



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:40 PM GMT

PDB ID : 1KQS
Title : The Haloarcula marismortui 50S Complexed with a Pretranslocational Intermediate in Protein Synthesis
Authors : Schmeing, T.M.; Seila, A.C.; Hansen, J.L.; Freeborn, B.; Soukup, J.K.; Scaringe, S.A.; Strobel, S.A.; Moore, P.B.; Steitz, T.A.
Deposited on : 2002-01-07
Resolution : 3.10 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

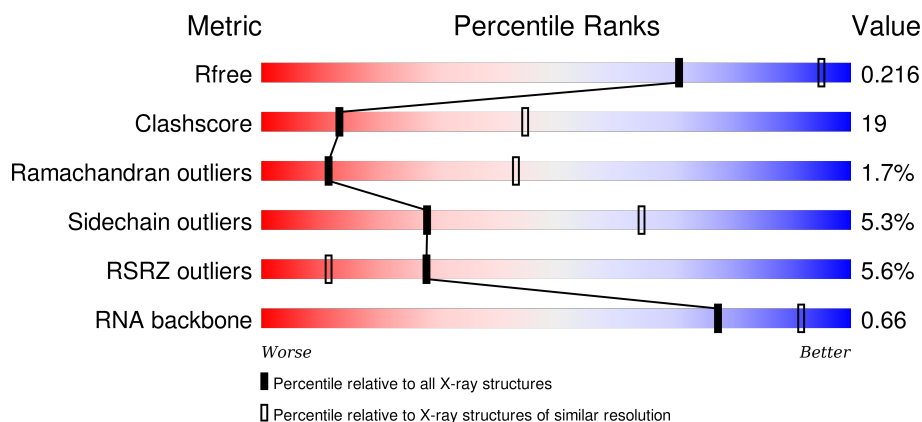
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



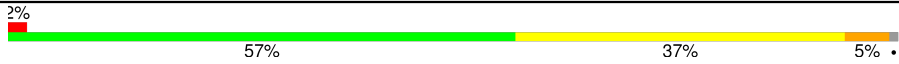


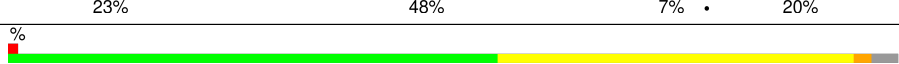

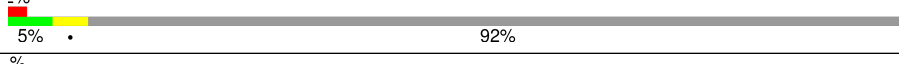
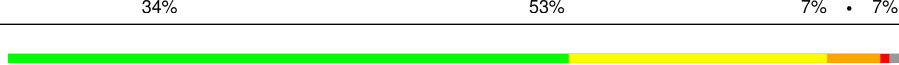


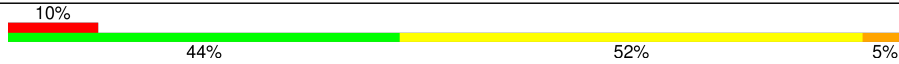
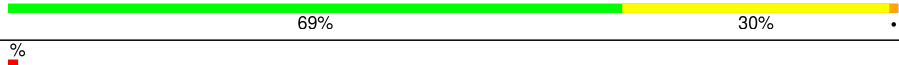
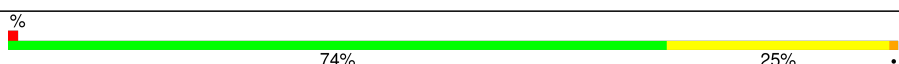

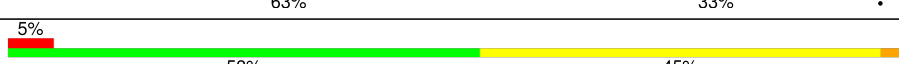
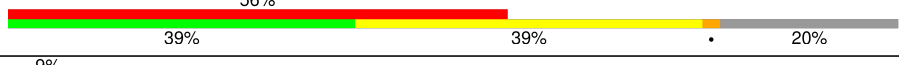


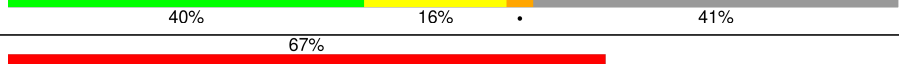



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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. 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>2%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>5% • 6%</div> </div> </div>
2	9	122	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>38%</div> <div>9% •</div> </div> </div>
3	3	3	<div> <div></div> <div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>
4	4	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
5	A	239	
6	B	337	
7	C	246	
8	D	176	
9	E	177	
10	F	119	
11	G	348	
12	H	167	
13	I	145	
14	J	132	
15	K	164	
16	L	194	
17	M	186	
18	N	115	
19	O	148	
20	P	95	
21	Q	154	
22	R	84	
23	S	119	
24	T	66	
25	U	70	
26	V	154	
27	W	91	
28	X	240	
29	Y	73	

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Mol	Chain	Length	Quality of chain
30	Z	56	
31	1	48	
32	2	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
33	MG	0	8053	-	-	-	X
33	MG	0	8064	-	-	-	X
33	MG	2	8078	-	-	-	X
33	MG	Y	8105	-	-	-	X
34	K	0	8201	-	-	-	X
34	K	0	8202	-	-	-	X
35	NA	0	8303	-	-	-	X
35	NA	0	8308	-	-	-	X
35	NA	0	8310	-	-	-	X
35	NA	0	8321	-	-	-	X
35	NA	0	8323	-	-	-	X
35	NA	0	8325	-	-	-	X
35	NA	0	8326	-	-	-	X
35	NA	0	8331	-	-	-	X
35	NA	0	8332	-	-	-	X
35	NA	0	8340	-	-	-	X
35	NA	0	8350	-	-	-	X
35	NA	0	8356	-	-	-	X
35	NA	0	8361	-	-	-	X
35	NA	0	8362	-	-	-	X
35	NA	0	8364	-	-	-	X
35	NA	0	8371	-	-	-	X
35	NA	0	8372	-	-	-	X
35	NA	0	8373	-	-	-	X
35	NA	0	8374	-	-	-	X
35	NA	0	8376	-	-	-	X
35	NA	0	8379	-	-	-	X
35	NA	0	8381	-	-	-	X
35	NA	0	8382	-	-	-	X
35	NA	9	8383	-	-	-	X
35	NA	Q	8386	-	-	-	X
36	CL	0	8505	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CL	0	8515	-	-	-	X
36	CL	2	8504	-	-	-	X
36	CL	B	8519	-	-	-	X
36	CL	N	8508	-	-	-	X
39	ACA	4	78	-	-	-	X
40	BTN	4	79	-	-	-	X
41	CD	2	8404	-	-	-	X
41	CD	T	8401	-	-	-	X
41	CD	Y	8403	-	-	-	X

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 98688 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

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

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

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 CCA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			

- Molecule 4 is a RNA chain called CC-Pmn-pcb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	2	Total	C	N	O	P	0	0	0
			37	18	6	12	1			

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L3.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	DELETION	UNP P20279
B	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L4.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L7AE.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L10E.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	145	Total	C	N	O	S	0	0	0
			1114	668	222	224				

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L15E.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L19E.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37Ae.

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

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L37E.

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

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	1	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	ARG	DELETION	UNP P22452

- Molecule 32 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	110	Total	Mg	0	0
			110	110		
33	J	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	X	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	S	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	73	Total	Na	0	0
			73	73		
35	P	1	Total	Na	0	0
			1	1		
35	Q	3	Total	Na	0	0
			3	3		

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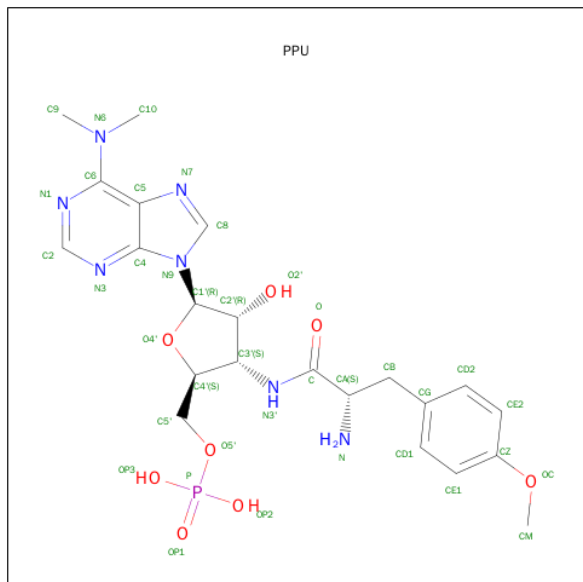
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	K	1	Total 1	Na 1	0	0
35	H	1	Total 1	Na 1	0	0
35	I	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	A	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	L	1	Total 1	Na 1	0	0

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

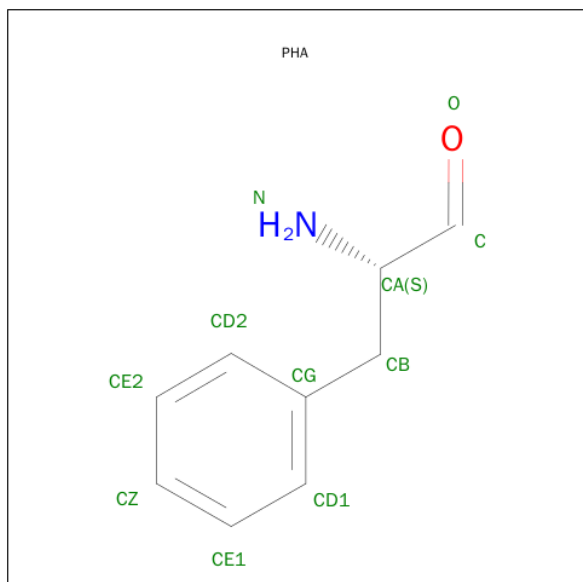
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	0	0
36	Q	1	Total 1	Cl 1	0	0
36	K	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	I	3	Total 3	Cl 3	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	X	1	Total 1	Cl 1	0	0
36	2	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

- Molecule 37 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: $C_{22}H_{30}N_7O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	4	1	Total	C	N	O	P	0	0
			37	22	7	7	1		

- Molecule 38 is PHENYLALANINAL (three-letter code: PHA) (formula: $C_9H_{11}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	4	1	Total	C	N	O	0	0
			11	9	1	1		

- ACA
-
- The chemical structure of 4-aminopentanoic acid (ACA) is shown. It consists of a five-carbon chain. The first carbon (C1) is part of a carboxylic acid group, with a double-bonded oxygen (O1) and a single-bonded hydroxyl group (O2, H). The fifth carbon (C6) is bonded to an amino group (H2N, N6). The carbons are labeled C1, C2, C3, C4, C5, and C6. The amino group is labeled H2N and N6. The carboxylic acid group is labeled O1 and O2.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	Z	1	Total Cd 1 1	0	0
41	Y	1	Total Cd 1 1	0	0
41	T	1	Total Cd 1 1	0	0
41	2	1	Total Cd 1 1	0	0
41	N	1	Total Cd 1 1	0	0

