



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 03:12 PM EST

PDB ID : 4V6Q
EMDB ID : EMD-5363
Title : Structural characterization of mRNA-tRNA translocation intermediates (class 5 of the six classes)
Authors : Agirrezabala, X.; Liao, H.; Schreiner, E.; Fu, J.; Ortiz-Meoz, R.F.; Schulten, K.; Green, R.; Frank, J.
Deposited on : 2011-12-08
Resolution : 11.50 Å (reported)
Based on initial model : 2I2U

This is a wwPDB EM 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/EMValidationReportHelp>

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:

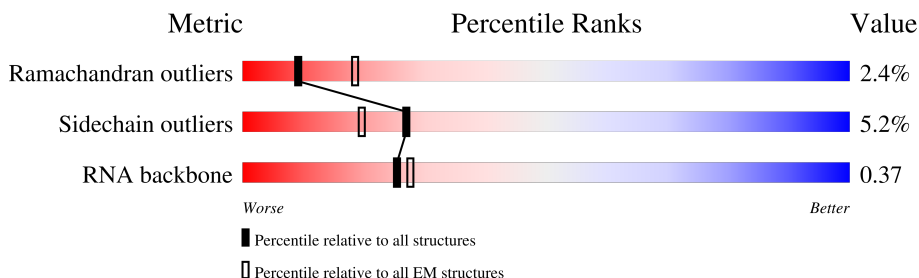
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 11.50 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.




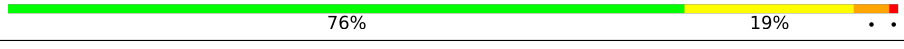
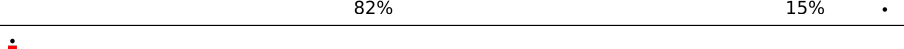
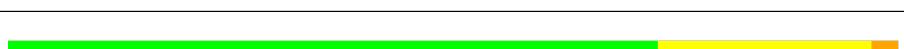



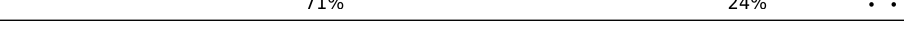



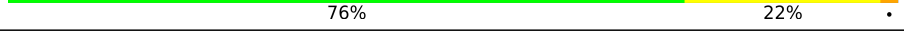

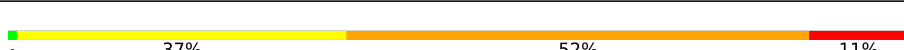


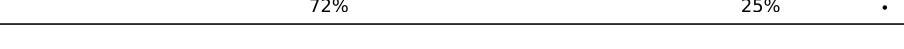







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1542	
2	AB	76	
3	AC	47	
4	AD	77	
5	AE	240	
6	AF	232	
7	AG	205	
8	AH	166	

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Mol	Chain	Length	Quality of chain
9	AI	135	
10	AJ	178	
11	AK	129	
12	AL	129	
13	AM	103	
14	AN	128	
15	AO	123	
16	AP	117	
17	AQ	100	
18	AR	88	
19	AS	82	
20	AT	83	
21	AU	74	
22	AV	91	
23	AW	86	
24	AX	70	
25	BA	120	
26	BB	2904	
27	BC	234	
28	BD	272	
29	BE	209	
30	BF	201	
31	BG	178	
32	BH	176	
33	BI	149	

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Mol	Chain	Length	Quality of chain
34	BJ	164	
35	BK	141	
36	BL	142	
37	BM	123	
38	BN	144	
39	BO	136	
40	BP	127	
41	BQ	117	
42	BR	114	
43	BS	117	
44	BT	103	
45	BU	110	
46	BV	100	
47	BW	103	
48	BX	94	
49	BY	84	
50	BZ	77	
51	B0	63	
52	B1	58	
53	B2	70	
54	B3	56	
55	B4	54	
56	B5	46	
57	B6	64	
58	B7	38	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 152351 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1542	Total	C	N	O	P	0	0
			33089	14767	6064	10717	1541		

- Molecule 2 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AB	76	Total	C	N	O	P	S	0	0
			1627	731	287	532	75	2		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	47	Total	C	N	O	P	0	0
			993	445	167	335	46		

- Molecule 4 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	AD	77	Total	C	N	O	P	S	0	0
			1641	734	297	533	76	1		

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	240	Total	C	N	O	S	0	0
			1872	1180	332	352	8		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	232	Total	C	N	O	S	0	0
			1822	1149	346	323	4		

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	166	Total	C	N	O	S	0	0
			1225	761	232	226	6		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	178	Total	C	N	O	S	0	0
			1400	874	269	253	4		

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	103	Total	C	N	O	S	0	0
			825	514	158	151	2		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	91	Total	C	N	O	S	0	0
			727	464	139	122	2		

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 24 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	120	Total	C	N	O	P	0	0
			2566	1144	468	835	119		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	2904	Total	C	N	O	P	0	0
			62351	27824	11469	20155	2903		

- Molecule 27 is a protein called 50S ribosomal protein L1.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BD	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BJ	164	Total	C	N	O	S	0	0
			1233	776	220	231	6		

- Molecule 35 is a protein called 50S ribosomal protein L11.

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

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BM	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 39 is a protein called 50S ribosomal protein L16.

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

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BP	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BQ	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	103	Total	C	N	O		0	0
			789	498	148	143			

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B0	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B2	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	B4	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 56 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

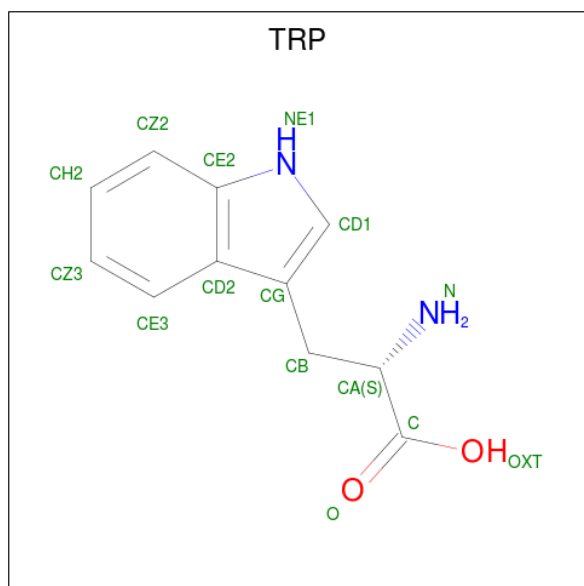
- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B6	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 58 is a protein called 50S ribosomal protein L36.

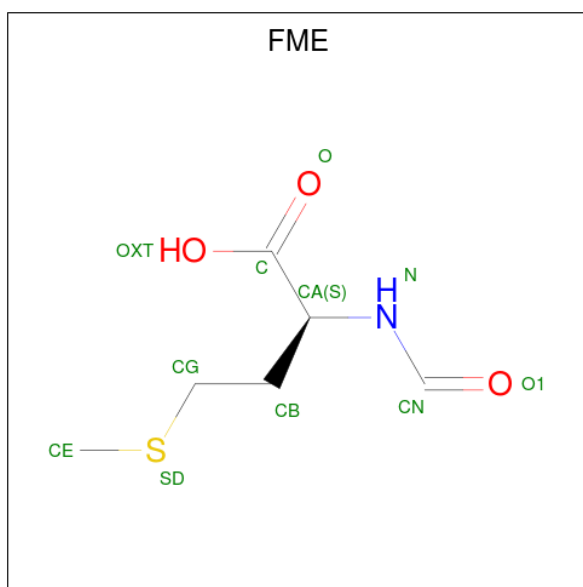
Mol	Chain	Residues	Atoms					AltConf	Trace
58	B7	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 59 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
59	AB	1	Total	C	N	O	0
			14	11	2	1	

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).

