



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:55 PM GMT

PDB ID : 1YIT  
Title : Crystal Structure Of Virginiamycin M and S Bound To The 50S Ribosomal Subunit Of Haloarcula Marismortui  
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2005-01-13  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



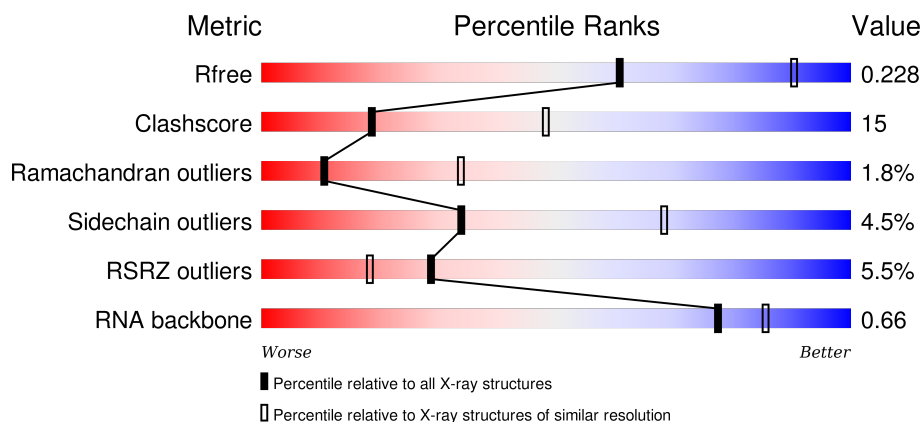
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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>59%</div> <div>30%</div> <div>5%</div> <div>6%</div> </div>
2	1	57	<div> <div>67%</div> <div>32%</div> <div>.</div> </div>
3	2	50	<div> <div>16%</div> <div>44%</div> <div>48%</div> <div>8%</div> </div>
4	3	92	<div> <div>12%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	8	7	
6	9	122	
7	A	240	
8	B	338	
9	C	246	
10	D	177	
11	E	178	
12	F	120	
13	G	348	
14	H	177	
15	I	162	
16	J	145	
17	K	132	
18	L	165	
19	M	195	
20	N	187	
21	O	116	
22	P	149	
23	Q	96	
24	R	155	
25	S	85	
26	T	120	
27	U	66	
28	V	71	
29	W	154	

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Mol	Chain	Length	Quality of chain
30	X	92	
31	Y	241	
32	Z	83	

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	8002	-	-	-	X
33	MG	0	8003	-	-	-	X
33	MG	0	8004	-	-	-	X
33	MG	0	8006	-	-	-	X
33	MG	0	8008	-	-	-	X
33	MG	0	8010	-	-	-	X
33	MG	0	8012	-	-	-	X
33	MG	0	8013	-	-	-	X
33	MG	0	8015	-	-	-	X
33	MG	0	8017	-	-	-	X
33	MG	0	8018	-	-	-	X
33	MG	0	8019	-	-	-	X
33	MG	0	8020	-	-	-	X
33	MG	0	8032	-	-	-	X
33	MG	0	8035	-	-	-	X
33	MG	0	8038	-	-	-	X
33	MG	0	8044	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8049	-	-	-	X
33	MG	0	8052	-	-	-	X
33	MG	0	8053	-	-	-	X
33	MG	0	8054	-	-	-	X
33	MG	0	8058	-	-	-	X
33	MG	0	8060	-	-	-	X
33	MG	0	8071	-	-	-	X
33	MG	0	8072	-	-	-	X
33	MG	0	8077	-	-	-	X
33	MG	0	8080	-	-	-	X
33	MG	0	8084	-	-	-	X
33	MG	0	8091	-	-	-	X
33	MG	0	8096	-	-	-	X
33	MG	0	8109	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8111	-	-	-	X
33	MG	0	8117	-	-	-	X
33	MG	A	8065	-	-	-	X
33	MG	B	8055	-	-	-	X
33	MG	B	8056	-	-	-	X
33	MG	K	8069	-	-	-	X
33	MG	Y	8108	-	-	-	X
34	K	0	8402	-	-	-	X
35	NA	0	8502	-	-	-	X
35	NA	0	8503	-	-	-	X
35	NA	0	8505	-	-	-	X
35	NA	0	8510	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8523	-	-	-	X
35	NA	0	8525	-	-	-	X
35	NA	0	8526	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8531	-	-	-	X
35	NA	0	8532	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8566	-	-	-	X
35	NA	0	8570	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	0	8572	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	0	8575	-	-	-	X
35	NA	0	8576	-	-	-	X
35	NA	0	8577	-	-	-	X
35	NA	9	8582	-	-	-	X
35	NA	A	8545	-	-	-	X
35	NA	L	8579	-	-	-	X
35	NA	M	8547	-	-	-	X
35	NA	R	8585	-	-	-	X
36	CL	0	8815	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	VIR	0	9000	-	-	-	X



## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 91326 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	26349	10873	19054	2745			

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 5 is a protein called VIRGINIAMYCIN S1.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	8	7	Total	C	N	O	0	0	0
			60	43	7	10			

- Molecule 6 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L2P.

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

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L3P.

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

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L4E.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L5P.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L6P.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L7AE.



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

- Molecule 13 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L13P.

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

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	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 18 is a protein called 50S RIBOSOMAL PROTEIN L15P.



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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L18P.

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

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L18E.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L19E.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L21E.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L22P.



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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L23P.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24P.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L24E.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29P.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30P.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31E.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32E.



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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	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 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	109	Total	Mg	0	0
			109	109		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	A	1	Total	Mg	0	0
			1	1		
33	T	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	3	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	1	Total	K	0	0
			1	1		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	73	Total Na 73 73	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	A	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

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

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

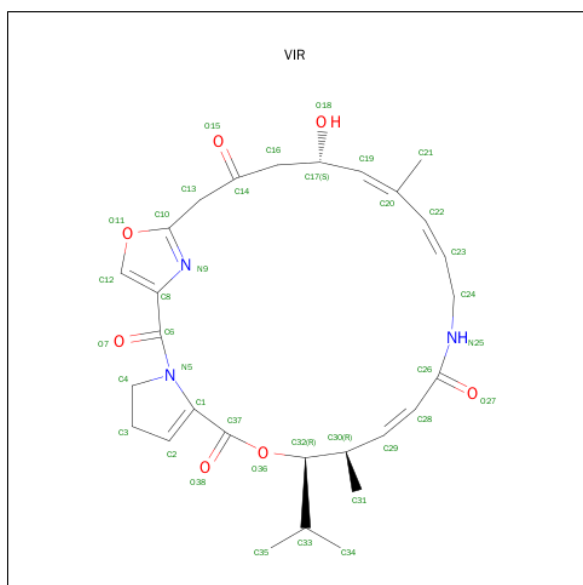
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	3	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0

- Molecule 37 is VIRGINIAMYCIN M1 (three-letter code: VIR) (formula:  $C_{28}H_{35}N_3O_7$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	1	Total C N O 38 28 3 7	0	0

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

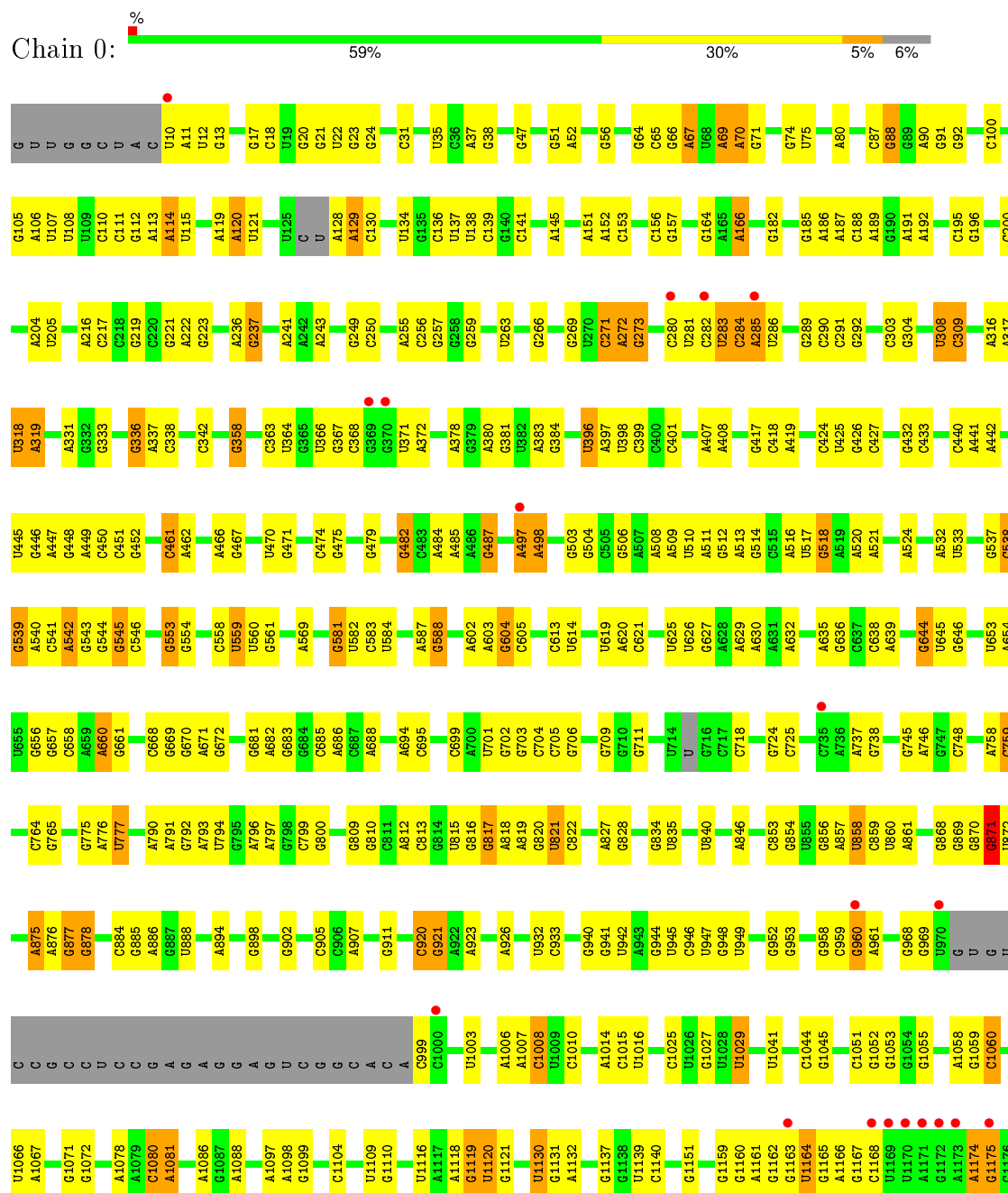
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	O	1	Total Cd 1 1	0	0
38	Z	1	Total Cd 1 1	0	0
38	1	1	Total Cd 1 1	0	0
38	3	1	Total Cd 1 1	0	0
38	U	1	Total Cd 1 1	0	0



