



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:21 PM UTC

PDB ID : 8QCQ / pdb_00008qcq
EMDB ID : EMD-18332
Title : B. subtilis ApdA-stalled ribosomal complex
Authors : Morici, M.; Wilson, D.N.
Deposited on : 2023-08-28
Resolution : 2.30 Å(reported)

This is a Full wwPDB EM Validation 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
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

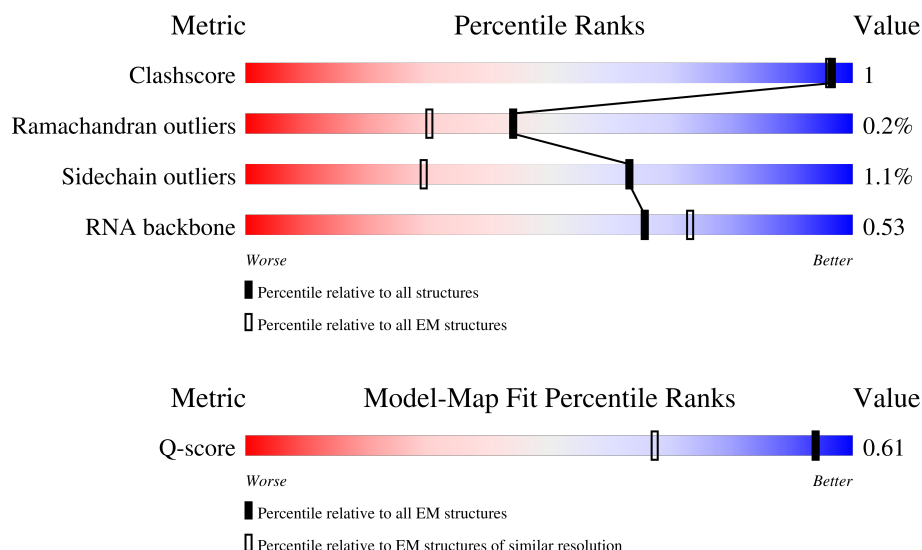
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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	0	59	17% 86% 7% 7%
2	1	49	80% 98% .
3	2	44	5% 98% .

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Mol	Chain	Length	Quality of chain
4	3	66	
5	4	37	
6	6	65	
7	A	2925	
8	B	119	
9	C	277	
10	D	209	
11	E	207	
12	F	179	
13	G	179	
14	J	145	
15	K	122	
16	L	146	
17	M	144	
18	N	120	
19	O	120	
20	P	115	
21	Q	119	
22	R	102	
23	S	113	
24	T	95	
25	U	103	
26	W	94	
27	X	62	
28	Y	66	

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Mol	Chain	Length	Quality of chain
29	Z	59	
30	a	1554	
31	e	166	
32	k	131	
33	l	138	
34	o	89	
35	q	87	
36	t	88	
37	w	77	
37	y	77	
38	8	6	
39	c	206	
40	g	156	
41	i	130	
42	j	102	
43	m	121	
44	n	61	
45	s	92	
46	h	132	
47	r	79	
48	f	95	
49	7	9	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 136664 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 protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	55	Total	C	N	O	S	0	0
			433	267	87	72	7		

- Molecule 2 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			403	245	81	74	3		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	65	Total	C	N	O	S	0	0
			522	327	109	84	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 6 is a protein called Large ribosomal subunit protein bL31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			356	222	63	66	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	?	-	GLN	deletion	UNP Q03223

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	2745	Total	C	N	O	P	0	0
			58964	26308	10911	19002	2743		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	273	Total	C	N	O	S	0	0
			2094	1302	412	374	6		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	207	Total	C	N	O	S	0	0
			1575	988	290	292	5		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	206	Total	C	N	O	S	0	0
			1567	983	290	292	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	178	Total	C	N	O	S	0	0
			1405	893	245	260	7		

- Molecule 13 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	144	Total	C	N	O	S	0	0
			1142	720	211	206	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	119	Total	C	N	O	S	0	0
			954	583	186	181	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	120	Total	C	N	O	S	0	0
			913	564	176	172	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	115	Total	C	N	O	S	0	0
			945	600	185	159	1		

- Molecule 21 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	118	Total	C	N	O	S	0	0
			950	597	191	158	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	102	Total	C	N	O	S	0	0
			795	506	140	148	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	110	Total	C	N	O	S	0	0
			850	530	165	151	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	89	Total	C	N	O	S	0	0
			716	447	133	133	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	102	Total	C	N	O	S	0	0
			770	482	143	141	4		

- Molecule 26 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	85	Total	C	N	O	0	0
			650	401	127	122		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	61	Total	C	N	O	S	0	0
			468	289	98	79	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	65	Total	C	N	O	S	0	0
			532	329	103	99	1		

- Molecule 29 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	58	Total	C	N	O	S	0	0
			456	281	89	85	1		

- Molecule 30 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	1533	Total	C	N	O	P	0	0
			32891	14667	6034	10657	1533		

- Molecule 31 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	158	Total	C	N	O	S	0	0
			1170	737	215	216	2		

- Molecule 32 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	115	Total	C	N	O	S	0	0
			847	520	166	159	2		

- Molecule 33 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	135	Total	C	N	O	S	0	0
			1047	650	210	185	2		

- Molecule 34 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	87	Total	C	N	O	S	0	0
			730	448	149	132	1		

- Molecule 35 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q	85	Total	C	N	O	S	0	0
			699	441	129	127	2		

- Molecule 36 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	t	86	Total	C	N	O	S	0	0
			658	402	134	121	1		

- Molecule 37 is a RNA chain called Pro-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	y	77	Total	C	N	O	P	0	0
			1645	733	293	542	77		
37	w	77	Total	C	N	O	P	0	0
			1645	733	293	542	77		

- Molecule 38 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	8	6	Total	C	N	O	P	0	0
			120	54	16	44	6		

- Molecule 39 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	204	Total	C	N	O	S	0	0
			1607	1003	302	299	3		

- Molecule 40 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1199	751	225	217	6		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	128	Total	C	N	O	S	0	0
			994	615	198	180	1		

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	98	Total	C	N	O	S	0	0
			788	497	144	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	118	Total	C	N	O	S	0	0
			942	578	194	170			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total	C	N	O	S	0	0
			498	317	98	78	5		

- Molecule 45 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	83	Total	C	N	O	S	0	0
			668	429	122	115	2		

- Molecule 46 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	h	122	Total	C	N	O	S	0	0
			958	601	181	174	2		

- Molecule 47 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	65	Total	C	N	O	S	0	0
			522	334	97	89	2		

- Molecule 48 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	f	92	Total	C	N	O	S	0	0
			755	476	132	146	1		

- Molecule 49 is a protein called ApdA nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	7	9	Total	C	N	O	0	0
			67	41	15	11		

- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
50	0	1	Total	Zn	0
			1	1	
50	1	1	Total	Zn	0
			1	1	
50	4	1	Total	Zn	0
			1	1	
50	6	1	Total	Zn	0
			1	1	
50	n	1	Total	Zn	0
			1	1	

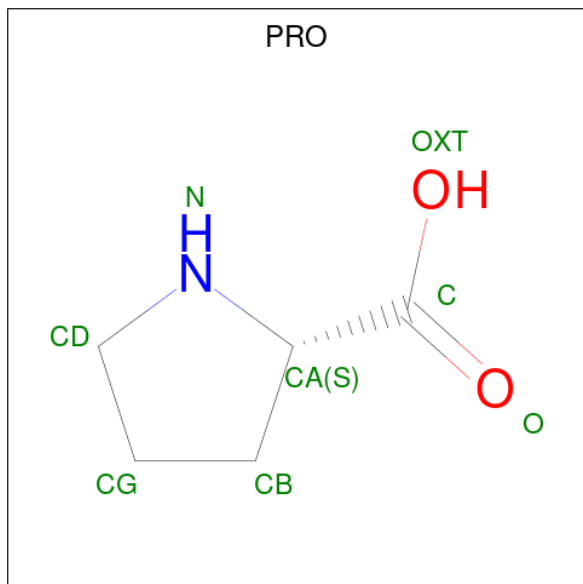
- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	A	155	Total	Mg	0
			155	155	
51	B	1	Total	Mg	0
			1	1	
51	C	1	Total	Mg	0
			1	1	
51	D	1	Total	Mg	0
			1	1	
51	a	40	Total	Mg	0
			40	40	
51	w	1	Total	Mg	0
			1	1	

- Molecule 52 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
52	A	40	Total	K	0
			40	40	
52	C	2	Total	K	0
			2	2	
52	U	1	Total	K	0
			1	1	

- Molecule 53 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				AltConf
53	y	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 54 is water.

Mol	Chain	Residues	Atoms		AltConf
54	3	3	Total	O	0
			3	3	
54	A	811	Total	O	0
			811	811	
54	B	5	Total	O	0
			5	5	
54	C	15	Total	O	0
			15	15	
54	D	1	Total	O	0
			1	1	
54	E	5	Total	O	0
			5	5	

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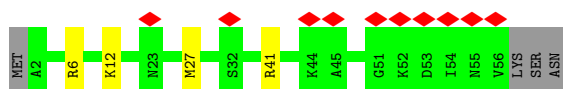
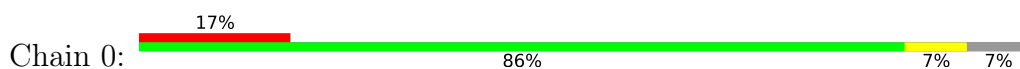
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Mol	Chain	Residues	Atoms		AltConf
54	L	5	Total 5	O 5	0
54	N	3	Total 3	O 3	0
54	P	3	Total 3	O 3	0
54	Q	3	Total 3	O 3	0
54	T	1	Total 1	O 1	0
54	a	132	Total 132	O 132	0
54	k	1	Total 1	O 1	0
54	y	3	Total 3	O 3	0
54	w	21	Total 21	O 21	0
54	i	1	Total 1	O 1	0
54	j	1	Total 1	O 1	0
54	7	8	Total 8	O 8	0

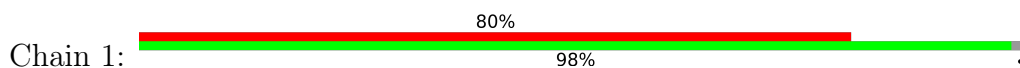
3 Residue-property plots [i](#)

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: 50S ribosomal protein L32



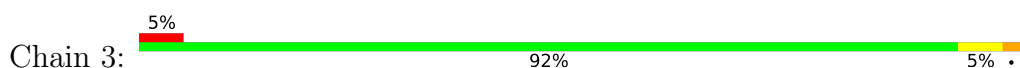
- Molecule 2: 50S ribosomal protein L33 1



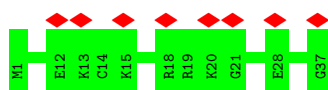
- Molecule 3: 50S ribosomal protein L34



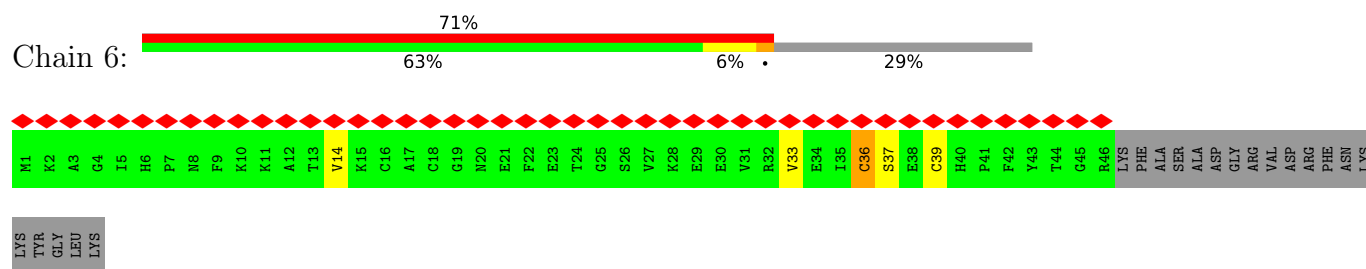
- Molecule 4: 50S ribosomal protein L35



- Molecule 5: 50S ribosomal protein L36



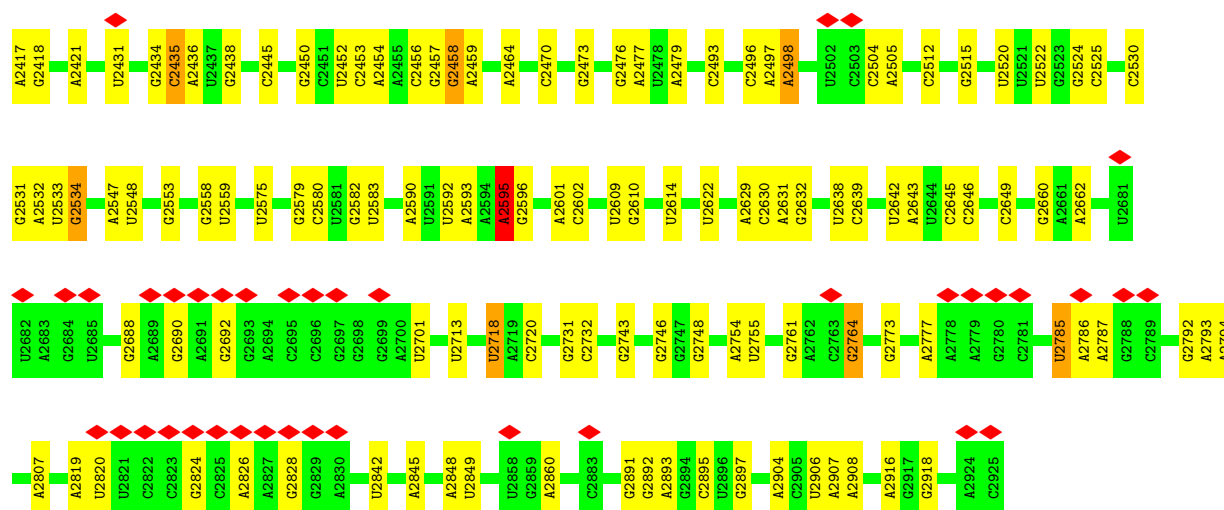
- Molecule 6: Large ribosomal subunit protein bL31-A



