



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 03:46 pm BST

PDB ID : 1YJ9
Title : Crystal Structure Of The Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui Containing a three residue deletion in L22
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-13
Resolution : 2.80 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 : 2.11
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) : 2.11

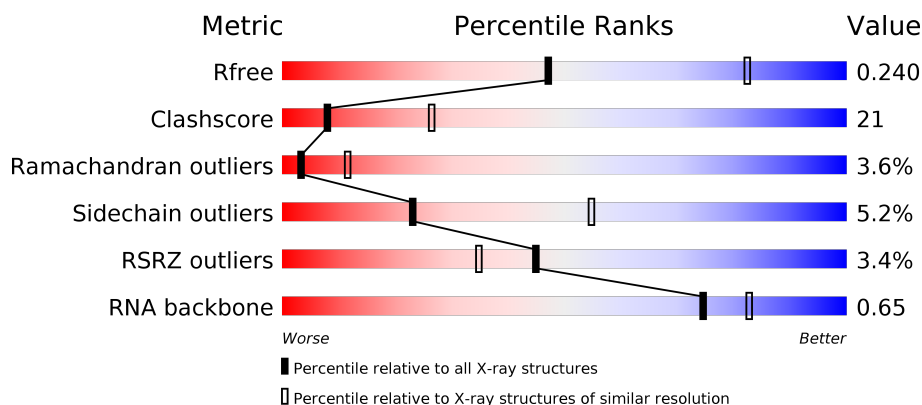
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



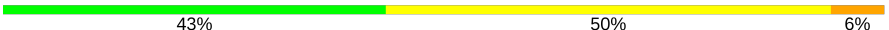
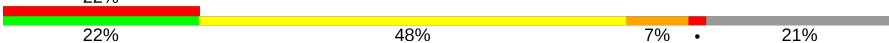

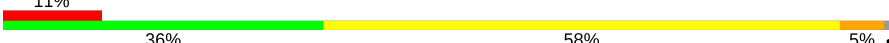



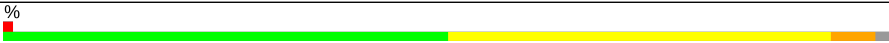

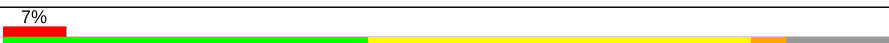


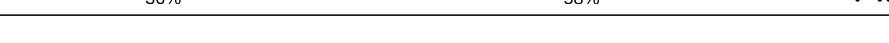
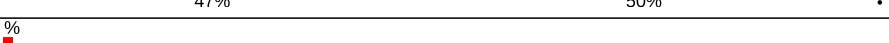
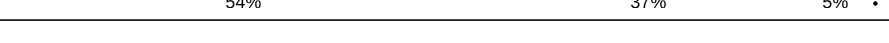




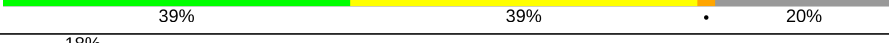



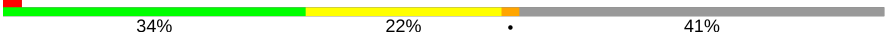

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>51%</div> <div>38%</div> <div>5%</div> <div>6%</div> </div>
2	9	122	<div>2%</div> <div>38%</div> <div>53%</div> <div>8%</div> <div>.</div>
3	A	240	<div>3%</div> <div>50%</div> <div>41%</div> <div>7%</div> <div>.</div>
4	B	338	<div>%</div> <div>43%</div> <div>49%</div> <div>8%</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	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	152	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
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
34	NA	0	8526	-	-	-	X
34	NA	0	8552	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8563	-	-	-	X
34	NA	0	8568	-	-	-	X
34	NA	R	8586	-	-	-	X
35	CL	0	8815	-	-	-	X
35	CL	J	8801	-	-	X	-
35	CL	J	8802	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 99031 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	1	0
			59041	26358	10875	19062	2746			

There are 5 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	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 L4E.

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

- 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 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	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	S	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
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 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	S	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	147	Total	C	N	O	S	0	0	0
			1123	699	204	216	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	GLN	DELETION	UNP P10970
R	?	-	GLN	DELETION	UNP P10970
R	?	-	GLY	DELETION	UNP P10970

- 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	S	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	GB 55231162

- 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	49	Total	C	N	O	S	0	0	0
			421	254	93	73	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	107	Total	Mg	0	0
			107	107		
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	2	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		
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	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	74	Total	Na	0	0
			74	74		

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	9	Total 9	Cl 9	0	0
35	J	3	Total 3	Cl 3	0	0
35	Q	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	5866	Total 5866	O 5866	0	0
37	9	143	Total 143	O 143	0	0
37	A	119	Total 119	O 119	0	0
37	B	148	Total 148	O 148	0	0
37	C	180	Total 180	O 180	0	0
37	D	46	Total 46	O 46	0	0
37	E	45	Total 45	O 45	0	0
37	F	27	Total 27	O 27	0	0
37	G	19	Total 19	O 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	69	Total 69	O 69	0	0
37	I	9	Total 9	O 9	0	0
37	J	57	Total 57	O 57	0	0
37	K	54	Total 54	O 54	0	0
37	L	84	Total 84	O 84	0	0
37	M	130	Total 130	O 130	0	0
37	N	64	Total 64	O 64	0	0
37	O	45	Total 45	O 45	0	0
37	P	64	Total 64	O 64	0	0
37	Q	53	Total 53	O 53	0	0
37	R	58	Total 58	O 58	0	0
37	S	34	Total 34	O 34	0	0
37	T	32	Total 32	O 32	0	0
37	U	26	Total 26	O 26	0	0
37	V	14	Total 14	O 14	0	0
37	W	72	Total 72	O 72	0	0
37	X	24	Total 24	O 24	0	0
37	Y	104	Total 104	O 104	0	0
37	Z	34	Total 34	O 34	0	0
37	1	63	Total 63	O 63	0	0
37	2	32	Total 32	O 32	0	0

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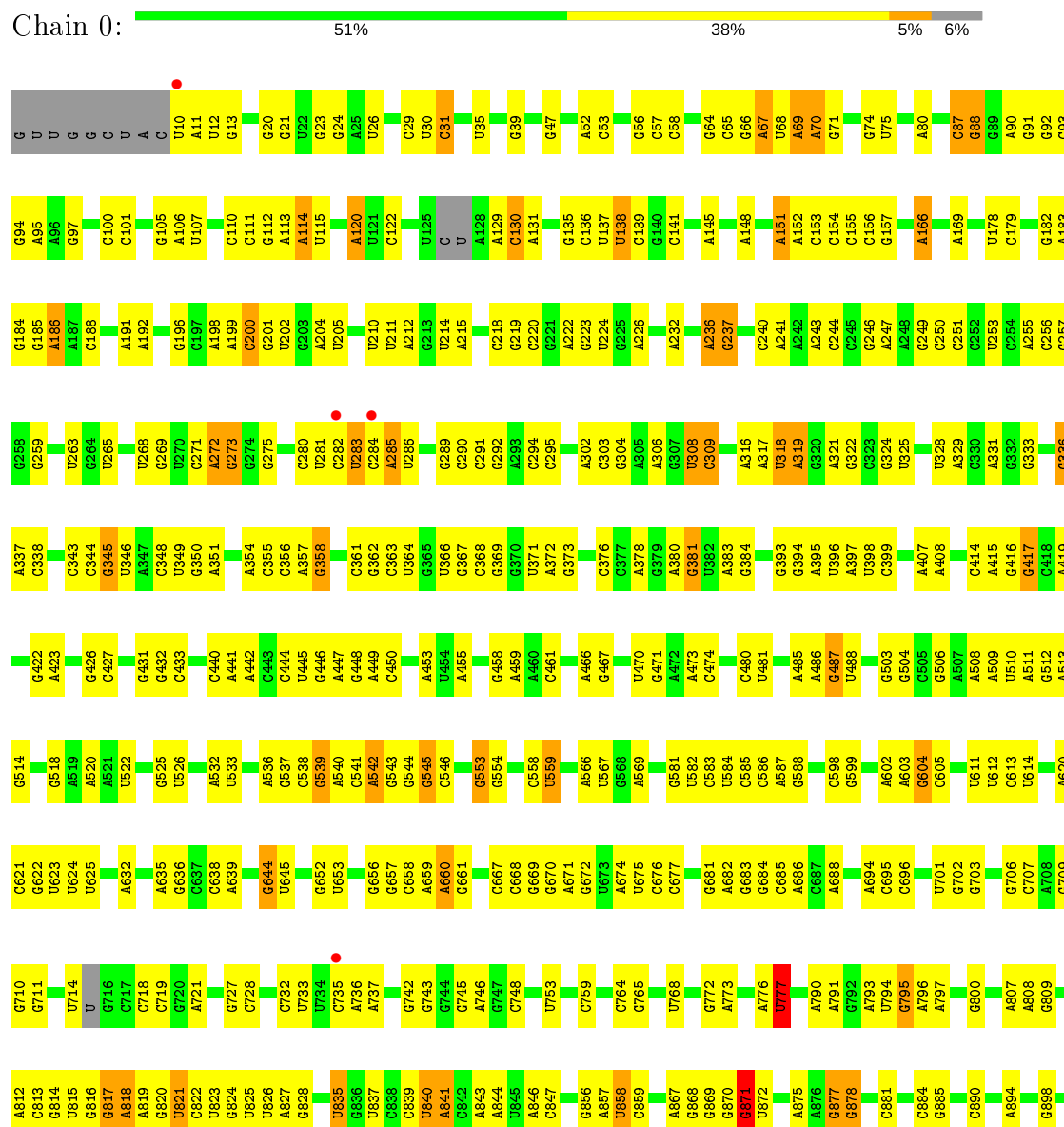
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	3	69	Total	O	0	0
			69	69		