### 3 Residue-property plots

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

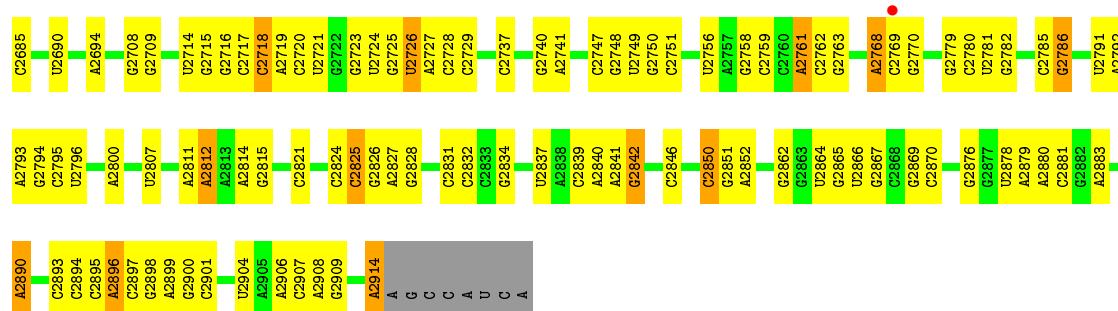
#### • Molecule 1: 23S RIBOSOMAL RNA



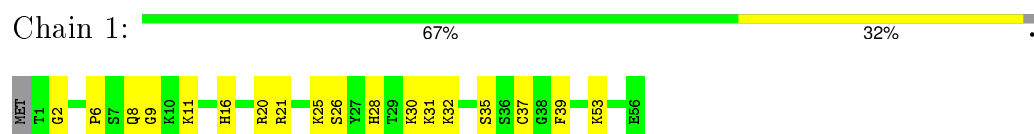


C2594	G2270	G2211	G2270	A1919	A1821	G1723	A1807	U1503	G1376	C1268	A1177
U2595	G2271	A	C	C1920	A1822	U1724	C1617	A1504	C1377	G1269	U1180
A2596	C	G	A	A1921	U1825	C1725	U1625	U1505	U1380	C1273	A1181
C2493	C	G	C	G1925	C1826	G1730	A1626	U1506	G1384	A1278	C1183
C2498	C	U	C	G1926	A1829	U1731	U1630	C1514	U1279	U1279	C1184
U2499	C	U	C	A1927	C1830	A1732	A1631	A1515	U1285	U1285	U1186
A2502	G	C	U	C1928	C1831	A1733	A1632	U1516	U1286	A1286	U1187
C2503	G	C	U	G1929	C1834	C1735	A1633	U1524	A1287	U1288	U1188
A2504	C	C	C	A1930	U1835	U1741	C1634	G1525	A1289	U1289	U1189
G2505	C	C	C	G1931	A1839	A1742	U1635	G1526	C1283	G1290	G1190
A2506	C	C	C	G1932	A1840	A1747	G1636	A1527	G1398	A1191	U1192
G2507	C	C	C	A1934	C1841	U1751	A1637	G1529	A1193	U1293	U1198
C2508	C	C	C	C1940	A1842	G1752	A1641	U1535	U1407	A1294	A1199
A2414	U	U	U	A1941	U1845	U1753	A1642	C1536	U1408	G1295	U1205
A2415	U	U	U	A1942	U1846	C1753	C1643	U1544	U1418	U1304	U1206
U2419	U	U	U	C1943	A1847	A1754	C1644	G1557	U1419	U1305	U1207
G2411	U	U	U	G1947	G1848	G1755	U1645	C1558	G1420	A1307	C1208
G2412	U	U	U	G1948	U1850	G1756	C1652	U1544	U1421	A1308	C1209
A2413	U	U	U	G1951	G1851	C1762	C1653	C1545	U1422	G1311	G1211
A2414	U	U	U	U	A1852	C1763	U1654	G1555	U1423	U1314	G1212
A2415	U	U	U	A	C1853	U1766	G1855	G1556	U1424	G1315	G1213
U2424	U	U	U	A	C1854	A1767	A1656	G1557	U1425	G1316	G1214
A2433	U	U	U	A	C1855	C1768	A1657	C1558	U1426	A1321	A1215
A2434	U	U	U	A	C1856	C1769	A1658	U	U1441	G1322	G1216
A2435	U	U	U	A	C1857	U1770	C1666	A1572	A1442	U1329	C1229
U2436	U	U	U	A	C1858	U1771	A1667	A1573	U1443	U1234	U1235
U2437	U	U	U	A	C1859	G1772	U1668	U1577	U1461	G1236	U1236
U2438	U	U	U	A	C1860	G1773	U1669	C1579	C1462	U1237	U1237
U2439	U	U	U	A	C1861	A1778	C1675	A1580	U1463	C1238	C1238
U2440	U	U	U	A	C1862	U1779	C1676	U1587	U1471	G1239	G1239
U2441	U	U	U	A	C1863	A1783	G1681	G1588	C1472	A1242	A1242
U2442	U	U	U	A	C1864	U1784	A1882	G1589	U1473	C1243	C1243
U2443	U	U	U	A	C1865	G1785	G1682	C1592	C1474	U1244	C1245
U2444	U	U	U	A	C1866	C1786	A1883	C1593	C1477	A1246	A1246
U2445	U	U	U	A	C1867	C1787	U1884	C1594	U1483	U1249	U1249
U2446	U	U	U	A	C1868	U1788	C1687	C1595	G1484	C1250	C1250
U2447	U	U	U	A	C1869	G1789	C1692	C1596	U1485	C1251	C1251
U2448	U	U	U	A	C1870	C1790	A1701	C1597	U1488	G1351	C1254
U2449	U	U	U	A	C1871	U1791	U1702	C1598	U1494	A1352	U1266
U2450	U	U	U	A	C1872	G1798	G1706	C1599	C1495	C1360	C1267
U2451	U	U	U	A	C1873	U1805	G1707	C1599	A1496	U1375	
U2452	U	U	U	A	C1874	G1806	C1708	C1599	U1345		
U2453	U	U	U	A	C1875	U1903	G1709	C1599	U1346		
U2454	U	U	U	A	C1876	U1904	A1710	C1599	G1351		
U2455	U	U	U	A	C1877	U1905	A1711	C1599	A1352		
U2456	U	U	U	A	C1878	G1812	A1712	C1599	C1353		
U2457	U	U	U	A	C1879	U1815	A1717	C1599	C1360		
U2458	U	U	U	A	C1880	G1819	A1722	C1599	U1500		
U2459	U	U	U	A	C1881	G1820		C1599			
U2460	U	U	U	A	C1882			C1599			
U2461	U	U	U	A	C1883			C1599			
U2462	U	U	U	A	C1884			C1599			
U2463	U	U	U	A	C1885			C1599			
U2464	U	U	U	A	C1886			C1599			
U2465	U	U	U	A	C1887			C1599			
U2466	U	U	U	A	C1888			C1599			
U2467	U	U	U	A	C1889			C1599			
U2468	U	U	U	A	C1890			C1599			
U2469	U	U	U	A	C1891			C1599			
U2470	U	U	U	A	C1892			C1599			
U2471	U	U	U	A	C1893			C1599			
U2472	U	U	U	A	C1894			C1599			
U2473	U	U	U	A	C1895			C1599			
U2474	U	U	U	A	C1896			C1599			
U2475	U	U	U	A	C1897			C1599			
U2476	U	U	U	A	C1898			C1599			
U2477	U	U	U	A	C1899			C1599			
U2478	U	U	U	A	C1900			C1599			
U2479	U	U	U	A	C1901			C1599			
U2480	U	U	U	A	C1902			C1599			
U2481	U	U	U	A	C1903			C1599			
U2482	U	U	U	A	C1904			C1599			
U2483	U	U	U	A	C1905			C1599			
U2484	U	U	U	A	C1906			C1599			
U2485	U	U	U	A	C1907			C1599			
U2486	U	U	U	A	C1908			C1599			
U2487	U	U	U	A	C1909			C1599			
U2488	U	U	U	A	C1910			C1599			
U2489	U	U	U	A	C1911			C1599			
U2490	U	U	U	A	C1912			C1599			
U2491	U	U	U	A	C1913			C1599			
U2492	U	U	U	A	C1914			C1599			
U2493	U	U	U	A	C1915			C1599			
U2494	U	U	U	A	C1916			C1599			
U2495	U	U	U	A	C1917			C1599			
U2496	U	U	U	A	C1918			C1599			
U2497	U	U	U	A	C1919			C1599			
U2498	U	U	U	A	C1920			C1599			
U2499	U	U	U	A	C1921			C1599			
U2500	U	U	U	A	C1922			C1599			
U2501	U	U	U	A	C1923			C1599			
U2502	U	U	U	A	C1924			C1599			
U2503	U	U	U	A	C1925			C1599			
U2504	U	U	U	A	C1926			C1599			
U2505	U	U	U	A	C1927			C1599			
U2506	U	U	U	A	C1928			C1599			
U2507	U	U	U	A	C1929			C1599			
U2508	U	U	U	A	C1930			C1599			
U2509	U	U	U	A	C1931			C1599			
U2510	U	U	U	A	C1932			C1599			
U2511	U	U	U	A	C1933			C1599			
U2512	U	U	U	A	C1934			C1599			
U2513	U	U	U	A	C1935			C1599			
U2514	U	U	U	A	C1936			C1599			
U2515	U	U	U	A	C1937			C1599			
U2516	U	U	U	A	C1938			C1599			
U2517	U	U	U	A	C1939			C1599			
U2518	U	U	U	A	C1940			C1599			
U2519	U	U	U	A	C1941			C1599			
U2520	U	U	U	A	C1942			C1599			
U2521	U	U	U	A	C1943			C1599			
U2522	U	U	U	A	C1944			C1599			
U2523	U	U	U	A	C1945			C1599			
U2524	U	U	U	A	C1946			C1599			
U2525	U	U	U	A	C1947			C1599			
U2526	U	U	U	A	C1948			C1599			
U2527	U	U	U	A	C1949			C1599			
U2528	U	U	U	A	C1950			C1599			
U2529	U	U	U	A	C1951			C1599			
U2530	U	U	U	A	C1952			C1599			
U2531	U	U	U	A	C1953			C1599			
U2532	U	U	U	A	C1954			C1599			
U2533	U	U	U	A	C1955			C1599			
U2534	U	U	U	A	C1956			C1599			
U2535	U	U	U	A	C1957			C1599			
U2536	U	U	U	A	C1958			C1599			
U2537	U	U	U	A	C1959			C1599			
U2538	U	U	U	A	C1960			C1599			
U2539	U	U	U	A	C1961			C1599			
U2540	U	U	U	A	C1962			C1599			
U2541	U	U	U	A	C1963			C1599			
U2542	U	U	U	A	C1964			C1599			
U2543	U	U	U	A	C1965			C1599			
U2544	U	U	U	A	C1966			C1599			
U2545	U	U	U	A	C1967			C1599			
U2546	U	U	U	A	C1968			C1599			
U2547	U	U	U	A	C1969			C1599			
U2548	U	U	U	A	C1970			C1599			
U2549	U	U	U	A	C1971			C1599			
U2550	U	U	U	A	C1972			C1599			
U2551	U	U	U	A	C1973			C1599			
U2552	U	U	U	A	C1974			C1599			
U2553	U	U	U	A	C1975			C1			

