



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:25 PM UTC

PDB ID : 3CCR / pdb_00003ccr
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488C. Density for anisomycin is visible but not included in the model.
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

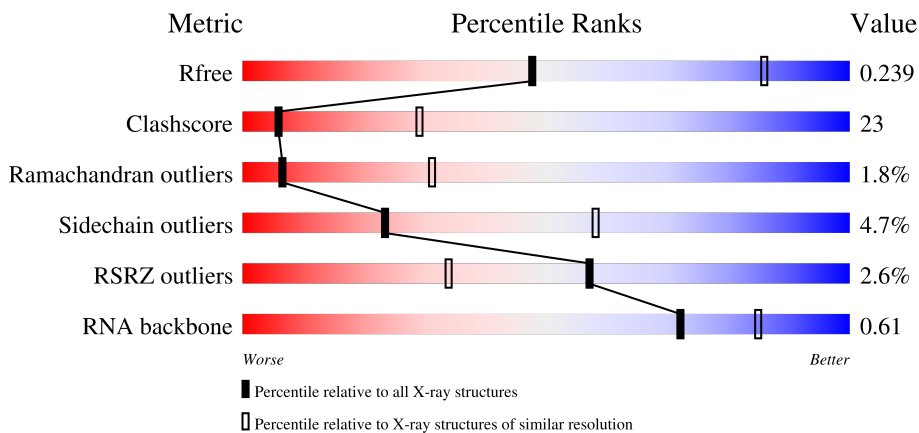
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



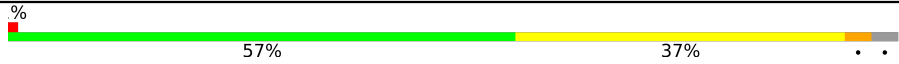



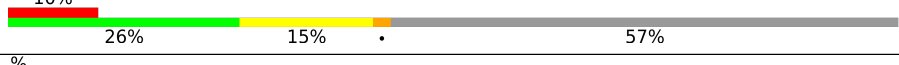
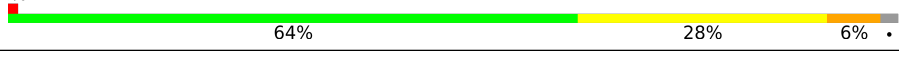



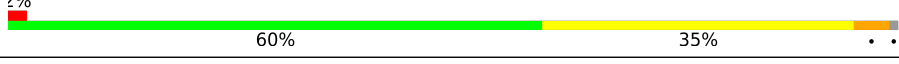

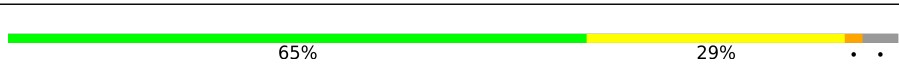
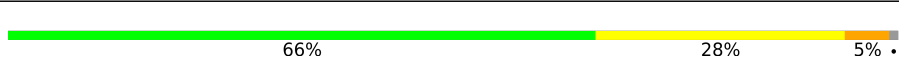

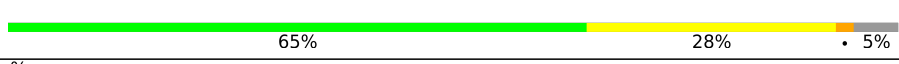

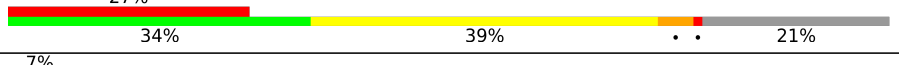

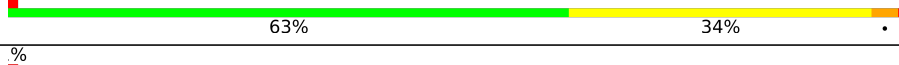

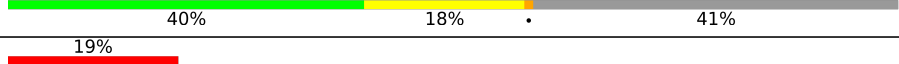


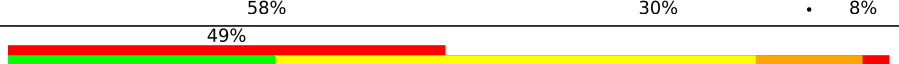
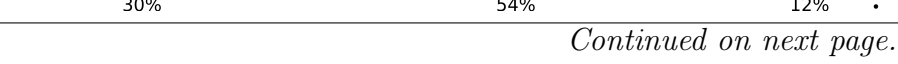
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	240	 2% 60% 33% 6%
2	B	338	 5% 55% 40% 5%
3	C	246	 63% 30% 6%
4	D	177	 5% 41% 35% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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	CL	3	8804	-	-	X	-
33	CL	B	8819	-	-	X	-
33	CL	M	8818	-	-	X	-
35	NA	0	8528	-	-	-	X
35	NA	0	8559	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99120 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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	246	1860	1130	345	384	1	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

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

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	132	994	609	189	192	4	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	194	1558	943	333	281	1	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59018	26348	10871	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		
32	0	84	Total	Mg	0	0
			84	84		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	J	3	Total Cl 3 3	0	0
33	K	1	Total Cl 1 1	0	0
33	L	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	0	9	Total Cl 9 9	0	0

- Molecule 34 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	3	Total Sr 3 3	0	0
34	B	2	Total Sr 2 2	0	0
34	F	1	Total Sr 1 1	0	0
34	R	1	Total Sr 1 1	0	0
34	S	1	Total Sr 1 1	0	0
34	1	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	93	Total Sr 93 93	0	0
34	9	3	Total Sr 3 3	0	0

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0
35	0	66	Total Na 66 66	0	0
35	9	2	Total Na 2 2	0	0

- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	M	1	Total K 1 1	0	0
36	0	1	Total K 1 1	0	0

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	1	1	Total 1	Cd 1	0	0
37	3	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	121	Total 121	O 121	0	0
38	B	145	Total 145	O 145	0	0
38	C	166	Total 166	O 166	0	0
38	D	46	Total 46	O 46	0	0
38	E	43	Total 43	O 43	0	0
38	F	31	Total 31	O 31	0	0
38	G	17	Total 17	O 17	0	0
38	H	72	Total 72	O 72	0	0
38	I	5	Total 5	O 5	0	0
38	J	52	Total 52	O 52	0	0
38	K	52	Total 52	O 52	0	0
38	L	81	Total 81	O 81	0	0
38	M	133	Total 133	O 133	0	0
38	N	56	Total 56	O 56	0	0
38	O	41	Total 41	O 41	0	0
38	P	63	Total 63	O 63	0	0
38	Q	52	Total 52	O 52	0	0

Continued on next page...

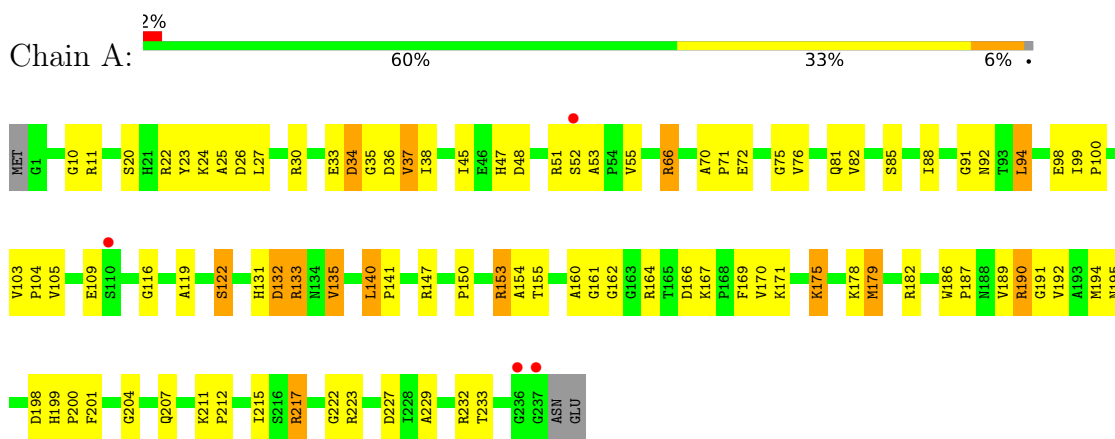
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	R	75	Total 75	O 75	0	0
38	S	37	Total 37	O 37	0	0
38	T	40	Total 40	O 40	0	0
38	U	28	Total 28	O 28	0	0
38	V	15	Total 15	O 15	0	0
38	W	69	Total 69	O 69	0	0
38	X	22	Total 22	O 22	0	0
38	Y	100	Total 100	O 100	0	0
38	Z	28	Total 28	O 28	0	0
38	1	61	Total 61	O 61	0	0
38	2	45	Total 45	O 45	0	0
38	3	76	Total 76	O 76	0	0
38	0	5897	Total 5897	O 5897	0	0
38	9	154	Total 154	O 154	0	0