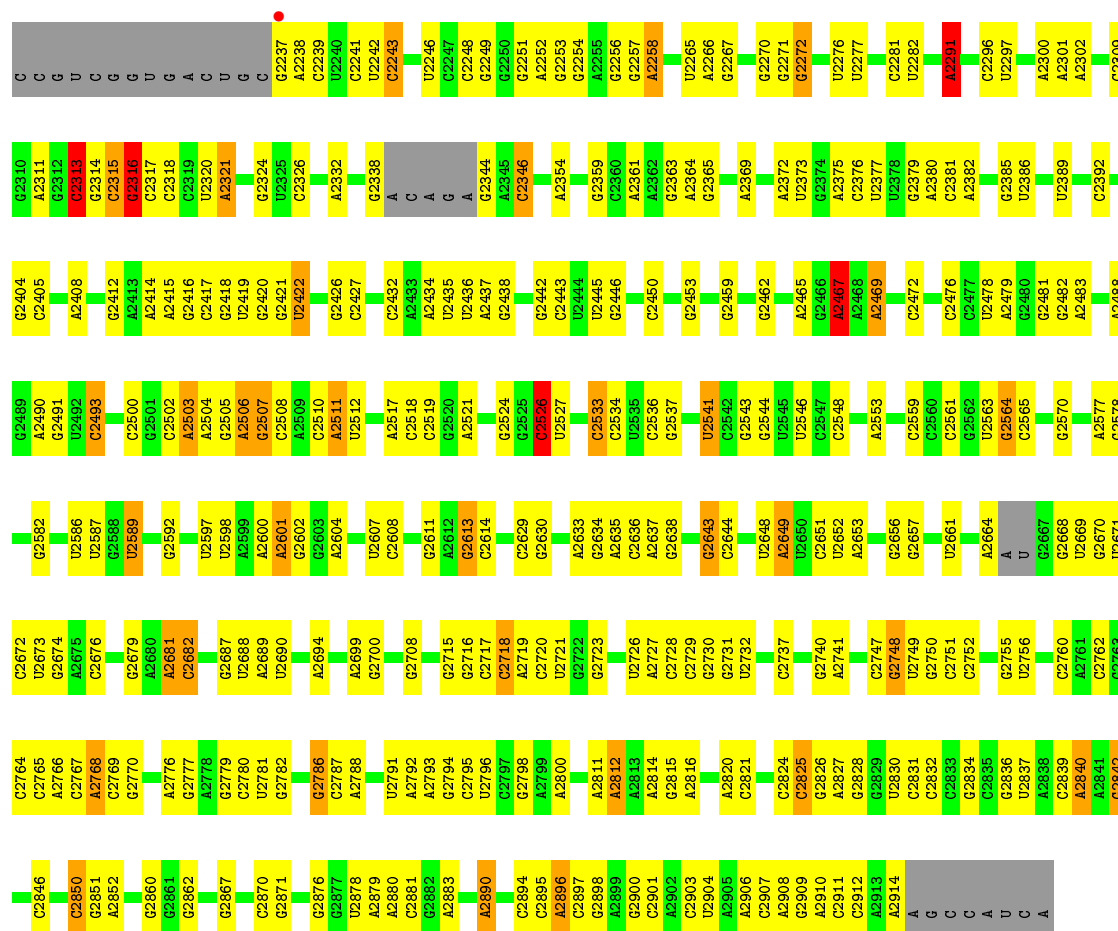
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

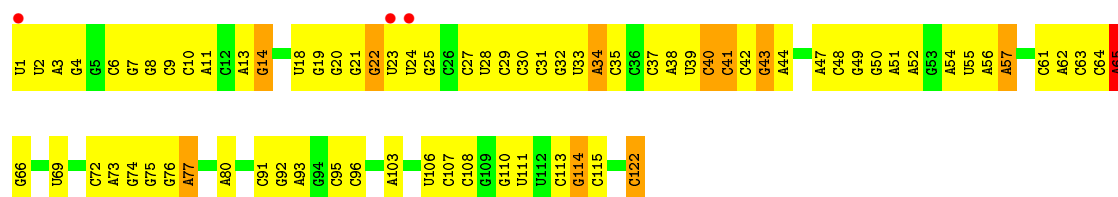
• Molecule 1: 23S Ribosomal RNA



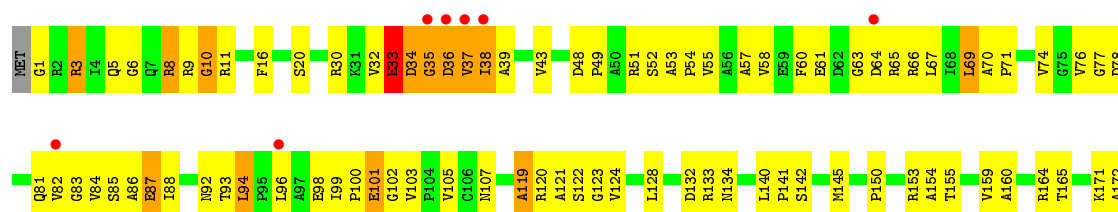
U	C2084	G1979	U1905	G1819	G1743	U1548	U1463	C1360	G1172	G1072	G902
A	A2085	U1980	A1909	G1820	A1746	C1549	G1468	C1361	A1173	A1078	U903
G	A2089	U1996	A1910	A1821	A1747	G1552	G1469	C1362	A1174	A1079	U904
G	G2090	A1997	G1823	A1822	G1751	C1553	A1470	C1366	G1175	C1080	C905
A	G2091		G1824	G1824	G1752	C1554	A1471	C1366	A1176	A1081	G906
U	G2094	G2000	G1916	U1825		G1555	C1472	G1370			A907
C	A2094	G2001	G1917	U1826		G1556	U1473	U1371	U1180	A1086	
C	A2095	U1918	U1918	G1827	A1755	G1557	C1474	U1372	U1181	A1087	G911
U	A2096	U1919	A1919	G1828	U1757	C1558	U1475	C1377	C1182	A1088	U919
U		U2003	G1920	A1829	U1758	C1559	C1477	G1378	C1183		C920
U		U2004	A1921	C1830	U1759	U		A1379	C1184	U1091	G921
C	A2101	G2005	G1922	U1830	U1760	U1561	C1483	U1388	U1185	A1092	A922
C	G2102	G2006	G1923	G1834		C1562	G1484	A1399	C1186		A923
A		U2008	A1924	U1835	U1761		A1485	U1276	U1187	A1097	
G	C2105		G1925	U1836	U1762	G1568	A1486	U1277	A1188		A926
G	C2106		G1926	C1762	C1763	U1569	U1487	G1278	A1189	U1109	
A	A2108	A2011	A1927	U1838	U1766		U1488	A1279	A1190	G1110	U932
G	U2109	U2012	A1930	U1840	U1767	A1572		U1285	U1192	U1116	A939
U	G2014	G2013	A1931	C1841	U1767	A1573		C1395	A1193	A1117	G940
U	A2015	A2015	G1932	A1845	U1769	U1576	A1494	C1396	A1194	A1118	G941
C	U2016	U2016	A1933	U1846	U1770	U1577	C1495	C1397	G1195	U1120	U942
C			A1934	A1847	C1771		G1497	G1290	C1196	G1121	A943
G	U2028	C2028	U1937	G1848	C1772	A1580		G1398	G1197		G944
C			G1938	G1849	G1773		U1500	U1297	U1198		U945
G	G2121	U2032	U1939	U1850	G1774	U1587	U1503	U1298	A1199	C1127	U946
U		G2033	C1940	A1851		G1588	U1504	G1299	A1200	U1128	U947
U	G2111	U2034	A1941	A1852	A1778	G1589	U1505	U1304	C1201	G1023	U948
C		U2035	C1942	C1853	A1779	G1592	U1506	C1305	C1202	G1024	G949
C	U2115	C2036	C1943	G1854	G1782	C1593	C1507		U1205	U1131	G950
C	U2116			G1855	A1783	C1594	C1508	G1311	U1206	A1132	A951
G		A2039	G1947	C1856	U1784	G1595	U1509	G1312	A1207	G1137	G952
G	A2135	G2044	G1950	A1857		U1596	C1513	G1313	C1208	U1028	G953
C			G1951	A1858	G1787	A1597	C1514	U1314	C1209	U1029	G958
C	A	C2047	U	A1859	U1788	A1598	C1515	G1315		G1039	C959
C	G		A	C1861	G1789	U1599	A1516	G1316			G960
C	U	G2050	A	C1862	C1790	G1600	U1517	G1319		G1145	A961
C	G		C	C1863	U1791	G1601	A1518		G1216	C1044	C962
C	U2133	G2053	U	C1864	G1794	G1602	G1523	A1328	U1149	G1045	C963
C	G2134		A			A1603	U1524	G1329	A1150		
G	A2136	U2057	A	G1868	C1798	G1604	U1525	A1329	G1151	G1051	G969
C			U			G1605	A1526	A1330	G1052	U970	
C	A	U2063	G	C1872			A1527	G1331	G1053		
A	C	U2064	A	G1873	A1803	C1613	A1528	G1332	G1054	U	
A	G		C	U1874	G1804	G1614	A1529	U1333	G1055	G	
C	U2135	A2067	C	A1875	G1805		G1529	U1334	U1056	U	
U	U2136	G2068	U1964	G1876	G1806	C1617	G1535	C1335	C1157	C	
U			C1965	G1877	U1807		U1536		G1158	U	
U			U1966	U1878	C1808	A1624	C1537	G1340	G1159	G	
G	C2071	G2072	U1967	U1879	G1809	U1625	C1538	A1341	G1160	C	
A	C	G2073	A1968	C1880	A1810	A1626	C1539	C1342	A1161	C	
A	A	A2074		C1882	G1811		G1540	C1343	G1162	U	
U	C		G1971	U1883	G1812	A1632		U1164	G1163	C	
U	A	U2078	C1972	G1884		C1633		U1165	U1064	C	
C	U	G2079	A1973	G1884	A1815	G1634	U1544	G1350	G1065	C	
U	A	G2080	G1974	C1894	C1816	U1635	C1545	G1351	U1066	G	
A		A2081		U1817	C1817	U1636	G1546	A1352	A1067	A	
C	G		A1978	A1904	C1818	A1637	A1547	C1353	A1070	G	
									G1071	A	

