



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 12:47 pm GMT

PDB ID : 1VQK  
Title : The structure of CCDA-PHE-CAP-BIO bound to the a site of the ribosomal subunit of haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

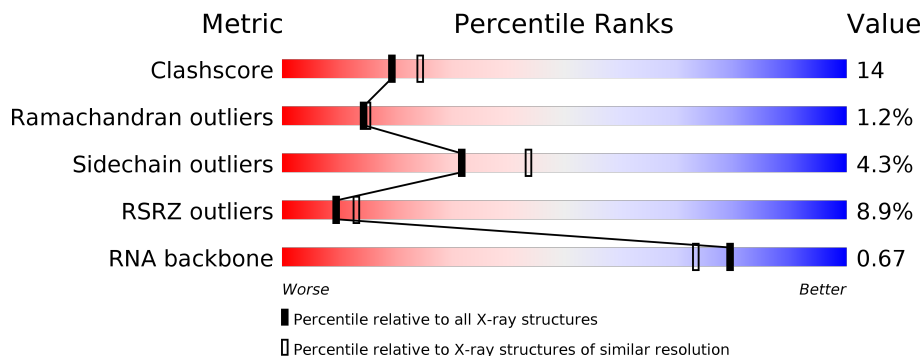
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)
RNA backbone	2636	1004 (2.76-1.84)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>3%</div> <div>65% 24% 5% 6%</div> </div>
2	9	122	<div> <div>5%</div> <div>57% 34% 8%</div> </div>
3	4	5	<div> <div>20%</div> <div>40% 60%</div> </div>
4	A	240	<div> <div>8%</div> <div>63% 32%</div> </div>
5	B	338	<div> <div>4%</div> <div>59% 35% 6%</div> </div>
6	C	246	<div> <div>2%</div> <div>63% 32%</div> </div>

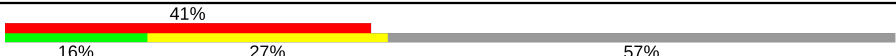
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Mol	Chain	Length	Quality of chain
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	

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Mol	Chain	Length	Quality of chain
32	I	162	

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
3	ACA	4	78	-	-	-	X
33	MG	0	8022	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8082	-	-	-	X
33	MG	0	8092	-	-	-	X
35	NA	0	9122	-	-	-	X
35	NA	0	9129	-	-	-	X
35	NA	0	9164	-	-	-	X
37	SR	0	9500	-	-	-	X
37	SR	0	9547	-	-	-	X
37	SR	0	9601	-	-	-	X
37	SR	B	9521	-	-	-	X

## 2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 99036 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

- 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 RNA chain called 5'-R(\*CP\*CP\*(DA)\*(PHE)\*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	5	Total	C	N	O	P	0	0	0
			73	40	12	19	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

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

- Molecule 6 is a protein called 50S ribosomal protein L4E.

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

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- 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
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	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	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			
			735	450	141	144	0	0	0

- 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		
			1149	713	209	223	4	0	0

- 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		
			641	389	111	138	3	0	0

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

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

- 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		
			410	244	75	86	5	0	0

- 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		
			499	304	94	100	1	0	0

- 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		
			1196	737	209	244	6	0	0

- 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	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 a protein called 50S RIBOSOMAL PROTEIN L11P.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	87	Total	Mg	0	0
			87	87		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	64	Total	Na	0	0
			64	64		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	D	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	3	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	3	Total 3	Na 3	0	0
35	9	1	Total 1	Na 1	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

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

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

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total 98	Sr 98	0	0
37	1	2	Total 2	Sr 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	1	Total 1	Sr 1	0	0
37	B	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0
37	A	3	Total 3	Sr 3	0	0
37	R	1	Total 1	Sr 1	0	0
37	9	3	Total 3	Sr 3	0	0
37	L	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	F	1	Total 1	Sr 1	0	0

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total 1	Cd 1	0	0
38	Z	1	Total 1	Cd 1	0	0
38	1	1	Total 1	Cd 1	0	0
38	3	1	Total 1	Cd 1	0	0
38	U	1	Total 1	Cd 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5769	Total 5769	O 5769	0	0
39	9	140	Total 140	O 140	0	0
39	A	121	Total 121	O 121	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	B	144	Total 144	O 144	0	0
39	C	177	Total 177	O 177	0	0
39	D	48	Total 48	O 48	0	0
39	E	44	Total 44	O 44	0	0
39	F	27	Total 27	O 27	0	0
39	G	17	Total 17	O 17	0	0
39	H	69	Total 69	O 69	0	0
39	J	52	Total 52	O 52	0	0
39	K	57	Total 57	O 57	0	0
39	L	81	Total 81	O 81	0	0
39	M	130	Total 130	O 130	0	0
39	N	61	Total 61	O 61	0	0
39	O	40	Total 40	O 40	0	0
39	P	64	Total 64	O 64	0	0
39	Q	49	Total 49	O 49	0	0
39	R	82	Total 82	O 82	0	0
39	S	32	Total 32	O 32	0	0
39	T	37	Total 37	O 37	0	0
39	U	29	Total 29	O 29	0	0
39	V	14	Total 14	O 14	0	0
39	W	69	Total 69	O 69	0	0

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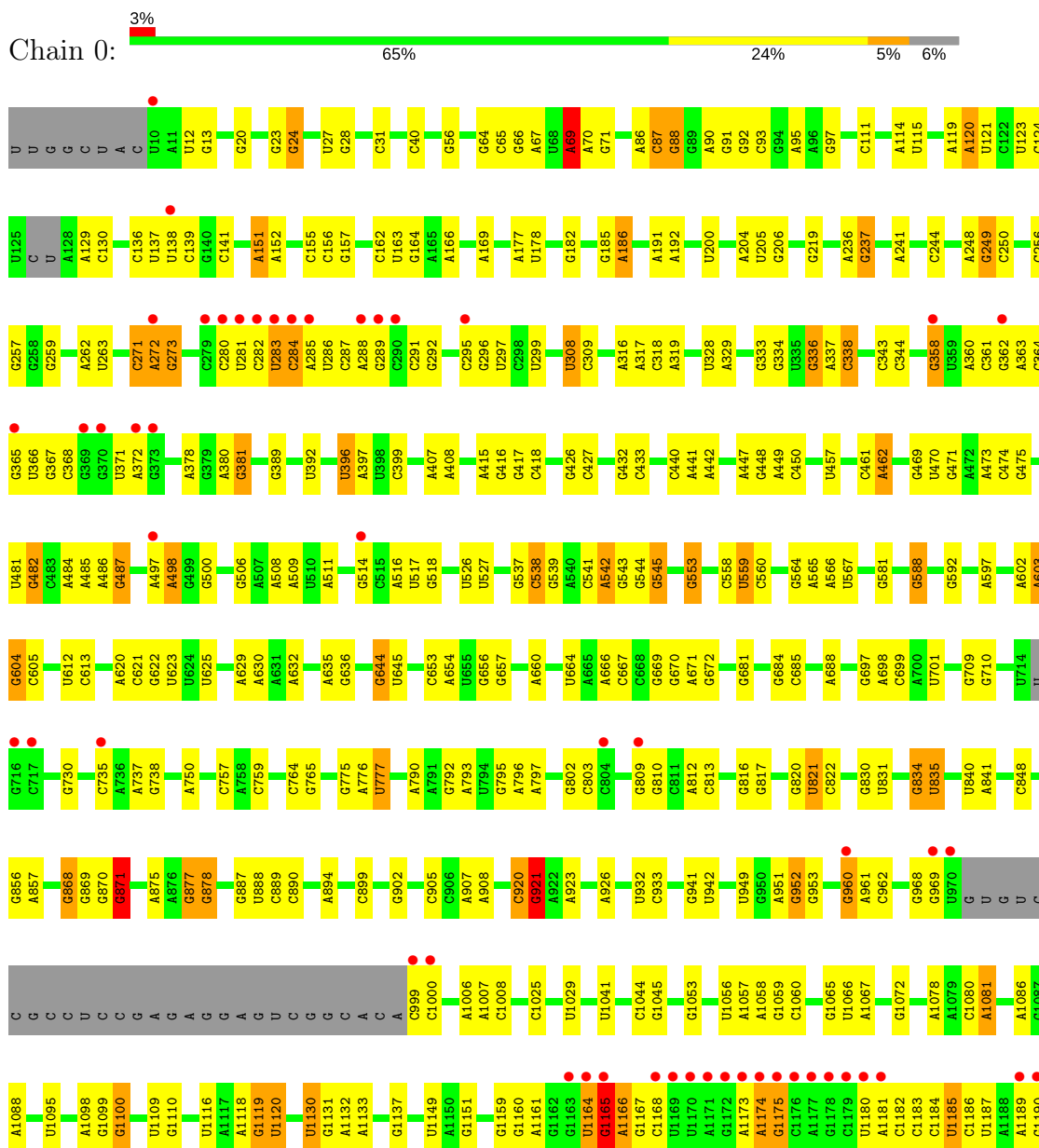
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	24	Total 24	O 24	0	0
39	Y	96	Total 96	O 96	0	0
39	Z	31	Total 31	O 31	0	0
39	1	50	Total 50	O 50	0	0
39	2	40	Total 40	O 40	0	0
39	3	67	Total 67	O 67	0	0
39	I	7	Total 7	O 7	0	0

### 3 Residue-property plots [i](#)

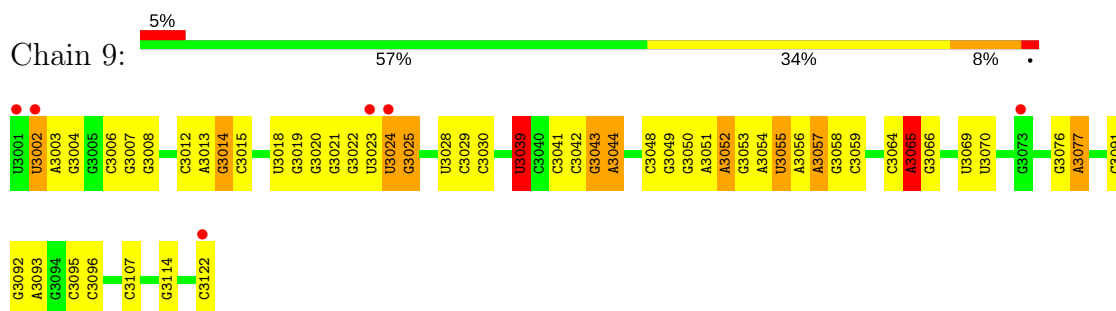
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