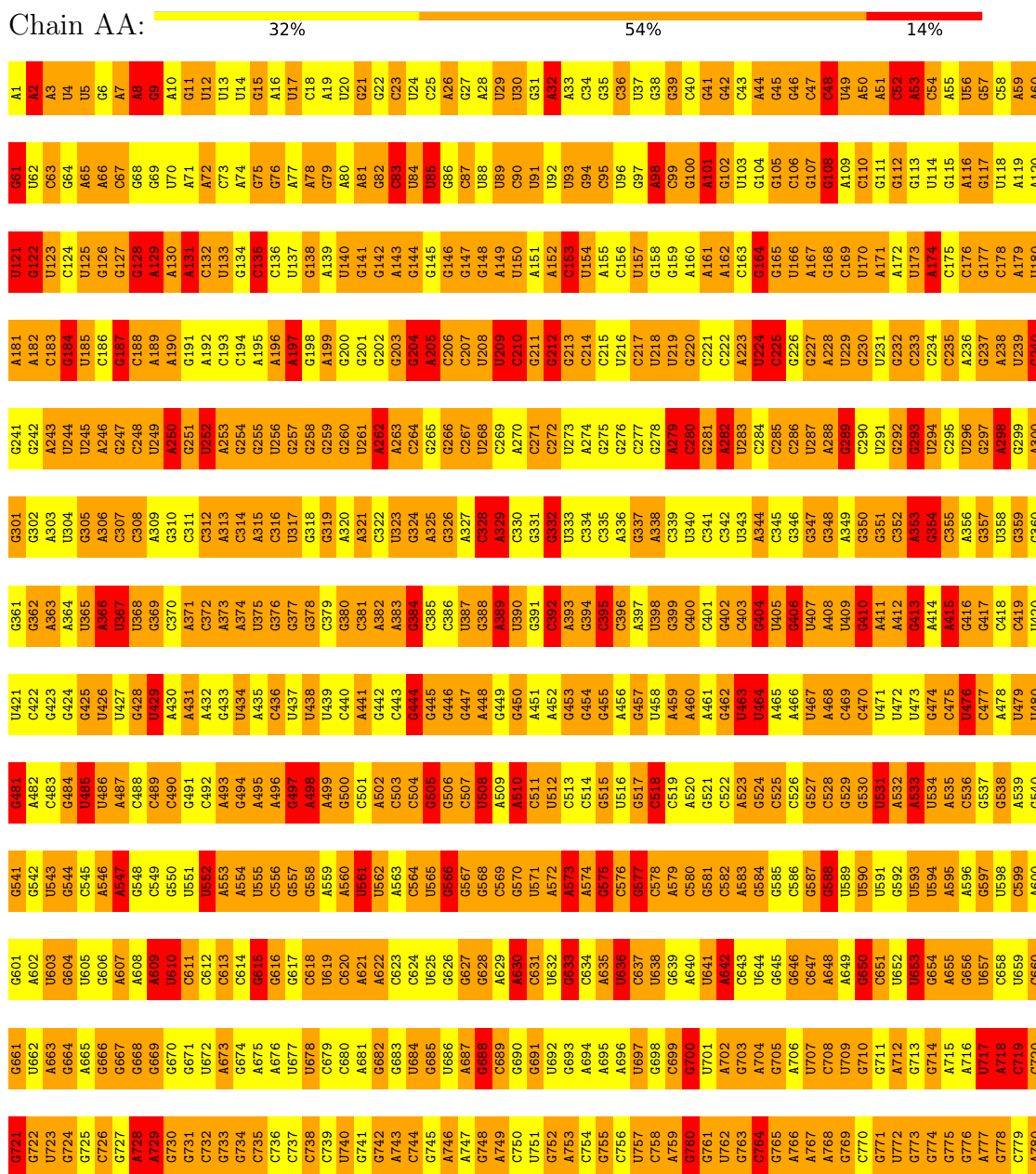


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	BB	1	10	6	1	2	1	0

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 16S ribosomal RNA




C1501	A1441	U1381	U1321	A1261	A1201	C1141	A1081	A1021	U961	A901	C841	A781
A1502	C1442	C1382	C1322	C1262	U1202	C1142	A1082	A1022	C962	G902	U842	C782
A1503	C1443	C1383	C1323	C1263	C1203	C1143	U1083	A1023	G963	G903	U843	C783
C1504	U1444	C1384	U1264	C1264	A1204	A1144	U1084	U1024	A964	U904	G844	A784
C1505	U1445	C1385	C1325	C1265	U1205	A1145	U1085	U1025	U965	U905	A845	A785
C1506	A1446	C1386	U1326	C1266	G1206	A1146	U1086	G1026	G966	A906	G846	C786
A1507	U1447	C1387	C1327	C1267	G1207	C1147	U1087	C1027	C967	A907	G847	A787
A1508	C1448	C1388	C1328	C1268	A1208	U1148	U1088	C1028	A968	A908	U848	U788
C1509	A1449	C1389	A1329	A1269	C1209	C1149	U1089	U1029	A969	A909	G849	U789
C1510	U1450	U1390	C1270	C1270	C1210	A1150	U1090	U1030	C970	C910	U850	A790
C1511	U1451	C1391	G1311	A1271	U1211	A1151	U1091	C1031	G971	U911	G851	C791
C1512	C1452	C1392	A1332	C1272	U1212	A1152	A1092	G1032	C972	C912	G852	A792
A1513	C1453	U1393	A1333	C1273	A1213	G1153	A1093	G1033	G973	A913	C853	C793
C1514	U1454	A1394	C1334	A1274	C1214	C1154	U1094	A1034	A974	A914	U854	A794
C1515	A1455	C1395	U1335	A1275	G1215	A1155	U1095	A1035	A975	A915	U855	C795
C1516	A1456	A1396	C1336	C1276	A1216	A1156	C1096	A1036	G976	U916	C856	A796
C1517	C1457	C1397	G1337	C1277	C1217	A1157	U1097	C1037	A977	G917	C857	C797
A1518	U1458	A1398	C1338	C1278	C1218	C1158	U1098	C1038	A978	A918	G858	U798
C1519	C1459	C1399	A1339	C1279	A1219	U1159	U1099	G1039	C979	A919	G859	C799
C1520	A1460	U1400	A1340	A1280	C1220	G1160	C1100	U1040	C980	U920	A860	G800
C1521	C1461	G1401	U1341	C1281	G1221	C1161	A1101	C1041	U981	U921	C861	A801
C1522	A1462	C1402	C1342	C1282	C1222	A1162	A1102	A1042	U982	G922	C862	U802
C1523	U1463	C1403	G1343	U1283	C1223	A1163	C1103	C1043	A983	A923	U863	G803
C1524	U1464	C1404	C1344	C1284	U1224	G1164	G1104	A1044	C984	G924	A864	U804
A1525	A1465	U1405	U1345	A1285	A1225	U1165	A1105	C1045	C985	G925	A865	C805
C1526	C1466	U1406	A1346	U1286	C1226	G1166	C1106	A1046	U986	G926	C866	C806
C1527	C1467	C1407	G1347	A1287	C1227	A1167	C1107	G1047	G987	G927	G867	A807
C1528	A1468	A1408	U1348	A1288	C1228	U1168	G1108	C1048	U988	G928	C868	G808
C1529	C1469	C1409	A1349	A1289	A1229	U1169	C1109	U1049	U989	G929	G869	G809
A1530	U1470	A1410	A1350	C1290	C1230	A1170	A1110	G1050	C990	C930	U870	C810
C1531	C1471	C1411	U1351	U1291	G1231	A1171	A1111	C1051	U991	C931	U871	C811
C1532	C1472	C1412	C1352	C1292	U1232	C1172	C1112	U1052	U992	C932	A872	C812
A1533	U1473	A1413	G1353	C1293	C1233	U1173	C1113	C1053	G993	G933	A873	U813
C1534	C1474	C1414	U1354	C1294	A1234	G1174	C1114	A1054	A994	A934	C874	A814
C1535	G1475	G1415	G1355	U1295	U1235	G1175	U1115	A1055	C995	A935	U875	A815
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C1537	C1477	C1417	U1357	C1297	C1237	G1177	A1117	G1057	U997	A937	G877	C817
C1538	U1478	A1418	U1358	U1298	A1238	G1178	U1118	C1058	C998	A938	A878	A818
C1539	C1479	C1419	C1359	A1299	A1239	A1179	C1119	C1059	C999	G939	C879	A819
U1540	A1480	U1420	A1360	U1300	U1240	A1180	C1120	U1060	A1000	C940	C880	U820
C1541	U1481	G1421	G1361	U1301	G1241	G1181	U1121	G1061	C1001	G941	G881	G821
A1542	C1482	C1422	A1362	C1302	G1242	G1182	U1122	U1062	G1002	G942	C882	U822
	A1483	A1423	C1363	C1303	C1243	U1183	U1123	C1063	G1003	U943	C883	C823
	C1484	U1424	U1364	C1304	G1244	G1184	G1124	G1064	A1004	G944	U884	G824
	A1485	U1425	G1365	G1305	C1245	G1185	U1125	U1065	A1005	G945	G885	A825
	C1486	G1426	C1366	A1306	A1246	G1186	U1126	C1066	G1006	A946	G886	C826
	C1487	C1427	C1367	U1307	U1247	G1187	G1127	A1067	U1007	G947	G887	U827
	G1488	A1428	A1368	U1308	A1248	A1188	C1128	G1068	U1008	C948	G888	U828
	C1489	C1429	C1369	C1309	C1249	U1189	C1129	C1069	U1009	A949	A889	G829
	U1490	A1430	C1370	G1310	A1250	G1190	A1130	U1070	C1010	U950	G890	A830
	A1491	C1431	G1371	A1311	A1251	A1191	G1131	C1071	C1011	U951	U891	A831
	A1492	C1432	U1372	G1312	G1252	G1192	C1132	G1072	A1012	U952	A892	G832
	A1493	A1433	G1373	U1313	G1253	G1193	G1133	U1073	G1013	G953	C893	G833
	C1494	A1434	A1374	C1314	A1254	U1194	G1134	G1074	A1014	U954	G894	U834
	U1495	U1435	A1375	U1315	G1255	A1195	U1135	U1075	G1015	U955	G895	U835
	C1496	U1436	U1376	C1316	A1256	A1196	C1136	U1076	A1016	U956	C896	G836
	C1497	C1437	A1377	C1317	A1257	A1197	C1137	G1077	U1017	U957	C897	U837
	U1498	A1438	C1378	A1318	G1258	G1198	G1138	U1078	G1018	U958	G898	G838
	A1499	C1439	A1379	A1319	C1259	U1199	G1139	G1079	A1019	A959	C899	C839
	C1500	U1440	U1380	C1260	A1260	C1160	C1140	A1080	C960	A900	G840	A780

• Molecule 2: A site tRNA

Chain AB:  38% 39% 22%

A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13	A14	A15	A16	A17	A18	A19	A20	A21	A22	A23	A24	A25	A26	A27	A28	A29	A30	A31	A32	A33	A34	A35	A36	A37	A38	A39	A40	A41	A42	A43	A44	A45	A46	A47	A48	A49	A50	A51	A52	A53	A54	A55	A56	A57	A58	A59	A60
C61	C62	C63	C64	C65	C66	C67	C68	C69	C70	C71	C72	C73	C74	C75	C76	C77	C78	C79	C80	C81	C82	C83	C84	C85	C86	C87	C88	C89	C90	C91	C92	C93	C94	C95	C96	C97	C98	C99	C100	C101	C102	C103	C104	C105	C106	C107	C108	C109	C110	C111	C112	C113	C114	C115	C116	C117	C118	C119	C120

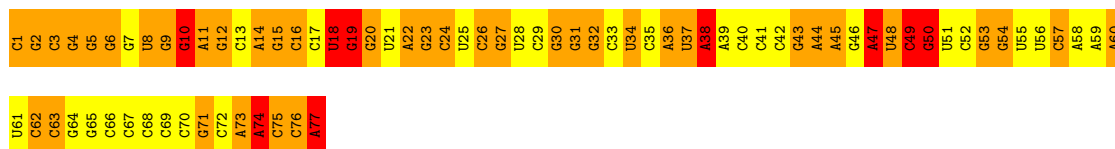
• Molecule 3: mRNA

Chain AC:  9% 19% 49% 32%



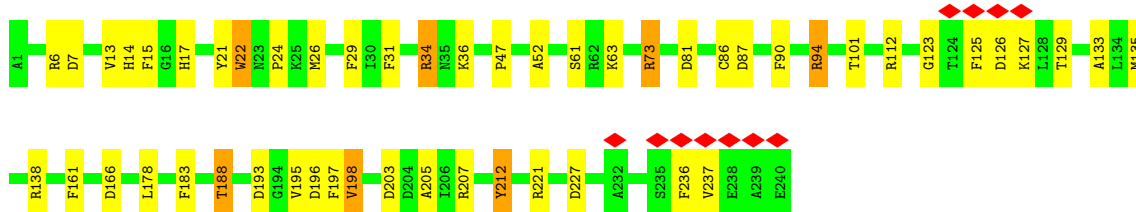
• Molecule 4: P site tRNA

Chain AD: 38% 51% 12%



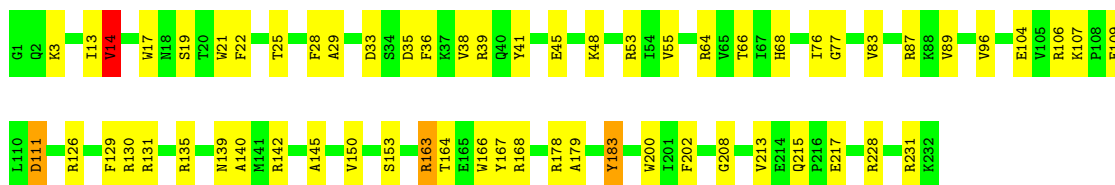
• Molecule 5: 30S ribosomal protein S2

Chain AE: 5% 78% 19%



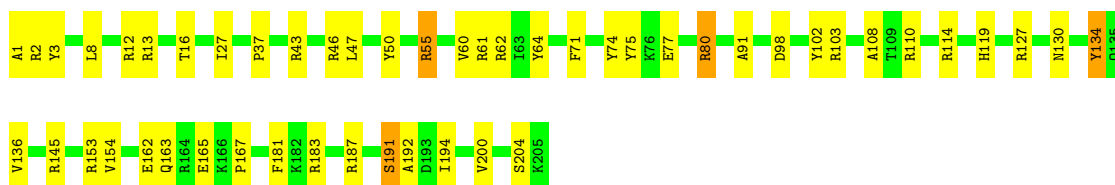
• Molecule 6: 30S ribosomal protein S3

Chain AF: 74% 25%



• Molecule 7: 30S ribosomal protein S4

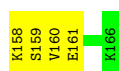
Chain AG: 76% 22%



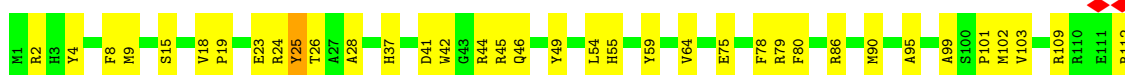
• Molecule 8: 30S ribosomal protein S5

Chain AH: 78% 20%

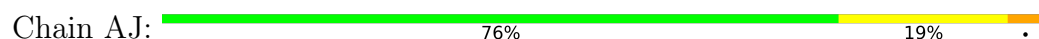




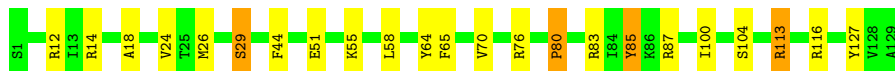
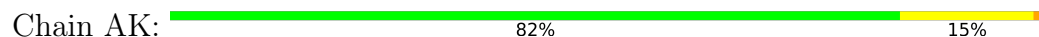
- Molecule 9: 30S ribosomal protein S6



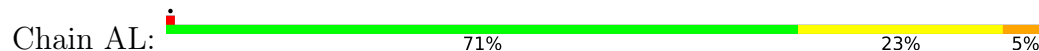
- Molecule 10: 30S ribosomal protein S7



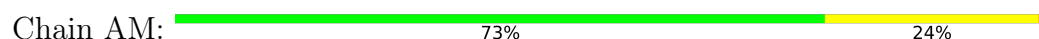
- Molecule 11: 30S ribosomal protein S8




- Molecule 12: 30S ribosomal protein S9



- Molecule 13: 30S ribosomal protein S10



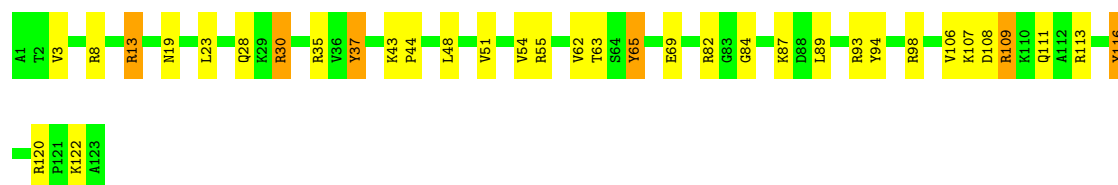
- Molecule 14: 30S ribosomal protein S11

Chain AN:  80% 19%



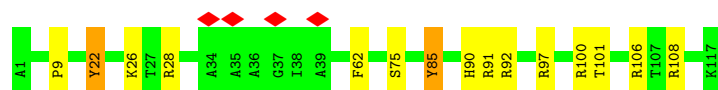
- Molecule 15: 30S ribosomal protein S12

Chain AO:  72% 24% 5%



- Molecule 16: 30S ribosomal protein S13

Chain AP:  87% 11%




- Molecule 17: 30S ribosomal protein S14

Chain AQ:  71% 24%



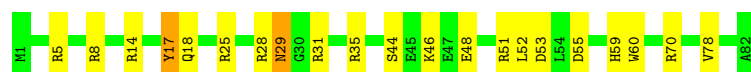
- Molecule 18: 30S ribosomal protein S15

Chain AR:  78% 18%




- Molecule 19: 30S ribosomal protein S16

Chain AS:  74% 23%



- Molecule 20: 30S ribosomal protein S17

Chain AT:  80% 20%



- Molecule 21: 30S ribosomal protein S18

Chain AU: 72% 23%



- Molecule 22: 30S ribosomal protein S19

Chain AV: 76% 22%



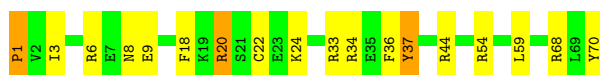
- Molecule 23: 30S ribosomal protein S20

