



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2020 – 12:08 PM BST

PDB ID : 2QA4
Title : A more complete structure of the the L7/L12 stalk of the Haloarcula marismortui 50S large ribosomal subunit
Authors : Steitz, T.A.; Kavran, J.M.
Deposited on : 2007-06-14
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

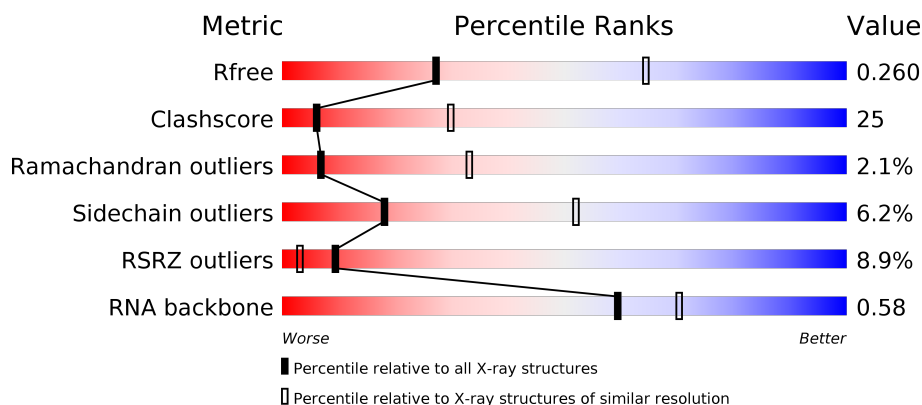
1 Overall quality at a glance

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))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>28%</div> <div>57%</div> <div>9%</div> <div>6%</div> </div>
2	9	122	<div> <div>17%</div> <div>69%</div> <div>13%</div> </div>
3	A	240	<div> <div>10%</div> <div>61%</div> <div>34%</div> </div>
4	B	338	<div> <div>4%</div> <div>59%</div> <div>36%</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	196	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	67	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	92	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	
31	3	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
32	MG	0	2971	-	-	-	X
32	MG	0	2973	-	-	-	X
32	MG	0	2980	-	-	-	X
32	MG	0	2984	-	-	-	X
32	MG	0	2998	-	-	-	X
32	MG	0	3006	-	-	-	X
32	MG	0	3025	-	-	-	X
32	MG	0	3026	-	-	-	X
32	MG	0	3028	-	-	-	X
32	MG	0	3029	-	-	-	X
32	MG	3	93	-	-	-	X
32	MG	A	240	-	-	-	X
32	MG	B	338	-	-	-	X
32	MG	K	133	-	-	-	X
32	MG	Y	241	-	-	-	X
33	K	0	3031	-	-	-	X
33	K	M	196	-	-	-	X
34	NA	0	3033	-	-	-	X
34	NA	0	3034	-	-	-	X
34	NA	0	3039	-	-	-	X
34	NA	0	3044	-	-	-	X
34	NA	0	3050	-	-	-	X
34	NA	0	3052	-	-	-	X
34	NA	0	3057	-	-	-	X
34	NA	0	3059	-	-	-	X
34	NA	0	3075	-	-	-	X
34	NA	0	3077	-	-	-	X
34	NA	0	3082	-	-	-	X
34	NA	0	3084	-	-	-	X
34	NA	0	3094	-	-	-	X
34	NA	0	3098	-	-	-	X
34	NA	0	3099	-	-	-	X
34	NA	0	3100	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	0	3103	-	-	-	X
34	NA	S	85	-	-	-	X
35	CL	0	3106	-	-	-	X
35	CL	0	3109	-	-	-	X
35	CL	0	3112	-	-	-	X
35	CL	3	95	-	-	X	X
35	CL	J	147	-	-	X	-
35	CL	J	149	-	-	X	-
35	CL	O	117	-	-	-	X
35	CL	Q	97	-	-	-	X
36	CD	O	116	-	-	-	X

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 92248 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	2753	Total	C	N	O	P	0	0	0
			58979	26332	10869	19036	2742			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	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	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

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

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

- Molecule 5 is a protein called 50S ribosomal protein L4P.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	CONFLICT	UNP P12735

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

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	125	Total	C	N	O	S	0	0	0
			959	592	162	203	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	CONFLICT	UNP P15825

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	INSERTION	UNP P60617
H	165	SER	LYS	CONFLICT	UNP P60617
H	166	SER	VAL	CONFLICT	UNP P60617
H	167	PRO	GLU	CONFLICT	UNP P60617
H	168	ALA	ARG	CONFLICT	UNP P60617
H	?	-	GLU	DELETION	UNP P60617
H	?	-	GLU	DELETION	UNP P60617
H	?	-	LEU	DELETION	UNP P60617
H	?	-	LEU	DELETION	UNP P60617
H	170	ASN	ILE	CONFLICT	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	118	Total	C	N	O	S	0	0	0
			876	548	135	192	1			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	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 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1559	943	332	283	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	UNP P60618
M	194	ALA	GLY	CONFLICT	UNP P60618

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19e.

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24e.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L31E.

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

- Molecule 27 is a protein called 50S ribosomal protein L32e.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	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	UNP P60619

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	108	Total	Mg	0	0
			108	108		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	3	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	1	Total	K	0	0
			1	1		
33	M	1	Total	K	0	0
			1	1		

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	73	Total	Na	0	0
			73	73		
34	J	1	Total	Na	0	0
			1	1		
34	Q	1	Total	Na	0	0
			1	1		
34	H	1	Total	Na	0	0
			1	1		
34	C	1	Total	Na	0	0
			1	1		
34	A	1	Total	Na	0	0
			1	1		
34	R	2	Total	Na	0	0
			2	2		
34	9	3	Total	Na	0	0
			3	3		
34	L	1	Total	Na	0	0
			1	1		
34	S	1	Total	Na	0	0
			1	1		
34	M	1	Total	Na	0	0
			1	1		

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	8	Total	Cl	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	J	3	Total 3	Cl 3	0	0
35	Q	1	Total 1	Cl 1	0	0
35	K	1	Total 1	Cl 1	0	0
35	B	1	Total 1	Cl 1	0	0
35	A	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

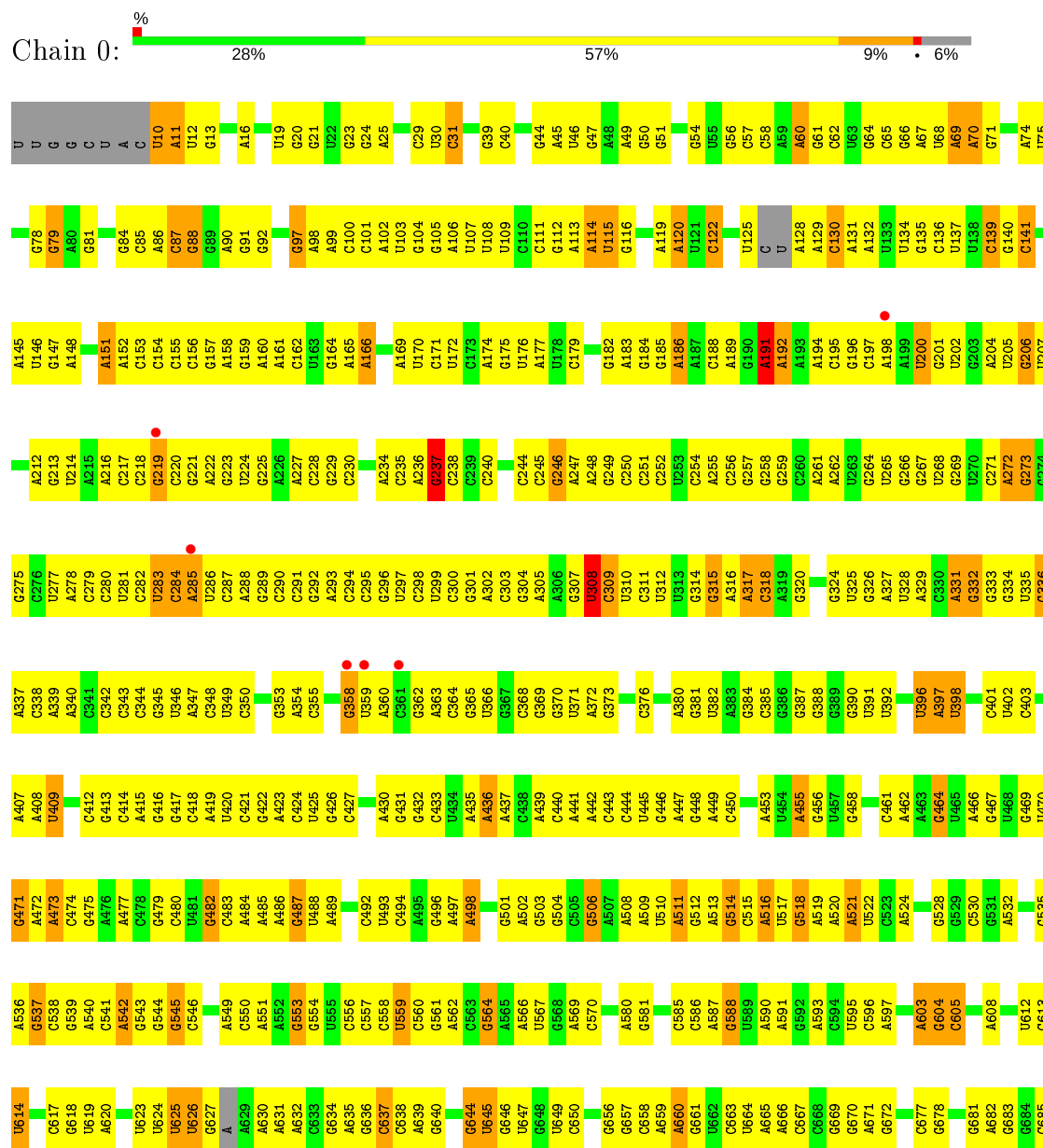
- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