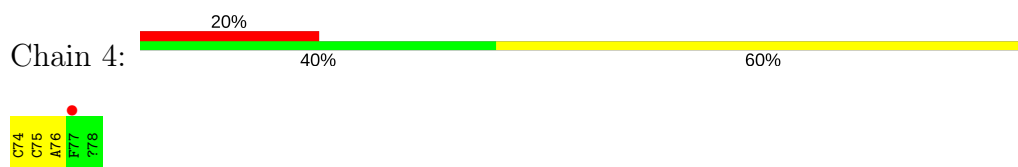


G2842	G2764	A2635	A2521	A2414	A2391	G2136	U2003	C1882	A1767	G1855	U1478	G1311	A1191
G2851	G2755	C2636	G2524	A2416	A2302	A	G2005	G1902	C1768	A1856	C1496	G1314	A1192
U2853	U2756	A2637	G2525	G2417	C2309	C	C2006	U1903	C1769	A1659	G1496	U1314	A1193
A2856	A2761	C2644	C2526	G2418	C2313	U	A2007	A1919	A1778	G1660	A1501	A1328	G1196
C2857	C2762	U2645	U2531	G2419	G2314	G	U2008	C1920	A1779	C1666	A1502	A1331	G1197
U2858	U2765	A2649	A2532	G2420	C2315	U	A2011	A1921	C1786	A1667	U1503	A1332	A1199
U2866	A2768	U2652	C2533	G2421	C2316	C	U2012	A1922	C1787	U1668	A1504	C1332	A1200
C2867	C2769	A2653	G2534	G2422	C2317	U	G2013	G1926	U1788	U1681	U1505	U1333	C1201
G2868	G2770	C2644	C2535	G2426	C2317	C	G2014	G1927	G1789	G1681	U1506	C1334	A1202
G2869	U2771	U2661	C2536	C2427	U2320	C	A2015	A1927	G1794	A1682	U1524	C1335	G1203
U2870	U2772	G2662	A2537	U2428	A2321	A	U2016	G1928	G1795	A1683	G1525	G1340	C1204
U2871	U2773	U2663	C2443	U2429	U2322	C	U2032	G1929	G1796	A1684	G1526	A1341	U1205
U2872	U2774	U2664	U2444	G2430	U2323	U	G2033	U1937	A1796	A1685	A1527	A1342	U1206
U2873	U2775	A	G2445	U2431	U2324	G	U2034	G1938	A1797	A1686	A1528	C1343	A1207
U2874	U2776	U	U2446	G2432	C2329	U	C2035	U1939	C1798	C1687	G1529	U1350	G1208
U2875	U2777	G2667	G2453	U2433	U2330	A	G2036	C1940	G1799	C1692	G1530	U1351	C1209
U2876	U2778	U2668	A2456	U2434	G2338	A	U2042	A1941	G1809	C1700	G1531	A1352	G1210
U2877	U2779	U2669	U2457	U2435	A	G	U2043	A1942	C1818	A1701	G1532	C1353	G1211
U2878	U2780	U2670	U2458	U2436	C	C	G2044	C1943	C1819	U1702	G1533	G1360	C1212
U2879	U2781	U2671	G2462	U2437	U2331	U	U2045	G1944	G1820	A1559	G1534	G1361	G1216
U2880	U2782	U2672	U2463	U2438	U2332	A	G2046	G1945	A1821	U	G1535	G1362	G1217
U2881	U2783	U2673	A2464	U2439	U2333	A	G2047	G1946	A1822	U1561	G1536	G1363	U1218
U2882	U2784	U2674	A2465	U2440	U2334	G	U2048	G1947	A1823	C1562	G1537	A1372	U1219
U2883	U2785	U2675	G2466	U2441	U2335	C	G2049	G1948	C1824	C1563	G1538	G1377	G1226
U2884	U2786	U2676	U2467	U2442	U2336	U	U2050	G1949	A1825	C1564	G1539	C1378	C1227
U2885	U2787	U2677	A2468	U2443	U2337	A	U2051	G1950	U1835	A1573	G1540	G1379	C1228
U2886	U2788	U2678	U2469	U2444	U2338	C	U2052	G1951	U1836	C1574	G1541	C1380	C1229
U2887	U2789	U2679	U2470	U2445	U2339	G	U2053	U1952	U1837	G1575	G1542	A1231	A1230
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U2890	U2792	U2682	U2473	U2448	U2342	U	U2056	U1955	U1840	C1593	G1545	A1234	A1233
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U2892	U2794	U2684	U2475	U2450	U2344	C	U2058	U1957	U1842	C1595	G1547	U1236	U1235
U2893	U2795	U2685	U2476	U2451	U2345	U	G2059	U1958	U1843	C1596	G1548	U1237	U1236
U2894	U2796	U2686	U2477	U2452	U2346	C	U2060	U1959	U1844	C1597	G1549	C1238	C1237
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U2902	U2804	U2694	U2485	U2460	U2354	U	U2068	U1967	U1852	A1618	G1557	U1431	A1247
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U2904	U2806	U2696	U2487	U2462	U2356	G	U2070	U1969	U1854	A1620	G1559	G1427	A1249
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U2906	U2808	U2698	U2489	U2464	U2358	C	U2072	U1971	U1856	A1622	G1561	C1429	C1251
U2907	U2809	U2699	U2490	U2465	U2359	A	U2073	U1972	U1857	A1623	G1562	U1429	A1252
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G2936	U2838	U2728	U2519	U2494	U2388	C	U2102	U2001	U1886	A1652	G1591	U1452	A1281
G2937	U2839	U2729	U2520	U2495	U2389	C	U2103	U2002	U1887	A1653	G1592	U1453	A1282
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G2942	U2844	U2734	U2525	U2500	U2394	C	U2108	U2007	U1892	A1658	G1597	U1458	A1287
G2943	U2845	U2735	U2526	U2501	U2395	C	U2109	U2008	U1893	A1659	G1598	U1459	A1288
G2944	U2846	U2736	U2527	U2502	U2396	C	U2110	U2009	U1894	A1660	G1599	U1460	A1289
G2945	U2847	U2737	U2528	U2503	U2397	C	U2111	U2010	U1895	A1661	G1600	U1461	A1290
G2946	U2848	U2738	U2529	U2504	U2398	C	U2112	U2011	U1896	A1662	G1601	U1462	A1291
G2947	U2849	U2739	U2530	U2505	U2399	C	U2113	U2012	U1897	A1663	G1602	U1463	A1292
G2948	U2850	U2740	U2531	U2506	U2400	C	U2114	U2013	U1898	A1664	G1603	U1464	A1293
G2949	U2851	U2741	U2532	U2507	U2401	C	U2115	U2014	U1899	A1665	G1604	U1465	A1294
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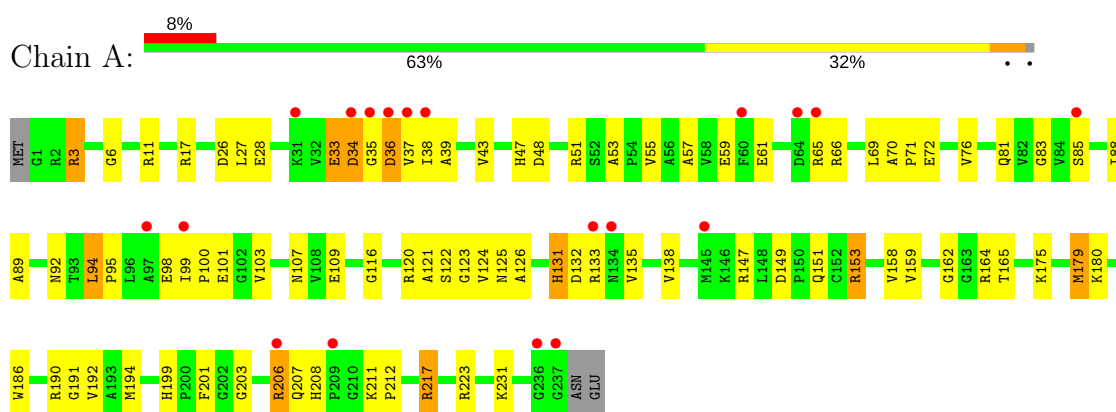
- Molecule 2: 5S ribosomal RNA



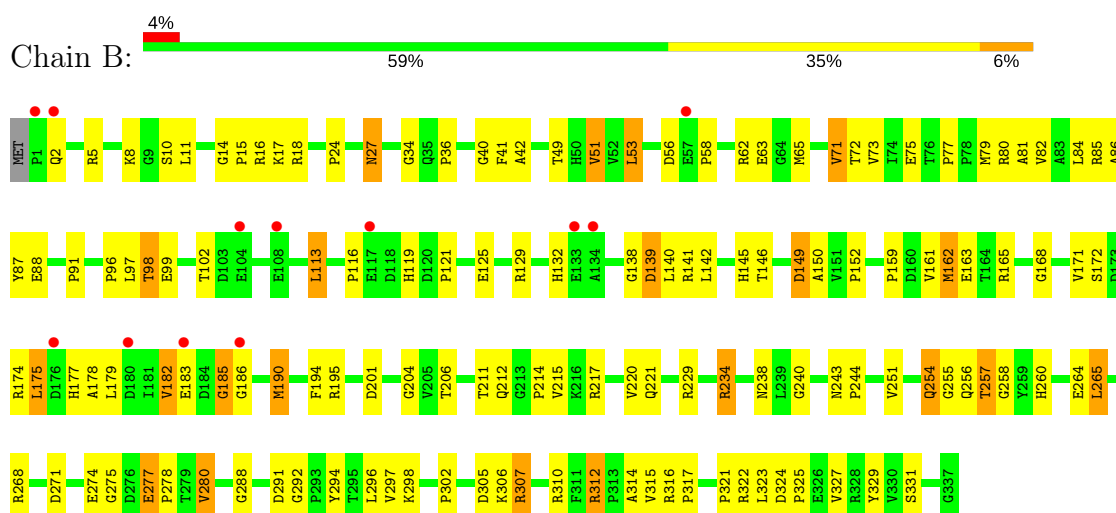
- Molecule 3: 5'-R(\*CP\*CP\*(DA)\*(PHE)\*(ACA))-3'



