



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 11:24 PM UTC

PDB ID : 6S0X / pdb_00006s0x
EMDB ID : EMD-10076
Title : Erythromycin Resistant Staphylococcus aureus 70S ribosome (delta R88 A89 uL22) in complex with erythromycin.
Authors : Halfon, Y.; Matozv, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Kjeldgaard, J.; Ingmer, H.; Yonath, A.
Deposited on : 2019-06-18
Resolution : 2.42 Å(reported)

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:

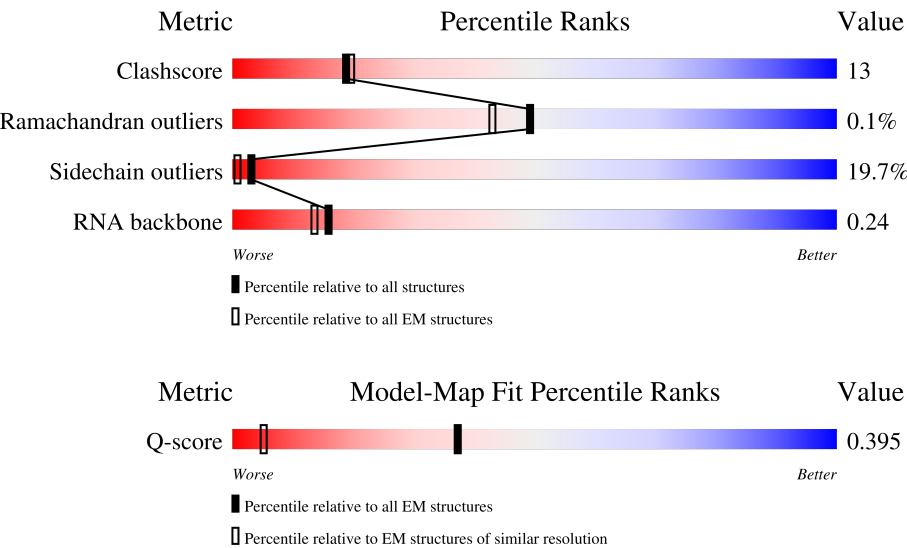
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.42 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.



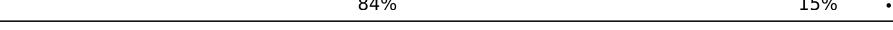
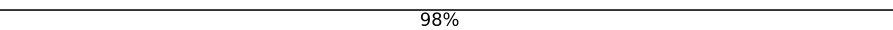
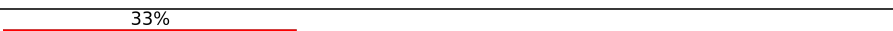
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5720 (1.93 - 2.92)

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	A	2905	
2	B	115	
3	C	274	

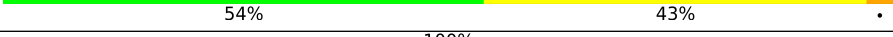
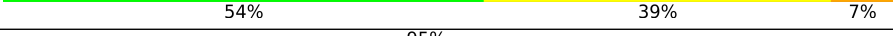
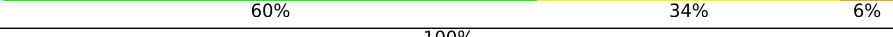
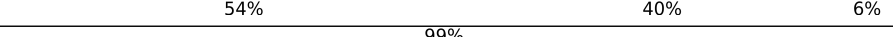
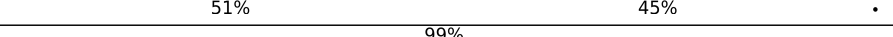
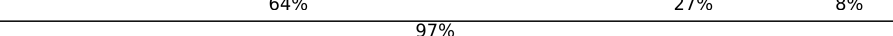
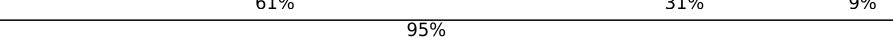
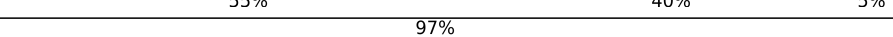
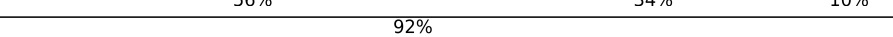
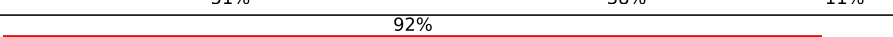
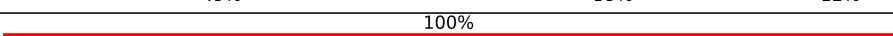
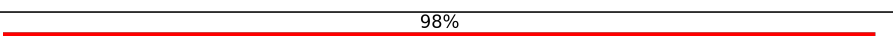
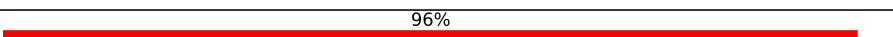
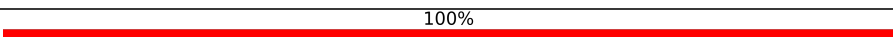
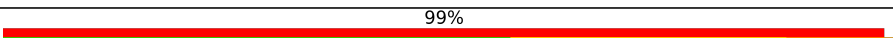
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Mol	Chain	Length	Quality of chain
4	D	215	
5	E	206	
6	F	173	
7	G	173	
8	H	145	
9	I	122	
10	J	146	
11	K	137	
12	L	120	
13	M	118	
14	N	114	
15	O	116	
16	P	102	
17	Q	110	
18	R	89	
19	S	103	
20	T	94	
21	U	77	
22	V	49	
23	W	67	
24	X	58	
25	Y	59	
26	Z	48	
27	1	47	
28	2	43	

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Mol	Chain	Length	Quality of chain
29	3	64	
30	4	37	
31	a	1539	
32	b	226	
33	c	202	
34	d	198	
35	e	156	
36	f	95	
37	g	152	
38	h	131	
39	i	127	
40	j	97	
41	k	114	
42	l	135	
43	m	104	
44	n	60	
45	o	88	
46	p	89	
47	q	80	
48	r	54	
49	s	80	
50	t	81	
51	u	52	
52	v	162	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	ERY	A	3001	X	-	-	-

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 140672 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2905	Total	C	N	O	P	0	0
			62277	27803	11387	20182	2905		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	115	Total	C	N	O	P	0	0
			2445	1094	436	801	114		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	274	Total	C	N	O	S	0	0
			2090	1301	415	369	5		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	173	Total	C	N	O	S	0	0
			1315	831	225	253	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	173	Total	C	N	O	S	0	0
			1248	780	236	229	3		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	145	Total	C	N	O	S	0	0
			1149	717	211	218	3		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	137	Total	C	N	O	S	0	0
			1079	694	204	177	4		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	118	Total	C	N	O	0	0
			883	552	173	158		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	114	Total	C	N	O	0	0
			889	563	175	151		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	110	Total	C	N	O	S	0	0
			838	525	159	151	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	ARG	deletion	UNP A0A077UKF9
Q	?	-	ALA	deletion	UNP A0A077UKF9

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	94	Total	C	N	O	0	0
			722	463	130	129		

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	77	Total	C	N	O	0	0
			587	363	115	109		

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	49	Total	C	N	O	0	0
			379	234	82	63		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	67	Total	C	N	O	0	0
			541	333	102	106		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	58	Total	C	N	O	0	0
			449	280	85	84		

- Molecule 25 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	59	Total	C	N	O	S	0	0
			370	225	68	76	1		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	48	Total	C	N	O	S	0	0
			360	222	77	59	2		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	37	Total	C	N	O	S	0	0
			295	186	60	44	5		

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1539	Total	C	N	O	P	0	0
			32969	14719	6017	10694	1539		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	226	Total	C	N	O	S	0	0
			1819	1159	317	335	8		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	202	Total	C	N	O	S	0	0
			1501	945	284	271	1		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	198	Total	C	N	O	S	0	0
			1497	952	275	268	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	156	Total	C	N	O	S	0	0
			1145	723	211	209	2		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	95	Total	C	N	O	S	0	0
			778	493	138	145	2		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	152	Total	C	N	O	S	0	0
			1161	722	218	217	4		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	131	Total	C	N	O	S	0	0
			1026	650	183	189	4		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	127	Total	C	N	O	S	0	0
			922	576	179	166	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	97	Total	C	N	O	S	0	0
			752	475	140	136	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	114	Total	C	N	O	S	0	0
			810	498	151	159	2		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	135	Total	C	N	O	S	0	0
			1037	646	211	178	2		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	104	Total	C	N	O	S	0	0
			727	453	139	135			

- Molecule 44 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total	C	N	O	S	0	0
			487	307	98	77	5		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			723	448	150	124	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	89	Total	C	N	O	S	0	0
			694	436	128	129	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	80	Total	C	N	O	S	0	0
			621	392	112	117			

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	54	Total	C	N	O	S	0	0
			445	284	86	73	2		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	80	Total	C	N	O	S	0	0
			636	410	113	111	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	81	Total	C	N	O	S	0	0
			591	358	117	115	1		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	u	52	Total	C	N	O	0	0
			400	249	79	72		

- Molecule 52 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	162	Total	C	N	O	S	0	0
			1333	835	242	254	2		

There are 24 discrepancies between the modelled and reference sequences:

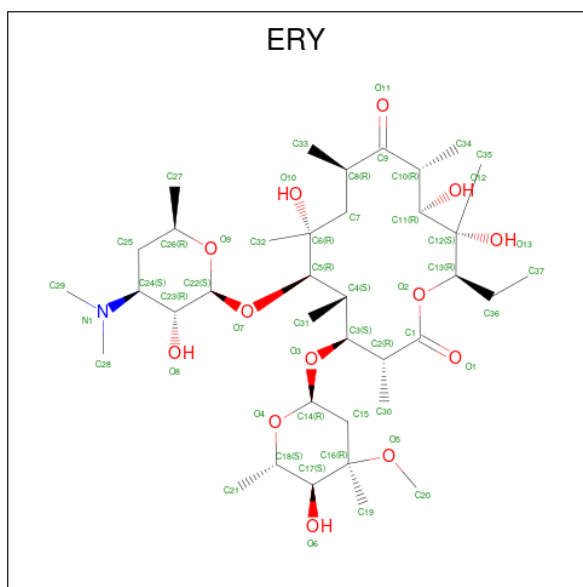
Chain	Residue	Modelled	Actual	Comment	Reference
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	PHE	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	ALA	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	LEU	deletion	UNP W8USK0
v	?	-	GLN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0
v	?	-	MET	deletion	UNP W8USK0
v	?	-	GLN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0

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Chain	Residue	Modelled	Actual	Comment	Reference
v	?	-	THR	deletion	UNP W8USK0
v	?	-	GLN	deletion	UNP W8USK0
v	?	-	VAL	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASN	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ALA	deletion	UNP W8USK0
v	?	-	TYR	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASP	deletion	UNP W8USK0
v	?	-	ASN	deletion	UNP W8USK0
v	?	-	GLU	deletion	UNP W8USK0

- Molecule 53 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$).