- Molecule 42 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	0	5873	Total O 5873 5873	0	0
42	9	140	Total O 140 140	0	0
42	3	4	Total O 4 4	0	0
42	4	4	Total O 4 4	0	0
42	A	132	Total O 132 132	0	0
42	B	143	Total O 143 143	0	0
42	C	176	Total O 176 176	0	0
42	D	51	Total O 51 51	0	0
42	E	44	Total O 44 44	0	0
42	F	29	Total O 29 29	0	0
42	G	22	Total O 22 22	0	0
42	H	78	Total O 78 78	0	0
42	I	57	Total O 57 57	0	0
42	J	61	Total O 61 61	0	0
42	K	84	Total O 84 84	0	0

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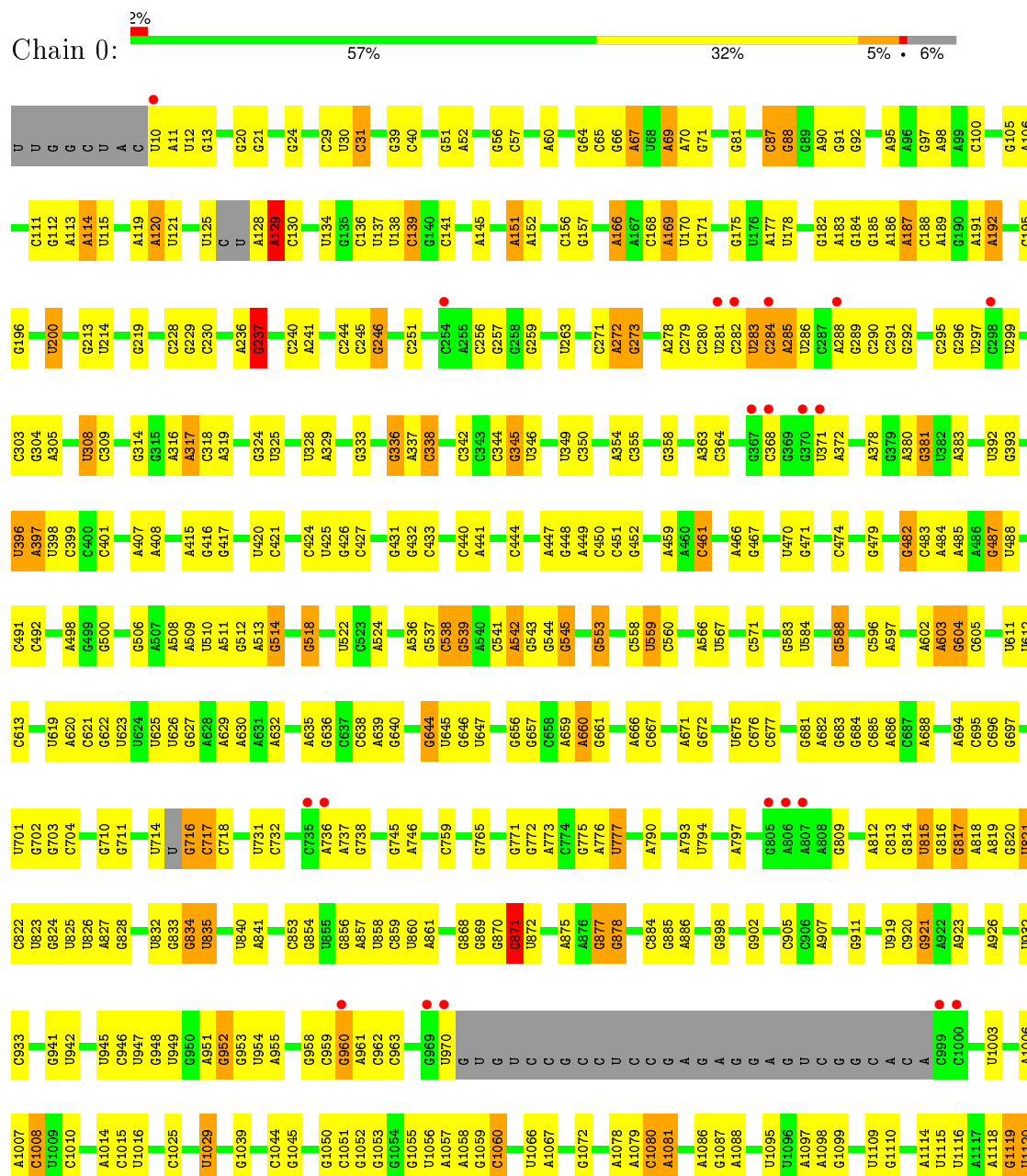
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	L	138	Total 138	O 138	0	0
42	M	70	Total 70	O 70	0	0
42	N	42	Total 42	O 42	0	0
42	O	67	Total 67	O 67	0	0
42	P	56	Total 56	O 56	0	0
42	Q	87	Total 87	O 87	0	0
42	R	36	Total 36	O 36	0	0
42	S	37	Total 37	O 37	0	0
42	T	26	Total 26	O 26	0	0
42	U	16	Total 16	O 16	0	0
42	V	66	Total 66	O 66	0	0
42	W	30	Total 30	O 30	0	0
42	X	96	Total 96	O 96	0	0
42	Y	33	Total 33	O 33	0	0
42	Z	55	Total 55	O 55	0	0
42	1	42	Total 42	O 42	0	0
42	2	76	Total 76	O 76	0	0