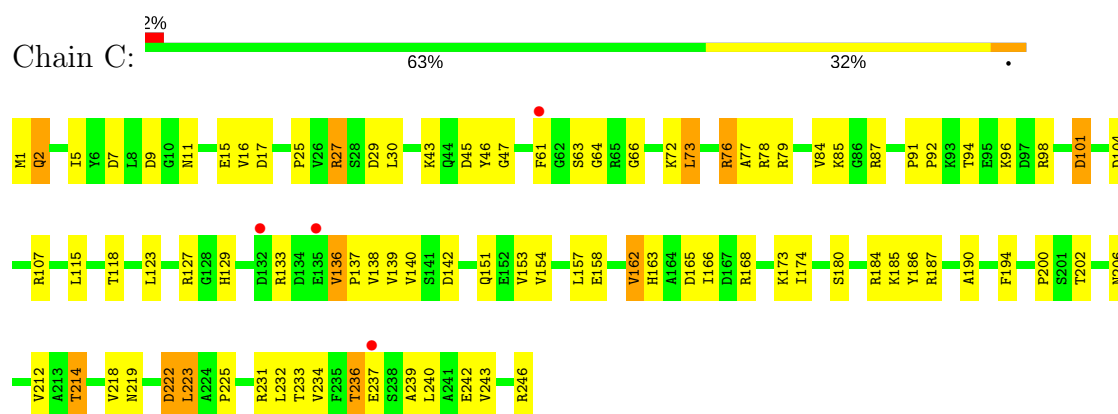
- Molecule 4: 50S ribosomal protein L2P



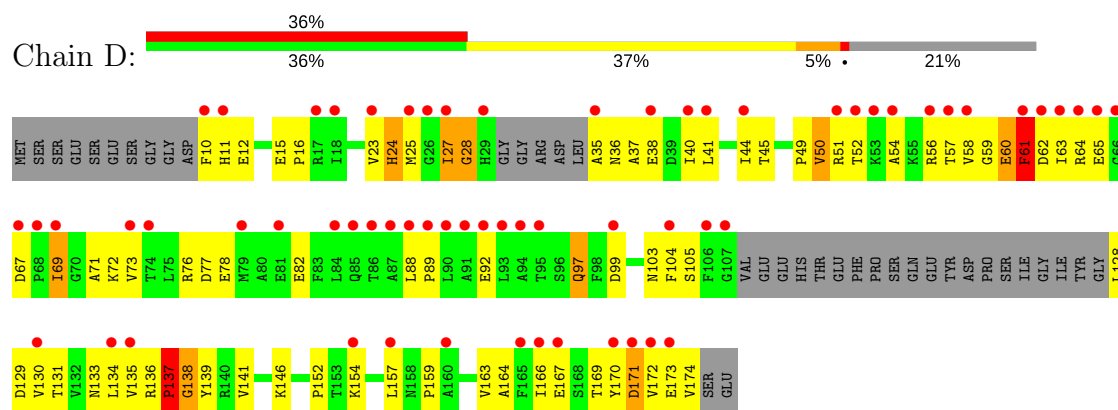
- Molecule 5: 50S ribosomal protein L3P



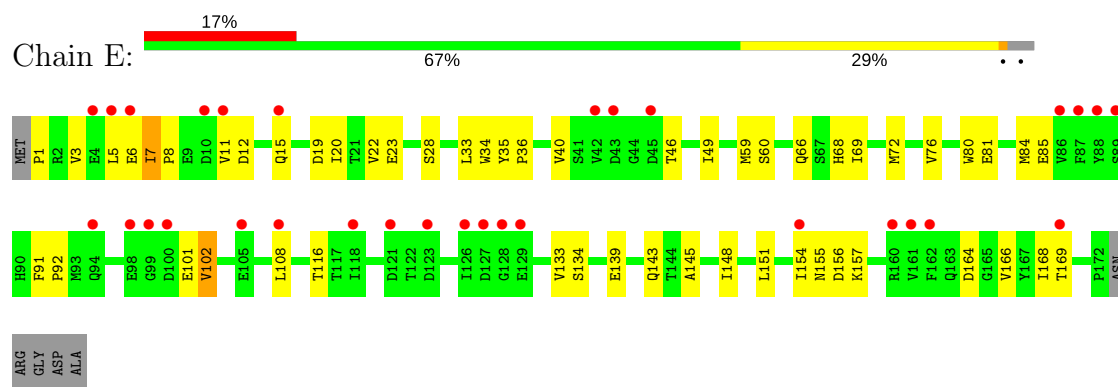
- Molecule 6: 50S ribosomal protein L4E



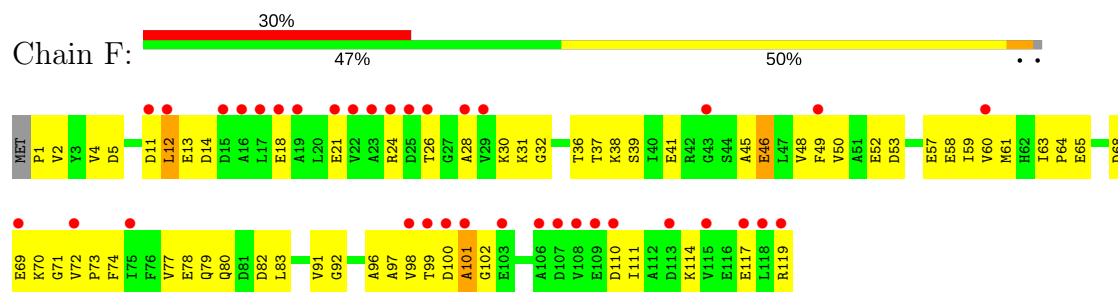
• Molecule 7: 50S ribosomal protein L5P



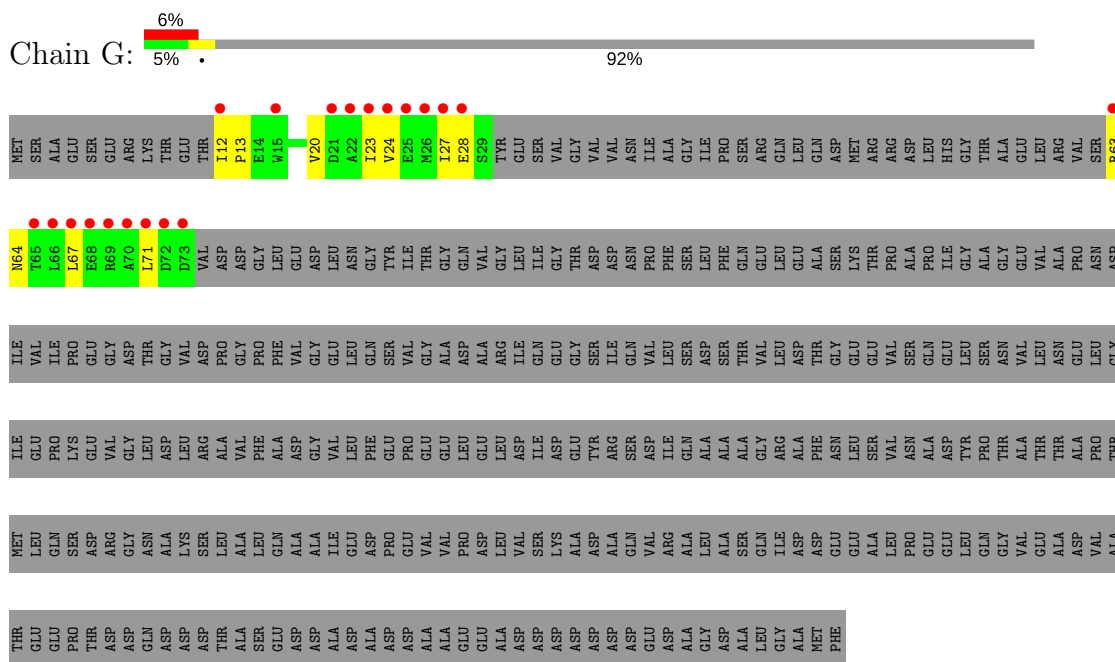
• Molecule 8: 50S ribosomal protein L6P



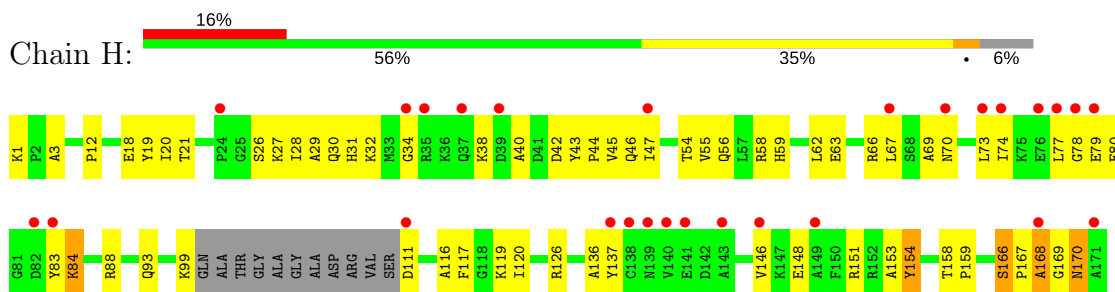
• Molecule 9: 50S ribosomal protein L7AE



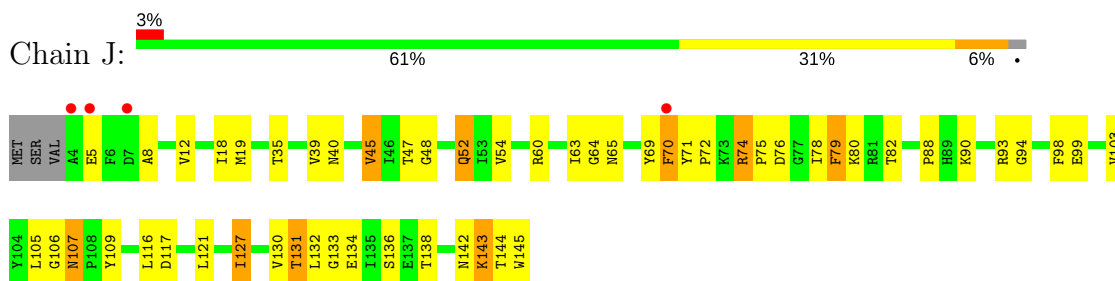
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