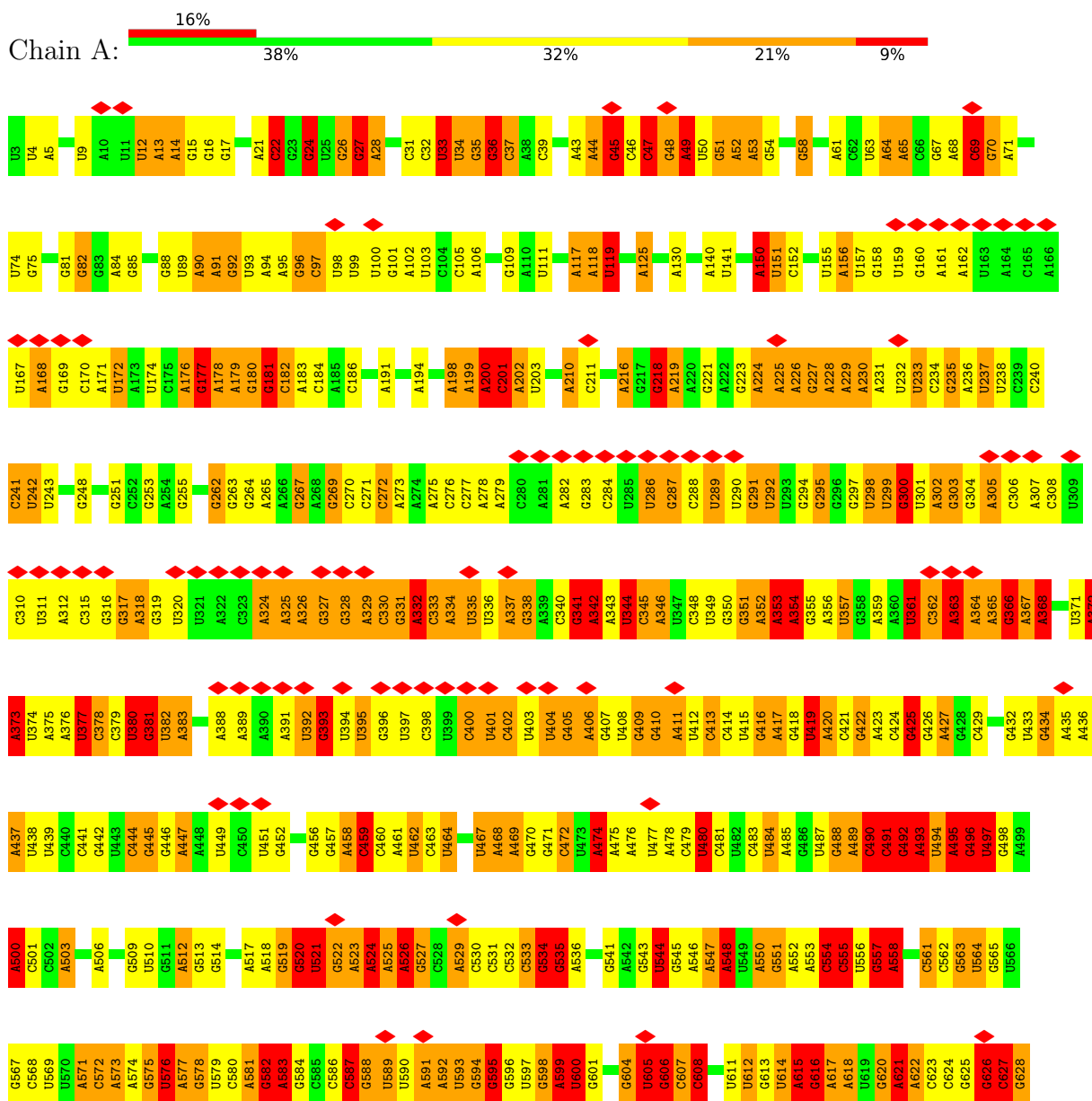


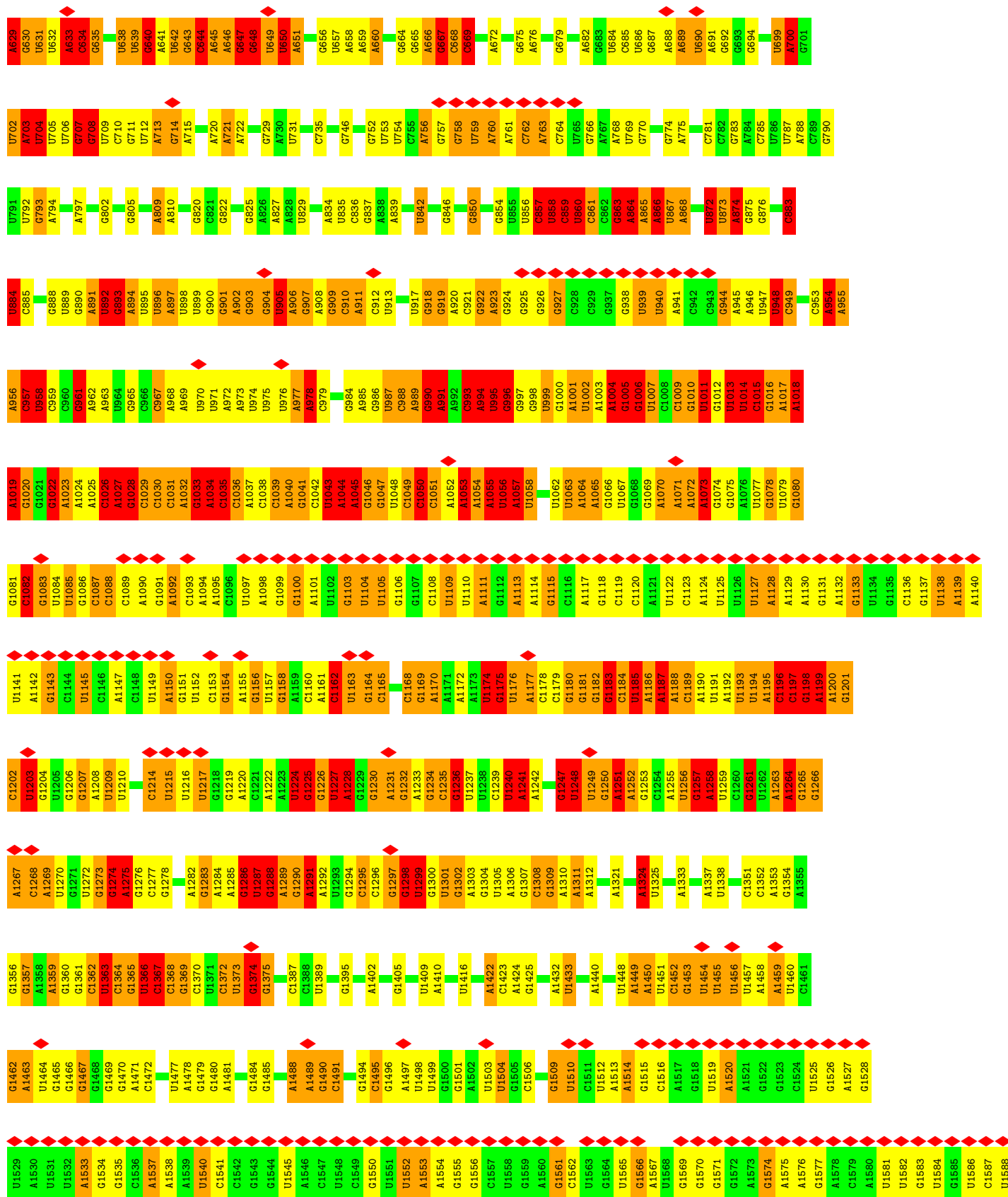
Mol	Chain	Residues	Atoms				AltConf
53	A	1	Total	C	N	O	0
			51	37	1	13	

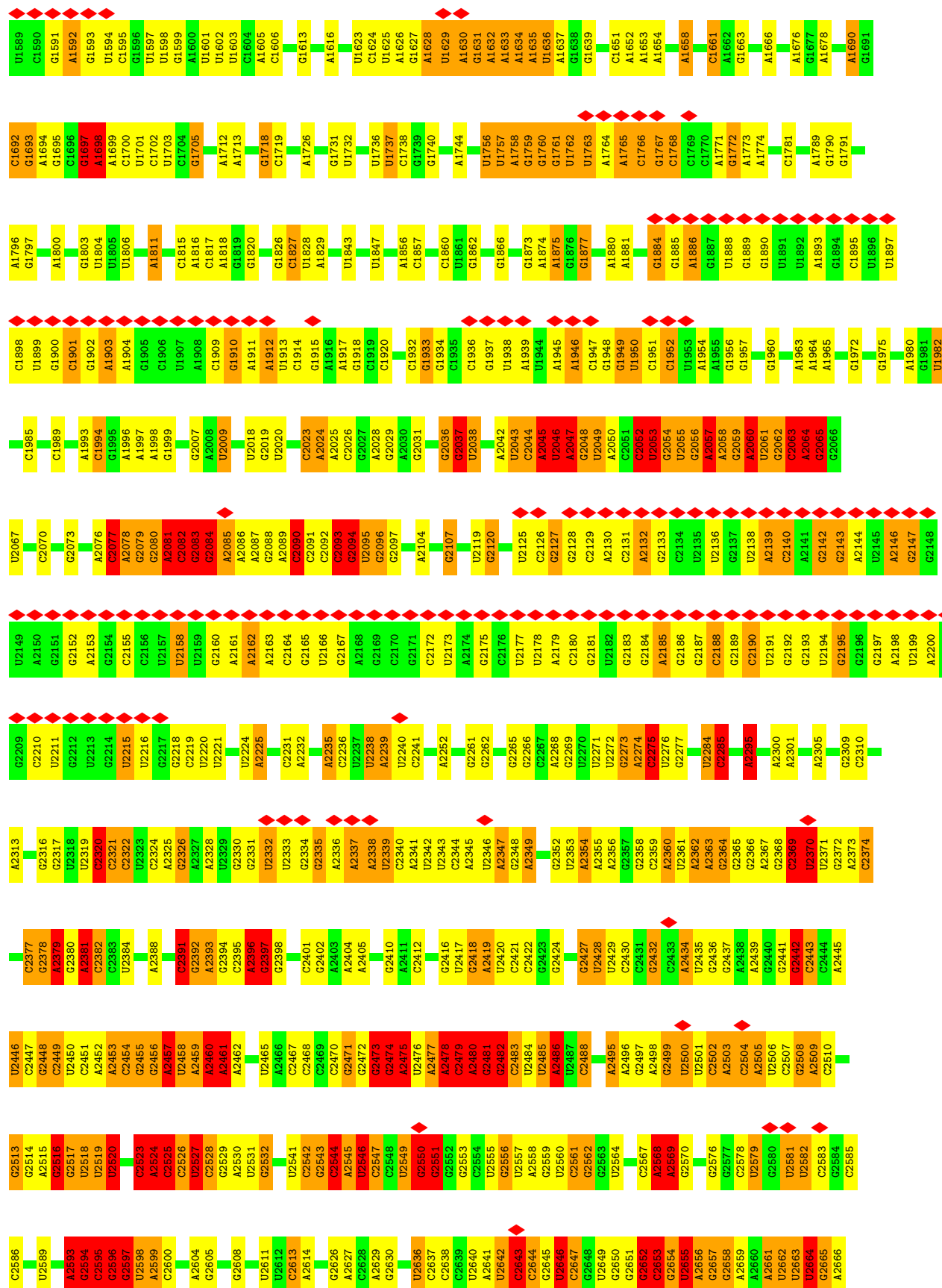
3 Residue-property plots

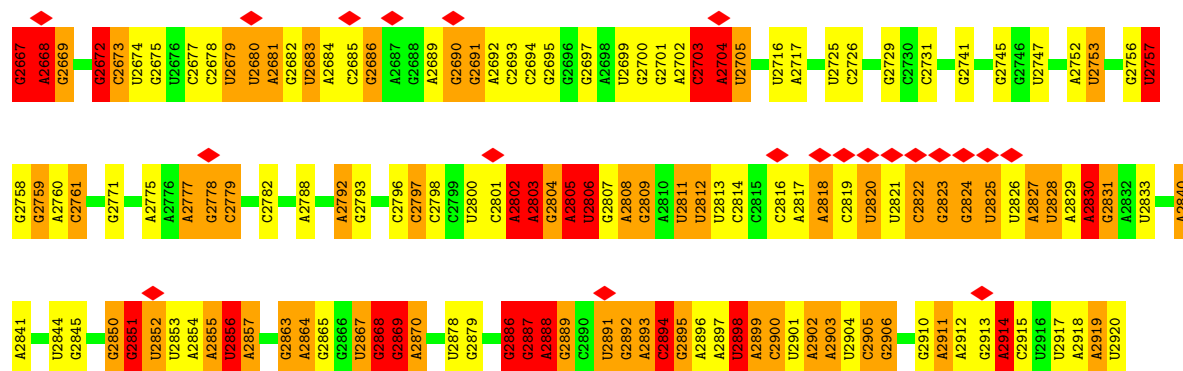
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S ribosomal RNA