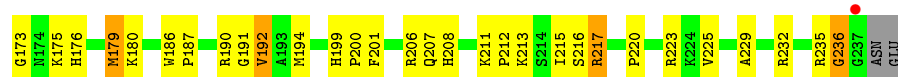


• Molecule 2: 5S Ribosomal RNA

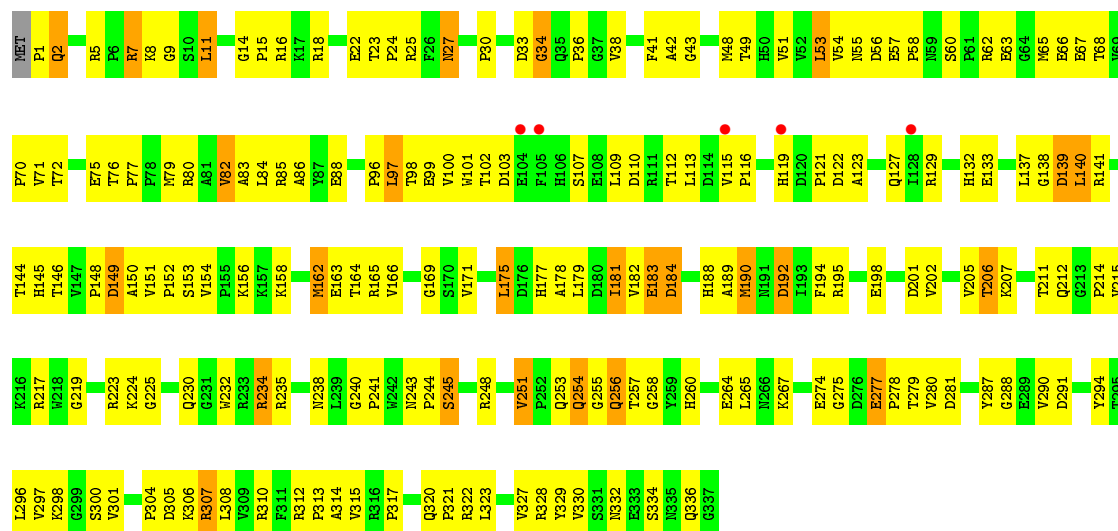


• Molecule 3: 50S ribosomal protein L2P

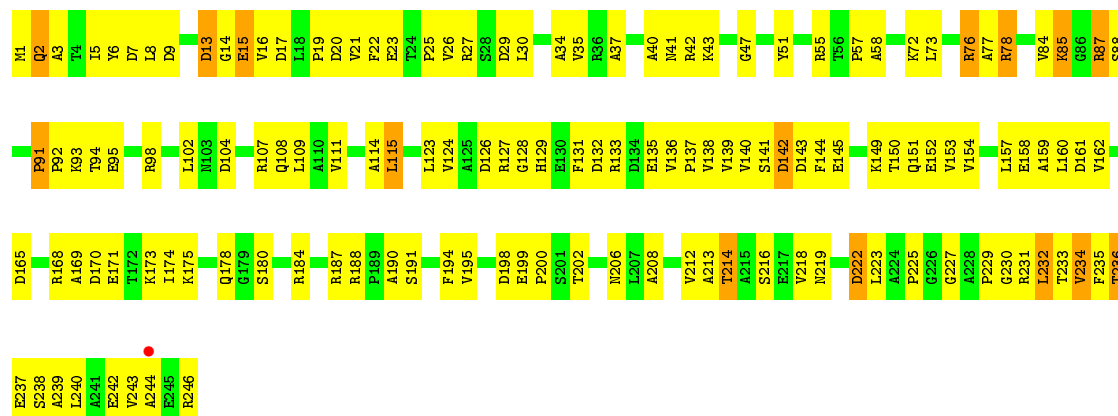




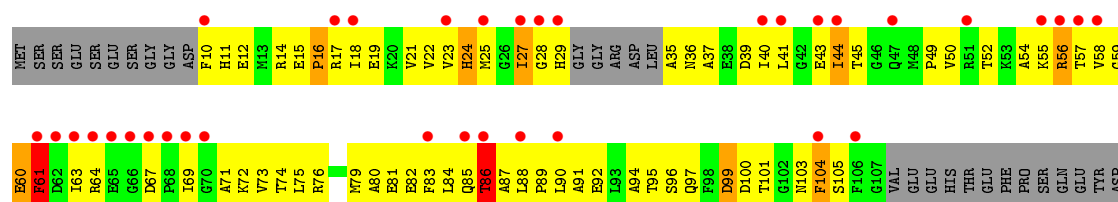
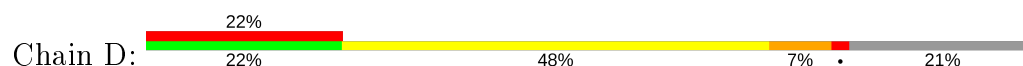
• Molecule 4: 50S ribosomal protein L3P

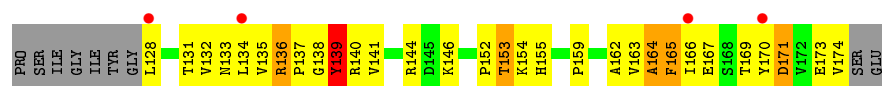


• Molecule 5: 50S ribosomal protein L4E

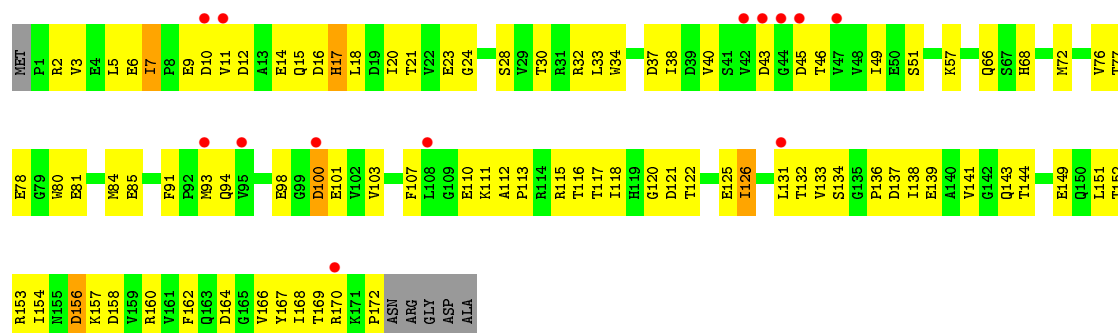


• Molecule 6: 50S ribosomal protein L5P

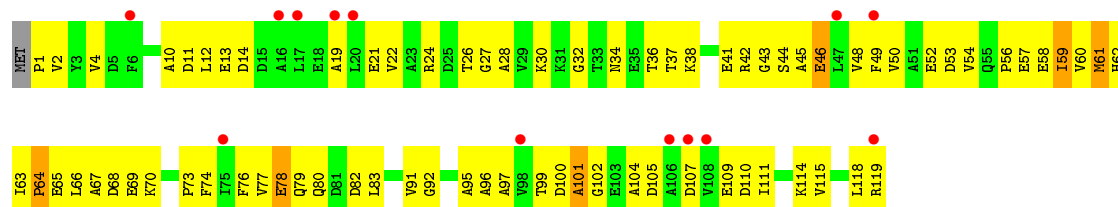




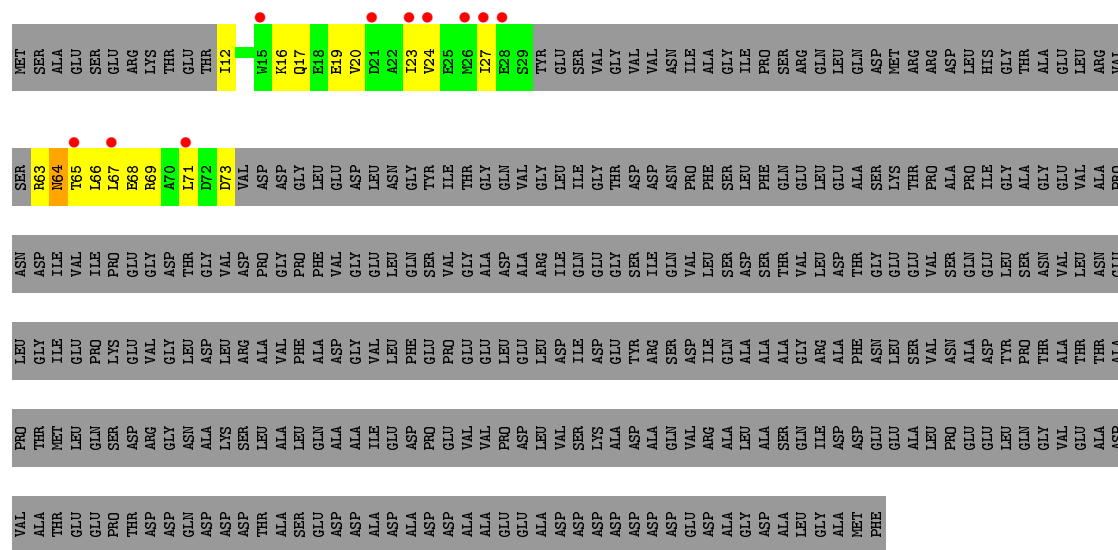
• Molecule 7: 50S ribosomal protein L6P



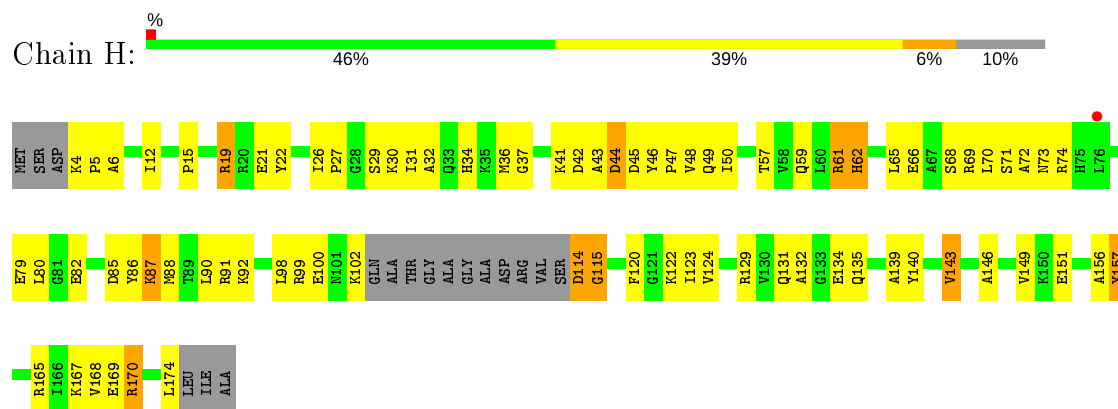
• Molecule 8: 50S ribosomal protein L7AE