Chain AW: 88% 10%



- Molecule 24: 30S ribosomal protein S21

Chain AX: 74% 21%



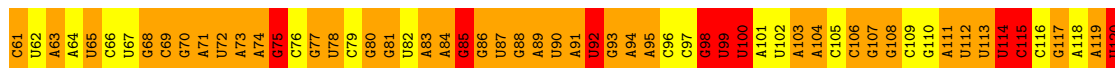
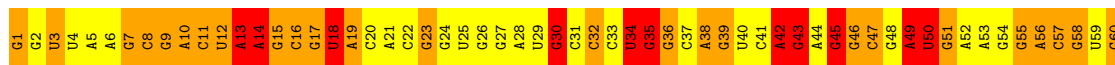
- Molecule 25: 5S ribosomal RNA

Chain BA: 37% 52% 11%



- Molecule 26: 23S ribosomal RNA

Chain BB: 33% 54% 12%




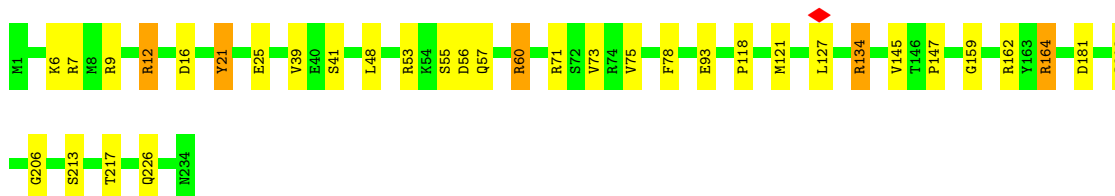
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A1142	U1082	G1022	G962	C902	U942	A782	A722	G662	A602	C542	G482	A422	A362	C302	G242	A182	G122
A1143	U1083	U1023	U963	C903	A943	A783	C723	G663	A603	G543	A483	A423	G363	C303	U243	A183	G123
A1144	A1084	A1024	C964	G904	A944	G784	U724	G664	A604	C544	G484	G784	C364	C304	A244	C184	G124
C1145	A1085	G1025	C965	A905	A945	G785	G725	U665	G605	U545	C485	G425	U365	C305	G245	G185	A125
C1146	A1086	U1026	G966	U906	U946	G786	G726	A666	U606	U546	C486	C426	C366	U306	C246	G186	A126
A1147	G1087	A1027	U967	G907	U947	C787	A727	U667	U607	A547	G487	U427	G367	G307	G247	G187	A127
U1148	A1088	A1028	C968	C908	C948	A788	G728	A668	A608	G548	G488	A428	A368	C308	G248	G188	C128
G1149	A1089	A1029	G969	A909	A949	G789	G729	G669	A609	G549	G489	A429	U369	A309	C249	G189	C129
C1150	A1090	C1030	U970	A910	U950	U790	A730	A670	C610	C550	A490	A430	G370	A310	G250	A190	A130
A1151	G1091	G1031	G971	A911	C951	U791	C731	G671	C611	G551	G491	U431	A371	A311	A251	A191	A131
C1152	C1092	A1032	A972	C912	U952	A792	G732	C672	G612	U552	A492	A432	G372	G312	G252	C192	G132
C1153	G1093	U1033	A973	C913	G953	A793	G733	C673	A613	G553	G493	C433	U373	G313	C253	U193	G133
G1154	U1094	G1034	C974	G914	C954	A794	A734	G674	A614	U554	G494	U434	A374	C314	G254	G194	G134
A1155	U1095	U1035	A975	C915	G955	C795	A735	A675	U615	G555	G495	A435	G375	G315	A255	A195	U135
A1156	A1096	U1036	G976	C916	G956	C796	G736	A676	A616	A556	G496	C436	G376	C316	A256	A196	G136
G1157	U1097	G1037	G977	A917	G957	G797	C737	A677	C617	C557	A497	U437	G377	G317	C257	A197	U137
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U1159	G1099	A1039	A979	U919	G959	G799	A739	C679	C619	G559	U499	A439	G379	G319	G259	A199	U139
G1160	C1100	A1040	A980	A920	U960	A800	C740	C680	G620	C560	G500	C440	G380	A320	G260	U200	C140
C1161	U1101	G1041	A981	C921	U961	G801	U741	C681	A621	G561	A501	U441	G381	U321	G261	C201	G141
G1162	C1102	C1042	C982	C922	A962	A802	A742	G682	C622	U562	A502	A442	A382	A322	A262	U202	A142
C1163	A1103	G1043	A983	G923	A963	U803	A743	U683	C623	A563	A503	A443	C383	C323	G263	A203	C143
C1164	C1104	C1044	A984	G924	C964	A804	U744	G684	C624	C564	A504	C444	A384	A324	C264	A204	C144
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G1166	G1106	A1046	C986	G926	A966	C806	U746	U686	A626	U566	G506	C446	G386	G326	C266	U206	A146
C1167	U1107	G1047	G987	A927	C967	U807	U747	C687	A627	U567	A507	A447	U387	G327	C267	A207	C147
G1168	U1108	A1048	A988	A928	U968	G808	G748	U688	C628	U568	A508	U448	C388	C328	C268	C208	U148
A1169	C1109	U1049	G989	U929	G969	G809	A749	A689	C629	U569	C509	A449	G389	G329	C269	C209	A149
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A1171	A1111	G1051	C991	U931	U971	U811	A751	C691	A631	U571	U511	U451	A391	C331	G271	C211	C151
C1172	U1112	C1052	C992	U932	U972	G812	A752	C692	A632	A572	G512	A452	U392	A332	A272	G212	A152
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C1174	C1114	A1054	C994	C934	G974	C814	U754	U694	C634	A574	A514	A454	C394	C334	C274	G214	U154
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C1183	C1123	G1063	G1003	A943	G983	G823	G763	U703	A643	G583	C523	G463	U403	C343	G283	A223	C163
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G1185	G1125	U1065	C1005	A945	C985	A825	C765	A705	C645	G585	U525	A465	U405	A345	G285	C225	A165
G1186	A1126	U1066	C1006	C946	A986	U826	U766	A706	U646	A586	A526	A466	G406	A346	U286	A226	U166
C1187	U1127	A1067	C1007	A947	U987	U827	U767	G707	G647	C587	A527	C467	A407	A347	G287	A227	A167
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C1193	A1133	A1073	C1013	G953	C993	A833	U773	G713	U653	U593	G533	C473	C413	C353	U293	A233	A173
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C1200	C1140	A1080	A1020	A960	A900	C940	G780	U720	C660	G600	C540	A480	C420	U360	A300	C240	G180

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A2169	U2109	G2049	G1989	G1929	G1869	A1809	A1749	G1689	U1629	U1569	A1509	G1449	G1389	U1329	A1269	U1209
A2170	G2110	C2050	G1990	U1930	A1870	A1810	U1750	A1690	A1630	A1570	G1510	G1450	A1390	C1330	G1270	G1210
A2171	U2111	A2051	U1991	U1931	A1871	A1811	U1751	A1691	G1631	A1571	G1511	C1451	A1391	G1331	C1271	C1211
U2172	G2112	A2052	G1992	A1932	A1872	U1812	G1752	U1692	A1632	A1572	G1512	G1452	A1392	G1332	A1272	G1212
A2173	U2113	G2053	U1993	G1933	G1873	A1813	G1753	U1693	A1633	A1573	G1513	A1453	A1393	G1333	U1273	A1213
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U2181	G2121	G2061	C2001	C1941	C1881	A1821	C1761	A1701	A1641	G1581	G1521	C1461	A1401	G1341	G1281	C1221
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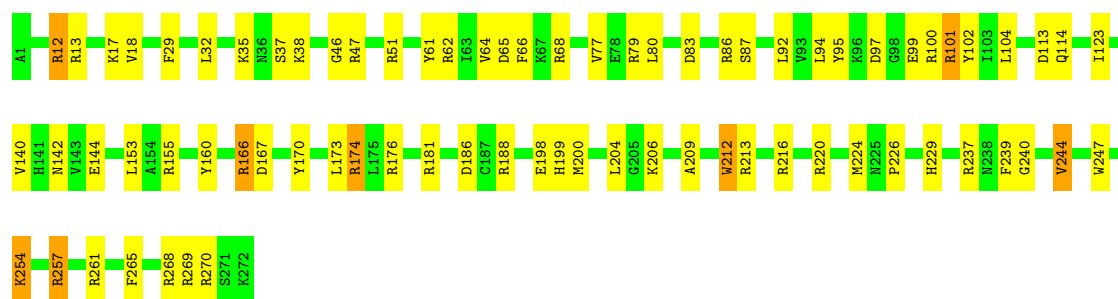
- Molecule 27: 50S ribosomal protein L1