3 Residue-property plots

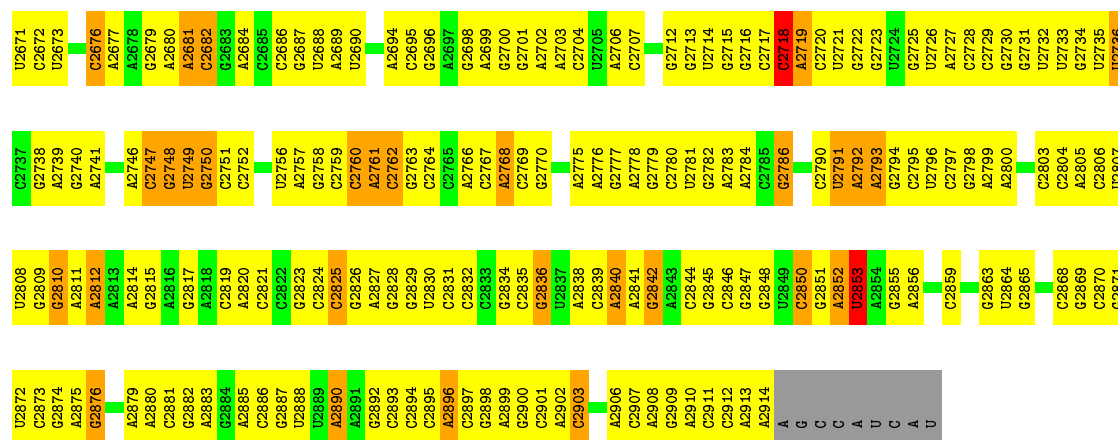
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S RIBOSOMAL RNA

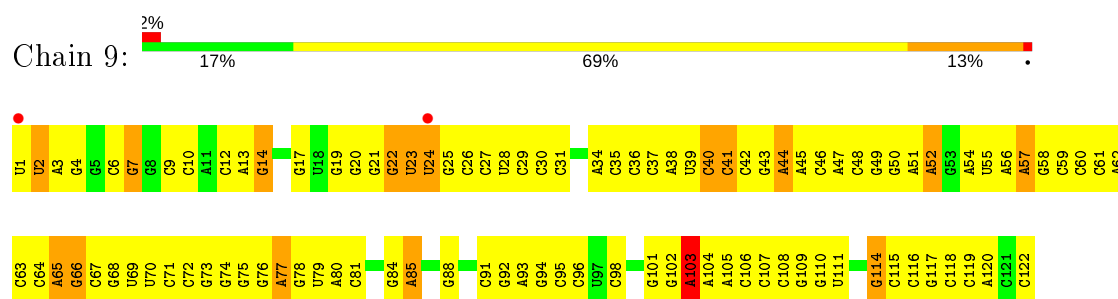


A1607	G1543	U1473	A1328	G1257	G1121	C1051	A908	U840	A761	A686
G1608	U1544	C1474	A1329	C1257	C1126	C1052	U909	A841	C764	C687
G1609	G1475	G1475	A1330	G1258	G1126	G1052	C910	C842	A765	A688
G1610	C1545	A1476	A1331	A1259	C1127	G1059	G911	A843	G766	G689
G1611	U1548	A1477	C1332	G1260	U1128	C1060	A912	A844	A766	G690
A1612	C1549	U1478	C1333	A1261	C1129	G1069	A913	U845	A767	
	A1550	A1479	C1334	C1262	U1130	G1063	A914	A846		A684
A1615	C1551		C1335	C1263	G1131	U1064	C915	C847	G772	C685
A1616	G1552	A1482	U1336	U1264	A1132	U1064	C920	C848	A773	C686
C1617	C1553	G1483	A1337	U1265	A1133	G1065	C921	C849	G774	G697
G1618	U1554	G1484	U1338	U1266	G1134	U1066	G921	U850	G775	A698
	G1555	A1485		C1267	G1135	A1202	A922		A776	C699
G1621	G1556	A1486	C1342	C1268	U1136	C1069	A923	C853	U777	A700
G1622	G1557	A1487	C1343	G1269	G1137	A1070	G924	C854	C778	U701
C1623	C1558	U1488	G1344	U1270	G1138	A1071	C925	U855	U779	G702
A1624	A1559		A1345		G1072	G1072	A926	C856	A780	G703
U1625	U	A1493	U1346	C1273	C1140	G1075	U927	U857	C781	C704
A1626	A1561	A1494	C1347			C1076		U858		C705
G1627	C1562	C1495	U1347	A1278	A1144	G1076	U932	C859	G786	G710
	G1563	A1496	A1348	U1279	G1145	G1077		U860	G787	G711
A1630	G1564	G1497	C1349	A1280	G1146	A1078	G935	A861		
A1631	C1565	U1498	U1350		C1147	A1079	C936	U866	A790	U714
A1632	C1566	U1499	G1351	G1283	C1148	C1080	C937	A867	G792	G716
C1633	C1567	U1500	A1352	U1284	U1149	A1081	G938	A868	A793	C717
G1634	A1567	A1501	C1353	U1285	A1150	A1082	U939	G869	U794	C718
U1635	G1568	A1502			G1151	C1083	G940	U870	G795	C719
G1636	C1570	U1503	A1358	C1289	C1152	A1084	G941	A871	A796	C720
A1637	A1571	A1504	C1360	U1219	C1153	C1085	U942	G872	A797	A721
	U1505	U1506	G1363	U1218	G1154	A1086	G943	U873	G800	G722
C1640	A1572	U1507	G1364	A1291	C1155	A1087	U944	A874		
A1641	C1573	C1507	C1365	U1292	G1156	A1088	U945	A875	A806	G723
A1642	C1574	C1508	C1366	U1293	C1157	G1089	U946	A876	A807	G727
C1643	C1575	U1509	U1366	G1295	G1158	A1090	C946	A877	A808	
C1644		G1510		U1296	G1159	U1091		G878	G809	G730
U1645	C1579	U1511	G1370	U1297	A1161	A1013	U949			U731
G1646	A1580	C1512		U1298	G1162	C1015	G951	A832		C732
		G1513	A1375	U1299	U1163	U1015	G952	U833	C813	U733
	U1583	C1514	C1376	G1300	U1164	U1016	U954	C884	G814	U734
	C1584		C1377	C1301	G1165	U1017	G955	G885	U815	
U1654	C1585	U1517	G1378	G1302	A1166	A1097	G956	A886	A736	C735
G1655	G1586	A1518	A1379		G1167	G1099	A957		A737	
A1656	U1587	U1519	U1380	C1305	C1168	U1101	G958	C890	A818	G738
A1657	G1588	G1520	A1381	U1306	U1169	C1102	G959	G891	A819	
A1658	G1589	C1521	C1382	A1307	U1170	G1103	C960	G892	G820	C740
A1659		A1522	U1383	U1308	A1171	C1104	A961	C893	U821	G741
G1660	G1592	U1523	C1384	U1309	G1172	A1107	C962	A894	C822	
	C1593	G1524	G1385	U1310	A1173	U1108	C963	A895	U823	G743
A1664	C1594	U1525	G1386	G1311	A1174	U1109	G964	C896	G824	
G1665	G1595	A1526	G1387	G1312	G1175	U1110		A897	U825	G744
C1666	U1596	U1527	U1388	A1313	C1176	U1111	U967	G898	U826	
A1667	A1597	A1528	G1389	U1314		A1032	G968	C899	U827	A746
U1668	A1598	G1529		G1315	C1182	C1033	G969	G900	U832	G747
A1669	U1599		A1392	G1316	C1183	G1112	U970	G901	G748	
G1670	G1600	G1536	A1393	A1317	C1184	A1114	G	U902	G833	
U1671	G1601	C1536	C1394	A1317	U1185	U1115	U	G903	G834	G755
G1672	C1602	C1537	C1395	G1322	U1186	U1116	G	U904	U835	A756
U1673	A1603	C1538	C1396	G1323	U1187	A1117	U	C905		
C1674	G1604	U1539	C1397	G1324	A1188	G1118	U	C906	C838	C759
C1675	G1605	G1540	C1398	G1327	A1189	G1119	C	C907	C1044	
G1676	A1606		A1399		G1190	U1120	C	A907	C839	G760