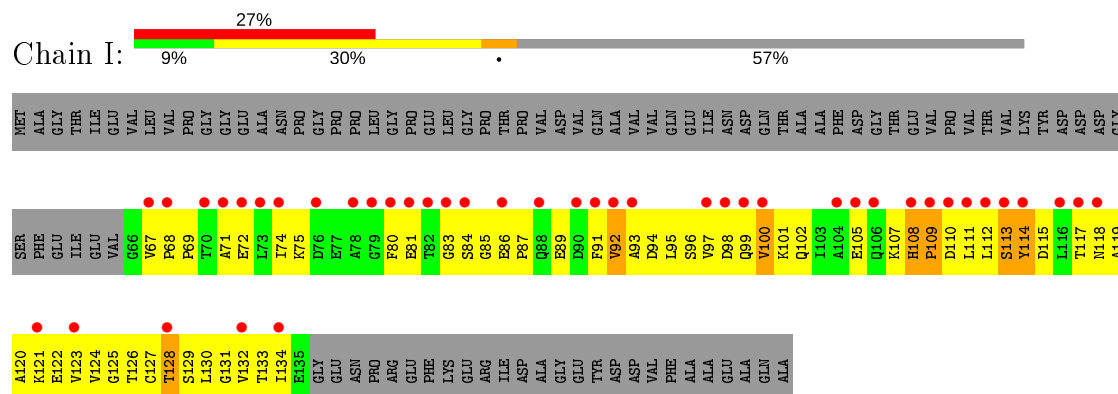
• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



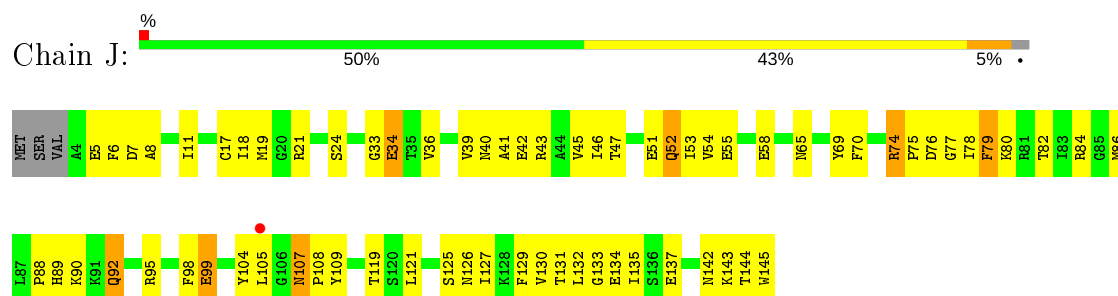
• Molecule 10: 50S RIBOSOMAL PROTEIN L10E



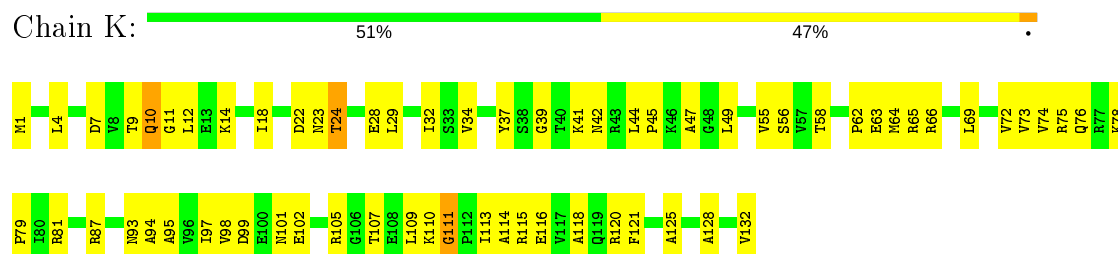
- Molecule 11: 50S RIBOSOMAL PROTEIN L11P



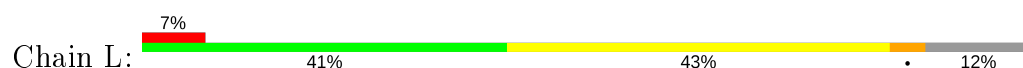
- Molecule 12: 50S ribosomal protein L13P



- Molecule 13: 50S ribosomal protein L14P



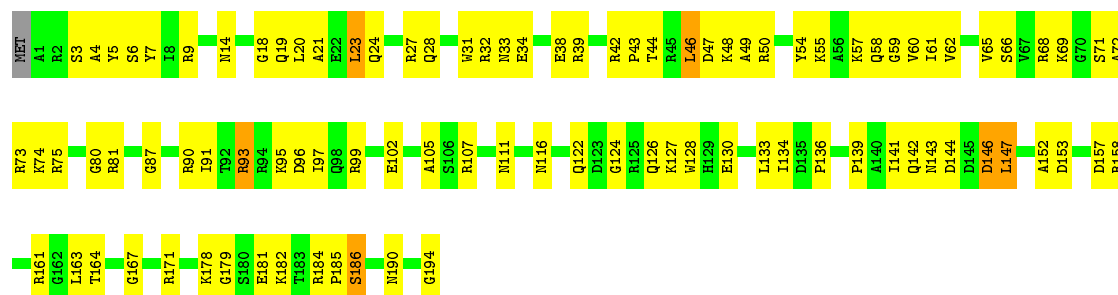
- Molecule 14: 50S ribosomal protein L15P





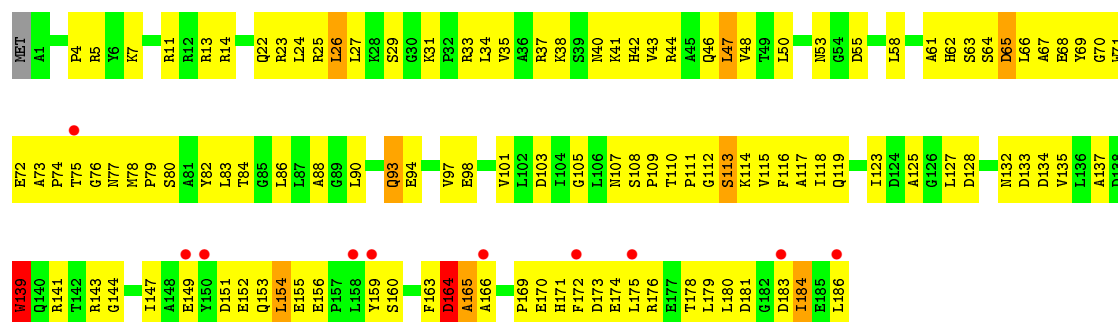
• Molecule 15: 50S Ribosomal Protein L15E

Chain M: 51% 46%



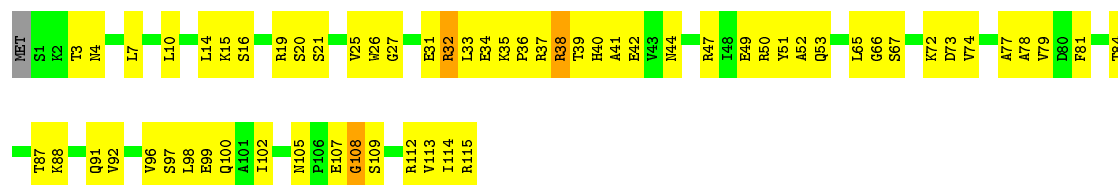
• Molecule 16: 50S ribosomal protein L18P

Chain N: 5% 36% 58%



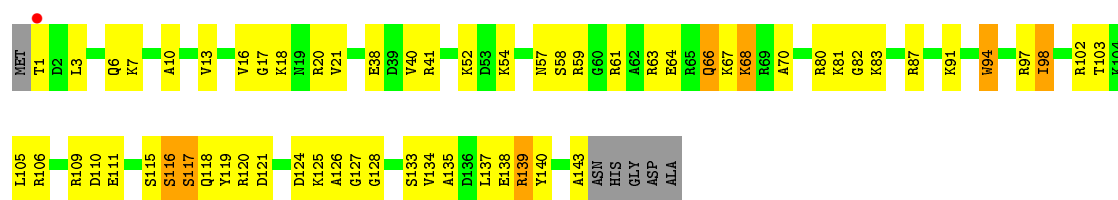
• Molecule 17: 50S ribosomal protein L18e

Chain O: 47% 50%



• Molecule 18: 50S ribosomal protein L19E

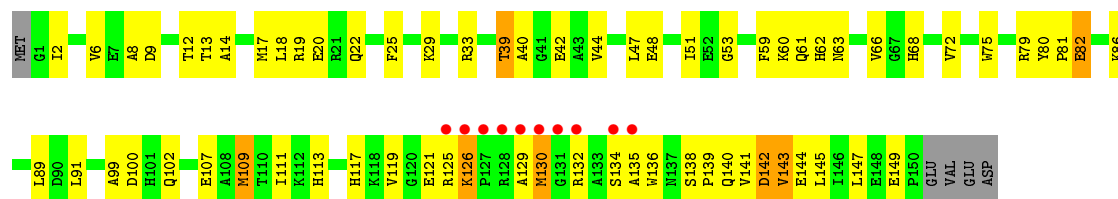
Chain P: 54% 37% 5%



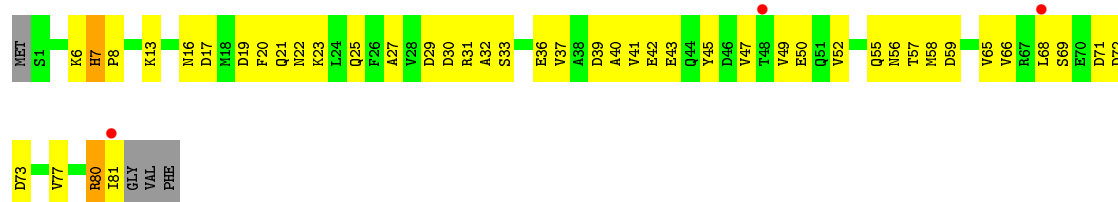
- Molecule 19: 50S ribosomal protein L21e