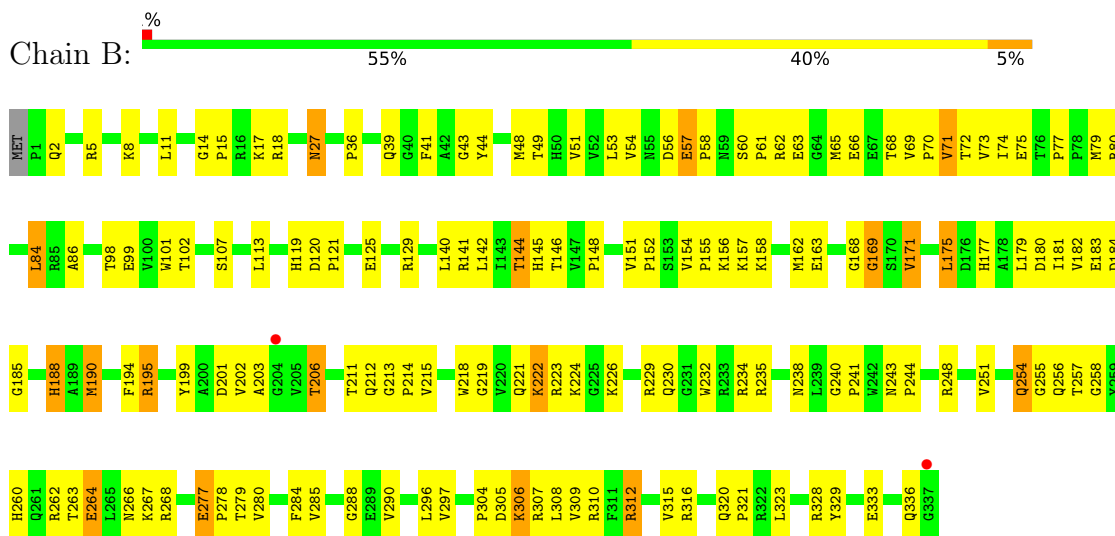
3 Residue-property plots

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

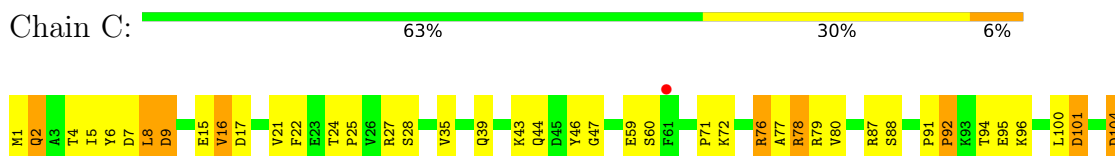
- Molecule 1: 50S ribosomal protein L2P



- Molecule 2: 50S ribosomal protein L3P

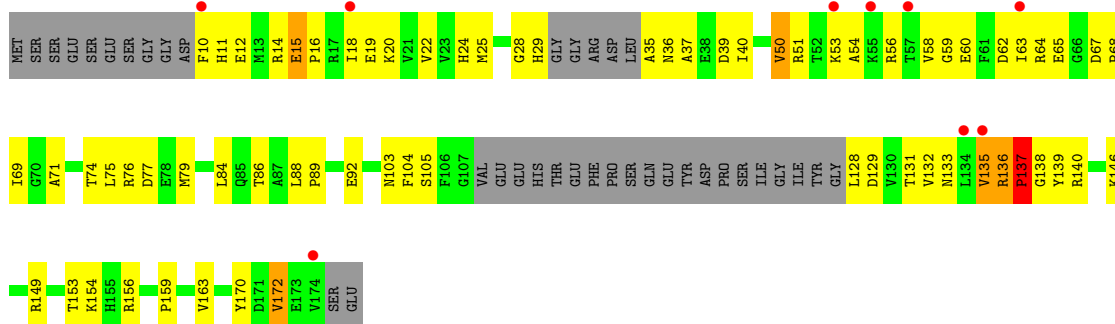
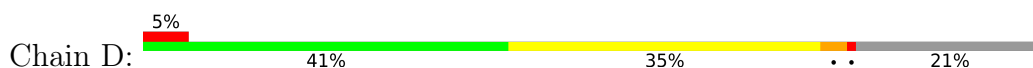


- Molecule 3: 50S ribosomal protein L4P

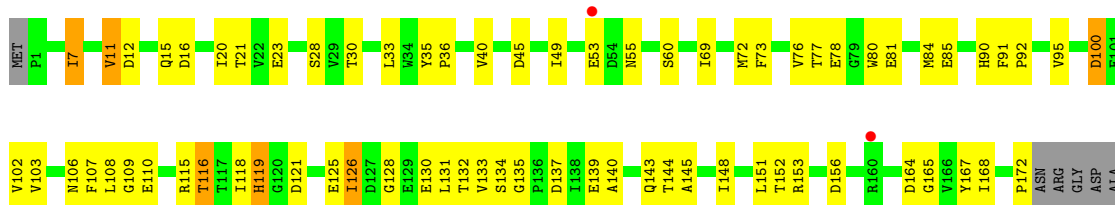




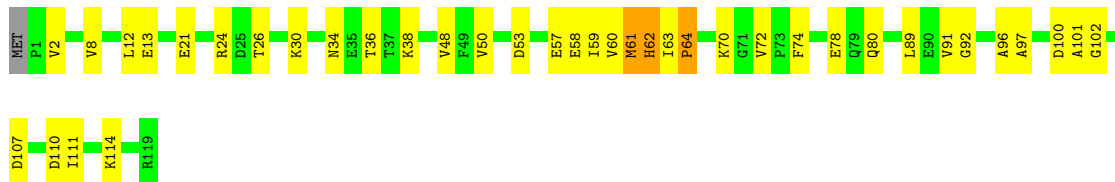
- Molecule 4: 50S ribosomal protein L5P



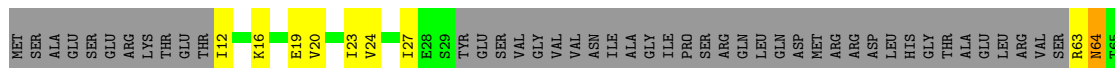
- Molecule 5: 50S ribosomal protein L6P



- Molecule 6: 50S ribosomal protein L7Ae

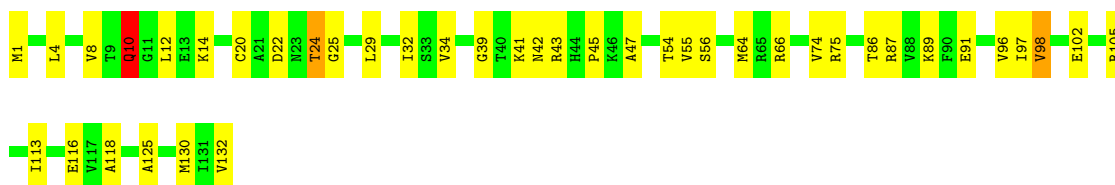


- Molecule 7: 50S ribosomal protein L10E



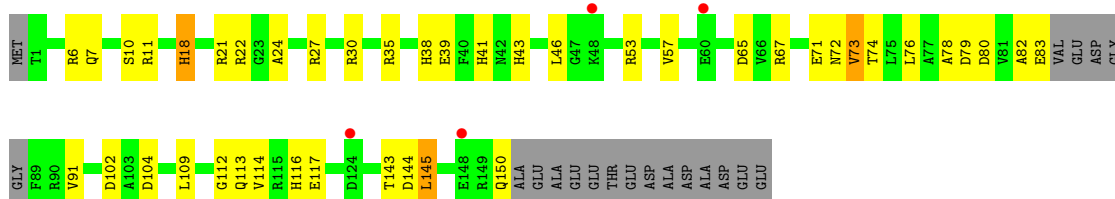
- Molecule 11: 50S ribosomal protein L14P

Chain K:  69% 29% ..



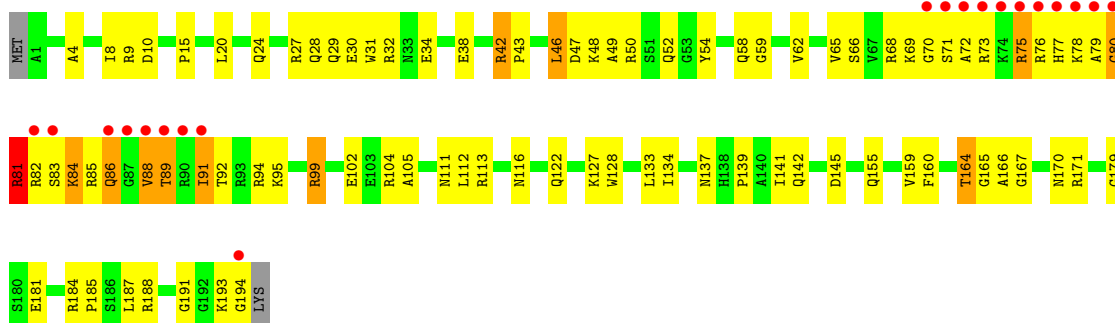
- Molecule 12: 50S ribosomal protein L15P

Chain L:  2% 62% 24% 12%



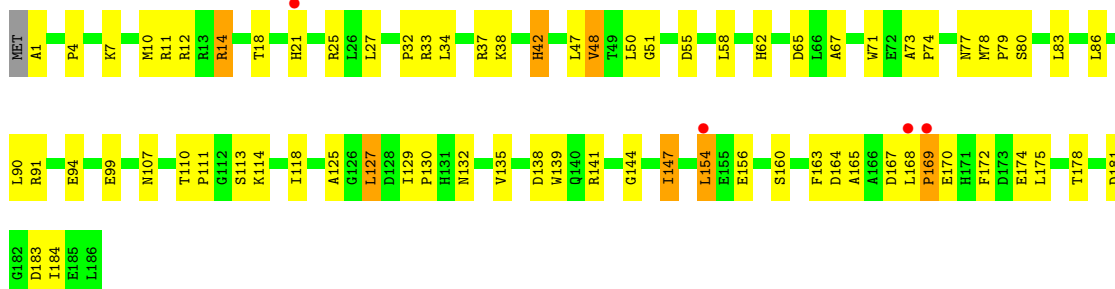
- Molecule 13: 50S ribosomal protein L15e

Chain M:  10% 54% 39% 6% ..

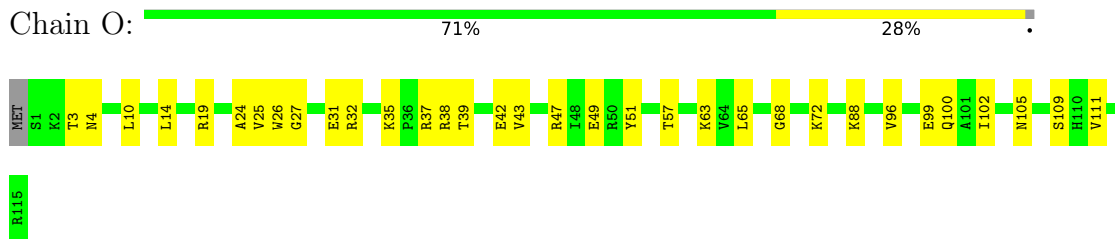


- Molecule 14: 50S ribosomal protein L18P

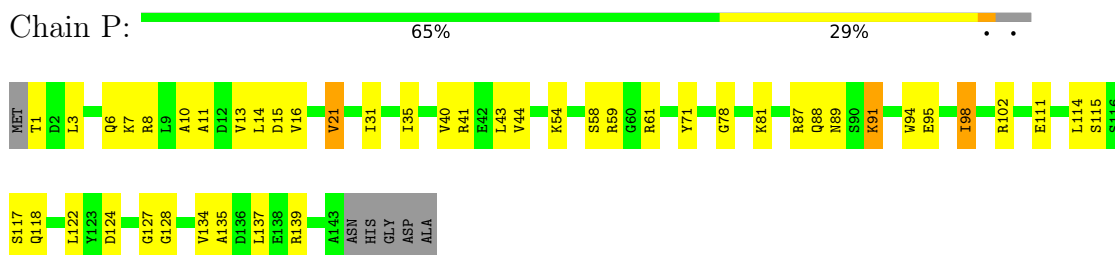
Chain N:  2% 60% 35% ..