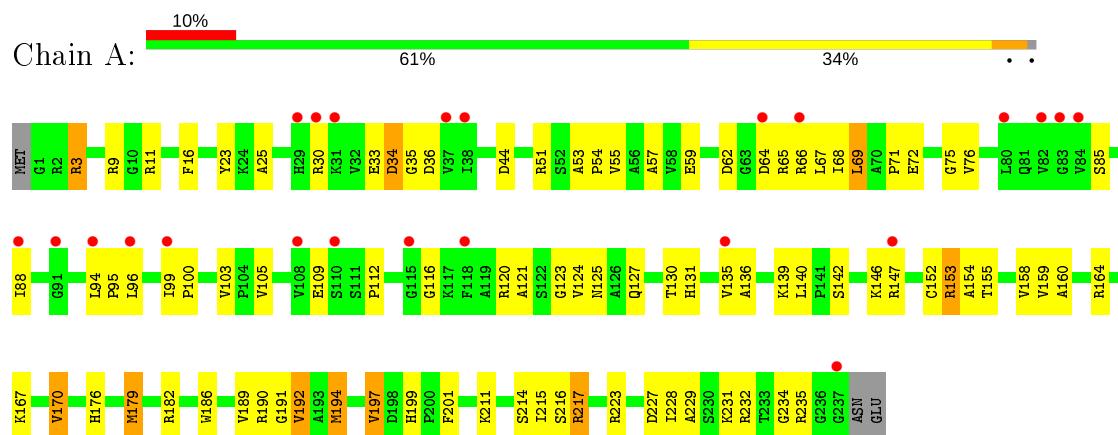




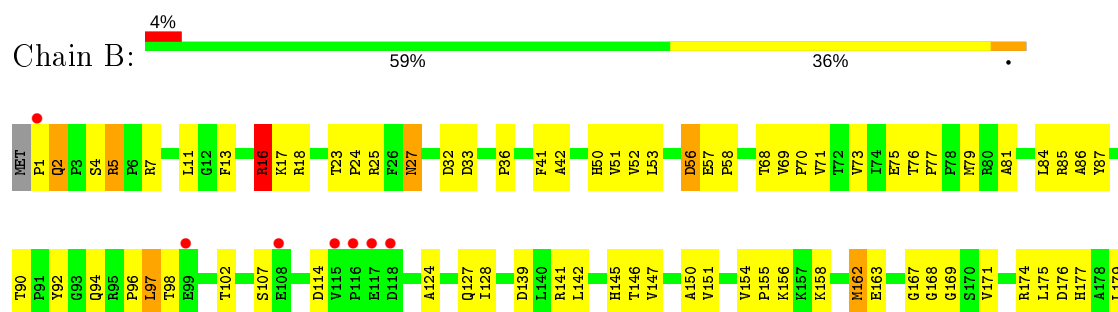
• Molecule 2: 5S RIBOSOMAL RNA

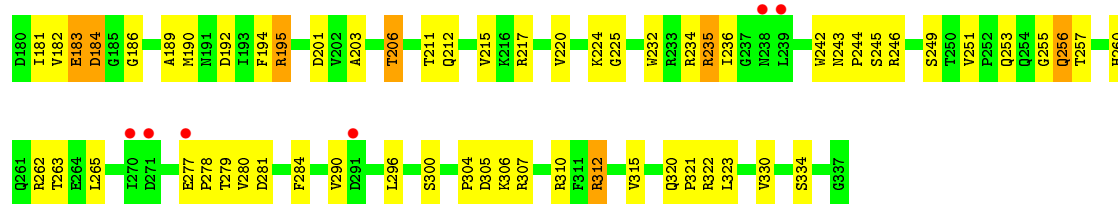


• Molecule 3: 50S ribosomal protein L2P

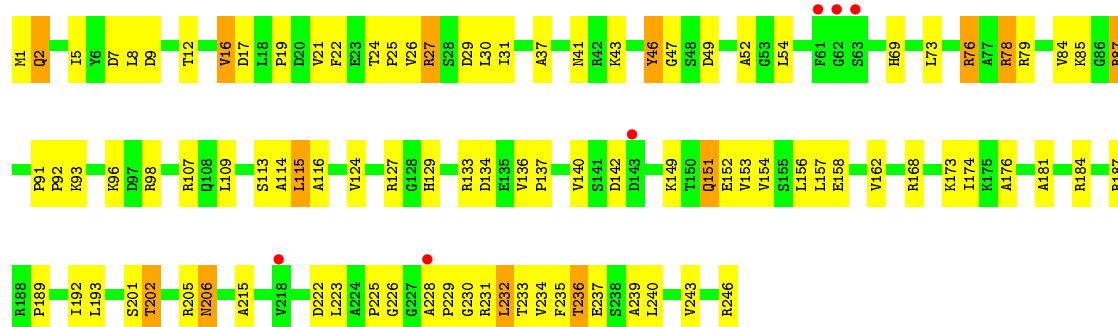


• Molecule 4: 50S ribosomal protein L3P

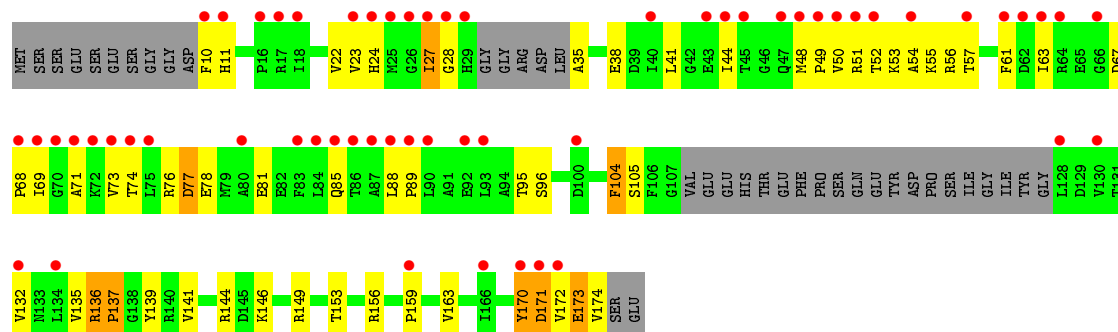




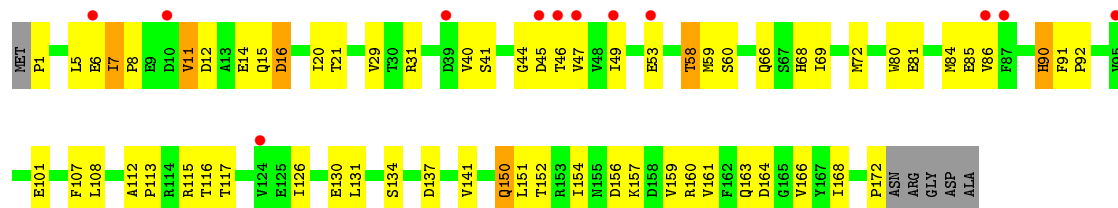
• Molecule 5: 50S ribosomal protein L4P



• Molecule 6: 50S ribosomal protein L5P

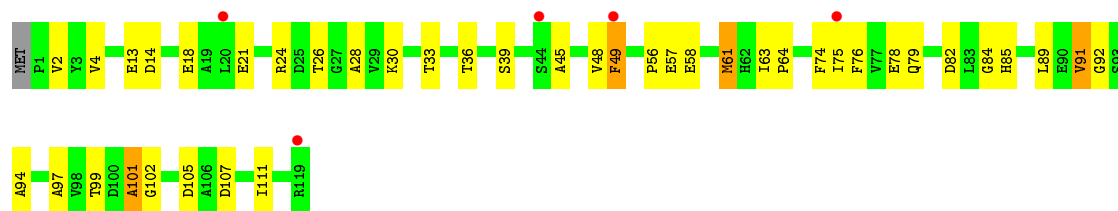


• Molecule 7: 50S ribosomal protein L6P

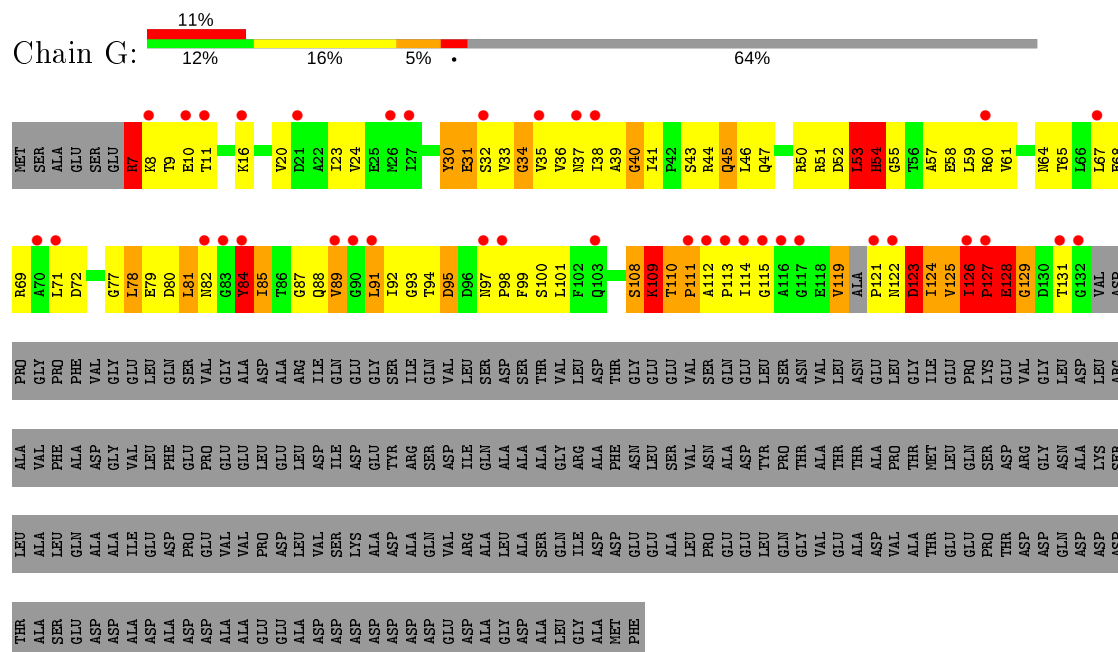


• Molecule 8: 50S ribosomal protein L7Ae

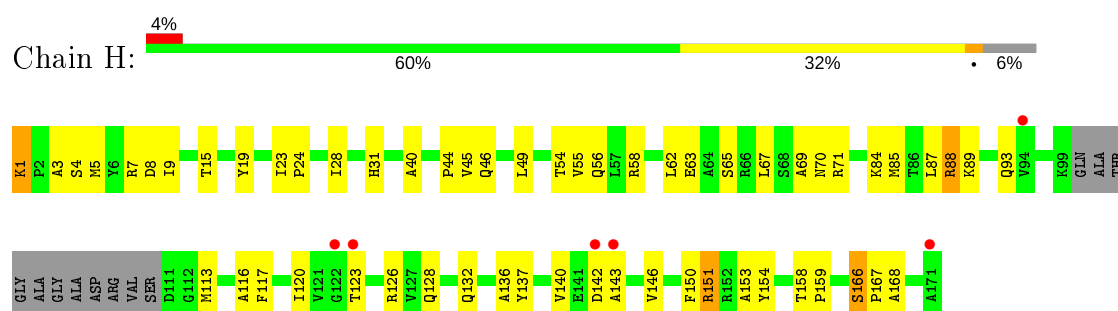




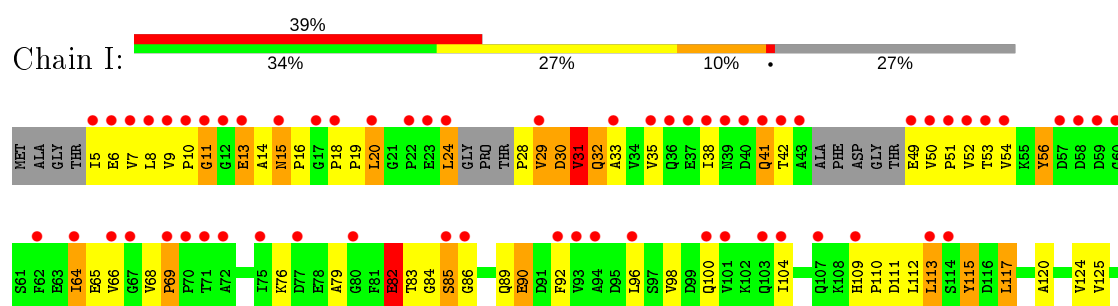
• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMO