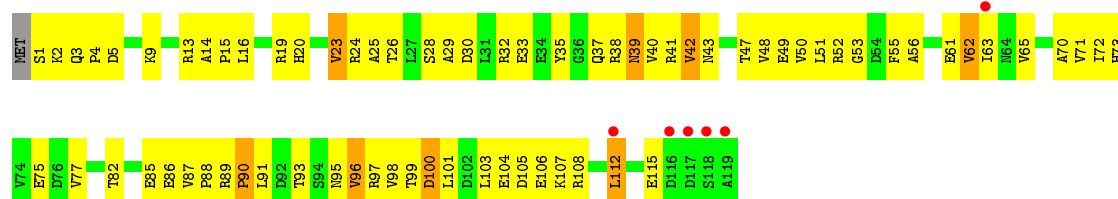
- Molecule 20: 50S ribosomal protein L22P



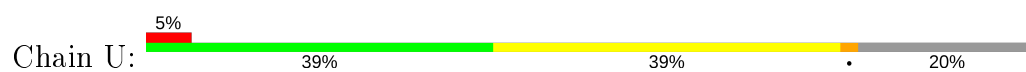
- Molecule 21: 50S ribosomal protein L23P



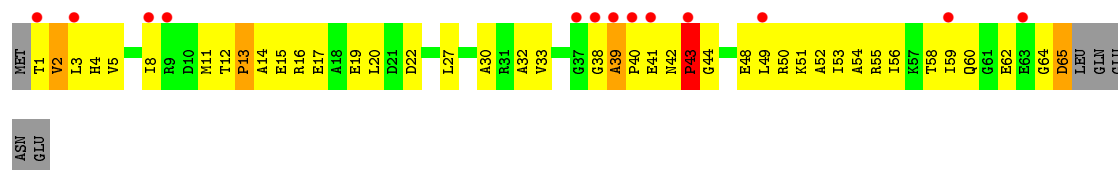
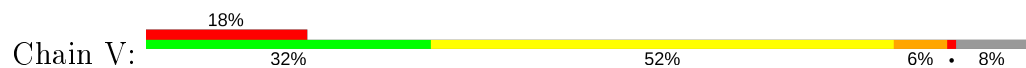
- Molecule 22: 50S ribosomal protein L24P



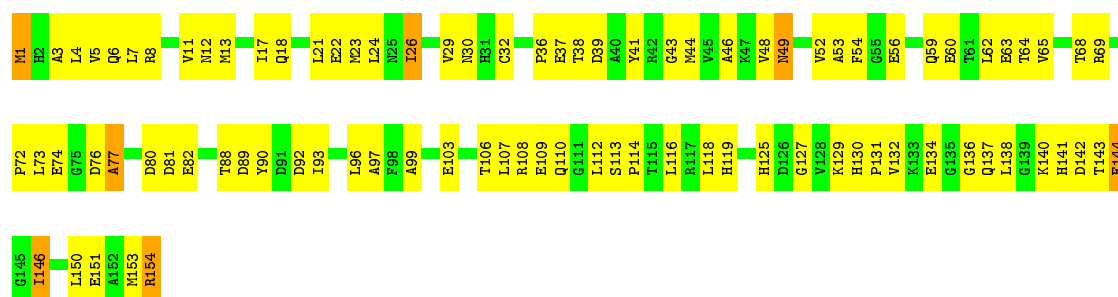
- Molecule 23: 50S ribosomal protein L24E



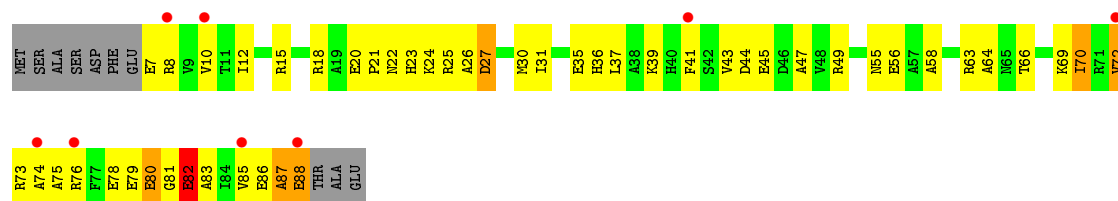
• Molecule 24: 50S ribosomal protein L29P



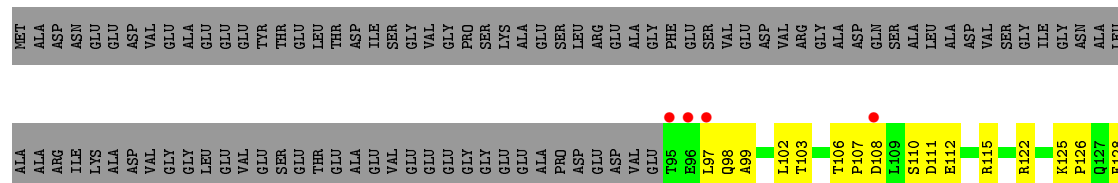
• Molecule 25: 50S ribosomal protein L30P

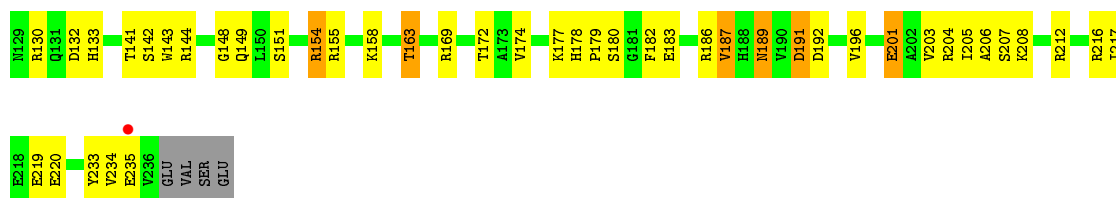


• Molecule 26: 50S ribosomal protein L31e

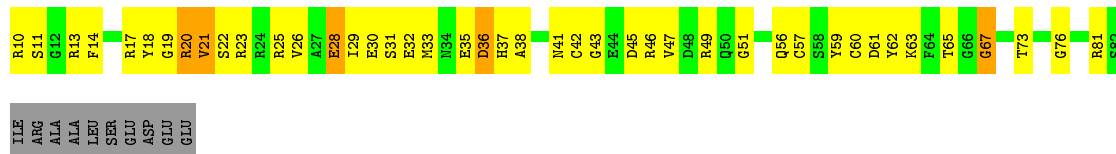
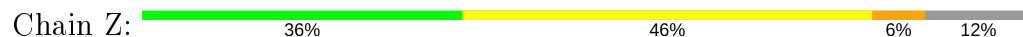


• Molecule 27: 50S ribosomal protein L32E

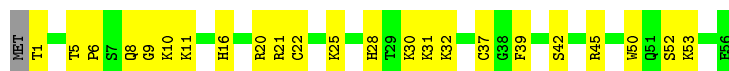




- Molecule 28: 50S ribosomal protein L37Ae



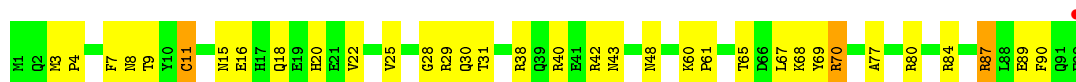
- Molecule 29: 50S ribosomal protein L37e



- 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	213.08Å 300.75Å 575.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.80 49.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.3 (29.94-2.80) 89.2 (49.56-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.184 , 0.242 0.185 , 0.240	Depositor DCC
R_{free} test set	3987 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99031	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, CD, OMU, UR3, 1MA, 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	0.42	0/65980	0.69	13/102903 (0.0%)
2	9	0.38	0/2904	0.70	1/4526 (0.0%)
3	A	0.35	0/1786	0.66	0/2408
4	B	0.35	0/2690	0.66	0/3652
5	C	0.39	0/1884	0.66	0/2551
6	D	0.33	0/1111	0.57	0/1498
7	E	0.35	0/1382	0.59	0/1880
8	F	0.34	0/901	0.59	0/1224
9	G	0.31	0/241	0.53	0/324
10	H	0.38	0/1302	0.70	1/1743 (0.1%)
11	I	0.31	0/526	0.59	0/716
12	J	0.40	0/1136	0.61	0/1530
13	K	0.37	0/1001	0.69	0/1347
14	L	0.36	0/1130	0.65	0/1509
15	M	0.36	0/1582	0.62	1/2117 (0.0%)
16	N	0.32	0/1474	0.64	0/1999
17	O	0.35	0/874	0.58	0/1181
18	P	0.37	0/1147	0.55	0/1528
19	Q	0.40	0/749	0.74	1/1005 (0.1%)
20	R	0.42	0/1146	0.63	0/1544
21	S	0.36	0/648	0.59	0/875
22	T	0.34	0/958	0.64	0/1289
23	U	0.34	0/417	0.58	0/562
24	V	0.31	0/502	0.56	0/675
25	W	0.37	0/1219	0.65	0/1655
26	X	0.36	0/664	0.62	0/895
27	Y	0.38	0/1146	0.65	0/1536
28	Z	0.38	0/589	0.63	0/787
29	1	0.40	0/438	0.64	0/578
30	2	0.41	0/427	0.61	0/566
31	3	0.40	0/771	0.58	0/1024
All	All	0.40	0/98725	0.68	17/147627 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	46
2	9	0	1
All	All	0	47

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1942	A	C5'-C4'-C3'	7.17	127.47	116.00
1	0	1504	A	C1'-O4'-C4'	-6.38	104.80	109.90
1	0	2291	A	N9-C1'-C2'	6.19	122.05	114.00
19	Q	68	GLY	N-CA-C	-5.89	98.36	113.10
1	0	1504	A	N9-C1'-C2'	5.75	121.48	114.00