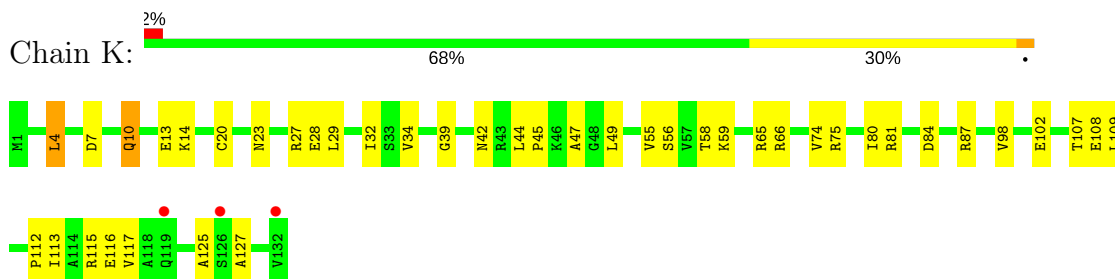
- Molecule 11: 50S RIBOSOMAL PROTEIN L10E



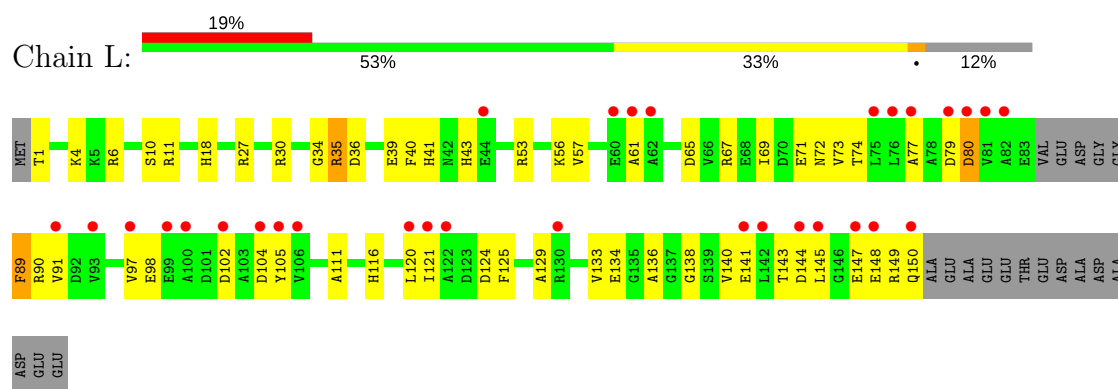
- Molecule 12: 50S ribosomal protein L13P



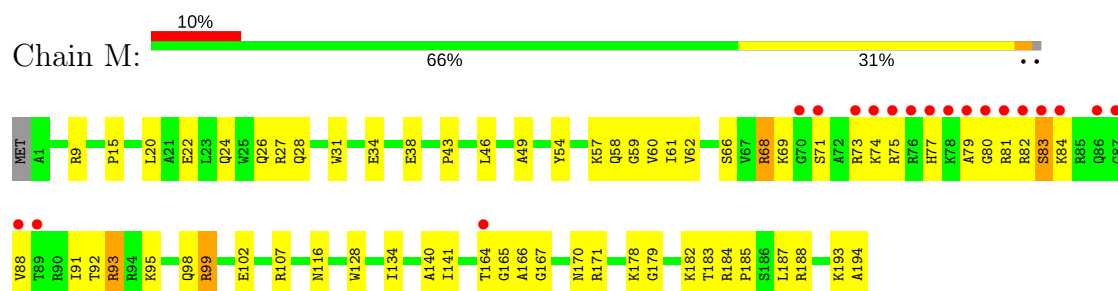
- Molecule 13: 50S ribosomal protein L14P



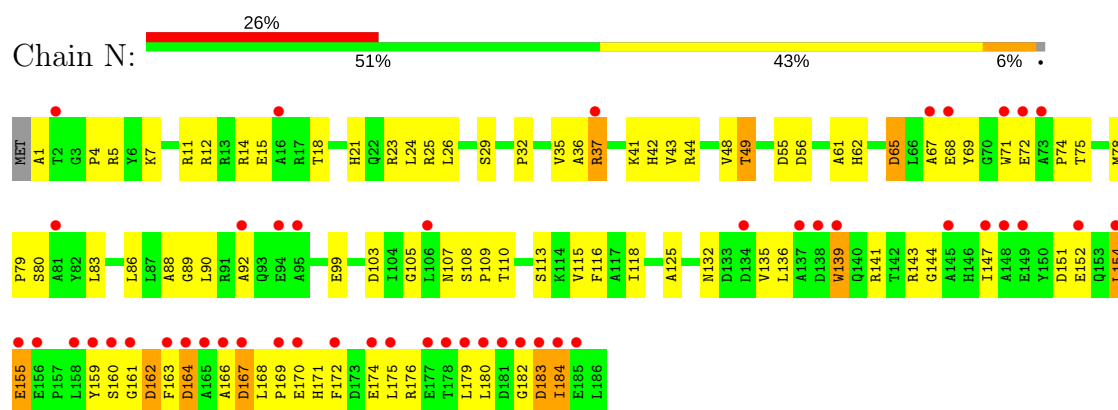
- Molecule 14: 50S ribosomal protein L15P



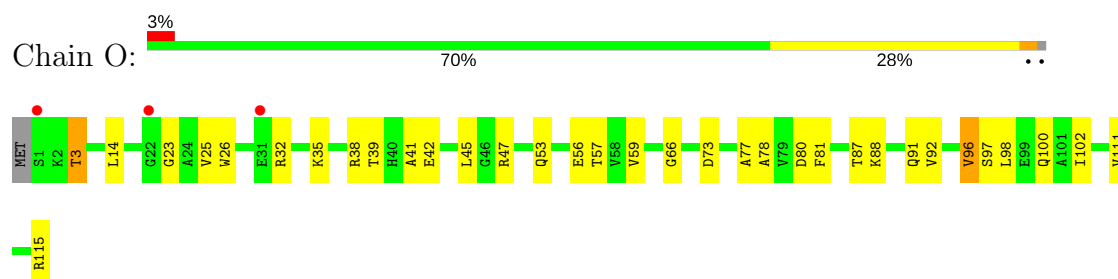
• Molecule 15: 50S Ribosomal Protein L15E