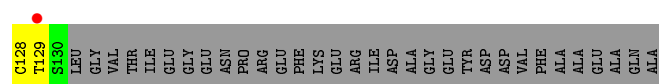


• Molecule 10: 50S ribosomal protein L10e



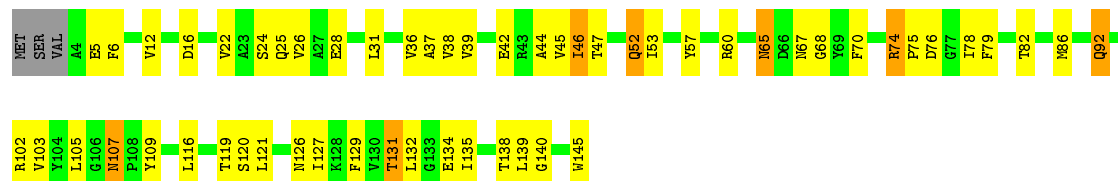
• Molecule 11: 50S ribosomal protein L11P





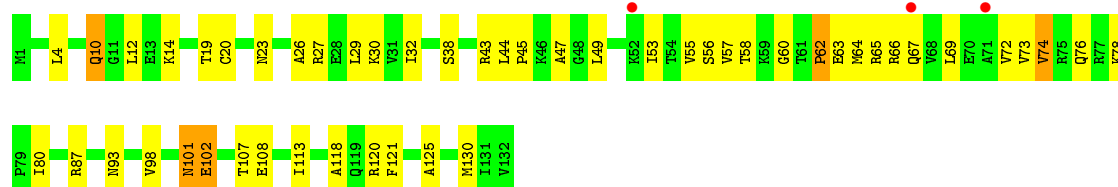
• Molecule 12: 50S ribosomal protein L13P

Chain J: 60% 33% 5%



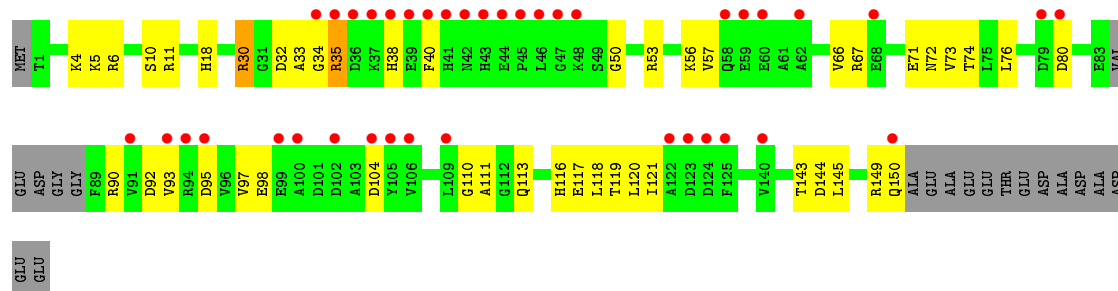
• Molecule 13: 50S ribosomal protein L14P

Chain K: 2% 62% 34%



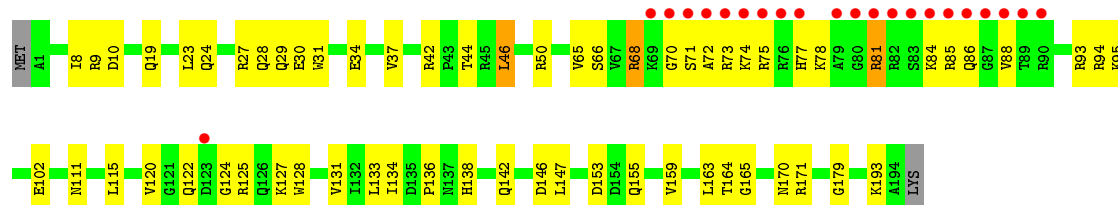
• Molecule 14: 50S ribosomal protein L15P

Chain L: 24% 60% 27% 12%

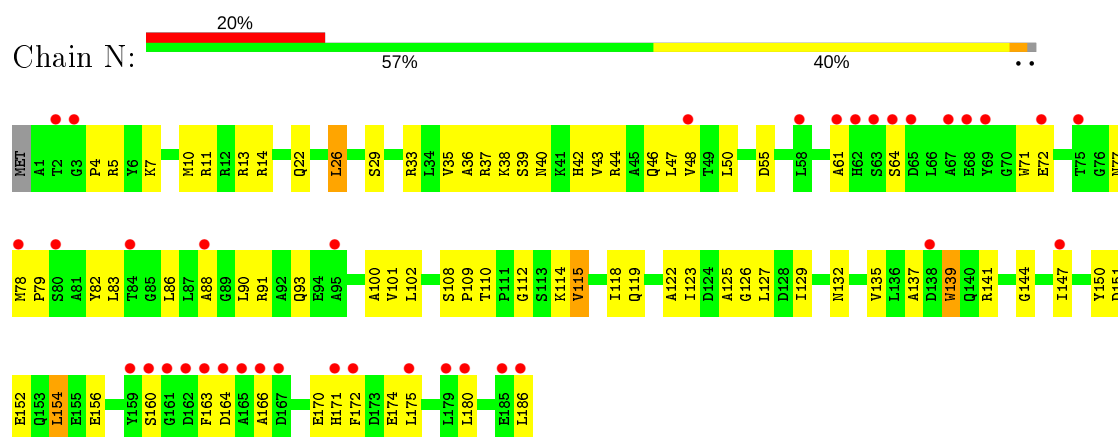


• Molecule 15: 50S ribosomal protein L15e

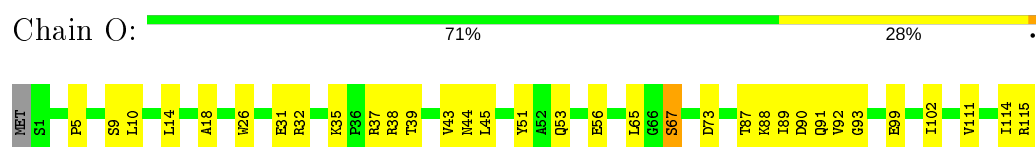
Chain M: 11% 67% 31%



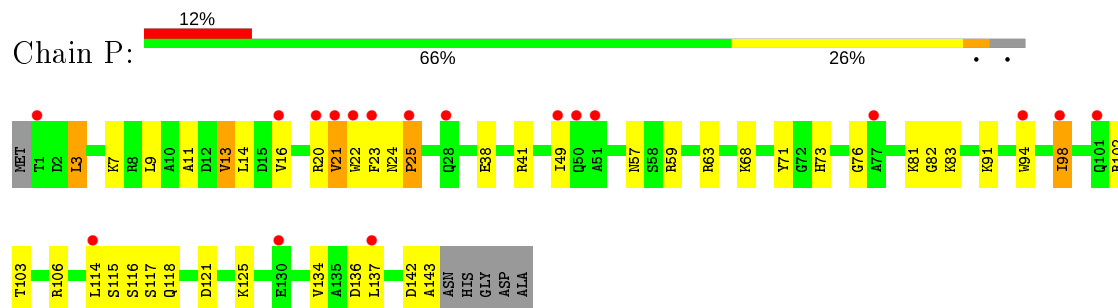
• Molecule 16: 50S ribosomal protein L18P



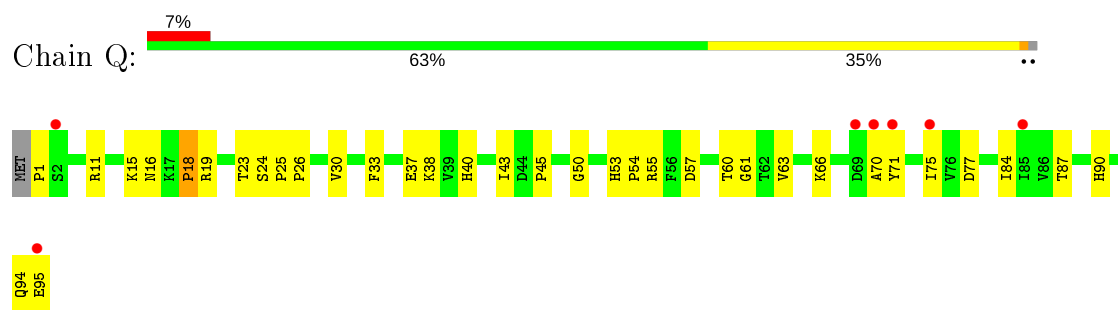
- Molecule 17: 50S ribosomal protein L18e



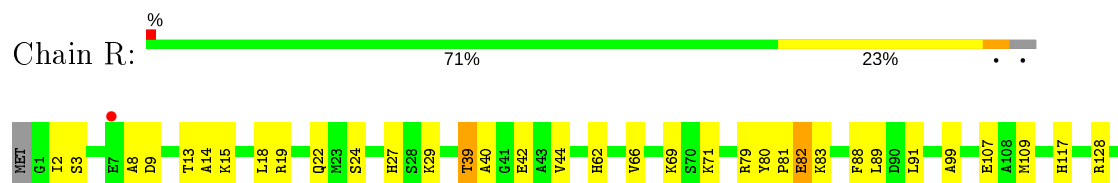
- Molecule 18: 50S ribosomal protein L19e



- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P

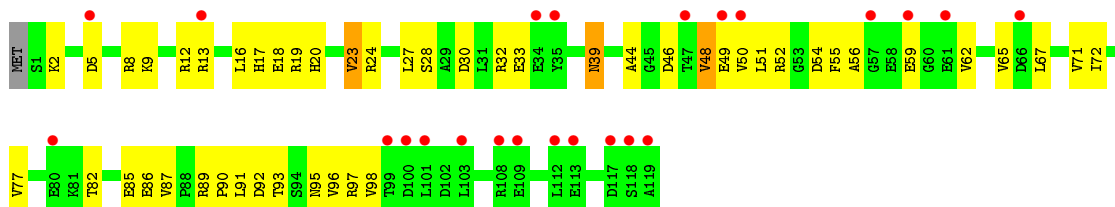




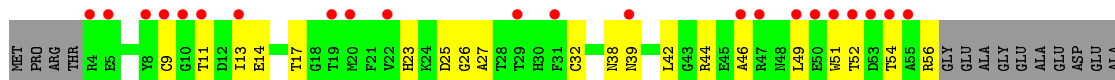
- Molecule 21: 50S ribosomal protein L23P



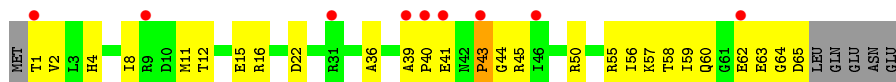
- Molecule 22: 50S ribosomal protein L24P



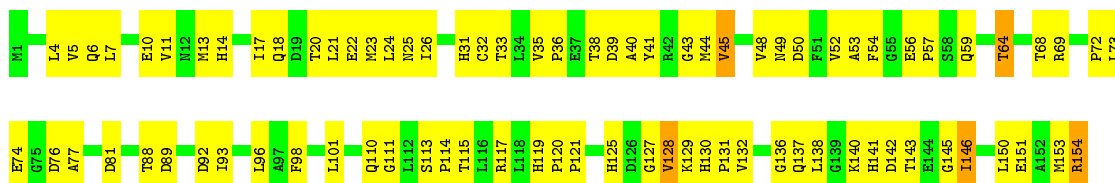
- Molecule 23: 50S ribosomal protein L24e



- Molecule 24: 50S ribosomal protein L29P

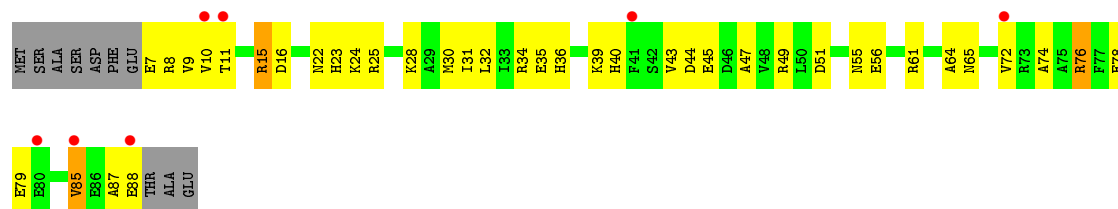


- Molecule 25: 50S ribosomal protein L30P

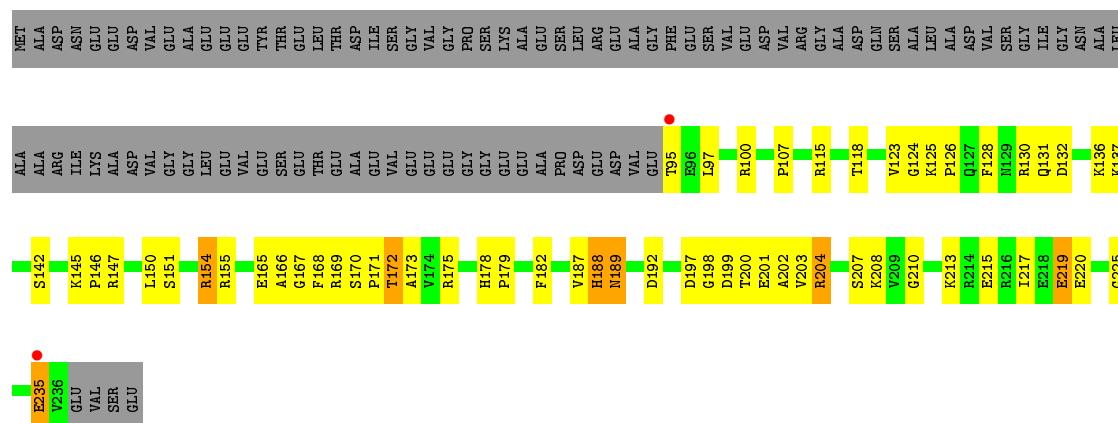


- Molecule 26: 50S RIBOSOMAL PROTEIN L31E

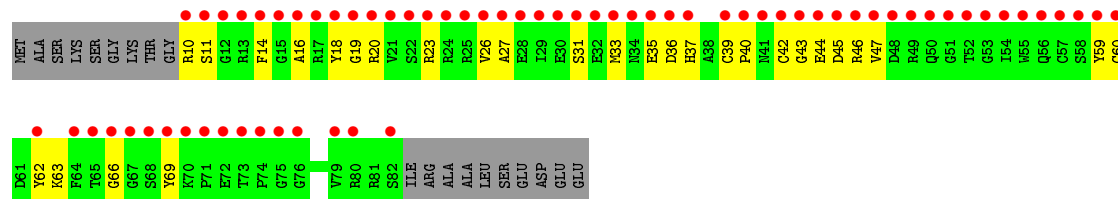




• Molecule 27: 50S ribosomal protein L32e



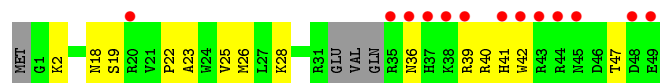
• Molecule 28: 50S ribosomal protein L37Ae



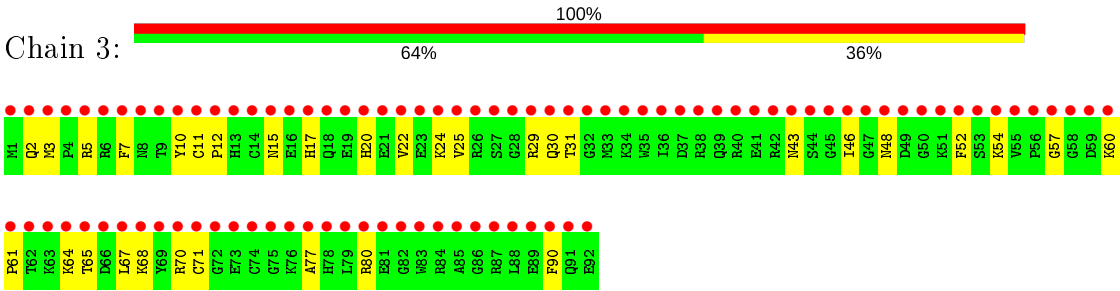
• Molecule 29: 50S ribosomal protein L37e



• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	214.49Å 302.43Å 578.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.83 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-3.00) 96.9 (49.83-3.01)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.288 0.259 , 0.260	Depositor DCC
R_{free} test set	18014 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	92248	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, CD, OMU, UR3, 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	0.56	0/65932	0.75	36/102817 (0.0%)
2	9	0.42	0/2905	0.72	1/4528 (0.0%)
3	A	0.39	0/1786	0.69	0/2408
4	B	0.46	0/2690	0.76	0/3652
5	C	0.47	0/1884	0.76	1/2551 (0.0%)
6	D	0.36	0/1111	0.60	0/1498
7	E	0.45	0/1382	0.68	0/1880
8	F	0.34	0/901	0.58	0/1224
9	G	1.36	5/971 (0.5%)	1.67	22/1317 (1.7%)
10	H	0.41	0/1287	0.70	0/1725
11	I	4.03	6/890 (0.7%)	2.13	7/1216 (0.6%)
12	J	0.50	0/1136	0.70	0/1530
13	K	0.46	0/1001	0.77	0/1347
14	L	0.39	0/1130	0.68	0/1509
15	M	0.42	0/1583	0.68	0/2119
16	N	0.34	0/1474	0.66	0/1999
17	O	0.45	0/874	0.70	0/1181
18	P	0.42	0/1147	0.60	0/1528
19	Q	0.38	0/749	0.68	0/1005
20	R	0.50	0/1172	0.75	0/1578
21	S	0.42	0/648	0.64	0/875
22	T	0.42	0/958	0.71	0/1289
23	U	0.35	0/417	0.61	0/562
24	V	0.39	0/502	0.61	0/675
25	W	0.47	0/1219	0.77	0/1655
26	X	0.51	0/664	0.72	0/895
27	Y	0.48	0/1146	0.74	0/1536
28	Z	0.36	0/589	0.55	0/787
29	1	0.50	0/438	0.71	0/578
30	2	0.40	0/401	0.60	0/529
31	3	0.35	0/771	0.57	0/1024
All	All	0.66	11/99758 (0.0%)	0.77	67/149017 (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	6	93
2	9	0	1
9	G	0	8
11	I	2	4
All	All	8	106

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	24	LEU	CA-CB	82.97	3.44	1.53
11	I	24	LEU	CG-CD2	57.61	3.65	1.51
11	I	24	LEU	CG-CD1	50.48	3.38	1.51
11	I	24	LEU	CB-CG	34.68	2.53	1.52
9	G	54	HIS	CB-CG	28.65	2.01	1.50

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	24	LEU	CB-CA-C	-36.47	40.91	110.20
11	I	24	LEU	CD1-CG-CD2	-30.12	20.15	110.50
11	I	24	LEU	CB-CG-CD1	-29.18	61.40	111.00
11	I	24	LEU	CB-CG-CD2	-25.73	67.26	111.00
11	I	24	LEU	CA-CB-CG	-25.40	56.88	115.30