Chain BC:  85% 13%



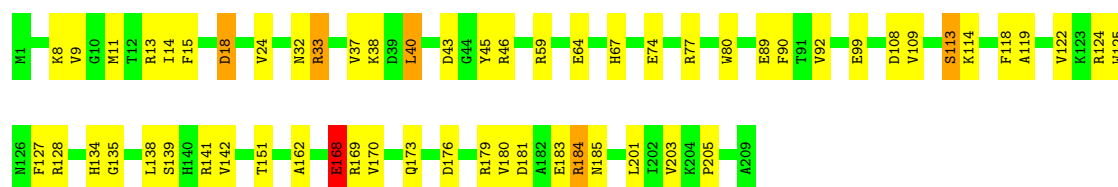
- Molecule 28: 50S ribosomal protein L2

Chain BD:  72% 25%



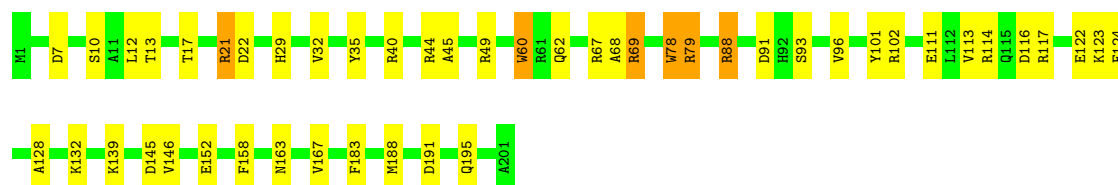
- Molecule 29: 50S ribosomal protein L3

Chain BE: 72% 25%



- Molecule 30: 50S ribosomal protein L4

Chain BF: 76% 21%



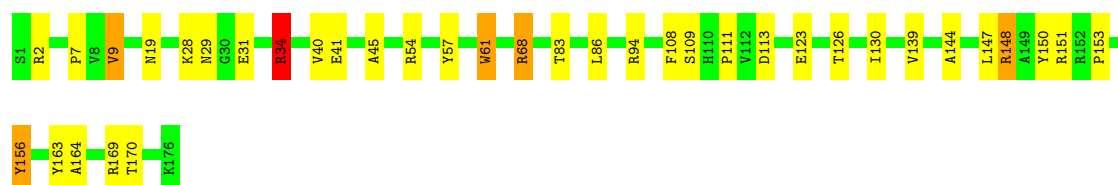
- Molecule 31: 50S ribosomal protein L5

Chain BG: 69% 25% 5%

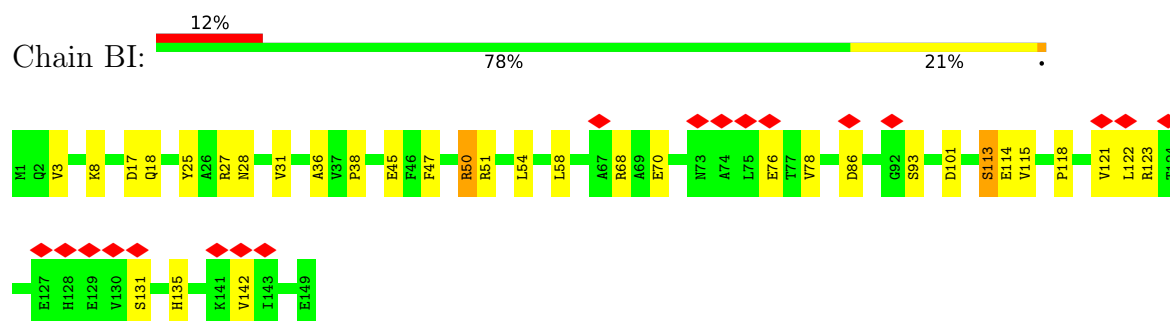


- Molecule 32: 50S ribosomal protein L6

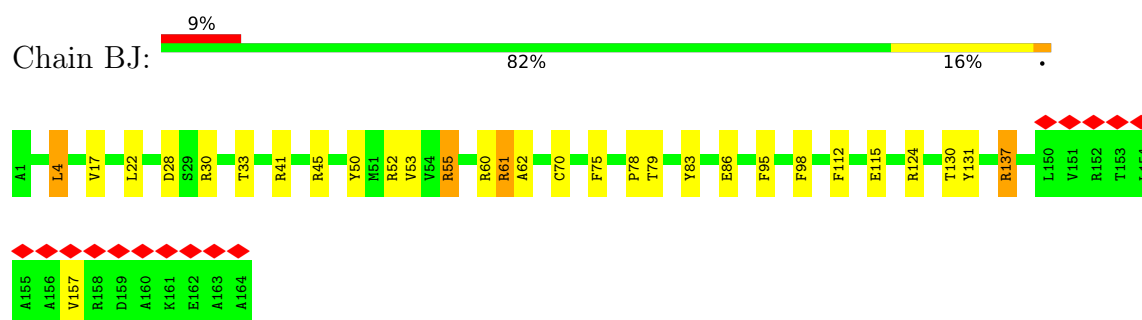
Chain BH: 79% 18%



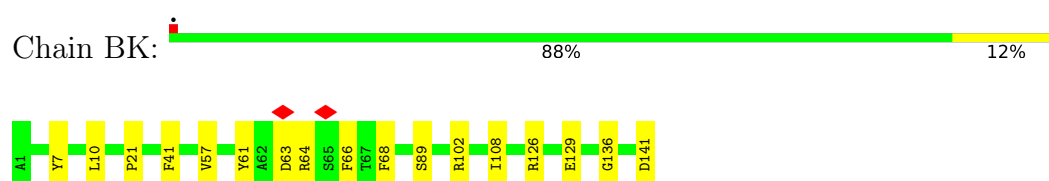
- Molecule 33: 50S ribosomal protein L9



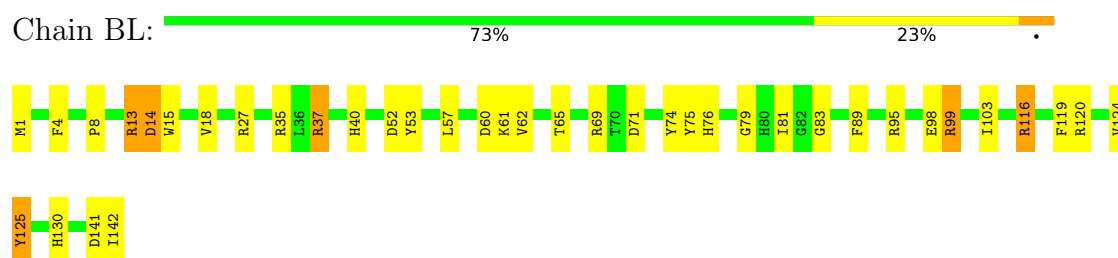
- Molecule 34: 50S ribosomal protein L10



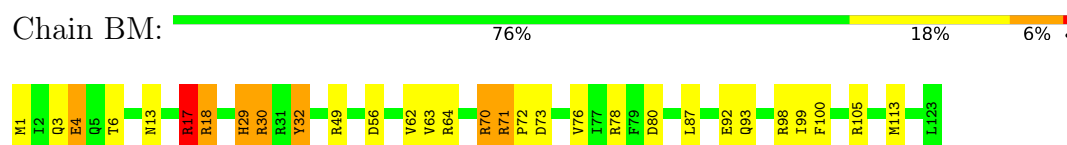
- Molecule 35: 50S ribosomal protein L11



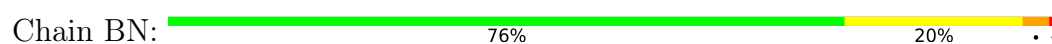
- Molecule 36: 50S ribosomal protein L13

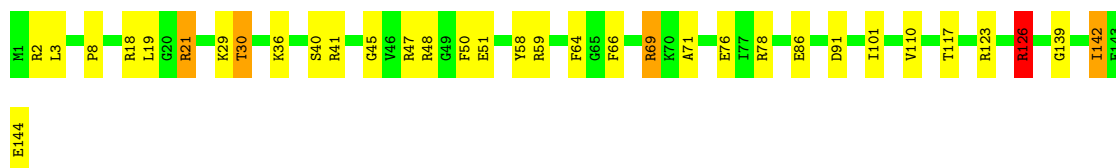


- Molecule 37: 50S ribosomal protein L14



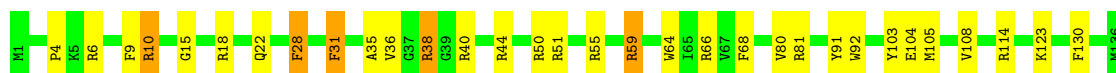
- Molecule 38: 50S ribosomal protein L15





- Molecule 39: 50S ribosomal protein L16

Chain BO: 76% 20% .



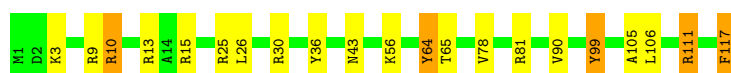
- Molecule 40: 50S ribosomal protein L17

Chain BP: 76% 20% .



- Molecule 41: 50S ribosomal protein L18

Chain BQ: 82% 14% .



- Molecule 42: 50S ribosomal protein L19

Chain BR: 73% 25% ..



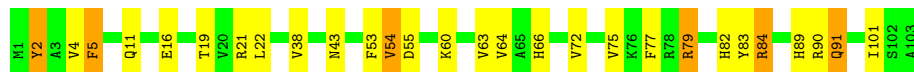
- Molecule 43: 50S ribosomal protein L20

Chain BS: 75% 21% .




- Molecule 44: 50S ribosomal protein L21

Chain BT: 73% 21% 6%




- Molecule 45: 50S ribosomal protein L22

Chain BU:  77% 18% 5%




- Molecule 46: 50S ribosomal protein L23

Chain BV:  74% 22% 4%




- Molecule 47: 50S ribosomal protein L24

Chain BW:  83% 16% 1%




- Molecule 48: 50S ribosomal protein L25

Chain BX:  80% 17% 3%



- Molecule 49: 50S ribosomal protein L27

Chain BY:  77% 18% 5%




- Molecule 50: 50S ribosomal protein L28

Chain BZ:  71% 23% 6%




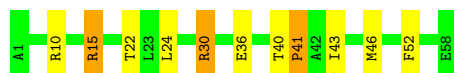
- Molecule 51: 50S ribosomal protein L29

Chain B0:  78% 17% 5%




- Molecule 52: 50S ribosomal protein L30

Chain B1:  81% 14% 5%




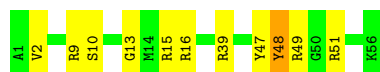
- Molecule 53: 50S ribosomal protein L31

Chain B2:  74% 23% .




- Molecule 54: 50S ribosomal protein L32

Chain B3:  80% 18% .



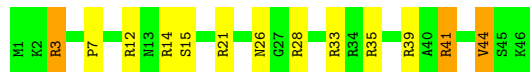
- Molecule 55: 50S ribosomal protein L33

Chain B4:  80% 17% .




- Molecule 56: 50S ribosomal protein L34

Chain B5:  72% 22% 7%




- Molecule 57: 50S ribosomal protein L35

Chain B6:  80% 17% .



- Molecule 58: 50S ribosomal protein L36

Chain B7:  76% 18% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Volumes were CTF-corrected in defocus groups	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	58269	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	1.481	Depositor
Minimum map value	-0.504	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.201	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	375.0, 375.0, 375.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5, 1.5, 1.5	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 6MZ, UR3, MIA, OMG, 4OC, 1MG, CH, OMC, OMU, 2MA, H2U, 3TD, 4SU, 2MG, 5MU, MA6, 7MG, PSU, FME

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	AA	3.07	3887/36769 (10.6%)	3.55	8401/57354 (14.6%)
2	AB	3.08	186/1600 (11.6%)	3.55	373/2492 (15.0%)
3	AC	3.05	112/1108 (10.1%)	3.41	210/1724 (12.2%)
4	AD	2.99	170/1721 (9.9%)	3.48	380/2683 (14.2%)
5	AE	1.48	5/1904 (0.3%)	1.91	50/2565 (1.9%)
6	AF	1.48	11/1852 (0.6%)	2.01	58/2490 (2.3%)
7	AG	1.54	5/1665 (0.3%)	2.05	55/2227 (2.5%)
8	AH	1.53	5/1239 (0.4%)	1.91	30/1664 (1.8%)
9	AI	1.54	5/1121 (0.4%)	2.02	30/1509 (2.0%)
10	AJ	1.54	9/1422 (0.6%)	1.97	38/1908 (2.0%)
11	AK	1.50	3/989 (0.3%)	1.90	19/1326 (1.4%)
12	AL	1.58	6/1048 (0.6%)	2.12	34/1394 (2.4%)
13	AM	1.49	3/835 (0.4%)	2.05	23/1127 (2.0%)
14	AN	1.52	4/982 (0.4%)	1.95	24/1323 (1.8%)
15	AO	1.56	7/969 (0.7%)	2.02	29/1300 (2.2%)
16	AP	1.50	1/919 (0.1%)	1.82	17/1226 (1.4%)
17	AQ	1.53	3/817 (0.4%)	1.97	28/1088 (2.6%)
18	AR	1.49	0/724	1.90	16/966 (1.7%)
19	AS	1.57	5/659 (0.8%)	1.97	17/884 (1.9%)
20	AT	1.52	3/681 (0.4%)	1.93	13/913 (1.4%)
21	AU	1.49	2/637 (0.3%)	2.13	17/851 (2.0%)
22	AV	1.46	2/744 (0.3%)	2.10	18/995 (1.8%)
23	AW	1.47	1/676 (0.1%)	1.92	14/895 (1.6%)
24	AX	1.61	3/598 (0.5%)	2.14	16/792 (2.0%)
25	BA	3.11	315/2869 (11.0%)	3.52	638/4474 (14.3%)
26	BB	3.08	7296/69257 (10.5%)	3.51	15472/108040 (14.3%)
27	BC	1.41	4/1748 (0.2%)	1.90	27/2355 (1.1%)
28	BD	1.59	15/2131 (0.7%)	2.01	74/2863 (2.6%)
29	BE	1.50	7/1586 (0.4%)	1.92	42/2134 (2.0%)
30	BF	1.47	2/1571 (0.1%)	2.10	41/2113 (1.9%)
31	BG	1.54	6/1444 (0.4%)	2.14	52/1937 (2.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BH	1.49	5/1343 (0.4%)	1.94	26/1816 (1.4%)
33	BI	1.46	2/1122 (0.2%)	1.88	25/1515 (1.7%)
34	BJ	1.52	5/1247 (0.4%)	1.92	29/1679 (1.7%)
35	BK	1.50	2/1046 (0.2%)	1.73	13/1410 (0.9%)
36	BL	1.52	7/1152 (0.6%)	2.06	33/1551 (2.1%)
37	BM	1.43	3/956 (0.3%)	1.98	28/1279 (2.2%)
38	BN	1.60	7/1062 (0.7%)	1.94	30/1413 (2.1%)
39	BO	1.54	7/1093 (0.6%)	2.13	38/1460 (2.6%)
40	BP	1.50	3/1021 (0.3%)	2.07	33/1364 (2.4%)
41	BQ	1.52	4/910 (0.4%)	1.97	21/1219 (1.7%)
42	BR	1.55	5/929 (0.5%)	2.02	27/1242 (2.2%)
43	BS	1.52	4/960 (0.4%)	2.00	27/1278 (2.1%)
44	BT	1.50	4/829 (0.5%)	1.93	22/1107 (2.0%)
45	BU	1.44	2/864 (0.2%)	1.98	24/1156 (2.1%)
46	BV	1.49	0/794	1.92	23/1060 (2.2%)
47	BW	1.45	2/797 (0.3%)	1.79	10/1062 (0.9%)
48	BX	1.47	5/766 (0.7%)	1.99	18/1025 (1.8%)
49	BY	1.47	1/642 (0.2%)	2.11	19/848 (2.2%)
50	BZ	1.47	2/635 (0.3%)	2.07	22/848 (2.6%)
51	B0	1.50	1/510 (0.2%)	2.11	15/677 (2.2%)
52	B1	1.54	6/453 (1.3%)	1.89	7/605 (1.2%)
53	B2	1.45	1/559 (0.2%)	2.22	15/745 (2.0%)
54	B3	1.51	3/450 (0.7%)	1.94	7/599 (1.2%)
55	B4	1.48	2/448 (0.4%)	2.10	7/594 (1.2%)
56	B5	1.48	0/380	2.06	15/498 (3.0%)
57	B6	1.56	7/513 (1.4%)	1.97	12/676 (1.8%)
58	B7	1.49	1/303 (0.3%)	1.91	6/397 (1.5%)
All	All	2.69	12174/164069 (7.4%)	3.17	26808/244735 (11.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	907
2	AB	0	36
3	AC	0	31
4	AD	0	44
5	AE	0	5
6	AF	0	2
7	AG	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	AH	0	6
9	AI	0	5
10	AJ	0	5
11	AK	0	2
12	AL	0	6
13	AM	0	1
14	AN	0	1
15	AO	0	7
16	AP	0	1
17	AQ	0	3
18	AR	0	5
19	AS	0	2
21	AU	0	5
22	AV	0	3
23	AW	0	1
24	AX	0	3
25	BA	0	66
26	BB	0	1683
27	BC	0	3
28	BD	0	10
29	BE	0	5
30	BF	0	3
31	BG	0	9
32	BH	0	4
33	BI	0	2
34	BJ	0	5
35	BK	0	1
36	BL	0	9
37	BM	0	7
38	BN	0	5
39	BO	0	2
40	BP	0	3
41	BQ	0	4
42	BR	0	2
43	BS	0	2
44	BT	0	2
45	BU	0	4
46	BV	0	2
47	BW	0	2
48	BX	0	1
49	BY	0	7
50	BZ	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
52	B1	0	1
53	B2	0	4
54	B3	0	2
55	B4	0	2
56	B5	0	1
57	B6	0	1
58	B7	0	1
All	All	0	2945

The worst 5 of 12174 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BB	2297	A	N3-C4	17.57	1.45	1.34
26	BB	764	A	N3-C4	15.94	1.44	1.34
26	BB	453	A	N3-C4	15.86	1.44	1.34
1	AA	914	A	N3-C4	15.76	1.44	1.34
26	BB	1972	G	C8-N7	15.68	1.40	1.30

The worst 5 of 26808 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	28	A	O4'-C1'-N9	21.28	125.23	108.20
53	B2	63	ARG	NE-CZ-NH1	21.04	130.82	120.30
26	BB	2041	U	O4'-C1'-N1	20.83	124.87	108.20
1	AA	1323	G	N9-C4-C5	20.57	113.63	105.40
1	AA	1142	G	C8-N9-C4	-20.50	98.20	106.40

There are no chirality outliers.