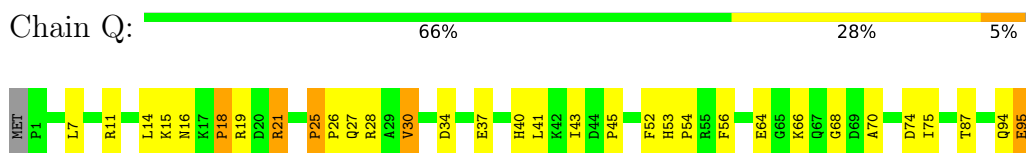
- Molecule 15: 50S ribosomal protein L18e



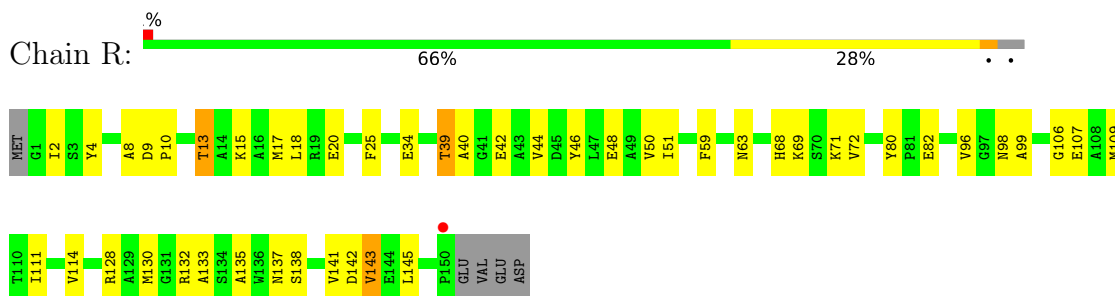
- Molecule 16: 50S ribosomal protein L19e



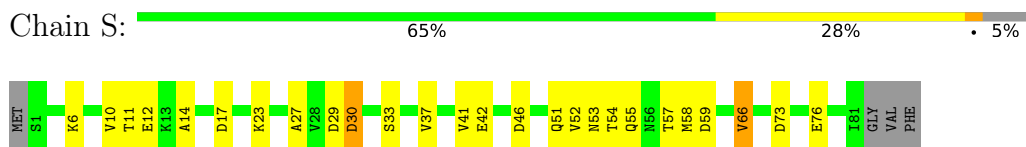
- Molecule 17: 50S ribosomal protein L21e



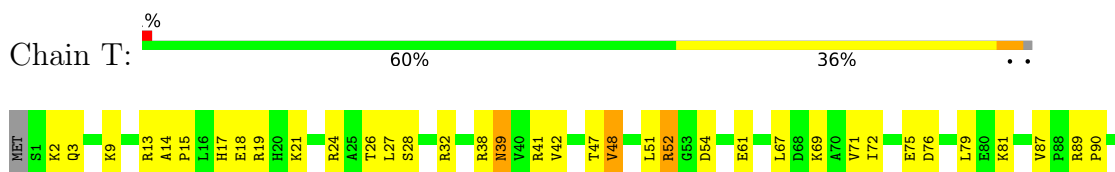
- Molecule 18: 50S ribosomal protein L22P

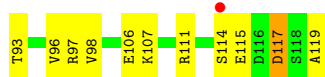


- Molecule 19: 50S ribosomal protein L23P

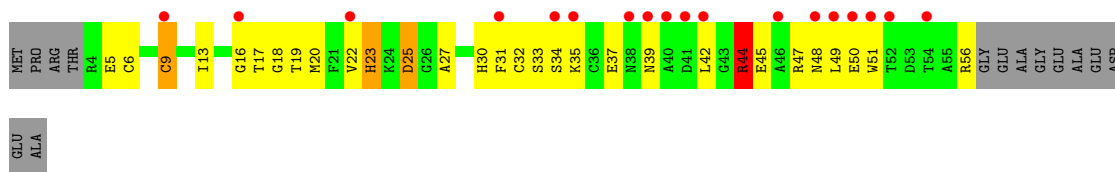


- Molecule 20: 50S ribosomal protein L24P





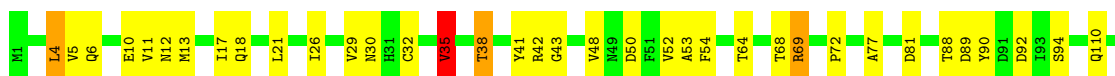
• Molecule 21: 50S ribosomal protein L24e



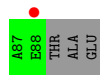
• Molecule 22: 50S ribosomal protein L29P



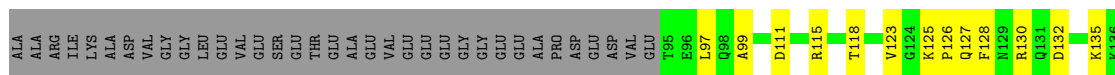
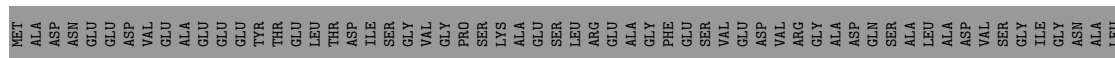
• Molecule 23: 50S ribosomal protein L30P



• Molecule 24: 50S ribosomal protein L31e

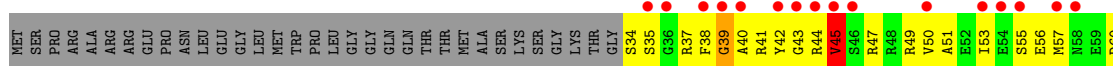
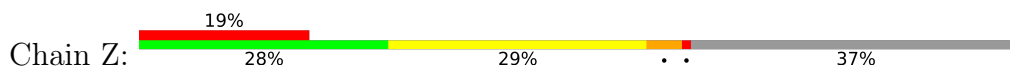


• Molecule 25: 50S ribosomal protein L32e





- Molecule 26: 50S ribosomal protein L37Ae



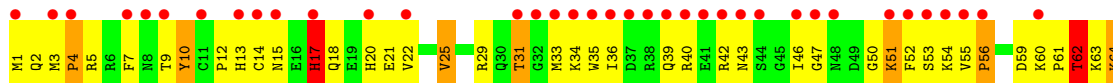
- Molecule 27: 50S ribosomal protein L37e



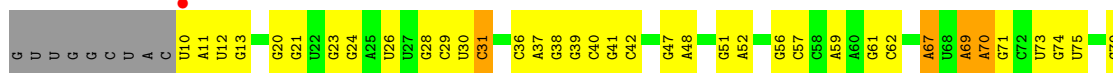
- Molecule 28: 50S ribosomal protein L39e



- Molecule 29: 50S ribosomal protein L44E



- Molecule 30: 23S RIBOSOMAL RNA



C1182	C1183	C1184	C1185	C1186	C1187	C1188	C1189	G1190	A1191	A1192	A1193	A1194	G1195	C1196	C1197	C1198	C1199	A1199	C1200	C1201	C1202	C1203	C1204	U1205	U1206	A1207	C1208	C1209	G1210	G1211	G1212	C1213	G1214	A1215	C1216	G1217	G1218	U1219	U1220	G1224	C1225	G1226	C1227	C1228	C1229	A1233	U1234	G1235	A1236	U1237	C1238	G1239	G1240	C1241	A1242	C1243	U1244	C1245																																																																																																																																																																																																									
G1108	U1109	U1110	U1111	G1112	U1115	U1116	A1117	U1118	A1119	A1120	U1121	C1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	G1131	A1132	A1133	G1134	G1137	U1138	U1139	C1140	U1149	G1150	G1151	A1154	G1155	C1156	C1157	G1158	G1159	G1160	A1161	G1162	G1163	G1164	G1165	A1166	G1167	C1168	U1169	U1170	A1171	G1172	A1173	A1174	G1175	C1176	A1177	G1178	U1179	U1180	A1181																																																																																																																																																																																																								
C1025	U1026	G1027	U1028	U1029	U1030	G1031	A1032	U1041	U1042	U1043	C1044	G1045	U1046	U1047	G1052	G1053	G1054	U1055	U1056	A1057	A1058	G1059	C1060	C1061	U1062	G1063	U1066	A1067	C1068	C1069	A1070	G1071	G1072	A1073	G1074	A1079	C1080	A1081	G1087	A1088	G1089	U1095	U1096	A1097	A1098	G1099	C1100	C1101	A1102	A1103	A1104	C1105	U1106	U1107	A1108	G1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121																																																																																																																																																																																															
G687	U688	C689	C690	G696	G697	A698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	U801	C802	A806	A807	A808	C809	C810	C811	C812	C813																																																																																																																																													
G614	U615	C616	C617	A618	A619	C620	U621	C622	U623	G624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732																																																																																																																																													
U330	U331	U332	U333	U334	U335	U336	U337	U338	U339	U340	U341	U342	U343	U344	U345	U346	U347	U348	U349	U350	U351	U352	U353	U354	U355	U356	U357	U358	U359	U360	U361	U362	U363	U364	U365	U366	U367	U368	U369	U370	U371	U372	U373	U374	U375	U376	U377	U378	U379	U380	U381	U382	U383	U384	U385	U386	U387	U388	U389	U390	U391	U392	U393	U394	U395	U396	U397	U398	U399	U400	U401	U402	U403	U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589
G292	A293	C294	C295	G296	U297	C298	C301	A302	C303	G304	G307	U308	C309	U310	C311	U312	U313	G314	G315	A316	U317	U318	A319	G320	C254	A255	C256	G257	U258	G259	A262	U263	G264	U265	A266	G267	U268	C269	U270	A271	C272	G273	G274	U277	A278	C279	C280	U281	C282	U283	C284	A285	U286	C287	C290	U364																																																																																																																																																																																																											
G365	U366	C367	C368	G369	G370	U371	A372	G373	U374	G378	U379	A380	G381	U382	A383	G384	C385	G386	G387	U388	U389	G392	U393	A394	A395	U396	A397	U398	G399	C400	U401	G402	U403	G404	U405	U406	A407	A408	C412	G413	G416	C417	C418	A419	U420	C421	U422	A423	C424	U425	U426	G427	U428	U429	U430	G432	U433	U434	A435	A436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589																																														
C440	A441	A442	C443	C444	U445	U446	A447	U448	A449	C450	C451	U452	A453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589																																																																																																														
A590	A591	C594	U595	C596	A597	C598	U599	G600	A603	G604	C605	U611	U612	U613	U614	U615	U616	C617	U618	U619	A620	C621	G622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732																																																																																																																														
G669	C670	A671	U672	U673	U674	U675	C676	U677	U678	G681	U684	C685	A686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732																																																																																																																																																																																																								
U733	U734	C735	A736	U737	U738	U739	C741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	C759	U763	C764	U765	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U806	U807	U808	U809	U810	U811	U812	U813																																																																																																																																																																																																							
G814	U815	C816	C817	A818	A819	C820	U821	C822	U823	G824	U																																																																																																																																																																																																																																																								