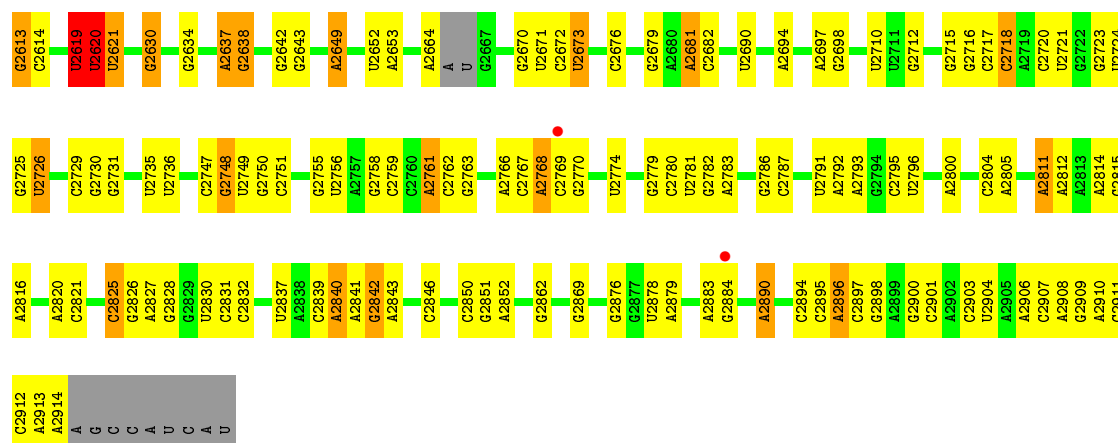
3 Residue-property plots

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

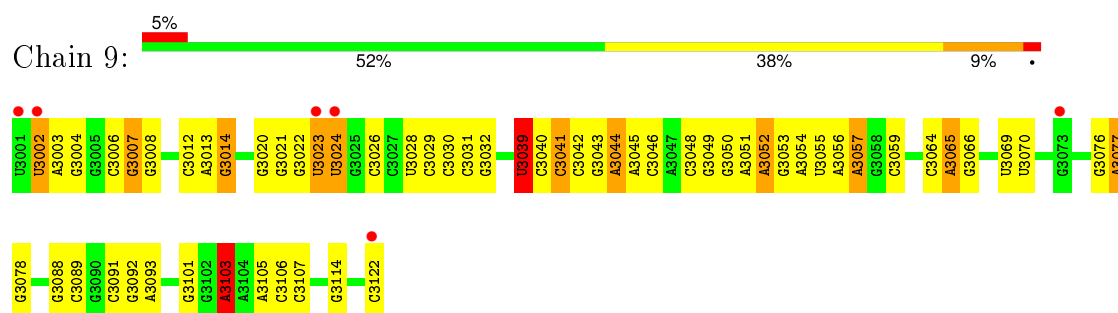
• Molecule 1: 23S rRNA



A2511	C2431	G2336	C2241	G2113	G2009	A1904	A1767	G1666	U	G1441	G1316	U1206	G1121
C2432	U2242	G2338	U2242	C2114	A2010	A1909	C1768	U1667	U1561	G1442	G1316	A1207	U1122
A2433	C2247	A	C2247	U2115	A2011	A1910	C1769	U1668	G1562	A1208	G1325	C1209	A1123
U2435	G2248	C	G2248	U2116	U2012	A1911	U1770	U1669	C1564	C1450	G1325	G1210	U1130
U2436	G2249	C	G2249	C2119	G2013	A1912	U1771	G1670	C1564	C1451	A1328	G1211	U1131
A2437	G2250	C	G2250	U2120	A2015	C1913	G1772	U1677	G1568	G1460	A1329	C1212	A1132
G2438	G2251	C	G2251	G2121	U2016	A1919	A1778	A1678	U1569	U1461	A1330	G1213	A1133
C2439	G2252	C	G2252	A2123	A2019	G1923	A1779	C1679	A1572	C1462	A1331	G1214	G1134
C2440	G2253	C	G2253	G2122	G2019	A1924	U1784	G1680	A1573	A1463	A1332	G1215	G1135
G2441	G2254	C	G2254	A2123	A2019	G1925	U1784	A1682	A1580	U1464	A1333	G1216	U1136
U2442	G2255	A	G2255	U2128	G2033	A1924	A1783	G1681	A1580	G1340	G1340	G1224	G1137
U2443	G2256	U	G2256	U2129	U2034	G1925	U1784	A1682	A1580	G1340	G1340	G1225	G1151
U2445	A2258	G	A2258	U2133	A2039	A1930	C1787	G1683	G1588	A1470	G1340	C1225	G1151
G2446	U2265	C	U2265	G2134	A2039	A1931	U1788	A1684	G1589	A1471	A1341	C1229	G1158
G2453	A2266	G	A2266	A2135	G2044	A1931	U1788	A1685	G1589	C1472	A1342	G1229	G1159
C2454	G2267	G	G2267	G2136	G2045	C1940	C1798	C1686	G1592	U1473	G1343	U1234	G1160
U2457	G2268	C	G2268	A	G2046	A1941	C1798	C1687	G1593	C1474	A1344	G1235	A1161
U2458	C2269	C	C2269	C	C2047	A1942	A1804	C1692	C1594	C1477	A1345	A1236	G1162
G2459	G2270	A	G2270	G	G2050	C1943	G1805	C1699	C1595	U1478	A1346	U1237	G1163
G2460	G2271	C	G2271	C	G2050	G1948	G1806	C1700	U1596	C1483	A1352	G1238	G1164
G2461	C2272	C	C2272	U	A2054	G1948	C1810	A1701	A1597	C1484	G1353	G1239	G1165
U2462	A2273	G	A2273	G	A2054	G1948	C1810	U1702	A1598	A1485	G1353	A1242	G1166
G2463	G2274	A	G2274	U	U2064	G1981	A1815	U1710	A1603	G1360	G1360	G1243	G1167
A2464	G2275	G	G2275	C	U2064	G1981	C1816	A1710	A1604	C1366	C1366	U1244	C1168
C2465	U2276	C	U2276	G	G2068	A	U1817	A1711	C1495	U1170	C1245	U1244	U1169
A2466	U2277	C	U2277	C	G2068	C	C1818	A1712	C1496	A1171	A1246	A1246	U1170
G2467	C2281	A	C2281	C	G2072	C	G1819	A1717	G1497	A1372	A1372	U1249	G1172
U2468	U2282	A	U2282	U	G2073	U	G1820	U1717	G1498	A1377	A1377	C1250	A1173
A2469	G2285	G	G2285	G	A2074	U	G1828	U1722	U1499	C1378	C1378	C1251	A1174
U2472	G2286	G	G2286	G	U2078	A	A1829	G1723	U1503	U1380	U1380	C1252	G1175
C2473	A2291	U	A2291	U	G2079	C	C1830	U1724	U1504	C1384	C1384	C1253	A1177
A2474	G2300	A	G2300	C	A2081	C	C1834	C1725	U1505	G1385	G1385	U1266	U1180
C2475	A2301	A	A2301	C	G2084	U1984	U1835	G1730	U1506	C1388	C1388	C1267	A1181
G2476	A2302	U	A2302	C	A2085	A1989	A1840	C1731	A1624	C1268	C1268	C1269	C1182
U2477	C2303	C	C2303	U	C2088	G1970	C1856	A1732	U1625	C1183	C1183	G1269	C1183
A2478	G2308	U	G2308	U	G2088	G1971	C1856	C1734	A1626	C1184	C1184	C1273	C1184
G2479	G2310	A	G2310	G	A2089	A1972	G1868	C1735	G1627	U1185	U1185	C1273	C1185
U2480	A2311	C	A2311	C	G2090	A1973	U1878	A1736	C1633	C1186	C1186	U1279	C1186
A2483	G2312	C	G2312	U	G2091	G1974	U1879	U1741	G1634	A1392	A1392	A1287	A1187
G2488	C2313	C	C2313	A	G2093	A1978	U1878	A1742	U1635	A1393	A1393	U1288	A1188
A2489	G2314	G	G2314	G	G2094	G1979	U1879	G1743	G1636	C1394	C1394	A1289	A1189
U2490	G2315	U	G2315	G	A2095	A1980	U1879	G1743	A1527	G1398	G1398	C1289	G1190
G2493	G2316	C	G2316	A	A2096	U1980	U1880	G1751	A1528	A1399	A1399	U1298	A1192
C2493	C2317	G	C2317	A	A2096	U1982	C1880	G1752	G1529	A1407	A1407	U1298	A1193
U2494	U2320	U	U2320	C	G2099	U1982	C1881	C1753	G1535	U1304	U1304	G1299	G1197
G2495	A2321	G	A2321	C	A2100	C1983	C1882	G1753	C1536	U1305	U1305	U1304	U1198
U2496	G2324	A	G2324	A	A2101	A1994	U1883	A1759	U1654	A1306	A1306	U1305	U1199
A2497	C2325	C	C2325	C	G2102	G1995	G1884	U1760	C1545	U1422	U1422	U1306	C1200
G2498	G2326	U	G2326	U	A2103	U1996	A1885	U1761	G1546	C1423	C1423	A1307	A1201
U2499	C2327	C	C2327	C	G2110	U2004	U1887	C1762	G1557	A1308	A1308	A1308	A1202
A2499	G2237	C	G2237	A	G2111	G2005	G1902	C1763	C1558	G1311	G1311	G1312	G1203
C2499	A2430	A	A2430	A	A2112	U2008	U1903	U1766	A1559	C1436	C1436	G1312	U1205