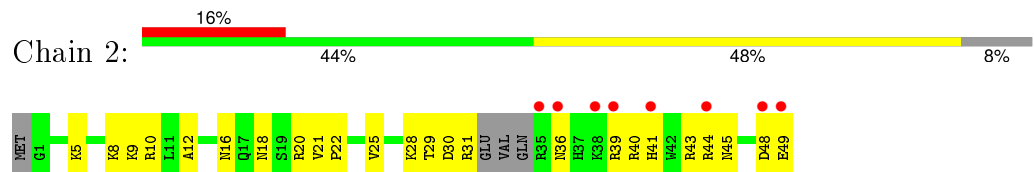




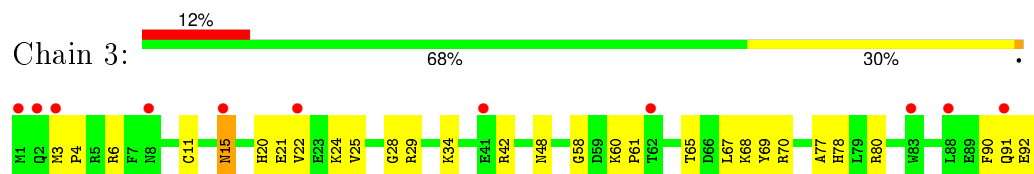
• Molecule 2: 50S RIBOSOMAL PROBLEM L37E



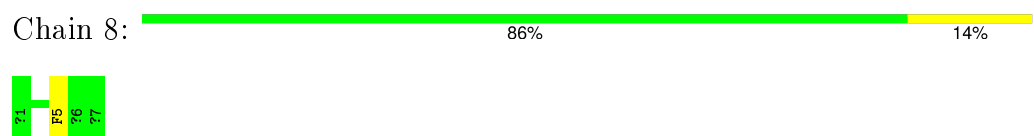
• Molecule 3: 50S RIBOSOMAL PROBLEM L39E



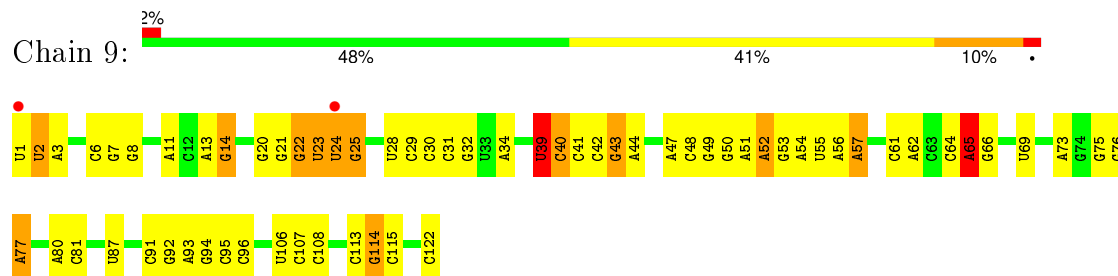
• Molecule 4: 50S RIBOSOMAL PROBLEM L44E



• Molecule 5: VIRGINIAMYCIN S1



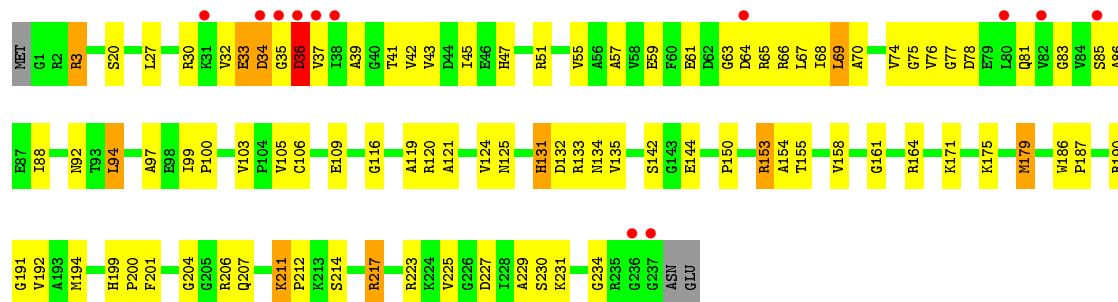
• Molecule 6: 5S RIBOSOMAL RNA



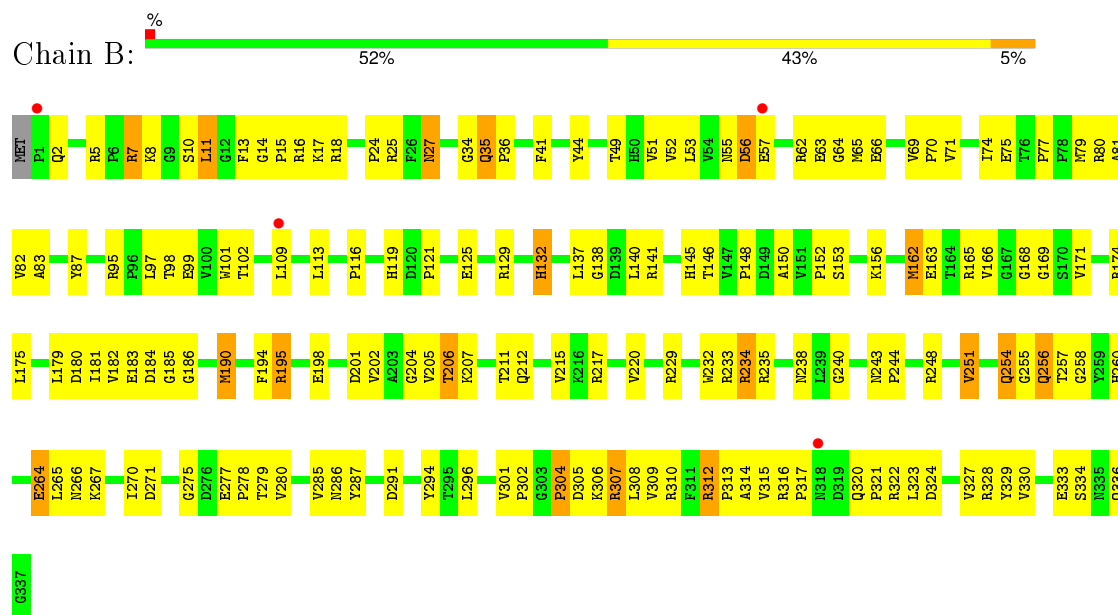
• Molecule 7: 50S RIBOSOMAL PROBLEM L2P



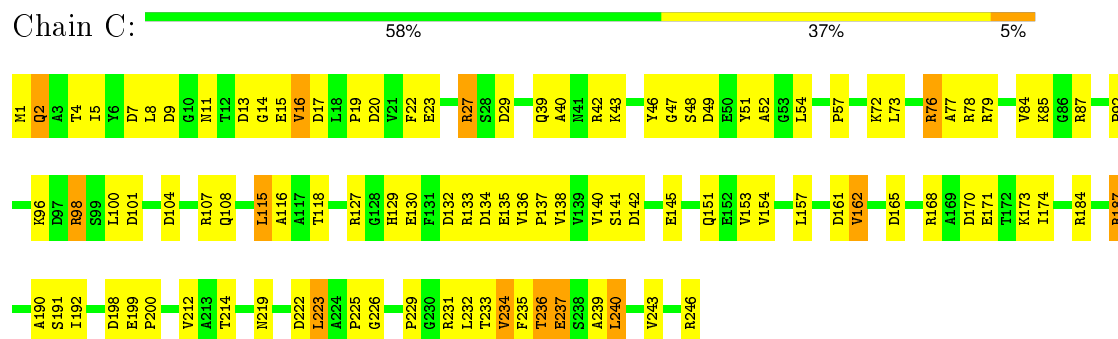




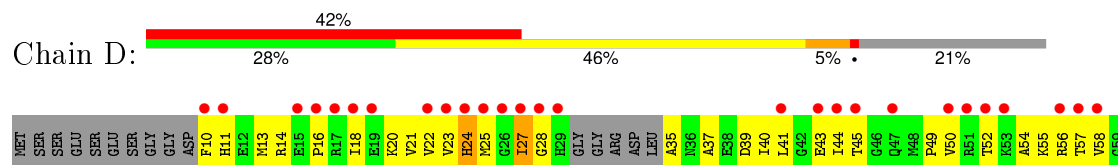
### • Molecule 8: 50S RIBOSOMAL PROTEIN L3P



