95	0.08	-	44,44,44,44	0
33	NA	A	8370	1/1	0.89	0.23	-	55,55,55,55	0
33	NA	B	8351	1/1	0.86	0.13	-	49,49,49,49	0
31	MG	A	8031	1/1	0.98	0.03	-	22,22,22,22	0
33	NA	A	8384	1/1	0.39	0.56	-	59,59,59,59	0
34	CL	Z	8520	1/1	0.84	0.16	-	39,39,39,39	0
31	MG	A	8037	1/1	0.91	0.06	-	39,39,39,39	0
33	NA	A	8355	1/1	0.86	0.62	-	57,57,57,57	0
33	NA	A	8363	1/1	0.83	0.33	-	64,64,64,64	0
33	NA	J	8322	1/1	0.75	0.37	-	63,63,63,63	0
31	MG	A	8092	1/1	0.96	0.13	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	A	8314	1/1	0.96	0.08	-	28,28,28,28	0
31	MG	L	8069	1/1	0.97	0.08	-	64,64,64,64	0
31	MG	A	8076	1/1	0.85	0.18	-	71,71,71,71	0
33	NA	A	8375	1/1	0.89	0.24	-	48,48,48,48	0
33	NA	A	8385	1/1	0.88	0.35	-	45,45,45,45	0
31	MG	A	8061	1/1	0.95	0.09	-	35,35,35,35	0
31	MG	A	8036	1/1	0.98	0.03	-	39,39,39,39	0
31	MG	A	8114	1/1	0.80	0.13	-	52,52,52,52	0
33	NA	A	8369	1/1	0.85	0.26	-	51,51,51,51	0
31	MG	A	8106	1/1	0.91	0.17	-	51,51,51,51	0
31	MG	A	8048	1/1	0.97	0.06	-	43,43,43,43	0
31	MG	A	8090	1/1	0.92	0.22	-	46,46,46,46	0
31	MG	A	8028	1/1	0.88	0.08	-	28,28,28,28	0
33	NA	A	8318	1/1	0.94	0.17	-	53,53,53,53	0
31	MG	A	8097	1/1	0.96	0.09	-	46,46,46,46	0
31	MG	A	8081	1/1	0.93	0.07	-	47,47,47,47	0
34	CL	O	8507	1/1	0.96	0.19	-	61,61,61,61	0
34	CL	C	8509	1/1	0.94	0.19	-	67,67,67,67	0
34	CL	S	8506	1/1	0.98	0.12	-	43,43,43,43	0
31	MG	A	8051	1/1	0.89	0.13	-	61,61,61,61	0
31	MG	A	8016	1/1	0.98	0.10	-	27,27,27,27	0
31	MG	A	8116	1/1	0.98	0.10	-	60,60,60,60	0
33	NA	A	8349	1/1	0.95	0.22	-	37,37,37,37	0
31	MG	A	8046	1/1	0.89	0.08	-	45,45,45,45	0
31	MG	1	8105	1/1	0.88	0.24	-	28,28,28,28	0
33	NA	A	8334	1/1	0.94	0.05	-	27,27,27,27	0
31	MG	B	8095	1/1	0.86	0.14	-	61,61,61,61	0
31	MG	A	8087	1/1	0.82	0.24	-	71,71,71,71	0
31	MG	A	8082	1/1	0.91	0.13	-	66,66,66,66	0
34	CL	A	8503	1/1	0.85	0.22	-	49,49,49,49	0
31	MG	A	8102	1/1	0.92	0.18	-	60,60,60,60	0
31	MG	A	8023	1/1	0.94	0.07	-	36,36,36,36	0
31	MG	A	8111	1/1	0.92	0.09	-	54,54,54,54	0
31	MG	A	8026	1/1	0.98	0.09	-	27,27,27,27	0
33	NA	A	8316	1/1	0.88	0.28	-	53,53,53,53	0
34	CL	K	8501	1/1	0.97	0.18	-	61,61,61,61	0
34	CL	A	8513	1/1	0.96	0.11	-	52,52,52,52	0
33	NA	A	8329	1/1	0.67	0.24	-	48,48,48,48	0
31	MG	A	8094	1/1	0.94	0.12	-	61,61,61,61	0
33	NA	A	8313	1/1	0.94	0.21	-	66,66,66,66	0
33	NA	A	8306	1/1	0.87	0.34	-	51,51,51,51	0
33	NA	A	8342	1/1	0.85	0.24	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	A	8011	1/1	0.95	0.07	-	35,35,35,35	0
31	MG	A	8086	1/1	0.98	0.18	-	35,35,35,35	0
33	NA	A	8354	1/1	0.94	0.14	-	32,32,32,32	0
31	MG	A	8063	1/1	0.91	0.07	-	74,74,74,74	0
31	MG	A	8062	1/1	0.95	0.10	-	58,58,58,58	0
33	NA	A	8377	1/1	0.78	0.70	-	66,66,66,66	0
34	CL	K	8502	1/1	0.72	0.23	-	72,72,72,72	0
31	MG	A	8117	1/1	0.97	0.09	-	25,25,25,25	0
33	NA	A	8340	1/1	0.81	0.60	-	41,41,41,41	0
33	NA	A	8357	1/1	0.58	0.17	-	56,56,56,56	0
31	MG	A	8089	1/1	0.76	0.13	-	68,68,68,68	0
31	MG	A	8098	1/1	0.97	0.13	-	29,29,29,29	0
31	MG	A	8050	1/1	0.80	0.17	-	79,79,79,79	0
33	NA	A	8367	1/1	0.95	0.08	-	42,42,42,42	0
31	MG	A	8103	1/1	0.84	0.17	-	56,56,56,56	0
33	NA	A	8319	1/1	0.91	0.11	-	40,40,40,40	0
31	MG	A	8079	1/1	0.99	0.09	-	36,36,36,36	0
31	MG	A	8025	1/1	0.98	0.09	-	47,47,47,47	0
33	NA	T	8312	1/1	0.81	0.16	-	44,44,44,44	0
34	CL	R	8511	1/1	0.95	0.13	-	49,49,49,49	0

## 6.5 Other polymers

There are no such residues in this entry.