• Molecule 2: 5S RRNA



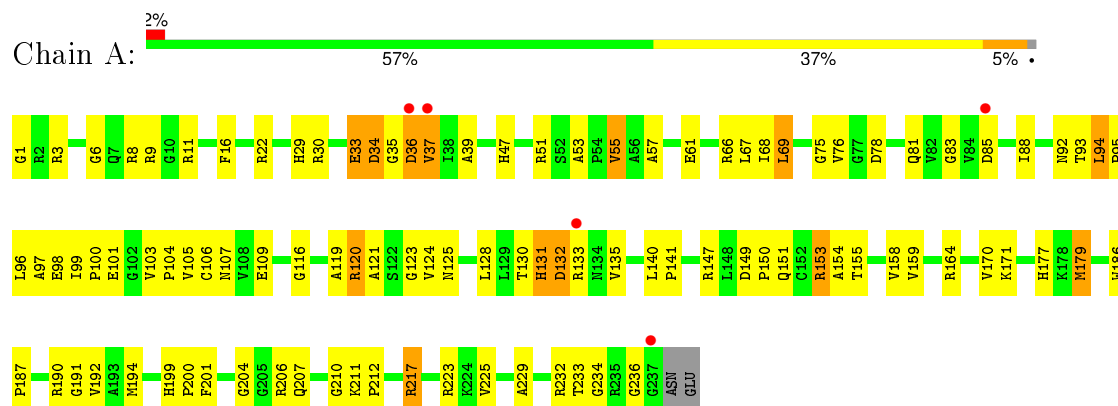
• Molecule 3: CCA



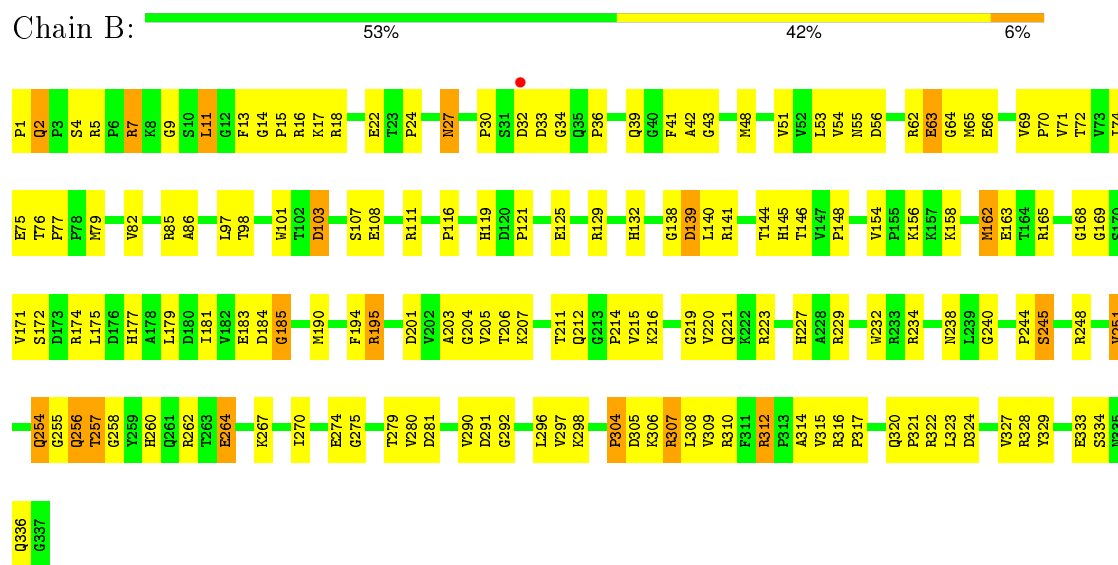
• Molecule 4: CC-Pmn-pcb



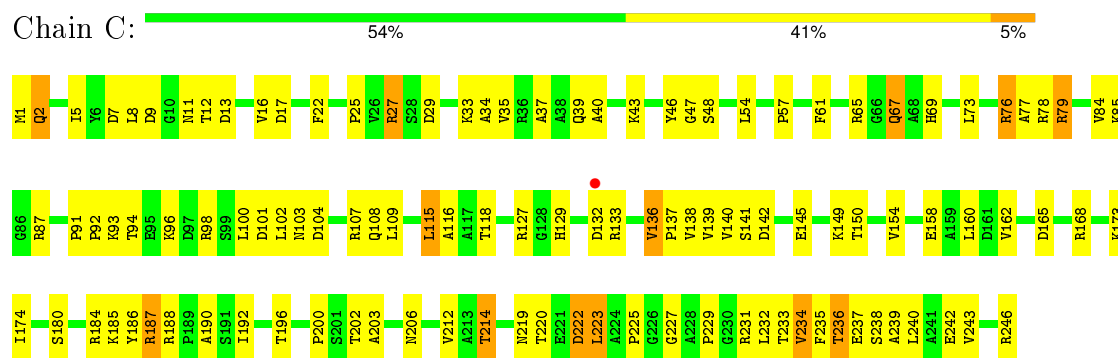
• Molecule 5: RIBOSOMAL PROTEIN L2



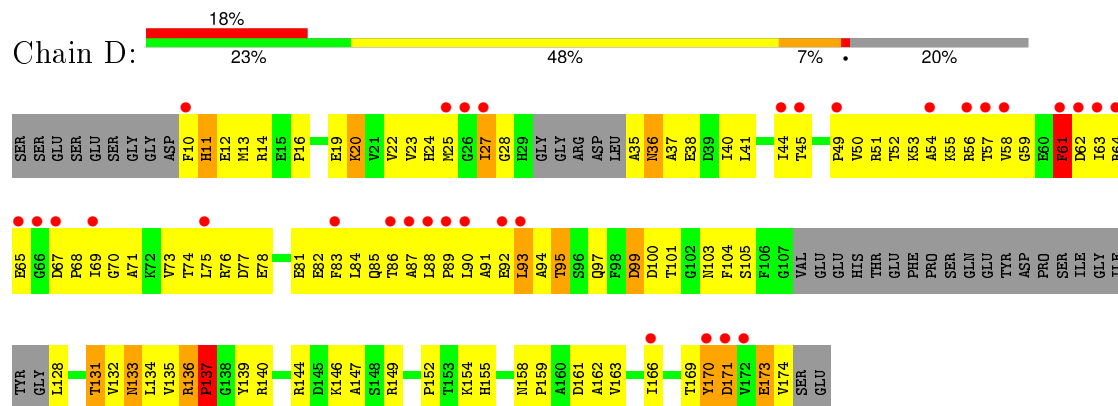
• Molecule 6: RIBOSOMAL PROTEIN L3



• Molecule 7: RIBOSOMAL PROTEIN L4

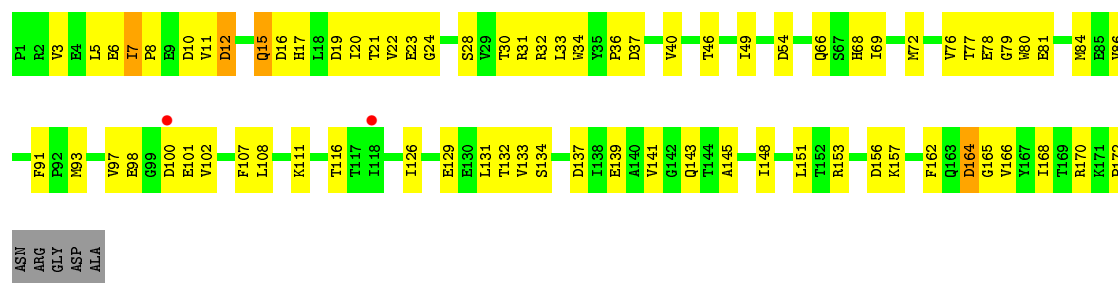


• Molecule 8: RIBOSOMAL PROTEIN L5

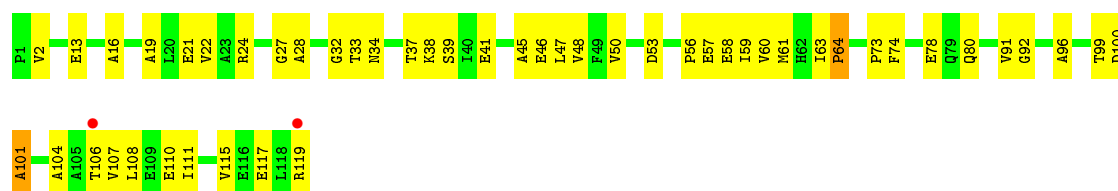


• Molecule 9: RIBOSOMAL PROTEIN L6

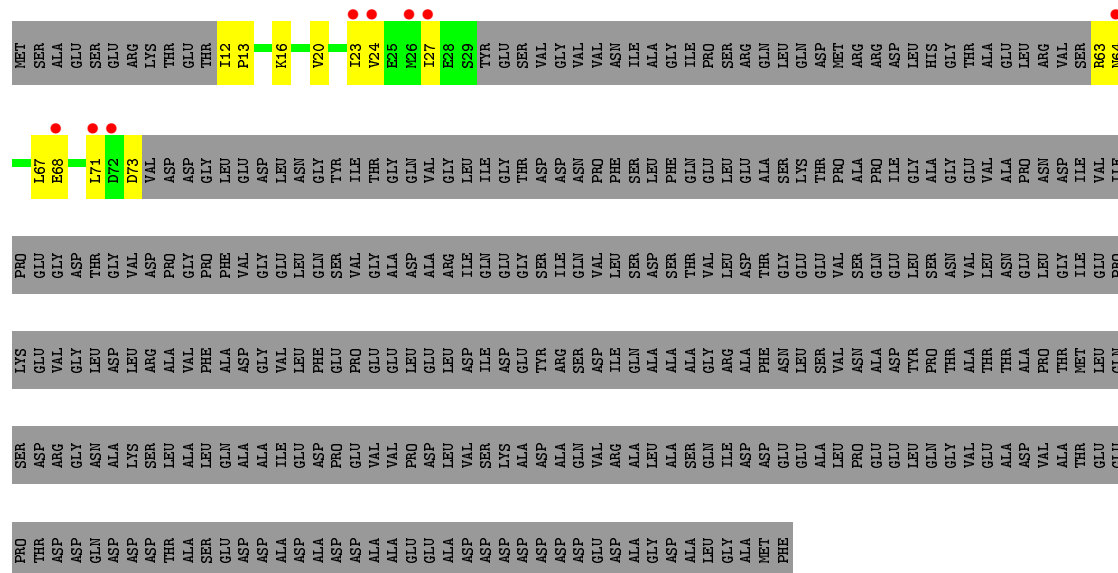




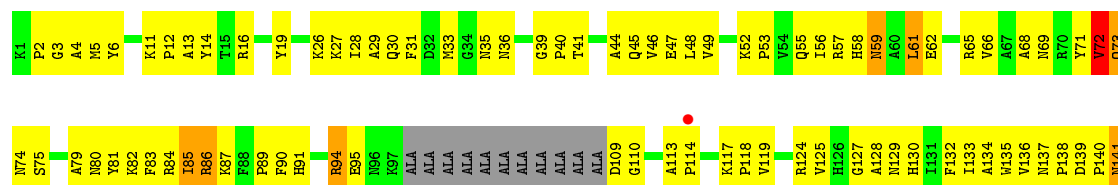
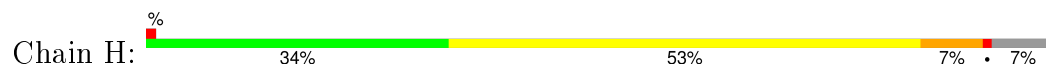
• Molecule 10: RIBOSOMAL PROTEIN L7AE