C2247	U2120	G2056	A1981	H1918	G1849	U1770	G1697	G1617	A1547	C1469	C1397	G1326	A1246
C2248	G2121	U2057	U1986	A1919	U1850	U1771	U1701	G1618	U1548	A1470	G1398	G1327	A1247
G2249	C2122	G2058	U1985	C1920	G1851	G1772	A1702	G1619	U1549	A1471	A1399	A1328	A1248
G2250	U	U2059	G1986	A1921	G1852	G1773	G1703	G1620	G1552	C1472	C1400	G1329	U1249
A2251	A	A2060	C1987	A1922	C1854	G1774	G1704	G1621	C1553	A1473	G1401	A1330	C1250
G2253	C	G2061	C1988	G1923	C1855	G1775	G1705	G1622	C1554	C1474	G1402	C1251	
G2254	C	A2062	G1989	A1924	C1856	U1776	C1706	C1623	G1555	G1475	U1405	U1333	
A2255	G	U2063	U1992	G1925	A1857	A1778	G1707	A1624	G1556	A1476	A1406	C1334	A1256
G2256	G	C1993	A1993	A1927	A1858	U1788	C1708	U1625	G1557	C1477	A1407	G1337	
G2257	C	G1994	U1994	U1860	U1859	G1788	C1709	A1626	C1558	U1478	U1409	U1338	G1260
A2258	A	G1995	C1987	C1861	U1860	G1789	A1710	A1627	A1559	U1479	G1410	G1339	A1261
C2259	C	A1997	G1862	C1862	C1862	C1790	A1711	U1628	U	G1484	G1410	G1340	
A2260	U	A1998	G1863	G1863	G1863	U1791	A1712	A1630	U1561	U1485	G1413	A1341	U1264
G2263	C	G2070	C1864	G1932	C1864	U1792	G1713	A1631	C1562	G1490	A1413	C1342	G1266
A2264	G	C2071	A1865	G1933	A1865	A1796	G1714	A1632	U1563	G1491	A1414	C1343	U1267
U2265	A	G2072	A1866	A1934	A1866	G1797	A1716	G1633	G1566	C1495	G1415	G1344	C1267
A2266	C	C2073	G1867	C1935	G1867	G1798	A1717	U1634	G1567	A1496	G1416	G1345	C1268
C2269	C	A2074	G1868	C1936	G1868	G1799	G1718	U1635	G1568	G1497	G1417	G1346	G1269
C2270	C	U2004	U1871	U1837	U1871	G1800	G1719	A1641	U1569	U1500	U1419	U1350	U1270
G2271	A	C2005	C1872	G1938	C1872	A1801	U1722	A1642	A1572	U1501	C1420	G1351	U1271
G2272	A	A2006	G1873	U1939	G1873	G1802	G1723	C1643	A1573	U1503	C1421	C1353	C1272
C2273	C	G2007	C1874	C1940	C1874	C1803	U1724	C1644	A1574	U1504	C1422	G1354	C1273
A2274	G	U2008	U1874	C1941	U1874	A1804	G1725	U1645	C1574	A1505	C1423	A1355	A1274
G2275	U	G2009	A1875	A1942	A1875	G1805	C1725	G1649	C1575	U1506	G1424	A1356	C1275
G2276	U	A2010	C1876	C1943	C1876	G1806	U1730	G1649	G1576	U1507	G1425	A1357	U1276
A2277	G	U2011	G1877	U1947	G1877	U1807	G1731	A1653	U1577	C1507	C1426	A1358	C1277
U2277	G	A2012	U1878	G1948	U1878	G1808	C1731	U1654	C1578	U1511	A1427	A1359	U1278
C2281	A	G2013	C1880	G1949	C1880	G1809	A1732	U1655	U1583	U1512	C1428	C1360	U1279
U2282	A	U2016	A1881	G1950	A1881	C1810	G1734	G1656	C1584	C1513	G1430	G1361	G1284
G2283	U	U2017	C1882	G1951	C1882	G1812	C1735	A1656	C1585	G1514	G1430	G1362	U1285
C2284	C	A2018	U1883	U	U1883	U1813	A1736	C1662	G1586	U1515	A1434	G1363	U1286
G2285	A	G2019	A1884	A	A1884	G1814	U1741	G1663	U1587	U1516	U1435	A1287	U1287
A2286	A	A2020	C1885	A	C1885	A1815	A1742	A1664	G1588	U1517	C1436	C1366	U1288
C2287	C	C2021	A1886	C	A1886	C1816	G1743	G1665	G1589	A1518	A1437	A1367	C1289
G2288	C	C2026	C1889	U	C1889	U1817	G1744	C1666	G1590	U1519	G1438	G1368	G1290
C2289	C	A2026	U1890	A	U1890	C1818	G1744	A1667	A1591	G1520	C1439	A1369	
G2294	G	U2032	C1894	G	C1894	G1819	G1745	U1668	C1592	C1521	U1440	G1370	U1293
C2295	G	G2033	G1898	U1902	G1898	U1820	U1748	G1669	C1593	A1522	G1441	U1371	A1294
G2296	C	U2034	C1899	C	C1899	U1825	U1749	A1670	C1594	G1523	A1442	A1372	
C2298	C	C2037	G1902	U1964	G1902	C1827	G1752	U1671	A1596	U1524	G1444	G1377	U1298
A2300	G	A2038	C1965	U1966	C1965	G1828	C1753	G1675	A1597	U1525	G1444	G1378	G1299
A2301	A	A2039	U1966	U1966	U1966	A1829	A1754	G1676	A1598	A1526	U1446	A1379	G1300
A2302	U	C2040	U1967	U1967	U1967	C1830	A1755	U1677	U1599	A1527	U1447	U1380	C1303
A2303	C	G2041	A1904	U1967	A1904	U1831	G1756	A1678	G1600	A1528	A1448	A1381	C1304
C2304	C	U2042	U1905	A1968	U1905	G1832	U1757	C1679	G1601	G1529	G1449	G1382	C1305
U2107	A	U2043	C1906	A1969	C1906	U1833	U1758	C1680	G1602	U1533	C1450	U1383	
U2108	A	G2044	U1907	A1970	U1907	U1834	A1759	G1681	A1603	U1534	C1451	C1384	U1309
U2109	A	G2045	G1908	G1971	G1908	C1834	A1759	A1682	G1604	C1537	G1452	G1385	U1310
G2046	G	G2046	U1909	U1972	U1909	U1835	G1760	G1683	G1605	C1538	G1453	G1389	U1311
G2111	G	C2047	A1910	A1973	A1910	A1840	C1761	A1684	A1606	U1539	U1454	A1390	G1312
A2112	A	G2050	C1913	G1974	C1913	C1841	C1762	A1685	A1607	G1540	G1460	G1391	A1313
G2114	C	G2051	C1914	U1977	C1914	C1844	C1763	A1686	G1608	G1541	U1461	A1392	U1314
A2118	C	A2053	U1915	A1978	U1915	A1845	G1765	C1687	C1613	G1543	C1462	A1393	G1315
C2119	G	A2055	U1916	G1979	U1916	A1845	U1766	A1691	G1614	U1544	U1463	C1394	G1316
U2246	G	A2055	U1980	U1980	U1980	G1848	C1769	C1692	A1616	U1545	C1464	C1395	G1324
G2237	C	G2237	U1980	U1980	U1980	G1848	C1769	C1692	A1616	U1545	C1464	C1395	G1324
A2244	C	A2244	U1980	U1980	U1980	G1848	C1769	C1692	A1616	U1545	C1464	C1395	G1324
G2238	C	G2238	U1980	U1980	U1980	G1848	C1769	C1692	A1616	U1545	C1464	C1395	G1324
G2239	C	G2239	U1980	U1980	U1980	G1848	C1769	C1692	A1616	U1545	C1464	C1395	G1324
U2240	C	U2240	U1980	U1980	U1980	G1848	C1769	C1692	A1616	U1545	C1464	C1395	G1324
C2241	C	C2241	U1980	U1980	U1980	G1848	C1769	C1692	A1616	U1545	C1464	C1395	G1324
G2243	C	G2243	U1980	U1980	U1980	G1848	C1769	C1692	A1616	U1545	C1464	C1395	G1324
A2244	C	A2244	U1980	U1980	U1980	G1848	C1769	C1692	A1616	U1545	C1464	C1395	G1324
G2245	C	G2245	U1980	U1980	U1980	G1848	C1769	C1692	A1616	U1545	C1464	C1395	G1324
U2320	G	U2320	U1980	U1980	U1980	G1848	C1769	C1692	A1616	U1545	C1464	C1395	G1324