• Molecule 16: 50S ribosomal protein L18P

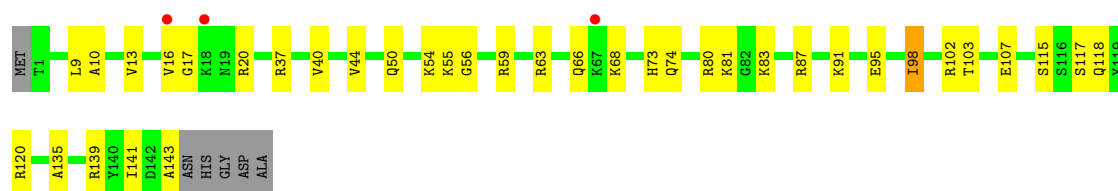


• Molecule 17: 50S ribosomal protein L18e

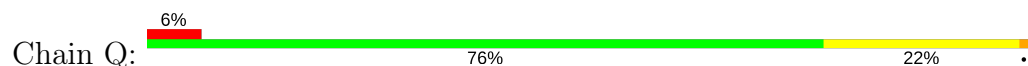


• Molecule 18: 50S ribosomal protein L19E





- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P



- Molecule 22: 50S ribosomal protein L24P

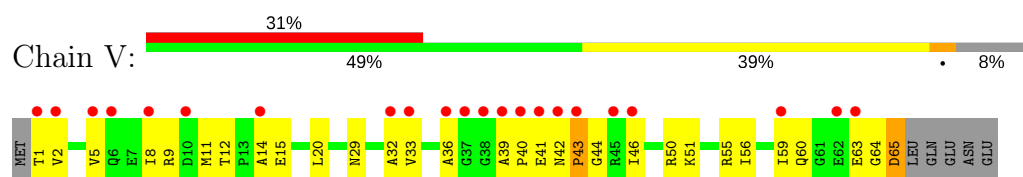


- Molecule 23: 50S ribosomal protein L24E

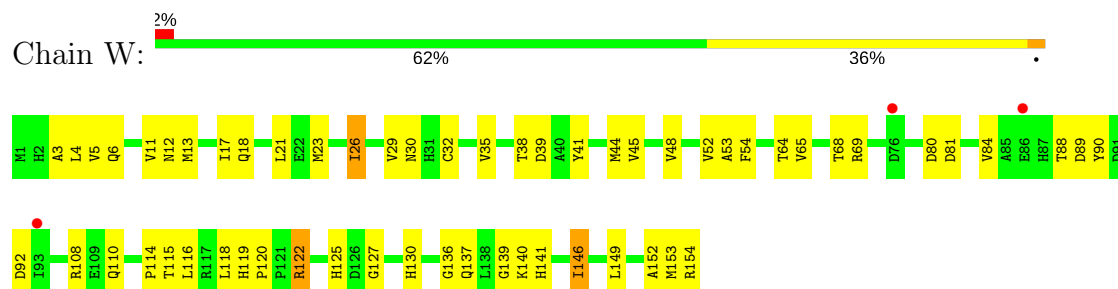


- Molecule 24: 50S ribosomal protein L29P

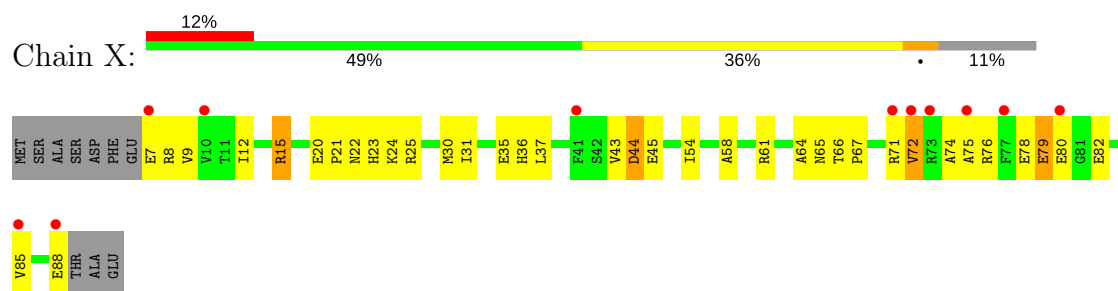




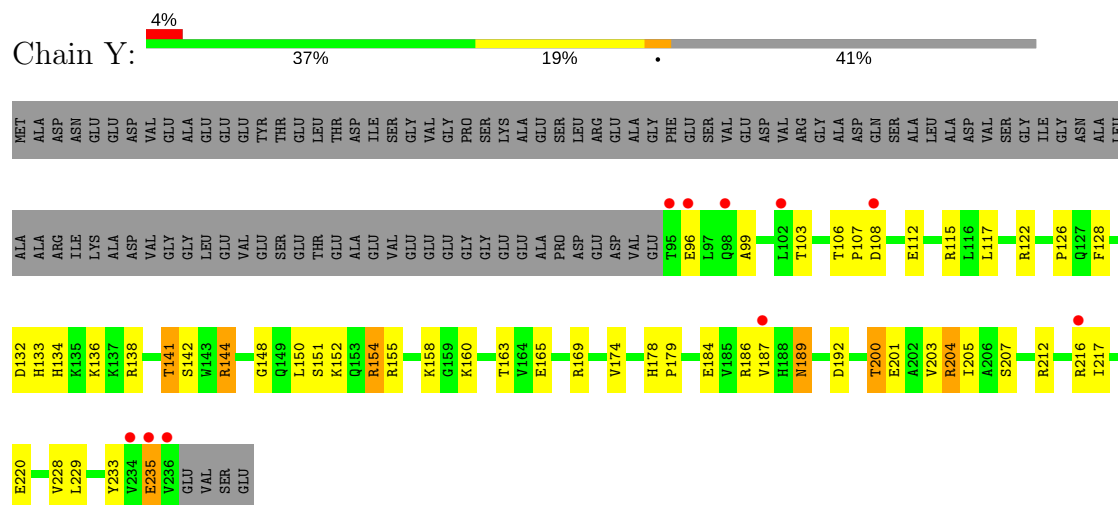
- Molecule 25: 50S ribosomal protein L30P



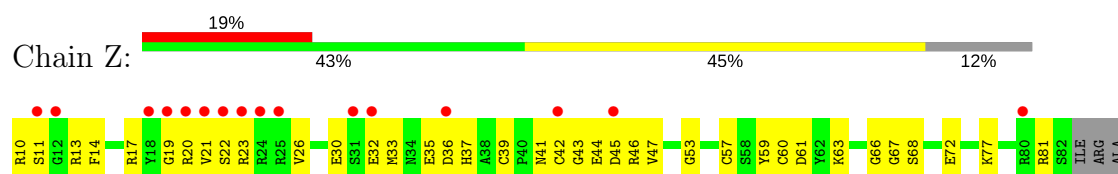
- Molecule 26: 50S ribosomal protein L31e



- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae

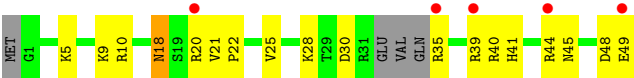


ALA  
LEU  
SER  
GLU  
ASP  
GLU  
GLU

• Molecule 29: 50S ribosomal protein L37e



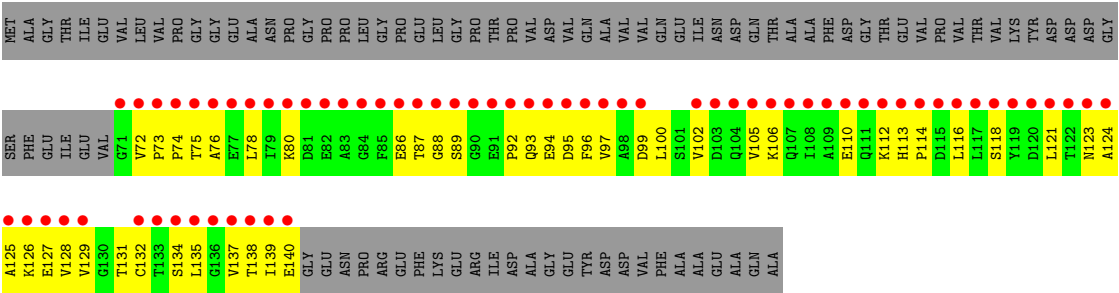
• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.87Å 298.57Å 575.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.30) 89.6 (49.73-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.69 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.250 0.205 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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, SR, NA, K, ACA, 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	0.37	0/65959	0.70	26/102870 (0.0%)
2	9	0.33	0/2905	0.71	1/4528 (0.0%)
3	4	0.52	0/75	0.73	0/110
4	A	0.34	0/1786	0.66	0/2408
5	B	0.33	0/2690	0.66	0/3652
6	C	0.38	0/1884	0.64	1/2551 (0.0%)
7	D	0.29	0/1111	0.54	0/1498
8	E	0.32	0/1382	0.57	0/1880
9	F	0.31	0/901	0.54	0/1224
10	G	0.27	0/241	0.47	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.35	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.34	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.60	0/1999
17	O	0.33	0/874	0.59	1/1181 (0.1%)
18	P	0.34	0/1147	0.56	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.35	0/1172	0.67	0/1578
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.31	0/958	0.63	0/1289
23	U	0.35	0/417	0.58	0/562
24	V	0.27	0/502	0.53	0/675
25	W	0.34	0/1219	0.60	0/1655
26	X	0.33	0/664	0.60	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.34	0/589	0.61	0/787
29	1	0.43	0/438	0.66	0/578
30	2	0.35	0/401	0.60	0/529
31	3	0.38	0/771	0.58	0/1024
32	I	0.28	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.36	0/98767	0.67	30/147687 (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	1	39
2	9	0	2
All	All	1	41

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.69	130.83	109.50
2	9	3039	U	N1-C1'-C2'	7.45	123.68	114.00
1	0	1942	A	C5'-C4'-C3'	7.27	127.63	116.00
1	0	1819	G	C5'-C4'-C3'	6.86	126.98	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	24	G	Sidechain
1	0	396	U	Sidechain
1	0	462	A	Sidechain
1	0	469	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	59021	0	29813	722	0
2	9	2600	0	1326	50	0
3	4	73	0	44	2	0
4	A	1753	0	1766	101	0
5	B	2625	0	2532	145	0
6	C	1859	0	1816	106	0
7	D	1094	0	1085	79	0
8	E	1357	0	1266	45	0
9	F	890	0	843	57	0
10	G	240	0	231	11	0
11	H	1266	0	1268	68	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	53	0
14	L	1118	0	1076	61	0
15	M	1560	0	1568	63	0
16	N	1445	0	1401	97	0
17	O	865	0	873	40	0
18	P	1136	0	1123	35	0
19	Q	735	0	729	18	0
20	R	1149	0	1122	37	0
21	S	641	0	605	16	0
22	T	950	0	923	47	0
23	U	410	0	364	26	0
24	V	499	0	511	38	0
25	W	1196	0	1137	82	0
26	X	654	0	653	35	0
27	Y	1130	0	1133	57	0
28	Z	578	0	539	28	0
29	1	431	0	426	22	0
30	2	396	0	413	26	0
31	3	755	0	728	26	0
32	I	519	0	500	51	0
33	0	87	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	64	0	0	0	0
35	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	9	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5769	0	0	106	0
39	1	50	0	0	2	0
39	2	40	0	0	3	0
39	3	67	0	0	4	0
39	9	140	0	0	6	0
39	A	121	0	0	11	0
39	B	144	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	C	177	0	0	18	0
39	D	48	0	0	10	0
39	E	44	0	0	1	0
39	F	27	0	0	4	0
39	G	17	0	0	1	0
39	H	69	0	0	7	0
39	I	7	0	0	1	0
39	J	52	0	0	4	0
39	K	57	0	0	6	0
39	L	81	0	0	14	0
39	M	130	0	0	3	0
39	N	61	0	0	9	0
39	O	40	0	0	5	0
39	P	64	0	0	2	0
39	Q	49	0	0	5	0
39	R	82	0	0	3	0
39	S	32	0	0	1	0
39	T	37	0	0	3	0
39	U	29	0	0	3	0
39	V	14	0	0	2	0
39	W	69	0	0	5	0
39	X	24	0	0	6	0
39	Y	96	0	0	9	0
39	Z	31	0	0	2	0
All	All	99036	0	59943	2083	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 14.

The worst 5 of 2083 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)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.29	1.14
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.29	1.10
6:C:236:THR:HG22	6:C:239:ALA:H	1.19	1.07
1:O:656:G:H5'	17:O:3:THR:HG22	1.38	1.05
1:O:1160:G:H5'	1:O:1161:A:H5'	1.40	1.04

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	209 (89%)	23 (10%)	3 (1%)	13	13
5	B	335/338 (99%)	314 (94%)	17 (5%)	4 (1%)	14	15
6	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
7	D	134/177 (76%)	105 (78%)	17 (13%)	12 (9%)	1	0
8	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
9	F	117/120 (98%)	100 (86%)	15 (13%)	2 (2%)	10	9
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	140 (90%)	14 (9%)	2 (1%)	13	13
12	J	140/145 (97%)	131 (94%)	6 (4%)	3 (2%)	8	6
13	K	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
14	L	141/165 (86%)	118 (84%)	22 (16%)	1 (1%)	24	29
15	M	192/195 (98%)	182 (95%)	8 (4%)	2 (1%)	17	19
16	N	184/187 (98%)	163 (89%)	12 (6%)	9 (5%)	2	1
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
18	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
21	S	79/85 (93%)	76 (96%)	2 (2%)	1 (1%)	13	13
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	19	22
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	11	10
25	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	61 (86%)	7 (10%)	3 (4%)	3	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	1 (1%)	1 (1%)	16	17
32	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	11	11
All	All	3705/4431 (84%)	3430 (93%)	229 (6%)	46 (1%)	14	15

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	27	LEU
4	A	37	VAL
5	B	139	ASP
7	D	137	PRO
9	F	101	ALA

