



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:05 PM BST

PDB ID : 4V7I
EMDB ID: : EMD-1484
Title : Ribosome-SecY complex.
Authors : Gumbart, J.C.; Trabuco, L.G.; Schreiner, E.; Villa, E.; Schulten, K.
Deposited on : 2009-10-21
Resolution : 9.60 Å(reported)
Based on PDB ID : 2I2V, 3BO0

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

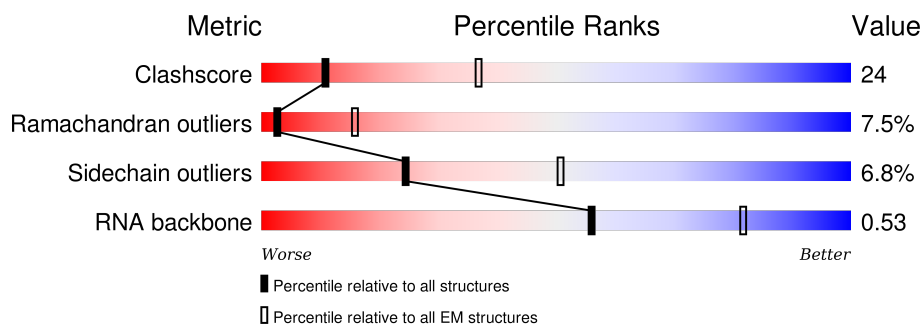
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.60 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.














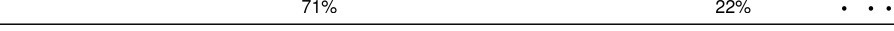







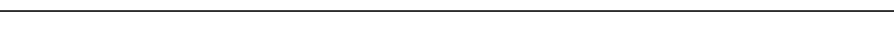

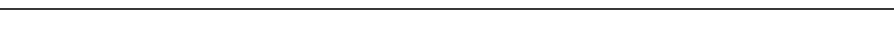
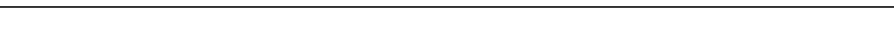


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A7	120	8% 40% 50% .
2	A8	2904	10% 42% 48%
3	AA	442	87% 9% .
4	AB	65	82% 12% 6%
5	AC	53	58% . 40%
6	A5	234	77% 21% .
7	A6	273	61% 31% 6% ..
8	AD	209	63% 25% 10% .









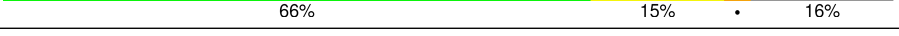

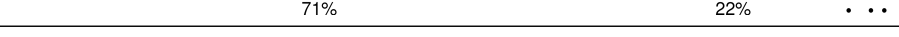
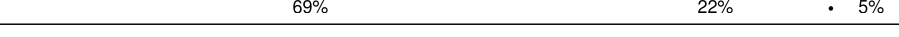

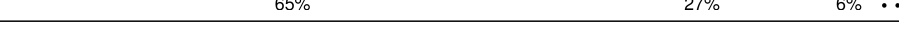




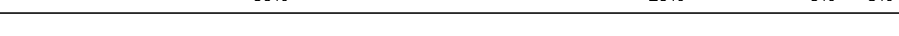



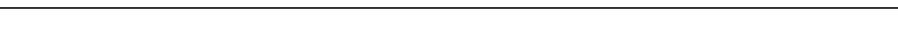
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Mol	Chain	Length	Quality of chain
9	AE	201	 73% 22% 5%
10	AF	179	 68% 23% 7% ..
11	AG	177	 66% 26% 7% ..
12	AH	149	 70% 26% .
13	AI	142	 74% 20% 6% .
14	AJ	142	 65% 27% 6% .
15	AK	123	 68% 24% 6% ..
16	AL	144	 74% 17% 6% ..
17	AM	136	 55% 35% 9% .
18	AN	127	 60% 28% 5% . 6%
19	AO	117	 79% 18% ..
20	AP	115	 71% 22% . . .
21	AQ	118	 69% 22% 8% .
22	AR	103	 62% 29% 9%
23	AS	110	 66% 25% 6% .
24	AT	100	 58% 27% 6% . 7%
25	AU	104	 66% 24% 5% . .
26	AV	94	 65% 31% . .
27	AW	85	 48% 29% 12% . 7%
28	AX	78	 55% 38% . . .
29	AY	63	 86% 14%
30	AZ	59	 68% 25% . . .
31	A0	57	 65% 25% 9% .
32	A1	55	 55% 27% 5% . 9%
33	A2	46	 65% 28% 7%

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Mol	Chain	Length	Quality of chain
34	A3	65	
35	A4	38	
36	BA	1542	
37	BB	241	
38	BC	233	
39	BD	206	
40	BE	167	
41	BF	135	
42	BG	179	
43	BH	130	
44	BI	130	
45	BJ	103	
46	BK	129	
47	BL	124	
48	BM	118	
49	BN	101	
50	BO	89	
51	BP	82	
52	BQ	84	
53	BR	75	
54	BS	92	
55	BT	87	
56	BU	71	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 148250 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A7	117	Total	C	N	O	P	0	0
			2507	1116	459	815	117		

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A8	2903	Total	C	N	O	P	0	0
			62321	27801	11467	20150	2903		

- Molecule 3 is a protein called PREPROTEIN TRANSLOCASE SECY SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AA	442	Total	C	N	O	S	0	0
			3408	2266	547	577	18		

- Molecule 4 is a protein called PREPROTEIN TRANSLOCASE SECE SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	AB	65	Total	C	N	O	0	0
			505	332	88	85		

- Molecule 5 is a protein called Preprotein translocase subunit secG.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AC	32	Total	C	N	O	0	0
			257	172	42	43		

- Molecule 6 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A6	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AH	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AK	121	Total	C	N	O	S	0	0
			930	582	179	164	5		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AN	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 19 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	AO	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 21 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	AQ	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 22 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 23 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 24 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AT	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	AU	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AV	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AW	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 28 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AX	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AZ	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 31 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	A1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 33 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 34 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	A3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 35 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	A4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 36 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BA	1530	Total	C	N	O	P	0	0
			32831	14642	6024	10635	1530		

- Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BB	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 38 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 39 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 40 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BE	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 41 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BF	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BG	150	Total	C	N	O	S	0	0
			1174	730	226	214	4		

- Molecule 43 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 44 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BJ	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 46 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 47 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 48 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BM	113	Total	C	N	O	S	0	0
			876	541	177	155	3		

- Molecule 49 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BN	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 50 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BO	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 51 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BP	80	Total	C	N	O	S	0	0
			638	400	126	111	1		

- Molecule 52 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	BR	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BS	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 56 is a protein called 30S ribosomal protein S21.

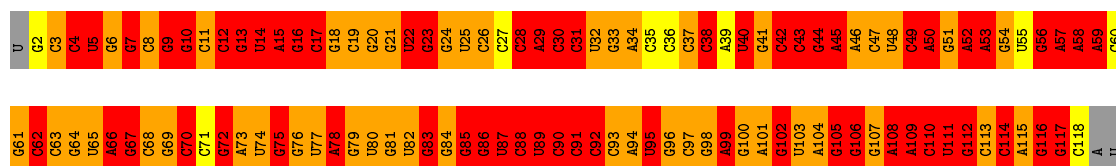
Mol	Chain	Residues	Atoms					AltConf	Trace
56	BU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

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. 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. 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.