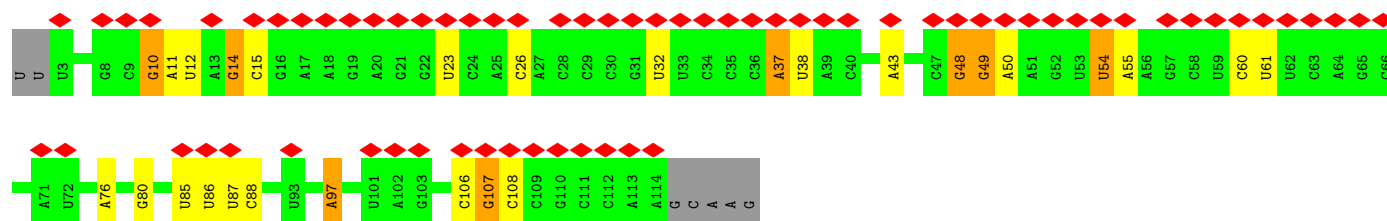
- Molecule 7: 23S rRNA



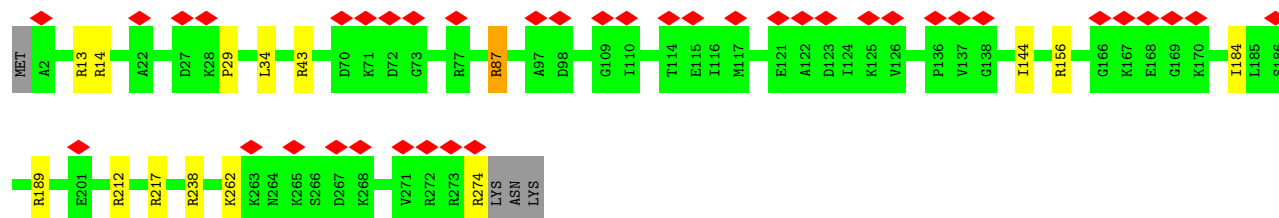




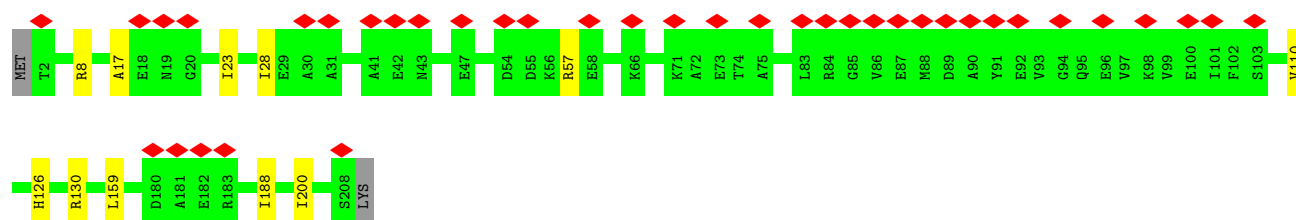
• Molecule 8: 5S rRNA



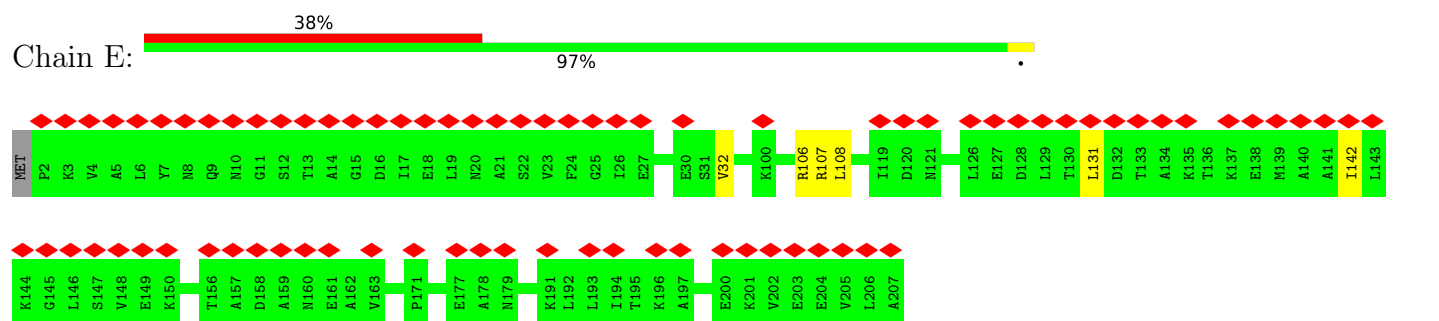
• Molecule 9: 50S ribosomal protein L2



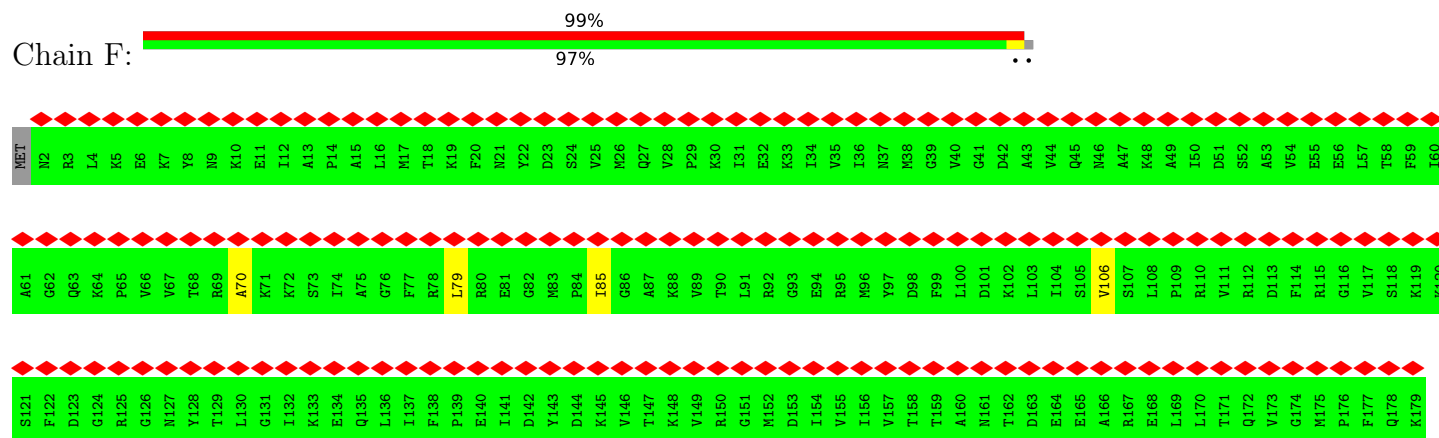
• Molecule 10: 50S ribosomal protein L3



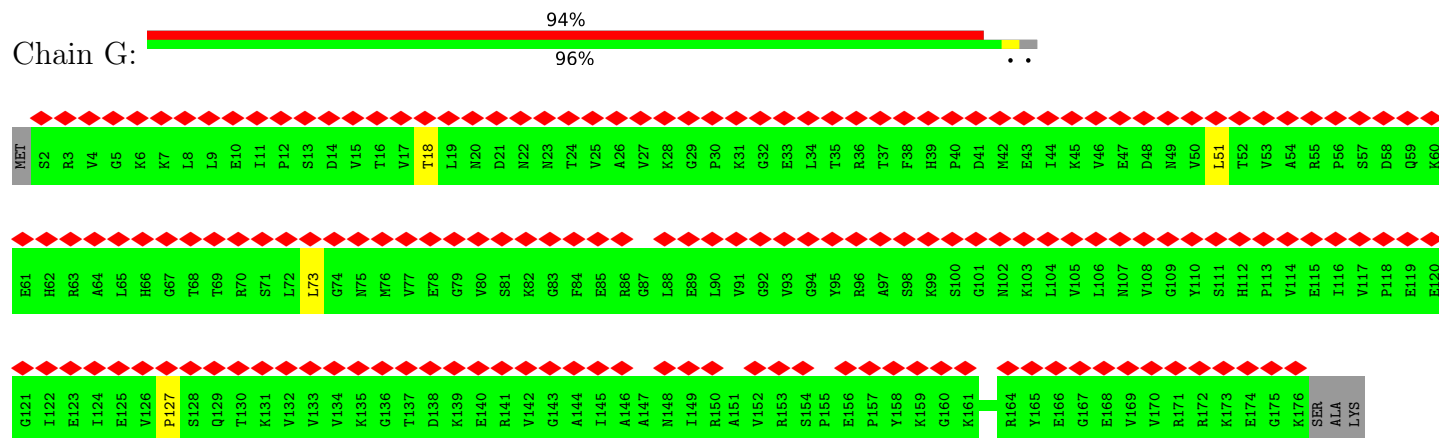
• Molecule 11: 50S ribosomal protein L4



• Molecule 12: 50S ribosomal protein L5



• Molecule 13: Large ribosomal subunit protein uL6

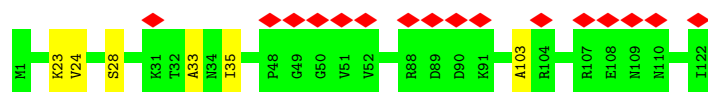


• Molecule 14: 50S ribosomal protein L13

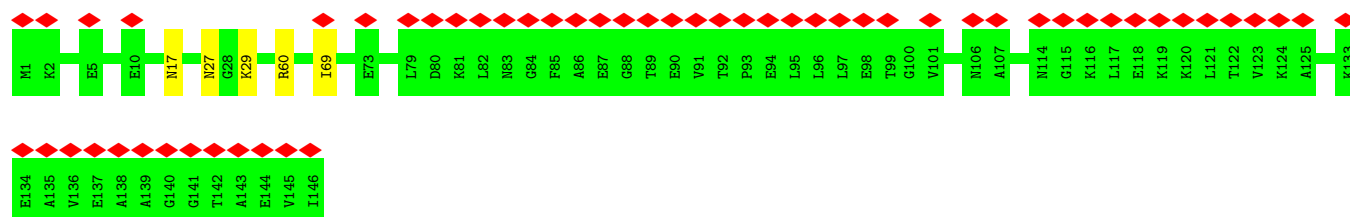
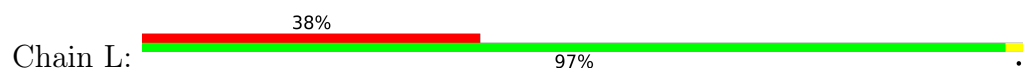


• Molecule 15: 50S ribosomal protein L14

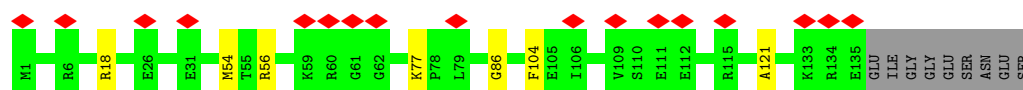
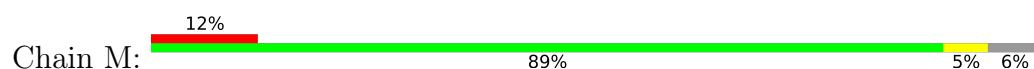




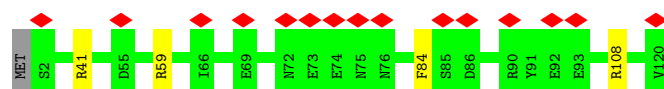
- Molecule 16: 50S ribosomal protein L15



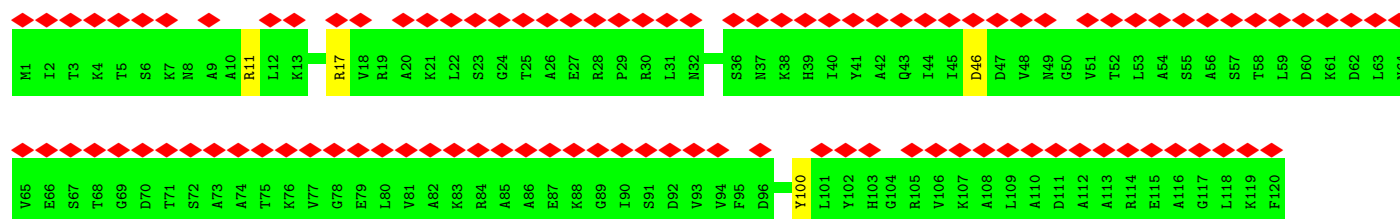
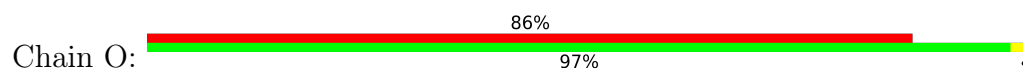
- Molecule 17: 50S ribosomal protein L16



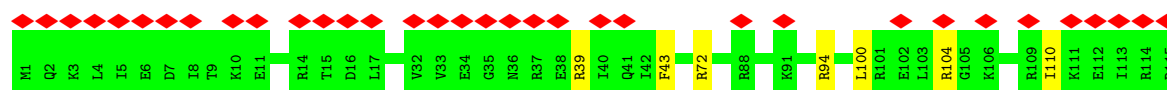
- Molecule 18: 50S ribosomal protein L17



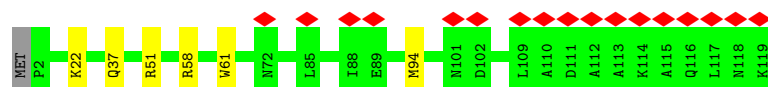
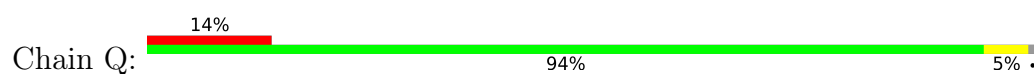
- Molecule 19: 50S ribosomal protein L18



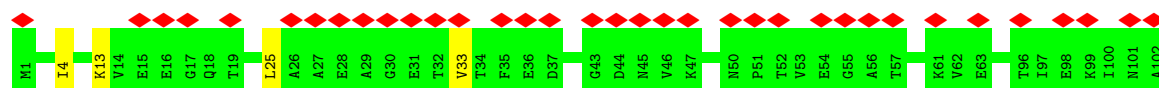
- Molecule 20: 50S ribosomal protein L19



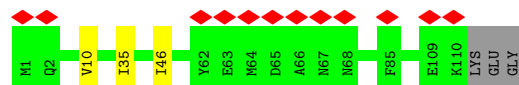
- Molecule 21: Large ribosomal subunit protein bL20