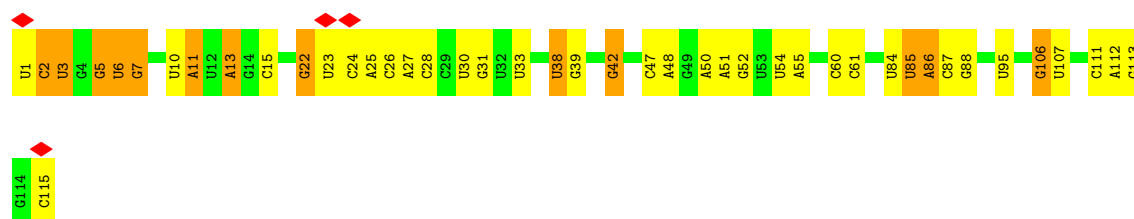






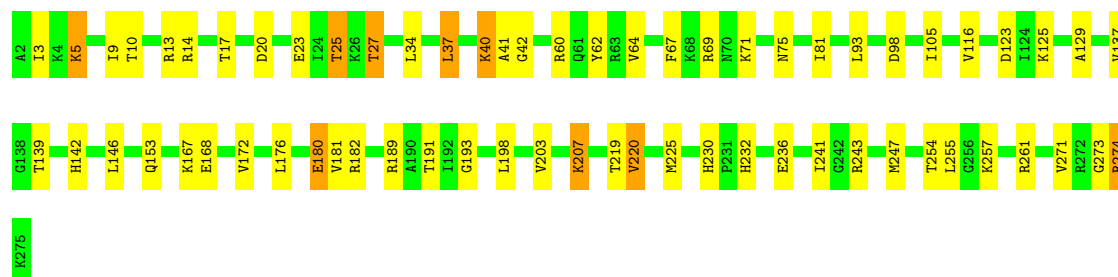
- Molecule 2: 5S ribosomal RNA

Chain B: 62% 27% 11%



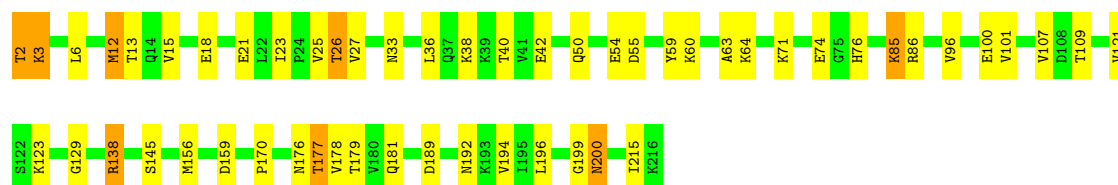
- Molecule 3: 50S ribosomal protein L2

Chain C: 76% 20% 4%



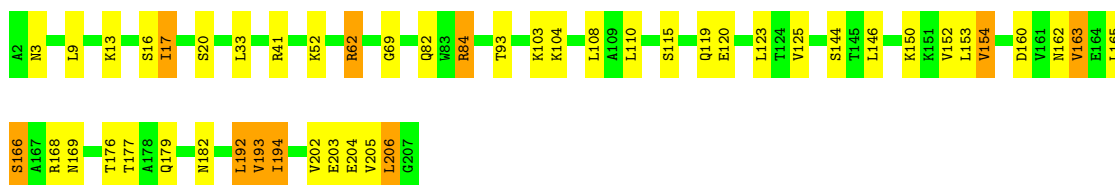
- Molecule 4: 50S ribosomal protein L3

Chain D: 75% 21% 4%

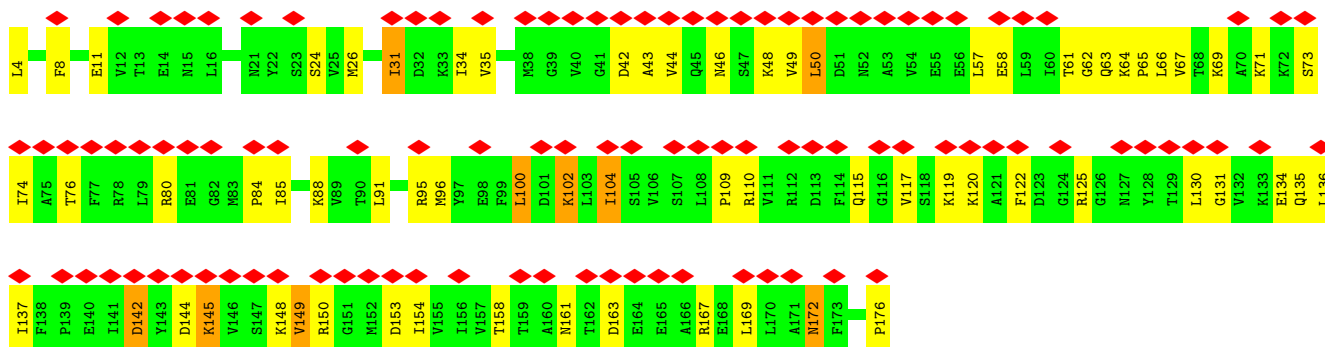


- Molecule 5: 50S ribosomal protein L4

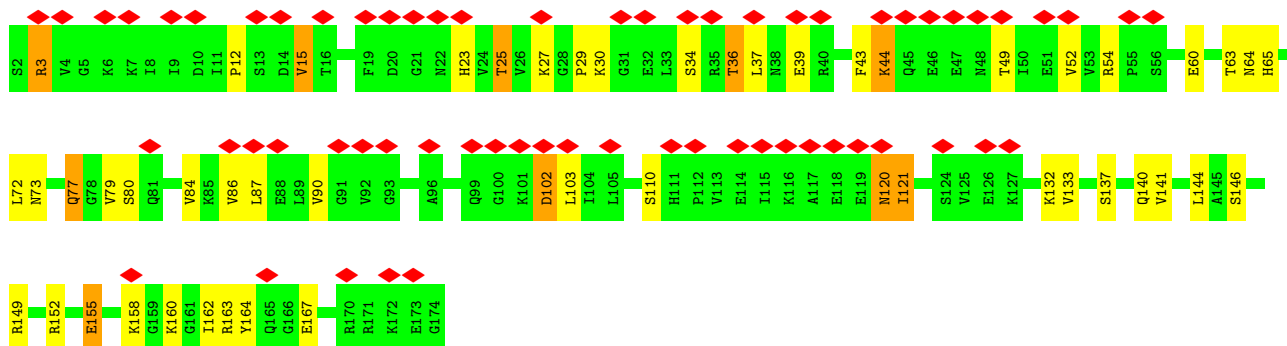
Chain E: 77% 18% 5%



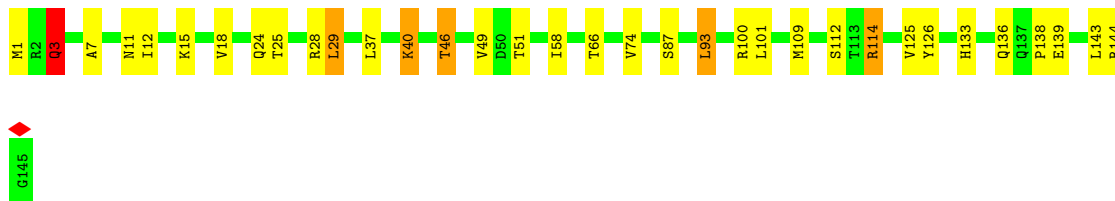
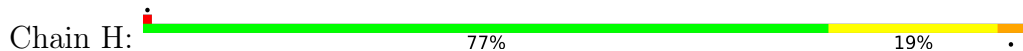
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L13



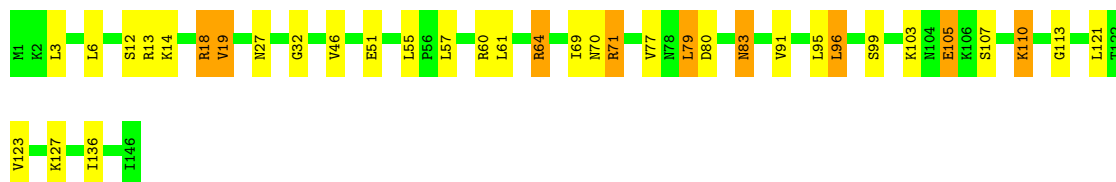
• Molecule 9: 50S ribosomal protein L14





- Molecule 10: 50S ribosomal protein L15

Chain J: 75% 18% 6%



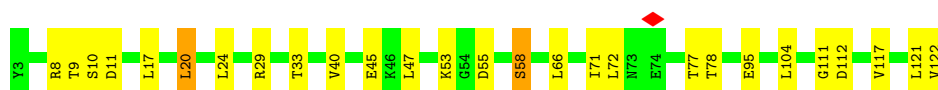
- Molecule 11: 50S ribosomal protein L16

Chain K: 76% 24%



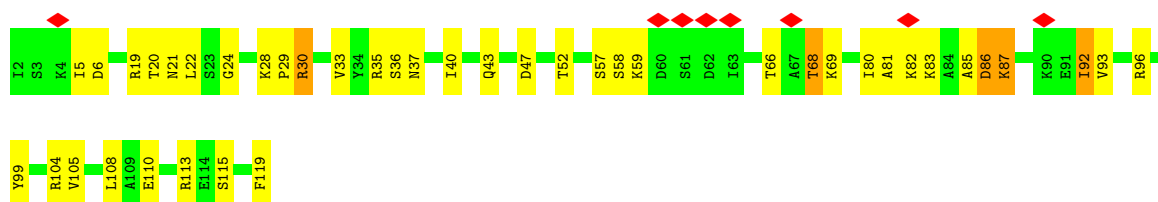
- Molecule 12: 50S ribosomal protein L17

Chain L: 78% 21% .



- Molecule 13: 50S ribosomal protein L18

Chain M: 7% 64% 31% .



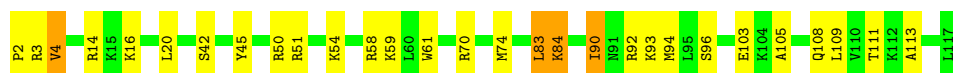
- Molecule 14: 50S ribosomal protein L19

Chain N: 83% 15% .



- Molecule 15: 50S ribosomal protein L20

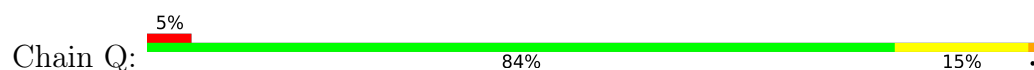
Chain O: 75% 22% .



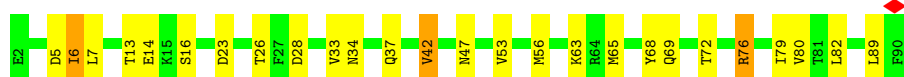
- Molecule 16: 50S ribosomal protein L21



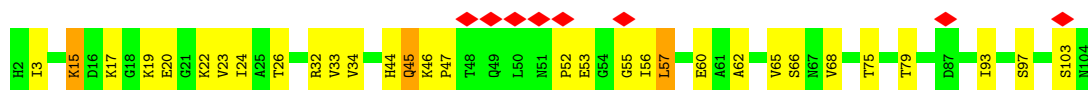
- Molecule 17: 50S ribosomal protein L22



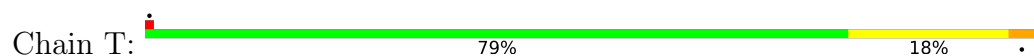
- Molecule 18: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L24



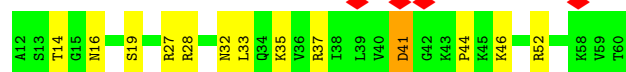
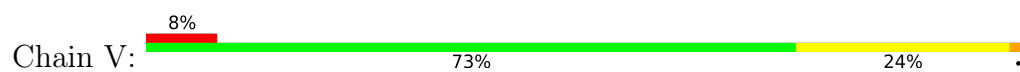
- Molecule 20: 50S ribosomal protein L25



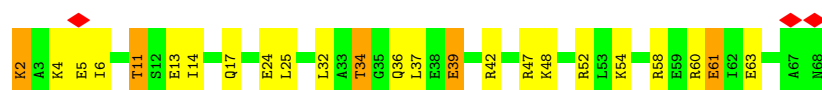
- Molecule 21: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L28



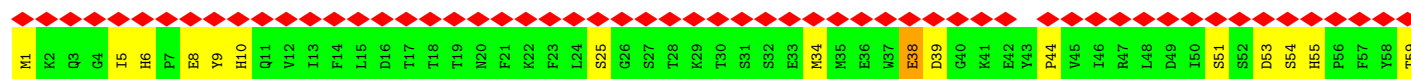
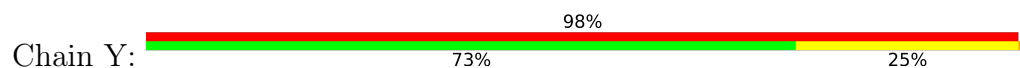
- Molecule 23: 50S ribosomal protein L29



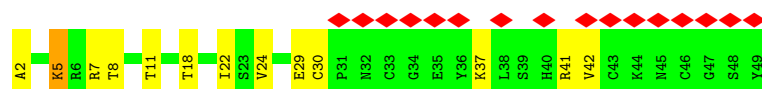
- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L31 type B



- Molecule 26: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L33

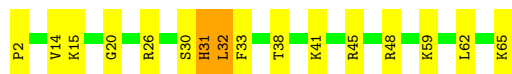


- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35

Chain 3:  75% 22% .

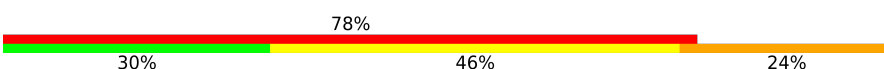


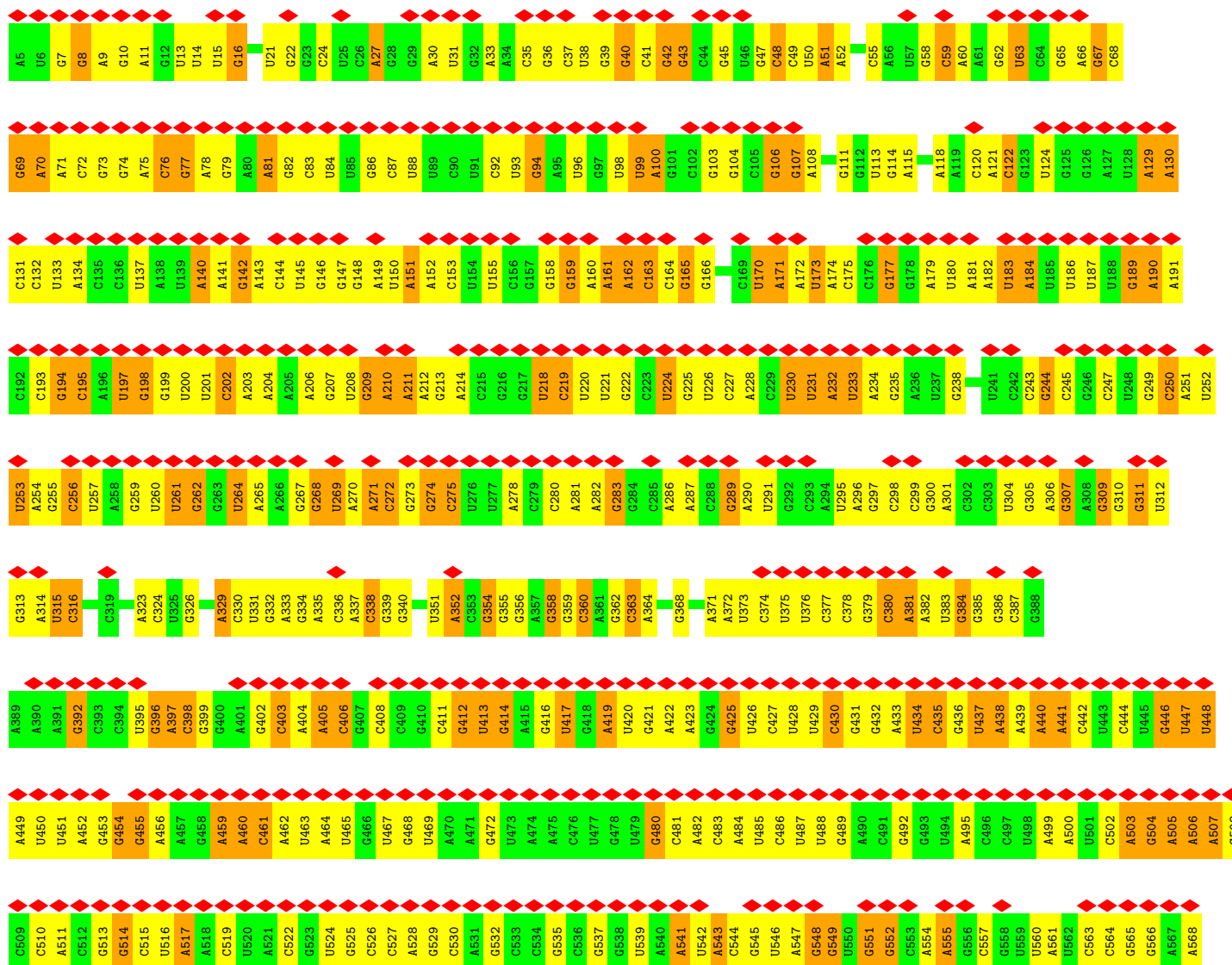
- Molecule 30: 50S ribosomal protein L36