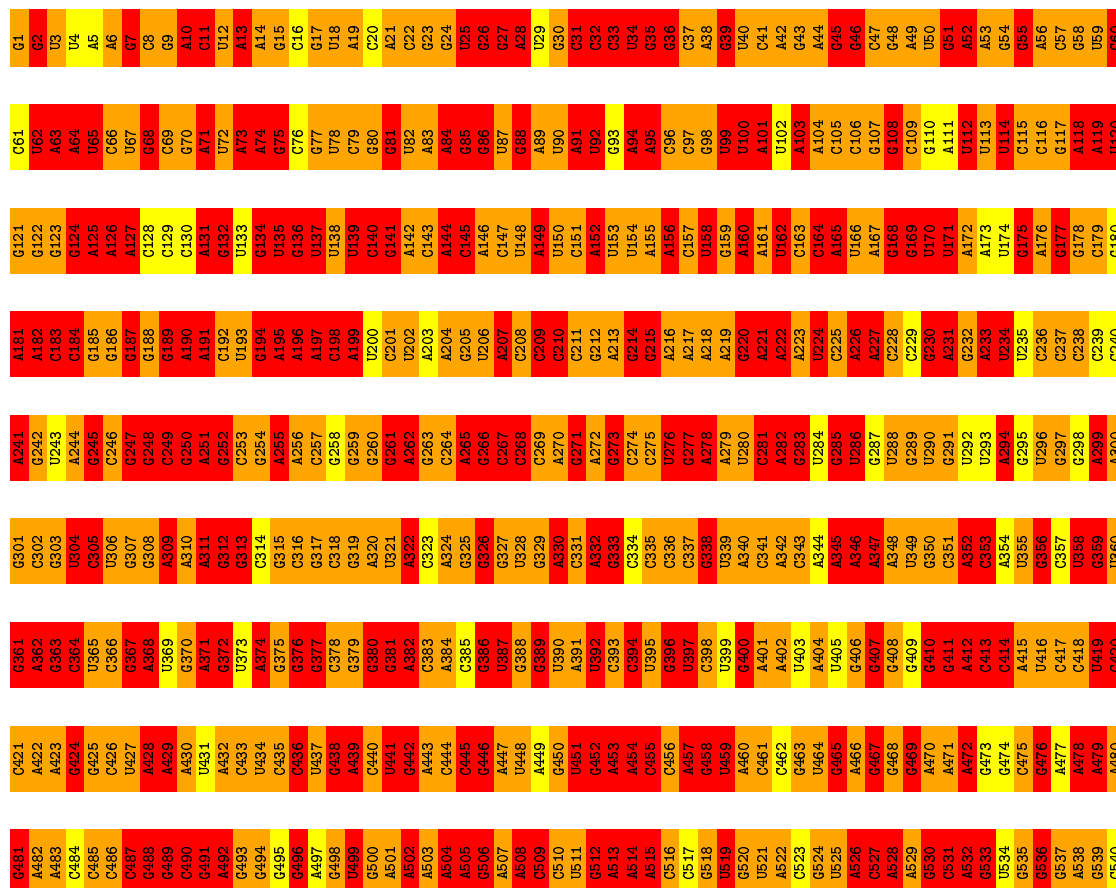
• Molecule 1: 5S ribosomal RNA

Chain A7: 



• Molecule 2: 23S ribosomal RNA

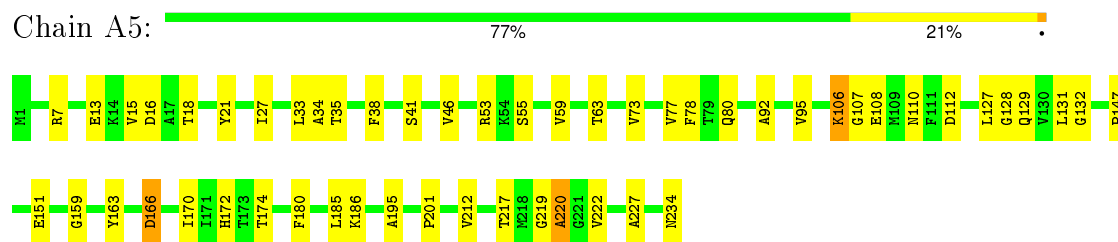
Chain A8: 



G1441	G1381	A1321	C1261	U1201	U1141	U1081	A1021	C961	C901	G841	A781	A721	A661	C601	A541
G1442	G1382	A1322	A1262	G1202	A1142	U1082	G1022	G962	C902	U842	A782	A722	A662	A602	C542
G1443	A1383	G1323	U1263	U1203	A1143	U1083	U1023	G963	C903	G843	A783	C723	G663	A603	G543
G1444	A1384	G1324	A1264	A1204	A1144	A1084	G1024	C964	G904	A844	A784	C724	G664	G604	C544
G1445	A1385	A1325	A1265	A1205	C1145	A1085	G1025	C965	A905	A845	A785	G725	U665	G605	U545
G1446	C1386	U1326	G1266	G1206	G1146	A1086	G1026	G966	U906	U846	A786	G726	U666	U606	U546
G1447	A1387	A1327	U1267	C1207	A1147	G1087	A1027	U967	G907	U847	C787	A727	U667	U607	A547
G1448	G1388	A1328	A1268	C1208	U1148	A1088	A1028	C968	C908	C848	A788	G728	A668	A608	G548
G1449	G1389	A1329	A1269	U1209	G1149	A1089	A1029	G969	G909	C849	A789	G729	G669	A609	G549
G1450	U1390	C1270	C1270	G1210	C1150	A1090	C1030	U970	A910	A850	A790	A730	A670	C610	C550
G1451	U1391	G1271	A1271	C1211	C1151	G1091	G1031	G971	A911	C851	C791	C731	C671	C611	G551
G1452	A1392	A1272	G1332	G1212	C1152	C1092	A1032	A972	G912	U852	A792	G732	C672	G612	U552
G1453	A1393	A1273	C1333	C1153	C1153	G1093	U1033	G973	U913	C853	A793	G733	C673	C613	G553
G1454	U1394	A1274	G1334	A1214	G1154	U1094	G1034	G974	G914	C854	A794	G734	C674	A614	U554
G1455	A1395	C1335	A1275	G1215	A1155	A1095	U1035	A975	C915	G855	A795	G735	C675	U615	G555
G1456	U1396	A1276	A1276	G1216	A1156	A1096	G1036	G976	G916	G856	A796	G736	A676	A616	A556
G1457	U1397	G1277	G1277	U1217	C1157	U1097	G1037	G977	A917	G857	C797	G737	A677	G617	C557
G1458	C1398	G1338	C1278	G1218	G1158	A1098	G1038	G978	A918	G858	G798	G738	C678	G618	U558
G1459	C1399	G1279	U1159	U1219	U1159	G1099	A1039	A979	U919	G859	G799	A739	C679	G619	G559
U1460	U1400	G1280	G1280	G1220	G1160	C1100	A1040	A980	A920	U860	A800	C740	C680	G620	C560
C1461	G1341	G1281	C1281	C1221	C1161	U1101	G1041	A981	C921	A861	G801	U741	C681	A621	G561
G1462	U1402	U1282	U1282	G1222	G1162	C1102	G1042	C982	C922	G862	A802	A742	G682	C622	U562
C1463	G1343	G1283	G1283	G1223	G1163	A1103	C1043	A983	G923	A863	U803	A743	U683	C623	A563
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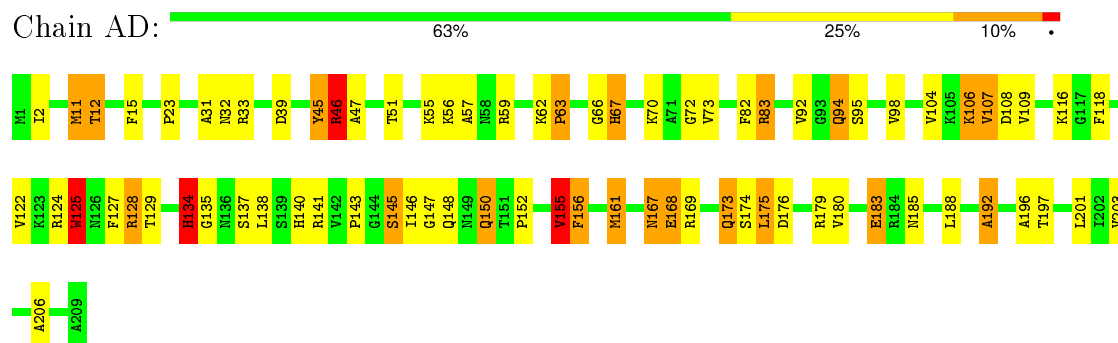