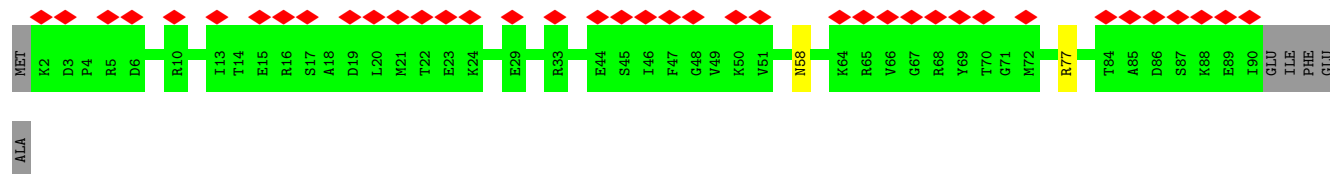
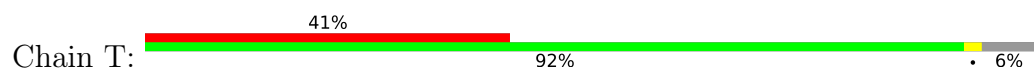
- Molecule 22: 50S ribosomal protein L21



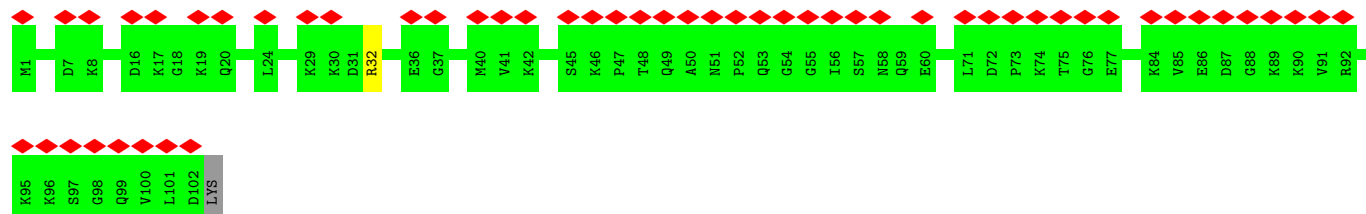
- Molecule 23: 50S ribosomal protein L22



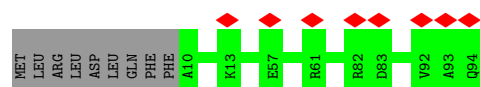
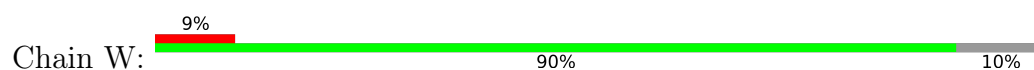
- Molecule 24: Large ribosomal subunit protein uL23



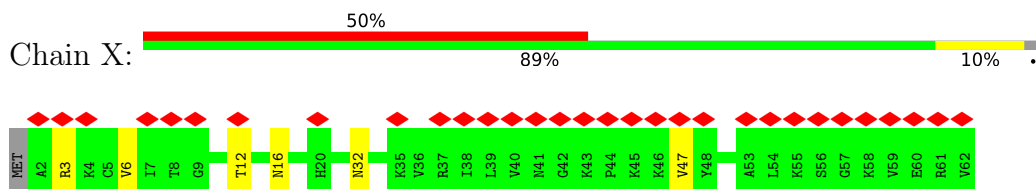
- Molecule 25: 50S ribosomal protein L24



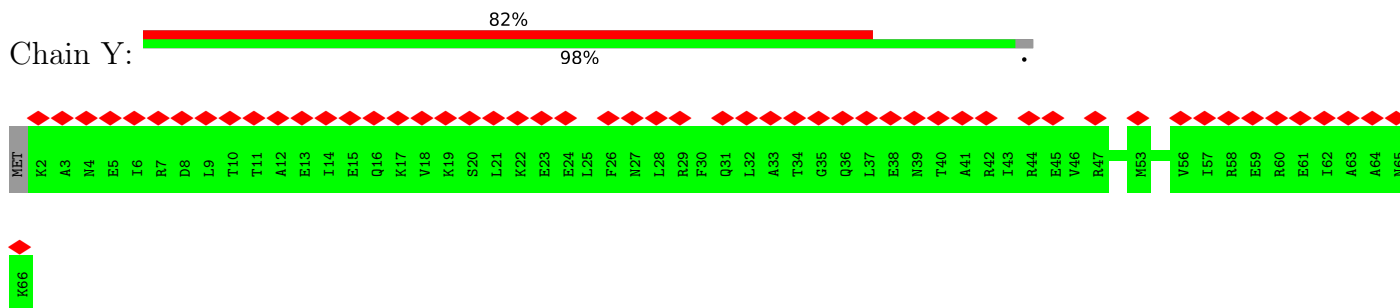
- Molecule 26: Large ribosomal subunit protein bL27



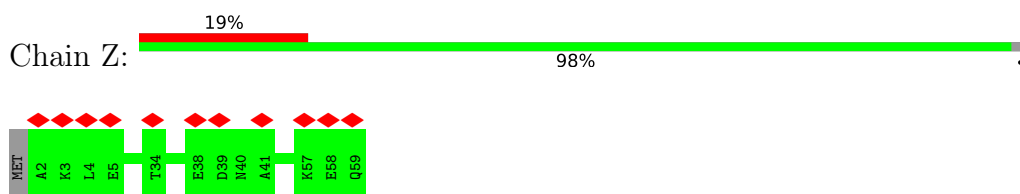
- Molecule 27: 50S ribosomal protein L28



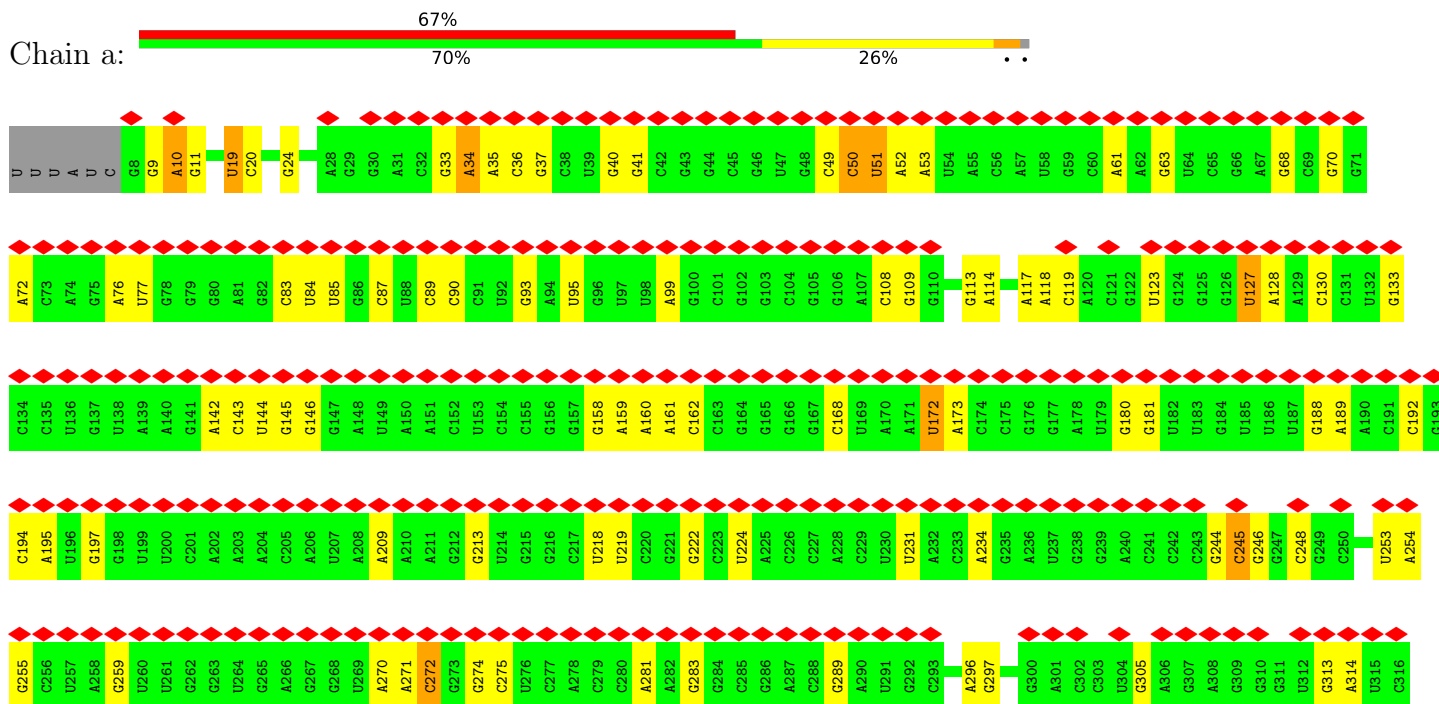
- Molecule 28: 50S ribosomal protein L29



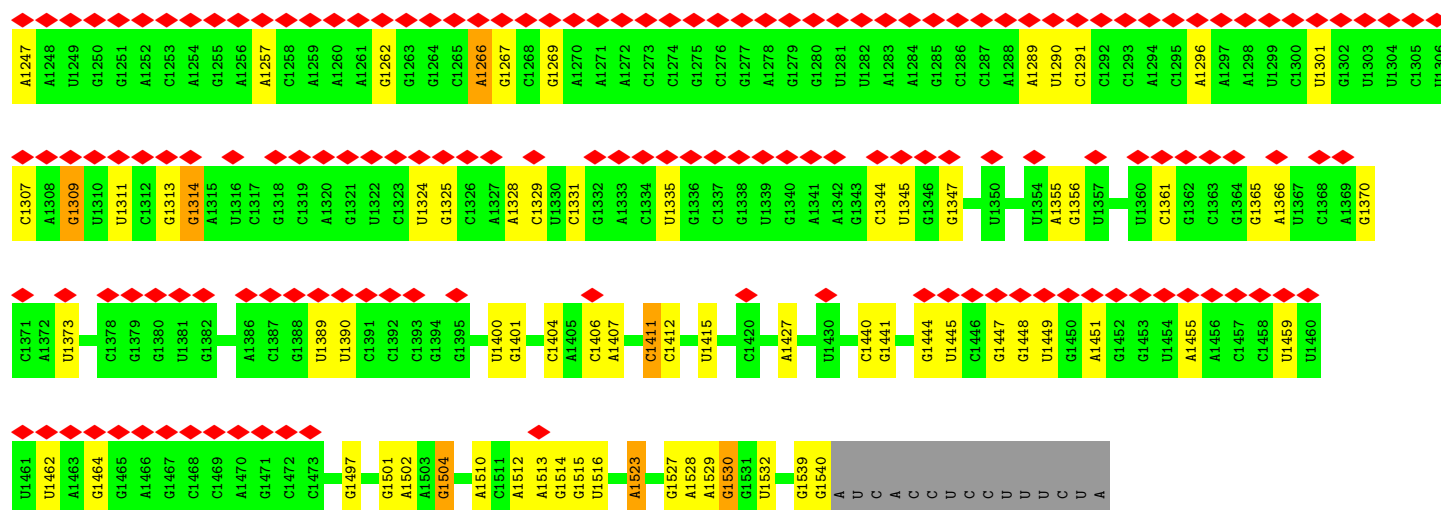
- Molecule 29: Large ribosomal subunit protein uL30