### • Molecule 9: 50S RIBOSOMAL PROTEIN L4E



### • Molecule 10: 50S RIBOSOMAL PROTEIN L5P

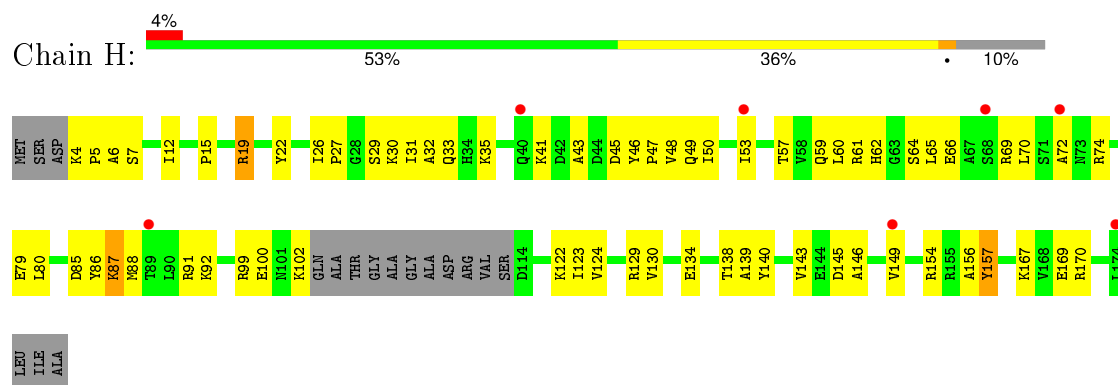




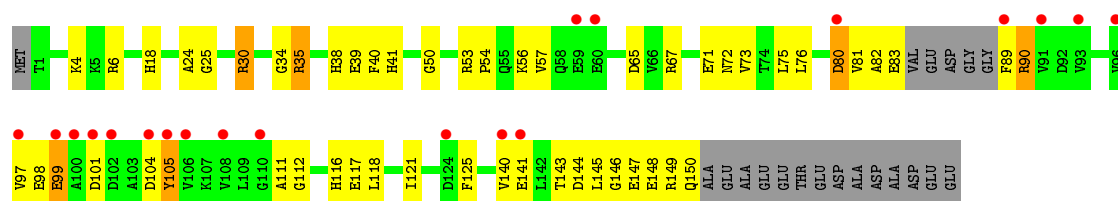




- Molecule 14: 50S RIBOSOMAL PROTEIN L10E

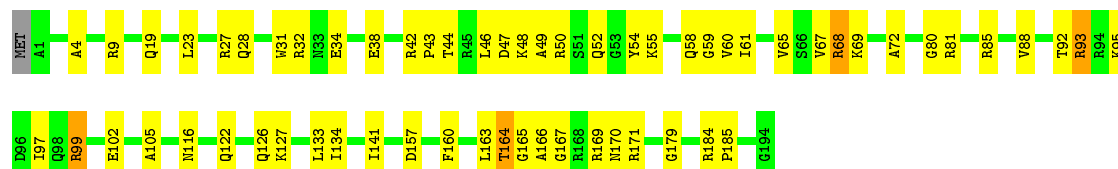






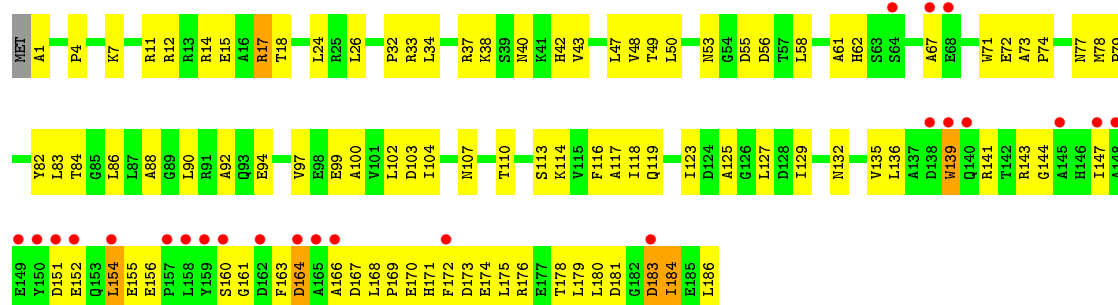
• Molecule 19: 50S RIBOSOMAL PROTEIN L15E

Chain M: 68% 29% ..



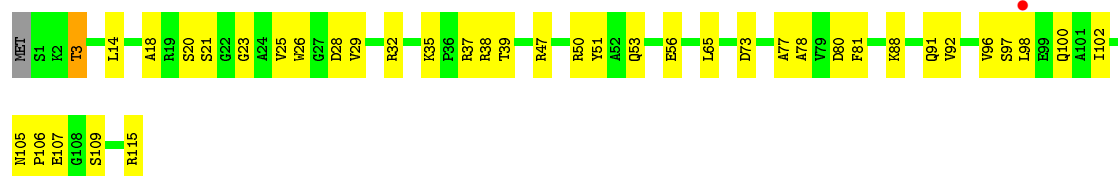
• Molecule 20: 50S RIBOSOMAL PROTEIN L18P

Chain N: 13% 47% 49% ..



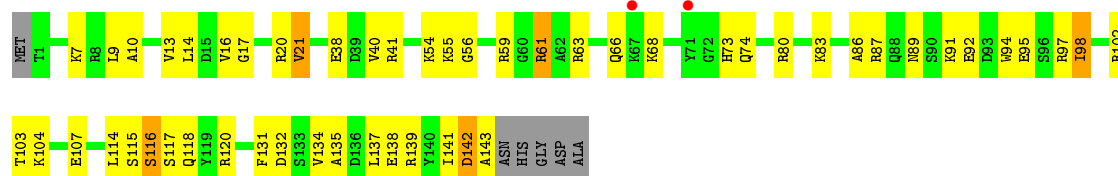
• Molecule 21: 50S RIBOSOMAL PROTEIN L18E

Chain O: % 66% 33% ..



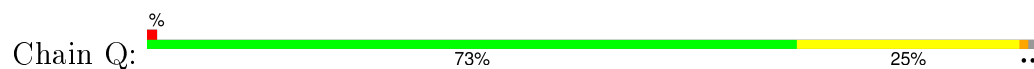
• Molecule 22: 50S RIBOSOMAL PROTEIN L19E

Chain P: % 60% 32% ..

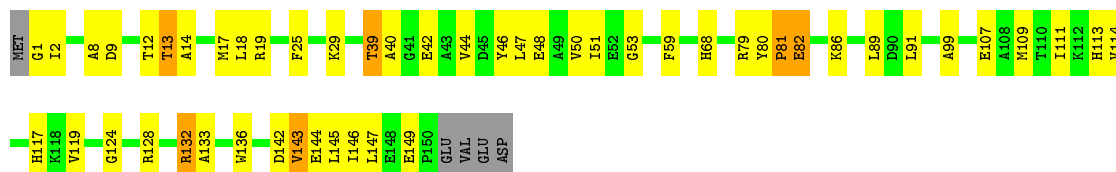


• Molecule 23: 50S RIBOSOMAL PROTEIN L21E





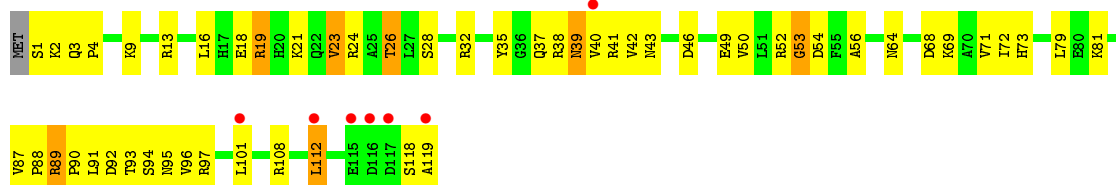
- Molecule 24: 50S RIBOSOMAL PROTEIN L22P



- Molecule 25: 50S RIBOSOMAL PROTEIN L23P



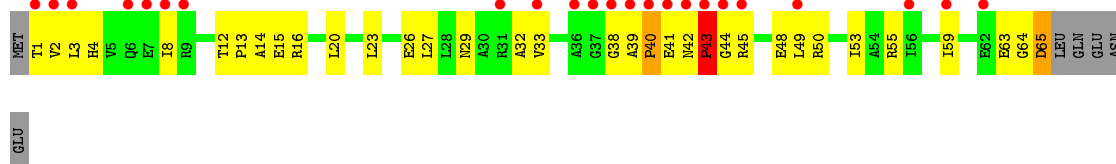
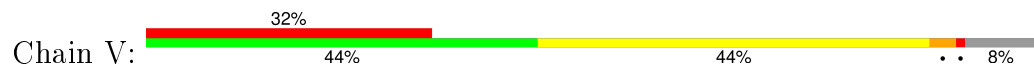
- Molecule 26: 50S RIBOSOMAL PROTEIN L24P