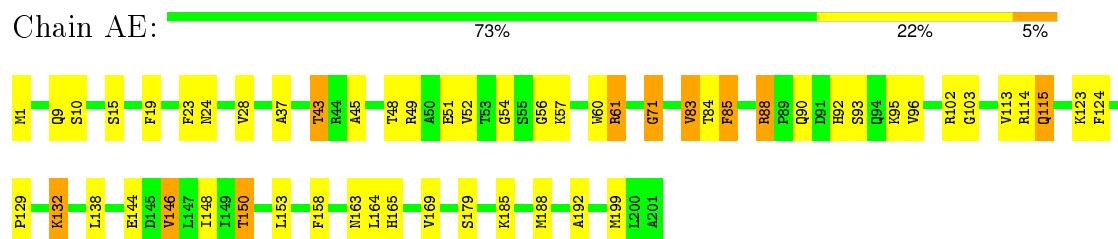
- Molecule 7: 50S ribosomal protein L2



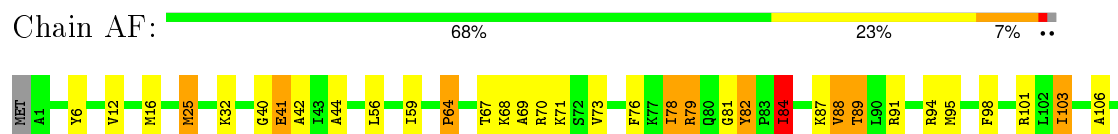
- Molecule 8: 50S ribosomal protein L3



- Molecule 9: 50S ribosomal protein L4



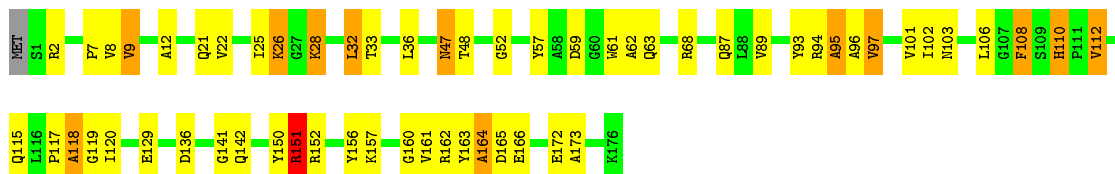
- Molecule 10: 50S ribosomal protein L5





- Molecule 11: 50S ribosomal protein L6

Chain AG: 66% 26% 7% ..



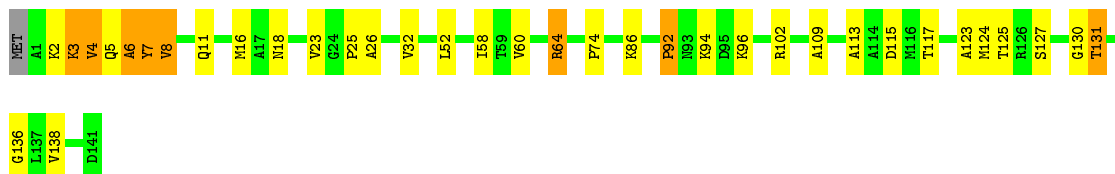
- Molecule 12: 50S ribosomal protein L9

Chain AH: 70% 26% .



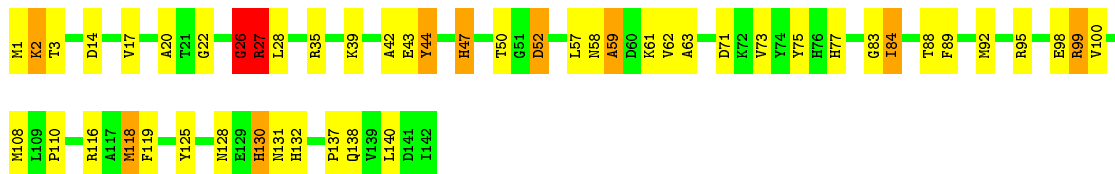
- Molecule 13: 50S ribosomal protein L11

Chain AI: 74% 20% 6% .



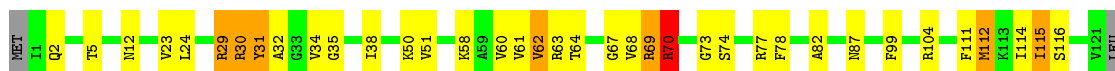
- Molecule 14: 50S ribosomal protein L13

Chain AJ: 65% 27% 6% .

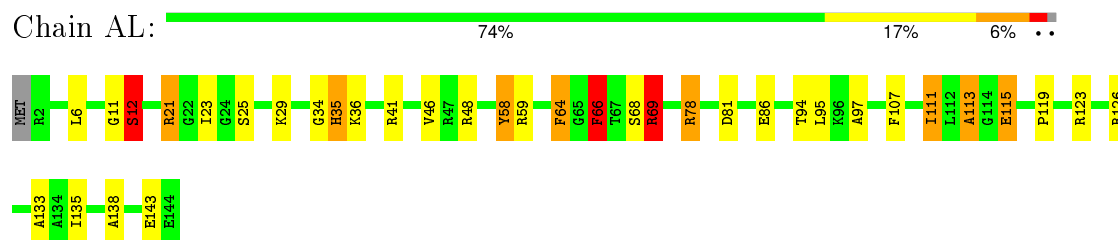


- Molecule 15: 50S ribosomal protein L14

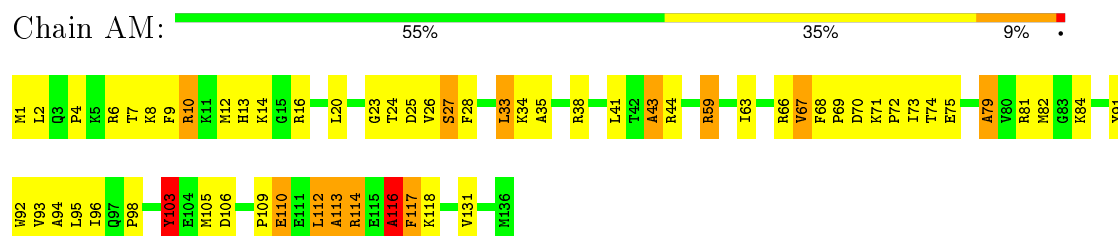
Chain AK: 68% 24% 6% ..



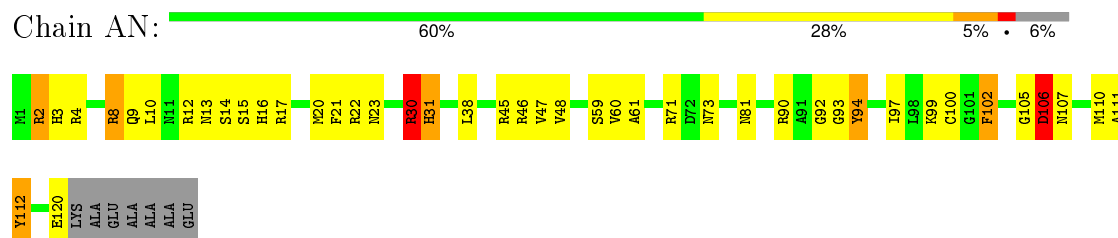
- Molecule 16: 50S ribosomal protein L15



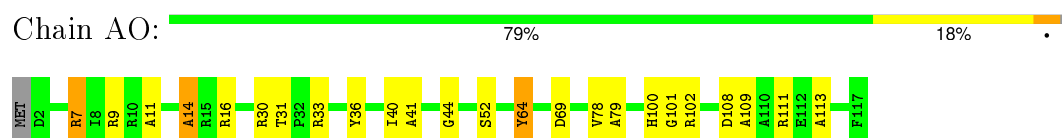
- Molecule 17: 50S ribosomal protein L16