A2321	U2457	G2520	U2597	A	U2735	C2806	G2869
U2322	U2458	A2521	U2598	U	U2736	U2807	C2870
G2323	U2387	G2522	A2599	G2667	G2737	U2808	C2871
G2324	U2388	U2523	A2599	G2668	C2737	G2809	U2872
U2325	U2389	G2524	A2600	U2669	G2744	G2810	G2873
C2326	U2390	U2525	A2601	U2670	G2745	A2811	G2874
	G2397	C2526	G2602	U2671	C2746	A2812	A2875
U2328	A2401	U2527	A2604	C2672	G2747	A2813	A2876
C2329	A2402	U2531	U2607	U2673	G2748	A2814	G2877
U2330	A2403	U2532	A2467	C2674	G2750	G2815	A2878
C2331	C2403	U2533	A2468	A2675	C2751	A2816	A2879
A2332	G2404	C2534	A2469	C2676	C2752	G2817	A2883
G2333	G2407	U2535	U2470	A2681	G2755	G2818	
C2334	A2408	U2536	G2471	C2682	U2756	C2819	C2886
C2335	C2409	G2537	C2472	G2611	A2757	A2820	C2887
G2337	G2410	U2538	U2473	G2612	A2758	G2821	G2888
G2338	G2411	U2539	A2474	C2613	G2759	G2822	U2889
A	G2412	U2540	C2475	U2614	C2759	G2823	A2890
C	A2413	U2541	C2476	U2615	C2760	C2824	A2891
A	A2414	U2544	C2477	G2616	A2761	C2825	G2892
G	A2415	C2548	C2478	G2617	C2762	G2826	C2893
A	G2416	C2549	U2479	U2618	A2766	A2827	C2894
A2344	G2417	C2548	A2480	U2619	C2767	G2828	C2895
A2345	C2418	C2548	G2481	U2620	A2768	A2829	A2896
C2346	U2419	C2549	G2482	U2621	C2769	G2830	C2897
	G2420		U2483	A2624	G2770	C2831	G2898
	C2421		U2484	C2625	G2771	C2832	A2899
	U2422		C2485	C2626	G2772	G2833	C2900
	C2423		U2486	G2627	G2773	G2834	C2901
	G2424		C2487	G2628	U2774	G2835	C2902
	U2425		C2487	G2629	A2775	G2836	C2903
	G2426		A2490	G2630	A2776	U2837	U2904
			G2491	A2633	G2776	A2840	A2905
			U2492	G2634	G2777	G2841	A2906
			C2493	A2635	A2778	G2842	A2907
			G2494	C2636	G2779	A2843	C2908
				A2637	C2780		C2909
				G2638	U2781		A2910
				U2640	G2782		C2911
				C2641	U2710		C2912
				G2642	G2711		A2913
				U2643	U2712		
				G2643	G2713		
				U2644	U2714		
				C2646	G2715		
				C2647	C2716		
				U2648	G2717		
				A2649	C2718		
				U2650	A2718		
				G2651	C2719		
				U2652	C2720		
				A2653			
				C2654			
				U2655			
				G2656			
				U2657			
				G2658			
				U2659			
				G2660			
				U2661			
				G2662			
				U2663			
				G2664			
				U2665			
				G2666			
				U2667			
				G2668			
				U2669			
				G2670			
				U2671			
				G2672			
				U2673			
				G2674			
				U2675			
				G2676			
				U2677			
				G2678			
				U2679			
				G2680			
				U2681			
				G2682			
				U2683			
				G2684			
				U2685			
				G2686			
				U2687			
				G2688			
				U2689			
				G2690			
				U2691			
				G2692			
				U2693			
				G2694			
				U2695			
				G2696			
				U2697			
				G2698			
				U2699			
				G2700			
				U2701			
				G2702			
				U2703			
				G2704			
				U2705			
				G2706			
				U2707			
				G2708			
				U2709			
				G2710			
				U2711			
				G2712			
				U2713			
				G2714			
				U2715			
				G2716			
				U2717			
				G2718			
				U2719			
				G2720			
				U2721			
				G2722			
				U2723			
				G2724			
				U2725			
				G2726			
				U2727			
				G2728			
				U2729			
				G2730			
				U2731			
				G2732			
				U2733			
				G2734			
				U2735			
				G2736			
				U2737			
				G2738			
				U2739			
				G2740			
				U2741			
				G2742			
				U2743			
				G2744			
				U2745			
				G2746			
				U2747			
				G2748			
				U2749			
				G2750			
				U2751			
				G2752			
				U2753			
				G2754			
				U2755			
				G2756			
				U2757			
				G2758			
				U2759			
				G2760			
				U2761			
				G2762			
				U2763			
				G2764			
				U2765			
				G2766			
				U2767			
				G2768			
				U2769			
				G2770			
				U2771			
				G2772			
				U2773			
				G2774			
				U2775			
				G2776			
				U2777			
				G2778			
				U2779			
				G2780			
				U2781			
				G2782			
				U2783			
				G2784			
				U2785			
				G2786			
				U2787			
				G2788			
				U2789			
				G2790			
				U2791			
				G2792			
				U2793			
				G2794			
				U2795			
				G2796			
				U2797			
				G2798			
				U2799			
				G2800			
				U2801			
				G2802			
				U2803			
				G2804			
				U2805			
				G2806			
				U2807			
				G2808			

● Molecule 31: 5S RIBOSOMAL RNA



U1	A62	U2	C63	A3	C64	G4	A65	G5	G66	C67	G68	G69	C9	C72	A73	G74	G75	G76	A77	C81	U82	G83	G83	G20	U87	G88	G89	U23	C89	G90	C91	G92	A93	U105	U106	C107	C108	G109	G110	C35	U111	C36	U112	C37	C37	A38	U39	C41	C42	C42	G43	A44	A47	C48	C49	G50	A51	A52	G53	A54	U55	A56	A57	G58	C59	C60	G61
----	-----	----	-----	----	-----	----	-----	----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	------	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.41Å 299.52Å 574.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 3.00 49.81 – 3.00	Depositor EDS
% Data completeness (in resolution range)	77.8 (49.81-3.00) 77.8 (49.81-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.180 , 0.247 0.178 , 0.239	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtrriage
Anisotropy	0.446	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 80.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99120	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, CL, OMU, CD, K, PSU, 1MA, MG, NA, OMG, SR

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	A	0.45	0/1786	1.03	8/2408 (0.3%)
2	B	0.44	0/2690	1.02	17/3652 (0.5%)
3	C	0.49	0/1885	1.02	11/2552 (0.4%)
4	D	0.39	0/1111	1.02	8/1498 (0.5%)
5	E	0.42	0/1382	0.93	5/1880 (0.3%)
6	F	0.41	0/901	0.97	3/1224 (0.2%)
7	G	0.37	0/241	0.81	0/324
8	H	0.41	0/1302	1.00	6/1743 (0.3%)
9	I	0.42	0/526	0.92	3/716 (0.4%)
10	J	0.44	0/1136	0.99	4/1530 (0.3%)
11	K	0.44	0/1004	1.00	3/1351 (0.2%)
12	L	0.39	0/1130	0.93	3/1509 (0.2%)
13	M	0.49	0/1582	0.96	3/2116 (0.1%)
14	N	0.39	0/1474	1.07	8/1999 (0.4%)
15	O	0.46	0/874	0.96	3/1181 (0.3%)
16	P	0.42	0/1147	0.90	1/1528 (0.1%)
17	Q	0.42	0/749	1.08	6/1005 (0.6%)
18	R	0.49	0/1172	0.97	1/1578 (0.1%)
19	S	0.44	0/648	0.92	4/875 (0.5%)
20	T	0.43	0/958	1.03	5/1289 (0.4%)
21	U	0.54	0/417	1.13	5/562 (0.9%)
22	V	0.42	0/502	0.95	0/675
23	W	0.49	0/1219	1.03	4/1655 (0.2%)
24	X	0.47	0/664	1.06	4/895 (0.4%)
25	Y	0.45	0/1146	0.94	2/1536 (0.1%)
26	Z	0.55	0/584	1.05	3/781 (0.4%)
27	1	0.47	0/438	0.87	0/578
28	2	0.45	0/401	0.90	1/529 (0.2%)
29	3	0.63	0/771	1.14	7/1024 (0.7%)
30	0	0.40	0/65954	0.60	9/102862 (0.0%)
31	9	0.40	0/2904	0.58	0/4526
All	All	0.42	0/98698	0.73	137/147581 (0.1%)

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
23	W	0	1
30	0	0	18
31	9	0	1
All	All	0	20

There are no bond length outliers.

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	3	25	VAL	N-CA-C	9.17	121.79	108.58
14	N	51	GLY	CA-C-N	8.79	128.38	119.24
14	N	51	GLY	C-N-CA	8.79	128.38	119.24
20	T	52	ARG	N-CA-C	8.62	124.73	114.04
4	D	136	ARG	CA-C-N	8.19	130.08	119.84

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	214	U	Sidechain
30	0	324	G	Sidechain
30	0	393	G	Sidechain
30	0	435	A	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	A	1753	0	1766	100	0
2	B	2625	0	2532	133	0
3	C	1860	0	1813	74	0
4	D	1094	0	1085	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1357	0	1266	56	0
6	F	890	0	843	28	0
7	G	240	0	231	11	0
8	H	1282	0	1292	55	0
9	I	519	0	500	26	0
10	J	1120	0	1098	45	0
11	K	994	0	1027	40	0
12	L	1118	0	1076	30	0
13	M	1558	0	1573	102	0
14	N	1445	0	1401	61	0
15	O	865	0	873	33	0
16	P	1136	0	1123	45	0
17	Q	735	0	729	21	0
18	R	1149	0	1122	39	0
19	S	641	0	605	16	0
20	T	950	0	924	35	0
21	U	410	0	368	39	0
22	V	499	0	511	20	0
23	W	1196	0	1137	55	0
24	X	654	0	653	24	0
25	Y	1130	0	1133	44	0
26	Z	573	0	535	65	0
27	1	431	0	426	20	0
28	2	396	0	413	22	0
29	3	755	0	732	95	0
30	0	59018	0	29810	2254	0
31	9	2599	0	1325	160	0
32	0	84	0	0	0	0
32	2	1	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	9	0	0	2	0
33	3	1	0	0	3	0
33	A	1	0	0	1	0
33	B	1	0	0	2	0
33	J	3	0	0	2	0
33	K	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	L	1	0	0	1	0
33	M	1	0	0	2	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	1	0	0	0	0
36	M	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5897	0	0	323	0
38	1	61	0	0	3	0
38	2	45	0	0	1	0
38	3	76	0	0	7	0
38	9	154	0	0	11	0
38	A	121	0	0	3	0
38	B	145	0	0	20	0
38	C	166	0	0	13	0
38	D	46	0	0	7	0
38	E	43	0	0	4	0
38	F	31	0	0	1	0
38	G	17	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	72	0	0	10	0
38	I	5	0	0	2	0
38	J	52	0	0	4	0
38	K	52	0	0	3	0
38	L	81	0	0	4	0
38	M	133	0	0	12	0
38	N	56	0	0	6	0
38	O	41	0	0	2	0
38	P	63	0	0	5	0
38	Q	52	0	0	1	0
38	R	75	0	0	2	0
38	S	37	0	0	0	0
38	T	40	0	0	3	0
38	U	28	0	0	5	0
38	V	15	0	0	1	0
38	W	69	0	0	7	0
38	X	22	0	0	4	0
38	Y	100	0	0	5	0
38	Z	28	0	0	5	0
All	All	99120	0	59922	3426	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 23.