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	148	A	Sidechain
1	0	26	U	Sidechain
1	0	333	G	Sidechain
1	0	398	U	Sidechain
1	0	458	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	59041	0	29817	1161	0
2	9	2599	0	1325	86	0
3	A	1753	0	1766	148	0
4	B	2625	0	2533	200	0
5	C	1859	0	1816	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1094	0	1085	138	0
7	E	1357	0	1266	77	0
8	F	890	0	843	79	0
9	G	240	0	231	22	0
10	H	1282	0	1292	95	0
11	I	519	0	500	63	0
12	J	1120	0	1098	80	0
13	K	992	0	1031	77	0
14	L	1118	0	1076	81	0
15	M	1558	0	1566	98	0
16	N	1445	0	1401	147	0
17	O	865	0	873	62	0
18	P	1136	0	1123	71	0
19	Q	735	0	729	37	0
20	R	1123	0	1099	69	0
21	S	641	0	605	39	0
22	T	950	0	923	99	0
23	U	410	0	364	31	0
24	V	499	0	511	44	0
25	W	1196	0	1137	120	0
26	X	654	0	653	57	0
27	Y	1130	0	1133	66	0
28	Z	578	0	539	39	0
29	1	431	0	426	36	0
30	2	421	0	437	35	0
31	3	755	0	728	31	0
32	0	107	0	0	0	0
32	2	1	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	2	0	0	0	0
34	0	74	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
34	T	1	0	0	0	0
35	0	9	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	4	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5866	0	0	246	0
37	1	63	0	0	8	0
37	2	32	0	0	2	0
37	3	69	0	0	8	0
37	9	143	0	0	12	0
37	A	119	0	0	21	0
37	B	148	0	0	31	0
37	C	180	0	0	34	0
37	D	46	0	0	17	0
37	E	45	0	0	10	0
37	F	27	0	0	8	0
37	G	19	0	0	2	0
37	H	69	0	0	12	0
37	I	9	0	0	5	0
37	J	57	0	0	8	0
37	K	54	0	0	10	0
37	L	84	0	0	17	0
37	M	130	0	0	10	0
37	N	64	0	0	22	0
37	O	45	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	P	64	0	0	10	0
37	Q	53	0	0	7	0
37	R	58	0	0	5	0
37	S	34	0	0	3	0
37	T	32	0	0	9	0
37	U	26	0	0	3	0
37	V	14	0	0	5	0
37	W	72	0	0	12	0
37	X	24	0	0	5	0
37	Y	104	0	0	15	0
37	Z	34	0	0	3	0
All	All	99031	0	59926	3232	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 21.

The worst 5 of 3232 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)
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.66	1.09
5:C:236:THR:HG22	5:C:239:ALA:H	0.95	1.08
1:O:1160:G:H5'	1:O:1161:A:H5'	1.13	1.07
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.36	1.04
29:1:25:LYS:HD2	30:2:49:GLU:H	1.20	1.03

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%)	191 (81%)	31 (13%)	13 (6%)	2 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	335/338 (99%)	291 (87%)	35 (10%)	9 (3%)	5	17
5	C	244/246 (99%)	201 (82%)	32 (13%)	11 (4%)	2	8
6	D	134/177 (76%)	85 (63%)	31 (23%)	18 (13%)	0	0
7	E	170/178 (96%)	150 (88%)	15 (9%)	5 (3%)	4	15
8	F	117/120 (98%)	93 (80%)	17 (14%)	7 (6%)	1	4
9	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
10	H	156/177 (88%)	134 (86%)	17 (11%)	5 (3%)	4	13
11	I	68/162 (42%)	49 (72%)	14 (21%)	5 (7%)	1	2
12	J	140/145 (97%)	121 (86%)	14 (10%)	5 (4%)	3	11
13	K	130/132 (98%)	111 (85%)	17 (13%)	2 (2%)	10	33
14	L	141/165 (86%)	114 (81%)	25 (18%)	2 (1%)	11	34
15	M	192/195 (98%)	169 (88%)	20 (10%)	3 (2%)	9	31
16	N	184/187 (98%)	149 (81%)	23 (12%)	12 (6%)	1	3
17	O	113/116 (97%)	102 (90%)	8 (7%)	3 (3%)	5	17
18	P	141/149 (95%)	125 (89%)	12 (8%)	4 (3%)	5	17
19	Q	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	6	22
20	R	145/152 (95%)	122 (84%)	18 (12%)	5 (3%)	3	13
21	S	79/85 (93%)	69 (87%)	9 (11%)	1 (1%)	12	36
22	T	117/120 (98%)	92 (79%)	19 (16%)	6 (5%)	2	6
23	U	51/66 (77%)	43 (84%)	7 (14%)	1 (2%)	7	24
24	V	63/71 (89%)	50 (79%)	9 (14%)	4 (6%)	1	3
25	W	152/154 (99%)	136 (90%)	14 (9%)	2 (1%)	12	36
26	X	80/92 (87%)	69 (86%)	8 (10%)	3 (4%)	3	10
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	56 (79%)	10 (14%)	5 (7%)	1	3
29	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
30	2	47/50 (94%)	44 (94%)	1 (2%)	2 (4%)	2	8
31	3	90/92 (98%)	84 (93%)	6 (7%)	0	100	100
All	All	3707/4434 (84%)	3148 (85%)	424 (11%)	135 (4%)	3	11

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	34	ASP
4	B	34	GLY
4	B	139	ASP
4	B	206	THR
5	C	8	LEU

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%)	171 (96%)	8 (4%)	27	60
4	B	282/283 (100%)	258 (92%)	24 (8%)	10	31
5	C	193/193 (100%)	182 (94%)	11 (6%)	20	50
6	D	117/148 (79%)	109 (93%)	8 (7%)	16	42
7	E	152/156 (97%)	147 (97%)	5 (3%)	38	72
8	F	93/94 (99%)	90 (97%)	3 (3%)	39	73
9	G	27/283 (10%)	26 (96%)	1 (4%)	34	68
10	H	134/145 (92%)	125 (93%)	9 (7%)	16	43
11	I	58/130 (45%)	55 (95%)	3 (5%)	23	55
12	J	118/121 (98%)	111 (94%)	7 (6%)	19	49
13	K	106/106 (100%)	104 (98%)	2 (2%)	57	85
14	L	113/127 (89%)	108 (96%)	5 (4%)	28	61
15	M	158/159 (99%)	151 (96%)	7 (4%)	28	61
16	N	149/150 (99%)	143 (96%)	6 (4%)	31	65
17	O	93/94 (99%)	88 (95%)	5 (5%)	22	53
18	P	113/117 (97%)	107 (95%)	6 (5%)	22	54
19	Q	79/80 (99%)	77 (98%)	2 (2%)	47	80
20	R	114/120 (95%)	109 (96%)	5 (4%)	28	61
21	S	71/74 (96%)	66 (93%)	5 (7%)	15	40
22	T	105/106 (99%)	99 (94%)	6 (6%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	44/52 (85%)	41 (93%)	3 (7%)	16	42
24	V	51/57 (90%)	48 (94%)	3 (6%)	19	49
25	W	130/130 (100%)	125 (96%)	5 (4%)	33	67
26	X	66/74 (89%)	60 (91%)	6 (9%)	9	27
27	Y	120/196 (61%)	114 (95%)	6 (5%)	24	56
28	Z	60/68 (88%)	58 (97%)	2 (3%)	38	72
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	45/46 (98%)	42 (93%)	3 (7%)	16	43
31	3	79/79 (100%)	75 (95%)	4 (5%)	24	55
All	All	3095/3617 (86%)	2935 (95%)	160 (5%)	23	55

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	46	ILE
15	M	93	ARG
27	Y	187	VAL
12	J	74	ARG
14	L	18	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	24	GLN
18	P	66	GLN
30	2	16	ASN
15	M	58	GLN
16	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2744/2922 (93%)	247 (9%)	26 (0%)
2	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2865/3044 (94%)	264 (9%)	27 (0%)

5 of 264 RNA backbone outliers are listed below:

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

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1506	U
1	0	2718	C
1	0	1377	C
1	0	857	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	UR3	0	2619	1	14,22,23	0.77	0	15,32,35	0.57	0
1	PSU	0	2621	1	17,21,22	1.48	3 (17%)	20,30,33	5.42	4 (20%)
1	OMG	0	2588	1	18,26,27	1.09	2 (11%)	20,38,41	2.60	5 (25%)
1	OMU	0	2587	1	14,22,23	0.95	1 (7%)	14,31,34	1.16	1 (7%)
1	1MA	0	628	1	15,25,26	0.76	0	15,37,40	1.37	1 (6%)

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	UR3	0	2619	1	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.36	1.48	1.52
1	0	2588	OMG	C6-N1	3.47	1.39	1.33
1	0	2621	PSU	C2-N1	2.77	1.43	1.38
1	0	2621	PSU	C4-N3	2.74	1.37	1.33
1	0	2587	OMU	C4-N3	2.31	1.37	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.41	114.59	128.43
1	0	2621	PSU	C4-N3-C2	14.20	127.13	115.14
1	0	2588	OMG	C5-C6-N1	-8.57	111.71	123.43
1	0	2621	PSU	C5-C4-N3	-7.93	115.14	125.36
1	0	2588	OMG	C6-N1-C2	5.80	125.14	115.93