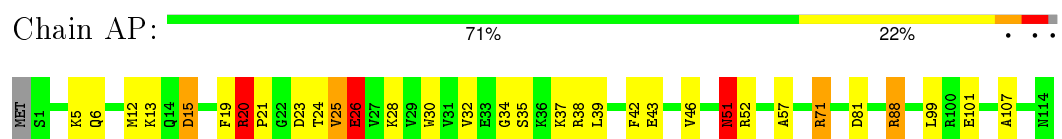
- Molecule 18: 50S ribosomal protein L17



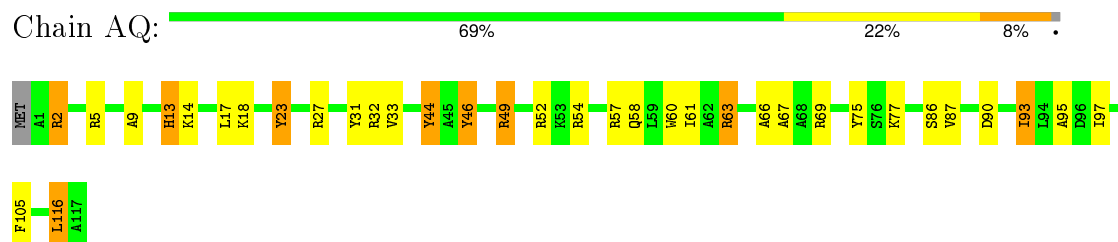
- Molecule 19: 50S ribosomal protein L18



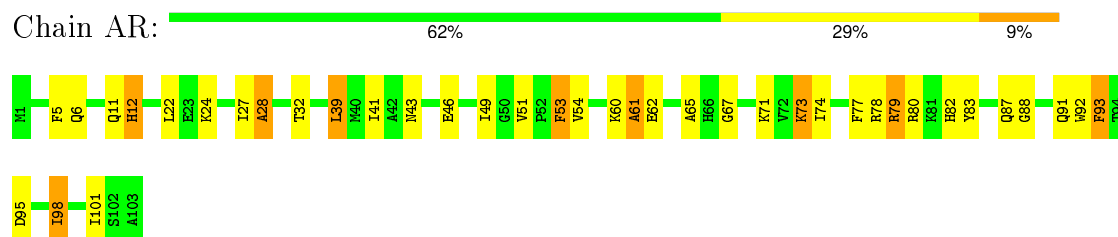
- Molecule 20: 50S ribosomal protein L19



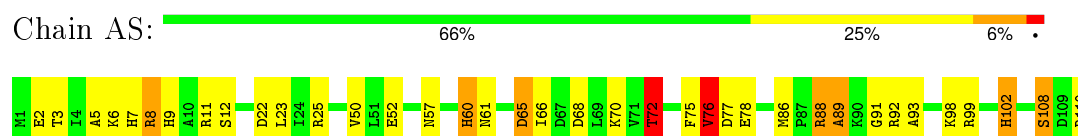
- Molecule 21: 50S ribosomal protein L20



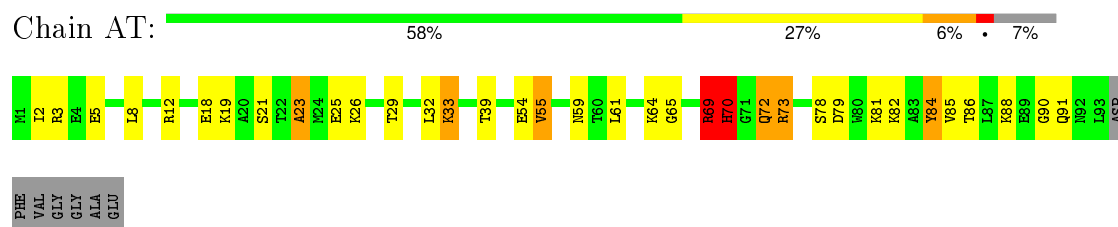
- Molecule 22: 50S ribosomal protein L21



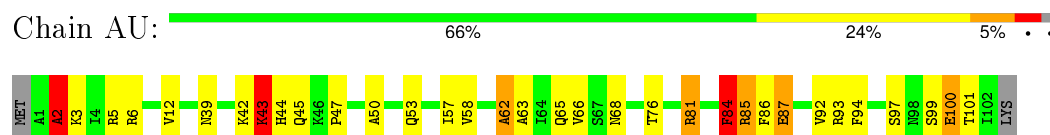
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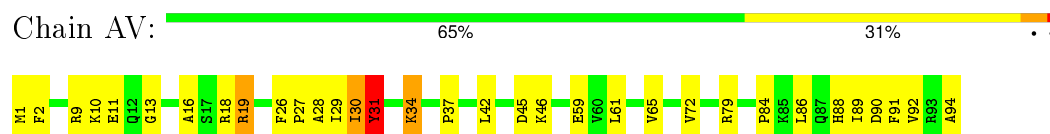
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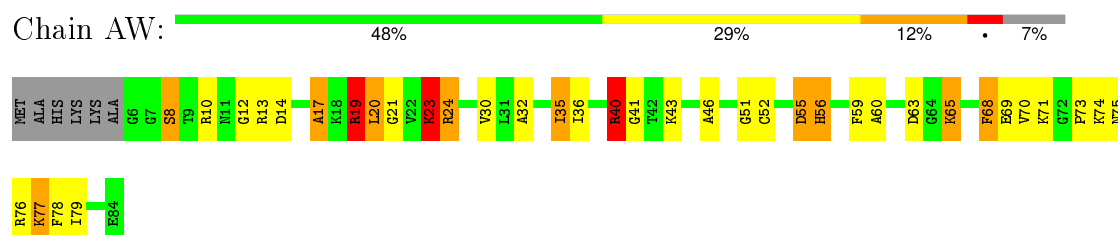
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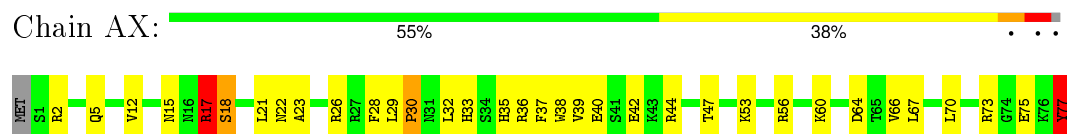
- Molecule 26: 50S ribosomal protein L25



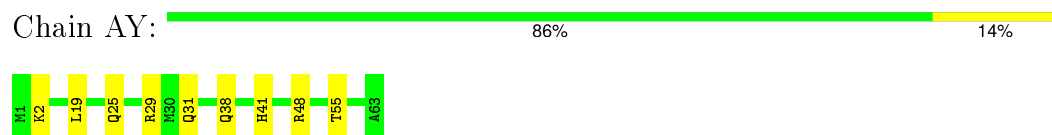
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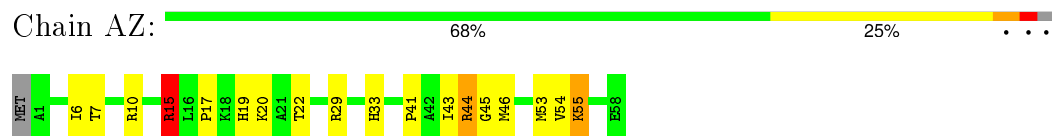
- Molecule 28: 50S ribosomal protein L28



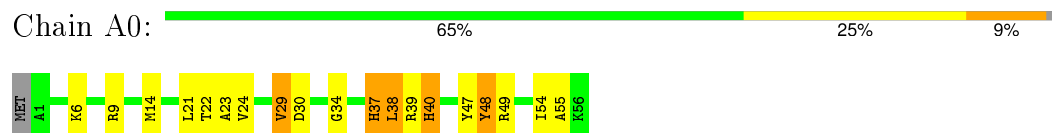
- Molecule 29: 50S ribosomal protein L29