The worst 5 of 3426 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)
30:0:871:G:C8	30:0:871:G:H5'	1.74	1.22
30:0:1160:G:H5'	30:0:1161:A:C5'	1.70	1.20
30:0:1160:G:C5'	30:0:1161:A:H5'	1.73	1.18
30:0:1278:A:H4'	30:0:1279:U:C4	1.81	1.16
13:M:171:ARG:HD3	30:0:156:C:H5''	1.15	1.13

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	
1	A	235/240 (98%)	200 (85%)	30 (13%)	5 (2%)	5	27
2	B	335/338 (99%)	305 (91%)	23 (7%)	7 (2%)	5	27
3	C	244/246 (99%)	216 (88%)	26 (11%)	2 (1%)	16	50
4	D	134/177 (76%)	105 (78%)	23 (17%)	6 (4%)	2	12
5	E	170/178 (96%)	158 (93%)	11 (6%)	1 (1%)	21	56
6	F	117/120 (98%)	97 (83%)	16 (14%)	4 (3%)	3	17
7	G	25/348 (7%)	22 (88%)	3 (12%)	0	100	100
8	H	156/177 (88%)	139 (89%)	16 (10%)	1 (1%)	21	56
9	I	68/162 (42%)	49 (72%)	16 (24%)	3 (4%)	2	12
10	J	140/145 (97%)	128 (91%)	10 (7%)	2 (1%)	9	36
11	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16	50
12	L	141/165 (86%)	116 (82%)	22 (16%)	3 (2%)	5	27
13	M	192/196 (98%)	171 (89%)	17 (9%)	4 (2%)	5	27
14	N	184/187 (98%)	163 (89%)	17 (9%)	4 (2%)	5	26
15	O	113/116 (97%)	106 (94%)	7 (6%)	0	100	100
16	P	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
17	Q	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	5	26
18	R	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	18	53
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
21	U	51/67 (76%)	44 (86%)	6 (12%)	1 (2%)	6	28
22	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	7	34
23	W	152/154 (99%)	142 (93%)	9 (6%)	1 (1%)	18	53
24	X	80/92 (87%)	72 (90%)	6 (8%)	2 (2%)	4	23
25	Y	140/241 (58%)	132 (94%)	7 (5%)	1 (1%)	18	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	55 (78%)	12 (17%)	4 (6%)	1	8
27	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	64 (71%)	17 (19%)	9 (10%)	0	2
All	All	3705/4472 (83%)	3292 (89%)	348 (9%)	65 (2%)	6	31

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	206	THR
2	B	306	LYS
4	D	137	PRO
6	F	61	MET
6	F	101	ALA

5.3.2 Protein sidechains [i](#)

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	
1	A	179/182 (98%)	169 (94%)	10 (6%)	19	52
2	B	282/283 (100%)	265 (94%)	17 (6%)	17	50
3	C	193/193 (100%)	178 (92%)	15 (8%)	11	39
4	D	117/148 (79%)	110 (94%)	7 (6%)	17	50
5	E	152/156 (97%)	147 (97%)	5 (3%)	33	67
6	F	93/94 (99%)	92 (99%)	1 (1%)	65	83
7	G	27/282 (10%)	25 (93%)	2 (7%)	13	42
8	H	134/145 (92%)	124 (92%)	10 (8%)	12	41
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	108 (92%)	10 (8%)	10	36
11	K	106/106 (100%)	102 (96%)	4 (4%)	29	63
12	L	113/127 (89%)	107 (95%)	6 (5%)	20	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	148 (94%)	10 (6%)	16	48
14	N	149/150 (99%)	145 (97%)	4 (3%)	39	71
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	110 (97%)	3 (3%)	39	71
17	Q	79/80 (99%)	73 (92%)	6 (8%)	12	41
18	R	117/122 (96%)	113 (97%)	4 (3%)	32	66
19	S	71/74 (96%)	70 (99%)	1 (1%)	59	80
20	T	105/106 (99%)	100 (95%)	5 (5%)	23	57
21	U	44/53 (83%)	43 (98%)	1 (2%)	44	74
22	V	51/57 (90%)	51 (100%)	0	100	100
23	W	130/130 (100%)	125 (96%)	5 (4%)	29	63
24	X	66/74 (89%)	62 (94%)	4 (6%)	17	49
25	Y	120/196 (61%)	115 (96%)	5 (4%)	26	61
26	Z	60/94 (64%)	58 (97%)	2 (3%)	33	67
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	43	73
29	3	79/79 (100%)	71 (90%)	8 (10%)	7	29
All	All	3095/3646 (85%)	2949 (95%)	146 (5%)	23	58

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	T	39	ASN
29	3	62	THR
20	T	117	ASP
25	Y	118	THR
4	D	172	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	132	ASN
19	S	53	ASN
29	3	13	HIS
16	P	50	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	94	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	245 (8%)	22 (0%)
31	9	121/122 (99%)	19 (15%)	2 (1%)
All	All	2866/3045 (94%)	264 (9%)	24 (0%)

5 of 264 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1352	A
30	0	2011	A
30	0	1970	G
30	0	2536	C
30	0	644	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMG	0	2588	30	23,26,27	0.34	0	32,38,41	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	UR3	0	2619	30	19,22,23	0.42	0	26,32,35	0.66	1 (3%)
30	OMU	0	2587	35,30	19,22,23	0.32	0	25,31,34	0.40	0
30	1MA	0	628	35,30	21,25,26	0.75	1 (4%)	30,37,40	0.68	1 (3%)
30	PSU	0	2621	30	18,21,22	1.56	2 (11%)	21,30,33	1.38	3 (14%)

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
30	OMG	0	2588	30	-	0/9/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	35,30	-	0/9/27/28	0/2/2/2
30	1MA	0	628	35,30	-	0/7/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	5.10	1.43	1.36
30	0	2621	PSU	C6-C5	2.99	1.38	1.35
30	0	628	1MA	C6-N6	2.51	1.34	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C6-C5-C4	3.53	120.55	118.17
30	0	2621	PSU	C6-N1-C2	-3.12	119.80	122.69
30	0	2621	PSU	O2-C2-N1	3.01	125.89	122.79
30	0	628	1MA	N1-C2-N3	2.84	129.36	126.00
30	0	2619	UR3	C4-N3-C2	2.73	126.78	124.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	628	1MA	3	0
30	0	2621	PSU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	237/240 (98%)	-0.04	4 (1%) 69 45	29, 65, 98, 115	0
2	B	337/338 (99%)	-0.06	2 (0%) 85 69	31, 59, 87, 97	0
3	C	246/246 (100%)	-0.33	1 (0%) 88 76	23, 47, 69, 80	0
4	D	140/177 (79%)	0.71	9 (6%) 25 13	74, 109, 132, 140	0
5	E	172/178 (96%)	-0.01	2 (1%) 76 55	50, 74, 97, 103	0
6	F	119/120 (99%)	0.04	0 100 100	50, 73, 106, 113	0
7	G	29/348 (8%)	0.44	1 (3%) 48 27	75, 96, 105, 109	0
8	H	160/177 (90%)	0.00	5 (3%) 51 30	48, 67, 99, 109	0
9	I	70/162 (43%)	1.26	17 (24%) 2 1	134, 152, 167, 169	0
10	J	142/145 (97%)	-0.18	2 (1%) 73 51	40, 58, 75, 97	0
11	K	132/132 (100%)	-0.33	0 100 100	39, 55, 81, 86	0
12	L	145/165 (87%)	0.31	4 (2%) 55 32	35, 72, 113, 129	0
13	M	194/196 (98%)	0.10	20 (10%) 12 6	31, 46, 99, 106	0
14	N	186/187 (99%)	0.26	4 (2%) 62 39	60, 80, 126, 132	0
15	O	115/116 (99%)	-0.16	0 100 100	43, 56, 74, 80	0
16	P	143/149 (95%)	-0.13	0 100 100	40, 59, 79, 85	0
17	Q	95/96 (98%)	-0.15	0 100 100	44, 56, 72, 88	0
18	R	150/155 (96%)	-0.39	1 (0%) 84 66	33, 49, 70, 83	0
19	S	81/85 (95%)	-0.17	0 100 100	40, 62, 82, 92	0
20	T	119/120 (99%)	-0.17	1 (0%) 82 64	40, 59, 87, 116	0
21	U	53/67 (79%)	1.66	18 (33%) 1 1	107, 117, 125, 126	0
22	V	65/71 (91%)	0.18	5 (7%) 19 10	46, 74, 118, 123	0
23	W	154/154 (100%)	-0.15	1 (0%) 85 69	39, 54, 73, 87	0
24	X	82/92 (89%)	0.05	1 (1%) 76 55	46, 65, 94, 108	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.34	0 100 100	30, 49, 71, 92	0
26	Z	73/116 (62%)	1.69	22 (30%) 1 1	98, 116, 126, 130	0
27	1	56/57 (98%)	-0.65	0 100 100	28, 36, 43, 48	0
28	2	46/50 (92%)	0.21	2 (4%) 40 21	31, 66, 97, 104	0
29	3	92/92 (100%)	2.17	45 (48%) 0 0	104, 119, 130, 134	0
30	0	2749/2923 (94%)	-0.76	4 (0%) 92 86	23, 51, 96, 175	0
31	9	122/122 (100%)	-0.45	2 (1%) 70 47	45, 75, 103, 154	0
All	All	6646/7517 (88%)	-0.27	173 (2%) 57 34	23, 57, 116, 175	0