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	2588	OMG	C3'-C2'-O2'-CM2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.26	14 (0%) 91 88	29, 55, 100, 157	0
2	9	122/122 (100%)	-0.22	3 (2%) 57 47	44, 68, 95, 159	0
3	A	237/240 (98%)	0.12	8 (3%) 45 35	34, 62, 95, 116	0
4	B	337/338 (99%)	-0.06	5 (1%) 73 68	32, 64, 90, 97	0
5	C	246/246 (100%)	-0.21	1 (0%) 92 91	29, 58, 81, 90	0
6	D	140/177 (79%)	1.27	39 (27%) 0 0	62, 107, 129, 138	0
7	E	172/178 (96%)	0.58	13 (7%) 13 7	52, 75, 97, 101	0
8	F	119/120 (99%)	0.64	13 (10%) 5 3	65, 84, 105, 117	0
9	G	29/348 (8%)	1.78	10 (34%) 0 0	76, 98, 106, 107	0
10	H	160/177 (90%)	-0.02	1 (0%) 89 86	40, 61, 96, 107	0
11	I	70/162 (43%)	2.71	43 (61%) 0 0	112, 126, 144, 147	0
12	J	142/145 (97%)	-0.21	1 (0%) 87 84	43, 58, 82, 95	0
13	K	132/132 (100%)	-0.05	0 100 100	40, 61, 84, 89	0
14	L	145/165 (87%)	0.28	11 (7%) 13 7	29, 75, 115, 126	0
15	M	194/195 (99%)	-0.24	0 100 100	40, 55, 69, 79	0
16	N	186/187 (99%)	0.25	10 (5%) 25 17	46, 71, 115, 125	0
17	O	115/116 (99%)	-0.05	0 100 100	47, 65, 81, 83	0
18	P	143/149 (95%)	0.20	1 (0%) 87 84	44, 66, 80, 86	0
19	Q	95/96 (98%)	-0.12	0 100 100	39, 51, 64, 79	0
20	R	147/152 (96%)	0.24	10 (6%) 17 10	41, 56, 114, 128	0
21	S	81/85 (95%)	0.21	3 (3%) 41 31	52, 72, 88, 95	0
22	T	119/120 (99%)	0.51	6 (5%) 28 19	51, 69, 94, 111	0
23	U	53/66 (80%)	0.13	3 (5%) 23 15	51, 64, 79, 85	0
24	V	65/71 (91%)	0.99	13 (20%) 1 0	63, 85, 118, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.20	0 100 100	41, 56, 76, 85	0
26	X	82/92 (89%)	0.38	8 (9%) 7 4	49, 66, 87, 101	0
27	Y	142/241 (58%)	0.04	5 (3%) 44 34	31, 53, 79, 95	0
28	Z	73/83 (87%)	-0.11	0 100 100	53, 69, 86, 102	0
29	1	56/57 (98%)	-0.42	0 100 100	35, 43, 49, 58	0
30	2	49/50 (98%)	0.20	3 (6%) 21 13	40, 66, 94, 104	0
31	3	92/92 (100%)	0.07	1 (1%) 80 75	42, 63, 76, 91	0
All	All	6646/7478 (88%)	-0.00	225 (3%) 45 35	29, 61, 106, 159	0