Chain 4:  76% 19% 5%

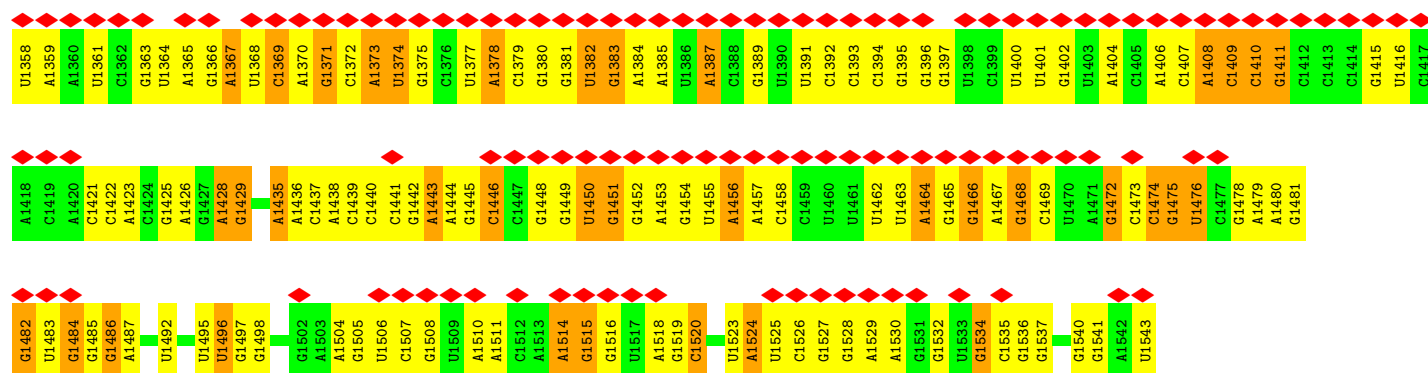


- Molecule 31: 16S ribosomal RNA

Chain a:  30% 78% 46% 24%



A1298	C1238	G1058	U998	A938	U872	U812	C752	U692	C631	U569
A1299	A1239	G1059	C999	C939	C875	C814	U753	G693	C632	U570
G1300	C1240	U1060	U1000	C940	C876	C815	G754	U694	A571	A571
U1301	G1241	G1061	U1001	C941	C877	C816	U755	A695	U572	U572
U1302	U1242	U1062	G1002	G942	A878	C916	A756	G696	U573	U573
G1303	C1243	U1063	A1003	C943	U879	G817	A757	G697	G574	G574
U1304	U1244	G1064	C1004	A944	U880	C818	C758	G698	G575	G575
U1305	U1245	C1065	A1005	C945	A881	G820	U759	G699	C577	C577
C1306	A1246	A1066	U1006	A946	A882	G821	U760	U700	A581	A581
U1307	C1247	U1067	C1007	A947	G883	A822	A761	G701	A582	A582
C1308	A1248	G1068	C1008	G948	C884	A823	C762	A702	G583	G583
A1309	U1249	G1069	U1009	C949	G885	A824	G763	A703	C584	C584
G1310	U1250	U1070	U1010	G950	A886	C825	C764	A704	G585	G585
U1311	C1251	U1071	G1011	G951	U887	G826	U765	U705	C586	C586
U1312	G1252	G1072	G1012	U952	U888	A827	G766	G706	G587	G587
C1313	U1133	U1073	A1013	G953	C889	G828	A767	C707	C588	C588
G1314	A1134	C1074	C1014	G954	G890	G829	U768	G708	G589	G589
G1315	G1135	G1075	A1015	G955	C891	A830	G769	C709	U590	U590
A1316	U1136	U1076	A1016	G956	C892	G831	U770	A710	A591	A591
U1317	G1137	C1077	C1017	G957	U893	U832	C772	G711	G592	G592
U1318	A1138	A1078	U1018	A958	G894	G833	G773	A712	C594	C594
G1319	U1139	G1079	C1019	U959	A898	C834	A774	A714	G595	G595
U1320	C1260	C1080	U1020	G960	G899	U835	A775	U715	G596	G596
G1321	A1261	U1081	A1021	U961	U900	A836	A776	A716	U597	U597
U1322	A1262	C1082	G1022	G962	A901	A837	C777	A717	U598	U598
C1323	G1263	U1083	A1023	G963	A904	G838	G778	U717	U599	U599
C1324	G1264	U1084	G1024	U964	A905	U839	U779	G718	U600	U600
U1325	G1265	G1085	A1025	U965	C906	G840	U780	G719	U601	U601
G1326	C1266	U1086	U1026	U966	G907	U841	G781	A720	U602	U602
C1327	A1267	C1087	A1027	A967	C908	U842	G782	G721	A603	A603
A1328	G1268	U1088	G1028	A968	C909	A843	G783	G722	A604	A604
A1329	C1269	U1089	A1029	U969	C910	G844	G784	G723	G605	G605
C1330	G1270	G1090	U1030	U970	G911	G845	A785	A724	U606	U606
U1331	A1271	A1091	C1031	C971	U914	G846	U786	C725	C607	C607
G1332	C1272	G1092	C1032	G972	G915	U847	C787	A726	U608	U608
A1333	A1273	A1093	U1033	A973	A916	G848	A788	C727	G609	G609
C1335	C1274	U1094	C1034	A974	A917	U849	A789	G728	A610	A610
U1336	G1275	G1095	U1035	G975	A918	U850	A790	C729	U611	U611
A1337	G1276	U1096	C1036	C976	C921	U851	C791	A730	U612	U612
C1338	C1277	U1097	C1037	A977	A922	C852	A792	G731	U613	U613
A1339	U1278	G1098	U1038	G978	A923	C853	G793	G732	G614	G614
U1340	A1279	U1099	C1039	C979	A924	G854	A794	G733	A615	A615
G1341	G1280	G1100	U1040	G980	G925	C855	U795	C734	A616	A616
A1342	U1281	U1101	C1041	C981	G926	C856	U796	G735	A617	A617
C1343	U1282	A1102	G1042	G982	G927	C857	A797	A736	G618	G618
G1344	C1283	A1103	G1043	A983	A928	C858	G799	A737	C619	C619
C1345	A1284	A1104	G1044	A984	U929	C859	U800	G738	C620	C620
U1346	U1285	G1105	G1045	G985	U930	U860	U801	C740	C621	C621
G1347	C1286	U1106	G1046	A986	G931	U861	A802	G741	A622	A622
A1348	U1287	C1107	A1047	A987	A932	G862	C903	G742	C623	C623
C1349	A1288	C1108	C1048	C988	G934	U863	C904	C743	G624	G624
A1349	U1289	C1109	A1049	C989	G935	G864	C905	U744	G625	G625
U1350	A1350	G1110	G1050	U990	G936	C865	U806	U745	C626	C626
G1351	U1291	C1111	A1051	U991	G937	U866	G907	U746	U627	U627
C1352	C1292	A1112	G1052	A992	C967	U867	U808	C747	C628	C628
G1353	G1293	A1113	U1053	C993	C968	A868	U809	C748	A629	A629
C1354	C1294	C1114	G1054	C994	A869	U869	A810	G749	U690	U690
U1355	A1295	G1115	A1055	A995	G870	C871	G911	U751	G691	G691
A1356	U1296	A1116	C1056	A996	C871	C871	C911	U751		
G1357	A1297	G1117	A1057	A997	C871	C871	C911	U751		



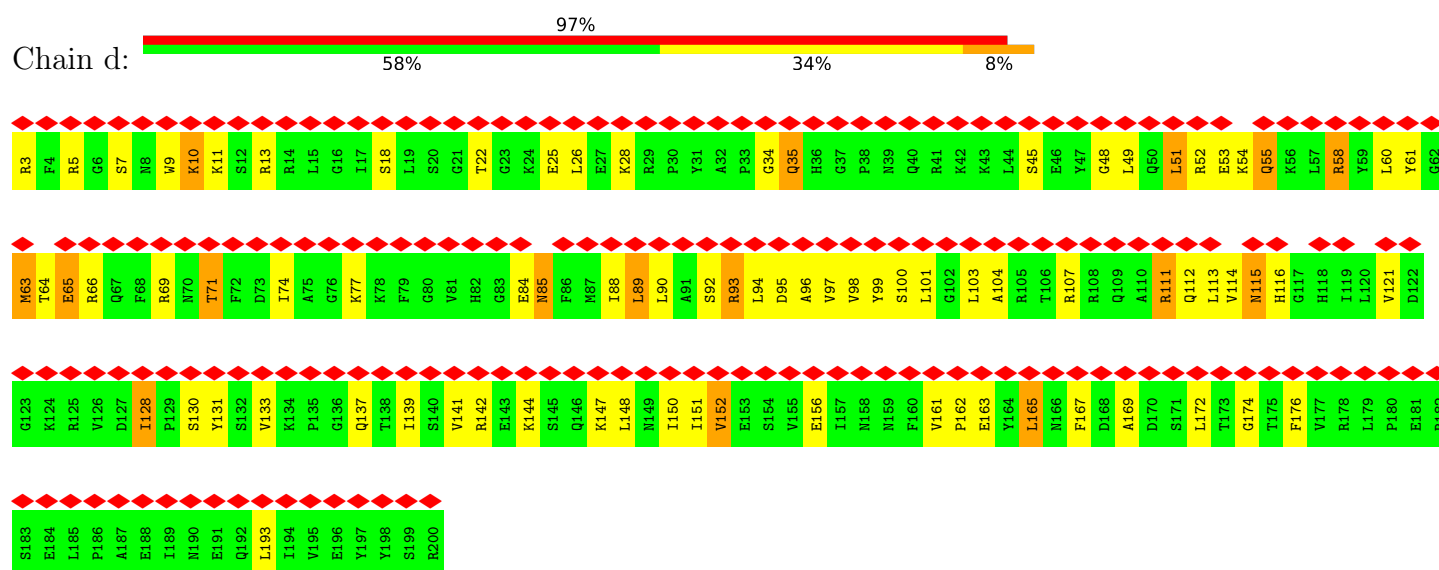
• Molecule 32: 30S ribosomal protein S2



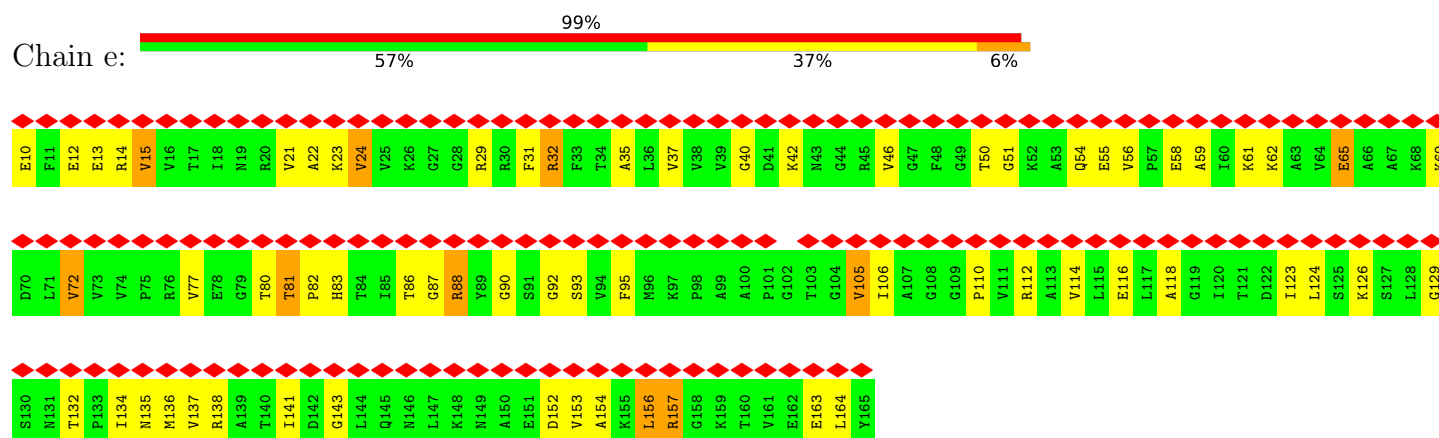
• Molecule 33: 30S ribosomal protein S3



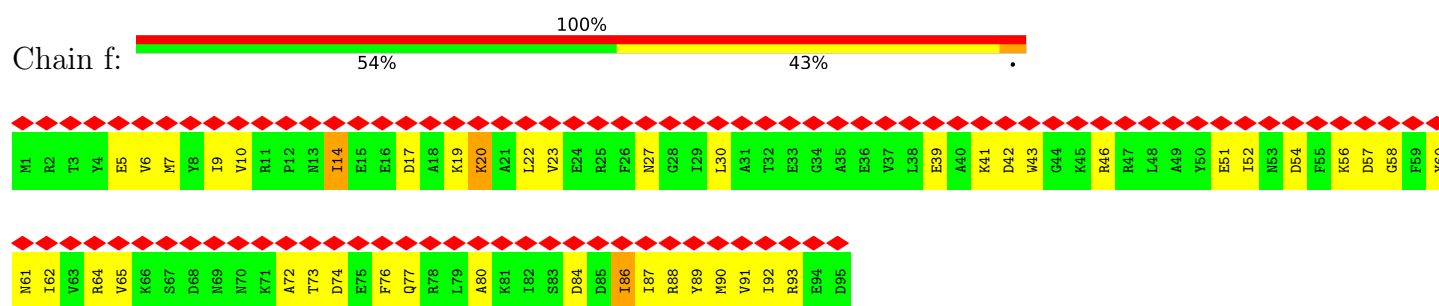
• Molecule 34: 30S ribosomal protein S4



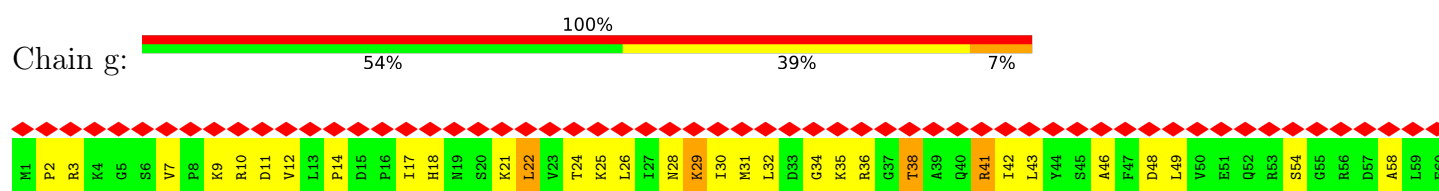
• Molecule 35: 30S ribosomal protein S5

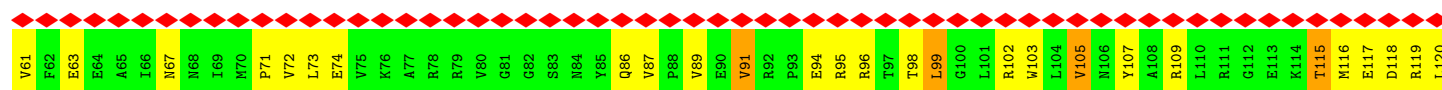


• Molecule 36: 30S ribosomal protein S6

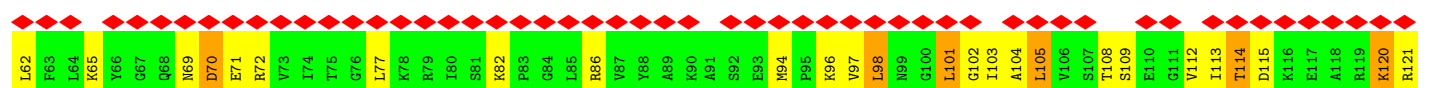


• Molecule 37: 30S ribosomal protein S7





• Molecule 38: 30S ribosomal protein S8



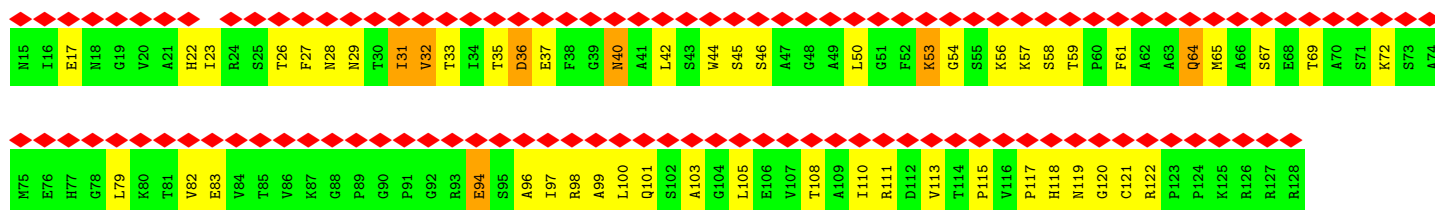
• Molecule 39: 30S ribosomal protein S9



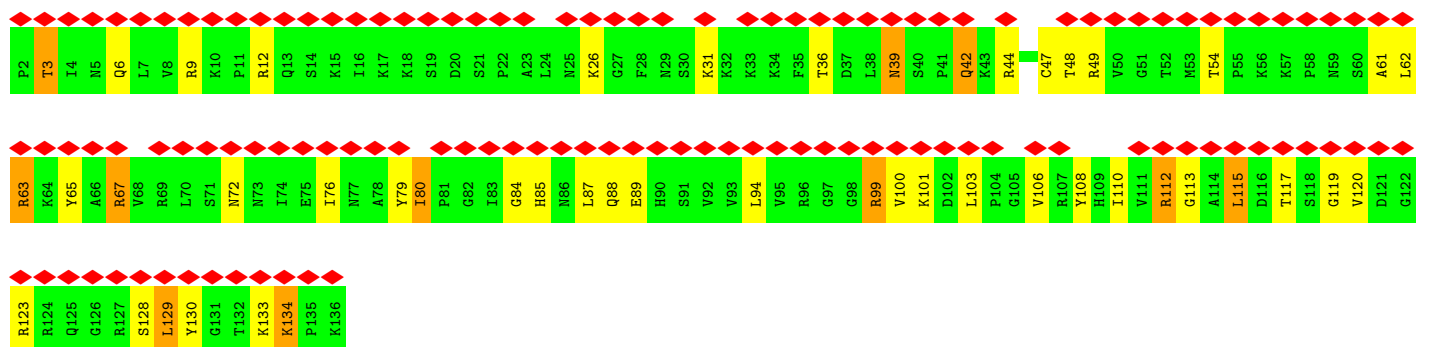
• Molecule 40: 30S ribosomal protein S10