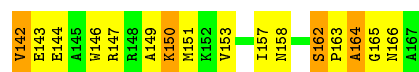


• Molecule 11: RIBOSOMAL PROTEIN L10



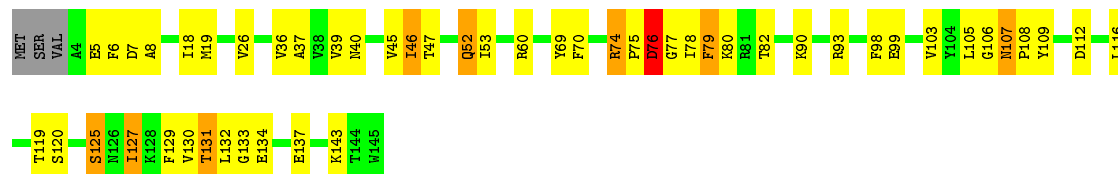
• Molecule 12: RIBOSOMAL PROTEIN L10E





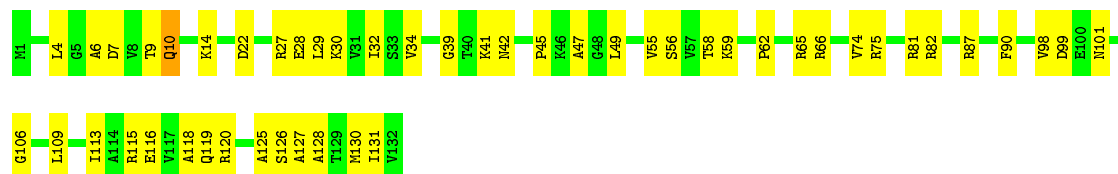
• Molecule 13: RIBOSOMAL PROTEIN L13

Chain I: 63% 29% 6% ••



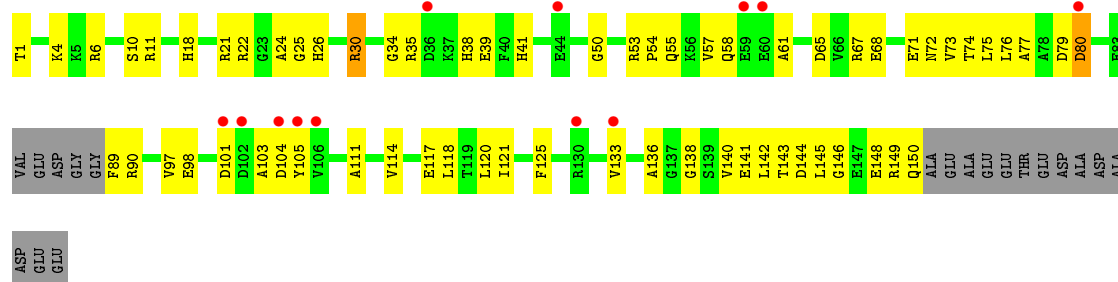
• Molecule 14: RIBOSOMAL PROTEIN L14

Chain J: 63% 36% •



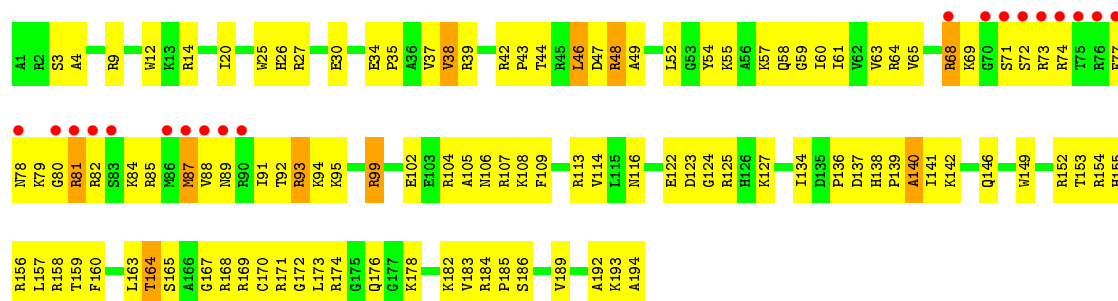
• Molecule 15: RIBOSOMAL PROTEIN L15

Chain K: 7% 49% 38% • 12%

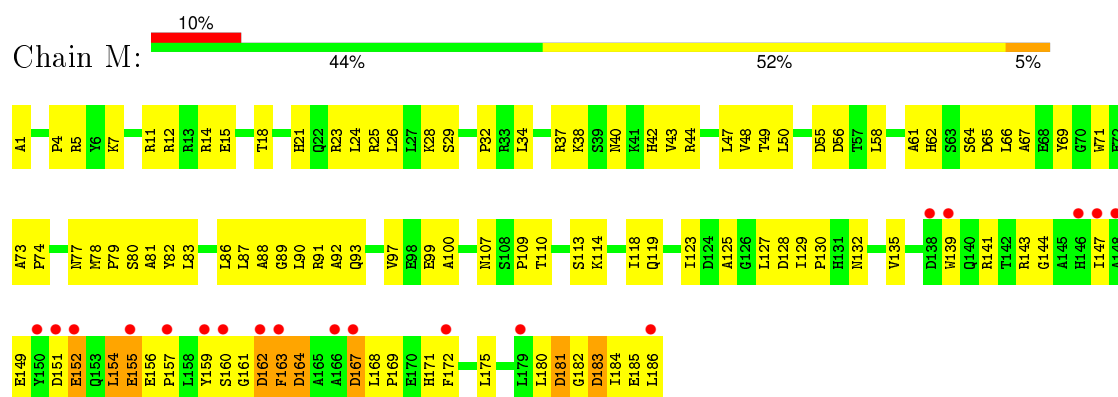


• Molecule 16: RIBOSOMAL PROTEIN L15E

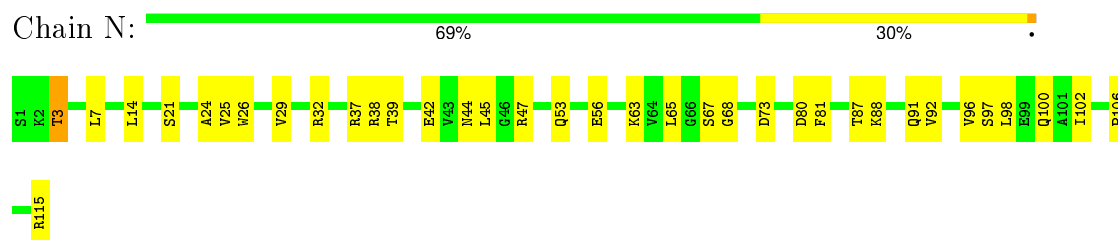
Chain L: 10% 42% 53% 5%



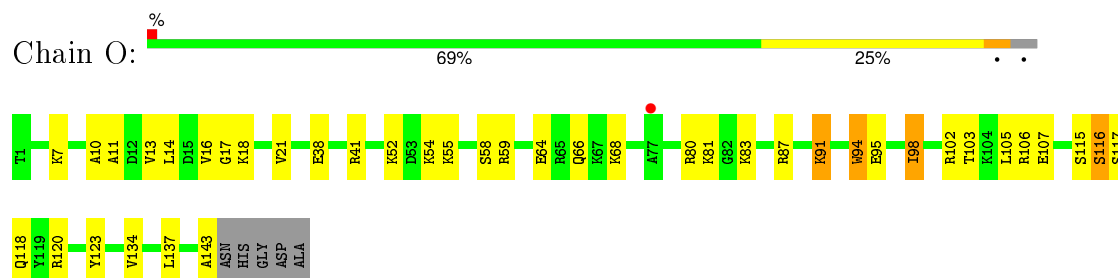
• Molecule 17: RIBOSOMAL PROTEIN L18



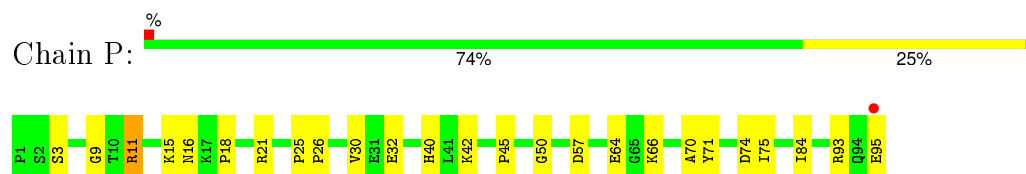
• Molecule 18: RIBOSOMAL PROTEIN L18E



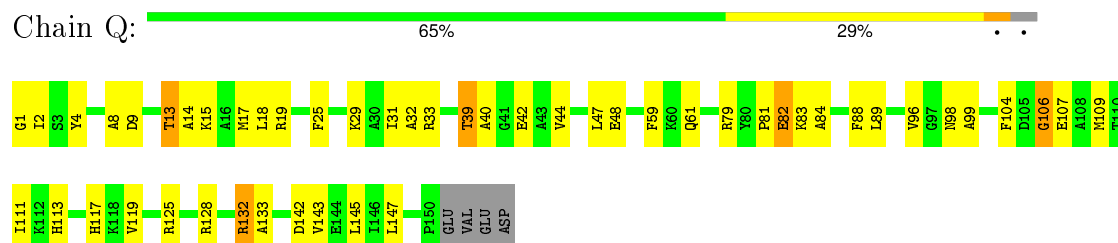
• Molecule 19: RIBOSOMAL PROTEIN L19E



• Molecule 20: RIBOSOMAL PROTEIN L21E



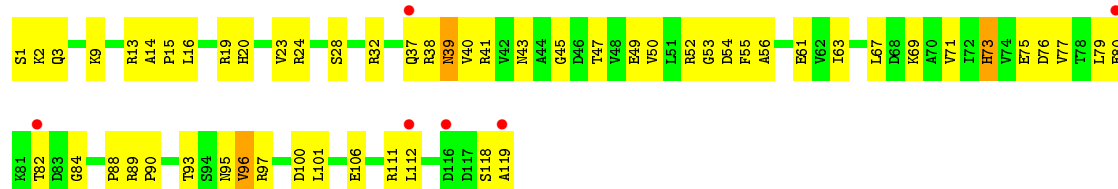
• Molecule 21: RIBOSOMAL PROTEIN L22



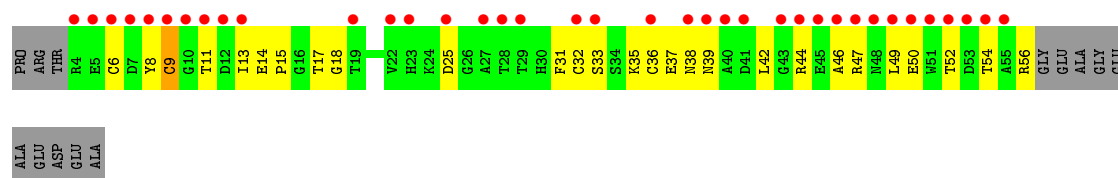
• Molecule 22: RIBOSOMAL PROTEIN L23



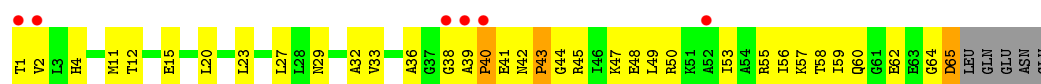
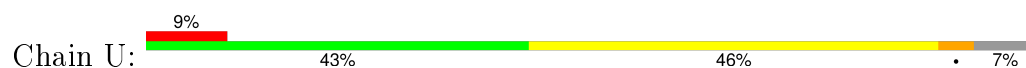
• Molecule 23: RIBOSOMAL PROTEIN L24



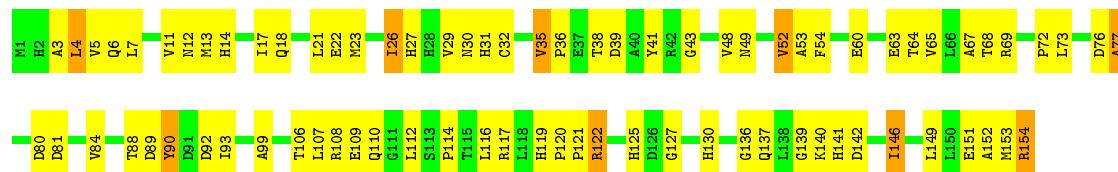
• Molecule 24: RIBOSOMAL PROTEIN L24E



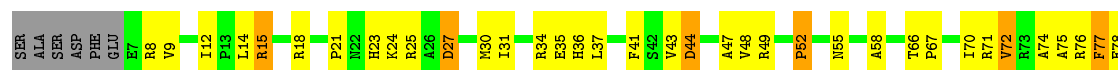
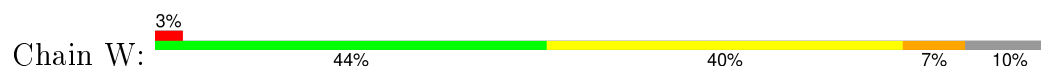
• Molecule 25: RIBOSOMAL PROTEIN L29



• Molecule 26: RIBOSOMAL PROTEIN L30



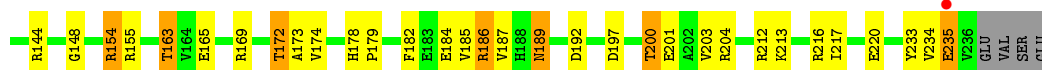
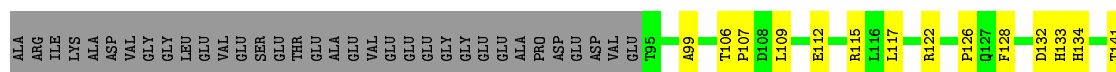
• Molecule 27: RIBOSOMAL PROTEIN L31E





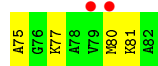
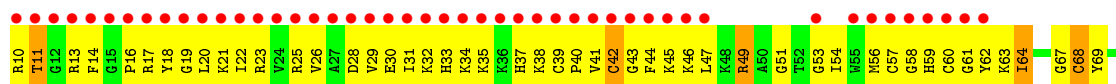
• Molecule 28: RIBOSOMAL PROTEIN L32E

Chain X: 40% 16% 41%



• Molecule 29: RIBOSOMAL PROTEIN L37Ae

Chain Y: 27% 67% 66% 7%



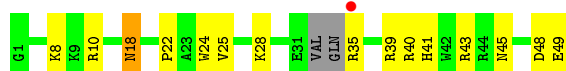
• Molecule 30: RIBOSOMAL PROTEIN L37E

Chain Z: 68% 32%



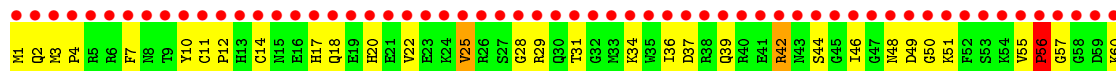
• Molecule 31: RIBOSOMAL PROTEIN L39E

Chain 1: 2% 65% 29%



• Molecule 32: RIBOSOMAL PROTEIN L44E

Chain 2: 42% 100% 53%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.78Å 300.35Å 574.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 44.78 – 3.06	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.10) 95.4 (44.78-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.173 , 0.220 0.172 , 0.216	Depositor DCC
R_{free} test set	3206 reflections (1.02%)	DCC
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 340532 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	98688	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.41	2/66076 (0.0%)	0.70	27/103052 (0.0%)
2	9	0.39	0/2905	0.75	2/4528 (0.0%)
3	3	0.82	0/65	0.87	0/99
4	4	0.49	0/40	0.62	0/60
5	A	0.34	0/1787	0.66	0/2409
6	B	0.35	0/2689	0.64	0/3652
7	C	0.39	0/1883	0.64	0/2551
8	D	0.32	0/1111	0.59	0/1498
9	E	0.34	0/1382	0.58	0/1880
10	F	0.33	0/896	0.56	0/1219
11	G	0.29	0/241	0.48	0/324
12	H	0.39	0/1246	0.76	2/1686 (0.1%)
13	I	0.38	0/1135	0.62	0/1530
14	J	0.35	0/1003	0.66	0/1351
15	K	0.34	0/1126	0.65	0/1504
16	L	0.41	0/1633	0.71	0/2180
17	M	0.29	0/1473	0.63	0/1999
18	N	0.35	0/873	0.62	0/1181
19	O	0.35	0/1143	0.54	0/1521
20	P	0.36	0/748	0.66	0/1005
21	Q	0.37	0/1172	0.66	0/1578
22	R	0.34	0/648	0.58	0/875
23	S	0.34	0/957	0.64	0/1289
24	T	0.34	0/417	0.56	0/562
25	U	0.30	0/502	0.57	0/675
26	V	0.37	0/1218	0.64	0/1655
27	W	0.35	0/664	0.61	0/895
28	X	0.38	0/1146	0.65	0/1536
29	Y	0.34	0/575	0.66	0/763
30	Z	0.41	0/437	0.64	0/578
31	1	0.32	0/398	0.54	0/527
32	2	0.39	0/771	0.57	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.40	2/98360 (0.0%)	0.69	31/147186 (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	37
2	9	0	1
26	V	0	1
All	All	1	39

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	U	O5'-C5'	-7.09	1.31	1.42
1	0	2620	U	C2'-O2'	6.66	1.50	1.41