The worst 5 of 225 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	9.6
20	R	131	GLY	7.2
22	T	119	ALA	6.8
6	D	69	ILE	6.4
20	R	134	SER	6.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	UR3	0	2619	21/22	0.98	0.14	40,42,43,46	0
1	OMG	0	2588	24/25	0.98	0.14	40,42,44,44	0
1	PSU	0	2621	20/21	0.98	0.14	40,41,43,44	0
1	OMU	0	2587	21/22	0.98	0.14	39,42,43,46	0
1	1MA	0	628	23/24	0.99	0.16	32,37,39,39	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	8568	1/1	0.49	0.46	84,84,84,84	0
34	NA	0	8513	1/1	0.60	0.18	72,72,72,72	0
34	NA	R	8586	1/1	0.61	0.50	81,81,81,81	0
34	NA	0	8526	1/1	0.64	0.83	78,78,78,78	0
35	CL	0	8815	1/1	0.70	0.76	112,112,112,112	0
32	MG	0	8031	1/1	0.70	0.19	34,34,34,34	0
34	NA	0	8556	1/1	0.71	0.69	58,58,58,58	0
34	NA	0	8552	1/1	0.73	0.65	62,62,62,62	0
34	NA	0	8571	1/1	0.75	0.28	61,61,61,61	0
32	MG	0	8104	1/1	0.78	0.29	61,61,61,61	0
34	NA	0	8563	1/1	0.79	0.46	51,51,51,51	0
32	MG	0	8050	1/1	0.80	0.11	97,97,97,97	0
34	NA	0	8507	1/1	0.82	0.46	61,61,61,61	0
32	MG	9	8095	1/1	0.82	0.09	54,54,54,54	0
34	NA	0	8564	1/1	0.83	0.17	40,40,40,40	0
32	MG	0	8038	1/1	0.84	0.21	38,38,38,38	0
34	NA	9	8551	1/1	0.85	0.19	46,46,46,46	0
34	NA	0	8572	1/1	0.85	0.31	69,69,69,69	0
34	NA	L	8580	1/1	0.85	0.72	72,72,72,72	0
34	NA	0	8585	1/1	0.86	0.53	60,60,60,60	0
34	NA	0	8530	1/1	0.86	0.30	72,72,72,72	0
34	NA	0	8567	1/1	0.86	0.17	70,70,70,70	0
34	NA	0	8582	1/1	0.86	0.25	78,78,78,78	0
34	NA	0	8538	1/1	0.87	0.09	61,61,61,61	0
34	NA	0	8541	1/1	0.87	0.24	53,53,53,53	0
35	CL	0	8816	1/1	0.87	0.47	79,79,79,79	0
34	NA	0	8524	1/1	0.87	0.26	68,68,68,68	0
32	MG	0	8041	1/1	0.87	0.22	59,59,59,59	0
32	MG	0	8097	1/1	0.87	0.19	51,51,51,51	0
34	NA	R	8537	1/1	0.87	0.14	51,51,51,51	0
34	NA	0	8528	1/1	0.88	0.74	61,61,61,61	0
34	NA	0	8522	1/1	0.88	0.19	68,68,68,68	0
34	NA	0	8532	1/1	0.88	0.36	47,47,47,47	0
32	MG	0	8043	1/1	0.88	0.12	62,62,62,62	0
35	CL	N	8807	1/1	0.88	0.33	74,74,74,74	0
32	MG	0	8099	1/1	0.88	0.14	62,62,62,62	0
34	NA	0	8508	1/1	0.89	0.23	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	CL	0	8817	1/1	0.89	0.17	74,74,74,74	0
35	CL	R	8806	1/1	0.89	0.18	63,63,63,63	0
35	CL	0	8805	1/1	0.89	0.23	77,77,77,77	0
34	NA	C	8504	1/1	0.89	0.34	48,48,48,48	0
32	MG	0	8107	1/1	0.89	0.19	65,65,65,65	0
34	NA	0	8506	1/1	0.89	0.71	51,51,51,51	0
34	NA	9	8583	1/1	0.89	0.64	71,71,71,71	0
32	MG	0	8114	1/1	0.90	0.16	47,47,47,47	0
32	MG	0	8049	1/1	0.90	0.31	70,70,70,70	0
32	MG	0	8040	1/1	0.90	0.12	57,57,57,57	0
32	MG	0	8082	1/1	0.91	0.10	76,76,76,76	0
34	NA	0	8581	1/1	0.91	0.14	52,52,52,52	0
34	NA	0	8569	1/1	0.91	0.59	66,66,66,66	0
32	MG	T	8073	1/1	0.91	0.21	68,68,68,68	0
32	MG	0	8115	1/1	0.91	0.14	70,70,70,70	0
35	CL	B	8819	1/1	0.91	0.40	74,74,74,74	0
32	MG	0	8085	1/1	0.91	0.13	62,62,62,62	0
34	NA	0	8566	1/1	0.91	0.33	68,68,68,68	0
32	MG	0	8092	1/1	0.92	0.24	80,80,80,80	0
32	MG	2	8076	1/1	0.92	0.17	69,69,69,69	0
34	NA	0	8579	1/1	0.92	0.27	62,62,62,62	0
35	CL	3	8804	1/1	0.92	0.29	74,74,74,74	0
34	NA	S	8512	1/1	0.92	0.14	48,48,48,48	0
35	CL	Y	8820	1/1	0.92	0.14	55,55,55,55	0
32	MG	0	8103	1/1	0.92	0.16	67,67,67,67	0
35	CL	0	8822	1/1	0.92	0.20	79,79,79,79	0
36	CD	3	8704	1/1	0.93	0.08	72,72,72,72	0
34	NA	0	8511	1/1	0.93	0.13	43,43,43,43	0
34	NA	0	8560	1/1	0.93	0.65	61,61,61,61	0
35	CL	J	8802	1/1	0.93	0.12	75,75,75,75	0
34	NA	0	8510	1/1	0.93	0.24	40,40,40,40	0
34	NA	0	8540	1/1	0.93	0.24	40,40,40,40	0
34	NA	0	8570	1/1	0.93	0.16	66,66,66,66	0
32	MG	0	8062	1/1	0.93	0.13	65,65,65,65	0
34	NA	0	8529	1/1	0.93	0.15	79,79,79,79	0
34	NA	0	8559	1/1	0.93	0.41	66,66,66,66	0
34	NA	0	8574	1/1	0.93	0.79	63,63,63,63	0
34	NA	0	8550	1/1	0.93	0.26	56,56,56,56	0
35	CL	0	8814	1/1	0.94	0.17	71,71,71,71	0
35	CL	A	8809	1/1	0.94	0.23	82,82,82,82	0
34	NA	M	8547	1/1	0.94	0.22	45,45,45,45	0
34	NA	0	8573	1/1	0.94	0.64	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	0	8533	1/1	0.94	0.14	49,49,49,49	0
35	CL	0	8803	1/1	0.94	0.20	80,80,80,80	0
32	MG	0	8111	1/1	0.94	0.07	48,48,48,48	0
34	NA	0	8557	1/1	0.94	0.11	65,65,65,65	0
34	NA	0	8561	1/1	0.94	0.34	50,50,50,50	0
34	NA	0	8578	1/1	0.94	0.58	77,77,77,77	0
34	NA	0	8535	1/1	0.94	0.20	73,73,73,73	0
32	MG	0	8070	1/1	0.94	0.12	54,54,54,54	0
35	CL	L	8810	1/1	0.94	0.13	73,73,73,73	0
32	MG	0	8112	1/1	0.94	0.18	64,64,64,64	0
34	NA	0	8584	1/1	0.94	0.17	70,70,70,70	0
34	NA	0	8576	1/1	0.95	0.18	51,51,51,51	0
35	CL	O	8808	1/1	0.95	0.40	99,99,99,99	0
34	NA	0	8521	1/1	0.95	0.38	73,73,73,73	0
32	MG	0	8044	1/1	0.95	0.16	51,51,51,51	0
35	CL	J	8801	1/1	0.95	0.10	67,67,67,67	0
34	NA	Q	8548	1/1	0.95	0.17	49,49,49,49	0
34	NA	0	8515	1/1	0.95	0.26	65,65,65,65	0
32	MG	0	8089	1/1	0.95	0.08	69,69,69,69	0
32	MG	0	8093	1/1	0.95	0.20	50,50,50,50	0
34	NA	0	8514	1/1	0.95	0.09	39,39,39,39	0
32	MG	0	8024	1/1	0.95	0.14	45,45,45,45	0
32	MG	0	8015	1/1	0.95	0.06	41,41,41,41	0
34	NA	0	8549	1/1	0.95	0.16	54,54,54,54	0
32	MG	0	8042	1/1	0.95	0.11	55,55,55,55	0
32	MG	0	8109	1/1	0.95	0.05	33,33,33,33	0
32	MG	K	8069	1/1	0.95	0.09	62,62,62,62	0
32	MG	0	8113	1/1	0.95	0.12	49,49,49,49	0
34	NA	0	8505	1/1	0.96	0.17	49,49,49,49	0
34	NA	0	8523	1/1	0.96	0.10	37,37,37,37	0
32	MG	0	8068	1/1	0.96	0.05	70,70,70,70	0
32	MG	0	8027	1/1	0.96	0.09	63,63,63,63	0
33	K	0	8401	1/1	0.96	0.41	91,91,91,91	0
32	MG	0	8087	1/1	0.96	0.10	81,81,81,81	0
32	MG	0	8063	1/1	0.96	0.23	73,73,73,73	0
34	NA	0	8575	1/1	0.96	0.25	58,58,58,58	0
32	MG	0	8048	1/1	0.96	0.09	62,62,62,62	0
33	K	0	8402	1/1	0.96	0.13	69,69,69,69	0
32	MG	0	8004	1/1	0.96	0.07	43,43,43,43	0
32	MG	0	8059	1/1	0.96	0.10	44,44,44,44	0
34	NA	A	8545	1/1	0.96	0.10	46,46,46,46	0
35	CL	Q	8811	1/1	0.96	0.16	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	0	8562	1/1	0.96	0.31	81,81,81,81	0
32	MG	0	8051	1/1	0.96	0.15	67,67,67,67	0
34	NA	0	8536	1/1	0.96	0.09	52,52,52,52	0
34	NA	0	8554	1/1	0.96	0.15	38,38,38,38	0
34	NA	0	8517	1/1	0.96	0.10	52,52,52,52	0
34	NA	0	8516	1/1	0.96	0.23	61,61,61,61	0
32	MG	0	8091	1/1	0.96	0.13	53,53,53,53	0
32	MG	Y	8108	1/1	0.96	0.15	48,48,48,48	0
34	NA	0	8577	1/1	0.96	0.20	72,72,72,72	0
34	NA	T	8543	1/1	0.96	0.14	43,43,43,43	0
32	MG	0	8014	1/1	0.96	0.10	20,20,20,20	0
32	MG	0	8003	1/1	0.96	0.10	47,47,47,47	0
32	MG	0	8100	1/1	0.96	0.13	66,66,66,66	0
32	MG	0	8088	1/1	0.96	0.10	34,34,34,34	0
32	MG	0	8052	1/1	0.96	0.06	44,44,44,44	0
32	MG	0	8025	1/1	0.97	0.12	58,58,58,58	0
32	MG	0	8105	1/1	0.97	0.08	63,63,63,63	0
35	CL	0	8813	1/1	0.97	0.10	67,67,67,67	0
34	NA	0	8518	1/1	0.97	0.18	32,32,32,32	0
32	MG	3	8078	1/1	0.97	0.07	43,43,43,43	0
32	MG	0	8081	1/1	0.97	0.14	74,74,74,74	0
32	MG	0	8007	1/1	0.97	0.09	29,29,29,29	0
32	MG	0	8046	1/1	0.97	0.06	55,55,55,55	0
32	MG	0	8016	1/1	0.97	0.13	48,48,48,48	0
34	NA	0	8544	1/1	0.97	0.07	33,33,33,33	0
34	NA	0	8542	1/1	0.97	0.20	51,51,51,51	0
32	MG	0	8033	1/1	0.97	0.13	37,37,37,37	0
34	NA	0	8527	1/1	0.97	0.12	69,69,69,69	0
32	MG	0	8102	1/1	0.97	0.19	71,71,71,71	0
34	NA	0	8525	1/1	0.97	0.10	50,50,50,50	0
32	MG	0	8116	1/1	0.97	0.08	39,39,39,39	0
32	MG	0	8074	1/1	0.97	0.06	40,40,40,40	0
32	MG	0	8096	1/1	0.97	0.11	53,53,53,53	0
34	NA	0	8503	1/1	0.97	0.20	70,70,70,70	0
34	NA	0	8539	1/1	0.97	0.10	26,26,26,26	0
35	CL	0	8812	1/1	0.97	0.14	65,65,65,65	0
34	NA	0	8502	1/1	0.97	0.23	49,49,49,49	0
32	MG	0	8094	1/1	0.97	0.04	67,67,67,67	0
34	NA	0	8509	1/1	0.97	0.12	37,37,37,37	0
35	CL	J	8821	1/1	0.97	0.10	54,54,54,54	0
34	NA	0	8534	1/1	0.97	0.11	55,55,55,55	0
34	NA	0	8519	1/1	0.97	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8053	1/1	0.97	0.15	47,47,47,47	0
34	NA	0	8501	1/1	0.97	0.11	29,29,29,29	0
32	MG	0	8008	1/1	0.97	0.08	35,35,35,35	0
34	NA	0	8558	1/1	0.97	0.70	107,107,107,107	0
32	MG	0	8064	1/1	0.97	0.19	43,43,43,43	0
32	MG	0	8101	1/1	0.97	0.09	70,70,70,70	0
34	NA	0	8531	1/1	0.98	0.17	55,55,55,55	0
32	MG	0	8057	1/1	0.98	0.20	67,67,67,67	0
32	MG	0	8010	1/1	0.98	0.10	45,45,45,45	0
32	MG	0	8022	1/1	0.98	0.06	42,42,42,42	0
32	MG	0	8086	1/1	0.98	0.07	46,46,46,46	0
32	MG	0	8013	1/1	0.98	0.16	54,54,54,54	0
32	MG	0	8036	1/1	0.98	0.08	44,44,44,44	0
32	MG	0	8035	1/1	0.98	0.03	58,58,58,58	0
32	MG	0	8028	1/1	0.98	0.06	48,48,48,48	0
32	MG	0	8075	1/1	0.98	0.09	54,54,54,54	0
34	NA	0	8520	1/1	0.98	0.06	33,33,33,33	0
32	MG	0	8083	1/1	0.98	0.04	52,52,52,52	0
32	MG	0	8037	1/1	0.98	0.08	51,51,51,51	0
32	MG	0	8084	1/1	0.98	0.07	54,54,54,54	0
32	MG	A	8066	1/1	0.98	0.06	88,88,88,88	0
32	MG	0	8047	1/1	0.98	0.09	59,59,59,59	0
34	NA	J	8546	1/1	0.98	0.11	48,48,48,48	0
32	MG	0	8110	1/1	0.98	0.04	59,59,59,59	0
36	CD	O	8705	1/1	0.98	0.08	98,98,98,98	0
35	CL	M	8818	1/1	0.98	0.19	60,60,60,60	0
32	MG	0	8045	1/1	0.98	0.10	59,59,59,59	0
32	MG	0	8018	1/1	0.98	0.11	50,50,50,50	0
32	MG	0	8011	1/1	0.98	0.11	32,32,32,32	0
32	MG	0	8029	1/1	0.98	0.12	55,55,55,55	0
32	MG	0	8077	1/1	0.98	0.07	32,32,32,32	0
34	NA	0	8565	1/1	0.98	0.29	49,49,49,49	0
32	MG	0	8032	1/1	0.98	0.07	32,32,32,32	0
32	MG	0	8090	1/1	0.99	0.10	59,59,59,59	0
32	MG	0	8071	1/1	0.99	0.08	80,80,80,80	0
32	MG	0	8019	1/1	0.99	0.03	39,39,39,39	0
32	MG	0	8080	1/1	0.99	0.09	47,47,47,47	0
32	MG	B	8055	1/1	0.99	0.07	46,46,46,46	0
32	MG	0	8106	1/1	0.99	0.09	38,38,38,38	0
32	MG	0	8021	1/1	0.99	0.10	31,31,31,31	0
34	NA	0	8555	1/1	0.99	0.23	67,67,67,67	0
32	MG	0	8012	1/1	0.99	0.10	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8006	1/1	0.99	0.06	37,37,37,37	0
32	MG	A	8065	1/1	0.99	0.08	43,43,43,43	0
32	MG	0	8061	1/1	0.99	0.10	36,36,36,36	0
32	MG	0	8079	1/1	0.99	0.11	43,43,43,43	0
32	MG	0	8023	1/1	0.99	0.07	42,42,42,42	0
32	MG	0	8005	1/1	0.99	0.09	45,45,45,45	0
32	MG	0	8026	1/1	0.99	0.09	28,28,28,28	0
32	MG	0	8009	1/1	0.99	0.04	36,36,36,36	0
32	MG	0	8017	1/1	0.99	0.04	33,33,33,33	0
36	CD	U	8701	1/1	0.99	0.10	76,76,76,76	0
32	MG	0	8034	1/1	0.99	0.10	36,36,36,36	0
32	MG	0	8030	1/1	0.99	0.13	34,34,34,34	0
34	NA	0	8553	1/1	0.99	0.10	36,36,36,36	0
32	MG	0	8098	1/1	0.99	0.11	30,30,30,30	0
32	MG	0	8001	1/1	0.99	0.09	33,33,33,33	0
32	MG	0	8056	1/1	0.99	0.11	49,49,49,49	0
32	MG	0	8060	1/1	0.99	0.13	50,50,50,50	0
32	MG	0	8054	1/1	0.99	0.10	43,43,43,43	0
32	MG	0	8072	1/1	0.99	0.11	61,61,61,61	0
32	MG	0	8002	1/1	0.99	0.06	35,35,35,35	0
36	CD	Z	8703	1/1	0.99	0.11	71,71,71,71	0
32	MG	0	8020	1/1	1.00	0.06	31,31,31,31	0
32	MG	0	8058	1/1	1.00	0.09	46,46,46,46	0
36	CD	1	8702	1/1	1.00	0.07	68,68,68,68	0
32	MG	0	8039	1/1	1.00	0.07	44,44,44,44	0
32	MG	0	8067	1/1	1.00	0.07	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.