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1161	A	C1'
1	0	1167	G	C3',C1'
1	0	1193	A	C4',C3',C1'
11	I	24	LEU	CA
11	I	30	ASP	CA

5 of 106 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	116	G	Sidechain
1	0	191	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	206	G	Sidechain
1	0	49	A	Sidechain
1	0	79	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	0	58979	0	29793	2515	0
2	9	2600	0	1326	157	0
3	A	1753	0	1766	73	0
4	B	2625	0	2533	110	0
5	C	1859	0	1816	84	0
6	D	1094	0	1085	50	0
7	E	1357	0	1266	46	0
8	F	890	0	843	31	0
9	G	959	0	928	154	0
10	H	1266	0	1268	49	0
11	I	876	0	835	60	0
12	J	1120	0	1098	49	0
13	K	992	0	1031	44	0
14	L	1118	0	1076	34	0
15	M	1559	0	1567	63	0
16	N	1445	0	1401	73	0
17	O	865	0	873	28	0
18	P	1136	0	1123	39	0
19	Q	735	0	728	27	0
20	R	1149	0	1122	44	0
21	S	641	0	605	13	0
22	T	950	0	924	50	0
23	U	410	0	367	15	0
24	V	499	0	511	21	0
25	W	1196	0	1137	72	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	51	0
28	Z	578	0	543	36	0
29	1	431	0	427	24	0
30	2	396	0	413	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	3	755	0	732	34	0
32	0	108	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	1	0	0	0	0
33	M	1	0	0	0	0
34	0	73	0	0	0	0
34	9	3	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	8	0	0	1	0
35	3	1	0	0	5	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	4	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	O	1	0	0	1	0
35	Q	1	0	0	1	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	1	1	0	0	1	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
All	All	92248	0	60923	3719	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 25.

The worst 5 of 3719 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)
9:G:54:HIS:CB	9:G:54:HIS:CG	2.01	1.43
9:G:108:SER:O	9:G:109:LYS:HE3	1.32	1.30
1:0:1167:G:H5'	1:0:1168:C:OP2	1.34	1.28
9:G:33:VAL:C	9:G:123:ASP:OD2	1.72	1.27
9:G:35:VAL:HG21	9:G:122:ASN:OD1	1.37	1.25

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	
3	A	235/240 (98%)	206 (88%)	24 (10%)	5 (2%)	7	33
4	B	335/338 (99%)	287 (86%)	38 (11%)	10 (3%)	4	24
5	C	244/246 (99%)	209 (86%)	28 (12%)	7 (3%)	4	24
6	D	134/177 (76%)	95 (71%)	34 (25%)	5 (4%)	3	19
7	E	170/178 (96%)	156 (92%)	12 (7%)	2 (1%)	13	48
8	F	117/120 (98%)	101 (86%)	13 (11%)	3 (3%)	5	27
9	G	121/348 (35%)	79 (65%)	29 (24%)	13 (11%)	0	2
10	H	156/171 (91%)	141 (90%)	11 (7%)	4 (3%)	5	27
11	I	112/162 (69%)	76 (68%)	28 (25%)	8 (7%)	1	5
12	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	11	43
13	K	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	10	42
14	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	22	60
15	M	192/196 (98%)	161 (84%)	31 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	184/187 (98%)	162 (88%)	19 (10%)	3 (2%)	9	40
17	O	113/116 (97%)	103 (91%)	9 (8%)	1 (1%)	17	55
18	P	141/149 (95%)	129 (92%)	11 (8%)	1 (1%)	22	60
19	Q	93/96 (97%)	85 (91%)	5 (5%)	3 (3%)	4	22
20	R	148/155 (96%)	129 (87%)	18 (12%)	1 (1%)	22	60
21	S	79/85 (93%)	65 (82%)	14 (18%)	0	100	100
22	T	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	17	55
23	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	9	40
25	W	152/154 (99%)	134 (88%)	17 (11%)	1 (1%)	22	60
26	X	80/92 (87%)	66 (82%)	13 (16%)	1 (1%)	12	45
27	Y	140/241 (58%)	130 (93%)	7 (5%)	3 (2%)	7	33
28	Z	71/92 (77%)	64 (90%)	7 (10%)	0	100	100
29	1	54/57 (95%)	45 (83%)	8 (15%)	1 (2%)	8	36
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	14	50
All	All	3845/4442 (87%)	3329 (87%)	436 (11%)	80 (2%)	7	33

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	16	ARG
6	D	27	ILE
8	F	91	VAL
9	G	127	PRO
11	I	11	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	164 (92%)	15 (8%)	11	38
4	B	282/283 (100%)	264 (94%)	18 (6%)	17	51
5	C	193/193 (100%)	174 (90%)	19 (10%)	8	30
6	D	117/148 (79%)	109 (93%)	8 (7%)	16	48
7	E	152/156 (97%)	142 (93%)	10 (7%)	16	49
8	F	93/94 (99%)	92 (99%)	1 (1%)	73	90
9	G	106/283 (38%)	95 (90%)	11 (10%)	7	27
10	H	132/138 (96%)	124 (94%)	8 (6%)	18	53
11	I	99/130 (76%)	84 (85%)	15 (15%)	3	14
12	J	118/121 (98%)	107 (91%)	11 (9%)	9	33
13	K	106/106 (100%)	98 (92%)	8 (8%)	13	43
14	L	113/127 (89%)	108 (96%)	5 (4%)	28	65
15	M	158/160 (99%)	150 (95%)	8 (5%)	24	60
16	N	149/150 (99%)	144 (97%)	5 (3%)	37	72
17	O	93/94 (99%)	89 (96%)	4 (4%)	29	66
18	P	113/117 (97%)	107 (95%)	6 (5%)	22	58
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	69
20	R	117/122 (96%)	113 (97%)	4 (3%)	37	72
21	S	71/74 (96%)	66 (93%)	5 (7%)	15	47
22	T	105/106 (99%)	99 (94%)	6 (6%)	20	56
23	U	44/53 (83%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	32	69
25	W	130/130 (100%)	121 (93%)	9 (7%)	15	48
26	X	66/74 (89%)	62 (94%)	4 (6%)	18	53
27	Y	120/196 (61%)	111 (92%)	9 (8%)	13	43
28	Z	60/74 (81%)	60 (100%)	0	100	100
29	1	46/47 (98%)	43 (94%)	3 (6%)	17	50
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	79
31	3	79/79 (100%)	78 (99%)	1 (1%)	69	89
All	All	3213/3620 (89%)	3014 (94%)	199 (6%)	18	52

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	9	VAL
12	J	79	PHE
26	X	76	ARG
11	I	15	ASN
11	I	90	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	24	GLN
16	N	107	ASN
27	Y	189	ASN
15	M	58	GLN
16	N	40	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2741/2922 (93%)	291 (10%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	4 (3%)
All	All	2862/3044 (94%)	307 (10%)	39 (1%)

5 of 307 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1506	U
2	9	43	G
1	0	1377	C
1	0	1450	C

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

4 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	14,22,23	0.93	1 (7%)	14,31,34	1.24	1 (7%)
1	UR3	0	2619	1	14,22,23	0.82	1 (7%)	15,32,35	0.66	0
1	PSU	0	2621	1	17,21,22	1.68	3 (17%)	20,30,33	5.51	5 (25%)
1	OMG	0	2588	1	18,26,27	1.14	2 (11%)	20,38,41	2.59	4 (20%)

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	-	0/7/27/28	0/2/2/2
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	1/5/27/28	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.14	1.47	1.52
1	0	2588	OMG	C6-N1	3.56	1.39	1.33
1	0	2621	PSU	C4-N3	2.86	1.38	1.33
1	0	2621	PSU	C2-N1	2.82	1.43	1.38
1	0	2587	OMU	C4-N3	2.54	1.37	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.70	114.36	128.43
1	0	2621	PSU	C4-N3-C2	14.29	127.20	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C5-C6-N1	-8.57	111.71	123.43
1	0	2621	PSU	C5-C4-N3	-8.15	114.86	125.36
1	0	2588	OMG	C6-N1-C2	5.63	124.87	115.93

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	2588	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	5	0
1	0	2619	UR3	1	0
1	0	2621	PSU	1	0
1	0	2588	OMG	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 231 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	G	2
1	0	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	0	1207:A	O3'	1208:C	P	2.51
1	G	53:LEU	C	54:HIS	N	1.63
1	G	54:HIS	C	55:GLY	N	0.99

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.18	16 (0%) 89 72	17, 56, 120, 184	0
2	9	122/122 (100%)	-0.01	2 (1%) 72 44	41, 89, 136, 181	0
3	A	237/240 (98%)	0.56	23 (9%) 7 2	34, 90, 133, 148	0
4	B	337/338 (99%)	0.15	13 (3%) 39 15	25, 60, 100, 112	0
5	C	246/246 (100%)	0.16	6 (2%) 59 30	29, 58, 91, 106	0
6	D	140/177 (79%)	1.95	58 (41%) 0 0	89, 146, 170, 178	0
7	E	172/178 (96%)	0.48	12 (6%) 16 5	46, 73, 100, 109	0
8	F	119/120 (99%)	0.37	5 (4%) 36 14	74, 110, 150, 166	0
9	G	125/348 (35%)	1.41	37 (29%) 0 0	100, 133, 165, 168	0
10	H	160/171 (93%)	0.34	6 (3%) 40 16	51, 76, 109, 120	0
11	I	118/162 (72%)	2.78	63 (53%) 0 0	20, 181, 199, 200	0
12	J	142/145 (97%)	-0.05	0 100 100	31, 54, 83, 99	0
13	K	132/132 (100%)	0.19	3 (2%) 60 31	33, 61, 98, 103	0
14	L	145/165 (87%)	1.49	39 (26%) 0 0	49, 111, 158, 162	0
15	M	194/196 (98%)	0.77	22 (11%) 5 1	2, 62, 161, 180	0
16	N	186/187 (99%)	1.18	37 (19%) 1 0	62, 106, 176, 189	0
17	O	115/116 (99%)	0.10	0 100 100	48, 70, 88, 91	0
18	P	143/149 (95%)	0.79	18 (12%) 3 1	44, 68, 103, 109	0
19	Q	95/96 (98%)	0.67	7 (7%) 14 4	52, 74, 87, 100	0
20	R	150/155 (96%)	0.04	1 (0%) 87 69	30, 48, 74, 81	0
21	S	81/85 (95%)	0.40	2 (2%) 57 29	56, 87, 108, 123	0
22	T	119/120 (99%)	0.99	23 (19%) 1 0	51, 74, 106, 139	0
23	U	53/67 (79%)	1.90	22 (41%) 0 0	96, 108, 126, 133	0
24	V	65/71 (91%)	0.84	9 (13%) 2 1	66, 105, 145, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.02	0 100 100	38, 55, 81, 95	0
26	X	82/92 (89%)	0.57	7 (8%) 10 3	43, 63, 84, 95	0
27	Y	142/241 (58%)	0.26	2 (1%) 75 49	23, 51, 87, 106	0
28	Z	73/92 (79%)	6.73	67 (91%) 0 0	164, 174, 200, 200	0
29	1	56/57 (98%)	0.06	0 100 100	28, 43, 56, 65	0
30	2	46/50 (92%)	1.29	13 (28%) 0 0	48, 87, 150, 152	0
31	3	92/92 (100%)	11.33	92 (100%) 0 0	184, 198, 200, 200	0
All	All	6790/7486 (90%)	0.51	605 (8%) 9 3	2, 67, 162, 200	0