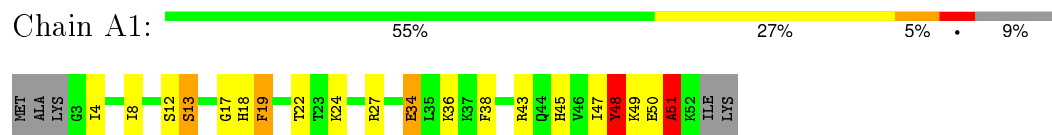
- Molecule 30: 50S ribosomal protein L30



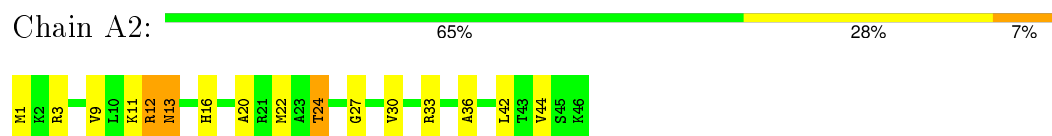
- Molecule 31: 50S ribosomal protein L32



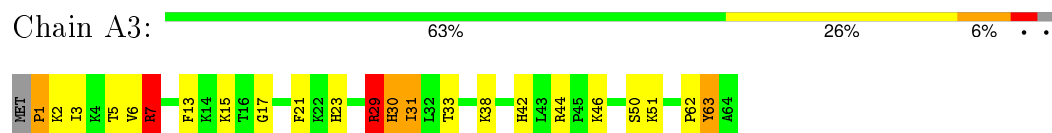
- Molecule 32: 50S ribosomal protein L33



- Molecule 33: 50S ribosomal protein L34



- Molecule 34: 50S ribosomal protein L35



- Molecule 35: 50S ribosomal protein L36





● Molecule 36: 16S ribosomal RNA

Chain BA: 12% 45% 42%

C841	A781	G721	G661	G601	G541	G481	U421	G361	G301	G241	A181	U121	G61
U842	A782	G722	U662	A602	G542	A482	G422	G362	G302	G242	A182	G122	U62
A843	U783	U723	A663	A603	U543	C483	G423	A363	A303	A243	C183	U123	C63
G844	A784	G724	G664	G604	G544	G484	G424	A364	U304	U244	G184	G124	G64
A845	G785	G725	A665	U605	C545	U485	G425	U365	G365	U245	U185	U125	A65
G846	G786	G726	G666	G606	A546	U486	U426	A366	A306	A246	C186	G126	G66
A847	A787	G727	G667	A607	A547	C487	U427	U367	C307	G247	G187	G127	A67
C848	U788	U728	G668	A608	G548	C488	G428	U368	C308	C248	C188	G128	G68
G849	A789	G729	G669	A609	C489	C489	U429	G369	A309	U249	A189	A129	G69
U850	U790	U730	G670	U610	G550	C490	A430	C370	G310	A250	A190	A130	U70
G851	G791	G731	G671	C611	U551	G491	A431	A371	C311	G251	G191	A131	A71
G852	A792	G732	U672	C612	U552	C492	A432	G372	C312	U252	A192	C132	A72
C853	U793	G733	A673	C613	A553	C493	G433	A373	A313	G253	A193	U133	U73
A854	A794	G734	G674	C614	A554	G494	A434	A374	C314	G254	A194	G134	A74
U855	U795	U735	A675	G615	U555	A495	A435	U375	A315	G255	A195	C135	G75
G856	G796	G736	A676	G616	C556	A496	G436	G376	C316	U256	A196	U136	G76
C857	U797	U737	U677	G617	G557	G497	U437	U377	U317	G257	A197	U137	A77
G858	U798	C738	U678	C618	G558	A498	U438	G378	G318	G258	G198	G138	A78
A859	G799	G739	C679	U619	A559	A499	U439	C379	G319	G259	A199	A139	U79
U860	U800	U740	C680	C620	A560	G500	A440	C380	A320	G260	G200	U140	A80
G861	U801	G741	A681	C621	U561	C501	A441	A381	A321	U261	G201	G141	A81
C862	A802	G742	G682	A622	A502	A502	G442	A382	C322	A262	G202	G142	G82
U863	G803	A743	G683	C623	C503	C503	A443	A383	U323	A263	G203	A143	C83
A864	U804	C744	U684	C624	C504	C504	G444	G384	G324	G264	G204	U144	U84
G865	C805	G745	G685	U625	U565	G505	G445	C385	A325	G265	G205	G145	U85
C866	C806	A746	U686	G626	G566	G506	G446	C386	G326	G266	C206	G146	G86
G867	A807	U747	A687	G627	G567	C507	G447	U387	A327	C267	C207	G147	C87
C868	C808	G748	G688	G628	U568	U508	A448	C388	C328	U268	U208	G148	U88
G869	G809	U749	C689	A629	C569	A509	A449	A389	A329	C268	U209	A149	U89
U870	U810	C750	C690	A630	G570	A510	G450	U390	C330	A270	G210	U150	C90
A871	C811	U751	G691	C631	U571	C511	A451	G391	G331	C271	G211	A151	G91
U872	U812	G752	U692	U632	A572	U512	G452	C392	G332	C272	G212	A152	U92
G873	A813	A753	G693	G633	C513	C513	G453	A393	U333	U273	G213	C153	U93
C874	A814	G754	A694	C634	A574	C514	G454	G394	C334	A274	C214	U154	G94
U875	A815	G755	A695	A635	G575	G515	G455	C395	C335	G275	C215	A155	C95
A876	U816	C756	A696	U636	C576	U516	A456	C396	A336	G276	U216	C156	C96
G877	C817	U757	U697	C637	G577	G517	G457	A397	G337	C277	C217	U157	G97
U878	A818	A758	G698	U638	G578	C518	U458	U398	A338	G278	U218	G158	C98
C879	U819	G759	C699	G639	A579	C519	A459	G399	C339	A279	U219	G159	C99
U880	C820	U760	U700	A640	C580	A520	A460	C400	U340	G280	G220	A160	C40
G881	G821	G761	U701	U641	G581	G521	A461	C401	C341	C281	C221	A161	A41
C882	U822	U762	A702	A642	C582	C522	G462	G402	C342	A282	C222	A162	G42
G883	C823	G763	G703	C643	A583	A523	U463	C403	U343	U283	A223	C163	C43
U884	G824	C764	A704	U644	G584	G524	U464	A404	A344	C284	U224	G164	A44
A885	A825	G765	G705	G645	G585	C525	A465	U405	C345	C285	G225	G165	G45
G886	C826	A766	A706	G646	C586	C526	A466	A406	G346	C286	C226	U166	C46
C887	U827	U767	U707	C647	G587	G527	U467	U407	G347	U287	G227	A167	C47
G888	U828	A768	C708	A648	U588	C528	U468	A408	C348	A288	A228	G168	C48
A889	G829	G769	U709	A649	U589	G529	C469	U409	A349	G289	U229	C169	A49
U890	U830	C770	G710	G650	U590	G530	A470	A410	G350	C290	U230	U170	A50
G891	A831	U771	G711	C651	U591	U531	U471	A411	C351	U291	G231	A171	A51
C892	C832	U772	A712	U652	G592	A532	U472	A412	C352	G292	G232	A172	C52
G893	G833	G773	G713	U653	U593	A533	U473	G413	A353	G293	C233	U173	A53
A894	U834	G774	G714	G654	U594	U534	A474	A414	C354	U294	C234	A174	C54
G895	U835	G775	A715	A655	A595	A535	A475	A415	C355	C295	G235	G175	A55
C896	C836	C776	A716	G656	A596	C536	U476	A416	A356	U296	A236	C176	U56
U897	U837	A777	U717	U657	G597	G537	C477	G417	G357	G297	G237	G177	C57
G898	C838	G778	A718	G658	U598	G538	A478	A418	U358	A298	A238	G178	C58
U899	U839	U779	C719	U659	A599	A539	U479	C419	G359	G299	U239	A179	A59
C900	C840	C780	U720	U660	C600	C540	U480	U400	C360	U300	G240	U120	A60



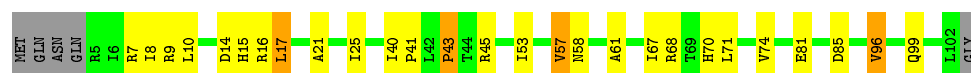
- Molecule 44: 30S ribosomal protein S9

Chain BI: 71% 22% . .