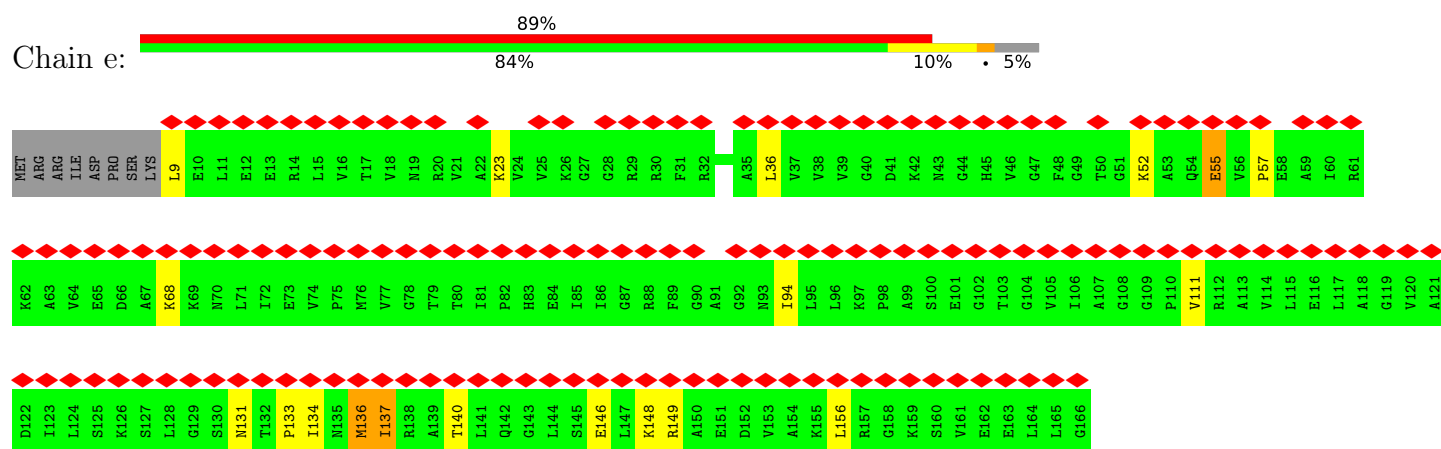
- Molecule 30: 16S rRNA



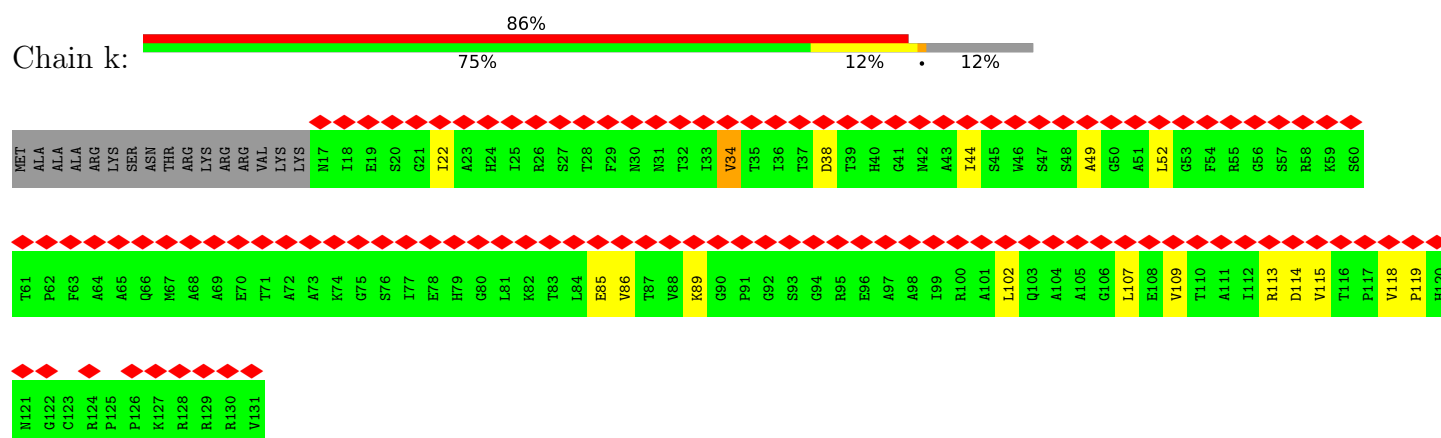
A1176	C1177	A1178	A1179	A1180	C1181	C1182	G1183	G1184	A1185	G1186	G1187	A1188	A1189	G1190	G1191	U1192	G1193	G1194	G1195	U1196	G1199	A1200	C1201	G1202	U1203	C1204	A1205	A1206	C1209	C1212	A1213	U1214	G1215	C1216	C1217	C1218	C1219	U1220	U1221	A1222	U1223	G1224	A1225	C1226	C1227	U1228	G1229	C1232	A1236	C1237	A1238	U1244								
C1116	C1117	A1120	A1121	C1122	C1123	C1124	U1125	U1126	G1127	A1128	U1129	C1130	U1131	U1132	A1133	G1134	U1135	U1136	G1137	C1138	C1139	A1140	G1141	C1142	A1143	U1144	U1145	U1146	A1147	G1148	U1149	U1150	G1151	G1152	G1153	C1154	A1155	C1156	U1157	C1158	U1159	A1160	A1161	G1162	G1163	U1164	G1165	A1166	C1167	U1168	G1169	C1170	C1171	G1172	U1173	U1174	G1175			
C1035	C1036	C1037	C1038	U1039	U1040	C1041	G1042	G1043	G1044	G1045	G1046	C1047	A1048	G1049	A1050	G1051	U1052	G1053	A1054	C1055	A1056	G1057	G1058	U1059	G1060	G1063	C1064	A1065	U1067	C1073	G1074	U1075	U1083	C1086	A1090	U1095	U1096	G1097	G1098	G1099	U1100	U1101	A1102	A1103	G1104	U1105	C1106	C1107	C1108	G1109	C1110	A1111	A1112	C1113						
U970	U971	A975	G976	C977	A978	A979	C980	G981	A985	G986	A987	A988	C989	C990	U991	C994	C995	A996	G997	G998	U999	C1000	U1001	U1002	G1003	A1004	C1005	A1006	U1007	C1008	C1009	U1010	C1011	U1012	G1013	A1014	C1015	A1016	A1017	U1018	C1019	C1020	U1021	A1022	G1023	A1024	U1025	A1026	U1027	A1028	G1029	G1030	A1031	C1032	G1033	U1034				
C853	C854	C855	C856	C857	C858	C859	U860	U861	A862	G865	C866	U867	G868	C869	A870	C876	U880	U881	A882	C885	A886	C887	C893	G896	A899	A923	A924	A925	C934	G935	G936	C940	C941	C942	C943	C944	A945	A947	A948	G955	A956	A959	U967	A968	A969															
U756	A757	A758	C759	U760	G761	A762	C763	G764	G767	A776	A777	G778	G782	G785	A786	G789	A793	G794	G795	A803	U807	C820	A824	A825	C826	G827	C830	A831	C832	C835	U836	A837	A838	C839	U840	G841	U842	C946	A947	A948	G846	G847	C848	C849	U850	U851	U852													
U686	U687	C688	C689	A690	C691	G692	U693	G694	U695	A696	G697	C698	G699	G700	U701	G702	U706	G707	C708	G709	U710	A711	G712	A713	G714	A715	U716	G717	U718	G719	G720	A721	G722	G723	A724	A725	C726	A727	C728	G729	A730	G731	U732	G733	A743	C744	U745	C746	U747	U748	U749	G750	U751	U752	C753	U754	G755			
G626	C627	U628	C629	A630	A631	C632	C633	G634	G635	G636	G637	A638	G639	G640	G641	U642	C643	A644	U645	U646	G647	G648	A649	A650	A651	C652	U653	G654	G655	U599	U599	U600	C601	U602	U603	A604	A605	G606	U607	C608	U609	G610	A611	U612	G613	U614	U615	A616	A617	U618	U619	C620	C621	G622	C623	C624	G625			
C558	G559	U560	U561	G562	U563	C564	C565	G566	G567	U568	A569	U570	U571	A572	U573	U574	G575	A581	A582	A583	G584	G585	G586	C587	U588	C589	G590	G596	G597	U598	U599	U600	C601	U602	U603	A604	A605	G606	U607	C608	U609	G610	A611	U612	G613	U614	U615	A616	A617	U618	U619	C620	C621	G622	C623	C624	G625			
A438	A439	A440	G441	C442	U443	C444	U445	G446	U447	U448	G449	U450	U451	A452	G453	G454	C394	U395	A456	A457	C458	G459	A460	C461	A462	A463	G464	U465	U466	C467	C468	G469	U470	U471	C472	G473	A474	A475	U476	A477	G478	G479	G480	C481	G482	A483	U484	A485	C486	U487	U488	U489	G490	A491	C492	G493	G494	U495	A496	C497
C378	G379	C380	A381	A382	U383	C384	G385	A386	C387	G388	A389	A390	A391	G392	U393	G394	C394	U395	A456	A457	C458	G459	A460	C461	A462	A463	G464	U465	U466	C467	C468	G469	U470	U471	C472	G473	A474	A475	U476	A477	G478	G479	G480	C481	G482	A483	U484	A485	C486	U487	U488	U489	G490	A491	C492	G493	G494	U495	A496	C497
G317	G318	C319	C320	A321	C324	U325	G326	G327	G328	A329	C330	U331	G332	A333	G334	A335	C336	A337	C338	G339	G340	C341	C342	C343	A344	G345	A346	C347	U348	C349	C350	U351	A352	C353	G354	G355	G356	A357	G358	G359	C360	A361	G362	C363	A364	G365	U366	A367	G368	G369	G370	A371	A372	U373	C374	U375	U376	C377		



• Molecule 31: 30S ribosomal protein S5

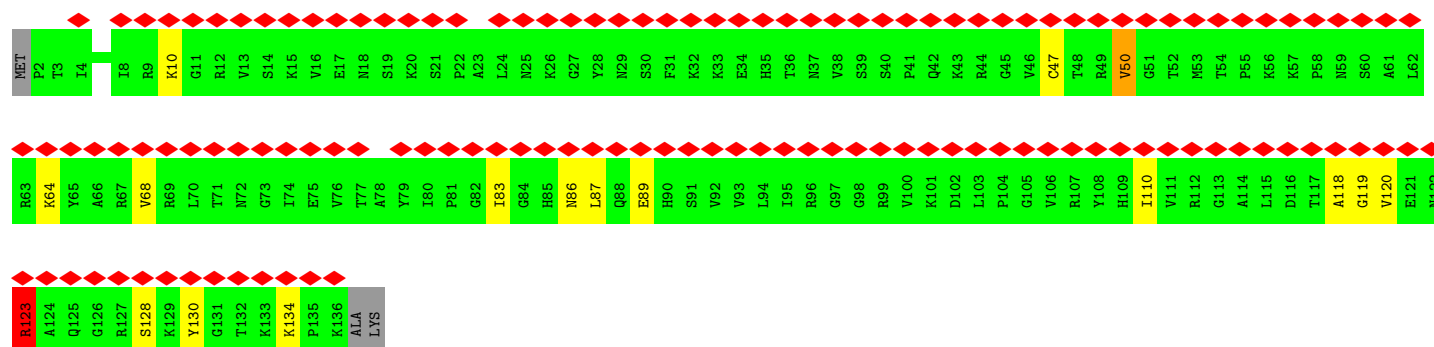


• Molecule 32: 30S ribosomal protein S11



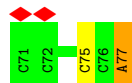
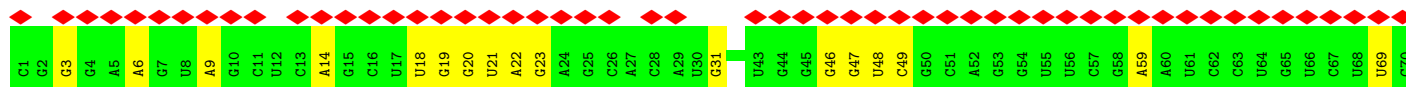
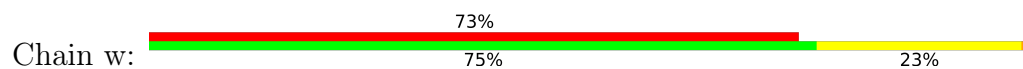
• Molecule 33: 30S ribosomal protein S12



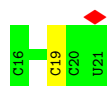
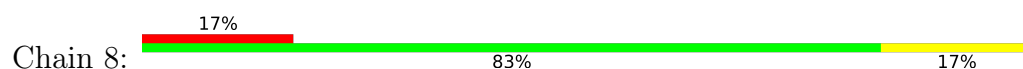




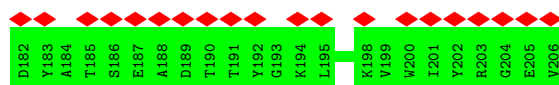
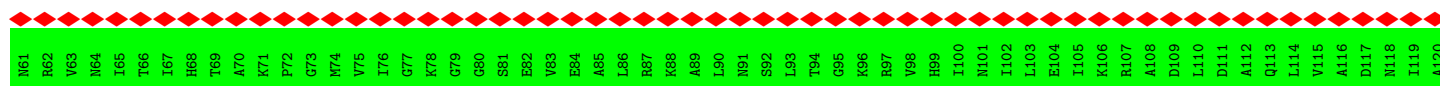
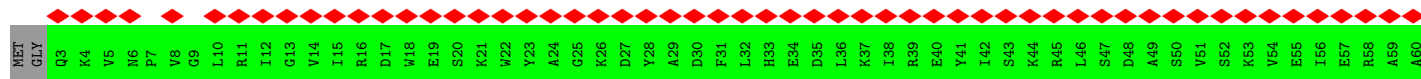
• Molecule 37: Pro-tRNA



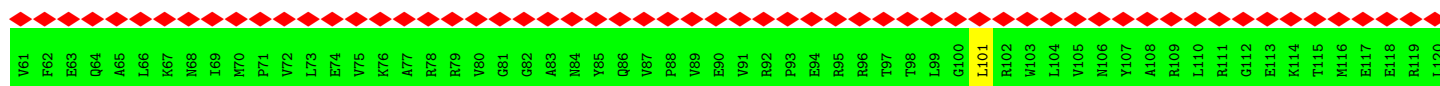
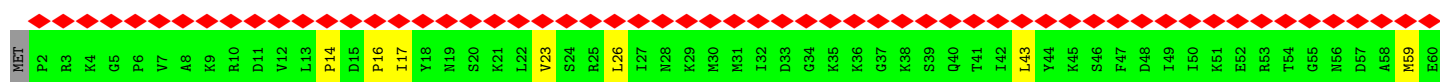
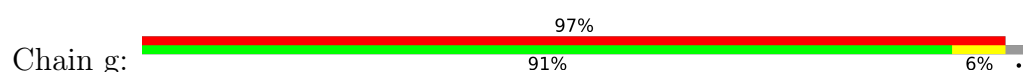
• Molecule 38: mRNA

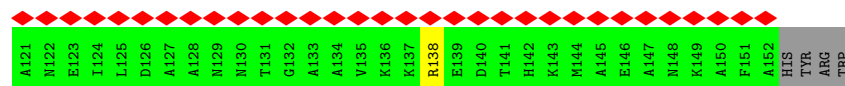


• Molecule 39: Small ribosomal subunit protein uS3



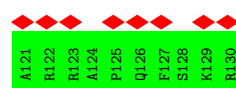
• Molecule 40: Small ribosomal subunit protein uS7





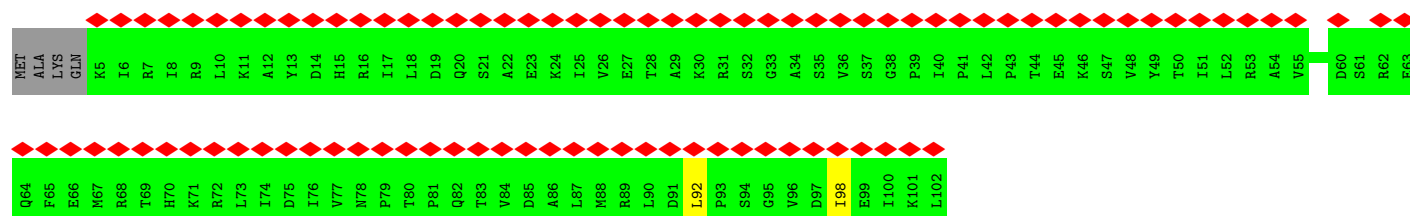
• Molecule 41: 30S ribosomal protein S9

Chain i:



• Molecule 42: 30S ribosomal protein S10

Chain j:



• Molecule 43: 30S ribosomal protein S13

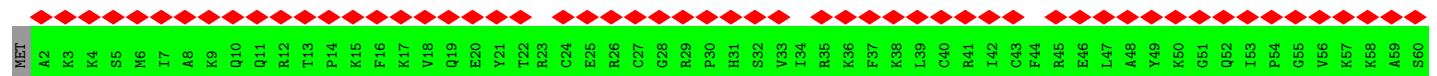
Chain m:



LYS

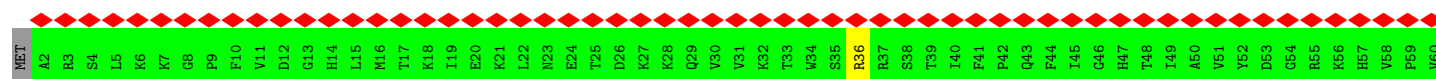
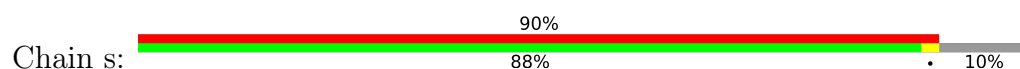
• Molecule 44: 30S ribosomal protein S14

Chain n:

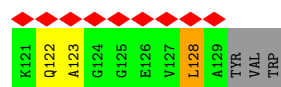
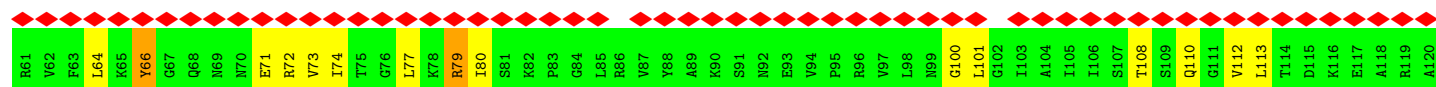
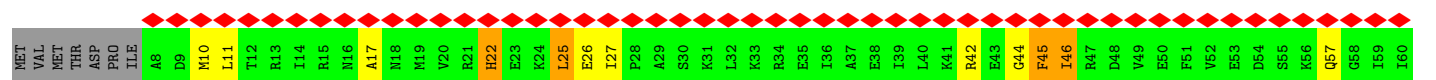
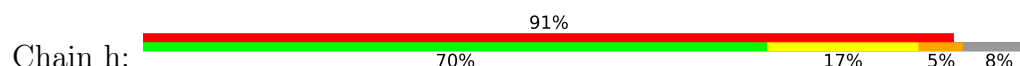




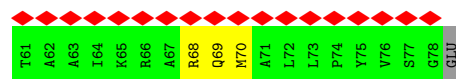
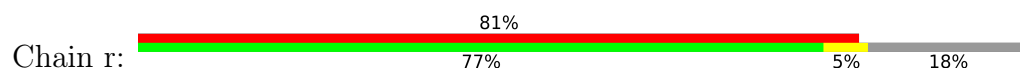
- Molecule 45: 30S ribosomal protein S19



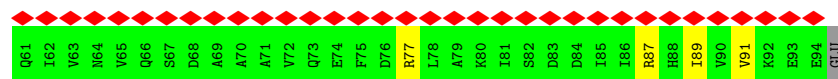
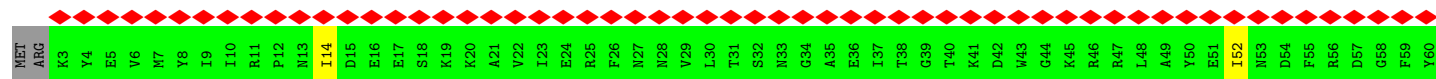
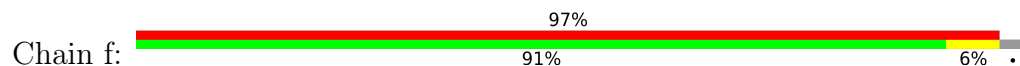
- Molecule 46: 30S ribosomal protein S8



- Molecule 47: 30S ribosomal protein S18

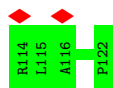


- Molecule 48: 30S ribosomal protein S6



- Molecule 49: ApdA nascent chain

Chain 7:  22% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142978	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75.6	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.342	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.052	Depositor
Map size (Å)	344.4, 344.4, 344.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, ZN, PSU, OMG, 2MA, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.60	0/440	1.06	0/584
2	1	0.47	0/408	0.86	0/541
3	2	0.61	0/371	0.89	0/483
4	3	0.66	0/529	1.01	0/691
5	4	0.55	0/300	0.96	0/393
6	6	0.55	0/363	1.04	0/485
7	A	0.52	0/65970	1.13	345/102904 (0.3%)
8	B	0.52	0/2675	1.07	15/4170 (0.4%)
9	C	0.58	0/2131	0.95	0/2859
10	D	0.56	0/1597	0.93	0/2140
11	E	0.56	0/1586	0.95	0/2139
12	F	0.47	0/1424	0.98	0/1910
13	G	0.51	0/1360	0.95	0/1832
14	J	0.55	0/1165	0.88	0/1566
15	K	0.53	0/928	0.94	0/1245
16	L	0.54	0/1094	0.96	0/1457
17	M	0.54	0/1099	0.92	0/1468
18	N	0.53	0/961	0.92	0/1284
19	O	0.51	0/922	0.94	1/1236 (0.1%)
20	P	0.52	0/958	0.94	0/1279
21	Q	0.60	0/962	0.98	0/1277
22	R	0.50	0/806	0.88	0/1080
23	S	0.59	0/859	0.96	0/1156
24	T	0.48	0/722	0.95	0/962
25	U	0.52	0/780	0.92	0/1043
26	W	0.53	0/658	0.89	0/873
27	X	0.69	0/472	0.99	0/627
28	Y	0.45	0/533	1.00	0/708
29	Z	0.51	0/458	0.91	0/613
30	a	0.56	0/36826	1.01	118/57450 (0.2%)
31	e	0.56	0/1181	1.10	1/1588 (0.1%)
32	k	0.62	0/861	1.04	0/1164

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	l	0.52	0/1064	0.97	1/1428 (0.1%)
34	o	0.47	0/738	1.07	0/985
35	q	0.50	0/707	0.92	0/944
36	t	0.49	0/661	1.21	0/882
37	w	0.57	0/1838	1.00	5/2864 (0.2%)
37	y	0.56	0/1838	0.96	4/2864 (0.1%)
38	8	0.68	0/131	0.86	0/200
39	c	0.49	0/1629	0.93	0/2192
40	g	0.58	0/1215	1.04	0/1629
41	i	0.53	0/1007	0.95	0/1351
42	j	0.52	0/800	0.93	0/1077
43	m	0.50	0/948	1.05	0/1267
44	n	0.49	0/508	0.95	0/672
45	s	0.53	0/685	0.94	0/920
46	h	0.55	0/966	1.11	0/1292
47	r	0.48	0/530	1.04	0/710
48	f	0.46	0/766	0.99	0/1031
49	7	0.58	0/67	1.06	0/89
All	All	0.54	0/147497	1.06	490/221604 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	2
3	2	0	1
4	3	0	1
7	A	0	5
9	C	0	10
10	D	0	3
11	E	0	2
16	L	0	1
19	O	0	1
20	P	0	2
21	Q	0	1
25	U	0	1
27	X	0	2
33	l	0	1
35	q	0	1
40	g	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	h	0	2
48	f	0	2
All	All	0	40

There are no bond length outliers.