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1164	U	OP1-P-O3'	-12.07	78.64	105.20
1	0	1164	U	OP2-P-O3'	-10.75	81.56	105.20
1	0	1165	G	O5'-P-OP2	9.72	122.36	110.70
1	0	1563	G	C2'-C3'-O3'	9.36	130.09	109.50
1	0	2619	U	C5'-C4'-C3'	-9.23	101.24	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	171	C	Sidechain
1	0	246	G	Sidechain
1	0	333	G	Sidechain
1	0	393	G	Sidechain
1	0	396	U	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	59017	0	29805	983	0
2	9	2600	0	1326	68	0
3	3	59	0	35	4	0
4	4	37	0	23	5	0
5	A	1754	0	1763	130	0
6	B	2624	0	2533	167	0
7	C	1858	0	1816	130	0
8	D	1094	0	1085	133	0
9	E	1357	0	1266	78	0
10	F	885	0	854	63	0
11	G	240	0	231	20	0
12	H	1215	0	1215	162	0
13	I	1119	0	1098	64	0
14	J	993	0	1027	58	0
15	K	1114	0	1072	64	0
16	L	1605	0	1676	164	0
17	M	1444	0	1401	139	0
18	N	864	0	873	33	0
19	O	1133	0	1127	43	0
20	P	734	0	729	23	0
21	Q	1149	0	1122	57	0
22	R	641	0	605	26	0
23	S	949	0	923	53	0
24	T	410	0	366	35	0
25	U	499	0	511	34	0
26	V	1195	0	1137	104	0
27	W	654	0	653	51	0
28	X	1130	0	1133	57	0
29	Y	563	0	601	72	0
30	Z	430	0	426	24	0
31	1	393	0	406	18	0
32	2	755	0	731	63	0
33	0	110	0	0	0	0
33	2	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	S	1	0	0	0	0
33	X	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	73	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	I	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	P	1	0	0	0	0
35	Q	3	0	0	0	0
35	R	1	0	0	0	0
36	0	10	0	0	0	0
36	2	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	I	3	0	0	1	0
36	K	1	0	0	0	0
36	L	1	0	0	1	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	Q	1	0	0	0	0
36	X	1	0	0	0	0
37	4	37	0	26	2	0
38	4	11	0	8	1	0
39	4	8	0	10	0	0
40	4	15	0	15	2	0
41	2	1	0	0	0	0
41	N	1	0	0	0	0
41	T	1	0	0	0	0
41	Y	1	0	0	0	0
41	Z	1	0	0	0	0
42	0	5873	0	0	207	0
42	1	42	0	0	3	0
42	2	76	0	0	7	0
42	3	4	0	0	3	0
42	4	4	0	0	0	0
42	9	140	0	0	11	0
42	A	132	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	B	143	0	0	23	0
42	C	176	0	0	35	0
42	D	51	0	0	19	0
42	E	44	0	0	10	0
42	F	29	0	0	12	0
42	G	22	0	0	5	0
42	H	78	0	0	22	0
42	I	57	0	0	4	0
42	J	61	0	0	9	0
42	K	84	0	0	19	0
42	L	138	0	0	22	0
42	M	70	0	0	15	0
42	N	42	0	0	7	0
42	O	67	0	0	6	0
42	P	56	0	0	3	0
42	Q	87	0	0	9	0
42	R	36	0	0	6	0
42	S	37	0	0	9	0
42	T	26	0	0	4	0
42	U	16	0	0	3	0
42	V	66	0	0	11	0
42	W	30	0	0	5	0
42	X	96	0	0	17	0
42	Y	33	0	0	12	0
42	Z	55	0	0	3	0
All	All	98688	0	59628	2828	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 19.

The worst 5 of 2828 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)
12:H:86:ARG:NH1	12:H:133:ILE:HG13	1.61	1.16
25:U:12:THR:HG22	25:U:15:GLU:HG3	1.34	1.09
7:C:236:THR:HG22	7:C:239:ALA:H	0.97	1.07
1:O:156:C:H5"	16:L:171:ARG:HD3	1.38	1.05
12:H:45:GLN:HB3	12:H:163:PRO:HD2	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	
5	A	235/239 (98%)	199 (85%)	32 (14%)	4 (2%)	11	43
6	B	335/337 (99%)	299 (89%)	29 (9%)	7 (2%)	9	37
7	C	244/246 (99%)	220 (90%)	22 (9%)	2 (1%)	24	63
8	D	134/176 (76%)	94 (70%)	26 (19%)	14 (10%)	1	3
9	E	170/177 (96%)	159 (94%)	11 (6%)	0	100	100
10	F	117/119 (98%)	104 (89%)	11 (9%)	2 (2%)	11	43
11	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
12	H	152/167 (91%)	132 (87%)	15 (10%)	5 (3%)	5	26
13	I	140/145 (97%)	127 (91%)	9 (6%)	4 (3%)	6	29
14	J	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	13	46
15	K	141/164 (86%)	124 (88%)	16 (11%)	1 (1%)	26	65
16	L	192/194 (99%)	174 (91%)	17 (9%)	1 (0%)	34	72
17	M	184/186 (99%)	166 (90%)	11 (6%)	7 (4%)	4	22
18	N	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
19	O	141/148 (95%)	138 (98%)	2 (1%)	1 (1%)	26	65
20	P	93/95 (98%)	86 (92%)	7 (8%)	0	100	100
21	Q	148/154 (96%)	136 (92%)	11 (7%)	1 (1%)	26	65
22	R	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
23	S	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
24	T	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
25	U	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	5	26
26	V	152/154 (99%)	143 (94%)	7 (5%)	2 (1%)	15	50
27	W	80/91 (88%)	71 (89%)	6 (8%)	3 (4%)	4	22
28	X	140/240 (58%)	140 (100%)	0	0	100	100
29	Y	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	14	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
31	1	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
32	2	90/92 (98%)	84 (93%)	3 (3%)	3 (3%)	5	26
All	All	3633/4235 (86%)	3293 (91%)	278 (8%)	62 (2%)	11	43

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	139	ASP
8	D	93	LEU
8	D	95	THR
8	D	173	GLU
10	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	
5	A	179/181 (99%)	166 (93%)	13 (7%)	17	52
6	B	282/282 (100%)	263 (93%)	19 (7%)	20	56
7	C	193/193 (100%)	177 (92%)	16 (8%)	14	46
8	D	117/147 (80%)	108 (92%)	9 (8%)	16	50
9	E	152/155 (98%)	146 (96%)	6 (4%)	39	75
10	F	92/92 (100%)	92 (100%)	0	100	100
11	G	27/283 (10%)	27 (100%)	0	100	100
12	H	122/122 (100%)	111 (91%)	11 (9%)	12	41
13	I	118/121 (98%)	107 (91%)	11 (9%)	11	39
14	J	106/106 (100%)	102 (96%)	4 (4%)	40	76
15	K	112/126 (89%)	108 (96%)	4 (4%)	42	77
16	L	166/166 (100%)	157 (95%)	9 (5%)	27	64
17	M	149/149 (100%)	145 (97%)	4 (3%)	52	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	N	93/93 (100%)	91 (98%)	2 (2%)	60	85
19	O	113/116 (97%)	109 (96%)	4 (4%)	43	78
20	P	79/79 (100%)	76 (96%)	3 (4%)	40	76
21	Q	117/121 (97%)	113 (97%)	4 (3%)	44	79
22	R	71/73 (97%)	71 (100%)	0	100	100
23	S	105/105 (100%)	102 (97%)	3 (3%)	50	81
24	T	44/52 (85%)	43 (98%)	1 (2%)	58	84
25	U	51/56 (91%)	49 (96%)	2 (4%)	39	75
26	V	130/130 (100%)	121 (93%)	9 (7%)	19	55
27	W	66/73 (90%)	61 (92%)	5 (8%)	16	51
28	X	120/195 (62%)	112 (93%)	8 (7%)	20	56
29	Y	56/56 (100%)	49 (88%)	7 (12%)	6	22
30	Z	46/46 (100%)	46 (100%)	0	100	100
31	1	42/44 (96%)	41 (98%)	1 (2%)	57	84
32	2	79/79 (100%)	75 (95%)	4 (5%)	29	66
All	All	3027/3441 (88%)	2868 (95%)	159 (5%)	28	64

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	H	94	ARG
15	K	30	ARG
28	X	235	GLU
13	I	46	ILE
13	I	112	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
15	K	58	GLN
19	O	73	HIS
31	1	16	ASN
16	L	26	HIS
17	M	107	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2747/2922 (94%)	244 (8%)	34 (1%)
2	9	121/122 (99%)	14 (11%)	4 (3%)
3	3	2/3 (66%)	1 (50%)	0
4	4	1/2 (50%)	0	0
All	All	2871/3049 (94%)	259 (9%)	38 (1%)

5 of 259 RNA backbone outliers are listed below:

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

5 of 38 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1450	C
1	0	1856	C
2	9	3023	U
1	0	1563	G
1	0	1979	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 236 ligands modelled in this entry, 232 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PPU	4	76	38,4	30,40,41	2.47	3 (10%)	37,57,60	1.23	3 (8%)
38	PHA	4	77	39,37	10,11,11	0.99	0	10,13,13	0.78	0
39	ACA	4	78	38,40	7,7,8	2.23	2 (28%)	5,6,8	1.30	1 (20%)
40	BTN	4	79	39	14,16,17	2.02	4 (28%)	13,21,23	1.24	1 (7%)

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
37	PPU	4	76	38,4	-	0/21/43/44	0/4/4/4
38	PHA	4	77	39,37	-	0/4/6/6	0/1/1/1
39	ACA	4	78	38,40	-	0/4/5/6	0/0/0/0
40	BTN	4	79	39	-	0/5/27/28	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	4	78	ACA	C3-C2	-5.26	1.32	1.52
37	4	76	PPU	OC-CM	-5.23	1.26	1.42
40	4	79	BTN	C9-C10	-4.04	1.36	1.52
40	4	79	BTN	C8-C7	-4.03	1.33	1.52
40	4	79	BTN	C3-N1	-3.39	1.30	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	4	76	PPU	C4'-C3'-N3'	-4.09	105.07	113.61
40	4	79	BTN	O3-C3-N2	-2.46	123.05	125.90
39	4	78	ACA	C4-C3-C2	-2.16	105.42	113.86
37	4	76	PPU	C-CA-N	2.20	118.52	108.73
37	4	76	PPU	C2-N1-C6	3.48	118.83	111.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	4	76	PPU	2	0
38	4	77	PHA	1	0
40	4	79	BTN	2	0