- Molecule 27: 50S RIBOSOMAL PROTEIN L24E

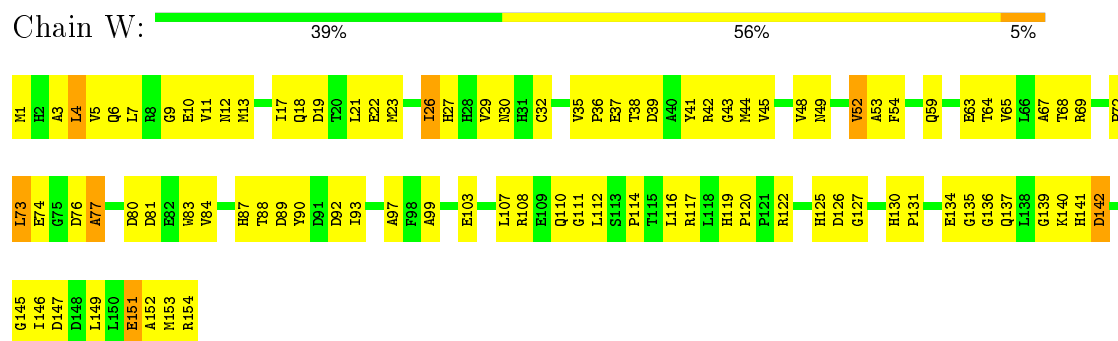


- Molecule 28: 50S RIBOSOMAL PROTEIN L29P

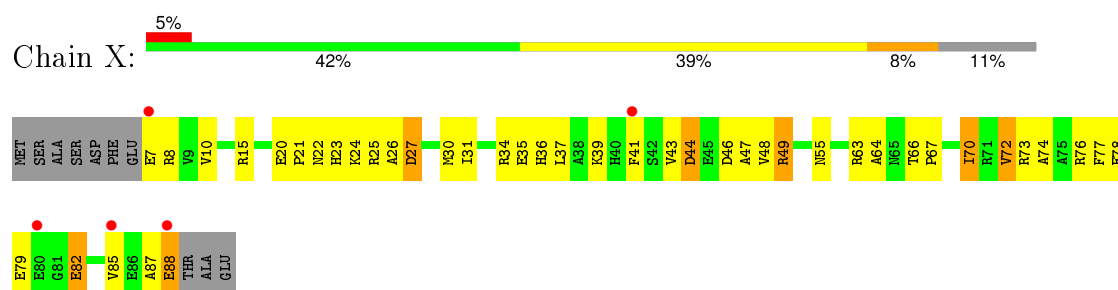


- Molecule 29: 50S RIBOSOMAL PROTEIN L30P

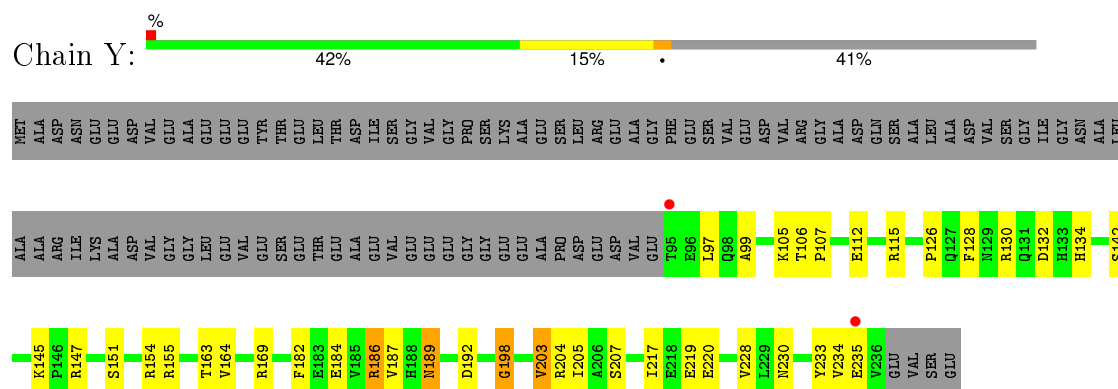




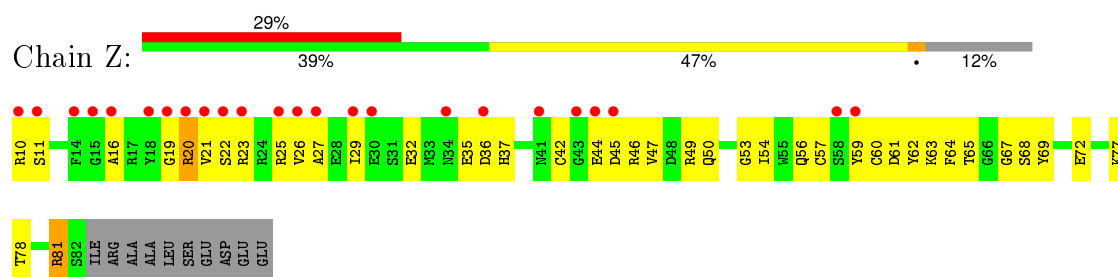
• Molecule 30: 50S RIBOSOMAL PROTEIN L31E



• Molecule 31: 50S RIBOSOMAL PROTEIN L32E



• Molecule 32: 50S RIBOSOMAL PROTEIN L37AE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.58 Å   299.76 Å   573.56 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.99 – 2.80 49.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.99-2.80) 93.7 (49.90-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.81 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.175   ,   0.221 0.209   ,   0.228	Depositor DCC
$R_{free}$ test set	4114 reflections (0.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 418145 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	91326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, DBB, CD, VIR, 1MA, UR3, OMU, 004, MHV, MEA, MHW, 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	0/65958	0.69	12/102869 (0.0%)
2	1	0.41	0/438	0.62	0/578
3	2	0.34	0/401	0.53	0/529
4	3	0.35	0/771	0.55	0/1024
5	8	1.13	0/13	1.01	0/15
6	9	0.33	0/2904	0.69	1/4526 (0.0%)
7	A	0.32	0/1786	0.64	0/2408
8	B	0.33	0/2690	0.64	0/3652
9	C	0.36	0/1884	0.63	0/2551
10	D	0.31	0/1111	0.53	0/1498
11	E	0.33	0/1382	0.58	0/1880
12	F	0.31	0/901	0.56	0/1224
13	G	0.29	0/241	0.47	0/324
14	H	0.34	0/1302	0.64	0/1743
15	I	0.29	0/526	0.55	0/716
16	J	0.37	0/1136	0.63	0/1530
17	K	0.34	0/1001	0.68	0/1347
18	L	0.32	0/1130	0.62	0/1509
19	M	0.33	0/1582	0.61	0/2117
20	N	0.29	0/1474	0.60	0/1999
21	O	0.33	0/874	0.59	0/1181
22	P	0.32	0/1147	0.54	0/1528
23	Q	0.36	0/749	0.69	0/1005
24	R	0.35	0/1172	0.64	0/1578
25	S	0.33	0/648	0.58	0/875
26	T	0.32	0/958	0.63	0/1289
27	U	0.33	0/417	0.58	0/562
28	V	0.28	0/502	0.58	0/675
29	W	0.35	0/1219	0.65	0/1655
30	X	0.34	0/664	0.59	0/895
31	Y	0.34	0/1146	0.65	0/1536
32	Z	0.32	0/589	0.59	0/787



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.36	0/98716	0.67	13/147605 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	38
6	9	0	4
All	All	0	42

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1942	A	C5'-C4'-C3'	7.56	128.09	116.00
1	0	871	G	C5'-C4'-O4'	-6.96	100.74	109.10
1	0	1504	A	C1'-O4'-C4'	-6.20	104.94	109.90
6	9	39	U	N1-C1'-C2'	6.08	121.90	114.00
1	0	2467	A	C1'-O4'-C4'	-5.61	105.42	109.90

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	22	U	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	462	A	Sidechain
1	0	471	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	29810	865	0
2	1	431	0	426	23	0
3	2	396	0	413	22	0
4	3	755	0	728	22	0
5	8	60	0	46	1	0
6	9	2599	0	1325	70	0
7	A	1753	0	1766	125	0
8	B	2625	0	2533	156	0
9	C	1859	0	1816	108	0
10	D	1094	0	1085	90	0
11	E	1357	0	1266	64	0
12	F	890	0	843	51	0
13	G	240	0	231	17	0
14	H	1282	0	1292	74	0
15	I	519	0	500	52	0
16	J	1120	0	1098	68	0
17	K	992	0	1031	62	0
18	L	1118	0	1076	47	0
19	M	1558	0	1566	60	0
20	N	1445	0	1401	105	0
21	O	865	0	873	29	0
22	P	1136	0	1123	54	0
23	Q	735	0	729	22	0
24	R	1149	0	1122	56	0
25	S	641	0	605	24	0
26	T	950	0	923	53	0
27	U	410	0	364	26	0
28	V	499	0	511	37	0
29	W	1196	0	1137	109	0
30	X	654	0	653	42	0
31	Y	1130	0	1133	43	0
32	Z	578	0	540	42	0
33	0	109	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	2	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	1	0	0	0	0
35	0	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	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	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	38	0	34	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
All	All	91326	0	59999	2318	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 15.

The worst 5 of 2318 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)
1:0:656:G:H5'	21:O:3:THR:HG22	1.23	1.16
1:0:871:G:H8	1:0:871:G:H5'	1.13	1.14
9:C:236:THR:HG22	9:C:239:ALA:H	1.13	1.07
1:0:871:G:C8	1:0:871:G:H5'	1.92	1.04
1:0:21:G:H5'	24:R:2:ILE:HA	1.40	1.04



There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
3	2	42/50 (84%)	39 (93%)	3 (7%)	0	100	100
4	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	17	50
5	8	2/7 (29%)	2 (100%)	0	0	100	100
7	A	235/240 (98%)	202 (86%)	28 (12%)	5 (2%)	9	29
8	B	335/338 (99%)	294 (88%)	35 (10%)	6 (2%)	11	34
9	C	244/246 (99%)	216 (88%)	27 (11%)	1 (0%)	39	74
10	D	134/177 (76%)	97 (72%)	28 (21%)	9 (7%)	1	4
11	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
12	F	117/120 (98%)	101 (86%)	11 (9%)	5 (4%)	3	10
13	G	25/348 (7%)	22 (88%)	3 (12%)	0	100	100
14	H	156/177 (88%)	142 (91%)	12 (8%)	2 (1%)	15	44
15	I	68/162 (42%)	43 (63%)	22 (32%)	3 (4%)	3	10
16	J	140/145 (97%)	127 (91%)	7 (5%)	6 (4%)	3	10
17	K	130/132 (98%)	119 (92%)	11 (8%)	0	100	100
18	L	141/165 (86%)	115 (82%)	23 (16%)	3 (2%)	9	29
19	M	192/195 (98%)	176 (92%)	15 (8%)	1 (0%)	34	69
20	N	184/187 (98%)	161 (88%)	17 (9%)	6 (3%)	5	16
21	O	113/116 (97%)	107 (95%)	5 (4%)	1 (1%)	21	55
22	P	141/149 (95%)	131 (93%)	6 (4%)	4 (3%)	6	21
23	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
24	R	148/155 (96%)	134 (90%)	13 (9%)	1 (1%)	26	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
26	T	117/120 (98%)	103 (88%)	12 (10%)	2 (2%)	11	36
27	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
28	V	63/71 (89%)	55 (87%)	6 (10%)	2 (3%)	5	17
29	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	15	44
30	X	80/92 (87%)	71 (89%)	7 (9%)	2 (2%)	7	24
31	Y	140/241 (58%)	131 (94%)	8 (6%)	1 (1%)	26	62
32	Z	71/83 (86%)	59 (83%)	9 (13%)	3 (4%)	3	11
All	All	3707/4444 (83%)	3293 (89%)	348 (9%)	66 (2%)	11	34