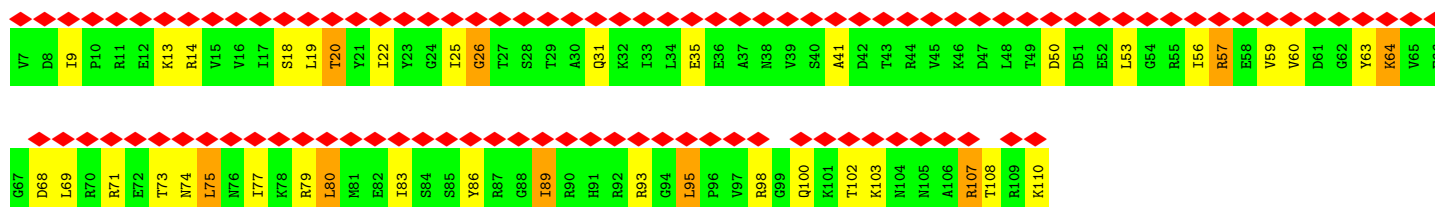
• Molecule 41: 30S ribosomal protein S11



• Molecule 42: 30S ribosomal protein S12



• Molecule 43: 30S ribosomal protein S13



• Molecule 44: 30S ribosomal protein S14 type Z

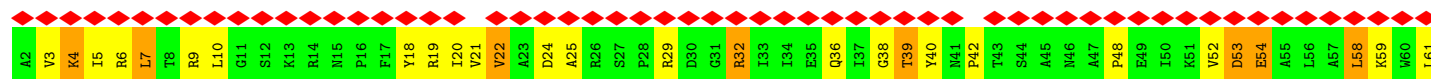
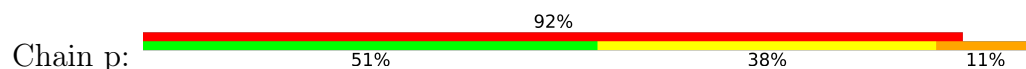


• Molecule 45: 30S ribosomal protein S15

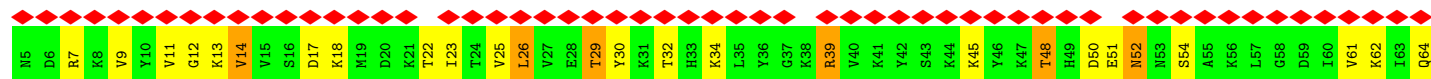
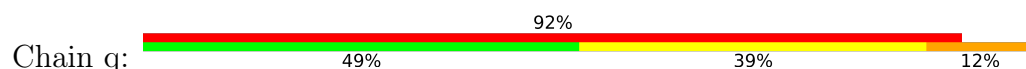




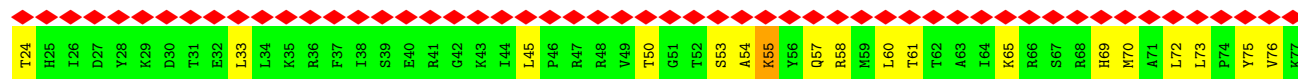
• Molecule 46: 30S ribosomal protein S16



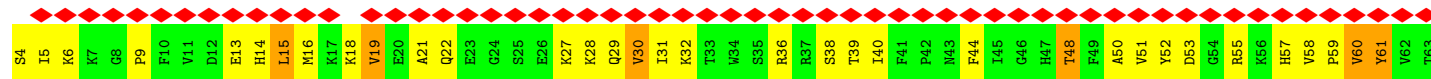
• Molecule 47: 30S ribosomal protein S17



• Molecule 48: 30S ribosomal protein S18

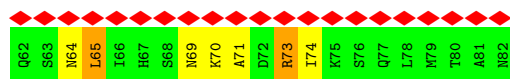


• Molecule 49: 30S ribosomal protein S19

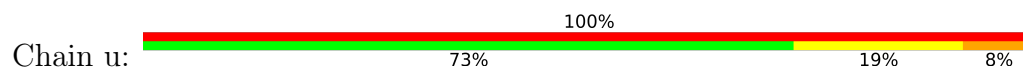


• Molecule 50: 30S ribosomal protein S20

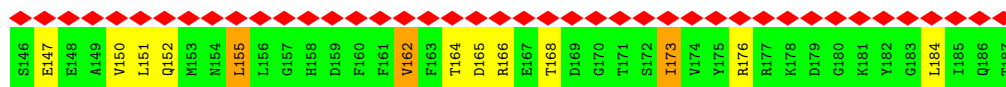
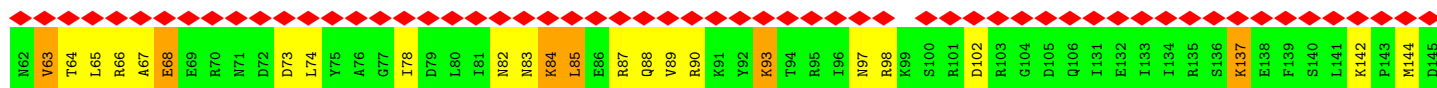




- Molecule 51: 30S ribosomal protein S21



- Molecule 52: Ribosome hibernation promoting factor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	378309	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.076	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.320	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	426.80002, 426.80002, 426.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ERY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.45	258/69740 (0.4%)	1.25	862/108755 (0.8%)
2	B	0.78	0/2733	0.66	1/4257 (0.0%)
3	C	1.17	0/2125	0.88	0/2853
4	D	1.19	0/1651	0.97	1/2215 (0.0%)
5	E	1.15	0/1595	0.98	2/2154 (0.1%)
6	F	0.36	0/1329	0.68	1/1791 (0.1%)
7	G	0.35	0/1266	0.56	0/1717
8	H	1.18	1/1171 (0.1%)	0.98	4/1577 (0.3%)
9	I	1.16	1/925 (0.1%)	0.98	3/1242 (0.2%)
10	J	1.11	0/1100	0.91	0/1467
11	K	1.02	1/1103 (0.1%)	0.78	0/1481
12	L	1.13	0/936	0.85	0/1253
13	M	0.64	0/892	0.71	0/1195
14	N	1.14	0/901	0.81	0/1209
15	O	1.30	0/955	0.93	0/1265
16	P	1.19	0/800	1.02	5/1070 (0.5%)
17	Q	1.11	0/846	0.89	0/1140
18	R	0.97	0/723	0.84	0/966
19	S	0.82	0/779	0.88	1/1043 (0.1%)
20	T	0.75	0/730	0.74	0/981
21	U	1.20	0/593	0.89	0/788
22	V	0.99	0/384	0.81	0/515
23	W	0.79	0/542	0.85	0/722
24	X	1.21	1/451 (0.2%)	0.90	0/606
25	Y	0.29	0/378	0.59	0/521
26	Z	1.12	0/366	0.96	0/489
27	1	0.45	0/395	0.55	0/530
28	2	1.35	0/371	1.00	0/484
29	3	1.12	0/526	0.85	0/690
30	4	0.72	0/298	0.73	0/392
31	a	0.30	0/36913	0.54	6/57564 (0.0%)
32	b	0.23	0/1846	0.59	2/2477 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.23	0/1523	0.60	0/2062
34	d	0.25	0/1526	0.67	1/2063 (0.0%)
35	e	0.25	0/1159	0.60	0/1566
36	f	0.26	0/789	0.65	0/1060
37	g	0.51	4/1176 (0.3%)	0.67	4/1588 (0.3%)
38	h	0.23	0/1038	0.56	0/1395
39	i	0.25	0/937	0.65	0/1269
40	j	0.23	0/764	0.60	0/1034
41	k	0.29	0/824	0.69	1/1119 (0.1%)
42	l	0.27	0/1054	0.57	0/1415
43	m	0.24	0/732	0.67	0/991
44	n	0.30	0/497	0.64	0/662
45	o	0.23	0/732	0.60	0/979
46	p	0.23	0/705	0.59	0/952
47	q	0.25	0/629	0.58	0/849
48	r	0.23	0/452	0.61	0/604
49	s	0.29	0/654	0.66	0/879
50	t	0.22	0/591	0.52	0/793
51	u	0.22	0/403	0.56	0/535
52	v	0.21	0/1350	0.56	0/1812
All	All	1.08	266/152898 (0.2%)	0.98	894/229036 (0.4%)

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	A	3	15
5	E	0	3
9	I	0	1
11	K	0	1
13	M	0	1
16	P	0	2
19	S	0	1
23	W	0	1
26	Z	0	1
29	3	0	1
43	m	0	1
49	s	0	3
All	All	3	31

The worst 5 of 266 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	G	C1'-N9	77.54	2.64	1.48
1	A	332	A	N9-C8	58.30	2.54	1.37
1	A	332	A	N7-C5	57.70	2.54	1.39
1	A	332	A	C8-N7	55.93	2.43	1.31
1	A	332	A	N9-C4	54.45	2.46	1.37

The worst 5 of 894 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	G	C8-N9-C4	-22.05	40.24	106.40
1	A	393	G	C5-N7-C8	-16.87	53.69	104.30
1	A	990	G	C5'-C4'-O4'	15.37	132.85	109.80
1	A	644	C	O4'-C1'-N1	12.94	127.91	108.50
1	A	393	G	N9-C1'-C2'	12.30	130.45	112.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	990	G	C4'
1	A	1289	A	C1'
1	A	2077	C	C1'

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	C	Sidechain
1	A	557	G	Sidechain
1	A	627	C	Sidechain
1	A	644	C	Sidechain
1	A	648	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	A	62277	0	30925	1220	0
2	B	2445	0	1240	16	0
3	C	2090	0	2201	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1627	0	1667	24	0
5	E	1572	0	1619	19	0
6	F	1315	0	1338	35	0
7	G	1248	0	1205	28	0
8	H	1149	0	1144	11	0
9	I	918	0	981	11	0
10	J	1086	0	1125	18	0
11	K	1079	0	1137	11	0
12	L	932	0	983	7	0
13	M	883	0	913	20	0
14	N	889	0	937	9	0
15	O	943	0	1014	23	0
16	P	790	0	830	13	0
17	Q	838	0	896	8	0
18	R	715	0	748	8	0
19	S	770	0	809	10	0
20	T	722	0	766	7	0
21	U	587	0	600	12	0
22	V	379	0	400	9	0
23	W	541	0	563	10	0
24	X	449	0	490	4	0
25	Y	370	0	243	9	0
26	Z	360	0	358	5	0
27	1	390	0	394	8	0
28	2	367	0	415	1	0
29	3	521	0	586	4	0
30	4	295	0	340	4	0
31	a	32969	0	16595	703	0
32	b	1819	0	1886	71	0
33	c	1501	0	1464	35	0
34	d	1497	0	1449	49	0
35	e	1145	0	1202	37	0
36	f	778	0	775	23	0
37	g	1161	0	1165	38	0
38	h	1026	0	1078	25	0
39	i	922	0	890	36	0
40	j	752	0	775	30	0
41	k	810	0	784	35	0
42	l	1037	0	1091	32	0
43	m	727	0	674	23	0
44	n	487	0	492	15	0
45	o	723	0	752	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	p	694	0	709	36	0
47	q	621	0	615	29	0
48	r	445	0	482	8	0
49	s	636	0	626	27	0
50	t	591	0	616	25	0
51	u	400	0	407	9	0
52	v	1333	0	1349	38	0
53	A	51	0	66	4	0
All	All	140672	0	92809	2714	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 13.