### 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	
4	A	179/182 (98%)	169 (94%)	10 (6%)	23	32
5	B	282/283 (100%)	261 (93%)	21 (7%)	15	19
6	C	193/193 (100%)	178 (92%)	15 (8%)	14	17
7	D	117/148 (79%)	112 (96%)	5 (4%)	32	43
8	E	152/156 (97%)	145 (95%)	7 (5%)	29	41
9	F	93/94 (99%)	91 (98%)	2 (2%)	55	72
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	30	42
12	J	118/121 (98%)	109 (92%)	9 (8%)	14	18
13	K	106/106 (100%)	103 (97%)	3 (3%)	47	63
14	L	113/127 (89%)	109 (96%)	4 (4%)	39	53
15	M	158/159 (99%)	153 (97%)	5 (3%)	42	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	149/150 (99%)	144 (97%)	5 (3%)	40	55
17	O	93/94 (99%)	91 (98%)	2 (2%)	55	72
18	P	113/117 (97%)	112 (99%)	1 (1%)	81	90
19	Q	79/80 (99%)	75 (95%)	4 (5%)	26	36
20	R	117/122 (96%)	114 (97%)	3 (3%)	49	66
21	S	71/74 (96%)	69 (97%)	2 (3%)	47	63
22	T	105/106 (99%)	101 (96%)	4 (4%)	36	50
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	58	75
25	W	130/130 (100%)	126 (97%)	4 (3%)	43	59
26	X	66/74 (89%)	60 (91%)	6 (9%)	10	12
27	Y	120/196 (61%)	110 (92%)	10 (8%)	12	15
28	Z	60/68 (88%)	59 (98%)	1 (2%)	63	79
29	1	46/47 (98%)	45 (98%)	1 (2%)	55	72
30	2	42/46 (91%)	41 (98%)	1 (2%)	52	69
31	3	79/79 (100%)	78 (99%)	1 (1%)	71	84
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2960 (96%)	133 (4%)	32	43

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	H	1	LYS
12	J	131	THR
27	Y	154	ARG
11	H	18	GLU
12	J	52	GLN

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	170	ASN
18	P	89	ASN
30	2	41	HIS
16	N	93	GLN

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Mol	Chain	Res	Type
17	O	100	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	238 (8%)	33 (1%)
2	9	121/122 (99%)	16 (13%)	2 (1%)
3	4	1/5 (20%)	0	0
All	All	2867/3049 (94%)	254 (8%)	35 (1%)

5 of 254 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 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1506	U
1	0	1692	C
1	0	2852	A
1	0	1563	G
1	0	1684	A

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

6 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	0.96	1 (7%)	18,31,34	3.70	2 (11%)
1	OMG	0	2588	1,3	19,26,27	1.05	2 (10%)	22,38,41	2.47	4 (18%)
1	UR3	0	2619	1	13,22,23	0.83	1 (7%)	15,32,35	0.66	0
1	PSU	0	2621	1	16,21,22	1.68	3 (18%)	20,30,33	5.36	4 (20%)
1	1MA	0	628	1,35	16,25,26	0.99	1 (6%)	12,37,40	1.22	1 (8%)
3	ACA	4	78	3	3,3,8	0.59	0	2,2,8	0.77	0

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	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3
3	ACA	4	78	3	-	0/0/1/6	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.99	1.47	1.52
1	0	2619	UR3	C6-C5	-2.11	1.33	1.38
1	0	2588	OMG	C8-N7	-2.05	1.30	1.34
1	0	2587	OMU	C4-N3	2.55	1.37	1.33
1	0	2621	PSU	C2-N1	2.74	1.43	1.38

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	-16.93	114.80	128.41
1	0	2588	OMG	C5-C6-N1	-8.39	111.54	123.47
1	0	2621	PSU	C5-C4-N3	-8.31	114.65	125.36
1	0	628	1MA	C2-N3-C4	-3.72	110.83	116.51
1	0	2587	OMU	C5-C4-N3	-3.67	114.66	123.17

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 311 ligands modelled in this entry, 311 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	-0.06	95 (3%) 44 51	22, 45, 89, 149	0
2	9	122/122 (100%)	0.18	6 (4%) 29 37	38, 63, 87, 149	0
3	4	4/5 (80%)	1.57	1 (25%) 0 0	61, 64, 71, 74	0
4	A	237/240 (98%)	0.57	19 (8%) 12 16	28, 50, 82, 104	0
5	B	337/338 (99%)	0.29	12 (3%) 42 49	28, 50, 75, 86	0
6	C	246/246 (100%)	0.12	4 (1%) 72 77	25, 46, 68, 80	0
7	D	140/177 (79%)	2.16	63 (45%) 0 0	58, 88, 120, 130	0
8	E	172/178 (96%)	0.93	31 (18%) 1 1	40, 62, 80, 86	0
9	F	119/120 (99%)	1.37	36 (30%) 0 0	44, 71, 100, 110	0
10	G	29/348 (8%)	2.90	20 (68%) 0 0	71, 89, 99, 100	0
11	H	160/171 (93%)	0.85	27 (16%) 1 2	43, 61, 93, 101	0
12	J	142/145 (97%)	0.12	4 (2%) 53 60	36, 47, 67, 89	0
13	K	132/132 (100%)	0.01	3 (2%) 60 67	33, 46, 67, 72	0
14	L	145/165 (87%)	0.95	31 (21%) 1 1	27, 64, 110, 120	0
15	M	194/195 (99%)	0.63	19 (9%) 7 10	31, 44, 77, 87	0
16	N	186/187 (99%)	1.20	48 (25%) 0 0	43, 63, 108, 113	0
17	O	115/116 (99%)	0.17	3 (2%) 56 63	39, 53, 67, 75	0
18	P	143/149 (95%)	0.22	3 (2%) 63 70	38, 51, 65, 76	0
19	Q	95/96 (98%)	0.26	6 (6%) 20 26	38, 47, 61, 76	0
20	R	150/155 (96%)	0.03	3 (2%) 65 71	29, 43, 61, 71	0
21	S	81/85 (95%)	0.49	7 (8%) 10 14	42, 58, 80, 95	0
22	T	119/120 (99%)	0.71	10 (8%) 11 15	40, 54, 81, 110	0
23	U	53/66 (80%)	0.31	2 (3%) 40 47	40, 50, 68, 79	0
24	V	65/71 (91%)	1.96	22 (33%) 0 0	52, 76, 110, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.17	3 (1%) 66 73	37, 49, 69, 78	0
26	X	82/92 (89%)	0.89	11 (13%) 3 4	40, 53, 82, 101	0
27	Y	142/241 (58%)	0.30	10 (7%) 16 22	29, 42, 63, 85	0
28	Z	73/83 (87%)	0.93	16 (21%) 0 1	48, 70, 85, 92	0
29	1	56/57 (98%)	-0.30	0 100 100	26, 32, 39, 49	0
30	2	46/50 (92%)	0.63	5 (10%) 5 8	33, 51, 67, 80	0
31	3	92/92 (100%)	0.37	4 (4%) 35 42	33, 55, 70, 83	0
32	I	70/162 (43%)	6.28	66 (94%) 0 0	111, 123, 141, 143	0
All	All	6650/7480 (88%)	0.38	590 (8%) 9 13	22, 50, 95, 149	0

The worst 5 of 590 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	17.6
7	D	63	ILE	15.2
24	V	1	THR	14.6
32	I	133	THR	13.9
32	I	79	ILE	12.9