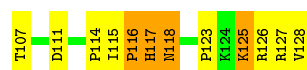
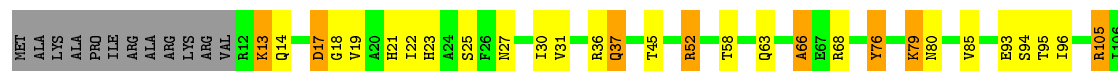
- Molecule 45: 30S ribosomal protein S10

Chain BJ: 69% 22% 5% .



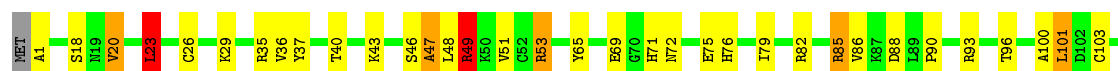
- Molecule 46: 30S ribosomal protein S11

Chain BK: 59% 22% 9% 9%



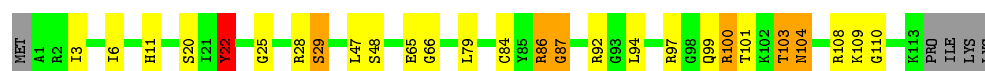
- Molecule 47: 30S ribosomal protein S12

Chain BL: 65% 27% 6% . .



- Molecule 48: 30S ribosomal protein S13

Chain BM: 73% 17% 5% . .

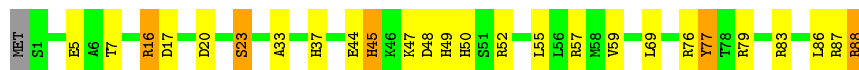


- Molecule 49: 30S ribosomal protein S14

Chain BN: 79% 15% . .



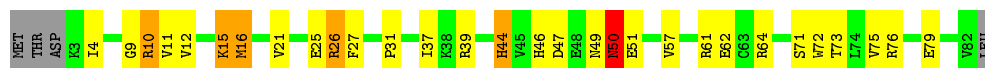
- Molecule 50: 30S ribosomal protein S15



- Molecule 51: 30S ribosomal protein S16



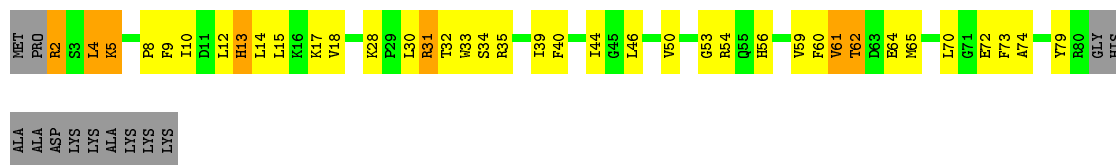
- Molecule 52: 30S ribosomal protein S17



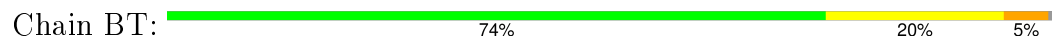
- Molecule 53: 30S ribosomal protein S18



- Molecule 54: 30S ribosomal protein S19

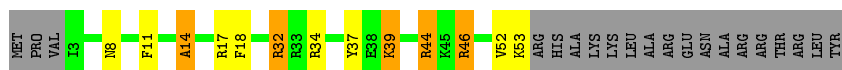


- Molecule 55: 30S ribosomal protein S20



- Molecule 56: 30S ribosomal protein S21





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EMAN- PHASE FLIPPING OF PARTICLES FORM THE SAME MICROGRAPH	Depositor
Microscope	TF20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1500.00	Depositor
Minimum defocus (nm)	-700.00	Depositor
Maximum defocus (nm)	-3000.00	Depositor
Magnification	50000	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 >2	RMSZ	# Z >2
1	A7	2.22	139/2803 (5.0%)	3.06	443/4371 (10.1%)
10	AF	1.11	0/1444	1.37	6/1937 (0.3%)
11	AG	1.09	0/1343	1.41	12/1816 (0.7%)
12	AH	1.05	0/1122	1.36	7/1515 (0.5%)
13	AI	0.96	0/1046	1.24	3/1410 (0.2%)
14	AJ	1.16	1/1152 (0.1%)	1.37	3/1551 (0.2%)
15	AK	1.21	0/939	1.35	4/1258 (0.3%)
16	AL	1.12	0/1054	1.30	7/1403 (0.5%)
17	AM	1.15	0/1093	1.46	12/1460 (0.8%)
18	AN	1.21	0/973	1.43	9/1301 (0.7%)
19	AO	1.16	0/902	1.30	3/1209 (0.2%)
2	A8	2.30	3372/69800 (4.8%)	3.05	10411/108892 (9.6%)
20	AP	1.16	0/929	1.38	5/1242 (0.4%)
21	AQ	1.24	0/960	1.45	8/1278 (0.6%)
22	AR	1.19	0/829	1.43	5/1107 (0.5%)
23	AS	1.11	0/864	1.40	9/1156 (0.8%)
24	AT	1.04	0/744	1.40	5/994 (0.5%)
25	AU	1.05	0/787	1.34	5/1051 (0.5%)
26	AV	1.11	0/766	1.38	4/1025 (0.4%)
27	AW	1.11	0/603	1.37	4/797 (0.5%)
28	AX	1.23	0/635	1.54	6/848 (0.7%)
29	AY	1.08	0/510	1.23	0/677
3	AA	0.95	0/3484	1.15	15/4732 (0.3%)
30	AZ	1.13	0/453	1.34	3/605 (0.5%)
31	A0	1.15	0/450	1.30	2/599 (0.3%)
32	A1	1.03	0/416	1.57	5/554 (0.9%)
33	A2	1.33	0/380	1.51	1/498 (0.2%)
34	A3	1.06	0/513	1.33	2/676 (0.3%)
35	A4	1.20	0/303	1.31	1/397 (0.3%)
36	BA	2.16	1315/36762 (3.6%)	2.97	5321/57350 (9.3%)
37	BB	1.01	0/1735	1.19	4/2338 (0.2%)
38	BC	1.04	0/1651	1.24	5/2225 (0.2%)
39	BD	1.09	0/1665	1.25	7/2227 (0.3%)
4	AB	0.98	0/514	1.20	1/694 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	BE	1.08	0/1118	1.32	5/1504 (0.3%)
41	BF	1.11	0/835	1.35	9/1128 (0.8%)
42	BG	1.06	0/1187	1.20	3/1591 (0.2%)
43	BH	1.08	0/989	1.39	5/1326 (0.4%)
44	BI	1.20	0/1034	1.33	4/1375 (0.3%)
45	BJ	1.08	0/796	1.25	2/1077 (0.2%)
46	BK	1.15	0/893	1.36	3/1205 (0.2%)
47	BL	1.21	0/969	1.41	5/1300 (0.4%)
48	BM	1.13	0/884	1.26	6/1181 (0.5%)
49	BN	1.10	0/817	1.34	5/1088 (0.5%)
5	AC	0.98	0/262	1.02	0/354
50	BO	1.19	0/724	1.33	3/966 (0.3%)
51	BP	1.14	0/648	1.29	6/870 (0.7%)
52	BQ	1.09	0/657	1.33	4/881 (0.5%)
53	BR	1.15	0/462	1.41	5/621 (0.8%)
54	BS	1.09	1/652 (0.2%)	1.36	7/877 (0.8%)
55	BT	1.13	0/671	1.30	3/888 (0.3%)
56	BU	1.21	0/430	1.26	2/570 (0.4%)
6	A5	0.98	0/1748	1.20	3/2355 (0.1%)
7	A6	1.15	0/2121	1.35	8/2852 (0.3%)
8	AD	1.10	0/1586	1.41	10/2134 (0.5%)
9	AE	1.05	0/1571	1.28	7/2113 (0.3%)
All	All	1.96	4828/160678 (3.0%)	2.65	16443/239449 (6.9%)