The worst 5 of 2714 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:G:N2	1:A:599:A:H8	1.18	1.39
1:A:1055:A:C6	1:A:1194:U:O4	1.77	1.37
1:A:272:C:O2	1:A:416:G:N2	1.59	1.34
1:A:583:A:N7	1:A:598:G:N2	1.75	1.31
1:A:1078:G:N2	1:A:1165:C:O2	1.63	1.31

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	
3	C	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	30	42
4	D	213/215 (99%)	194 (91%)	19 (9%)	0	100	100
5	E	204/206 (99%)	187 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	171/173 (99%)	142 (83%)	29 (17%)	0	100	100
7	G	171/173 (99%)	154 (90%)	17 (10%)	0	100	100
8	H	143/145 (99%)	130 (91%)	13 (9%)	0	100	100
9	I	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	J	144/146 (99%)	134 (93%)	10 (7%)	0	100	100
11	K	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
12	L	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
13	M	116/118 (98%)	103 (89%)	13 (11%)	0	100	100
14	N	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
15	O	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
16	P	100/102 (98%)	92 (92%)	7 (7%)	1 (1%)	12	18
17	Q	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
18	R	87/89 (98%)	78 (90%)	9 (10%)	0	100	100
19	S	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	12	18
20	T	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
21	U	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
22	V	47/49 (96%)	39 (83%)	8 (17%)	0	100	100
23	W	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
24	X	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
25	Y	57/59 (97%)	44 (77%)	13 (23%)	0	100	100
26	Z	46/48 (96%)	39 (85%)	7 (15%)	0	100	100
27	1	45/47 (96%)	45 (100%)	0	0	100	100
28	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	55 (89%)	6 (10%)	1 (2%)	7	10
30	4	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
32	b	224/226 (99%)	206 (92%)	18 (8%)	0	100	100
33	c	200/202 (99%)	174 (87%)	26 (13%)	0	100	100
34	d	196/198 (99%)	166 (85%)	30 (15%)	0	100	100
35	e	154/156 (99%)	133 (86%)	21 (14%)	0	100	100
36	f	93/95 (98%)	86 (92%)	7 (8%)	0	100	100
37	g	150/152 (99%)	142 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	h	129/131 (98%)	110 (85%)	19 (15%)	0	100	100
39	i	125/127 (98%)	99 (79%)	26 (21%)	0	100	100
40	j	95/97 (98%)	79 (83%)	16 (17%)	0	100	100
41	k	112/114 (98%)	94 (84%)	18 (16%)	0	100	100
42	l	133/135 (98%)	116 (87%)	17 (13%)	0	100	100
43	m	100/104 (96%)	84 (84%)	16 (16%)	0	100	100
44	n	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
45	o	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
46	p	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
47	q	78/80 (98%)	67 (86%)	11 (14%)	0	100	100
48	r	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
49	s	78/80 (98%)	63 (81%)	15 (19%)	0	100	100
50	t	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
51	u	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
52	v	158/162 (98%)	144 (91%)	14 (9%)	0	100	100
All	All	5487/5589 (98%)	4951 (90%)	532 (10%)	4 (0%)	49	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	41	ALA
16	P	51	PRO
19	S	52	PRO
29	3	20	GLY

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	C	220/221 (100%)	184 (84%)	36 (16%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	173/173 (100%)	146 (84%)	27 (16%)	2	3
5	E	168/168 (100%)	139 (83%)	29 (17%)	2	2
6	F	141/152 (93%)	112 (79%)	29 (21%)	1	1
7	G	122/151 (81%)	102 (84%)	20 (16%)	2	2
8	H	123/123 (100%)	103 (84%)	20 (16%)	2	2
9	I	100/100 (100%)	83 (83%)	17 (17%)	2	2
10	J	109/112 (97%)	85 (78%)	24 (22%)	1	1
11	K	110/114 (96%)	94 (86%)	16 (14%)	3	3
12	L	96/101 (95%)	76 (79%)	20 (21%)	1	1
13	M	85/94 (90%)	68 (80%)	17 (20%)	1	1
14	N	93/100 (93%)	80 (86%)	13 (14%)	3	4
15	O	96/96 (100%)	86 (90%)	10 (10%)	7	10
16	P	84/86 (98%)	65 (77%)	19 (23%)	1	1
17	Q	88/90 (98%)	80 (91%)	8 (9%)	9	13
18	R	78/80 (98%)	63 (81%)	15 (19%)	1	2
19	S	81/88 (92%)	63 (78%)	18 (22%)	1	1
20	T	78/82 (95%)	66 (85%)	12 (15%)	2	3
21	U	59/60 (98%)	47 (80%)	12 (20%)	1	1
22	V	39/41 (95%)	36 (92%)	3 (8%)	12	19
23	W	58/60 (97%)	46 (79%)	12 (21%)	1	1
24	X	52/52 (100%)	39 (75%)	13 (25%)	0	1
25	Y	23/56 (41%)	20 (87%)	3 (13%)	4	5
26	Z	35/44 (80%)	26 (74%)	9 (26%)	0	0
27	1	44/45 (98%)	39 (89%)	5 (11%)	5	8
28	2	39/39 (100%)	36 (92%)	3 (8%)	12	19
29	3	55/55 (100%)	45 (82%)	10 (18%)	2	2
30	4	35/35 (100%)	29 (83%)	6 (17%)	2	2
32	b	196/196 (100%)	157 (80%)	39 (20%)	1	1
33	c	138/164 (84%)	101 (73%)	37 (27%)	0	0
34	d	147/174 (84%)	117 (80%)	30 (20%)	1	1
35	e	118/122 (97%)	93 (79%)	25 (21%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	f	80/83 (96%)	63 (79%)	17 (21%)	1	1
37	g	118/128 (92%)	96 (81%)	22 (19%)	1	2
38	h	111/112 (99%)	86 (78%)	25 (22%)	1	1
39	i	86/105 (82%)	67 (78%)	19 (22%)	1	1
40	j	81/87 (93%)	64 (79%)	17 (21%)	1	1
41	k	82/90 (91%)	65 (79%)	17 (21%)	1	1
42	l	111/117 (95%)	88 (79%)	23 (21%)	1	1
43	m	62/92 (67%)	41 (66%)	21 (34%)	0	0
44	n	48/52 (92%)	33 (69%)	15 (31%)	0	0
45	o	77/80 (96%)	55 (71%)	22 (29%)	0	0
46	p	73/75 (97%)	57 (78%)	16 (22%)	1	1
47	q	65/75 (87%)	49 (75%)	16 (25%)	1	1
48	r	48/49 (98%)	38 (79%)	10 (21%)	1	1
49	s	67/70 (96%)	52 (78%)	15 (22%)	1	1
50	t	61/67 (91%)	52 (85%)	9 (15%)	3	3
51	u	40/48 (83%)	32 (80%)	8 (20%)	1	1
52	v	147/147 (100%)	103 (70%)	44 (30%)	0	0
All	All	4440/4751 (94%)	3567 (80%)	873 (20%)	3	1

5 of 873 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	b	221	ILE
36	f	93	ARG
49	s	19	VAL
33	c	94	THR
32	b	213	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
34	d	118	HIS
39	i	62	ASN
34	d	166	ASN
37	g	18	HIS

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Mol	Chain	Res	Type
41	k	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2899/2905 (99%)	1357 (46%)	256 (8%)
2	B	114/115 (99%)	33 (28%)	2 (1%)
31	a	1537/1539 (99%)	710 (46%)	0
All	All	4550/4559 (99%)	2100 (46%)	258 (5%)

5 of 2100 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	A
1	A	12	U
1	A	13	A
1	A	14	A

5 of 258 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2578	C
1	A	2665	G
1	A	858	U
1	A	809	A
1	A	2760	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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
53	ERY	A	3001	-	53,53,53	2.25	12 (22%)	82,82,82	5.03	38 (46%)

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
53	ERY	A	3001	-	3/3/21/21	30/72/107/107	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	3001	ERY	O2-C1	10.24	1.57	1.34
53	A	3001	ERY	O10-C6	-5.14	1.36	1.44
53	A	3001	ERY	O2-C13	-4.44	1.39	1.46
53	A	3001	ERY	C19-C16	3.94	1.60	1.52
53	A	3001	ERY	C10-C11	-3.77	1.49	1.54

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	3001	ERY	O5-C16-C15	-19.27	83.30	112.95
53	A	3001	ERY	O13-C12-C13	-15.29	83.86	107.24
53	A	3001	ERY	O10-C6-C32	-14.33	75.32	108.48
53	A	3001	ERY	O13-C12-C11	-12.96	83.82	108.88
53	A	3001	ERY	O13-C12-C35	-12.83	81.67	107.84

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	A	3001	ERY	C6
53	A	3001	ERY	C12
53	A	3001	ERY	C14

5 of 30 torsion outliers are listed below:

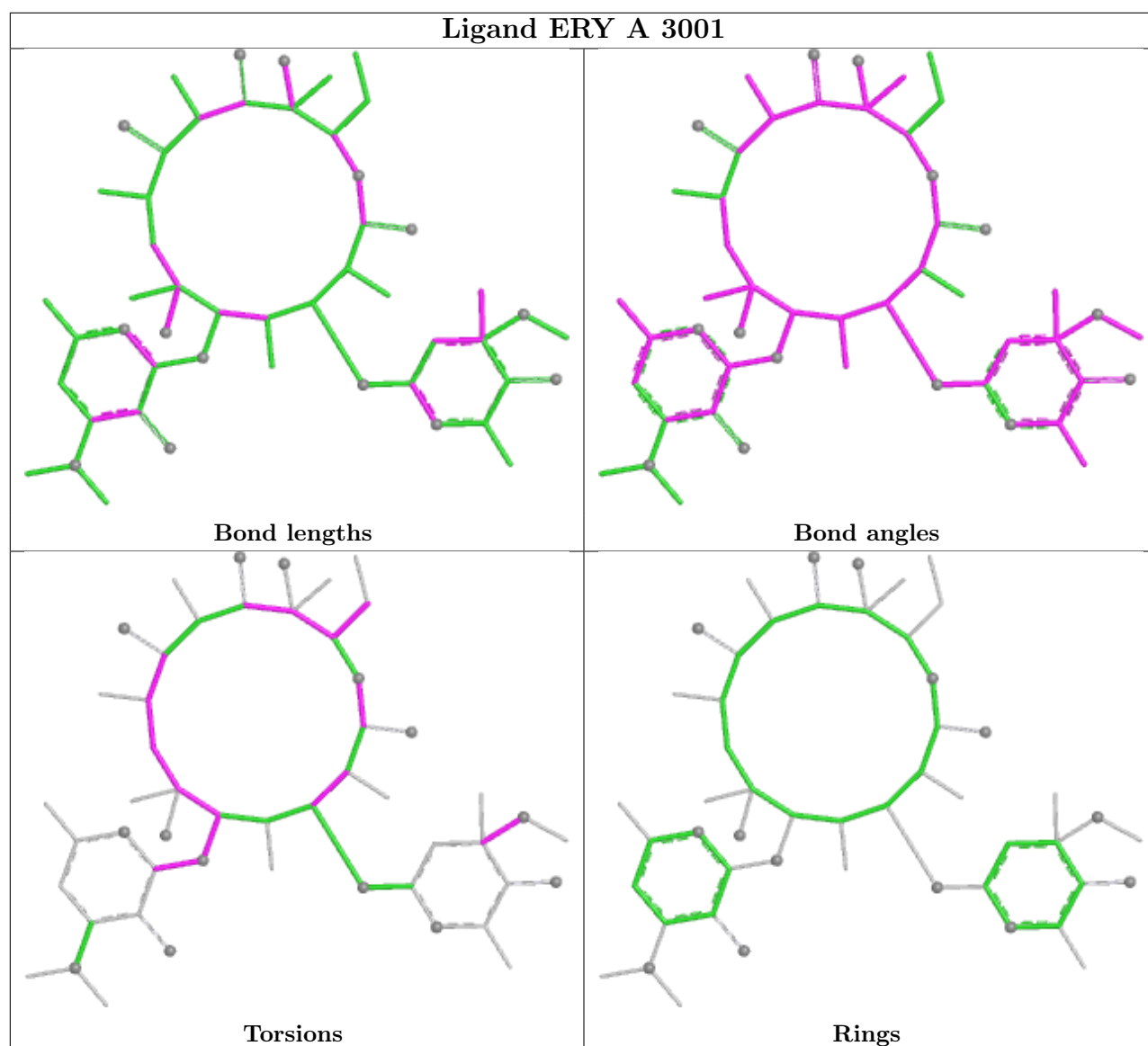
Mol	Chain	Res	Type	Atoms
53	A	3001	ERY	C10-C11-C12-C13
53	A	3001	ERY	C10-C11-C12-C35
53	A	3001	ERY	C10-C11-C12-O13
53	A	3001	ERY	O12-C11-C12-C13
53	A	3001	ERY	O12-C11-C12-C35

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	A	3001	ERY	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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
1	A	7
52	v	1
31	a	1
43	m	1

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Mol	Chain	Number of breaks
8	H	1
24	X	1
11	K	1

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	106:GLN	C	131:ILE	N	27.31
1	A	2207:U	O3'	2208:A	P	12.57
1	A	1939:A	O3'	1944:U	P	12.49
1	A	929:C	O3'	937:G	P	11.52
1	a	465:U	O3'	466:G	P	9.63

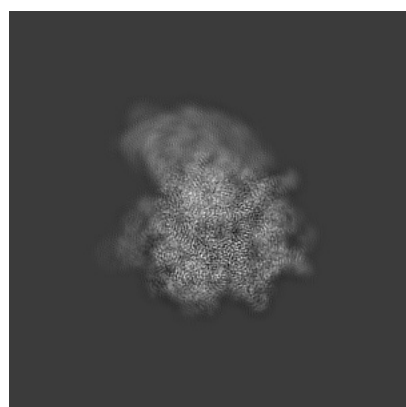
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10076. These allow visual inspection of the internal detail of the map and identification of artifacts.