5 of 2945 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	11	G	Sidechain
1	AA	2	A	Sidechain
1	AA	4	U	Sidechain
1	AA	8	A	Sidechain
1	AA	9	G	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	AA	33089	0	16596	0	0
2	AB	1627	0	840	0	0
3	AC	993	0	501	0	0
4	AD	1641	0	839	0	0
5	AE	1872	0	1885	0	0
6	AF	1822	0	1913	0	0
7	AG	1643	0	1710	0	0
8	AH	1225	0	1273	0	0
9	AI	1101	0	1050	0	0
10	AJ	1400	0	1449	0	0
11	AK	979	0	1034	0	0
12	AL	1036	0	1084	0	0
13	AM	825	0	865	0	0
14	AN	965	0	997	0	0
15	AO	955	0	1019	0	0
16	AP	910	0	981	0	0
17	AQ	805	0	847	0	0
18	AR	716	0	742	0	0
19	AS	649	0	666	0	0
20	AT	672	0	716	0	0
21	AU	626	0	651	0	0
22	AV	727	0	769	0	0
23	AW	670	0	722	0	0
24	AX	590	0	631	0	0
25	BA	2566	0	1295	0	0
26	BB	62351	0	31202	0	0
27	BC	1733	0	1824	0	0
28	BD	2092	0	2170	0	0
29	BE	1565	0	1616	0	0
30	BF	1552	0	1619	0	0
31	BG	1420	0	1460	0	0
32	BH	1323	0	1374	0	0
33	BI	1111	0	1148	0	0
34	BJ	1233	0	1283	0	0
35	BK	1032	0	1088	0	0
36	BL	1129	0	1162	0	0
37	BM	947	0	1023	0	0
38	BN	1053	0	1129	0	0
39	BO	1074	0	1157	0	0
40	BP	1008	0	1045	0	0
41	BQ	900	0	935	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BR	917	0	965	0	0
43	BS	947	0	1022	0	0
44	BT	816	0	839	0	0
45	BU	857	0	922	0	0
46	BV	787	0	846	0	0
47	BW	789	0	847	0	0
48	BX	753	0	780	0	0
49	BY	634	0	656	0	0
50	BZ	625	0	655	0	0
51	B0	509	0	543	0	0
52	B1	449	0	491	0	0
53	B2	549	0	552	0	0
54	B3	444	0	461	0	0
55	B4	441	0	485	0	0
56	B5	377	0	418	0	0
57	B6	504	0	574	0	0
58	B7	302	0	343	0	0
59	AB	14	0	9	0	0
60	BB	10	0	10	0	0
All	All	152351	0	103728	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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 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	
5	AE	238/240 (99%)	217 (91%)	14 (6%)	7 (3%)	4	29
6	AF	230/232 (99%)	217 (94%)	8 (4%)	5 (2%)	6	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	203/205 (99%)	187 (92%)	13 (6%)	3 (2%)	10	46
8	AH	164/166 (99%)	148 (90%)	14 (8%)	2 (1%)	13	50
9	AI	133/135 (98%)	122 (92%)	10 (8%)	1 (1%)	19	60
10	AJ	176/178 (99%)	165 (94%)	9 (5%)	2 (1%)	14	52
11	AK	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	60
12	AL	127/129 (98%)	112 (88%)	12 (9%)	3 (2%)	6	33
13	AM	101/103 (98%)	90 (89%)	6 (6%)	5 (5%)	2	20
14	AN	126/128 (98%)	111 (88%)	14 (11%)	1 (1%)	19	60
15	AO	121/123 (98%)	106 (88%)	14 (12%)	1 (1%)	19	60
16	AP	115/117 (98%)	109 (95%)	5 (4%)	1 (1%)	17	57
17	AQ	98/100 (98%)	84 (86%)	7 (7%)	7 (7%)	1	14
18	AR	86/88 (98%)	81 (94%)	4 (5%)	1 (1%)	13	50
19	AS	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
20	AT	81/83 (98%)	72 (89%)	8 (10%)	1 (1%)	13	50
21	AU	72/74 (97%)	61 (85%)	7 (10%)	4 (6%)	2	19
22	AV	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	14	52
23	AW	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
24	AX	68/70 (97%)	61 (90%)	4 (6%)	3 (4%)	2	22
27	BC	232/234 (99%)	216 (93%)	11 (5%)	5 (2%)	6	35
28	BD	270/272 (99%)	235 (87%)	25 (9%)	10 (4%)	3	24
29	BE	207/209 (99%)	174 (84%)	26 (13%)	7 (3%)	3	26
30	BF	199/201 (99%)	174 (87%)	15 (8%)	10 (5%)	2	20
31	BG	176/178 (99%)	151 (86%)	16 (9%)	9 (5%)	2	19
32	BH	174/176 (99%)	157 (90%)	12 (7%)	5 (3%)	4	29
33	BI	147/149 (99%)	130 (88%)	12 (8%)	5 (3%)	3	26
34	BJ	162/164 (99%)	157 (97%)	4 (2%)	1 (1%)	25	66
35	BK	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
36	BL	140/142 (99%)	120 (86%)	16 (11%)	4 (3%)	4	29
37	BM	121/123 (98%)	109 (90%)	8 (7%)	4 (3%)	4	26
38	BN	142/144 (99%)	124 (87%)	14 (10%)	4 (3%)	5	30
39	BO	134/136 (98%)	123 (92%)	10 (8%)	1 (1%)	22	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BP	125/127 (98%)	116 (93%)	8 (6%)	1 (1%)	19	60
41	BQ	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
42	BR	112/114 (98%)	98 (88%)	11 (10%)	3 (3%)	5	31
43	BS	115/117 (98%)	108 (94%)	4 (4%)	3 (3%)	5	31
44	BT	101/103 (98%)	90 (89%)	7 (7%)	4 (4%)	3	23
45	BU	108/110 (98%)	98 (91%)	6 (6%)	4 (4%)	3	24
46	BV	98/100 (98%)	76 (78%)	19 (19%)	3 (3%)	4	27
47	BW	101/103 (98%)	88 (87%)	10 (10%)	3 (3%)	4	28
48	BX	92/94 (98%)	87 (95%)	4 (4%)	1 (1%)	14	52
49	BY	82/84 (98%)	64 (78%)	16 (20%)	2 (2%)	6	33
50	BZ	75/77 (97%)	68 (91%)	4 (5%)	3 (4%)	3	23
51	B0	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	9	44
52	B1	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
53	B2	68/70 (97%)	65 (96%)	2 (3%)	1 (2%)	10	46
54	B3	54/56 (96%)	48 (89%)	4 (7%)	2 (4%)	3	24
55	B4	52/54 (96%)	49 (94%)	1 (2%)	2 (4%)	3	24
56	B5	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	2	22
57	B6	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	9	44
58	B7	36/38 (95%)	30 (83%)	3 (8%)	3 (8%)	1	12
All	All	6319/6423 (98%)	5706 (90%)	460 (7%)	153 (2%)	9	33

5 of 153 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	AF	163	ARG
8	AH	77	ASN
13	AM	57	VAL
14	AN	52	ARG
17	AQ	2	LYS

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	
5	AE	198/198 (100%)	189 (96%)	9 (4%)	27	52
6	AF	189/189 (100%)	178 (94%)	11 (6%)	20	45
7	AG	172/172 (100%)	166 (96%)	6 (4%)	36	59
8	AH	125/125 (100%)	116 (93%)	9 (7%)	14	39
9	AI	116/116 (100%)	111 (96%)	5 (4%)	29	53
10	AJ	146/146 (100%)	133 (91%)	13 (9%)	9	30
11	AK	104/104 (100%)	97 (93%)	7 (7%)	16	41
12	AL	106/106 (100%)	99 (93%)	7 (7%)	16	41
13	AM	90/90 (100%)	86 (96%)	4 (4%)	28	53
14	AN	98/98 (100%)	95 (97%)	3 (3%)	40	62
15	AO	103/103 (100%)	98 (95%)	5 (5%)	25	50
16	AP	95/95 (100%)	94 (99%)	1 (1%)	73	84
17	AQ	83/83 (100%)	80 (96%)	3 (4%)	35	59
18	AR	76/76 (100%)	72 (95%)	4 (5%)	22	47
19	AS	65/65 (100%)	61 (94%)	4 (6%)	18	43
20	AT	77/77 (100%)	74 (96%)	3 (4%)	32	56
21	AU	64/64 (100%)	61 (95%)	3 (5%)	26	51
22	AV	78/78 (100%)	74 (95%)	4 (5%)	24	48
23	AW	65/65 (100%)	64 (98%)	1 (2%)	65	80
24	AX	60/60 (100%)	57 (95%)	3 (5%)	24	49
27	BC	181/181 (100%)	171 (94%)	10 (6%)	21	47
28	BD	217/217 (100%)	207 (95%)	10 (5%)	27	52
29	BE	164/164 (100%)	150 (92%)	14 (8%)	10	33
30	BF	165/165 (100%)	157 (95%)	8 (5%)	25	51
31	BG	149/149 (100%)	137 (92%)	12 (8%)	11	35
32	BH	137/137 (100%)	124 (90%)	13 (10%)	8	27
33	BI	114/114 (100%)	110 (96%)	4 (4%)	36	59
34	BJ	122/122 (100%)	118 (97%)	4 (3%)	38	61
35	BK	109/109 (100%)	107 (98%)	2 (2%)	59	77
36	BL	116/116 (100%)	109 (94%)	7 (6%)	19	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BM	104/104 (100%)	100 (96%)	4 (4%)	33	57
38	BN	103/103 (100%)	100 (97%)	3 (3%)	42	64
39	BO	109/109 (100%)	103 (94%)	6 (6%)	21	47
40	BP	103/103 (100%)	99 (96%)	4 (4%)	32	56
41	BQ	87/87 (100%)	82 (94%)	5 (6%)	20	45
42	BR	99/99 (100%)	94 (95%)	5 (5%)	24	48
43	BS	89/89 (100%)	84 (94%)	5 (6%)	21	46
44	BT	84/84 (100%)	77 (92%)	7 (8%)	11	34
45	BU	93/93 (100%)	89 (96%)	4 (4%)	29	53
46	BV	84/84 (100%)	77 (92%)	7 (8%)	11	34
47	BW	84/84 (100%)	80 (95%)	4 (5%)	25	51
48	BX	78/78 (100%)	73 (94%)	5 (6%)	17	42
49	BY	62/62 (100%)	58 (94%)	4 (6%)	17	42
50	BZ	67/67 (100%)	63 (94%)	4 (6%)	19	44
51	B0	55/55 (100%)	50 (91%)	5 (9%)	9	29
52	B1	48/48 (100%)	46 (96%)	2 (4%)	30	54
53	B2	62/62 (100%)	59 (95%)	3 (5%)	25	51
54	B3	47/47 (100%)	47 (100%)	0	100	100
55	B4	48/48 (100%)	45 (94%)	3 (6%)	18	43
56	B5	38/38 (100%)	35 (92%)	3 (8%)	12	35
57	B6	51/51 (100%)	50 (98%)	1 (2%)	55	74
58	B7	34/34 (100%)	34 (100%)	0	100	100
All	All	5213/5213 (100%)	4940 (95%)	273 (5%)	27	48

5 of 273 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BU	95	ARG
46	BV	100	GLU
51	B0	59	GLU
22	AV	1	PRO
21	AU	4	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1538/1542 (99%)	309 (20%)	98 (6%)
2	AB	74/76 (97%)	28 (37%)	8 (10%)
25	BA	119/120 (99%)	16 (13%)	11 (9%)
26	BB	2898/2904 (99%)	534 (18%)	181 (6%)
3	AC	46/47 (97%)	21 (45%)	7 (15%)
4	AD	76/77 (98%)	13 (17%)	3 (3%)
All	All	4751/4766 (99%)	921 (19%)	308 (6%)

5 of 921 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	3	A
1	AA	5	U
1	AA	7	A
1	AA	8	A

5 of 308 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BB	1715	G
26	BB	2585	U
26	BB	1828	G
26	BB	2236	U
26	BB	2791	G