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	A7	0	56
10	AF	0	5
11	AG	0	6
12	AH	0	2
13	AI	0	3
14	AJ	0	6
15	AK	0	4
16	AL	0	4
17	AM	0	13
18	AN	0	4
19	AO	0	3
2	A8	0	1380

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	AP	0	5
21	AQ	0	7
22	AR	0	4
23	AS	0	2
24	AT	0	3
25	AU	0	4
26	AV	0	1
27	AW	0	1
28	AX	0	2
29	AY	0	2
3	AA	0	12
30	AZ	0	2
31	A0	0	3
32	A1	0	3
33	A2	0	1
34	A3	0	4
35	A4	0	1
36	BA	0	678
37	BB	0	5
38	BC	0	2
39	BD	0	12
4	AB	0	2
40	BE	0	1
41	BF	0	3
42	BG	0	3
43	BH	0	4
44	BI	0	1
45	BJ	0	1
46	BK	0	5
47	BL	0	9
48	BM	0	7
49	BN	0	4
50	BO	0	5
51	BP	0	3
52	BQ	0	1
53	BR	0	4
54	BS	0	2
55	BT	0	1
56	BU	0	3
6	A5	0	3
7	A6	0	18
8	AD	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	AE	0	6
All	All	0	2335

The worst 5 of 4828 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A8	2469	A	N7-C5	-14.86	1.30	1.39
2	A8	1689	A	N7-C5	-14.56	1.30	1.39
2	A8	2412	A	N7-C5	-13.83	1.30	1.39
2	A8	2860	A	N7-C5	-13.77	1.30	1.39
2	A8	633	A	N7-C5	-13.76	1.30	1.39

The worst 5 of 16443 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A8	1723	G	C5-C6-O6	-25.05	113.57	128.60
2	A8	2471	A	O4'-C1'-N9	24.02	127.42	108.20
2	A8	1723	G	N1-C6-O6	23.04	133.72	119.90
2	A8	2468	A	O4'-C1'-N9	21.60	125.48	108.20
2	A8	198	C	C6-N1-C2	-21.54	111.68	120.30

There are no chirality outliers.

5 of 2335 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A7	10	G	Sidechain
1	A7	4	C	Sidechain
1	A7	5	U	Sidechain
1	A7	7	G	Sidechain
1	A7	9	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	A7	2507	0	1270	171	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A8	62321	0	31344	3726	0
3	AA	3408	0	3619	13	0
4	AB	505	0	557	1	0
5	AC	257	0	272	1	0
6	A5	1733	0	1824	24	0
7	A6	2082	0	2157	50	0
8	AD	1565	0	1616	37	0
9	AE	1552	0	1619	31	0
10	AF	1420	0	1460	20	0
11	AG	1323	0	1374	22	0
12	AH	1111	0	1148	17	0
13	AI	1032	0	1088	26	0
14	AJ	1129	0	1162	29	0
15	AK	930	0	1003	20	0
16	AL	1045	0	1117	15	0
17	AM	1074	0	1157	24	0
18	AN	960	0	1000	32	0
19	AO	892	0	923	10	0
20	AP	917	0	965	10	0
21	AQ	947	0	1022	15	0
22	AR	816	0	839	17	0
23	AS	857	0	922	22	0
24	AT	738	0	807	14	0
25	AU	779	0	834	16	0
26	AV	753	0	780	23	0
27	AW	596	0	610	29	0
28	AX	625	0	655	19	0
29	AY	509	0	543	5	0
30	AZ	449	0	491	11	0
31	A0	444	0	461	9	0
32	A1	409	0	440	14	0
33	A2	377	0	418	7	0
34	A3	504	0	574	12	0
35	A4	302	0	343	10	0
36	BA	32831	0	16521	1593	0
37	BB	1704	0	1732	17	0
38	BC	1624	0	1699	19	0
39	BD	1643	0	1710	21	0
40	BE	1105	0	1148	22	0
41	BF	817	0	808	21	0
42	BG	1174	0	1230	12	0
43	BH	979	0	1034	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BI	1022	0	1070	17	0
45	BJ	786	0	828	13	0
46	BK	877	0	887	18	0
47	BL	955	0	1019	23	0
48	BM	876	0	937	7	0
49	BN	805	0	847	3	0
50	BO	716	0	742	10	0
51	BP	638	0	656	11	0
52	BQ	648	0	691	10	0
53	BR	455	0	478	6	0
54	BS	637	0	665	25	0
55	BT	665	0	714	7	0
56	BU	425	0	449	4	0
All	All	148250	0	102279	6042	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 24.

The worst 5 of 6042 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)
2:A8:1902:C:H1'	7:A6:242:HIS:CE1	2.14	0.83
36:BA:113:G:H1'	36:BA:354:G:H4'	1.61	0.83
2:A8:2121:G:H1	2:A8:2176:A:H61	1.27	0.82
36:BA:68:G:H1'	36:BA:151:A:H61	1.47	0.79
28:AX:18:SER:H	28:AX:22:ASN:H	1.30	0.79