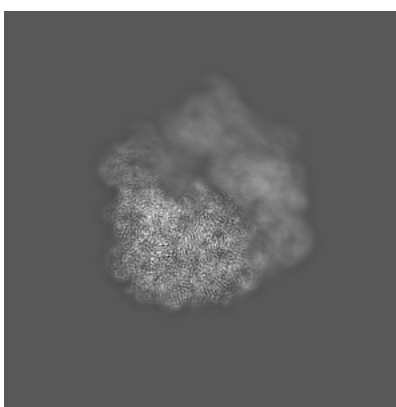
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

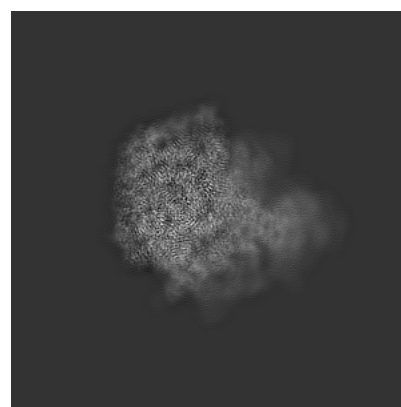
6.1.1 Primary map



X



Y

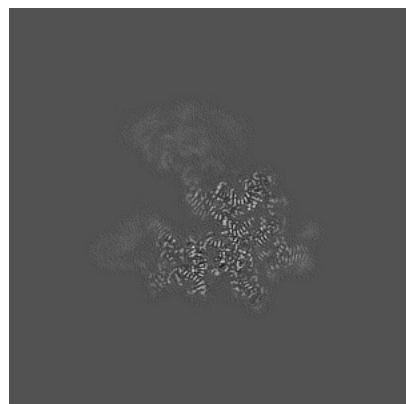


Z

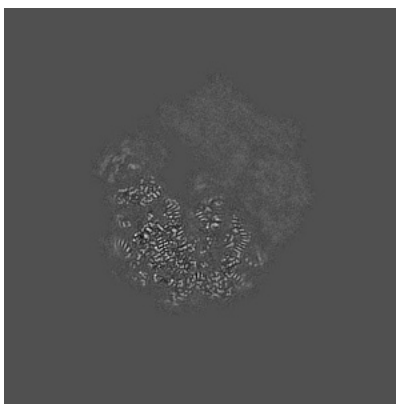
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

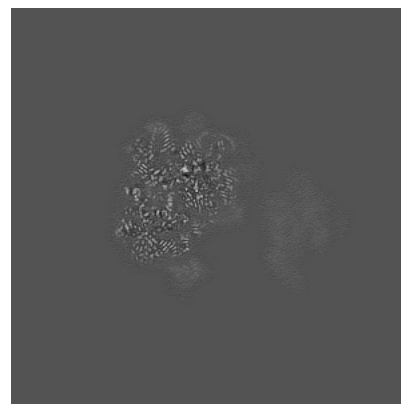
6.2.1 Primary map



X Index: 200



Y Index: 200

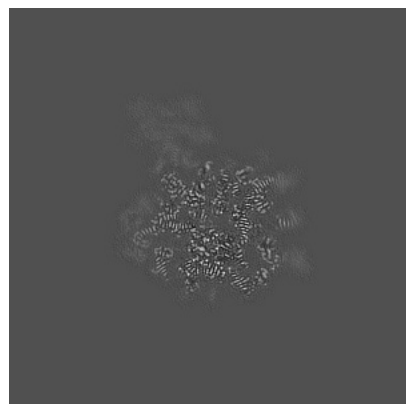


Z Index: 200

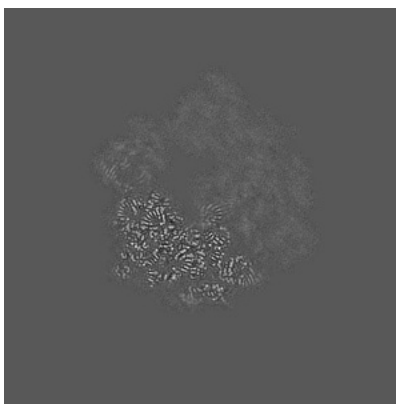
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

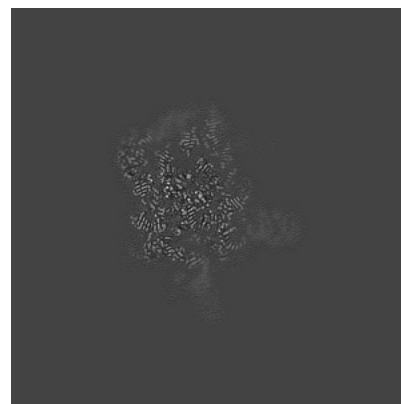
6.3.1 Primary map



X Index: 171



Y Index: 185

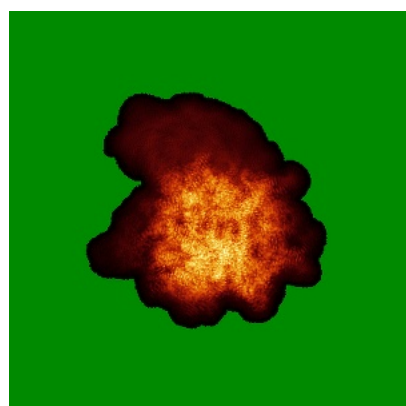


Z Index: 147

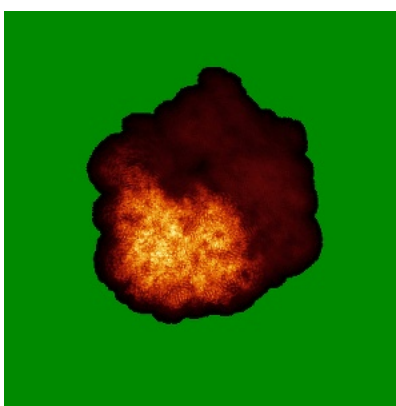
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

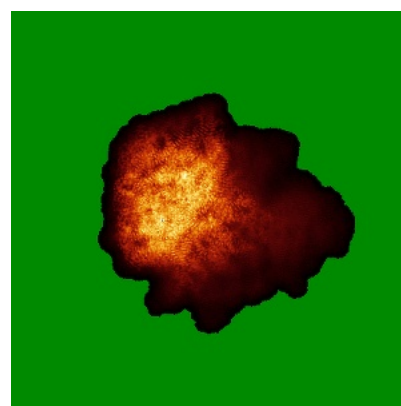
6.4.1 Primary map



X



Y

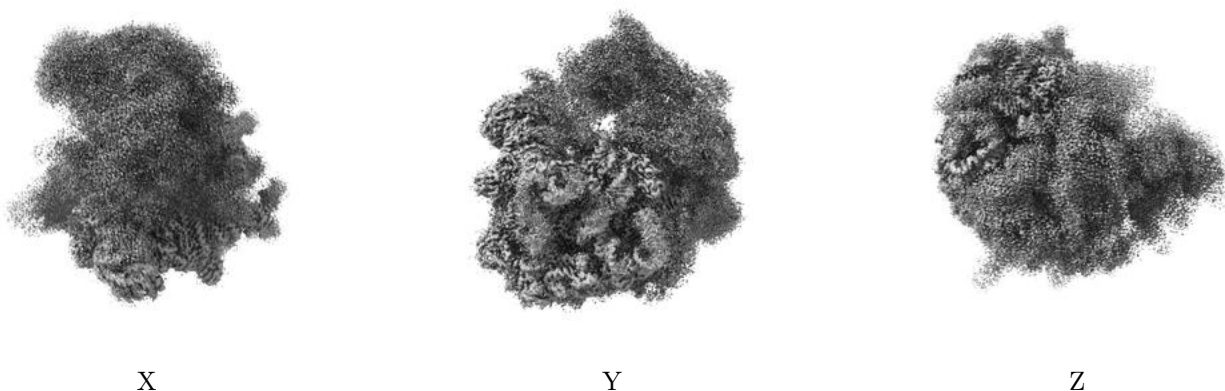


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

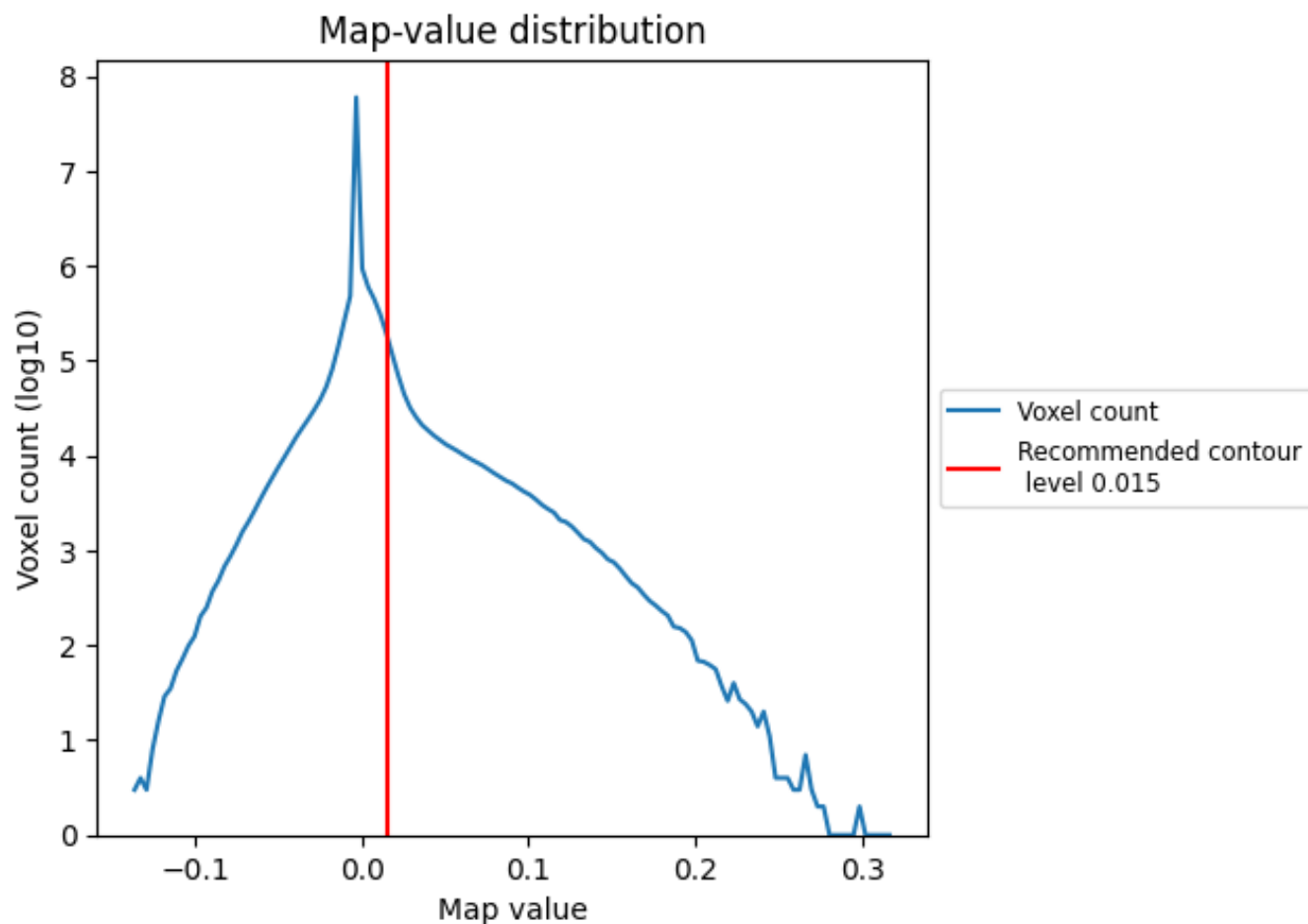
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

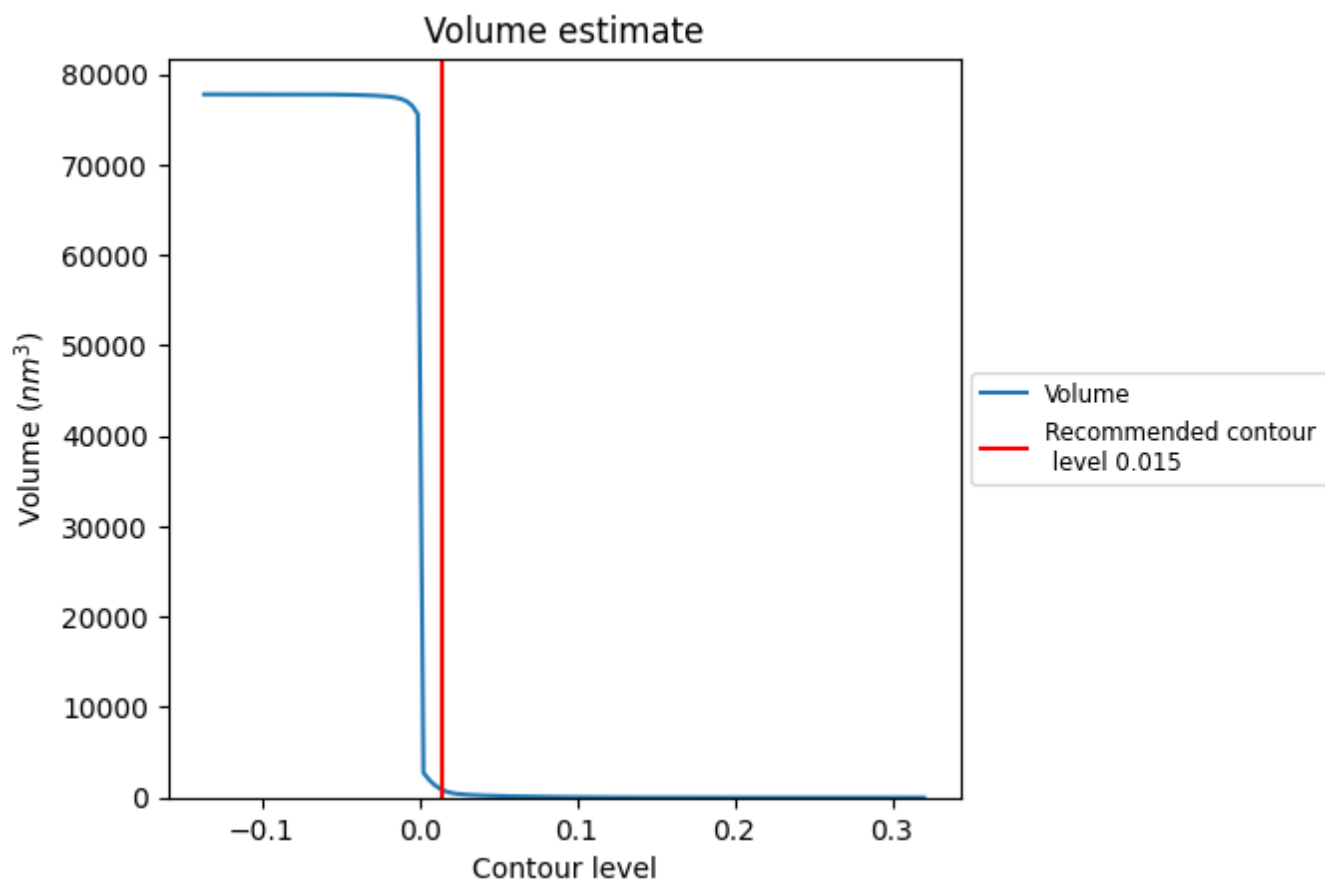
This section contains the results of statistical analysis of the map.

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.