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

49 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
2	7MG	AB	46	2	22,26,27	4.30	5 (22%)	29,39,42	1.72	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	5MC	BB	1962	26	18,22,23	1.75	4 (22%)	26,32,35	1.60	3 (11%)
26	PSU	BB	2605	26	18,21,22	1.79	4 (22%)	22,30,33	2.12	5 (22%)
2	PSU	AB	55	2	18,21,22	1.94	5 (27%)	22,30,33	1.65	6 (27%)
26	2MG	BB	1835	26	18,26,27	1.76	3 (16%)	16,38,41	1.56	2 (12%)
26	H2U	BB	2449	26	18,21,22	1.48	4 (22%)	21,30,33	1.11	3 (14%)
4	H2U	AD	21	4	18,21,22	1.37	2 (11%)	21,30,33	2.24	5 (23%)
4	PSU	AD	56	4	18,21,22	1.94	4 (22%)	22,30,33	1.26	1 (4%)
1	2MG	AA	1516	1	18,26,27	1.80	4 (22%)	16,38,41	1.43	2 (12%)
1	MA6	AA	1519	1	19,26,27	2.02	6 (31%)	18,38,41	2.60	5 (27%)
1	PSU	AA	516	1	18,21,22	1.61	4 (22%)	22,30,33	1.90	5 (22%)
1	7MG	AA	527	1	22,26,27	3.40	4 (18%)	29,39,42	1.46	1 (3%)
2	H2U	AB	17	2	18,21,22	1.65	4 (22%)	21,30,33	1.59	6 (28%)
4	5MU	AD	55	4	19,22,23	1.54	5 (26%)	28,32,35	1.48	5 (17%)
1	MA6	AA	1518	1	19,26,27	1.69	5 (26%)	18,38,41	1.38	4 (22%)
4	OMC	AD	33	4	19,22,23	1.02	2 (10%)	26,31,34	1.72	4 (15%)
26	PSU	BB	746	26	18,21,22	1.76	4 (22%)	22,30,33	1.83	7 (31%)
1	5MC	AA	967	1	18,22,23	1.43	2 (11%)	26,32,35	2.06	8 (30%)
1	5MC	AA	1407	1	18,22,23	1.41	3 (16%)	26,32,35	1.29	4 (15%)
26	PSU	BB	955	26	18,21,22	2.04	3 (16%)	22,30,33	2.17	5 (22%)
26	2MA	BB	2503	26	17,25,26	1.74	4 (23%)	17,37,40	1.81	5 (29%)
26	PSU	BB	2504	26	18,21,22	1.80	3 (16%)	22,30,33	2.21	5 (22%)
26	PSU	BB	2580	26	18,21,22	1.90	5 (27%)	22,30,33	1.83	5 (22%)
1	2MG	AA	1207	1	18,26,27	1.95	6 (33%)	16,38,41	1.13	1 (6%)
1	4OC	AA	1402	1	20,23,24	1.35	3 (15%)	26,32,35	1.46	5 (19%)
2	4SU	AB	8	2	18,21,22	2.03	5 (27%)	26,30,33	1.58	6 (23%)
26	3TD	BB	1915	26	18,22,23	1.94	4 (22%)	22,32,35	1.71	5 (22%)
26	2MG	BB	2445	26	18,26,27	1.81	3 (16%)	16,38,41	2.29	6 (37%)
26	7MG	BB	2069	26	22,26,27	4.31	6 (27%)	29,39,42	1.93	6 (20%)
26	OMC	BB	2498	26	19,22,23	1.15	4 (21%)	26,31,34	1.83	7 (26%)
2	H2U	AB	16	2	18,21,22	1.99	4 (22%)	21,30,33	1.58	4 (19%)
2	5MU	AB	54	2	19,22,23	1.54	4 (21%)	28,32,35	2.60	8 (28%)
26	1MG	BB	745	26	18,26,27	1.69	6 (33%)	19,39,42	2.35	9 (47%)
2	MIA	AB	37	2	24,31,32	3.06	4 (16%)	26,44,47	2.19	9 (34%)
26	6MZ	BB	2030	26	18,25,26	1.33	2 (11%)	16,36,39	2.52	6 (37%)
26	6MZ	BB	1618	26	18,25,26	1.94	4 (22%)	16,36,39	2.14	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PSU	BB	2457	26	18,21,22	1.64	4 (22%)	22,30,33	1.26	2 (9%)
26	OMU	BB	2552	26	19,22,23	0.97	2 (10%)	26,31,34	1.56	5 (19%)
1	2MG	AA	966	1	18,26,27	1.83	4 (22%)	16,38,41	1.81	3 (18%)
2	H2U	AB	20	2	18,21,22	1.42	4 (22%)	21,30,33	1.87	5 (23%)
4	4SU	AD	8	4	18,21,22	2.18	4 (22%)	26,30,33	2.45	10 (38%)
26	5MU	BB	747	26	19,22,23	1.64	3 (15%)	28,32,35	2.09	10 (35%)
26	PSU	BB	1911	26	18,21,22	1.76	4 (22%)	22,30,33	1.52	5 (22%)
26	PSU	BB	1917	26	18,21,22	1.83	4 (22%)	22,30,33	1.30	2 (9%)
2	OMC	AB	32	2	19,22,23	1.11	3 (15%)	26,31,34	1.74	7 (26%)
26	OMG	BB	2251	26	18,26,27	1.35	2 (11%)	19,38,41	1.83	6 (31%)
1	UR3	AA	1498	1	19,22,23	1.41	3 (15%)	26,32,35	2.06	12 (46%)
26	CH	BB	2575	26	16,21,22	1.57	1 (6%)	20,30,33	1.41	3 (15%)
26	5MU	BB	1939	26	19,22,23	1.33	2 (10%)	28,32,35	1.87	8 (28%)

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
2	7MG	AB	46	2	-	0/7/37/38	0/3/3/3
26	5MC	BB	1962	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	2605	26	-	1/7/25/26	0/2/2/2
2	PSU	AB	55	2	-	0/7/25/26	0/2/2/2
26	2MG	BB	1835	26	-	0/5/27/28	0/3/3/3
26	H2U	BB	2449	26	-	0/7/38/39	0/2/2/2
4	H2U	AD	21	4	-	0/7/38/39	0/2/2/2
4	PSU	AD	56	4	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	1/5/27/28	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	AA	516	1	-	1/7/25/26	0/2/2/2
1	7MG	AA	527	1	-	1/7/37/38	0/3/3/3
2	H2U	AB	17	2	-	2/7/38/39	0/2/2/2
4	5MU	AD	55	4	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
4	OMC	AD	33	4	-	0/9/27/28	0/2/2/2
26	PSU	BB	746	26	-	3/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PSU	BB	955	26	-	0/7/25/26	0/2/2/2
26	2MA	BB	2503	26	-	0/3/25/26	0/3/3/3
26	PSU	BB	2504	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	2580	26	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
2	4SU	AB	8	2	-	5/7/25/26	0/2/2/2
26	3TD	BB	1915	26	-	0/7/25/26	0/2/2/2
26	2MG	BB	2445	26	-	0/5/27/28	0/3/3/3
26	7MG	BB	2069	26	-	1/7/37/38	0/3/3/3
26	OMC	BB	2498	26	-	1/9/27/28	0/2/2/2
2	H2U	AB	16	2	-	0/7/38/39	0/2/2/2
2	5MU	AB	54	2	-	0/7/25/26	0/2/2/2
26	1MG	BB	745	26	-	0/3/25/26	0/3/3/3
2	MIA	AB	37	2	-	1/11/33/34	0/3/3/3
26	6MZ	BB	2030	26	-	1/5/27/28	0/3/3/3
26	6MZ	BB	1618	26	-	0/5/27/28	0/3/3/3
26	PSU	BB	2457	26	-	0/7/25/26	0/2/2/2
26	OMU	BB	2552	26	-	0/9/27/28	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
2	H2U	AB	20	2	-	0/7/38/39	0/2/2/2
4	4SU	AD	8	4	-	0/7/25/26	0/2/2/2
26	5MU	BB	747	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	1911	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	1917	26	-	1/7/25/26	0/2/2/2
2	OMC	AB	32	2	-	1/9/27/28	0/2/2/2
26	OMG	BB	2251	26	-	0/5/27/28	0/3/3/3
1	UR3	AA	1498	1	-	1/7/25/26	0/2/2/2
26	CH	BB	2575	26	-	0/5/25/26	0/2/2/2
26	5MU	BB	1939	26	-	0/7/25/26	0/2/2/2

The worst 5 of 184 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BB	2069	7MG	C8-N9	-18.96	1.35	1.46
2	AB	46	7MG	C8-N9	-18.04	1.35	1.46
1	AA	527	7MG	C8-N9	-14.09	1.38	1.46
2	AB	37	MIA	C2-S10	13.92	1.87	1.75
4	AD	8	4SU	C5-C4	-6.50	1.34	1.42

The worst 5 of 253 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	MA6	N1-C6-N6	7.78	125.25	117.06
2	AB	46	7MG	N9-C8-N7	6.87	113.21	103.38
26	BB	2069	7MG	N9-C8-N7	6.82	113.13	103.38
26	BB	1618	6MZ	C9-N6-C6	6.37	128.36	122.87
4	AD	21	H2U	O4'-C1'-N1	6.33	117.92	109.30

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1516	2MG	N3-C2-N2-CM2
2	AB	8	4SU	C2'-C1'-N1-C2
2	AB	32	OMC	C1'-C2'-O2'-CM2
26	BB	746	PSU	C2'-C1'-C5-C4
2	AB	8	4SU	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
59	TRP	AB	101	60,2	14,15,16	2.01	4 (28%)	13,20,22	1.64	3 (23%)
60	FME	BB	3001	59	8,9,10	0.98	0	7,9,11	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	TRP	AB	101	60,2	-	0/5/6/8	0/2/2/2
60	FME	BB	3001	59	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AB	101	TRP	OXT-C	-4.64	1.22	1.42
59	AB	101	TRP	CZ3-CE3	3.48	1.44	1.36
59	AB	101	TRP	C-CA	3.04	1.57	1.52
59	AB	101	TRP	CZ2-CE2	-2.19	1.38	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AB	101	TRP	OXT-C-CA	2.45	121.20	111.52
59	AB	101	TRP	CZ2-CE2-CD2	2.43	125.20	120.76
59	AB	101	TRP	CH2-CZ2-CE2	-2.25	116.84	120.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	BB	3001	FME	O1-CN-N-CA

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	BB	2
1	AA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BB	1872:A	O3'	1873:G	P	1.76
1	AA	1017:U	O3'	1018:G	P	1.75
1	BB	600:G	O3'	601:C	P	1.75

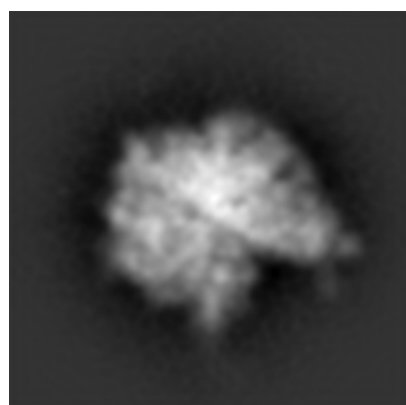
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5363. These allow visual inspection of the internal detail of the map and identification of artifacts.

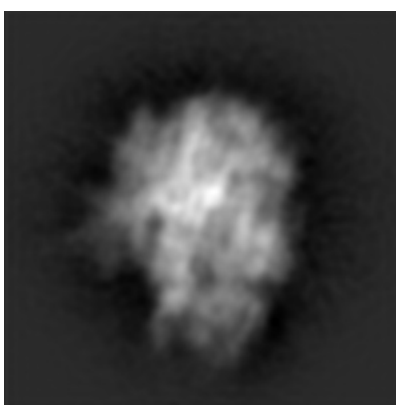
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

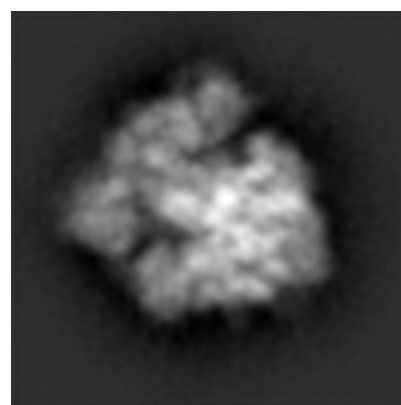
6.1.1 Primary map



X



Y

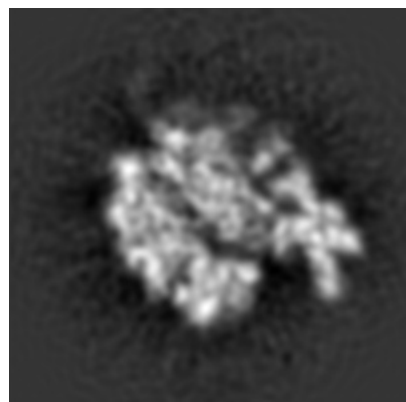


Z

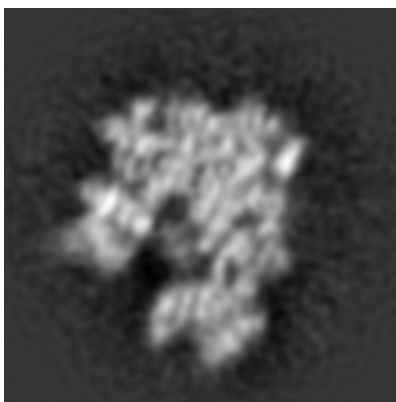
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