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACA	4	78	4/9	0.59	0.43	70,71,72,72	0
1	OMG	0	2588	24/25	0.97	0.12	32,34,38,40	0
1	1MA	0	628	23/24	0.98	0.14	31,33,36,39	0
1	UR3	0	2619	21/22	0.98	0.14	42,46,49,51	0
1	PSU	0	2621	20/21	0.98	0.12	33,36,44,45	0
1	OMU	0	2587	21/22	0.98	0.12	35,37,38,39	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	0	9129	1/1	-0.06	0.43	88,88,88,88	0
37	SR	0	9601	1/1	0.06	1.47	200,200,200,200	0
37	SR	0	9500	1/1	0.17	1.74	200,200,200,200	0
37	SR	B	9521	1/1	0.21	0.71	200,200,200,200	0
37	SR	0	9484	1/1	0.28	0.16	150,150,150,150	0
35	NA	0	9122	1/1	0.34	0.44	98,98,98,98	0
33	MG	0	8108	1/1	0.40	0.28	115,115,115,115	0
35	NA	S	9112	1/1	0.46	0.16	74,74,74,74	0
37	SR	0	9501	1/1	0.49	0.34	200,200,200,200	0
35	NA	0	9171	1/1	0.52	0.25	63,63,63,63	0
33	MG	0	8094	1/1	0.54	0.39	82,82,82,82	0
35	NA	0	9184	1/1	0.55	0.31	86,86,86,86	0
33	MG	0	8092	1/1	0.56	1.61	83,83,83,83	0
37	SR	0	9537	1/1	0.59	0.17	152,152,152,152	0
33	MG	0	8052	1/1	0.62	0.31	72,72,72,72	0
35	NA	0	9164	1/1	0.63	0.57	67,67,67,67	0
33	MG	0	8061	1/1	0.63	0.13	81,81,81,81	0
33	MG	0	8047	1/1	0.66	0.52	94,94,94,94	0
33	MG	0	8082	1/1	0.68	0.48	103,103,103,103	0
37	SR	0	9468	1/1	0.69	0.05	115,115,115,115	0
33	MG	0	8050	1/1	0.71	0.25	94,94,94,94	0
37	SR	0	9547	1/1	0.71	0.52	200,200,200,200	0
37	SR	0	9590	1/1	0.72	0.09	142,142,142,142	0
37	SR	0	9581	1/1	0.73	0.07	134,134,134,134	0
33	MG	0	8022	1/1	0.73	0.54	113,113,113,113	0
35	NA	0	9111	1/1	0.77	0.21	57,57,57,57	0
33	MG	0	8014	1/1	0.77	0.30	78,78,78,78	0
33	MG	0	8059	1/1	0.78	0.28	60,60,60,60	0
33	MG	0	8114	1/1	0.79	0.17	83,83,83,83	0
33	MG	0	8104	1/1	0.80	0.33	83,83,83,83	0
33	MG	0	8054	1/1	0.80	0.13	58,58,58,58	0
35	NA	0	9185	1/1	0.81	0.56	54,54,54,54	0
35	NA	0	9113	1/1	0.81	0.14	64,64,64,64	0
33	MG	0	8101	1/1	0.81	0.11	51,51,51,51	0
37	SR	0	9539	1/1	0.81	0.38	167,167,167,167	0
35	NA	0	9172	1/1	0.81	0.41	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9182	1/1	0.82	0.13	84,84,84,84	0
35	NA	0	9181	1/1	0.82	0.12	48,48,48,48	0
35	NA	9	9183	1/1	0.82	0.23	72,72,72,72	0
33	MG	0	8107	1/1	0.82	0.22	68,68,68,68	0
35	NA	0	9126	1/1	0.83	0.14	55,55,55,55	0
35	NA	J	9146	1/1	0.83	0.13	62,62,62,62	0
35	NA	0	9163	1/1	0.83	0.32	77,77,77,77	0
33	MG	B	8055	1/1	0.84	0.27	104,104,104,104	0
35	NA	0	9152	1/1	0.84	0.38	67,67,67,67	0
35	NA	0	9174	1/1	0.84	0.24	67,67,67,67	0
35	NA	0	9168	1/1	0.84	0.28	72,72,72,72	0
35	NA	0	9110	1/1	0.85	0.20	49,49,49,49	0
35	NA	0	9132	1/1	0.85	0.38	61,61,61,61	0
33	MG	0	8013	1/1	0.85	0.38	16,16,16,16	0
35	NA	0	9141	1/1	0.86	0.12	61,61,61,61	0
35	NA	0	9140	1/1	0.86	0.34	61,61,61,61	0
37	SR	9	9588	1/1	0.86	0.14	122,122,122,122	0
33	MG	0	8103	1/1	0.87	0.31	79,79,79,79	0
33	MG	0	8065	1/1	0.87	0.33	92,92,92,92	0
35	NA	0	9150	1/1	0.87	0.33	54,54,54,54	0
33	MG	0	8090	1/1	0.87	0.27	81,81,81,81	0
33	MG	9	8095	1/1	0.87	0.24	44,44,44,44	0
33	MG	0	8021	1/1	0.87	0.24	51,51,51,51	0
34	K	0	9001	1/1	0.87	0.48	95,95,95,95	0
33	MG	0	8040	1/1	0.88	0.34	94,94,94,94	0
33	MG	0	8024	1/1	0.88	0.93	90,90,90,90	0
33	MG	0	8057	1/1	0.88	0.39	79,79,79,79	0
37	SR	0	9452	1/1	0.89	0.20	114,114,114,114	0
33	MG	0	8032	1/1	0.89	0.11	36,36,36,36	0
33	MG	0	8042	1/1	0.90	0.06	53,53,53,53	0
35	NA	0	9125	1/1	0.90	1.07	106,106,106,106	0
35	NA	0	9170	1/1	0.90	0.33	75,75,75,75	0
35	NA	0	9173	1/1	0.90	0.39	66,66,66,66	0
37	SR	0	9529	1/1	0.90	0.09	116,116,116,116	0
33	MG	0	8091	1/1	0.90	0.07	56,56,56,56	0
33	MG	0	8025	1/1	0.90	0.34	23,23,23,23	0
34	K	0	9002	1/1	0.91	0.19	86,86,86,86	0
35	NA	D	9151	1/1	0.91	0.12	63,63,63,63	0
35	NA	0	9179	1/1	0.91	0.81	84,84,84,84	0
37	SR	0	9504	1/1	0.91	0.11	92,92,92,92	0
35	NA	0	9166	1/1	0.91	0.11	65,65,65,65	0
35	NA	0	9178	1/1	0.91	0.17	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9124	1/1	0.91	0.15	51,51,51,51	0
33	MG	0	8102	1/1	0.91	0.15	70,70,70,70	0
33	MG	0	8098	1/1	0.92	0.08	43,43,43,43	0
35	NA	R	9186	1/1	0.92	0.16	64,64,64,64	0
33	MG	0	8080	1/1	0.92	0.24	48,48,48,48	0
33	MG	0	8083	1/1	0.92	0.07	51,51,51,51	0
35	NA	0	9154	1/1	0.92	0.20	51,51,51,51	0
36	CL	B	9319	1/1	0.92	0.15	59,59,59,59	0
33	MG	0	8058	1/1	0.92	0.47	85,85,85,85	0
33	MG	0	8085	1/1	0.92	0.41	102,102,102,102	0
33	MG	0	8084	1/1	0.92	0.53	109,109,109,109	0
35	NA	0	9135	1/1	0.92	0.14	46,46,46,46	0
33	MG	0	8113	1/1	0.92	0.08	45,45,45,45	0
36	CL	J	9302	1/1	0.92	0.11	55,55,55,55	0
36	CL	0	9316	1/1	0.93	0.17	74,74,74,74	0
35	NA	0	9107	1/1	0.93	0.24	58,58,58,58	0
35	NA	3	9169	1/1	0.93	0.41	102,102,102,102	0
35	NA	0	9159	1/1	0.93	0.17	56,56,56,56	0
37	SR	0	9505	1/1	0.93	0.13	104,104,104,104	0
35	NA	0	9101	1/1	0.93	0.15	43,43,43,43	0
37	SR	0	9522	1/1	0.93	0.06	104,104,104,104	0
33	MG	0	8030	1/1	0.93	0.04	34,34,34,34	0
35	NA	0	9175	1/1	0.93	0.19	52,52,52,52	0
35	NA	0	9157	1/1	0.93	0.16	41,41,41,41	0
33	MG	0	8088	1/1	0.93	0.06	43,43,43,43	0
36	CL	N	9307	1/1	0.93	0.12	54,54,54,54	0
33	MG	0	8075	1/1	0.93	0.06	37,37,37,37	0
33	MG	0	8099	1/1	0.93	0.17	77,77,77,77	0
35	NA	0	9177	1/1	0.93	0.40	70,70,70,70	0
33	MG	0	8045	1/1	0.94	0.21	75,75,75,75	0
35	NA	0	9165	1/1	0.94	0.22	41,41,41,41	0
33	MG	0	8115	1/1	0.94	0.14	53,53,53,53	0
36	CL	0	9322	1/1	0.94	0.10	54,54,54,54	0
37	SR	0	9489	1/1	0.94	0.09	87,87,87,87	0
33	MG	0	8097	1/1	0.94	0.20	55,55,55,55	0
33	MG	0	8089	1/1	0.94	0.12	61,61,61,61	0
33	MG	0	8043	1/1	0.94	0.08	47,47,47,47	0
35	NA	0	9118	1/1	0.94	0.22	41,41,41,41	0
33	MG	0	8027	1/1	0.94	0.19	30,30,30,30	0
35	NA	0	9158	1/1	0.94	0.10	62,62,62,62	0
33	MG	0	8041	1/1	0.94	0.12	47,47,47,47	0
35	NA	0	9127	1/1	0.94	0.20	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	T	8073	1/1	0.94	0.14	42,42,42,42	0
35	NA	0	9160	1/1	0.94	0.15	42,42,42,42	0
35	NA	0	9120	1/1	0.94	0.30	61,61,61,61	0
37	SR	0	9482	1/1	0.94	0.19	118,118,118,118	0
33	MG	0	8072	1/1	0.95	0.25	74,74,74,74	0
38	CD	O	9205	1/1	0.95	0.04	85,85,85,85	0
35	NA	0	9134	1/1	0.95	0.07	47,47,47,47	0
35	NA	0	9161	1/1	0.95	0.30	57,57,57,57	0
35	NA	R	9137	1/1	0.95	0.11	32,32,32,32	0
33	MG	0	8009	1/1	0.95	0.07	31,31,31,31	0
35	NA	0	9115	1/1	0.95	0.24	43,43,43,43	0
33	MG	0	8060	1/1	0.95	0.10	81,81,81,81	0
33	MG	0	8093	1/1	0.95	0.14	42,42,42,42	0
37	SR	0	9495	1/1	0.95	0.11	88,88,88,88	0
37	SR	0	9530	1/1	0.95	0.12	94,94,94,94	0
35	NA	0	9130	1/1	0.95	0.08	45,45,45,45	0
33	MG	0	8076	1/1	0.95	0.21	55,55,55,55	0
35	NA	0	9102	1/1	0.95	0.20	58,58,58,58	0
33	MG	0	8051	1/1	0.95	0.29	22,22,22,22	0
36	CL	3	9304	1/1	0.95	0.11	59,59,59,59	0
35	NA	0	9149	1/1	0.95	0.14	41,41,41,41	0
37	SR	0	9626	1/1	0.95	0.30	140,140,140,140	0
37	SR	0	9459	1/1	0.96	0.07	96,96,96,96	0
37	SR	0	9490	1/1	0.96	0.11	105,105,105,105	0
33	MG	0	8046	1/1	0.96	0.08	40,40,40,40	0
35	NA	0	9106	1/1	0.96	0.20	37,37,37,37	0
35	NA	0	9131	1/1	0.96	0.10	47,47,47,47	0
33	MG	0	8063	1/1	0.96	0.07	74,74,74,74	0
33	MG	0	8039	1/1	0.96	0.04	56,56,56,56	0
33	MG	A	8066	1/1	0.96	0.18	53,53,53,53	0
35	NA	0	9108	1/1	0.96	0.12	34,34,34,34	0