All (490) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	732	A	O3'-P-O5'	-16.48	79.28	104.00
7	A	225	A	O3'-P-O5'	-15.08	81.38	104.00
7	A	1375	A	O3'-P-O5'	-14.66	82.00	104.00
7	A	490	A	O3'-P-O5'	-13.10	84.35	104.00
30	a	1313	G	O3'-P-O5'	-11.29	87.06	104.00
7	A	2382	G	O3'-P-O5'	-11.11	87.34	104.00
7	A	1277	A	O3'-P-O5'	-10.88	87.67	104.00
7	A	1340	A	O3'-P-O5'	-10.42	88.38	104.00
7	A	2308	G	O3'-P-O5'	-10.33	88.50	104.00
7	A	2764	G	O3'-P-O5'	-10.27	88.60	104.00
30	a	899	A	O3'-P-O5'	-10.03	88.96	104.00
7	A	619	A	O5'-P-OP1	-9.69	78.95	108.00
7	A	1606	A	O3'-P-O5'	-9.52	89.73	104.00
7	A	986	G	O3'-P-O5'	9.32	117.98	104.00
7	A	274	A	O3'-P-O5'	-9.28	90.08	104.00
7	A	1398	A	O3'-P-O5'	-9.25	90.12	104.00
30	a	1501	G	O3'-P-O5'	-9.13	90.31	104.00
7	A	1998	A	O3'-P-O5'	-9.05	90.42	104.00
8	B	54	U	O3'-P-O5'	-9.05	90.42	104.00
7	A	207	A	O3'-P-O5'	-9.02	90.48	104.00
7	A	373	A	O3'-P-O5'	-8.99	90.51	104.00
7	A	2340	A	O3'-P-O5'	-8.85	90.72	104.00
7	A	1374	C	O3'-P-O5'	-8.72	90.92	104.00
7	A	182	C	C4'-C3'-O3'	8.71	126.07	113.00
7	A	874	U	C2'-C3'-O3'	-8.70	100.65	113.70
7	A	2307	A	O3'-P-O5'	-8.67	91.00	104.00
7	A	2361	C	O3'-P-O5'	-8.63	91.05	104.00
7	A	2032	A	O3'-P-O5'	-8.62	91.07	104.00
7	A	119	U	O3'-P-O5'	-8.58	91.12	104.00
30	a	245	C	O3'-P-O5'	-8.57	91.14	104.00
30	a	566	G	O3'-P-O5'	-8.42	91.36	104.00
30	a	923	A	O3'-P-O5'	-8.41	91.38	104.00
30	a	1361	C	O3'-P-O5'	-8.41	91.39	104.00
7	A	2347	G	O3'-P-O5'	-8.38	91.42	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1884	G	O3'-P-O5'	-8.34	91.49	104.00
7	A	1934	C	O3'-P-O5'	-8.26	91.61	104.00
7	A	1417	A	O3'-P-O5'	-8.16	91.76	104.00
30	a	1313	G	C4'-C3'-O3'	-8.14	100.79	113.00
30	a	246	G	O3'-P-O5'	-8.03	91.95	104.00
7	A	958	A	O3'-P-O5'	-7.96	92.07	104.00
7	A	1886	G	O3'-P-O5'	-7.94	92.09	104.00
7	A	746	A	O3'-P-O5'	-7.89	92.16	104.00
30	a	581	A	O3'-P-O5'	-7.87	92.20	104.00
30	a	589	C	O3'-P-O5'	-7.86	92.21	104.00
7	A	1966	A	O3'-P-O5'	-7.84	92.24	104.00
30	a	1504	G	O3'-P-O5'	-7.82	92.27	104.00
7	A	2090	G	O5'-P-OP2	-7.77	84.68	108.00
7	A	470	A	O3'-P-O5'	-7.74	92.39	104.00
30	a	607	U	O3'-P-O5'	-7.62	92.56	104.00
8	B	10	G	O3'-P-O5'	-7.59	92.62	104.00
7	A	2456	C	O3'-P-O5'	-7.57	92.65	104.00
8	B	48	G	C2'-C3'-O3'	7.54	125.01	113.70
7	A	2601	A	C2'-C3'-O3'	-7.53	98.20	109.50
30	a	557	G	O3'-P-O5'	-7.48	92.77	104.00
30	a	985	A	C2'-C3'-O3'	7.45	120.67	109.50
7	A	2891	G	O3'-P-O5'	-7.44	92.84	104.00
7	A	2842	U	O3'-P-O5'	-7.40	92.91	104.00
7	A	673	A	O3'-P-O5'	-7.39	92.92	104.00
30	a	296	A	O3'-P-O5'	-7.38	92.93	104.00
30	a	673	G	O3'-P-O5'	-7.38	92.94	104.00
7	A	183	A	C1'-O4'-C4'	-7.35	102.35	109.70
30	a	1090	A	O3'-P-O5'	-7.30	93.04	104.00
7	A	123	G	O3'-P-O5'	-7.28	93.08	104.00
7	A	2414	C	O3'-P-O5'	-7.28	93.08	104.00
30	a	50	C	O3'-P-O5'	-7.28	93.09	104.00
7	A	1004	U	O3'-P-O5'	-7.27	93.09	104.00
7	A	44	A	O3'-P-O5'	-7.27	93.10	104.00
7	A	539	G	O3'-P-O5'	-7.27	93.10	104.00
7	A	132	C	O3'-P-O5'	-7.26	93.10	104.00
7	A	2524	G	O3'-P-O5'	7.26	114.88	104.00
7	A	2601	A	C4'-C3'-O3'	7.24	120.26	109.40
7	A	516	G	O3'-P-O5'	-7.21	93.19	104.00
30	a	896	G	O3'-P-O5'	-7.21	93.19	104.00
7	A	831	U	O3'-P-O5'	-7.20	93.21	104.00
7	A	1876	A	O3'-P-O5'	-7.20	93.21	104.00
7	A	564	G	C4'-C3'-O3'	-7.16	102.27	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	337	A	O3'-P-O5'	-7.14	93.29	104.00
7	A	378	C	O3'-P-O5'	-7.12	93.31	104.00
7	A	468	C	O3'-P-O5'	-7.11	93.34	104.00
7	A	2520	U	C4'-C3'-O3'	-7.10	102.35	113.00
7	A	1751	U	C2'-C3'-O3'	7.08	120.12	109.50
7	A	2746	G	O3'-P-O5'	-7.07	93.40	104.00
30	a	360	C	O3'-P-O5'	-7.06	93.41	104.00
7	A	1526	G	O3'-P-O5'	-7.06	93.41	104.00
30	a	664	A	O3'-P-O5'	-7.05	93.43	104.00
7	A	1199	C	O5'-P-OP2	-7.04	86.87	108.00
7	A	1704	U	O3'-P-O5'	-7.04	93.44	104.00
7	A	1424	A	O3'-P-O5'	-7.04	93.44	104.00
7	A	1866	C	O3'-P-O5'	-7.03	93.46	104.00
7	A	1958	G	O3'-P-O5'	-7.02	93.47	104.00
30	a	789	G	O3'-P-O5'	-7.00	93.50	104.00
7	A	1359	G	O3'-P-O5'	-6.99	93.51	104.00
7	A	1036	A	O3'-P-O5'	-6.99	93.52	104.00
7	A	1173	A	O3'-P-O5'	-6.99	93.52	104.00
7	A	1935	G	O3'-P-O5'	-6.96	93.56	104.00
7	A	2595	A	O3'-P-O5'	-6.94	93.59	104.00
7	A	2904	A	O3'-P-O5'	-6.92	93.62	104.00
7	A	810	G	O3'-P-O5'	-6.92	93.63	104.00
7	A	1177	G	O3'-P-O5'	-6.91	93.63	104.00
7	A	590	U	O3'-P-O5'	-6.91	93.64	104.00
7	A	1681	U	O5'-P-OP2	-6.87	87.40	108.00
30	a	882	A	O3'-P-O5'	-6.86	93.70	104.00
30	a	887	C	O3'-P-O5'	-6.86	93.71	104.00
7	A	2098	G	O3'-P-O5'	-6.82	93.77	104.00
7	A	2074	C	O3'-P-O5'	-6.81	93.78	104.00
7	A	354	A	O3'-P-O5'	-6.81	93.79	104.00
7	A	2639	C	O3'-P-O5'	-6.81	93.79	104.00
7	A	2049	A	O3'-P-O5'	-6.78	93.83	104.00
30	a	785	G	O3'-P-O5'	-6.78	93.83	104.00
7	A	1294	A	C4'-C3'-O3'	-6.74	102.89	113.00
7	A	733	U	O5'-P-OP1	6.73	128.19	108.00
7	A	2662	A	O3'-P-O5'	-6.72	93.92	104.00
37	w	46	G	O3'-P-O5'	-6.72	93.92	104.00
7	A	1167	C	O3'-P-O5'	-6.70	93.95	104.00
7	A	2629	A	O3'-P-O5'	-6.70	93.95	104.00
7	A	2030	A	O3'-P-O5'	-6.69	93.97	104.00
7	A	1480	A	O3'-P-O5'	-6.68	93.98	104.00
7	A	2473	G	O3'-P-O5'	-6.68	93.98	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2793	A	O3'-P-O5'	-6.66	94.01	104.00
30	a	545	C	C4'-C3'-O3'	6.64	119.36	109.40
7	A	1375	A	C4'-C3'-O3'	-6.61	103.08	113.00
7	A	2389	A	O3'-P-O5'	-6.61	94.09	104.00
7	A	188	C	O3'-P-O5'	-6.60	94.10	104.00
7	A	960	U	O3'-P-O5'	-6.59	94.12	104.00
7	A	2504	C	O3'-P-O5'	-6.59	94.12	104.00
7	A	1181	C	C4'-C3'-O3'	-6.58	103.14	113.00
7	A	1525	G	C2'-C3'-O3'	6.56	123.54	113.70
7	A	1644	C	O3'-P-O5'	-6.56	94.16	104.00
7	A	1690	G	O3'-P-O5'	-6.56	94.16	104.00
7	A	254	A	O3'-P-O5'	-6.54	94.19	104.00
37	w	75	C	O3'-P-O5'	-6.52	94.22	104.00
30	a	1514	G	O3'-P-O5'	-6.50	94.25	104.00
7	A	436	A	O3'-P-O5'	-6.49	94.26	104.00
7	A	1406	A	O3'-P-O5'	-6.49	94.27	104.00
30	a	987	A	O3'-P-O5'	-6.48	94.27	104.00
7	A	1559	C	O3'-P-O5'	-6.47	94.30	104.00
7	A	297	G	O3'-P-O5'	-6.46	94.31	104.00
7	A	2458	G	O3'-P-O5'	-6.46	94.31	104.00
30	a	254	A	O3'-P-O5'	-6.44	94.34	104.00
7	A	481	U	O3'-P-O5'	-6.43	94.35	104.00
7	A	543	A	O3'-P-O5'	-6.43	94.35	104.00
30	a	1148	G	C2'-C3'-O3'	6.43	119.14	109.50
7	A	1197	A	O3'-P-O5'	-6.42	94.36	104.00
7	A	679	A	O3'-P-O5'	6.42	113.63	104.00
7	A	1279	C	O3'-P-O5'	-6.41	94.39	104.00
7	A	583	G	O3'-P-O5'	-6.39	94.41	104.00
7	A	2271	G	O3'-P-O5'	-6.39	94.42	104.00
7	A	1501	U	O3'-P-O5'	-6.38	94.43	104.00
30	a	707	G	O3'-P-O5'	-6.38	94.43	104.00
7	A	2057	U	O3'-P-O5'	-6.38	94.44	104.00
7	A	2622	U	O3'-P-O5'	-6.37	94.44	104.00
7	A	1018	G	O3'-P-O5'	-6.35	94.47	104.00
7	A	1067	A	O3'-P-O5'	-6.35	94.47	104.00
7	A	679	A	C2'-C3'-O3'	-6.35	104.18	113.70
7	A	1666	U	O3'-P-O5'	-6.33	94.50	104.00
7	A	2534	G	O3'-P-O5'	-6.33	94.50	104.00
7	A	1893	U	O3'-P-O5'	-6.32	94.52	104.00
8	B	107	G	C4'-C3'-O3'	6.32	118.88	109.40
7	A	1613	C	O3'-P-O5'	-6.32	94.53	104.00
30	a	708	C	O3'-P-O5'	-6.32	94.53	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2024	U	C4'-C3'-O3'	-6.31	103.53	113.00
8	B	80	G	O3'-P-O5'	-6.31	94.54	104.00
7	A	830	A	O3'-P-O5'	-6.31	94.54	104.00
7	A	1433	U	O3'-P-O5'	-6.30	94.55	104.00
7	A	1381	A	O3'-P-O5'	-6.29	94.56	104.00
8	B	86	U	O3'-P-O5'	-6.29	94.56	104.00
7	A	1037	C	C4'-C3'-O3'	-6.28	103.58	113.00
30	a	925	A	O3'-P-O5'	-6.28	94.58	104.00
7	A	1787	G	O3'-P-O5'	-6.27	94.60	104.00
7	A	2493	C	O3'-P-O5'	-6.26	94.61	104.00
30	a	608	C	O3'-P-O5'	-6.26	94.61	104.00
7	A	828	A	O3'-P-O5'	-6.25	94.63	104.00
30	a	582	A	O3'-P-O5'	-6.25	94.63	104.00
7	A	1818	A	C4'-C3'-O3'	-6.24	103.64	113.00
7	A	2645	C	C3'-C2'-O2'	6.24	120.06	110.70
7	A	1416	G	C4'-C3'-O3'	-6.23	103.66	113.00
30	a	1266	A	C2'-C3'-O3'	6.23	118.84	109.50
7	A	2592	U	C4'-C3'-O3'	-6.20	103.70	113.00
7	A	2548	U	O3'-P-O5'	-6.20	94.71	104.00
30	a	885	C	O3'-P-O5'	-6.19	94.71	104.00
7	A	2639	C	C1'-C2'-O2'	-6.19	102.52	111.80
7	A	1999	A	C2'-C3'-O3'	6.17	118.76	109.50
7	A	2754	A	O3'-P-O5'	-6.15	94.77	104.00
7	A	2525	C	P-O5'-C5'	-6.14	111.69	120.90
7	A	803	C	O3'-P-O5'	-6.13	94.81	104.00
7	A	1988	G	O3'-P-O5'	-6.12	94.81	104.00
7	A	58	G	O3'-P-O5'	-6.12	94.81	104.00
30	a	1301	U	O3'-P-O5'	-6.12	94.82	104.00
7	A	1742	G	O3'-P-O5'	-6.11	94.84	104.00
7	A	723	A	O3'-P-O5'	-6.10	94.85	104.00
30	a	341	C	O3'-P-O5'	-6.10	94.85	104.00
7	A	1310	C	O3'-P-O5'	-6.09	94.86	104.00
7	A	158	C	O3'-P-O5'	-6.09	94.87	104.00
30	a	1026	A	O3'-P-O5'	-6.08	94.87	104.00
30	a	837	A	O3'-P-O5'	-6.08	94.88	104.00
7	A	889	A	O3'-P-O5'	-6.08	94.88	104.00
30	a	1075	U	O3'-P-O5'	-6.08	94.88	104.00
7	A	1708	U	O3'-P-O5'	-6.08	94.89	104.00
7	A	1543	U	C4'-C3'-O3'	6.07	118.50	109.40
30	a	549	G	O3'-P-O5'	-6.07	94.90	104.00
7	A	1690	G	C2'-C3'-O3'	-6.06	104.61	113.70
7	A	108	A	O3'-P-O5'	-6.05	94.92	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	840	U	O3'-P-O5'	-6.05	94.92	104.00
8	B	14	G	O3'-P-O5'	-6.05	94.93	104.00
7	A	724	A	C4'-C3'-O3'	-6.03	103.95	113.00
30	a	127	U	C2'-C3'-O3'	6.03	122.74	113.70
7	A	563	C	C4'-C3'-O3'	-6.01	103.98	113.00
7	A	183	A	C3'-C2'-O2'	-6.00	105.60	114.60
7	A	1433	U	C2'-C3'-O3'	-6.00	104.70	113.70
7	A	2059	A	O3'-P-O5'	-6.00	95.00	104.00
7	A	1369	C	P-O5'-C5'	-6.00	111.91	120.90
7	A	1199	C	O5'-P-OP1	5.99	125.97	108.00
7	A	1751	U	O3'-P-O5'	-5.98	95.03	104.00
7	A	267	C	O3'-P-O5'	-5.98	95.04	104.00
30	a	807	U	O3'-P-O5'	-5.96	95.06	104.00
7	A	432	C	C4'-C3'-O3'	-5.95	104.07	113.00
7	A	1062	C	O3'-P-O5'	-5.95	95.08	104.00
7	A	2907	A	O3'-P-O5'	-5.95	95.08	104.00
7	A	266	U	O3'-P-O5'	-5.94	95.08	104.00
30	a	245	C	C4'-C3'-O3'	-5.94	104.08	113.00
7	A	360	C	O3'-P-O5'	-5.92	95.12	104.00
7	A	1829	C	O3'-P-O5'	5.92	112.88	104.00
30	a	1528	A	O3'-P-O5'	-5.92	95.12	104.00
7	A	1044	C	O3'-P-O5'	-5.92	95.12	104.00
30	a	712	G	O3'-P-O5'	-5.92	95.12	104.00
8	B	37	A	C2'-C3'-O3'	5.91	122.57	113.70
7	A	484	C	O3'-P-O5'	-5.91	95.14	104.00
30	a	1189	A	O3'-P-O5'	-5.91	95.14	104.00
7	A	2080	A	C1'-C2'-O2'	-5.89	102.96	111.80
7	A	722	A	C4'-C3'-O3'	-5.89	104.17	113.00
7	A	174	U	O3'-P-O5'	-5.88	95.18	104.00
7	A	257	G	O3'-P-O5'	5.87	112.81	104.00
7	A	1244	A	O3'-P-O5'	-5.87	95.19	104.00
7	A	795	G	C1'-O4'-C4'	-5.87	104.03	109.90
7	A	1037	C	O3'-P-O5'	-5.86	95.21	104.00
7	A	1827	U	O3'-P-O5'	-5.86	95.21	104.00
30	a	795	G	O3'-P-O5'	-5.86	95.21	104.00
30	a	544	A	C2'-C3'-O3'	5.86	118.28	109.50
7	A	34	U	C2'-C3'-O3'	5.85	118.27	109.50
30	a	1309	G	O3'-P-O5'	-5.84	95.23	104.00
7	A	747	G	C4'-C3'-O3'	-5.84	104.24	113.00
30	a	981	G	O3'-P-O5'	-5.84	95.24	104.00
7	A	296	G	O3'-P-O5'	-5.83	95.25	104.00
7	A	540	G	C4'-C3'-O3'	-5.82	104.26	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	10	A	O3'-P-O5'	-5.81	95.28	104.00
7	A	998	G	O3'-P-O5'	-5.81	95.29	104.00
7	A	2364	A	C4'-C3'-O3'	-5.81	104.29	113.00
30	a	508	A	C2'-C3'-O3'	5.81	118.21	109.50
7	A	918	U	O3'-P-O5'	-5.80	95.30	104.00
7	A	986	G	C2'-C3'-O3'	-5.79	105.01	113.70
7	A	714	U	O3'-P-O5'	-5.79	95.31	104.00
7	A	2452	U	O3'-P-O5'	-5.79	95.32	104.00
7	A	1498	U	O3'-P-O5'	-5.77	95.34	104.00
7	A	1806	U	O3'-P-O5'	-5.77	95.34	104.00
7	A	1481	G	O3'-P-O5'	-5.77	95.35	104.00
7	A	1888	A	O3'-P-O5'	-5.76	95.36	104.00
30	a	1314	G	O3'-P-O5'	-5.76	95.36	104.00
8	B	60	C	O3'-P-O5'	-5.75	95.38	104.00
7	A	483	C	O3'-P-O5'	-5.74	95.39	104.00
30	a	405	A	O3'-P-O5'	-5.74	95.39	104.00
7	A	9	U	O3'-P-O5'	-5.74	95.40	104.00
7	A	13	A	O3'-P-O5'	-5.74	95.40	104.00
7	A	1695	A	O3'-P-O5'	-5.73	95.40	104.00
30	a	508	A	O3'-P-O5'	-5.73	95.41	104.00
7	A	1035	G	O3'-P-O5'	-5.73	95.41	104.00
7	A	2412	G	C4'-C3'-O3'	-5.72	104.42	113.00
7	A	2575	U	O3'-P-O5'	-5.71	95.43	104.00
7	A	1246	G	O4'-C4'-C3'	-5.71	98.29	104.00
7	A	54	G	O3'-P-O5'	-5.71	95.44	104.00
7	A	599	G	O3'-P-O5'	-5.71	95.44	104.00
30	a	793	A	O3'-P-O5'	-5.71	95.44	104.00
30	a	1356	G	O3'-P-O5'	-5.70	95.45	104.00
30	a	37	G	O3'-P-O5'	-5.70	95.45	104.00
30	a	709	G	O3'-P-O5'	-5.69	95.46	104.00
37	y	6	A	O3'-P-O5'	-5.68	95.48	104.00
7	A	2732	C	O3'-P-O5'	-5.68	95.48	104.00
7	A	635	C	O3'-P-O5'	-5.68	95.48	104.00
7	A	1072	A	O3'-P-O5'	-5.66	95.50	104.00
7	A	1625	C	O3'-P-O5'	-5.66	95.51	104.00
7	A	1179	A	O3'-P-O5'	-5.66	95.51	104.00
7	A	1448	U	O3'-P-O5'	-5.66	95.51	104.00
30	a	520	C	O3'-P-O5'	-5.66	95.51	104.00
30	a	289	G	O3'-P-O5'	-5.65	95.53	104.00
7	A	183	A	O4'-C4'-C3'	-5.64	100.46	106.10
7	A	217	G	O3'-P-O5'	-5.64	95.54	104.00
7	A	583	G	C4'-C3'-O3'	-5.63	104.55	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	659	A	O3'-P-O5'	-5.63	95.56	104.00
30	a	329	A	O3'-P-O5'	-5.62	95.57	104.00
7	A	2731	G	O3'-P-O5'	-5.61	95.59	104.00
30	a	1117	C	O3'-P-O5'	-5.61	95.59	104.00
30	a	321	A	O3'-P-O5'	-5.60	95.59	104.00
7	A	1379	U	C2'-C3'-O3'	-5.59	101.11	109.50
8	B	49	G	C2'-C3'-O3'	5.59	122.09	113.70
30	a	876	C	O3'-P-O5'	-5.59	95.62	104.00
7	A	2383	A	C4'-C3'-O3'	-5.58	104.62	113.00
30	a	584	G	O3'-P-O5'	-5.58	95.63	104.00
8	B	37	A	C4'-C3'-C2'	-5.57	97.03	102.60
7	A	458	G	O3'-P-O5'	5.56	112.34	104.00
7	A	2688	G	O3'-P-O5'	-5.56	95.66	104.00
7	A	1199	C	O5'-C5'-C4'	5.55	119.83	111.50
7	A	2553	G	O3'-P-O5'	-5.55	95.67	104.00
7	A	299	U	O3'-P-O5'	-5.55	95.68	104.00
7	A	1995	A	O3'-P-O5'	-5.55	95.68	104.00
7	A	482	C	O3'-P-O5'	-5.54	95.68	104.00
30	a	1154	C	C2'-C3'-O3'	-5.54	105.38	113.70
7	A	2646	C	C2'-C3'-O3'	-5.54	105.40	113.70
7	A	857	U	C4'-C3'-O3'	-5.53	104.70	113.00
30	a	1448	G	O3'-P-O5'	-5.53	95.70	104.00
7	A	1616	G	O3'-P-O5'	-5.52	95.72	104.00
30	a	142	A	O3'-P-O5'	-5.50	95.75	104.00
7	A	1992	C	C2'-C3'-O3'	5.50	117.75	109.50
30	a	117	A	O3'-P-O5'	-5.50	95.75	104.00
37	w	69	U	O3'-P-O5'	-5.50	95.75	104.00
7	A	2498	A	O3'-P-O5'	-5.49	95.77	104.00
7	A	1810	G	O3'-P-O5'	-5.48	95.78	104.00
30	a	1313	G	C2'-C3'-O3'	5.48	121.92	113.70
30	a	1411	C	C3'-C2'-O2'	5.46	118.89	110.70
30	a	1199	G	O3'-P-O5'	-5.46	95.81	104.00
8	B	26	C	O3'-P-O5'	-5.46	95.81	104.00
30	a	36	C	O3'-P-O5'	-5.45	95.83	104.00
30	a	305	G	O3'-P-O5'	-5.45	95.83	104.00
7	A	493	G	O3'-P-O5'	-5.45	95.83	104.00
37	y	46	G	O3'-P-O5'	-5.45	95.83	104.00
30	a	1057	G	O3'-P-O5'	-5.44	95.84	104.00
30	a	759	C	O3'-P-O5'	-5.44	95.84	104.00
30	a	118	A	O3'-P-O5'	-5.44	95.85	104.00
7	A	515	G	C4'-C3'-O3'	-5.43	104.86	113.00
7	A	1285	G	O3'-P-O5'	-5.42	95.87	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1983	G	O3'-P-O5'	-5.42	95.87	104.00
7	A	2792	G	O3'-P-O5'	-5.42	95.87	104.00
7	A	1029	A	C4'-C3'-O3'	-5.40	104.90	113.00
7	A	2579	G	O3'-P-O5'	-5.40	95.90	104.00
8	B	61	U	O3'-P-O5'	-5.40	95.90	104.00
7	A	1413	G	O3'-P-O5'	-5.40	95.91	104.00
8	B	32	U	O3'-P-O5'	-5.40	95.91	104.00
7	A	2530	C	O3'-P-O5'	-5.39	95.91	104.00
7	A	1289	U	C4'-C3'-O3'	-5.39	104.91	113.00
7	A	1751	U	P-O3'-C3'	5.38	128.28	120.20
7	A	1643	C	O3'-P-O5'	-5.38	95.94	104.00
7	A	2236	C	O3'-P-O5'	-5.37	95.95	104.00
7	A	1301	U	O3'-P-O5'	-5.37	95.95	104.00
7	A	491	C	O5'-P-OP1	5.36	124.08	108.00
30	a	270	A	O3'-P-O5'	-5.36	95.97	104.00
30	a	1530	G	O3'-P-O5'	-5.36	95.97	104.00
7	A	672	C	O3'-P-O5'	-5.35	95.97	104.00
30	a	587	C	O3'-P-O5'	-5.35	95.97	104.00
7	A	2713	U	O3'-P-O5'	-5.35	95.98	104.00
7	A	2457	G	O3'-P-O5'	-5.34	95.98	104.00
7	A	2512	C	O3'-P-O5'	-5.34	95.98	104.00
37	w	3	G	O3'-P-O5'	-5.34	95.99	104.00
7	A	1683	C	O3'-P-O5'	-5.34	95.99	104.00
30	a	767	G	C4'-C3'-O3'	-5.34	104.99	113.00
7	A	2077	G	O3'-P-O5'	-5.33	96.00	104.00
7	A	2099	G	C4'-C3'-O3'	-5.33	105.00	113.00
7	A	497	G	O3'-P-O5'	-5.33	96.01	104.00
7	A	956	A	O3'-P-O5'	-5.33	96.01	104.00
7	A	1239	U	O3'-P-O5'	-5.33	96.01	104.00
7	A	987	A	C2'-C3'-O3'	-5.33	105.71	113.70
7	A	1083	G	O3'-P-O5'	-5.33	96.01	104.00
7	A	2649	C	C3'-C2'-O2'	5.33	118.69	110.70
7	A	1006	A	O3'-P-O5'	5.32	111.99	104.00
7	A	1812	A	O3'-P-O5'	-5.32	96.02	104.00
7	A	831	U	C2'-C3'-O3'	-5.31	105.74	113.70
7	A	2580	C	O3'-P-O5'	-5.31	96.04	104.00
7	A	343	A	C4'-C3'-O3'	-5.31	105.04	113.00
7	A	2363	C	O3'-P-O5'	-5.31	96.04	104.00
30	a	830	G	O3'-P-O5'	-5.31	96.04	104.00
7	A	2630	C	O3'-P-O5'	-5.30	96.04	104.00
7	A	1897	C	O3'-P-O5'	-5.30	96.06	104.00
7	A	1315	G	O5'-P-OP2	-5.29	92.12	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2748	G	O3'-P-O5'	-5.29	96.06	104.00
7	A	1422	C	O3'-P-O5'	-5.29	96.06	104.00
37	w	6	A	O3'-P-O5'	-5.29	96.06	104.00
7	A	2761	G	C4'-C3'-O3'	-5.29	105.07	113.00
7	A	1616	G	C4'-C3'-O3'	-5.28	105.07	113.00
7	A	1231	G	C4'-C3'-C2'	-5.28	97.32	102.60
7	A	2609	U	C4'-C3'-O3'	-5.28	105.09	113.00
7	A	1186	C	C4'-C3'-O3'	-5.27	105.10	113.00
7	A	1627	A	O3'-P-O5'	-5.26	96.10	104.00
7	A	2067	G	O3'-P-O5'	-5.26	96.11	104.00
30	a	351	U	O3'-P-O5'	-5.26	96.11	104.00
30	a	967	U	O3'-P-O5'	-5.26	96.11	104.00
7	A	864	C	C4'-C3'-C2'	-5.26	97.34	102.60
7	A	2094	C	C2'-C3'-O3'	-5.26	105.81	113.70
7	A	2496	C	C4'-C3'-O3'	-5.25	105.13	113.00
30	a	1447	G	O3'-P-O5'	-5.25	96.13	104.00
7	A	1481	G	C4'-C3'-O3'	-5.24	105.14	113.00
7	A	1657	C	O3'-P-O5'	-5.24	96.14	104.00
30	a	37	G	C4'-C3'-O3'	-5.24	105.14	113.00
7	A	1328	C	O3'-P-O5'	-5.24	96.14	104.00
7	A	2582	G	C3'-C2'-O2'	5.24	118.55	110.70
7	A	2701	U	O3'-P-O5'	-5.24	96.15	104.00
30	a	1048	A	O3'-P-O5'	-5.23	96.15	104.00
7	A	826	U	C3'-C2'-O2'	5.23	118.55	110.70
7	A	1679	A	O3'-P-O5'	-5.23	96.16	104.00
7	A	2275	G	O3'-P-O5'	-5.22	96.16	104.00
7	A	411	G	O3'-P-O5'	-5.22	96.18	104.00
33	l	123	ARG	CG-CD-NE	5.21	123.46	112.00
7	A	988	G	O3'-P-O5'	-5.21	96.19	104.00
7	A	183	A	N9-C1'-C2'	5.20	121.81	114.00
7	A	612	U	O3'-P-O5'	-5.20	96.20	104.00
7	A	2052	A	O3'-P-O5'	-5.20	96.21	104.00
7	A	1488	G	O3'-P-O5'	-5.19	96.22	104.00
7	A	1785	G	O3'-P-O5'	-5.19	96.22	104.00
7	A	2051	U	O3'-P-O5'	-5.19	96.22	104.00
7	A	202	A	C1'-O4'-C4'	-5.18	104.52	109.70
7	A	1708	U	C4'-C3'-O3'	-5.18	105.23	113.00
30	a	985	A	O3'-P-O5'	5.18	111.77	104.00
7	A	1268	G	C4'-C3'-O3'	-5.18	105.23	113.00
7	A	2849	U	O3'-P-O5'	-5.17	96.24	104.00
7	A	1395	C	O3'-P-O5'	-5.17	96.25	104.00
7	A	1038	C	C4'-C3'-O3'	-5.17	105.25	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	820	C	C4'-C3'-O3'	-5.17	105.25	113.00
7	A	854	U	C4'-C3'-C2'	-5.17	97.44	102.60
7	A	73	A	O3'-P-O5'	-5.16	96.26	104.00
30	a	590	G	O3'-P-O5'	-5.16	96.26	104.00
37	y	69	U	O3'-P-O5'	-5.15	96.27	104.00
7	A	2227	A	O3'-P-O5'	-5.15	96.27	104.00
7	A	2522	U	O3'-P-O5'	-5.15	96.28	104.00
7	A	1246	G	C4'-C3'-C2'	-5.15	97.45	102.60
7	A	2253	G	C4'-C3'-O3'	-5.15	105.28	113.00
7	A	773	G	O3'-P-O5'	-5.14	96.28	104.00
7	A	1229	U	C4'-C3'-O3'	-5.14	105.29	113.00
7	A	1617	A	C4'-C3'-O3'	-5.14	105.29	113.00
19	O	46	ASP	CA-CB-CG	5.14	117.74	112.60
7	A	2418	G	C4'-C3'-O3'	-5.13	105.30	113.00
30	a	1209	C	O3'-P-O5'	-5.13	96.30	104.00
30	a	1523	A	O3'-P-O5'	-5.13	96.31	104.00
30	a	1262	G	O3'-P-O5'	-5.12	96.31	104.00
30	a	1335	U	O3'-P-O5'	-5.12	96.31	104.00
7	A	558	G	O4'-C1'-N9	5.12	115.88	108.20
7	A	2090	G	O5'-P-OP1	5.12	123.37	108.00
7	A	2341	U	O3'-P-O5'	-5.12	96.31	104.00
7	A	2438	G	O3'-P-O5'	-5.12	96.32	104.00
7	A	2614	U	O3'-P-O5'	-5.12	96.32	104.00
30	a	936	G	C4'-C3'-O3'	-5.12	105.32	113.00
7	A	1002	G	C4'-C3'-O3'	-5.12	105.32	113.00
30	a	1370	G	O3'-P-O5'	-5.11	96.33	104.00
7	A	1750	G	O3'-P-O5'	-5.11	96.33	104.00
7	A	2445	C	O3'-P-O5'	-5.11	96.34	104.00
30	a	1102	A	O3'-P-O5'	-5.11	96.34	104.00
7	A	1488	G	C2'-C3'-O3'	-5.10	106.05	113.70
30	a	172	U	O3'-P-O5'	-5.10	96.35	104.00
30	a	782	G	O3'-P-O5'	-5.10	96.35	104.00
7	A	1719	G	O3'-P-O5'	-5.10	96.35	104.00
7	A	1310	C	C2'-C3'-O3'	-5.09	106.06	113.70
7	A	2649	C	C4'-C3'-O3'	-5.09	105.36	113.00
37	y	3	G	O3'-P-O5'	-5.09	96.36	104.00
7	A	1181	C	OP2-P-O3'	-5.09	92.73	108.00
7	A	1651	G	C2'-C3'-O3'	-5.09	106.07	113.70
7	A	2895	C	C2'-C3'-O3'	-5.09	106.06	113.70
7	A	109	G	O3'-P-O5'	-5.09	96.37	104.00
30	a	756	U	O3'-P-O5'	-5.08	96.38	104.00
8	B	11	A	O3'-P-O5'	-5.08	96.38	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2916	A	O3'-P-O5'	-5.08	96.38	104.00
30	a	832	G	O3'-P-O5'	-5.08	96.39	104.00
30	a	1113	C	O3'-P-O5'	-5.07	96.39	104.00
7	A	2643	A	O3'-P-O5'	-5.07	96.39	104.00
7	A	2792	G	C4'-C3'-O3'	-5.07	105.39	113.00
30	a	1532	U	O3'-P-O5'	-5.07	96.39	104.00
30	a	1404	C	O3'-P-O5'	-5.07	96.40	104.00
7	A	192	G	O3'-P-O5'	-5.06	96.42	104.00
7	A	2660	G	O3'-P-O5'	-5.05	96.42	104.00
7	A	229	A	C4'-C3'-O3'	-5.05	105.43	113.00
7	A	866	A	O5'-P-OP1	-5.05	92.86	108.00
7	A	2359	G	O3'-P-O5'	-5.04	96.43	104.00
7	A	2908	A	C4'-C3'-O3'	-5.04	105.44	113.00
7	A	955	C	O3'-P-O5'	-5.04	96.44	104.00
7	A	2417	A	C4'-C3'-O3'	-5.04	105.44	113.00
30	a	532	A	O3'-P-O5'	-5.04	96.45	104.00
30	a	1212	C	O3'-P-O5'	-5.04	96.45	104.00
7	A	1327	U	C1'-C2'-O2'	-5.03	104.25	111.80
7	A	2080	A	O3'-P-O5'	-5.03	96.46	104.00
7	A	2434	G	O3'-P-O5'	5.03	111.54	104.00
30	a	548	A	O3'-P-O5'	-5.03	96.46	104.00
7	A	126	A	O3'-P-O5'	-5.02	96.47	104.00
7	A	129	C	O3'-P-O5'	-5.02	96.48	104.00
7	A	1031	C	C4'-C3'-O3'	-5.02	105.48	113.00
30	a	924	A	O3'-P-O5'	-5.02	96.48	104.00
7	A	467	C	O3'-P-O5'	-5.01	96.48	104.00
30	a	893	C	C4'-C3'-O3'	-5.01	105.48	113.00
30	a	19	U	C4'-C3'-C2'	-5.01	97.59	102.60
7	A	701	G	O3'-P-O5'	-5.01	96.48	104.00
7	A	1841	G	C4'-C3'-O3'	-5.01	105.48	113.00
30	a	395	U	O3'-P-O5'	-5.01	96.48	104.00
7	A	2271	G	C1'-C2'-O2'	5.01	115.91	108.40
7	A	386	U	O3'-P-O5'	-5.00	96.50	104.00
7	A	828	A	C4'-C3'-O3'	-5.00	105.50	113.00
7	A	1383	U	O3'-P-O5'	-5.00	96.50	104.00
31	e	55	GLU	CB-CG-CD	5.00	121.10	112.60