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	34	ASP
10	D	63	ILE
10	D	137	PRO
12	F	101	ALA
16	J	5	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	46/47 (98%)	46 (100%)	0	100	100
3	2	42/46 (91%)	40 (95%)	2 (5%)	31	66
4	3	79/79 (100%)	78 (99%)	1 (1%)	76	94
5	8	2/2 (100%)	2 (100%)	0	100	100
7	A	179/182 (98%)	169 (94%)	10 (6%)	26	59
8	B	282/283 (100%)	263 (93%)	19 (7%)	20	50
9	C	193/193 (100%)	176 (91%)	17 (9%)	12	35
10	D	117/148 (79%)	110 (94%)	7 (6%)	24	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	E	152/156 (97%)	147 (97%)	5 (3%)	45	79
12	F	93/94 (99%)	92 (99%)	1 (1%)	80	95
13	G	27/283 (10%)	26 (96%)	1 (4%)	41	76
14	H	134/145 (92%)	131 (98%)	3 (2%)	60	89
15	I	58/130 (45%)	57 (98%)	1 (2%)	68	92
16	J	118/121 (98%)	110 (93%)	8 (7%)	20	49
17	K	106/106 (100%)	103 (97%)	3 (3%)	51	84
18	L	113/127 (89%)	107 (95%)	6 (5%)	28	61
19	M	158/159 (99%)	152 (96%)	6 (4%)	40	74
20	N	149/150 (99%)	145 (97%)	4 (3%)	52	85
21	O	93/94 (99%)	90 (97%)	3 (3%)	46	80
22	P	113/117 (97%)	108 (96%)	5 (4%)	35	69
23	Q	79/80 (99%)	77 (98%)	2 (2%)	55	86
24	R	117/122 (96%)	112 (96%)	5 (4%)	35	70
25	S	71/74 (96%)	69 (97%)	2 (3%)	51	84
26	T	105/106 (99%)	99 (94%)	6 (6%)	25	58
27	U	44/52 (85%)	43 (98%)	1 (2%)	58	88
28	V	51/57 (90%)	49 (96%)	2 (4%)	39	74
29	W	130/130 (100%)	123 (95%)	7 (5%)	27	60
30	X	66/74 (89%)	59 (89%)	7 (11%)	8	24
31	Y	120/196 (61%)	116 (97%)	4 (3%)	45	79
32	Z	60/68 (88%)	60 (100%)	0	100	100
All	All	3097/3621 (86%)	2959 (96%)	138 (4%)	34	68

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	G	64	ASN
17	K	129	THR
30	X	15	ARG
14	H	87	LYS
16	J	52	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:



Mol	Chain	Res	Type
17	K	42	ASN
19	M	170	ASN
29	W	125	HIS
18	L	18	HIS
18	L	116	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	239 (8%)	27 (0%)
6	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	255 (8%)	28 (0%)

5 of 255 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 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1450	C
1	0	1856	C
1	0	2761	A
1	0	1506	U
1	0	1685	A

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

10 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	12,22,23	1.07	1 (8%)	19,31,34	3.15	2 (10%)
1	OMG	0	2588	1	17,26,27	0.99	1 (5%)	21,38,41	2.56	3 (14%)
1	UR3	0	2619	1	12,22,23	0.89	0	16,32,35	0.87	0
1	PSU	0	2621	1	13,21,22	1.49	2 (15%)	18,30,33	6.11	4 (22%)
1	1MA	0	628	1	14,25,26	1.02	1 (7%)	15,37,40	1.14	1 (6%)
5	MHW	8	1	33,5	9,9,10	1.78	3 (33%)	8,11,13	0.78	0
5	DBB	8	3	5	4,5,6	0.64	0	3,5,7	1.49	1 (33%)
5	MEA	8	5	5	10,12,13	1.65	4 (40%)	10,14,16	1.26	1 (10%)
5	MHV	8	6	5	7,9,10	1.14	1 (14%)	8,11,13	1.29	0
5	004	8	7	5	9,10,11	2.04	2 (22%)	10,12,14	2.28	3 (30%)

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	-	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	-	0/3/25/26	0/3/3/3
5	MHW	8	1	33,5	-	0/2/2/4	0/1/1/1
5	DBB	8	3	5	-	0/2/4/6	0/0/0/0
5	MEA	8	5	5	-	0/4/8/10	0/1/1/1
5	MHV	8	6	5	-	0/1/12/14	0/1/1/1
5	004	8	7	5	-	0/4/6/8	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.45	1.48	1.52
5	8	5	MEA	CE2-CZ	2.08	1.43	1.38
5	8	5	MEA	CA-N	2.14	1.51	1.47
5	8	7	004	CD2-CG2	2.21	1.43	1.38
1	0	2621	PSU	C4-N3	2.39	1.37	1.33

The worst 5 of 15 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.44	114.66	128.33
1	0	2588	OMG	C5-C6-N1	-8.78	111.58	123.59
1	0	628	1MA	C2-N3-C4	-3.59	110.83	116.40
1	0	2587	OMU	C5-C4-N3	-3.27	114.73	123.12
5	8	5	MEA	O-C-CA	-3.24	116.88	125.44

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
1	0	2587	OMU	2	0
1	0	2619	UR3	2	0
5	8	5	MEA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	VIR	0	9000	-	34,40,40	2.45	17 (50%)	37,55,55	1.91	8 (21%)

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	VIR	0	9000	-	-	0/42/58/58	0/1/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9000	VIR	C28-C29	-5.64	1.17	1.32
37	0	9000	VIR	C16-C17	-3.38	1.48	1.54
37	0	9000	VIR	C13-C14	-2.92	1.46	1.51
37	0	9000	VIR	C1-C37	-2.60	1.38	1.47
37	0	9000	VIR	C17-C19	-2.55	1.47	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9000	VIR	C28-C26-N25	-4.85	103.70	114.87
37	0	9000	VIR	C8-C6-N5	-2.98	111.19	118.55
37	0	9000	VIR	C12-C8-C6	-2.10	122.48	129.47
37	0	9000	VIR	O7-C6-C8	2.04	123.28	118.75
37	0	9000	VIR	C31-C30-C32	2.29	115.45	111.08

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%)	0.05	41 (1%) 76 68	20, 45, 89, 150	0
2	1	56/57 (98%)	-0.18	0 100 100	25, 32, 36, 40	0
3	2	46/50 (92%)	0.82	8 (17%) 2 1	28, 59, 93, 108	0
4	3	92/92 (100%)	0.98	11 (11%) 6 3	42, 60, 72, 82	0
5	8	2/7 (28%)	0.06	0 100 100	40, 40, 40, 41	0
6	9	122/122 (100%)	0.17	2 (1%) 74 66	35, 62, 88, 150	0
7	A	237/240 (98%)	0.29	12 (5%) 32 21	26, 53, 88, 108	0
8	B	337/338 (99%)	0.06	4 (1%) 81 73	25, 51, 77, 89	0
9	C	246/246 (100%)	0.03	0 100 100	21, 43, 68, 77	0
10	D	140/177 (79%)	2.38	74 (52%) 0 0	55, 98, 121, 131	0
11	E	172/178 (96%)	0.75	13 (7%) 17 9	42, 64, 86, 95	0
12	F	119/120 (99%)	0.54	9 (7%) 17 9	46, 69, 92, 107	0
13	G	29/348 (8%)	1.79	12 (41%) 0 0	70, 87, 93, 97	0
14	H	160/177 (90%)	0.46	7 (4%) 38 26	37, 56, 91, 103	0
15	I	70/162 (43%)	3.45	50 (71%) 0 0	105, 121, 139, 140	0
16	J	142/145 (97%)	0.09	1 (0%) 89 84	34, 48, 66, 85	0
17	K	132/132 (100%)	0.04	3 (2%) 64 52	28, 48, 68, 79	0
18	L	145/165 (87%)	0.79	20 (13%) 4 2	24, 64, 104, 118	0
19	M	194/195 (99%)	-0.15	0 100 100	28, 41, 57, 63	0
20	N	186/187 (99%)	0.69	24 (12%) 5 2	37, 63, 108, 116	0
21	O	115/116 (99%)	0.09	1 (0%) 85 79	35, 51, 70, 73	0
22	P	143/149 (95%)	0.18	2 (1%) 78 69	33, 53, 70, 75	0
23	Q	95/96 (98%)	0.04	1 (1%) 82 74	35, 42, 58, 75	0
24	R	150/155 (96%)	-0.06	0 100 100	30, 42, 61, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	S	81/85 (95%)	0.02	2 (2%) 61 48	40, 59, 77, 84	0
26	T	119/120 (99%)	0.46	7 (5%) 26 16	36, 54, 82, 98	0
27	U	53/66 (80%)	0.51	6 (11%) 7 3	40, 53, 70, 80	0
28	V	65/71 (91%)	1.79	23 (35%) 0 0	51, 72, 112, 117	0
29	W	154/154 (100%)	-0.21	0 100 100	32, 45, 62, 74	0
30	X	82/92 (89%)	0.37	5 (6%) 25 15	39, 54, 76, 93	0
31	Y	142/241 (58%)	-0.01	2 (1%) 78 69	24, 42, 64, 87	0
32	Z	73/83 (87%)	1.47	24 (32%) 0 0	64, 78, 91, 99	0
All	All	6648/7488 (88%)	0.28	364 (5%) 29 18	20, 50, 97, 150	0

The worst 5 of 364 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	V	1	THR	11.6
15	I	128	THR	9.0
28	V	40	PRO	8.6
10	D	18	ILE	7.7
10	D	63	ILE	7.7