The worst 5 of 605 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	3	9	THR	24.4
31	3	33	MET	23.0
31	3	69	TYR	22.4
31	3	78	HIS	20.9
31	3	25	VAL	20.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OMU	0	2587	21/22	0.94	0.18	33,36,42,43	0
1	OMG	0	2588	24/25	0.95	0.18	38,42,48,49	0
1	UR3	0	2619	21/22	0.96	0.18	34,42,44,47	0
1	PSU	0	2621	20/21	0.97	0.15	35,37,44,44	0

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	NA	0	3103	1/1	-0.15	0.88	198,198,198,198	0
34	NA	0	3050	1/1	-0.11	1.21	137,137,137,137	0
32	MG	0	3027	1/1	-0.00	0.96	110,110,110,110	0
32	MG	0	2946	1/1	0.09	0.34	200,200,200,200	0
32	MG	0	2971	1/1	0.18	0.41	200,200,200,200	0
34	NA	0	3100	1/1	0.30	1.21	56,56,56,56	0
35	CL	O	117	1/1	0.38	1.01	127,127,127,127	0
32	MG	0	3025	1/1	0.41	0.47	57,57,57,57	0
34	NA	0	3093	1/1	0.45	0.39	116,116,116,116	0
32	MG	0	2998	1/1	0.45	0.50	73,73,73,73	0
34	NA	0	3057	1/1	0.45	0.80	124,124,124,124	0
32	MG	0	3029	1/1	0.47	0.99	69,69,69,69	0
32	MG	3	93	1/1	0.49	0.51	69,69,69,69	0
34	NA	0	3054	1/1	0.50	0.34	63,63,63,63	0
35	CL	0	3109	1/1	0.53	0.61	135,135,135,135	0
34	NA	0	3047	1/1	0.55	0.36	53,53,53,53	0
35	CL	0	3106	1/1	0.56	1.27	120,120,120,120	0
34	NA	0	3082	1/1	0.56	0.48	43,43,43,43	0
36	CD	O	116	1/1	0.59	0.47	200,200,200,200	0
35	CL	0	3112	1/1	0.59	0.56	96,96,96,96	0
34	NA	S	85	1/1	0.59	0.67	64,64,64,64	0
34	NA	0	3052	1/1	0.60	0.52	72,72,72,72	0
35	CL	3	95	1/1	0.61	0.65	124,124,124,124	0
32	MG	0	2988	1/1	0.61	0.34	52,52,52,52	0
34	NA	0	3065	1/1	0.64	0.19	27,27,27,27	0
32	MG	0	3028	1/1	0.64	0.97	66,66,66,66	0
34	NA	0	3068	1/1	0.65	0.25	68,68,68,68	0
32	MG	Y	241	1/1	0.66	0.47	68,68,68,68	0
34	NA	0	3098	1/1	0.67	0.52	62,62,62,62	0
34	NA	0	3094	1/1	0.67	0.43	116,116,116,116	0
34	NA	0	3075	1/1	0.67	0.46	41,41,41,41	0
34	NA	0	3046	1/1	0.67	0.28	26,26,26,26	0
32	MG	B	338	1/1	0.68	0.59	43,43,43,43	0
32	MG	0	2964	1/1	0.69	0.34	50,50,50,50	0
34	NA	0	3038	1/1	0.69	0.32	67,67,67,67	0
34	NA	0	3059	1/1	0.69	0.42	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	2980	1/1	0.71	0.47	48,48,48,48	0
35	CL	0	3111	1/1	0.72	0.25	54,54,54,54	0
32	MG	A	240	1/1	0.72	0.48	56,56,56,56	0
33	K	M	196	1/1	0.73	0.42	127,127,127,127	0
34	NA	0	3044	1/1	0.73	0.85	46,46,46,46	0
34	NA	C	247	1/1	0.73	0.34	41,41,41,41	0
34	NA	A	242	1/1	0.74	0.28	55,55,55,55	0
34	NA	0	3077	1/1	0.74	0.55	119,119,119,119	0
34	NA	0	3092	1/1	0.74	0.25	45,45,45,45	0
32	MG	0	2987	1/1	0.75	0.16	35,35,35,35	0
32	MG	0	2984	1/1	0.75	0.51	59,59,59,59	0
34	NA	9	125	1/1	0.75	0.35	78,78,78,78	0
32	MG	0	2973	1/1	0.75	0.42	51,51,51,51	0
34	NA	R	156	1/1	0.76	0.33	53,53,53,53	0
34	NA	0	3034	1/1	0.76	0.77	91,91,91,91	0
34	NA	0	3099	1/1	0.76	0.90	56,56,56,56	0
34	NA	0	3064	1/1	0.77	0.30	60,60,60,60	0
32	MG	0	2969	1/1	0.77	0.40	38,38,38,38	0
32	MG	0	3007	1/1	0.78	0.29	54,54,54,54	0
34	NA	0	3058	1/1	0.78	0.26	61,61,61,61	0
32	MG	0	2985	1/1	0.78	0.29	34,34,34,34	0
32	MG	0	3006	1/1	0.78	0.42	49,49,49,49	0
34	NA	0	3039	1/1	0.79	0.63	29,29,29,29	0
34	NA	0	3033	1/1	0.79	0.45	60,60,60,60	0
33	K	0	3031	1/1	0.79	0.47	153,153,153,153	0
35	CL	Q	97	1/1	0.79	0.57	93,93,93,93	0
32	MG	0	3026	1/1	0.79	1.06	79,79,79,79	0
34	NA	9	124	1/1	0.79	0.16	34,34,34,34	0
32	MG	0	2974	1/1	0.79	0.19	51,51,51,51	0
34	NA	0	3084	1/1	0.79	0.43	62,62,62,62	0
34	NA	0	3051	1/1	0.80	0.33	49,49,49,49	0
34	NA	J	146	1/1	0.80	0.24	41,41,41,41	0
32	MG	0	3014	1/1	0.80	0.32	87,87,87,87	0
32	MG	0	3013	1/1	0.80	0.38	41,41,41,41	0
32	MG	A	241	1/1	0.80	0.38	142,142,142,142	0
34	NA	0	3056	1/1	0.80	0.33	42,42,42,42	0
32	MG	K	133	1/1	0.80	0.45	35,35,35,35	0
34	NA	0	3060	1/1	0.80	0.15	101,101,101,101	0
35	CL	0	3108	1/1	0.81	0.36	72,72,72,72	0
32	MG	0	2989	1/1	0.81	0.67	56,56,56,56	0
32	MG	0	2944	1/1	0.81	0.18	25,25,25,25	0
32	MG	0	3011	1/1	0.81	0.86	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	9	126	1/1	0.81	0.85	91,91,91,91	0
35	CL	R	157	1/1	0.81	0.24	55,55,55,55	0
32	MG	0	3030	1/1	0.82	0.18	46,46,46,46	0
34	NA	0	3061	1/1	0.82	0.12	39,39,39,39	0
34	NA	0	3043	1/1	0.82	0.38	115,115,115,115	0
32	MG	0	3018	1/1	0.82	0.35	78,78,78,78	0
35	CL	L	166	1/1	0.82	0.27	68,68,68,68	0
32	MG	0	3024	1/1	0.83	0.35	1,1,1,1	0
34	NA	0	3063	1/1	0.83	0.19	162,162,162,162	0
36	CD	Z	93	1/1	0.83	0.35	200,200,200,200	0
34	NA	0	3101	1/1	0.83	0.17	43,43,43,43	0
35	CL	A	243	1/1	0.83	0.40	90,90,90,90	0
32	MG	0	2962	1/1	0.84	0.48	60,60,60,60	0
34	NA	Q	96	1/1	0.84	0.24	64,64,64,64	0
34	NA	0	3067	1/1	0.85	0.30	47,47,47,47	0
32	MG	0	3004	1/1	0.85	0.53	27,27,27,27	0
32	MG	0	2949	1/1	0.85	0.35	45,45,45,45	0
32	MG	0	2993	1/1	0.85	0.44	78,78,78,78	0
35	CL	M	198	1/1	0.86	0.36	77,77,77,77	0
34	NA	0	3041	1/1	0.86	0.36	70,70,70,70	0
32	MG	0	3010	1/1	0.86	0.17	56,56,56,56	0
32	MG	0	2938	1/1	0.86	0.47	42,42,42,42	0
32	MG	0	2947	1/1	0.86	0.27	15,15,15,15	0
32	MG	0	3017	1/1	0.87	0.34	166,166,166,166	0
34	NA	0	3032	1/1	0.87	0.45	30,30,30,30	0
34	NA	0	3035	1/1	0.87	0.17	17,17,17,17	0
32	MG	0	2968	1/1	0.87	0.10	60,60,60,60	0
32	MG	0	3023	1/1	0.87	0.34	29,29,29,29	0
32	MG	0	2956	1/1	0.87	0.18	24,24,24,24	0
32	MG	0	3019	1/1	0.87	0.40	41,41,41,41	0
32	MG	0	2929	1/1	0.88	0.19	14,14,14,14	0
32	MG	0	3022	1/1	0.88	0.38	44,44,44,44	0