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	41	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	0	6	ARG	Sidechain
3	2	36	ARG	Sidechain
4	3	13	ARG	Sidechain
7	A	1363	G	Sidechain
7	A	2497	A	Sidechain
7	A	2593	A	Sidechain
7	A	510	G	Sidechain
7	A	558	G	Sidechain
9	C	13	ARG	Sidechain
9	C	14	ARG	Sidechain
9	C	156	ARG	Sidechain
9	C	189	ARG	Sidechain
9	C	212	ARG	Sidechain
9	C	217	ARG	Sidechain
9	C	238	ARG	Sidechain
9	C	274	ARG	Sidechain
9	C	43	ARG	Sidechain
9	C	87	ARG	Sidechain
10	D	130	ARG	Sidechain
10	D	57	ARG	Sidechain
10	D	8	ARG	Sidechain
11	E	106	ARG	Sidechain
11	E	107	ARG	Sidechain
16	L	60	ARG	Sidechain
19	O	17	ARG	Sidechain
20	P	104	ARG	Sidechain
20	P	94	ARG	Sidechain
21	Q	51	ARG	Sidechain
25	U	32	ARG	Sidechain
27	X	16	ASN	Peptide
27	X	3	ARG	Sidechain
48	f	77	ARG	Sidechain
48	f	87	ARG	Sidechain
40	g	138	ARG	Sidechain
40	g	14	PRO	Peptide
46	h	42	ARG	Sidechain
46	h	79	ARG	Sidechain
33	l	123	ARG	Sidechain
35	q	4	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	433	0	450	1	0
2	1	403	0	411	0	0
3	2	368	0	410	0	0
4	3	522	0	577	4	0
5	4	297	0	339	0	0
6	6	356	0	346	3	0
7	A	58964	0	29662	61	0
8	B	2392	0	1213	1	0
9	C	2094	0	2181	2	0
10	D	1575	0	1642	4	0
11	E	1567	0	1652	2	0
12	F	1405	0	1467	4	0
13	G	1342	0	1388	1	0
14	J	1142	0	1182	2	0
15	K	921	0	977	4	0
16	L	1082	0	1132	2	0
17	M	1076	0	1145	5	0
18	N	954	0	983	3	0
19	O	913	0	947	1	0
20	P	945	0	1020	3	0
21	Q	950	0	1018	5	0
22	R	795	0	838	3	0
23	S	850	0	911	2	0
24	T	716	0	764	1	0
25	U	770	0	824	0	0
26	W	650	0	662	0	0
27	X	468	0	514	3	0
28	Y	532	0	569	0	0
29	Z	456	0	491	0	0
30	a	32891	0	16559	43	0
31	e	1170	0	1247	9	0
32	k	847	0	860	7	0
33	l	1047	0	1107	8	0
34	o	730	0	759	1	0
35	q	699	0	739	0	0
36	t	658	0	715	0	0
37	w	1645	0	829	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	y	1645	0	829	0	0
38	8	120	0	65	0	0
39	c	1607	0	1644	5	0
40	g	1199	0	1256	2	0
41	i	994	0	1035	0	0
42	j	788	0	832	1	0
43	m	942	0	1006	3	0
44	n	498	0	529	0	0
45	s	668	0	682	1	0
46	h	958	0	1020	14	0
47	r	522	0	558	3	0
48	f	755	0	746	2	0
49	7	67	0	71	0	0
50	0	1	0	0	0	0
50	1	1	0	0	0	0
50	4	1	0	0	0	0
50	6	1	0	0	0	0
50	n	1	0	0	0	0
51	A	155	0	0	0	0
51	B	1	0	0	0	0
51	C	1	0	0	0	0
51	D	1	0	0	0	0
51	a	40	0	0	0	0
51	w	1	0	0	0	0
52	A	40	0	0	0	0
52	C	2	0	0	0	0
52	U	1	0	0	0	0
53	y	7	0	7	1	0
54	3	3	0	0	0	0
54	7	8	0	0	0	0
54	A	811	0	0	0	0
54	B	5	0	0	0	0
54	C	15	0	0	0	0
54	D	1	0	0	0	0
54	E	5	0	0	0	0
54	L	5	0	0	0	0
54	N	3	0	0	0	0
54	P	3	0	0	0	0
54	Q	3	0	0	0	0
54	T	1	0	0	0	0
54	a	132	0	0	0	0
54	i	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	j	1	0	0	0	0
54	k	1	0	0	0	0
54	w	21	0	0	0	0
54	y	3	0	0	0	0
All	All	136664	0	88810	188	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 1.