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AA	440/442 (100%)	383 (87%)	41 (9%)	16 (4%)	4	38
4	AB	63/65 (97%)	55 (87%)	3 (5%)	5 (8%)	1	19
5	AC	30/53 (57%)	29 (97%)	1 (3%)	0	100	100
6	A5	232/234 (99%)	199 (86%)	18 (8%)	15 (6%)	1	25
7	A6	269/273 (98%)	192 (71%)	55 (20%)	22 (8%)	1	18
8	AD	207/209 (99%)	144 (70%)	40 (19%)	23 (11%)	0	11
9	AE	199/201 (99%)	155 (78%)	29 (15%)	15 (8%)	1	21
10	AF	176/179 (98%)	120 (68%)	34 (19%)	22 (12%)	0	8
11	AG	174/177 (98%)	129 (74%)	24 (14%)	21 (12%)	0	8
12	AH	147/149 (99%)	102 (69%)	32 (22%)	13 (9%)	1	17
13	AI	139/142 (98%)	122 (88%)	11 (8%)	6 (4%)	3	34
14	AJ	140/142 (99%)	109 (78%)	22 (16%)	9 (6%)	2	25
15	AK	119/123 (97%)	87 (73%)	26 (22%)	6 (5%)	3	31
16	AL	141/144 (98%)	107 (76%)	18 (13%)	16 (11%)	0	10
17	AM	134/136 (98%)	91 (68%)	31 (23%)	12 (9%)	1	17
18	AN	118/127 (93%)	89 (75%)	21 (18%)	8 (7%)	1	23
19	AO	114/117 (97%)	94 (82%)	17 (15%)	3 (3%)	7	45
20	AP	112/115 (97%)	82 (73%)	20 (18%)	10 (9%)	1	17
21	AQ	115/118 (98%)	87 (76%)	20 (17%)	8 (7%)	1	22
22	AR	101/103 (98%)	84 (83%)	11 (11%)	6 (6%)	2	27
23	AS	108/110 (98%)	85 (79%)	17 (16%)	6 (6%)	2	28
24	AT	91/100 (91%)	60 (66%)	23 (25%)	8 (9%)	1	17
25	AU	100/104 (96%)	67 (67%)	17 (17%)	16 (16%)	0	5
26	AV	92/94 (98%)	73 (79%)	17 (18%)	2 (2%)	8	49
27	AW	77/85 (91%)	48 (62%)	13 (17%)	16 (21%)	0	3
28	AX	75/78 (96%)	49 (65%)	19 (25%)	7 (9%)	1	16
29	AY	61/63 (97%)	41 (67%)	19 (31%)	1 (2%)	12	56
30	AZ	56/59 (95%)	49 (88%)	6 (11%)	1 (2%)	11	53
31	A0	54/57 (95%)	41 (76%)	8 (15%)	5 (9%)	1	16
32	A1	48/55 (87%)	37 (77%)	6 (12%)	5 (10%)	1	12
33	A2	44/46 (96%)	33 (75%)	7 (16%)	4 (9%)	1	17
34	A3	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	A4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	1	18
37	BB	216/241 (90%)	165 (76%)	40 (18%)	11 (5%)	2	30
38	BC	204/233 (88%)	158 (78%)	30 (15%)	16 (8%)	1	20
39	BD	203/206 (98%)	163 (80%)	28 (14%)	12 (6%)	2	27
40	BE	148/167 (89%)	106 (72%)	32 (22%)	10 (7%)	1	23
41	BF	98/135 (73%)	71 (72%)	16 (16%)	11 (11%)	0	11
42	BG	148/179 (83%)	110 (74%)	26 (18%)	12 (8%)	1	19
43	BH	127/130 (98%)	87 (68%)	32 (25%)	8 (6%)	2	25
44	BI	125/130 (96%)	99 (79%)	16 (13%)	10 (8%)	1	19
45	BJ	96/103 (93%)	79 (82%)	9 (9%)	8 (8%)	1	18
46	BK	115/129 (89%)	87 (76%)	15 (13%)	13 (11%)	0	10
47	BL	121/124 (98%)	104 (86%)	13 (11%)	4 (3%)	5	40
48	BM	111/118 (94%)	83 (75%)	18 (16%)	10 (9%)	1	17
49	BN	98/101 (97%)	68 (69%)	21 (21%)	9 (9%)	1	17
50	BO	86/89 (97%)	76 (88%)	7 (8%)	3 (4%)	4	39
51	BP	78/82 (95%)	63 (81%)	9 (12%)	6 (8%)	1	20
52	BQ	78/84 (93%)	58 (74%)	12 (15%)	8 (10%)	1	12
53	BR	53/75 (71%)	44 (83%)	7 (13%)	2 (4%)	4	37
54	BS	77/92 (84%)	57 (74%)	16 (21%)	4 (5%)	2	30
55	BT	83/87 (95%)	71 (86%)	8 (10%)	4 (5%)	3	32
56	BU	49/71 (69%)	33 (67%)	11 (22%)	5 (10%)	1	13
All	All	6388/6779 (94%)	4900 (77%)	1008 (16%)	480 (8%)	3	21

5 of 480 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AA	239	LYS
3	AA	349	PRO
6	A5	55	SER
6	A5	59	VAL
7	A6	78	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AA	362/362 (100%)	341 (94%)	21 (6%)	25	61
4	AB	52/52 (100%)	46 (88%)	6 (12%)	7	32
5	AC	28/45 (62%)	28 (100%)	0	100	100
6	A5	181/181 (100%)	171 (94%)	10 (6%)	27	63
7	A6	216/218 (99%)	200 (93%)	16 (7%)	17	54
8	AD	164/164 (100%)	144 (88%)	20 (12%)	6	31
9	AE	165/165 (100%)	161 (98%)	4 (2%)	57	82
10	AF	149/150 (99%)	135 (91%)	14 (9%)	11	42
11	AG	137/138 (99%)	127 (93%)	10 (7%)	17	54
12	AH	114/114 (100%)	110 (96%)	4 (4%)	43	74
13	AI	109/110 (99%)	100 (92%)	9 (8%)	14	49
14	AJ	116/116 (100%)	106 (91%)	10 (9%)	13	47
15	AK	102/104 (98%)	95 (93%)	7 (7%)	19	56
16	AL	102/103 (99%)	94 (92%)	8 (8%)	16	51
17	AM	109/109 (100%)	97 (89%)	12 (11%)	8	34
18	AN	100/103 (97%)	91 (91%)	9 (9%)	12	44
19	AO	86/87 (99%)	83 (96%)	3 (4%)	43	74
20	AP	99/100 (99%)	94 (95%)	5 (5%)	29	66
21	AQ	89/90 (99%)	81 (91%)	8 (9%)	12	44
22	AR	84/84 (100%)	76 (90%)	8 (10%)	11	41
23	AS	93/93 (100%)	82 (88%)	11 (12%)	6	32
24	AT	80/84 (95%)	72 (90%)	8 (10%)	9	38
25	AU	83/85 (98%)	78 (94%)	5 (6%)	24	60
26	AV	78/78 (100%)	72 (92%)	6 (8%)	16	52
27	AW	59/63 (94%)	51 (86%)	8 (14%)	5	27
28	AX	67/68 (98%)	63 (94%)	4 (6%)	24	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	AY	55/55 (100%)	55 (100%)	0	100	100
30	AZ	48/49 (98%)	46 (96%)	2 (4%)	36	70
31	A0	47/48 (98%)	42 (89%)	5 (11%)	8	36
32	A1	45/49 (92%)	44 (98%)	1 (2%)	60	83
33	A2	38/38 (100%)	34 (90%)	4 (10%)	8	36
34	A3	51/52 (98%)	45 (88%)	6 (12%)	6	32
35	A4	34/34 (100%)	33 (97%)	1 (3%)	50	78
37	BB	180/199 (90%)	173 (96%)	7 (4%)	39	72
38	BC	170/190 (90%)	162 (95%)	8 (5%)	32	68
39	BD	172/173 (99%)	166 (96%)	6 (4%)	43	74
40	BE	113/126 (90%)	103 (91%)	10 (9%)	12	45
41	BF	87/116 (75%)	79 (91%)	8 (9%)	11	43
42	BG	123/147 (84%)	121 (98%)	2 (2%)	70	88
43	BH	104/105 (99%)	96 (92%)	8 (8%)	16	52
44	BI	105/107 (98%)	98 (93%)	7 (7%)	20	57
45	BJ	86/90 (96%)	83 (96%)	3 (4%)	43	74
46	BK	90/99 (91%)	81 (90%)	9 (10%)	9	38
47	BL	103/104 (99%)	93 (90%)	10 (10%)	10	40
48	BM	91/96 (95%)	88 (97%)	3 (3%)	45	76
49	BN	83/84 (99%)	79 (95%)	4 (5%)	31	67
50	BO	76/77 (99%)	73 (96%)	3 (4%)	39	72
51	BP	65/65 (100%)	61 (94%)	4 (6%)	23	60
52	BQ	74/78 (95%)	68 (92%)	6 (8%)	15	50
53	BR	48/65 (74%)	43 (90%)	5 (10%)	9	36
54	BS	70/79 (89%)	67 (96%)	3 (4%)	35	70
55	BT	65/66 (98%)	58 (89%)	7 (11%)	8	35
56	BU	44/61 (72%)	40 (91%)	4 (9%)	12	43
All	All	5291/5518 (96%)	4929 (93%)	362 (7%)	24	57

5 of 362 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	AP	24	THR

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Mol	Chain	Res	Type
24	AT	84	TYR
51	BP	18	GLN
21	AQ	13	HIS
22	AR	95	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
19	AO	19	GLN
26	AV	24	ASN
50	BO	49	HIS
19	AO	100	HIS
23	AS	7	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A7	116/120 (96%)	24 (20%)	4 (3%)
2	A8	2902/2904 (99%)	537 (18%)	109 (3%)
36	BA	1530/1542 (99%)	296 (19%)	51 (3%)
All	All	4548/4566 (99%)	857 (18%)	164 (3%)

5 of 857 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A7	9	G
1	A7	12	C
1	A7	13	G
1	A7	14	U
1	A7	15	A

5 of 164 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A8	1938	A
2	A8	2309	A
36	BA	1168	U
2	A8	2021	C
2	A8	2134	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.