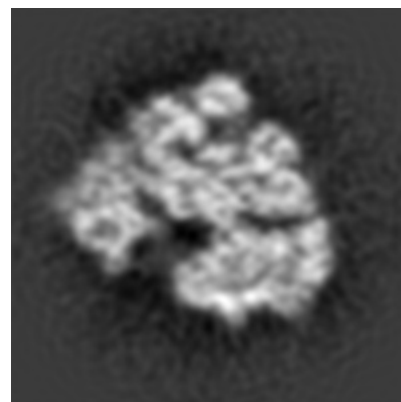
6.2.1 Primary map



X Index: 125



Y Index: 125

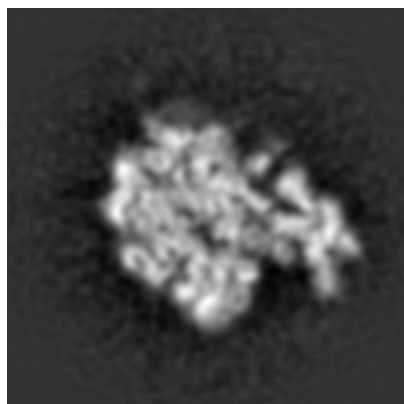


Z Index: 125

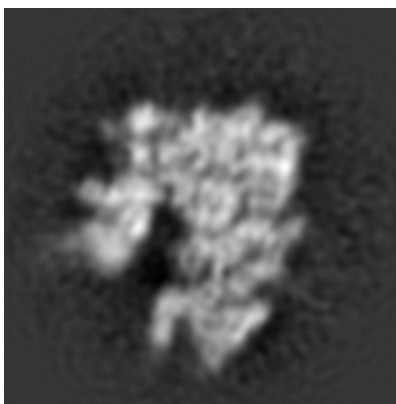
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

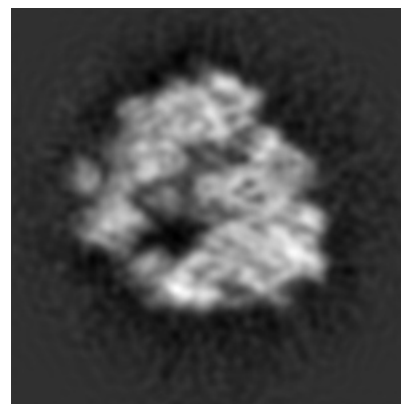
6.3.1 Primary map



X Index: 129



Y Index: 131

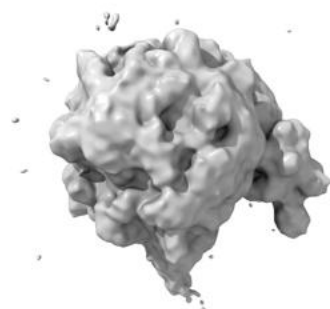


Z Index: 115

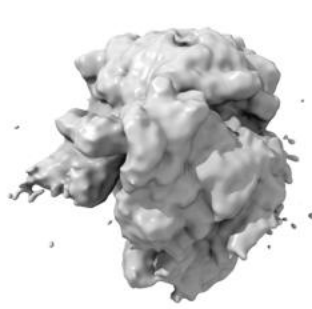
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

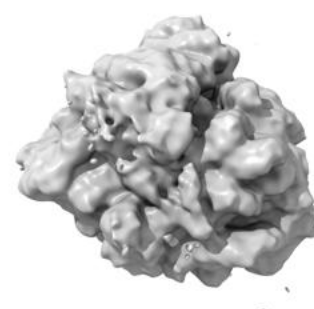
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

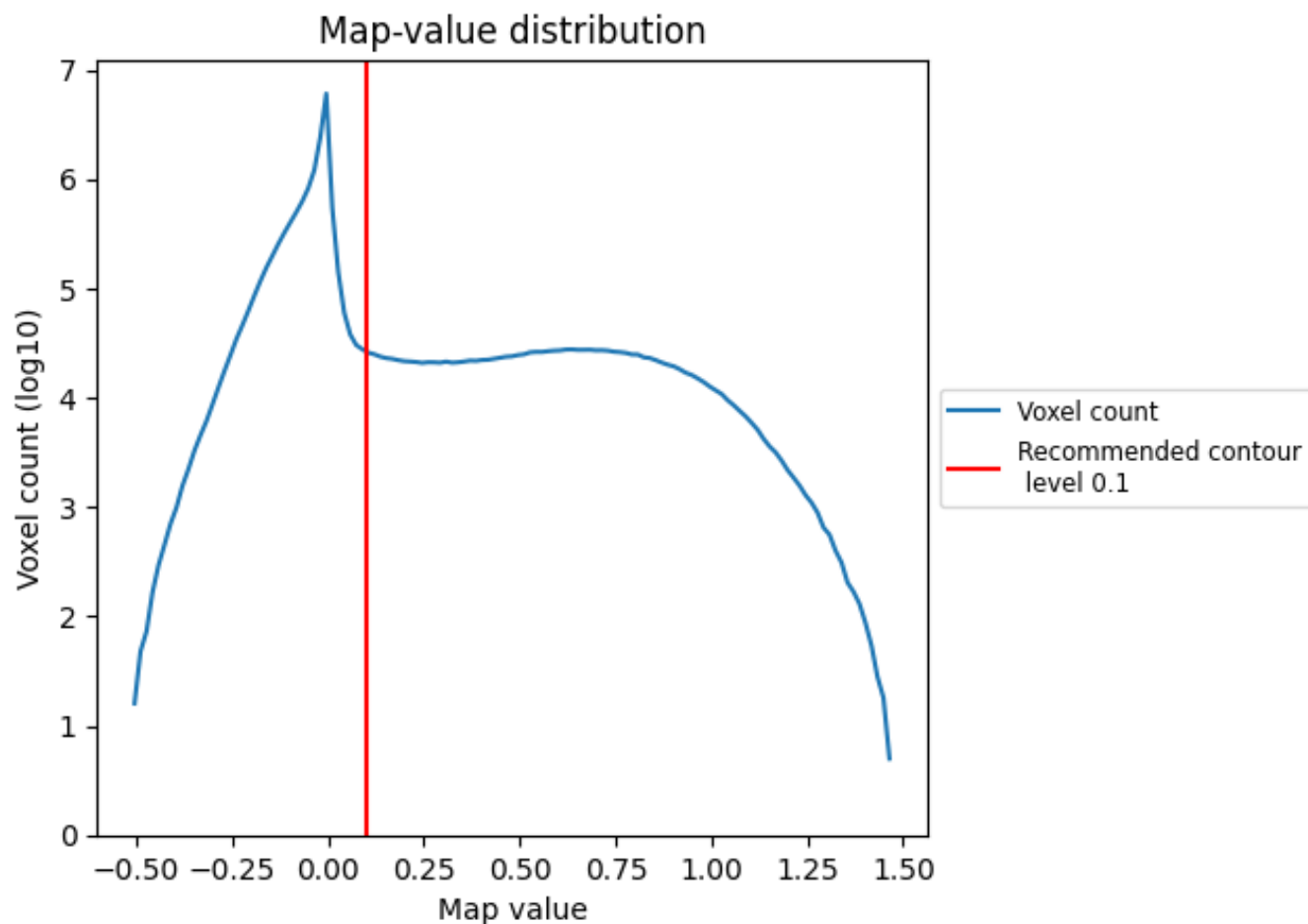
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

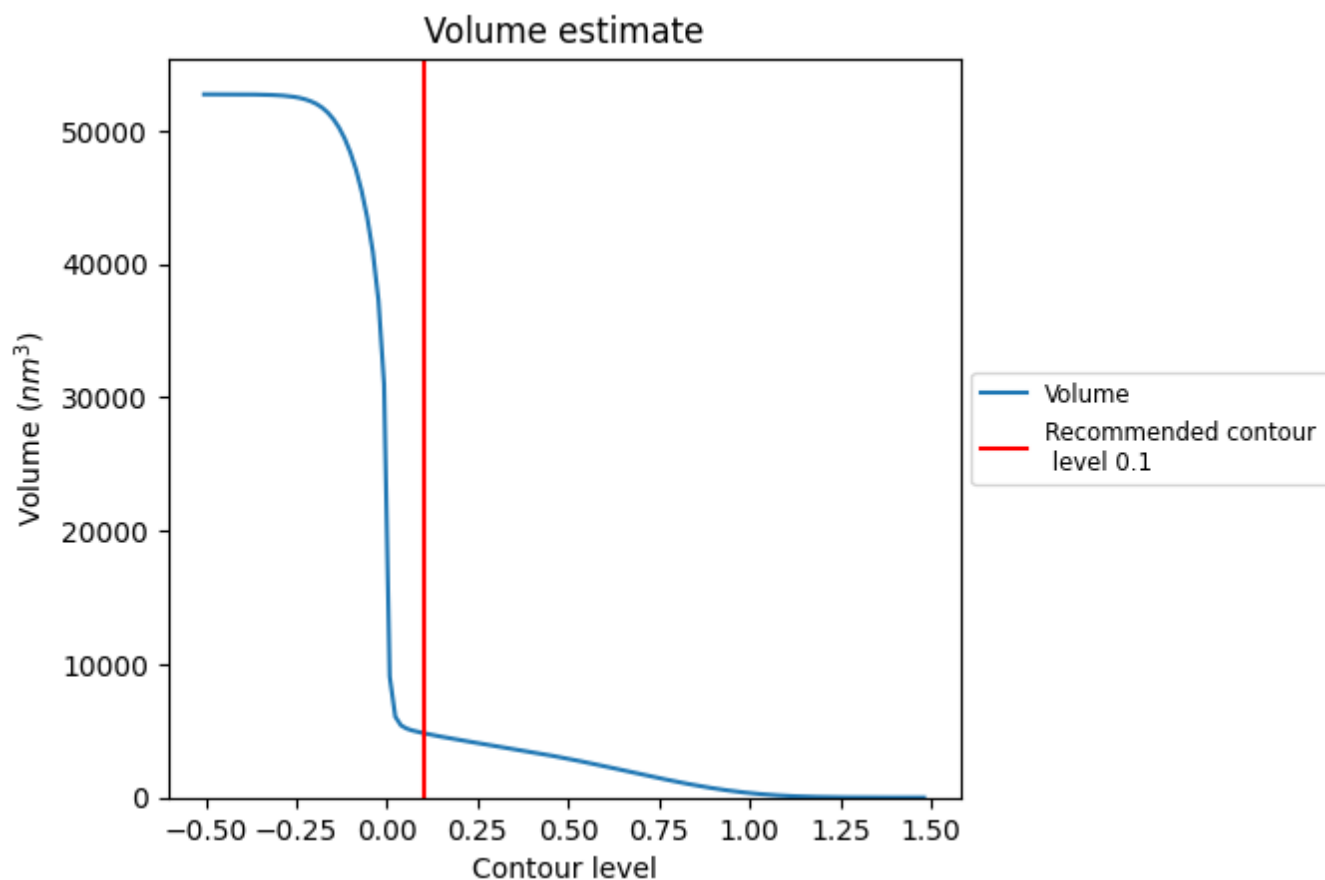
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

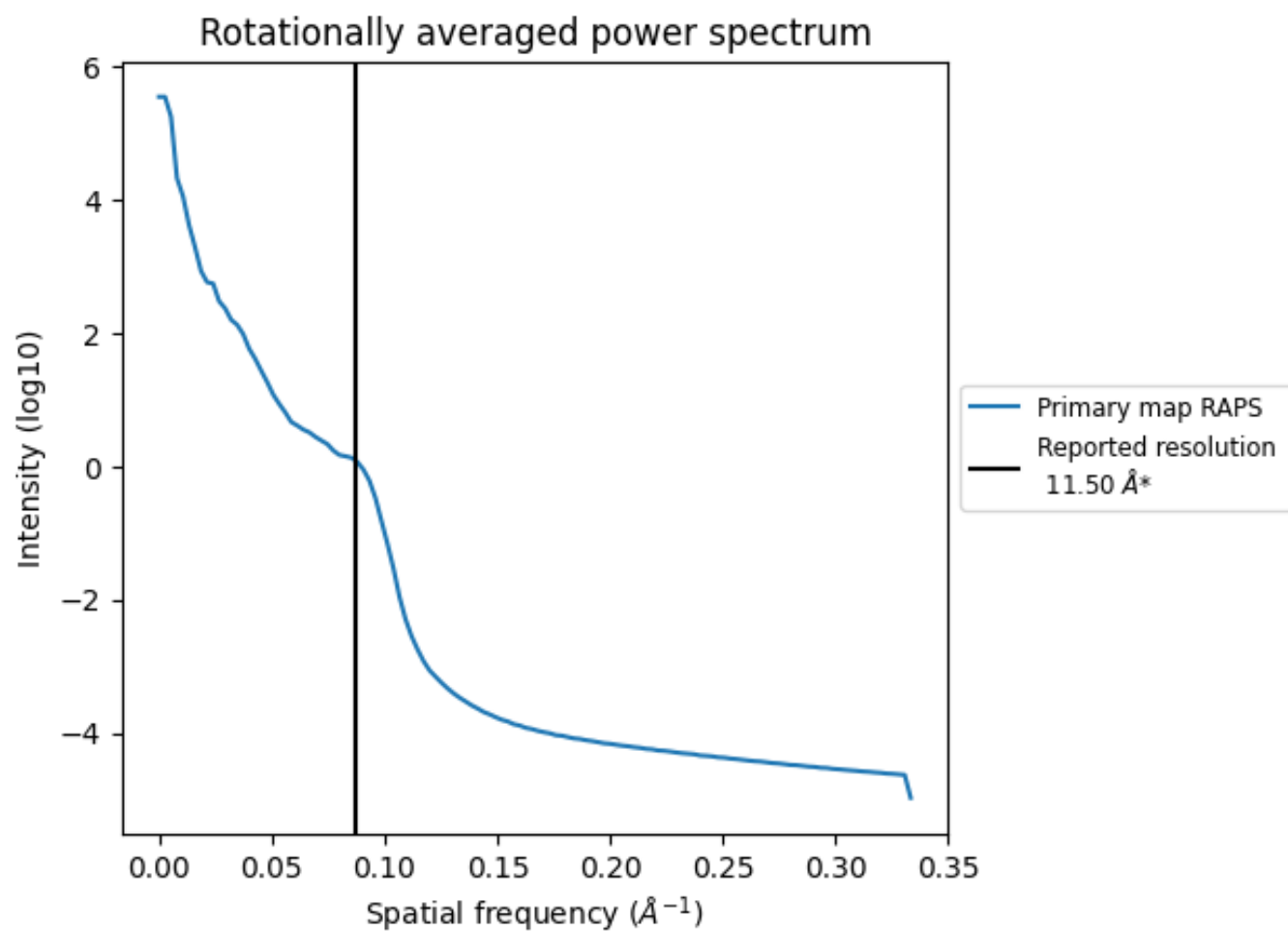
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4835 nm^3 ; this corresponds to an approximate mass of 4367 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.087 Å⁻¹