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, 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	2754/2922 (94%)	-0.18	61 (2%) 65 42	11, 39, 86, 141	0
2	9	122/122 (100%)	0.28	6 (4%) 33 14	28, 60, 91, 145	0
3	3	3/3 (100%)	1.49	0 100 100	44, 44, 46, 52	3 (100%)
4	4	2/2 (100%)	0.06	0 100 100	48, 48, 48, 56	0
5	A	237/239 (99%)	-0.17	5 (2%) 67 44	21, 53, 94, 113	0
6	B	337/337 (100%)	-0.33	1 (0%) 94 88	19, 45, 71, 81	0
7	C	246/246 (100%)	-0.39	1 (0%) 93 85	12, 37, 63, 71	0
8	D	140/176 (79%)	1.18	32 (22%) 1 0	55, 94, 120, 127	0
9	E	172/177 (97%)	0.19	2 (1%) 81 64	32, 56, 81, 87	0
10	F	119/119 (100%)	0.14	2 (1%) 73 52	41, 66, 94, 104	0
11	G	29/348 (8%)	1.58	8 (27%) 1 0	60, 79, 84, 89	0
12	H	156/167 (93%)	-0.00	1 (0%) 90 80	30, 48, 74, 81	0
13	I	142/145 (97%)	-0.41	0 100 100	26, 38, 60, 77	0
14	J	132/132 (100%)	-0.31	0 100 100	24, 44, 72, 76	0
15	K	145/164 (88%)	0.34	12 (8%) 14 5	16, 68, 97, 109	0
16	L	194/194 (100%)	0.06	19 (9%) 10 3	23, 39, 118, 128	0
17	M	186/186 (100%)	0.41	19 (10%) 9 3	36, 65, 109, 120	0
18	N	115/115 (100%)	-0.21	0 100 100	31, 47, 65, 69	0
19	O	143/148 (96%)	-0.05	1 (0%) 89 78	27, 47, 67, 77	0
20	P	95/95 (100%)	-0.26	1 (1%) 82 66	27, 40, 57, 79	0
21	Q	150/154 (97%)	-0.52	0 100 100	22, 35, 54, 65	0
22	R	81/84 (96%)	-0.03	2 (2%) 61 37	35, 53, 73, 80	0
23	S	119/119 (100%)	0.13	6 (5%) 32 13	33, 47, 75, 91	0
24	T	53/66 (80%)	3.01	37 (69%) 0 0	101, 113, 122, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	U	65/70 (92%)	0.72	6 (9%) 11 4	45, 69, 106, 112	0
26	V	154/154 (100%)	-0.41	0 100 100	25, 38, 56, 69	0
27	W	82/91 (90%)	0.18	3 (3%) 45 22	32, 49, 69, 89	0
28	X	142/240 (59%)	-0.27	1 (0%) 89 78	17, 36, 58, 77	0
29	Y	73/73 (100%)	4.11	49 (67%) 0 0	89, 118, 129, 133	0
30	Z	56/56 (100%)	-0.73	0 100 100	14, 26, 32, 39	0
31	1	46/48 (95%)	-0.02	1 (2%) 65 42	23, 52, 84, 96	0
32	2	92/92 (100%)	7.49	92 (100%) 0 0	122, 136, 142, 146	0
All	All	6582/7284 (90%)	0.08	368 (5%) 28 11	11, 45, 105, 146	3 (0%)