37	SR	0	9474	1/1	0.96	0.09	96,96,96,96	0
36	CL	0	9315	1/1	0.96	0.10	54,54,54,54	0
36	CL	J	9301	1/1	0.96	0.09	55,55,55,55	0
33	MG	0	8036	1/1	0.96	0.09	63,63,63,63	0
35	NA	0	9155	1/1	0.96	0.24	54,54,54,54	0
37	SR	0	9447	1/1	0.96	0.10	66,66,66,66	0
36	CL	L	9310	1/1	0.96	0.09	56,56,56,56	0
37	SR	0	9466	1/1	0.96	0.04	87,87,87,87	0
35	NA	0	9156	1/1	0.96	0.21	55,55,55,55	0
37	SR	0	9506	1/1	0.96	0.07	86,86,86,86	0
37	SR	0	9431	1/1	0.96	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9534	1/1	0.96	0.11	106,106,106,106	0
35	NA	0	9139	1/1	0.96	0.13	57,57,57,57	0
33	MG	0	8015	1/1	0.96	0.10	29,29,29,29	0
33	MG	0	8003	1/1	0.96	0.19	29,29,29,29	0
37	SR	9	9503	1/1	0.96	0.03	109,109,109,109	0
37	SR	H	9486	1/1	0.96	0.19	121,121,121,121	0
37	SR	0	9467	1/1	0.97	0.10	74,74,74,74	0
33	MG	0	8019	1/1	0.97	0.05	53,53,53,53	0
36	CL	Y	9320	1/1	0.97	0.10	42,42,42,42	0
37	SR	0	9570	1/1	0.97	0.07	96,96,96,96	0
37	SR	0	9421	1/1	0.97	0.10	65,65,65,65	0
37	SR	0	9405	1/1	0.97	0.14	54,54,54,54	0
37	SR	0	9475	1/1	0.97	0.14	77,77,77,77	0
37	SR	0	9585	1/1	0.97	0.08	86,86,86,86	0
36	CL	0	9311	1/1	0.97	0.10	56,56,56,56	0
37	SR	0	9629	1/1	0.97	0.10	69,69,69,69	0
35	NA	0	9167	1/1	0.97	0.07	50,50,50,50	0
37	SR	0	9454	1/1	0.97	0.09	73,73,73,73	0
35	NA	0	9116	1/1	0.97	0.26	45,45,45,45	0
35	NA	0	9143	1/1	0.97	0.07	38,38,38,38	0
37	SR	0	9509	1/1	0.97	0.12	83,83,83,83	0
37	SR	0	9560	1/1	0.97	0.08	97,97,97,97	0
35	NA	0	9114	1/1	0.97	0.19	51,51,51,51	0
35	NA	0	9136	1/1	0.97	0.11	31,31,31,31	0
37	SR	0	9433	1/1	0.97	0.11	73,73,73,73	0
37	SR	F	9595	1/1	0.97	0.14	95,95,95,95	0
33	MG	0	8116	1/1	0.97	0.04	51,51,51,51	0
33	MG	0	8020	1/1	0.97	0.18	30,30,30,30	0
37	SR	0	9477	1/1	0.97	0.10	82,82,82,82	0
37	SR	0	9446	1/1	0.97	0.10	80,80,80,80	0
35	NA	C	9104	1/1	0.97	0.17	27,27,27,27	0
37	SR	0	9465	1/1	0.97	0.08	96,96,96,96	0
33	MG	0	8079	1/1	0.97	0.14	30,30,30,30	0
33	MG	0	8096	1/1	0.97	0.13	44,44,44,44	0
37	SR	A	9437	1/1	0.97	0.13	64,64,64,64	0
37	SR	0	9517	1/1	0.97	0.06	96,96,96,96	0
36	CL	0	9314	1/1	0.97	0.05	47,47,47,47	0
33	MG	0	8001	1/1	0.97	0.22	17,17,17,17	0
37	SR	9	9481	1/1	0.98	0.06	83,83,83,83	0
33	MG	0	8110	1/1	0.98	0.13	46,46,46,46	0
33	MG	0	8031	1/1	0.98	0.13	48,48,48,48	0
37	SR	0	9442	1/1	0.98	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CL	J	9321	1/1	0.98	0.12	58,58,58,58	0
33	MG	0	8017	1/1	0.98	0.18	20,20,20,20	0
37	SR	0	9455	1/1	0.98	0.10	61,61,61,61	0
35	NA	0	9162	1/1	0.98	0.30	51,51,51,51	0
37	SR	0	9568	1/1	0.98	0.08	75,75,75,75	0
36	CL	0	9305	1/1	0.98	0.07	52,52,52,52	0
33	MG	0	8037	1/1	0.98	0.06	40,40,40,40	0
37	SR	0	9407	1/1	0.98	0.14	42,42,42,42	0
35	NA	0	9105	1/1	0.98	0.15	41,41,41,41	0
36	CL	O	9308	1/1	0.98	0.06	67,67,67,67	0
37	SR	0	9508	1/1	0.98	0.08	83,83,83,83	0
33	MG	0	8005	1/1	0.98	0.09	29,29,29,29	0
37	SR	B	9458	1/1	0.98	0.09	73,73,73,73	0
33	MG	0	8029	1/1	0.98	0.22	27,27,27,27	0
37	SR	0	9441	1/1	0.98	0.08	54,54,54,54	0
37	SR	0	9464	1/1	0.98	0.05	80,80,80,80	0
37	SR	0	9438	1/1	0.98	0.09	63,63,63,63	0
37	SR	0	9427	1/1	0.98	0.12	53,53,53,53	0
37	SR	0	9432	1/1	0.98	0.12	63,63,63,63	0
36	CL	0	9313	1/1	0.98	0.11	51,51,51,51	0
35	NA	Q	9148	1/1	0.98	0.13	50,50,50,50	0
33	MG	0	8002	1/1	0.98	0.13	22,22,22,22	0
37	SR	0	9478	1/1	0.98	0.07	70,70,70,70	0
37	SR	0	9426	1/1	0.98	0.08	66,66,66,66	0
37	SR	1	9460	1/1	0.98	0.12	49,49,49,49	0
37	SR	0	9483	1/1	0.98	0.08	67,67,67,67	0
37	SR	0	9566	1/1	0.98	0.07	75,75,75,75	0
33	MG	0	8028	1/1	0.98	0.10	34,34,34,34	0
37	SR	0	9448	1/1	0.98	0.07	62,62,62,62	0
37	SR	0	9453	1/1	0.98	0.09	68,68,68,68	0
33	MG	0	8117	1/1	0.98	0.11	39,39,39,39	0
33	MG	Y	8109	1/1	0.98	0.10	38,38,38,38	0
33	MG	0	8067	1/1	0.98	0.12	36,36,36,36	0
37	SR	0	9488	1/1	0.98	0.13	78,78,78,78	0
33	MG	0	8068	1/1	0.98	0.14	47,47,47,47	0
37	SR	A	9497	1/1	0.98	0.11	85,85,85,85	0
36	CL	0	9303	1/1	0.98	0.17	49,49,49,49	0
35	NA	M	9147	1/1	0.98	0.10	38,38,38,38	0
37	SR	0	9417	1/1	0.98	0.13	53,53,53,53	0
37	SR	0	9412	1/1	0.98	0.12	43,43,43,43	0
33	MG	0	8056	1/1	0.98	0.18	47,47,47,47	0
37	SR	0	9456	1/1	0.98	0.06	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9469	1/1	0.99	0.04	85,85,85,85	0
35	NA	0	9123	1/1	0.99	0.10	37,37,37,37	0
37	SR	0	9473	1/1	0.99	0.04	69,69,69,69	0
38	CD	Z	9203	1/1	0.99	0.07	75,75,75,75	0
33	MG	0	8004	1/1	0.99	0.12	27,27,27,27	0
37	SR	0	9450	1/1	0.99	0.08	64,64,64,64	0
36	CL	0	9317	1/1	0.99	0.08	49,49,49,49	0
35	NA	R	9138	1/1	0.99	0.08	52,52,52,52	0
37	SR	S	9470	1/1	0.99	0.14	95,95,95,95	0
33	MG	0	8074	1/1	0.99	0.21	20,20,20,20	0
37	SR	0	9425	1/1	0.99	0.09	71,71,71,71	0
37	SR	0	9445	1/1	0.99	0.10	62,62,62,62	0
37	SR	0	9422	1/1	0.99	0.12	53,53,53,53	0
37	SR	0	9461	1/1	0.99	0.04	73,73,73,73	0
37	SR	0	9451	1/1	0.99	0.09	63,63,63,63	0
33	MG	K	8069	1/1	0.99	0.21	23,23,23,23	0
36	CL	R	9306	1/1	0.99	0.17	46,46,46,46	0
38	CD	U	9201	1/1	0.99	0.09	56,56,56,56	0
33	MG	0	8106	1/1	0.99	0.03	37,37,37,37	0
37	SR	0	9498	1/1	0.99	0.06	63,63,63,63	0
37	SR	0	9449	1/1	0.99	0.09	59,59,59,59	0
37	SR	0	9423	1/1	0.99	0.11	51,51,51,51	0
37	SR	0	9457	1/1	0.99	0.10	47,47,47,47	0
37	SR	0	9435	1/1	0.99	0.07	68,68,68,68	0
37	SR	0	9424	1/1	0.99	0.15	43,43,43,43	0
33	MG	0	8112	1/1	0.99	0.04	44,44,44,44	0
37	SR	0	9440	1/1	0.99	0.04	63,63,63,63	0
35	NA	0	9128	1/1	0.99	0.13	40,40,40,40	0
33	MG	0	8026	1/1	0.99	0.18	26,26,26,26	0
37	SR	0	9414	1/1	0.99	0.13	53,53,53,53	0
35	NA	0	9117	1/1	0.99	0.16	32,32,32,32	0
37	SR	0	9532	1/1	0.99	0.05	100,100,100,100	0
37	SR	0	9408	1/1	0.99	0.15	38,38,38,38	0
36	CL	M	9318	1/1	0.99	0.16	37,37,37,37	0
37	SR	R	9418	1/1	0.99	0.15	53,53,53,53	0
33	MG	0	8070	1/1	0.99	0.18	21,21,21,21	0
37	SR	0	9429	1/1	0.99	0.11	63,63,63,63	0
38	CD	3	9204	1/1	0.99	0.06	58,58,58,58	0
37	SR	0	9413	1/1	0.99	0.12	44,44,44,44	0
37	SR	0	9515	1/1	0.99	0.19	100,100,100,100	0
37	SR	1	9419	1/1	0.99	0.12	38,38,38,38	0
36	CL	A	9309	1/1	0.99	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9545	1/1	0.99	0.05	67,67,67,67	0
37	SR	0	9480	1/1	0.99	0.06	86,86,86,86	0
33	MG	0	8038	1/1	0.99	0.26	13,13,13,13	0
37	SR	A	9436	1/1	0.99	0.06	57,57,57,57	0
37	SR	0	9434	1/1	0.99	0.15	58,58,58,58	0
37	SR	0	9420	1/1	0.99	0.15	60,60,60,60	0
37	SR	0	9462	1/1	0.99	0.13	66,66,66,66	0
37	SR	0	9443	1/1	0.99	0.10	59,59,59,59	0
33	MG	0	8044	1/1	0.99	0.06	42,42,42,42	0
37	SR	3	9439	1/1	0.99	0.06	63,63,63,63	0
37	SR	0	9411	1/1	0.99	0.16	42,42,42,42	0
33	MG	0	8008	1/1	0.99	0.22	14,14,14,14	0
33	MG	0	8012	1/1	0.99	0.26	37,37,37,37	0
37	SR	L	9409	1/1	1.00	0.12	36,36,36,36	0
37	SR	0	9430	1/1	1.00	0.14	41,41,41,41	0
36	CL	0	9312	1/1	1.00	0.08	45,45,45,45	0
37	SR	0	9428	1/1	1.00	0.07	43,43,43,43	0
37	SR	0	9406	1/1	1.00	0.17	33,33,33,33	0
37	SR	0	9415	1/1	1.00	0.11	50,50,50,50	0
37	SR	0	9416	1/1	1.00	0.09	45,45,45,45	0
38	CD	1	9202	1/1	1.00	0.04	51,51,51,51	0
37	SR	0	9410	1/1	1.00	0.15	34,34,34,34	0
37	SR	0	9444	1/1	1.00	0.09	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.