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	OMG	0	2588	24/25	0.98	0.15	-	28,30,34,36	0
1	OMU	0	2587	21/22	0.98	0.17	-	31,34,37,40	0
1	1MA	0	628	23/24	0.98	0.16	-	26,28,29,30	0
1	UR3	0	2619	21/22	0.98	0.17	-	26,32,37,38	0
5	MHV	8	6	9/10	0.96	0.17	-	42,43,45,48	0
5	MHW	8	1	9/10	0.92	0.21	-	37,40,43,44	0
5	MEA	8	5	12/13	0.95	0.21	-	39,40,43,43	0
1	PSU	0	2621	20/21	0.98	0.14	-	25,29,33,34	0
5	004	8	7	10/11	0.97	0.22	-	41,45,48,49	0
5	DBB	8	3	6/7	0.95	0.17	-	36,40,40,41	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	0	8573	1/1	0.94	0.84	59.27	68,68,68,68	0
35	NA	0	8561	1/1	0.86	0.61	52.62	59,59,59,59	0
33	MG	0	8071	1/1	0.55	0.67	46.04	68,68,68,68	0
35	NA	0	8535	1/1	0.46	0.59	41.56	44,44,44,44	0
33	MG	0	8038	1/1	0.90	0.54	41.23	26,26,26,26	0
33	MG	0	8060	1/1	0.67	0.51	39.62	51,51,51,51	0
35	NA	0	8572	1/1	0.85	0.60	36.84	58,58,58,58	0
35	NA	0	8563	1/1	0.72	0.34	32.27	44,44,44,44	0
33	MG	0	8072	1/1	0.86	0.50	31.99	63,63,63,63	0
33	MG	0	8091	1/1	0.66	0.39	31.76	55,55,55,55	0
33	MG	0	8084	1/1	0.49	0.48	30.80	43,43,43,43	0
33	MG	0	8111	1/1	0.60	0.48	30.55	42,42,42,42	0
35	NA	0	8571	1/1	0.71	0.55	28.71	62,62,62,62	0
33	MG	0	8096	1/1	0.53	0.35	28.64	46,46,46,46	0
33	MG	0	8018	1/1	0.78	0.41	28.30	43,43,43,43	0
33	MG	K	8069	1/1	0.89	0.45	27.42	45,45,45,45	0
35	NA	0	8526	1/1	0.93	0.68	25.76	51,51,51,51	0
33	MG	0	8012	1/1	0.60	0.57	22.67	36,36,36,36	0
35	NA	0	8502	1/1	0.80	0.30	22.67	44,44,44,44	0
33	MG	Y	8108	1/1	0.88	0.35	22.24	36,36,36,36	0
35	NA	0	8576	1/1	0.69	0.40	21.85	69,69,69,69	0
35	NA	9	8582	1/1	0.87	0.51	20.62	78,78,78,78	0
35	NA	0	8556	1/1	0.95	0.48	20.60	40,40,40,40	0
35	NA	0	8521	1/1	0.84	0.56	20.33	61,61,61,61	0
33	MG	0	8054	1/1	0.74	0.32	19.99	32,32,32,32	0
33	MG	0	8032	1/1	0.56	0.35	17.76	26,26,26,26	0
33	MG	0	8080	1/1	0.85	0.23	15.84	36,36,36,36	0
33	MG	0	8058	1/1	0.52	0.47	15.48	39,39,39,39	0
35	NA	0	8550	1/1	0.61	0.26	14.37	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8577	1/1	0.78	0.56	14.00	44,44,44,44	0
35	NA	0	8570	1/1	0.65	0.26	13.63	58,58,58,58	0
33	MG	0	8117	1/1	0.96	0.39	13.46	47,47,47,47	0
35	NA	0	8560	1/1	0.80	0.36	12.83	56,56,56,56	0
33	MG	0	8035	1/1	0.91	0.33	12.47	42,42,42,42	0
33	MG	0	8013	1/1	0.75	0.34	12.26	32,32,32,32	0
35	NA	0	8527	1/1	0.62	0.39	11.98	51,51,51,51	0
33	MG	0	8015	1/1	0.84	0.33	11.28	30,30,30,30	0
33	MG	0	8047	1/1	0.88	0.28	11.01	70,70,70,70	0
33	MG	0	8077	1/1	0.97	0.35	10.99	29,29,29,29	0
33	MG	0	8019	1/1	0.75	0.38	10.97	27,27,27,27	0
35	NA	L	8579	1/1	0.84	0.48	10.92	67,67,67,67	0
35	NA	0	8566	1/1	0.74	0.30	10.65	46,46,46,46	0
33	MG	0	8052	1/1	0.72	0.30	10.52	49,49,49,49	0
35	NA	0	8532	1/1	0.75	0.28	10.31	42,42,42,42	0
35	NA	0	8525	1/1	0.85	0.28	10.19	51,51,51,51	0
33	MG	0	8049	1/1	0.72	0.60	10.18	73,73,73,73	0
33	MG	A	8065	1/1	0.66	0.46	10.14	43,43,43,43	0
33	MG	0	8017	1/1	0.90	0.37	10.05	27,27,27,27	0
36	CL	0	8815	1/1	0.89	0.22	9.92	84,84,84,84	0
35	NA	0	8575	1/1	0.88	0.32	8.83	45,45,45,45	0
35	NA	0	8523	1/1	0.87	0.26	8.40	35,35,35,35	0
33	MG	0	8003	1/1	0.69	0.27	8.29	31,31,31,31	0
33	MG	0	8020	1/1	0.91	0.27	7.31	20,20,20,20	0
35	NA	0	8503	1/1	0.92	0.27	7.10	45,45,45,45	0
35	NA	0	8531	1/1	0.86	0.25	7.05	46,46,46,46	0
35	NA	0	8505	1/1	0.66	0.24	6.65	32,32,32,32	0
35	NA	0	8565	1/1	0.42	0.31	6.27	53,53,53,53	0
35	NA	A	8545	1/1	0.72	0.39	6.17	49,49,49,49	0
33	MG	B	8055	1/1	0.69	0.30	5.94	38,38,38,38	0
33	MG	0	8053	1/1	0.79	0.26	5.52	40,40,40,40	0
35	NA	0	8510	1/1	0.92	0.24	5.38	40,40,40,40	0
33	MG	B	8056	1/1	0.91	0.41	5.12	50,50,50,50	0
35	NA	M	8547	1/1	0.85	0.25	5.04	31,31,31,31	0
33	MG	0	8004	1/1	0.67	0.24	4.92	39,39,39,39	0
33	MG	0	8044	1/1	0.88	0.23	3.99	43,43,43,43	0
35	NA	R	8585	1/1	0.77	0.36	3.91	82,82,82,82	0
37	VIR	0	9000	38/38	0.96	0.22	3.84	24,36,40,44	0
33	MG	0	8109	1/1	0.67	0.21	3.64	20,20,20,20	0
35	NA	0	8564	1/1	0.92	0.39	3.51	45,45,45,45	0
35	NA	0	8553	1/1	0.87	0.30	3.35	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8006	1/1	0.87	0.22	2.86	32,32,32,32	0
33	MG	0	8002	1/1	0.90	0.20	2.72	28,28,28,28	0
34	K	0	8402	1/1	0.88	0.22	2.67	66,66,66,66	0
33	MG	0	8008	1/1	0.81	0.19	2.53	35,35,35,35	0
33	MG	0	8010	1/1	0.80	0.20	2.18	34,34,34,34	0
35	NA	0	8567	1/1	0.88	0.17	1.99	64,64,64,64	0
33	MG	0	8074	1/1	0.65	0.24	1.90	34,34,34,34	0
33	MG	0	8106	1/1	0.70	0.21	1.82	38,38,38,38	0
36	CL	0	8816	1/1	0.96	0.20	1.61	57,57,57,57	0
36	CL	B	8819	1/1	0.97	0.23	1.45	46,46,46,46	0
35	NA	R	8537	1/1	0.60	0.21	1.35	44,44,44,44	0
35	NA	C	8504	1/1	0.77	0.28	1.25	40,40,40,40	0
33	MG	0	8001	1/1	0.63	0.18	1.17	33,33,33,33	0
33	MG	0	8102	1/1	0.77	0.21	0.48	80,80,80,80	0
35	NA	Q	8548	1/1	0.85	0.21	0.33	32,32,32,32	0
33	MG	0	8086	1/1	0.78	0.24	0.11	47,47,47,47	0
35	NA	0	8520	1/1	0.83	0.17	0.02	28,28,28,28	0
36	CL	3	8804	1/1	0.93	0.28	-0.18	68,68,68,68	0
36	CL	O	8808	1/1	0.91	0.22	-0.38	84,84,84,84	0
33	MG	0	8007	1/1	0.87	0.15	-0.42	18,18,18,18	0
35	NA	0	8543	1/1	0.91	0.17	-0.46	46,46,46,46	0
33	MG	0	8033	1/1	0.81	0.15	-0.65	32,32,32,32	0
33	MG	3	8078	1/1	0.83	0.17	-1.00	45,45,45,45	0
35	NA	J	8546	1/1	0.86	0.16	-1.12	48,48,48,48	0
35	NA	0	8524	1/1	0.95	0.10	-1.31	43,43,43,43	0
35	NA	0	8538	1/1	0.93	0.12	-1.31	42,42,42,42	0
33	MG	0	8064	1/1	0.95	0.12	-1.48	30,30,30,30	0
36	CL	0	8805	1/1	0.90	0.14	-1.56	58,58,58,58	0
35	NA	0	8533	1/1	0.87	0.14	-1.56	43,43,43,43	0
35	NA	0	8517	1/1	0.84	0.12	-1.57	46,46,46,46	0
33	MG	0	8057	1/1	0.91	0.15	-1.64	38,38,38,38	0
36	CL	0	8812	1/1	0.94	0.12	-1.66	43,43,43,43	0
35	NA	0	8509	1/1	0.94	0.10	-1.79	38,38,38,38	0
38	CD	U	8701	1/1	1.00	0.09	-1.93	58,58,58,58	0
36	CL	M	8818	1/1	0.98	0.13	-1.98	40,40,40,40	0
36	CL	J	8821	1/1	0.98	0.10	-2.03	48,48,48,48	0