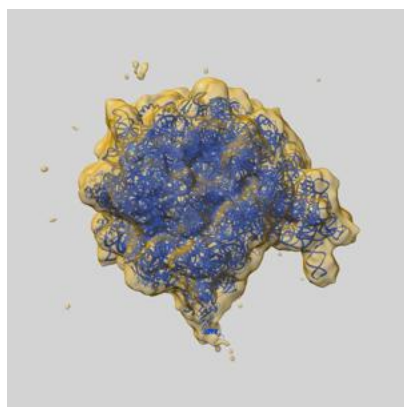
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

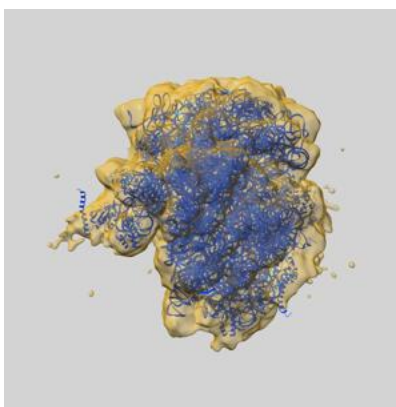
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5363 and PDB model 4V6Q. Per-residue inclusion information can be found in section 3 on page 15.

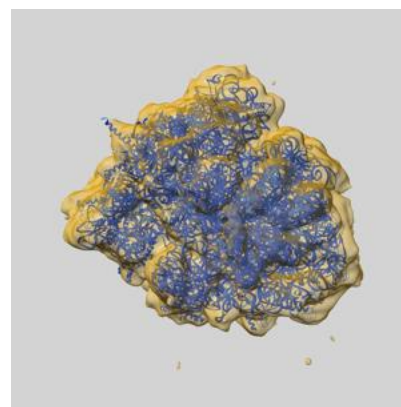
9.1 Map-model overlay [i](#)



X



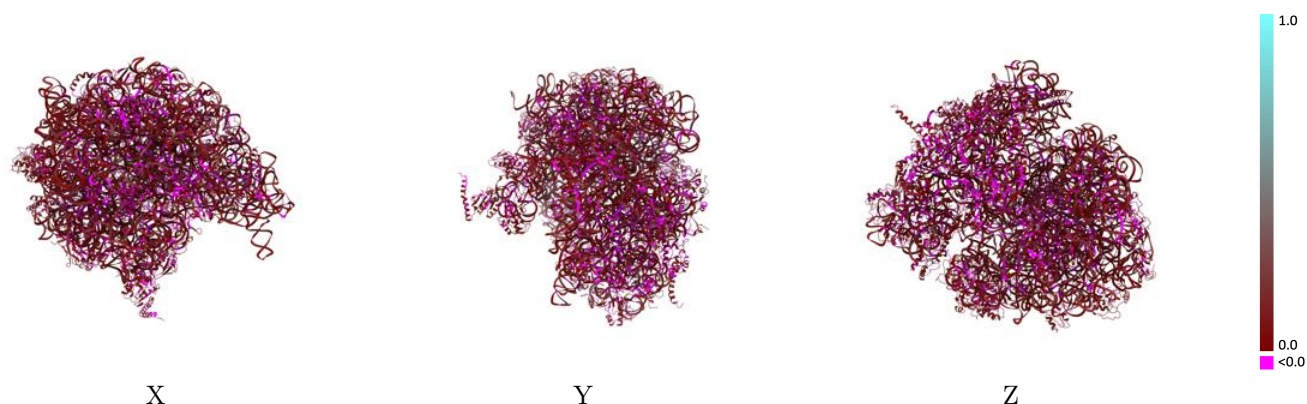
Y



Z

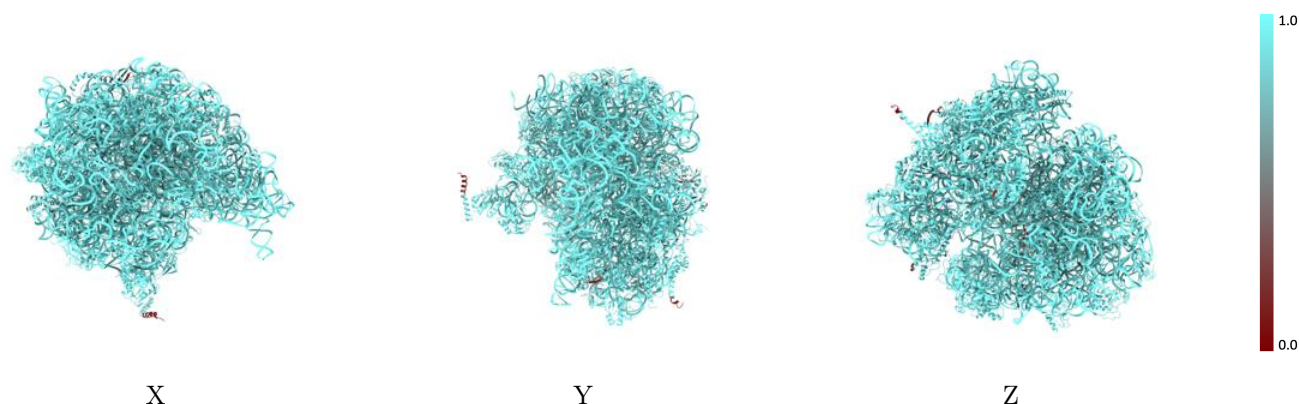
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



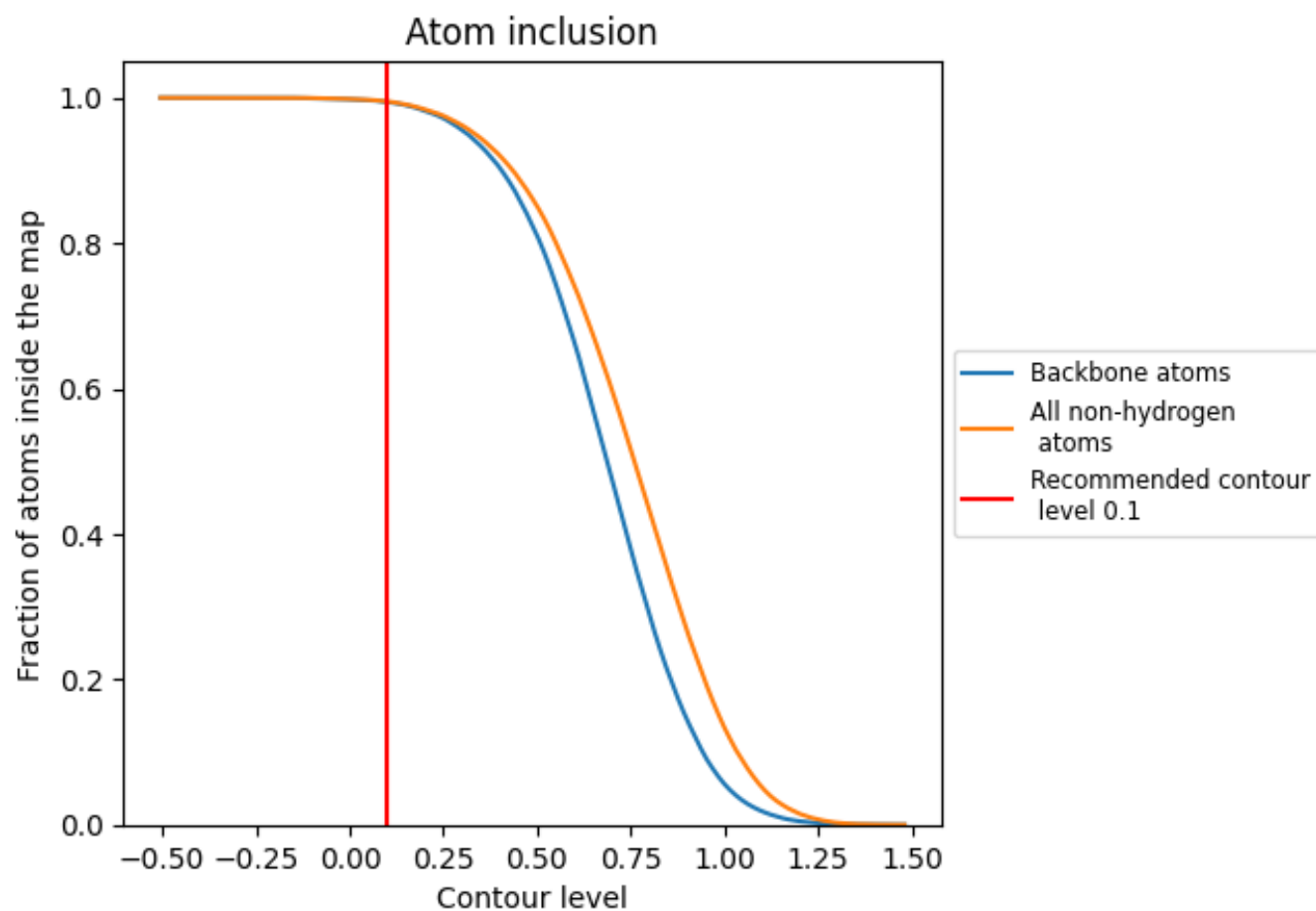
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

















































The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9950	 0.0740
AA	 0.9997	 0.0910
AB	 0.9860	 0.0530
AC	 0.8953	 0.0140
AD	 0.9939	 0.0980
AE	 0.9468	 0.0370
AF	 0.9994	 0.0630
AG	 0.9994	 0.0450
AH	 0.9925	 0.0430
AI	 0.9813	 0.0410
AJ	 0.9912	 0.0540
AK	 0.9979	 0.0400
AL	 0.9809	 0.0480
AM	 1.0000	 0.0220
AN	 0.9925	 0.0420
AO	 0.9891	 0.0400
AP	 0.9749	 0.0410
AQ	 1.0000	 0.0400
AR	 1.0000	 0.0540
AS	 0.9984	 0.0100
AT	 1.0000	 0.0570
AU	 1.0000	 0.0290
AV	 0.9789	 0.0360
AW	 1.0000	 0.0460
AX	 1.0000	 0.0290
B0	 1.0000	 0.0320
B1	 1.0000	 0.0430
B2	 0.9814	 0.0180
B3	 1.0000	 0.0280
B4	 0.9977	 0.0540
B5	 1.0000	 0.0030
B6	 1.0000	 0.0370
B7	 1.0000	 0.0320
BA	 1.0000	 0.1010
BB	 0.9997	 0.0910



Continued on next page...

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Chain	Atom inclusion	Q-score
BC	 0.9906	 0.0420
BD	 1.0000	 0.0180
BE	 0.9993	 0.0240
BF	 0.9993	 0.0650
BG	 0.9906	 0.0460
BH	 1.0000	 0.0250
BI	 0.8513	 0.0260
BJ	 0.8997	 0.0450
BK	 0.9726	 0.0380
BL	 1.0000	 0.0330
BM	 0.9957	 0.0600
BN	 0.9990	 0.0160
BO	 1.0000	 0.0440
BP	 1.0000	 0.0250
BQ	 0.9954	 0.0580
BR	 0.9977	 0.0280
BS	 0.9978	 0.0250
BT	 0.9950	 0.0480
BU	 0.9976	 0.0270
BV	 0.9987	 0.0330
BW	 1.0000	 0.0690
BX	 1.0000	 0.0740
BY	 0.9984	 0.0240
BZ	 1.0000	 0.0350