The worst 5 of 173 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	Z	46	SER	8.4
29	3	39	GLN	7.4
13	M	80	GLY	6.8
29	3	46	ILE	6.5
29	3	83	TRP	6.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	OMU	0	2587	21/22	0.97	0.07	41,44,50,50	0
30	OMG	0	2588	24/25	0.97	0.07	39,41,42,45	0
30	UR3	0	2619	21/22	0.97	0.07	39,43,45,48	0
30	PSU	0	2621	20/21	0.97	0.07	40,43,44,44	0
30	1MA	0	628	23/24	0.98	0.07	31,36,38,38	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	CD	U	8701	1/1	0.61	0.33	200,200,200,200	0
34	SR	0	8959	1/1	0.63	0.11	200,200,200,200	0
35	NA	0	8559	1/1	0.66	0.51	122,122,122,122	0
35	NA	0	8556	1/1	0.67	0.22	63,63,63,63	0
37	CD	3	8704	1/1	0.69	0.37	200,200,200,200	0
34	SR	3	8999	1/1	0.72	0.22	172,172,172,172	0
32	MG	0	8083	1/1	0.74	0.15	71,71,71,71	0
32	MG	B	8042	1/1	0.76	0.23	56,56,56,56	0
34	SR	9	8980	1/1	0.77	0.10	182,182,182,182	0
35	NA	0	8528	1/1	0.77	0.52	83,83,83,83	0
34	SR	0	8938	1/1	0.77	0.10	164,164,164,164	0
35	NA	0	8548	1/1	0.78	0.21	68,68,68,68	0
34	SR	0	8997	1/1	0.79	0.28	194,194,194,194	0
34	SR	0	8919	1/1	0.79	0.15	200,200,200,200	0
34	SR	0	8985	1/1	0.80	0.14	182,182,182,182	0
35	NA	0	8562	1/1	0.80	0.39	89,89,89,89	0
34	SR	0	9000	1/1	0.81	0.37	200,200,200,200	0
34	SR	0	8971	1/1	0.81	0.10	170,170,170,170	0
34	SR	0	8983	1/1	0.81	0.20	191,191,191,191	0
34	SR	0	9001	1/1	0.82	0.11	166,166,166,166	0
33	CL	3	8804	1/1	0.82	0.17	120,120,120,120	0
34	SR	0	8988	1/1	0.82	0.11	170,170,170,170	0
34	SR	A	8993	1/1	0.83	0.10	159,159,159,159	0
35	NA	0	8525	1/1	0.83	0.24	85,85,85,85	0
32	MG	0	8049	1/1	0.83	0.27	74,74,74,74	0
32	MG	T	8057	1/1	0.84	0.19	63,63,63,63	0
32	MG	0	8063	1/1	0.84	0.23	86,86,86,86	0
37	CD	Z	8703	1/1	0.84	0.25	200,200,200,200	0
34	SR	0	9006	1/1	0.84	0.31	180,180,180,180	0
35	NA	0	8573	1/1	0.85	0.10	55,55,55,55	0
34	SR	0	8989	1/1	0.85	0.22	200,200,200,200	0
34	SR	0	8977	1/1	0.85	0.12	181,181,181,181	0
33	CL	0	8816	1/1	0.85	0.21	94,94,94,94	0
35	NA	0	8553	1/1	0.86	0.21	70,70,70,70	0
34	SR	3	8932	1/1	0.86	0.14	158,158,158,158	0
35	NA	0	8557	1/1	0.86	0.12	59,59,59,59	0
34	SR	0	8991	1/1	0.87	0.13	193,193,193,193	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	SR	0	8953	1/1	0.87	0.17	200,200,200,200	0
34	SR	0	8998	1/1	0.87	0.20	184,184,184,184	0
35	NA	0	8565	1/1	0.87	0.15	70,70,70,70	0
32	MG	9	8074	1/1	0.87	0.09	63,63,63,63	0
35	NA	0	8574	1/1	0.87	0.29	54,54,54,54	0
33	CL	A	8809	1/1	0.87	0.30	100,100,100,100	0
35	NA	0	8554	1/1	0.87	0.46	65,65,65,65	0
32	MG	0	8080	1/1	0.87	0.11	68,68,68,68	0
35	NA	0	8555	1/1	0.88	0.23	50,50,50,50	0
34	SR	0	8969	1/1	0.88	0.24	192,192,192,192	0
34	SR	9	9003	1/1	0.88	0.10	177,177,177,177	0
35	NA	0	8518	1/1	0.88	0.31	75,75,75,75	0
34	SR	0	8957	1/1	0.88	0.16	200,200,200,200	0
35	NA	0	8564	1/1	0.88	0.10	57,57,57,57	0
34	SR	0	8975	1/1	0.88	0.11	171,171,171,171	0
35	NA	0	8535	1/1	0.88	0.18	64,64,64,64	0
35	NA	0	8546	1/1	0.88	0.19	80,80,80,80	0
32	MG	0	8075	1/1	0.88	0.17	83,83,83,83	0
34	SR	0	9002	1/1	0.88	0.12	157,157,157,157	0
34	SR	0	8979	1/1	0.88	0.15	198,198,198,198	0
34	SR	0	8947	1/1	0.89	0.14	194,194,194,194	0
34	SR	0	8974	1/1	0.89	0.19	164,164,164,164	0
35	NA	0	8547	1/1	0.89	0.14	47,47,47,47	0
32	MG	3	8090	1/1	0.89	0.25	80,80,80,80	0
33	CL	O	8808	1/1	0.89	0.10	87,87,87,87	0
32	MG	0	8081	1/1	0.89	0.15	80,80,80,80	0
35	NA	0	8523	1/1	0.89	0.10	51,51,51,51	0
34	SR	0	8968	1/1	0.89	0.17	177,177,177,177	0
34	SR	0	8944	1/1	0.89	0.13	165,165,165,165	0
34	SR	0	8976	1/1	0.90	0.14	197,197,197,197	0
35	NA	0	8570	1/1	0.90	0.05	25,25,25,25	0
35	NA	R	8575	1/1	0.90	0.08	89,89,89,89	0
33	CL	N	8807	1/1	0.90	0.14	99,99,99,99	0
32	MG	A	8051	1/1	0.90	0.10	101,101,101,101	0
34	SR	0	8964	1/1	0.90	0.09	129,129,129,129	0
32	MG	0	8030	1/1	0.90	0.33	86,86,86,86	0
32	MG	0	8038	1/1	0.91	0.06	61,61,61,61	0
34	SR	0	8915	1/1	0.91	0.10	118,118,118,118	0
35	NA	0	8541	1/1	0.91	0.11	54,54,54,54	0
35	NA	0	8544	1/1	0.91	0.11	41,41,41,41	0
35	NA	0	8563	1/1	0.91	0.23	65,65,65,65	0
35	NA	S	8510	1/1	0.91	0.07	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8508	1/1	0.91	0.19	61,61,61,61	0
35	NA	0	8566	1/1	0.91	0.13	62,62,62,62	0
32	MG	0	8029	1/1	0.91	0.18	68,68,68,68	0
35	NA	0	8571	1/1	0.91	0.06	46,46,46,46	0
35	NA	0	8551	1/1	0.91	0.14	55,55,55,55	0
35	NA	0	8552	1/1	0.91	0.15	58,58,58,58	0
35	NA	0	8519	1/1	0.91	0.13	51,51,51,51	0
34	SR	B	8987	1/1	0.91	0.25	200,200,200,200	0
32	MG	0	8036	1/1	0.91	0.08	37,37,37,37	0
34	SR	S	8961	1/1	0.92	0.08	126,126,126,126	0
34	SR	0	9004	1/1	0.92	0.23	200,200,200,200	0
34	SR	0	8995	1/1	0.92	0.15	140,140,140,140	0
32	MG	0	8033	1/1	0.92	0.10	40,40,40,40	0
34	SR	0	8951	1/1	0.92	0.07	139,139,139,139	0
35	NA	R	8532	1/1	0.92	0.05	37,37,37,37	0
34	SR	0	8939	1/1	0.92	0.18	152,152,152,152	0
34	SR	0	8955	1/1	0.92	0.19	200,200,200,200	0
32	MG	0	8037	1/1	0.93	0.30	76,76,76,76	0
33	CL	B	8819	1/1	0.93	0.15	59,59,59,59	0
35	NA	0	8522	1/1	0.93	0.09	45,45,45,45	0
34	SR	0	8973	1/1	0.93	0.07	112,112,112,112	0
34	SR	F	9005	1/1	0.93	0.08	131,131,131,131	0
32	MG	0	8018	1/1	0.93	0.12	34,34,34,34	0
32	MG	0	8066	1/1	0.93	0.20	75,75,75,75	0
32	MG	0	8092	1/1	0.93	0.10	44,44,44,44	0
33	CL	0	8811	1/1	0.93	0.21	79,79,79,79	0
34	SR	0	8982	1/1	0.93	0.26	200,200,200,200	0
34	SR	0	8958	1/1	0.93	0.06	114,114,114,114	0
32	MG	0	8039	1/1	0.93	0.08	71,71,71,71	0
34	SR	0	8963	1/1	0.93	0.05	123,123,123,123	0
36	K	0	8401	1/1	0.93	0.34	156,156,156,156	0
34	SR	0	8931	1/1	0.93	0.07	110,110,110,110	0
35	NA	0	8506	1/1	0.93	0.07	58,58,58,58	0
33	CL	0	8822	1/1	0.93	0.29	97,97,97,97	0
33	CL	L	8810	1/1	0.94	0.08	64,64,64,64	0
34	SR	0	8970	1/1	0.94	0.06	131,131,131,131	0
34	SR	B	8950	1/1	0.94	0.08	113,113,113,113	0
32	MG	0	8082	1/1	0.94	0.12	66,66,66,66	0
34	SR	0	8946	1/1	0.94	0.08	123,123,123,123	0
34	SR	0	9007	1/1	0.94	0.40	179,179,179,179	0
32	MG	0	8071	1/1	0.94	0.09	31,31,31,31	0
32	MG	0	8068	1/1	0.94	0.13	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	CL	J	8801	1/1	0.94	0.10	71,71,71,71	0
33	CL	0	8813	1/1	0.94	0.08	46,46,46,46	0
34	SR	0	8981	1/1	0.94	0.12	157,157,157,157	0
34	SR	0	8956	1/1	0.94	0.07	151,151,151,151	0
33	CL	0	8815	1/1	0.94	0.11	87,87,87,87	0
35	NA	0	8513	1/1	0.94	0.15	66,66,66,66	0
33	CL	J	8802	1/1	0.94	0.07	76,76,76,76	0
34	SR	0	8926	1/1	0.94	0.07	109,109,109,109	0
35	NA	0	8520	1/1	0.94	0.15	39,39,39,39	0
35	NA	0	8567	1/1	0.94	0.23	68,68,68,68	0
34	SR	0	8960	1/1	0.94	0.08	152,152,152,152	0
34	SR	0	8962	1/1	0.94	0.08	179,179,179,179	0
34	SR	0	8927	1/1	0.94	0.15	196,196,196,196	0
34	SR	0	8996	1/1	0.94	0.12	199,199,199,199	0
35	NA	0	8529	1/1	0.94	0.05	41,41,41,41	0
34	SR	0	8928	1/1	0.94	0.08	146,146,146,146	0
35	NA	0	8536	1/1	0.94	0.10	40,40,40,40	0
33	CL	K	8812	1/1	0.94	0.11	48,48,48,48	0
34	SR	0	8922	1/1	0.95	0.13	169,169,169,169	0
33	CL	0	8814	1/1	0.95	0.17	72,72,72,72	0
34	SR	0	8965	1/1	0.95	0.07	127,127,127,127	0
34	SR	0	8967	1/1	0.95	0.07	133,133,133,133	0
32	MG	2	8060	1/1	0.95	0.06	35,35,35,35	0
32	MG	0	8035	1/1	0.95	0.14	61,61,61,61	0