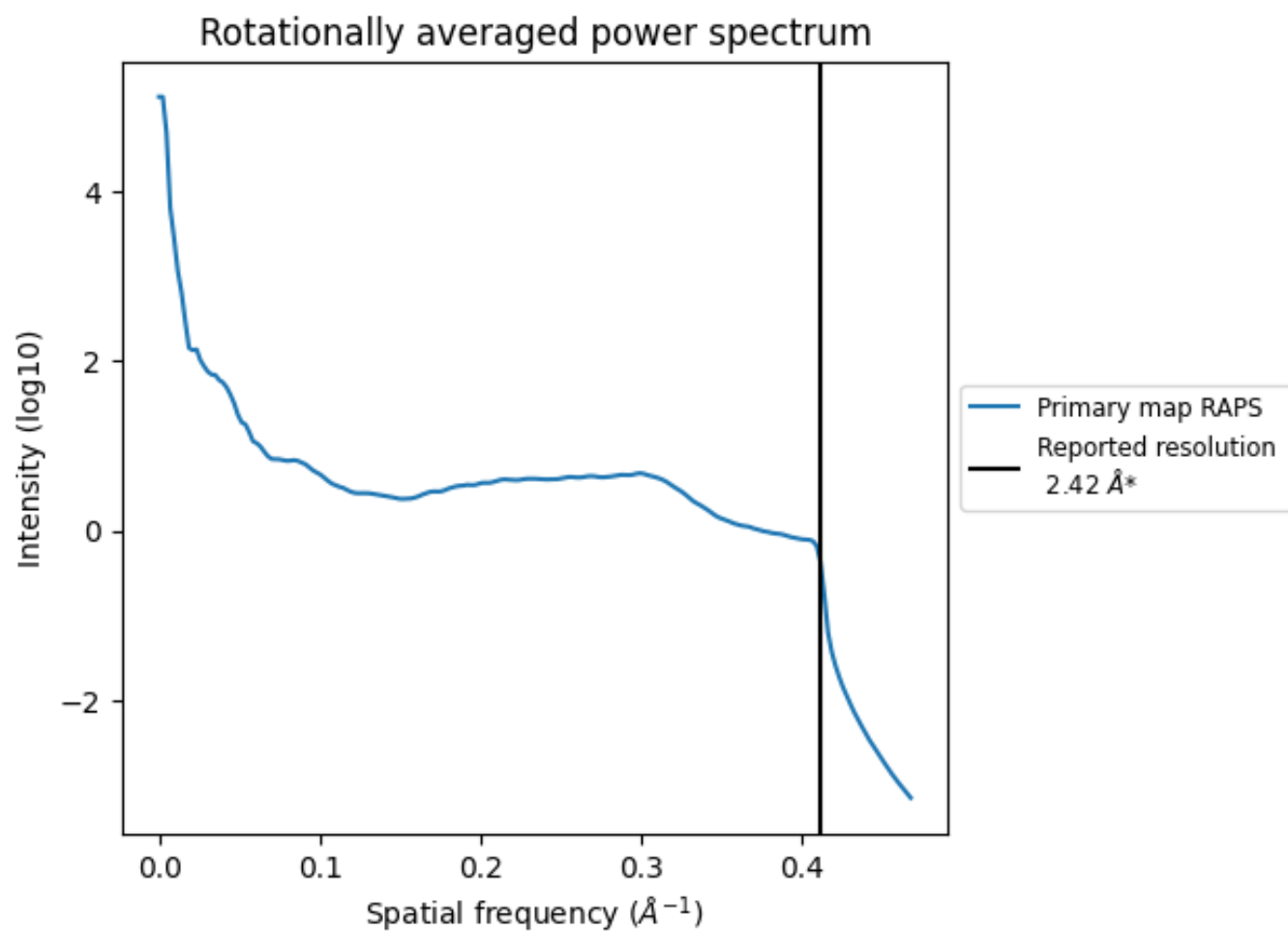
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 827 nm^3 ; this corresponds to an approximate mass of 747 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 0.412 Å⁻¹

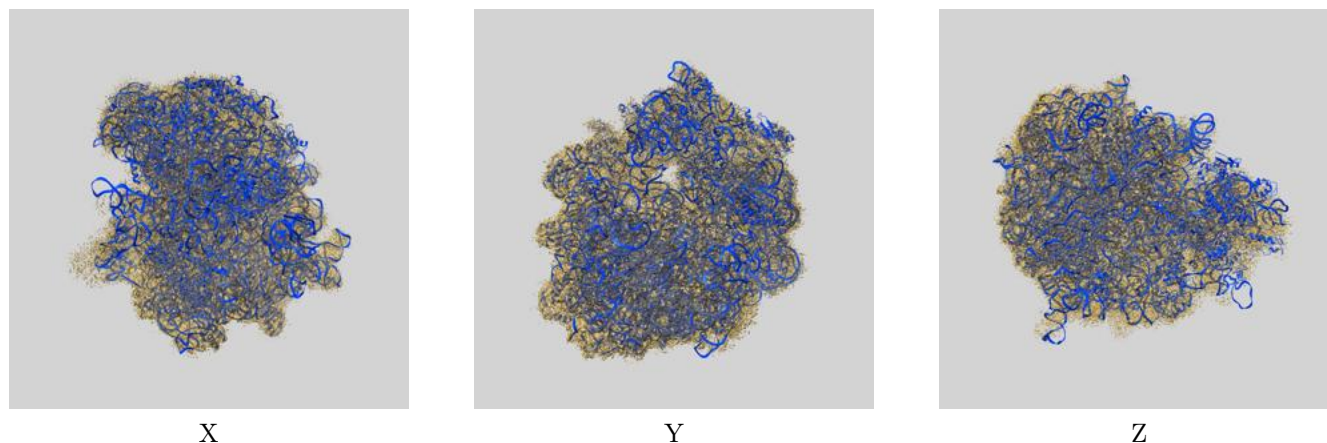
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

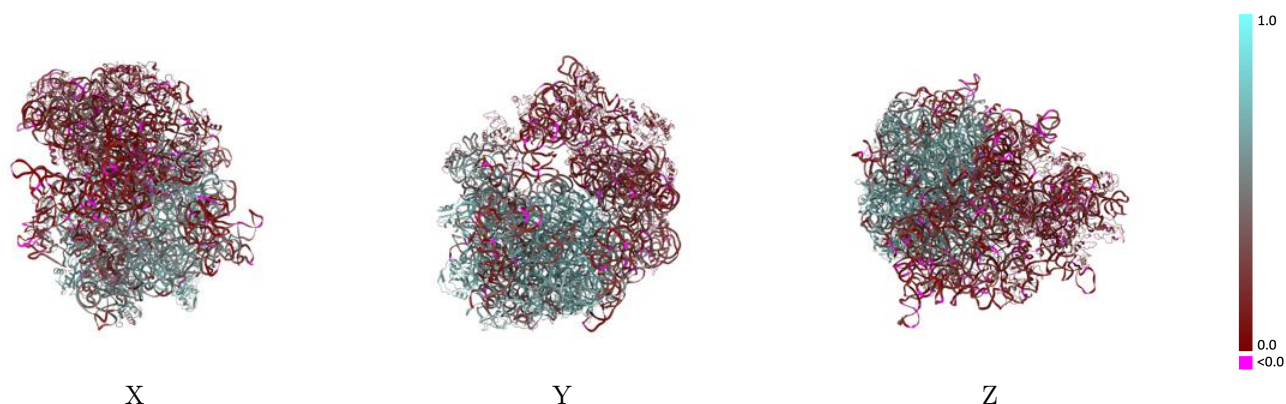
This section contains information regarding the fit between EMDB map EMD-10076 and PDB model 6S0X. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



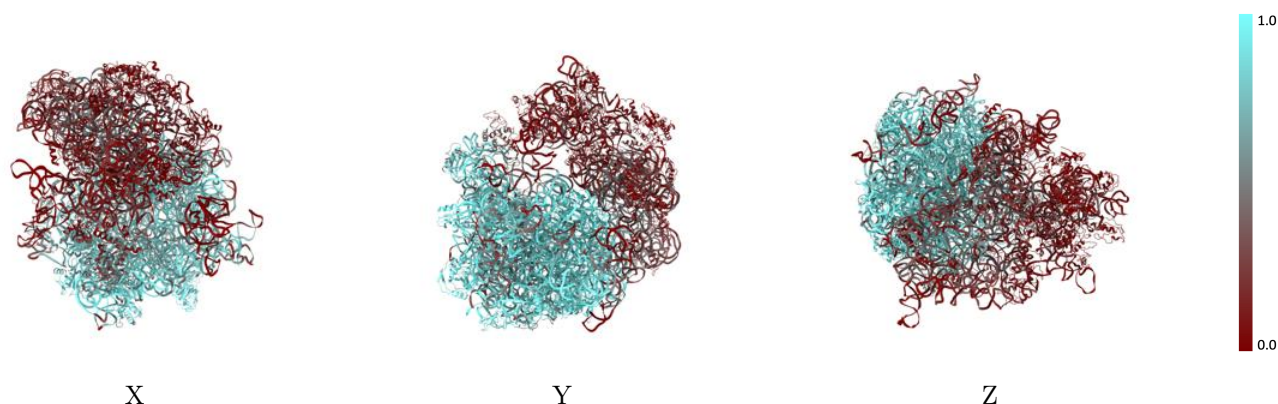
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



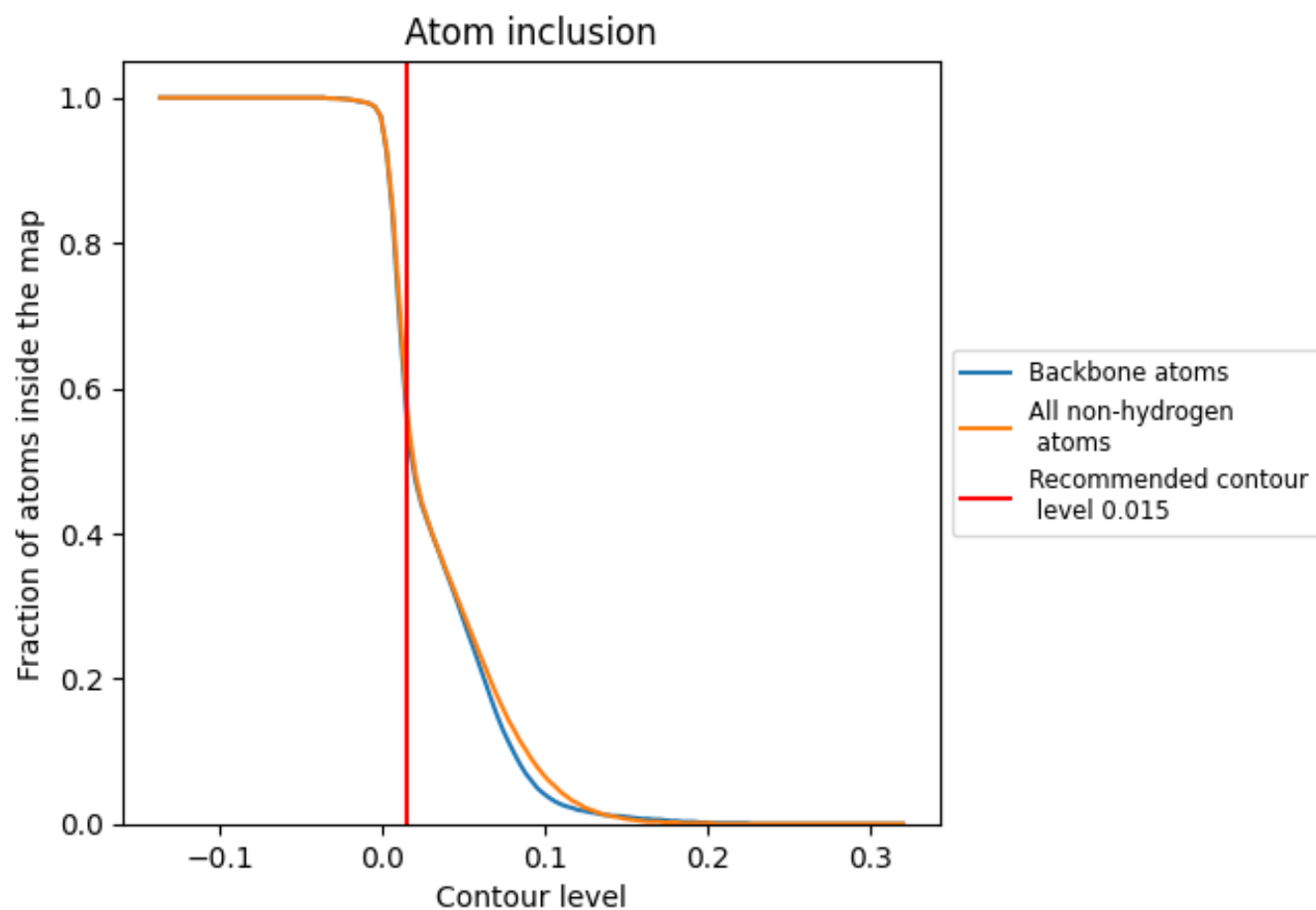
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 58% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5780	 0.3950
1	 0.6110	 0.5660
2	 0.9770	 0.7030
3	 0.9480	 0.6780
4	 0.8860	 0.6120
A	 0.7700	 0.4870
B	 0.8920	 0.5200
C	 0.9590	 0.6800
D	 0.9600	 0.6750
E	 0.9360	 0.6600
F	 0.3570	 0.2880
G	 0.5070	 0.4070
H	 0.9540	 0.6750
I	 0.9510	 0.6720
J	 0.9400	 0.6480
K	 0.9530	 0.6590
L	 0.9500	 0.6770
M	 0.7990	 0.5230
N	 0.9410	 0.6600
O	 0.9730	 0.6950
P	 0.9550	 0.6720
Q	 0.9110	 0.6470
R	 0.9100	 0.6290
S	 0.8170	 0.5610
T	 0.8420	 0.5900
U	 0.9530	 0.6660
V	 0.8880	 0.6150
W	 0.8340	 0.5500
X	 0.9460	 0.6750
Y	 0.1550	 0.2060
Z	 0.7230	 0.5340
a	 0.2680	 0.1630
b	 0.0630	 0.2110
c	 0.0760	 0.2020
d	 0.1300	 0.2350



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Chain	Atom inclusion	Q-score
e	 0.0970	 0.2040
f	 0.0780	 0.2010
g	 0.0390	 0.1850
h	 0.1500	 0.2220
i	 0.0530	 0.1810
j	 0.0980	 0.2040
k	 0.1200	 0.2060
l	 0.1700	 0.2810
m	 0.0920	 0.1990
n	 0.1240	 0.2100
o	 0.1210	 0.2160
p	 0.1990	 0.2480
q	 0.1880	 0.2290
r	 0.1380	 0.2430
s	 0.1150	 0.1900
t	 0.1290	 0.2400
u	 0.0540	 0.2300
v	 0.0240	 0.1830