38	CD	1	8702	1/1	0.99	0.05	-2.25	58,58,58,58	0
35	NA	0	8544	1/1	0.86	0.10	-2.31	24,24,24,24	0
38	CD	Z	8703	1/1	0.99	0.06	-2.53	84,84,84,84	0
38	CD	3	8704	1/1	0.97	0.07	-2.58	69,69,69,69	0
35	NA	0	8539	1/1	0.92	0.12	-2.73	35,35,35,35	0
36	CL	0	8813	1/1	0.99	0.11	-2.99	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	T	8073	1/1	0.90	0.07	-3.43	66,66,66,66	0
33	MG	0	8067	1/1	0.98	0.10	-7.30	44,44,44,44	0
33	MG	0	8040	1/1	0.62	0.52	-	56,56,56,56	0
36	CL	N	8807	1/1	0.87	0.22	-	62,62,62,62	0
35	NA	0	8514	1/1	0.73	0.17	-	33,33,33,33	0
33	MG	0	8085	1/1	0.73	0.32	-	53,53,53,53	0
33	MG	0	8062	1/1	0.56	0.37	-	61,61,61,61	0
35	NA	H	8522	1/1	0.87	0.16	-	55,55,55,55	0
33	MG	0	8014	1/1	0.60	0.32	-	22,22,22,22	0
33	MG	0	8094	1/1	0.78	0.28	-	72,72,72,72	0
36	CL	0	8803	1/1	0.98	0.13	-	54,54,54,54	0
33	MG	0	8115	1/1	0.52	0.33	-	49,49,49,49	0
35	NA	0	8549	1/1	0.81	0.28	-	46,46,46,46	0
33	MG	0	8113	1/1	0.67	0.24	-	52,52,52,52	0
35	NA	0	8501	1/1	0.91	0.33	-	23,23,23,23	0
36	CL	Y	8820	1/1	0.96	0.10	-	43,43,43,43	0
35	NA	0	8529	1/1	0.49	0.24	-	66,66,66,66	0
33	MG	0	8098	1/1	0.86	0.21	-	25,25,25,25	0
33	MG	2	8076	1/1	0.57	0.39	-	57,57,57,57	0
36	CL	0	8817	1/1	0.94	0.13	-	49,49,49,49	0
33	MG	0	8009	1/1	0.57	0.35	-	28,28,28,28	0
35	NA	0	8578	1/1	0.67	0.43	-	58,58,58,58	0
33	MG	0	8110	1/1	0.80	0.25	-	52,52,52,52	0
33	MG	0	8100	1/1	0.79	0.40	-	63,63,63,63	0
36	CL	A	8809	1/1	0.93	0.28	-	68,68,68,68	0
33	MG	0	8024	1/1	0.93	0.22	-	22,22,22,22	0
35	NA	0	8558	1/1	0.88	0.89	-	61,61,61,61	0
35	NA	0	8568	1/1	0.52	0.75	-	58,58,58,58	0
33	MG	0	8063	1/1	0.81	0.67	-	62,62,62,62	0
35	NA	0	8506	1/1	0.78	1.28	-	41,41,41,41	0
33	MG	0	8022	1/1	0.51	0.25	-	59,59,59,59	0
35	NA	0	8554	1/1	0.92	0.20	-	38,38,38,38	0
33	MG	0	8005	1/1	0.87	0.28	-	31,31,31,31	0
36	CL	L	8810	1/1	0.97	0.18	-	53,53,53,53	0
33	MG	0	8103	1/1	0.82	0.26	-	47,47,47,47	0
35	NA	0	8542	1/1	0.90	0.38	-	41,41,41,41	0
33	MG	0	8105	1/1	0.84	0.19	-	50,50,50,50	0
33	MG	0	8039	1/1	0.64	0.32	-	42,42,42,42	0
33	MG	0	8021	1/1	0.85	0.39	-	36,36,36,36	0
33	MG	0	8043	1/1	0.66	0.23	-	45,45,45,45	0
35	NA	0	8507	1/1	0.81	0.23	-	59,59,59,59	0
35	NA	0	8581	1/1	0.70	0.37	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8075	1/1	0.44	0.36	-	51,51,51,51	0
33	MG	0	8050	1/1	0.76	0.16	-	77,77,77,77	0
33	MG	0	8045	1/1	0.88	0.22	-	54,54,54,54	0
33	MG	0	8092	1/1	0.57	0.51	-	66,66,66,66	0
35	NA	0	8583	1/1	0.24	0.59	-	56,56,56,56	0
36	CL	0	8822	1/1	0.82	0.41	-	81,81,81,81	0
33	MG	0	8027	1/1	0.75	0.28	-	44,44,44,44	0
33	MG	0	8029	1/1	0.68	0.45	-	37,37,37,37	0
35	NA	0	8574	1/1	0.88	0.88	-	44,44,44,44	0
35	NA	0	8528	1/1	0.90	0.32	-	38,38,38,38	0
35	NA	0	8534	1/1	0.85	0.12	-	40,40,40,40	0
36	CL	0	8814	1/1	0.99	0.13	-	49,49,49,49	0
33	MG	0	8107	1/1	0.32	0.27	-	49,49,49,49	0
35	NA	0	8511	1/1	0.75	0.27	-	48,48,48,48	0
33	MG	0	8104	1/1	0.79	0.21	-	51,51,51,51	0
35	NA	0	8555	1/1	0.82	0.59	-	72,72,72,72	0
33	MG	0	8025	1/1	0.85	0.25	-	31,31,31,31	0
33	MG	0	8068	1/1	0.78	0.30	-	77,77,77,77	0
33	MG	0	8016	1/1	0.52	0.24	-	32,32,32,32	0
35	NA	0	8584	1/1	0.55	0.42	-	51,51,51,51	0
33	MG	0	8061	1/1	0.75	0.24	-	31,31,31,31	0
33	MG	0	8048	1/1	0.89	0.27	-	49,49,49,49	0
38	CD	O	8705	1/1	0.94	0.09	-	88,88,88,88	0
35	NA	0	8559	1/1	0.66	0.63	-	52,52,52,52	0
33	MG	0	8112	1/1	0.86	0.38	-	42,42,42,42	0
33	MG	0	8101	1/1	0.79	0.23	-	50,50,50,50	0
33	MG	0	8116	1/1	0.93	0.15	-	20,20,20,20	0
35	NA	0	8519	1/1	0.76	0.21	-	25,25,25,25	0
33	MG	0	8046	1/1	0.84	0.11	-	48,48,48,48	0
33	MG	0	8083	1/1	0.74	0.33	-	39,39,39,39	0
36	CL	J	8801	1/1	0.91	0.19	-	63,63,63,63	0
33	MG	0	8026	1/1	0.92	0.19	-	22,22,22,22	0
33	MG	9	8095	1/1	0.91	0.09	-	55,55,55,55	0
33	MG	0	8041	1/1	0.71	0.26	-	42,42,42,42	0
35	NA	0	8562	1/1	0.80	0.29	-	43,43,43,43	0
35	NA	0	8569	1/1	0.73	0.64	-	73,73,73,73	0
33	MG	0	8070	1/1	0.75	0.13	-	45,45,45,45	0
33	MG	0	8037	1/1	0.76	0.23	-	32,32,32,32	0
35	NA	0	8518	1/1	0.87	0.42	-	30,30,30,30	0
35	NA	0	8513	1/1	0.78	0.40	-	56,56,56,56	0
36	CL	0	8811	1/1	0.94	0.14	-	53,53,53,53	0
33	MG	0	8097	1/1	0.59	0.19	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8541	1/1	0.79	0.27	-	39,39,39,39	0
33	MG	0	8023	1/1	0.63	0.31	-	41,41,41,41	0
33	MG	0	8118	1/1	0.82	0.28	-	34,34,34,34	0
35	NA	0	8516	1/1	0.70	0.37	-	42,42,42,42	0
33	MG	0	8036	1/1	0.83	0.48	-	36,36,36,36	0
36	CL	J	8802	1/1	0.93	0.19	-	63,63,63,63	0
33	MG	0	8059	1/1	0.91	0.34	-	38,38,38,38	0
33	MG	0	8079	1/1	0.76	0.27	-	36,36,36,36	0
33	MG	0	8093	1/1	0.83	0.26	-	49,49,49,49	0
33	MG	0	8090	1/1	0.55	0.63	-	53,53,53,53	0
35	NA	0	8552	1/1	0.73	0.33	-	59,59,59,59	0
36	CL	R	8806	1/1	0.89	0.13	-	41,41,41,41	0
35	NA	0	8515	1/1	0.90	0.48	-	47,47,47,47	0
35	NA	S	8512	1/1	0.77	0.14	-	35,35,35,35	0
35	NA	0	8580	1/1	0.81	0.33	-	49,49,49,49	0
33	MG	0	8034	1/1	0.90	0.23	-	24,24,24,24	0
35	NA	0	8530	1/1	0.77	0.26	-	40,40,40,40	0
33	MG	0	8088	1/1	0.78	0.17	-	21,21,21,21	0
35	NA	0	8536	1/1	0.88	0.25	-	47,47,47,47	0
33	MG	0	8011	1/1	0.62	0.39	-	11,11,11,11	0
33	MG	0	8042	1/1	0.91	0.15	-	31,31,31,31	0
33	MG	0	8114	1/1	0.89	0.40	-	47,47,47,47	0
33	MG	0	8051	1/1	0.63	0.40	-	60,60,60,60	0
33	MG	0	8089	1/1	0.51	0.66	-	77,77,77,77	0
33	MG	0	8087	1/1	0.71	0.14	-	51,51,51,51	0
33	MG	0	8082	1/1	0.68	0.43	-	63,63,63,63	0
35	NA	0	8540	1/1	0.90	0.27	-	34,34,34,34	0
33	MG	0	8030	1/1	0.67	0.19	-	21,21,21,21	0
33	MG	0	8099	1/1	0.89	0.19	-	49,49,49,49	0
33	MG	0	8031	1/1	0.83	0.23	-	27,27,27,27	0
33	MG	0	8028	1/1	0.74	0.28	-	35,35,35,35	0
33	MG	0	8066	1/1	0.62	0.27	-	62,62,62,62	0
35	NA	0	8508	1/1	0.42	0.27	-	56,56,56,56	0
35	NA	0	8557	1/1	0.91	0.09	-	50,50,50,50	0
33	MG	0	8081	1/1	0.84	0.16	-	44,44,44,44	0
35	NA	9	8551	1/1	0.72	0.24	-	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.