The worst 5 of 368 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	2	37	ASP	17.5
32	2	78	HIS	17.4
32	2	82	GLY	17.2
32	2	11	CYS	14.7
29	Y	11	THR	13.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8356	1/1	0.95	0.65	41.33	59,59,59,59	0
34	K	0	8201	1/1	0.96	0.65	36.09	80,80,80,80	0
35	NA	0	8325	1/1	0.96	0.38	33.22	29,29,29,29	0
36	CL	0	8515	1/1	0.90	0.68	30.55	72,72,72,72	0
35	NA	Q	8386	1/1	0.42	0.80	24.66	62,62,62,62	0
35	NA	0	8332	1/1	0.84	0.38	19.43	57,57,57,57	0
35	NA	0	8361	1/1	0.97	0.46	18.20	40,40,40,40	0
35	NA	0	8350	1/1	0.94	0.42	17.84	26,26,26,26	0
35	NA	0	8374	1/1	0.91	0.52	16.49	49,49,49,49	0
35	NA	0	8371	1/1	0.76	0.47	14.89	47,47,47,47	0
35	NA	0	8372	1/1	0.74	0.38	14.80	73,73,73,73	0
35	NA	0	8340	1/1	0.86	0.26	12.84	48,48,48,48	0
35	NA	9	8383	1/1	0.71	0.65	12.76	57,57,57,57	0
35	NA	0	8323	1/1	0.98	0.26	12.50	34,34,34,34	0
40	BTN	4	79	15/16	0.88	0.31	12.31	91,104,104,105	0
35	NA	0	8364	1/1	0.90	0.26	11.73	47,47,47,47	0
35	NA	0	8362	1/1	0.95	0.27	9.98	63,63,63,63	0
35	NA	0	8379	1/1	0.93	0.23	9.95	25,25,25,25	0
35	NA	0	8321	1/1	0.97	0.33	9.30	58,58,58,58	0
35	NA	0	8308	1/1	0.92	0.21	9.26	44,44,44,44	0
35	NA	0	8310	1/1	0.89	0.31	9.22	16,16,16,16	0
36	CL	B	8519	1/1	0.96	0.24	8.51	51,51,51,51	0
36	CL	0	8505	1/1	0.95	0.33	8.41	57,57,57,57	0
33	MG	0	8064	1/1	0.98	0.28	8.40	17,17,17,17	0
39	ACA	4	78	8/9	0.95	0.24	8.32	67,73,85,88	0
35	NA	0	8331	1/1	0.89	0.32	7.94	69,69,69,69	0
35	NA	0	8381	1/1	0.95	0.24	6.94	71,71,71,71	0
35	NA	0	8376	1/1	0.97	0.22	5.33	50,50,50,50	0
35	NA	0	8382	1/1	0.79	0.30	5.14	57,57,57,57	0
33	MG	0	8053	1/1	0.93	0.20	5.13	38,38,38,38	0
35	NA	0	8326	1/1	0.83	0.27	3.47	38,38,38,38	0
35	NA	0	8303	1/1	0.94	0.17	3.06	33,33,33,33	0
36	CL	N	8508	1/1	0.96	0.31	2.66	82,82,82,82	0
35	NA	0	8373	1/1	0.85	0.23	2.27	51,51,51,51	0
41	CD	T	8401	1/1	0.80	0.77	2.01	200,200,200,200	0
35	NA	0	8365	1/1	0.85	0.30	1.83	42,42,42,42	0
34	K	0	8202	1/1	0.83	0.46	1.56	69,69,69,69	0
33	MG	X	8109	1/1	0.99	0.20	1.51	35,35,35,35	0
33	MG	0	8044	1/1	0.98	0.16	1.46	35,35,35,35	0
38	PHA	4	77	11/11	0.91	0.27	1.44	64,67,71,71	0
35	NA	0	8378	1/1	0.95	0.17	1.16	31,31,31,31	0
37	PPU	4	76	37/38	0.96	0.21	1.09	48,55,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	Y	8105	1/1	0.55	0.63	0.91	67,67,67,67	0
35	NA	Q	8337	1/1	0.88	0.19	0.40	41,41,41,41	0
35	NA	0	8368	1/1	0.92	0.14	0.24	41,41,41,41	0
35	NA	0	8324	1/1	0.88	0.18	0.17	39,39,39,39	0
35	NA	0	8366	1/1	0.92	0.17	0.13	20,20,20,20	0
33	MG	0	8067	1/1	0.95	0.15	-0.56	31,31,31,31	0
35	NA	C	8304	1/1	0.96	0.16	-0.61	25,25,25,25	0
36	CL	I	8521	1/1	0.95	0.13	-0.64	39,39,39,39	0
35	NA	0	8327	1/1	0.97	0.13	-0.76	16,16,16,16	0
35	NA	K	8380	1/1	0.96	0.17	-0.77	69,69,69,69	0
41	CD	Y	8403	1/1	0.85	0.52	-0.91	200,200,200,200	0
35	NA	0	8339	1/1	0.94	0.13	-1.06	8,8,8,8	0
35	NA	0	8333	1/1	0.91	0.11	-1.08	25,25,25,25	0
35	NA	P	8348	1/1	0.93	0.13	-1.12	45,45,45,45	0
33	MG	0	8055	1/1	0.93	0.12	-1.17	82,82,82,82	0
35	NA	0	8309	1/1	0.96	0.11	-1.17	24,24,24,24	0
33	MG	0	8052	1/1	0.97	0.13	-1.40	36,36,36,36	0
35	NA	0	8335	1/1	0.98	0.13	-1.43	47,47,47,47	0
41	CD	2	8404	1/1	0.77	0.87	-1.61	200,200,200,200	0
35	NA	0	8302	1/1	0.95	0.12	-1.72	18,18,18,18	0
33	MG	S	8073	1/1	0.95	0.21	-1.78	36,36,36,36	0
35	NA	0	8317	1/1	0.97	0.10	-1.78	23,23,23,23	0
36	CL	2	8504	1/1	0.74	0.43	-1.79	104,104,104,104	0
33	MG	0	8112	1/1	0.96	0.12	-1.79	34,34,34,34	0
35	NA	0	8305	1/1	0.99	0.11	-2.07	19,19,19,19	0
35	NA	I	8346	1/1	0.92	0.09	-2.07	20,20,20,20	0
33	MG	0	8059	1/1	0.95	0.13	-2.07	59,59,59,59	0
33	MG	2	8078	1/1	0.84	0.42	-2.16	73,73,73,73	0
33	MG	A	8065	1/1	0.95	0.09	-2.16	44,44,44,44	0
33	MG	0	8074	1/1	0.96	0.05	-2.25	27,27,27,27	0
36	CL	0	8512	1/1	0.99	0.10	-2.35	34,34,34,34	0
33	MG	0	8107	1/1	0.99	0.03	-2.72	24,24,24,24	0
33	MG	0	8101	1/1	0.92	0.12	-3.03	40,40,40,40	0
35	NA	Q	8338	1/1	1.00	0.07	-3.03	57,57,57,57	0
35	NA	L	8347	1/1	0.96	0.10	-3.15	7,7,7,7	0
36	CL	L	8518	1/1	0.96	0.12	-3.22	36,36,36,36	0
33	MG	0	8008	1/1	0.97	0.06	-3.25	42,42,42,42	0
33	MG	0	8032	1/1	0.99	0.06	-3.26	29,29,29,29	0
33	MG	0	8056	1/1	0.98	0.06	-3.32	35,35,35,35	0
33	MG	0	8110	1/1	0.98	0.09	-3.43	22,22,22,22	0
33	MG	0	8077	1/1	0.99	0.05	-3.46	21,21,21,21	0
35	NA	A	8345	1/1	0.97	0.11	-3.49	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8033	1/1	0.99	0.10	-3.93	18,18,18,18	0
33	MG	0	8039	1/1	0.98	0.06	-4.10	31,31,31,31	0
33	MG	0	8012	1/1	0.98	0.07	-4.17	26,26,26,26	0
35	NA	0	8353	1/1	0.98	0.07	-4.24	34,34,34,34	0
33	MG	0	8021	1/1	0.98	0.09	-4.29	26,26,26,26	0
33	MG	0	8014	1/1	0.98	0.07	-4.31	22,22,22,22	0
33	MG	0	8004	1/1	0.98	0.06	-4.34	30,30,30,30	0
35	NA	0	8344	1/1	0.97	0.06	-4.54	9,9,9,9	0
33	MG	0	8071	1/1	0.98	0.08	-4.82	66,66,66,66	0
33	MG	0	8091	1/1	0.98	0.06	-4.88	40,40,40,40	0
33	MG	0	8027	1/1	0.97	0.05	-5.00	37,37,37,37	0
33	MG	0	8108	1/1	0.98	0.06	-5.13	61,61,61,61	0
33	MG	0	8035	1/1	0.98	0.05	-5.15	39,39,39,39	0
41	CD	Z	8402	1/1	1.00	0.06	-5.22	49,49,49,49	0
35	NA	0	8320	1/1	0.98	0.07	-5.23	15,15,15,15	0
33	MG	0	8006	1/1	0.98	0.09	-5.25	28,28,28,28	0
33	MG	0	8038	1/1	0.99	0.04	-5.26	23,23,23,23	0
35	NA	0	8343	1/1	0.98	0.07	-5.54	17,17,17,17	0
33	MG	0	8017	1/1	0.99	0.03	-5.60	15,15,15,15	0
33	MG	0	8015	1/1	0.98	0.07	-5.74	29,29,29,29	0
33	MG	0	8084	1/1	0.98	0.07	-5.83	38,38,38,38	0
33	MG	0	8096	1/1	0.98	0.05	-6.39	33,33,33,33	0
33	MG	0	8057	1/1	0.98	0.10	-6.40	30,30,30,30	0
33	MG	0	8060	1/1	0.98	0.07	-6.80	32,32,32,32	0
33	MG	0	8062	1/1	0.98	0.04	-6.90	37,37,37,37	0
33	MG	0	8054	1/1	0.99	0.05	-7.00	28,28,28,28	0
33	MG	0	8010	1/1	0.97	0.05	-7.10	20,20,20,20	0
33	MG	0	8001	1/1	0.99	0.08	-7.31	21,21,21,21	0
33	MG	0	8058	1/1	0.96	0.06	-7.49	28,28,28,28	0
33	MG	0	8003	1/1	0.98	0.08	-7.56	22,22,22,22	0
33	MG	0	8020	1/1	1.00	0.07	-8.27	16,16,16,16	0
33	MG	0	8013	1/1	0.98	0.08	-8.37	25,25,25,25	0
33	MG	0	8080	1/1	0.99	0.07	-9.58	42,42,42,42	0
33	MG	0	8018	1/1	0.98	0.04	-9.65	32,32,32,32	0
33	MG	0	8002	1/1	0.99	0.05	-10.04	33,33,33,33	0
33	MG	0	8019	1/1	0.99	0.03	-10.72	13,13,13,13	0
33	MG	0	8007	1/1	0.99	0.05	-11.33	18,18,18,18	0
33	MG	0	8089	1/1	0.98	0.12	-	50,50,50,50	0
33	MG	0	8042	1/1	0.98	0.12	-	40,40,40,40	0
33	MG	0	8045	1/1	0.98	0.10	-	44,44,44,44	0
33	MG	0	8025	1/1	0.96	0.08	-	17,17,17,17	0
36	CL	X	8520	1/1	0.95	0.13	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8093	1/1	0.99	0.07	-	43,43,43,43	0
33	MG	0	8005	1/1	0.99	0.05	-	26,26,26,26	0
33	MG	0	8100	1/1	0.96	0.10	-	65,65,65,65	0
36	CL	0	8516	1/1	0.96	0.18	-	44,44,44,44	0
33	MG	0	8063	1/1	0.99	0.06	-	68,68,68,68	0
33	MG	0	8088	1/1	0.95	0.09	-	23,23,23,23	0
35	NA	0	8358	1/1	0.91	0.31	-	98,98,98,98	0
35	NA	0	8341	1/1	0.94	0.15	-	40,40,40,40	0
35	NA	0	8311	1/1	0.91	0.14	-	38,38,38,38	0
35	NA	9	8351	1/1	0.81	0.72	-	112,112,112,112	0
35	NA	0	8334	1/1	0.97	0.12	-	29,29,29,29	0
33	MG	0	8048	1/1	0.98	0.08	-	34,34,34,34	0
33	MG	0	8103	1/1	0.92	0.20	-	34,34,34,34	0
33	MG	0	8117	1/1	0.99	0.09	-	19,19,19,19	0
35	NA	0	8342	1/1	0.96	0.22	-	19,19,19,19	0
33	MG	0	8023	1/1	0.99	0.07	-	28,28,28,28	0
35	NA	0	8349	1/1	0.96	0.14	-	37,37,37,37	0
36	CL	I	8502	1/1	0.95	0.09	-	56,56,56,56	0
33	MG	0	8022	1/1	0.99	0.05	-	30,30,30,30	0
33	MG	0	8047	1/1	0.98	0.10	-	48,48,48,48	0
36	CL	0	8517	1/1	0.92	0.22	-	57,57,57,57	0
36	CL	0	8511	1/1	0.96	0.23	-	63,63,63,63	0
33	MG	0	8016	1/1	0.97	0.09	-	25,25,25,25	0
33	MG	0	8031	1/1	0.99	0.03	-	18,18,18,18	0
33	MG	0	8092	1/1	0.94	0.34	-	71,71,71,71	0
33	MG	0	8114	1/1	0.78	0.73	-	161,161,161,161	0
35	NA	0	8360	1/1	0.96	0.65	-	39,39,39,39	0
36	CL	Q	8506	1/1	0.99	0.11	-	43,43,43,43	0
33	MG	0	8076	1/1	0.84	0.18	-	70,70,70,70	0
33	MG	0	8113	1/1	0.96	0.20	-	36,36,36,36	0
36	CL	0	8513	1/1	0.95	0.11	-	52,52,52,52	0
35	NA	0	8330	1/1	0.98	0.19	-	21,21,21,21	0
33	MG	0	8079	1/1	0.98	0.05	-	27,27,27,27	0
36	CL	M	8507	1/1	0.93	0.15	-	54,54,54,54	0
33	MG	0	8082	1/1	0.94	0.13	-	43,43,43,43	0
35	NA	H	8322	1/1	0.86	0.25	-	48,48,48,48	0
35	NA	0	8377	1/1	0.83	0.28	-	59,59,59,59	0
33	MG	0	8036	1/1	0.97	0.10	-	32,32,32,32	0
35	NA	0	8385	1/1	0.65	0.39	-	52,52,52,52	0
33	MG	0	8043	1/1	0.96	0.07	-	34,34,34,34	0
35	NA	0	8319	1/1	0.96	0.09	-	50,50,50,50	0
33	MG	0	8086	1/1	0.95	0.10	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8097	1/1	0.98	0.14	-	30,30,30,30	0
33	MG	0	8085	1/1	0.97	0.30	-	103,103,103,103	0
33	MG	0	8081	1/1	0.98	0.08	-	36,36,36,36	0
35	NA	0	8306	1/1	0.90	0.68	-	21,21,21,21	0
35	NA	0	8359	1/1	0.98	0.18	-	42,42,42,42	0
33	MG	J	8069	1/1	0.98	0.08	-	47,47,47,47	0
33	MG	0	8099	1/1	0.94	0.18	-	37,37,37,37	0
35	NA	0	8355	1/1	0.93	0.60	-	60,60,60,60	0
33	MG	0	8116	1/1	0.91	0.10	-	64,64,64,64	0
33	MG	0	8090	1/1	0.97	0.11	-	65,65,65,65	0
36	CL	0	8514	1/1	0.98	0.12	-	44,44,44,44	0
33	MG	0	8111	1/1	0.91	0.10	-	49,49,49,49	0
33	MG	0	8046	1/1	0.92	0.09	-	40,40,40,40	0
33	MG	0	8104	1/1	0.95	0.16	-	41,41,41,41	0
33	MG	9	8095	1/1	0.93	0.14	-	72,72,72,72	0
35	NA	0	8328	1/1	0.89	0.49	-	41,41,41,41	0
35	NA	0	8315	1/1	0.98	0.15	-	32,32,32,32	0
35	NA	0	8313	1/1	0.99	0.15	-	59,59,59,59	0
33	MG	0	8098	1/1	0.98	0.29	-	24,24,24,24	0
33	MG	0	8040	1/1	0.98	0.09	-	107,107,107,107	0
33	MG	0	8009	1/1	0.99	0.04	-	18,18,18,18	0
33	MG	0	8068	1/1	0.98	0.08	-	58,58,58,58	0
35	NA	0	8384	1/1	0.35	1.14	-	87,87,87,87	0
33	MG	0	8102	1/1	0.85	1.14	-	135,135,135,135	0
35	NA	0	8357	1/1	0.93	0.11	-	53,53,53,53	0
33	MG	0	8050	1/1	0.95	0.23	-	78,78,78,78	0
35	NA	0	8336	1/1	0.93	0.08	-	30,30,30,30	0
33	MG	0	8011	1/1	0.98	0.20	-	1,1,1,1	0
35	NA	0	8363	1/1	0.64	0.74	-	40,40,40,40	0
33	MG	0	8034	1/1	0.99	0.03	-	22,22,22,22	0
35	NA	0	8301	1/1	0.94	0.11	-	28,28,28,28	0
33	MG	0	8066	1/1	0.94	0.14	-	60,60,60,60	0
33	MG	0	8029	1/1	0.98	0.05	-	23,23,23,23	0
33	MG	0	8087	1/1	0.94	0.10	-	36,36,36,36	0
36	CL	0	8503	1/1	0.94	0.18	-	49,49,49,49	0
33	MG	0	8028	1/1	0.97	0.06	-	23,23,23,23	0
35	NA	0	8316	1/1	0.97	0.19	-	28,28,28,28	0
35	NA	0	8369	1/1	0.89	0.36	-	67,67,67,67	0
35	NA	0	8329	1/1	0.23	0.56	-	62,62,62,62	0
35	NA	0	8370	1/1	0.96	0.28	-	48,48,48,48	0
33	MG	0	8049	1/1	0.87	0.29	-	73,73,73,73	0
33	MG	0	8051	1/1	0.89	0.17	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8106	1/1	0.95	0.09	-	64,64,64,64	0
33	MG	0	8030	1/1	0.99	0.11	-	29,29,29,29	0
36	CL	A	8509	1/1	0.90	0.25	-	76,76,76,76	0
36	CL	K	8510	1/1	0.84	0.23	-	70,70,70,70	0
35	NA	0	8318	1/1	0.99	0.08	-	22,22,22,22	0
33	MG	0	8075	1/1	0.97	0.06	-	50,50,50,50	0
36	CL	0	8522	1/1	0.85	0.37	-	76,76,76,76	0
33	MG	0	8072	1/1	0.97	0.10	-	43,43,43,43	0
35	NA	0	8367	1/1	0.96	0.20	-	36,36,36,36	0
35	NA	0	8307	1/1	0.92	0.23	-	40,40,40,40	0
35	NA	0	8354	1/1	0.81	0.37	-	29,29,29,29	0
33	MG	0	8024	1/1	0.86	0.68	-	109,109,109,109	0
35	NA	0	8314	1/1	0.94	0.16	-	33,33,33,33	0
41	CD	N	8405	1/1	0.92	0.06	-	111,111,111,111	0
35	NA	0	8375	1/1	0.97	0.20	-	40,40,40,40	0
35	NA	R	8312	1/1	0.55	0.65	-	84,84,84,84	0
33	MG	0	8083	1/1	0.99	0.05	-	38,38,38,38	0
33	MG	0	8061	1/1	0.99	0.07	-	28,28,28,28	0
33	MG	0	8037	1/1	0.99	0.05	-	34,34,34,34	0
36	CL	I	8501	1/1	0.98	0.13	-	60,60,60,60	0
33	MG	0	8115	1/1	0.94	0.12	-	58,58,58,58	0
33	MG	0	8094	1/1	0.97	0.06	-	54,54,54,54	0
33	MG	0	8026	1/1	0.99	0.08	-	25,25,25,25	0
33	MG	0	8041	1/1	0.95	0.28	-	50,50,50,50	0
35	NA	0	8352	1/1	0.85	0.26	-	28,28,28,28	0
33	MG	0	8070	1/1	0.98	0.44	-	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.