35	CL	N	187	1/1	0.88	0.29	64,64,64,64	0
32	MG	0	2981	1/1	0.88	0.50	44,44,44,44	0
32	MG	0	2950	1/1	0.88	0.23	17,17,17,17	0
34	NA	0	3088	1/1	0.88	0.26	33,33,33,33	0
34	NA	0	3089	1/1	0.88	0.14	51,51,51,51	0
35	CL	J	149	1/1	0.88	0.15	45,45,45,45	0
32	MG	0	2986	1/1	0.88	0.35	53,53,53,53	0
32	MG	0	2943	1/1	0.88	0.37	23,23,23,23	0
32	MG	0	2935	1/1	0.89	0.38	28,28,28,28	0
32	MG	0	3009	1/1	0.89	0.28	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	3015	1/1	0.89	0.49	53,53,53,53	0
32	MG	0	2963	1/1	0.89	0.15	72,72,72,72	0
32	MG	0	2951	1/1	0.89	0.38	11,11,11,11	0
32	MG	0	2979	1/1	0.89	0.23	20,20,20,20	0
32	MG	0	2975	1/1	0.90	0.16	45,45,45,45	0
34	NA	0	3102	1/1	0.90	0.31	47,47,47,47	0
34	NA	0	3078	1/1	0.90	0.16	78,78,78,78	0
34	NA	0	3080	1/1	0.90	0.41	57,57,57,57	0
36	CD	3	94	1/1	0.90	1.15	200,200,200,200	0
32	MG	0	2936	1/1	0.90	0.13	17,17,17,17	0
32	MG	0	3020	1/1	0.90	0.18	84,84,84,84	0
34	NA	0	3072	1/1	0.90	0.24	65,65,65,65	0
34	NA	0	3073	1/1	0.90	0.27	25,25,25,25	0
32	MG	0	2999	1/1	0.90	0.19	25,25,25,25	0
35	CL	0	3105	1/1	0.91	0.17	59,59,59,59	0
34	NA	H	172	1/1	0.91	0.16	43,43,43,43	0
34	NA	0	3055	1/1	0.91	0.14	36,36,36,36	0
32	MG	0	2945	1/1	0.91	0.32	27,27,27,27	0
35	CL	0	3110	1/1	0.91	0.55	56,56,56,56	0
35	CL	K	134	1/1	0.91	0.34	55,55,55,55	0
32	MG	0	2992	1/1	0.91	0.26	52,52,52,52	0
32	MG	9	123	1/1	0.91	0.17	37,37,37,37	0
34	NA	0	3081	1/1	0.91	0.18	49,49,49,49	0
34	NA	0	3090	1/1	0.91	0.29	81,81,81,81	0
32	MG	0	1	1/1	0.91	0.20	26,26,26,26	0
34	NA	0	3069	1/1	0.91	0.28	58,58,58,58	0
32	MG	0	2960	1/1	0.91	0.29	11,11,11,11	0
32	MG	0	3016	1/1	0.91	0.20	43,43,43,43	0
32	MG	0	2959	1/1	0.92	0.18	39,39,39,39	0
32	MG	0	2924	1/1	0.92	0.23	35,35,35,35	0
32	MG	0	3005	1/1	0.92	0.16	47,47,47,47	0
35	CL	B	339	1/1	0.92	0.46	61,61,61,61	0
32	MG	0	3001	1/1	0.92	0.15	38,38,38,38	0
35	CL	J	148	1/1	0.92	0.07	49,49,49,49	0
34	NA	0	3071	1/1	0.92	0.13	27,27,27,27	0
34	NA	0	3074	1/1	0.92	0.47	66,66,66,66	0
34	NA	M	197	1/1	0.92	0.16	28,28,28,28	0
34	NA	0	3040	1/1	0.92	0.18	29,29,29,29	0
32	MG	0	2970	1/1	0.92	0.19	32,32,32,32	0
34	NA	0	3066	1/1	0.92	0.11	9,9,9,9	0
34	NA	0	3085	1/1	0.92	0.41	15,15,15,15	0
32	MG	0	2930	1/1	0.92	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	0	3095	1/1	0.92	0.49	126,126,126,126	0
34	NA	R	155	1/1	0.93	0.21	31,31,31,31	0
34	NA	0	3083	1/1	0.93	0.17	27,27,27,27	0
35	CL	J	147	1/1	0.93	0.16	69,69,69,69	0
32	MG	0	2978	1/1	0.93	0.17	46,46,46,46	0
34	NA	0	3104	1/1	0.93	0.59	34,34,34,34	0
32	MG	0	2991	1/1	0.93	0.16	20,20,20,20	0
34	NA	0	3042	1/1	0.93	0.38	32,32,32,32	0
32	MG	0	3003	1/1	0.93	0.18	26,26,26,26	0
34	NA	0	3091	1/1	0.93	0.25	31,31,31,31	0
34	NA	0	3076	1/1	0.93	0.22	51,51,51,51	0
34	NA	0	3086	1/1	0.93	0.40	26,26,26,26	0
32	MG	0	2966	1/1	0.93	0.13	46,46,46,46	0
32	MG	0	2937	1/1	0.93	0.24	14,14,14,14	0
35	CL	Y	242	1/1	0.93	0.26	27,27,27,27	0
32	MG	0	2990	1/1	0.93	0.15	31,31,31,31	0
34	NA	0	3070	1/1	0.94	0.10	27,27,27,27	0
32	MG	0	2928	1/1	0.94	0.14	32,32,32,32	0
32	MG	0	3000	1/1	0.94	0.20	7,7,7,7	0
34	NA	0	3045	1/1	0.94	0.22	33,33,33,33	0
32	MG	0	3008	1/1	0.94	0.30	52,52,52,52	0
32	MG	0	2957	1/1	0.94	0.14	37,37,37,37	0
32	MG	0	2997	1/1	0.94	0.27	59,59,59,59	0
32	MG	0	3012	1/1	0.94	0.27	39,39,39,39	0
32	MG	0	2942	1/1	0.94	0.41	16,16,16,16	0
32	MG	0	2977	1/1	0.94	0.52	43,43,43,43	0
34	NA	0	3048	1/1	0.94	0.21	46,46,46,46	0
32	MG	0	2954	1/1	0.94	0.18	29,29,29,29	0
32	MG	0	2967	1/1	0.94	0.30	50,50,50,50	0
32	MG	0	2952	1/1	0.95	0.23	4,4,4,4	0
34	NA	0	3079	1/1	0.95	0.12	53,53,53,53	0
34	NA	0	3096	1/1	0.95	0.21	47,47,47,47	0
34	NA	0	3087	1/1	0.95	0.08	22,22,22,22	0
34	NA	0	3097	1/1	0.95	0.17	50,50,50,50	0
32	MG	0	2995	1/1	0.95	0.16	13,13,13,13	0
32	MG	0	2983	1/1	0.95	0.29	43,43,43,43	0
32	MG	0	2931	1/1	0.95	0.11	27,27,27,27	0
32	MG	0	2939	1/1	0.95	0.31	20,20,20,20	0
32	MG	0	2982	1/1	0.95	0.25	14,14,14,14	0
32	MG	0	2941	1/1	0.96	0.16	15,15,15,15	0
34	NA	L	165	1/1	0.96	0.07	42,42,42,42	0
36	CD	U	67	1/1	0.96	0.10	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	0	3037	1/1	0.96	0.34	61,61,61,61	0
32	MG	0	2932	1/1	0.96	0.14	10,10,10,10	0
35	CL	0	3107	1/1	0.96	0.15	55,55,55,55	0
34	NA	0	3062	1/1	0.96	0.07	38,38,38,38	0
32	MG	0	2994	1/1	0.96	0.20	14,14,14,14	0
32	MG	0	2925	1/1	0.96	0.19	5,5,5,5	0
32	MG	0	3021	1/1	0.96	0.23	20,20,20,20	0
32	MG	0	2976	1/1	0.96	0.18	19,19,19,19	0
32	MG	0	2933	1/1	0.96	0.32	1,1,1,1	0
34	NA	0	3049	1/1	0.97	0.27	28,28,28,28	0
32	MG	0	2958	1/1	0.97	0.43	33,33,33,33	0
32	MG	T	120	1/1	0.97	0.25	38,38,38,38	0
34	NA	0	3053	1/1	0.97	0.07	19,19,19,19	0
32	MG	0	2955	1/1	0.97	0.30	11,11,11,11	0
32	MG	0	2953	1/1	0.97	0.11	8,8,8,8	0
34	NA	0	3036	1/1	0.97	0.36	49,49,49,49	0
32	MG	0	2972	1/1	0.97	0.20	109,109,109,109	0
32	MG	0	2940	1/1	0.97	0.33	24,24,24,24	0
32	MG	0	2965	1/1	0.98	0.22	47,47,47,47	0
32	MG	0	2926	1/1	0.98	0.15	17,17,17,17	0
32	MG	0	3002	1/1	0.98	0.06	20,20,20,20	0
32	MG	0	2961	1/1	0.98	0.19	41,41,41,41	0
32	MG	0	2996	1/1	0.98	0.24	21,21,21,21	0
32	MG	0	2934	1/1	0.98	0.34	22,22,22,22	0
32	MG	0	2927	1/1	0.99	0.19	18,18,18,18	0
36	CD	1	57	1/1	0.99	0.06	76,76,76,76	0
32	MG	0	2948	1/1	0.99	0.27	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.