35	NA	0	8524	1/1	0.95	0.09	54,54,54,54	0
33	CL	0	8805	1/1	0.95	0.09	70,70,70,70	0
34	SR	A	8930	1/1	0.95	0.11	125,125,125,125	0
35	NA	C	8503	1/1	0.95	0.09	45,45,45,45	0
35	NA	M	8539	1/1	0.95	0.09	32,32,32,32	0
35	NA	Q	8540	1/1	0.95	0.33	67,67,67,67	0
34	SR	0	8972	1/1	0.95	0.13	150,150,150,150	0
34	SR	0	8914	1/1	0.95	0.07	105,105,105,105	0
35	NA	0	8545	1/1	0.95	0.10	33,33,33,33	0
34	SR	0	8941	1/1	0.95	0.07	122,122,122,122	0
35	NA	9	8543	1/1	0.95	0.20	38,38,38,38	0
35	NA	9	8572	1/1	0.95	0.05	71,71,71,71	0
35	NA	0	8501	1/1	0.95	0.12	43,43,43,43	0
35	NA	0	8505	1/1	0.95	0.17	53,53,53,53	0
32	MG	0	8065	1/1	0.95	0.06	50,50,50,50	0
32	MG	0	8032	1/1	0.95	0.05	27,27,27,27	0
33	CL	Y	8820	1/1	0.96	0.07	47,47,47,47	0
32	MG	0	8040	1/1	0.96	0.17	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	SR	0	8992	1/1	0.96	0.14	130,130,130,130	0
34	SR	0	8994	1/1	0.96	0.16	200,200,200,200	0
33	CL	0	8803	1/1	0.96	0.16	69,69,69,69	0
34	SR	0	8942	1/1	0.96	0.07	130,130,130,130	0
35	NA	0	8533	1/1	0.96	0.10	53,53,53,53	0
34	SR	0	8924	1/1	0.96	0.15	133,133,133,133	0
34	SR	0	8925	1/1	0.96	0.09	94,94,94,94	0
35	NA	0	8502	1/1	0.96	0.06	56,56,56,56	0
32	MG	0	8091	1/1	0.96	0.09	58,58,58,58	0
34	SR	A	8929	1/1	0.96	0.11	117,117,117,117	0
32	MG	0	8017	1/1	0.96	0.05	20,20,20,20	0
35	NA	0	8511	1/1	0.96	0.06	48,48,48,48	0
32	MG	0	8079	1/1	0.96	0.06	36,36,36,36	0
35	NA	0	8550	1/1	0.96	0.11	47,47,47,47	0
35	NA	0	8515	1/1	0.96	0.07	44,44,44,44	0
34	SR	0	8933	1/1	0.96	0.13	126,126,126,126	0
34	SR	0	8986	1/1	0.96	0.08	200,200,200,200	0
34	SR	0	8935	1/1	0.96	0.05	87,87,87,87	0
34	SR	0	8916	1/1	0.97	0.05	114,114,114,114	0
32	MG	0	8016	1/1	0.97	0.05	48,48,48,48	0
35	NA	0	8537	1/1	0.97	0.13	29,29,29,29	0
35	NA	J	8538	1/1	0.97	0.08	49,49,49,49	0
34	SR	0	8954	1/1	0.97	0.05	103,103,103,103	0
34	SR	0	8920	1/1	0.97	0.10	106,106,106,106	0
34	SR	0	8921	1/1	0.97	0.04	75,75,75,75	0
34	SR	0	8984	1/1	0.97	0.05	105,105,105,105	0
32	MG	B	8043	1/1	0.97	0.20	53,53,53,53	0
32	MG	0	8041	1/1	0.97	0.17	36,36,36,36	0
33	CL	0	8817	1/1	0.97	0.08	69,69,69,69	0
32	MG	0	8077	1/1	0.97	0.08	43,43,43,43	0
33	CL	J	8821	1/1	0.97	0.07	66,66,66,66	0
35	NA	0	8507	1/1	0.97	0.06	32,32,32,32	0
32	MG	0	8047	1/1	0.97	0.17	67,67,67,67	0
35	NA	0	8509	1/1	0.97	0.08	54,54,54,54	0
32	MG	0	8004	1/1	0.97	0.07	21,21,21,21	0
32	MG	0	8050	1/1	0.97	0.10	52,52,52,52	0
35	NA	0	8560	1/1	0.97	0.11	74,74,74,74	0
35	NA	0	8561	1/1	0.97	0.22	57,57,57,57	0
35	NA	0	8514	1/1	0.97	0.07	17,17,17,17	0
32	MG	0	8055	1/1	0.97	0.04	45,45,45,45	0
34	SR	0	8937	1/1	0.97	0.05	100,100,100,100	0
32	MG	0	8020	1/1	0.97	0.12	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8089	1/1	0.97	0.09	59,59,59,59	0
32	MG	0	8005	1/1	0.97	0.10	34,34,34,34	0
35	NA	0	8568	1/1	0.97	0.05	38,38,38,38	0
32	MG	0	8015	1/1	0.97	0.05	25,25,25,25	0
34	SR	0	8911	1/1	0.97	0.03	79,79,79,79	0
32	MG	0	8093	1/1	0.97	0.03	28,28,28,28	0
35	NA	0	8526	1/1	0.97	0.04	33,33,33,33	0
35	NA	0	8527	1/1	0.97	0.25	54,54,54,54	0
32	MG	0	8067	1/1	0.97	0.04	32,32,32,32	0
34	SR	9	8978	1/1	0.97	0.05	125,125,125,125	0
37	CD	O	8705	1/1	0.97	0.06	93,93,93,93	0
35	NA	0	8530	1/1	0.97	0.10	49,49,49,49	0
34	SR	0	8948	1/1	0.97	0.07	103,103,103,103	0
35	NA	0	8534	1/1	0.97	0.05	37,37,37,37	0
32	MG	0	8023	1/1	0.98	0.10	24,24,24,24	0
32	MG	0	8024	1/1	0.98	0.10	96,96,96,96	0
32	MG	0	8014	1/1	0.98	0.11	21,21,21,21	0
35	NA	0	8542	1/1	0.98	0.11	51,51,51,51	0
34	SR	0	8936	1/1	0.98	0.04	87,87,87,87	0
32	MG	0	8001	1/1	0.98	0.04	26,26,26,26	0
32	MG	0	8069	1/1	0.98	0.08	55,55,55,55	0
32	MG	0	8031	1/1	0.98	0.08	52,52,52,52	0
34	SR	R	8912	1/1	0.98	0.04	86,86,86,86	0
35	NA	0	8549	1/1	0.98	0.13	77,77,77,77	0
32	MG	0	8072	1/1	0.98	0.06	47,47,47,47	0
34	SR	0	8943	1/1	0.98	0.04	72,72,72,72	0
34	SR	1	8913	1/1	0.98	0.03	100,100,100,100	0
34	SR	0	8945	1/1	0.98	0.04	107,107,107,107	0
32	MG	K	8054	1/1	0.98	0.08	40,40,40,40	0
32	MG	0	8076	1/1	0.98	0.06	27,27,27,27	0
34	SR	0	8901	1/1	0.98	0.03	63,63,63,63	0
34	SR	0	8908	1/1	0.98	0.03	77,77,77,77	0
35	NA	0	8558	1/1	0.98	0.18	44,44,44,44	0
35	NA	0	8512	1/1	0.98	0.04	36,36,36,36	0
34	SR	0	8910	1/1	0.98	0.04	99,99,99,99	0
34	SR	0	8990	1/1	0.98	0.05	125,125,125,125	0
32	MG	Y	8086	1/1	0.98	0.02	37,37,37,37	0
35	NA	0	8516	1/1	0.98	0.07	20,20,20,20	0
33	CL	R	8806	1/1	0.98	0.04	47,47,47,47	0
32	MG	0	8078	1/1	0.98	0.10	51,51,51,51	0
32	MG	0	8034	1/1	0.98	0.05	53,53,53,53	0
35	NA	0	8521	1/1	0.98	0.09	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	SR	0	8917	1/1	0.98	0.05	109,109,109,109	0
35	NA	0	8569	1/1	0.98	0.11	67,67,67,67	0
32	MG	0	8052	1/1	0.98	0.03	51,51,51,51	0
32	MG	0	8009	1/1	0.98	0.08	24,24,24,24	0
32	MG	0	8056	1/1	0.98	0.07	75,75,75,75	0
32	MG	0	8059	1/1	0.98	0.07	53,53,53,53	0
32	MG	0	8085	1/1	0.98	0.10	67,67,67,67	0
32	MG	0	8061	1/1	0.98	0.06	19,19,19,19	0
36	K	M	8402	1/1	0.98	0.05	60,60,60,60	0
34	SR	0	8966	1/1	0.98	0.04	97,97,97,97	0
32	MG	0	8062	1/1	0.98	0.09	57,57,57,57	0
34	SR	0	9008	1/1	0.98	0.04	97,97,97,97	0
32	MG	0	8010	1/1	0.98	0.05	24,24,24,24	0
32	MG	0	8064	1/1	0.98	0.04	33,33,33,33	0
34	SR	0	8909	1/1	0.99	0.05	89,89,89,89	0
32	MG	0	8084	1/1	0.99	0.07	24,24,24,24	0
32	MG	0	8044	1/1	0.99	0.04	52,52,52,52	0
34	SR	0	8949	1/1	0.99	0.02	102,102,102,102	0
32	MG	0	8087	1/1	0.99	0.02	26,26,26,26	0
32	MG	0	8088	1/1	0.99	0.05	35,35,35,35	0
32	MG	0	8046	1/1	0.99	0.04	26,26,26,26	0
32	MG	0	8011	1/1	0.99	0.07	24,24,24,24	0
34	SR	0	8918	1/1	0.99	0.03	71,71,71,71	0
32	MG	0	8048	1/1	0.99	0.06	20,20,20,20	0
35	NA	0	8517	1/1	0.99	0.06	21,21,21,21	0
32	MG	0	8013	1/1	0.99	0.03	24,24,24,24	0
32	MG	0	8070	1/1	0.99	0.03	40,40,40,40	0
32	MG	0	8021	1/1	0.99	0.06	25,25,25,25	0
34	SR	0	8923	1/1	0.99	0.04	85,85,85,85	0
32	MG	0	8022	1/1	0.99	0.06	17,17,17,17	0
32	MG	0	8073	1/1	0.99	0.11	51,51,51,51	0
32	MG	0	8053	1/1	0.99	0.04	45,45,45,45	0
32	MG	0	8007	1/1	0.99	0.03	18,18,18,18	0
32	MG	0	8008	1/1	0.99	0.07	26,26,26,26	0
32	MG	0	8058	1/1	0.99	0.04	22,22,22,22	0
33	CL	M	8818	1/1	0.99	0.04	39,39,39,39	0
34	SR	0	8934	1/1	0.99	0.06	99,99,99,99	0
32	MG	0	8025	1/1	0.99	0.02	30,30,30,30	0
35	NA	0	8531	1/1	0.99	0.04	15,15,15,15	0
34	SR	1	8952	1/1	0.99	0.03	72,72,72,72	0
32	MG	0	8026	1/1	0.99	0.03	27,27,27,27	0
32	MG	0	8027	1/1	0.99	0.05	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8002	1/1	0.99	0.03	29,29,29,29	0
34	SR	0	8940	1/1	0.99	0.02	77,77,77,77	0
34	SR	0	8903	1/1	0.99	0.04	46,46,46,46	0
34	SR	0	8904	1/1	0.99	0.07	58,58,58,58	0
34	SR	0	8906	1/1	0.99	0.07	64,64,64,64	0
34	SR	0	8907	1/1	0.99	0.02	40,40,40,40	0
32	MG	0	8003	1/1	0.99	0.08	22,22,22,22	0
35	NA	0	8504	1/1	1.00	0.03	27,27,27,27	0
32	MG	0	8028	1/1	1.00	0.02	19,19,19,19	0
34	SR	0	8902	1/1	1.00	0.04	67,67,67,67	0
32	MG	0	8019	1/1	1.00	0.04	23,23,23,23	0
32	MG	0	8006	1/1	1.00	0.03	20,20,20,20	0
34	SR	0	8905	1/1	1.00	0.09	62,62,62,62	0
32	MG	0	8045	1/1	1.00	0.03	24,24,24,24	0
37	CD	1	8702	1/1	1.00	0.04	61,61,61,61	0
32	MG	0	8012	1/1	1.00	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.