All (188) 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)
21:Q:94:MET:HE1	22:R:13:LYS:HB2	1.61	0.81
53:y:101:PRO:N	37:w:77:A:HO2'	1.84	0.74
32:k:102:LEU:HB3	32:k:107:LEU:HD21	1.68	0.74
46:h:11:LEU:HD22	46:h:79:ARG:HD2	1.74	0.70
30:a:510:C:O2'	30:a:558:C:O2'	2.08	0.69
7:A:1808:U:H5	7:A:1813:A:N7	1.91	0.69
48:f:89:ILE:HD13	48:f:91:VAL:HG23	1.75	0.68
30:a:985:A:H4'	30:a:986:G:H5''	1.80	0.64
7:A:790:A:O2'	7:A:1704:U:OP1	2.13	0.64
30:a:509:G:H4'	30:a:556:A:C5	2.34	0.63
7:A:1411:U:HO2'	7:A:2241:A:H8	1.46	0.63
11:E:32:VAL:HG21	11:E:108:LEU:HD23	1.82	0.61
7:A:761:U:H2'	7:A:763:A:H2	1.66	0.61
17:M:77:LYS:NZ	17:M:86:GLY:O	2.34	0.60
39:c:141:MET:HE3	39:c:148:VAL:HG12	1.81	0.60
1:O:27:MET:HE1	23:S:35:ILE:HA	1.83	0.60
32:k:89:LYS:HD3	32:k:115:VAL:HG23	1.82	0.60
31:e:9:LEU:HD12	31:e:68:LYS:HE3	1.82	0.59
7:A:2435:C:C6	16:L:69:ILE:HD13	2.37	0.59
30:a:545:C:HO2'	30:a:546:G:H8	1.51	0.59
7:A:2906:U:O2	18:N:41:ARG:NH2	2.36	0.58
40:g:26:LEU:HD13	40:g:101:LEU:HD22	1.86	0.58
7:A:1327:U:H5	7:A:1365:U:O2	1.87	0.57
33:l:47:CYS:SG	33:l:50:VAL:HG13	2.44	0.57
27:X:6:VAL:HG21	27:X:47:VAL:HB	1.88	0.55
33:l:119:GLY:HA3	33:l:130:TYR:HB3	1.88	0.55
7:A:2595:A:N1	15:K:28:SER:OG	2.39	0.54
30:a:340:G:C2	30:a:341:C:C2	2.95	0.54
7:A:2590:A:N3	15:K:23:LYS:NZ	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:e:111:VAL:HG13	31:e:137:ILE:HG13	1.89	0.54
30:a:1444:G:H2'	30:a:1445:U:C6	2.43	0.54
32:k:89:LYS:HE2	32:k:113:ARG:HB2	1.90	0.53
33:l:64:LYS:HB2	33:l:87:LEU:HD13	1.91	0.52
43:m:29:THR:O	43:m:33:VAL:HG12	2.09	0.52
31:e:94:ILE:HB	31:e:136:MET:HE3	1.92	0.52
13:G:51:LEU:HD21	13:G:73:LEU:HD13	1.92	0.51
30:a:527:C:H2'	30:a:539:G:C8	2.46	0.51
30:a:1411:C:O2	30:a:1510:A:N1	2.44	0.51
31:e:94:ILE:HB	31:e:136:MET:CE	2.41	0.51
33:l:83:ILE:HG22	33:l:120:VAL:HG12	1.91	0.50
30:a:778:G:H4'	30:a:1523:A:H4'	1.94	0.50
7:A:761:U:H2'	7:A:763:A:C2	2.46	0.49
30:a:661:U:O4	30:a:761:G:O2'	2.30	0.49
17:M:54:MET:HE1	17:M:104:PHE:CG	2.47	0.49
21:Q:94:MET:HE2	22:R:4:ILE:HG12	1.94	0.49
7:A:840:A:OP2	7:A:2100:A:O2'	2.28	0.49
4:3:31:HIS:HD2	7:A:2450:G:N7	2.10	0.49
6:6:33:VAL:HG11	12:F:106:VAL:HG13	1.95	0.49
7:A:1028:C:O2	7:A:1028:C:O5'	2.30	0.49
20:P:39:ARG:NH2	30:a:354:G:OP1	2.45	0.48
7:A:1947:A:H8	7:A:1948:A:H62	1.62	0.48
30:a:244:G:H2'	30:a:245:C:O4'	2.14	0.48
46:h:11:LEU:HD13	46:h:79:ARG:HB3	1.96	0.48
30:a:723:G:H2'	30:a:724:A:C8	2.49	0.48
32:k:89:LYS:HG3	32:k:114:ASP:HA	1.96	0.48
7:A:1066:A:N1	7:A:1187:U:O2'	2.40	0.47
7:A:2785:U:H5	7:A:2787:A:N7	2.13	0.47
30:a:337:A:C6	30:a:340:G:C2	3.02	0.47
16:L:17:ASN:HD21	16:L:27:ASN:HD22	1.61	0.47
9:C:144:ILE:HG21	9:C:184:ILE:HD13	1.97	0.47
24:T:58:ASN:ND2	24:T:77:ARG:HH11	2.12	0.47
30:a:545:C:O2'	30:a:546:G:H8	1.98	0.47
30:a:955:G:C2	30:a:956:A:C8	3.03	0.47
30:a:51:U:O2	30:a:370:G:H1'	2.14	0.47
30:a:337:A:C2	30:a:340:G:C4	3.03	0.47
7:A:2320:U:OP1	7:A:2409:U:O2'	2.30	0.47
23:S:10:VAL:HG11	23:S:46:ILE:HG21	1.97	0.47
7:A:1681:U:H2'	7:A:1682:C:C6	2.50	0.47
46:h:77:LEU:HB3	46:h:79:ARG:HH12	1.80	0.47
10:D:110:VAL:HG13	10:D:200:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:140:A:N1	7:A:1640:G:O2'	2.44	0.46
40:g:16:PRO:C	40:g:17:ILE:HD12	2.40	0.46
7:A:2231:C:O2'	7:A:2233:C:OP1	2.28	0.46
30:a:19:U:H2'	30:a:20:C:C6	2.50	0.46
30:a:317:G:O2'	30:a:616:A:N1	2.49	0.46
7:A:1074:A:N3	7:A:2515:G:O2'	2.39	0.46
10:D:28:ILE:HD13	10:D:188:ILE:HD12	1.96	0.46
30:a:959:A:N7	43:m:105:ASN:ND2	2.63	0.46
30:a:1365:G:H2'	30:a:1366:A:C8	2.51	0.46
7:A:2229:C:O2	7:A:2255:C:N4	2.48	0.46
31:e:55:GLU:HG3	31:e:57:PRO:HD2	1.98	0.46
32:k:118:VAL:N	32:k:119:PRO:CD	2.79	0.46
45:s:36:ARG:NH2	45:s:75:ALA:O	2.49	0.46
7:A:999:A:OP2	17:M:18:ARG:NH2	2.49	0.46
7:A:2498:A:H4'	17:M:56:ARG:HD2	1.98	0.45
10:D:126:HIS:CD2	10:D:159:LEU:HB3	2.51	0.45
22:R:25:LEU:HD13	22:R:33:VAL:HG21	1.98	0.45
30:a:699:G:H2'	30:a:700:G:O4'	2.16	0.45
46:h:108:THR:HG23	46:h:123:ALA:N	2.31	0.45
30:a:676:G:H4'	34:o:51:HIS:CD2	2.51	0.45
33:l:123:ARG:HB2	33:l:123:ARG:NH1	2.31	0.45
7:A:1292:G:H1	21:Q:37:GLN:HE21	1.64	0.45
30:a:108:C:H2'	30:a:109:G:O4'	2.17	0.45
7:A:183:A:OP1	7:A:184:G:H5''	2.17	0.45
7:A:1074:A:N6	7:A:1171:G:H2'	2.32	0.45
46:h:22:HIS:O	46:h:72:ARG:NH1	2.50	0.45
6:6:14:VAL:HG11	12:F:106:VAL:HG21	1.98	0.45
7:A:909:G:H2'	7:A:910:A:O4'	2.17	0.45
7:A:1359:G:C2	7:A:1368:U:H5''	2.51	0.45
7:A:1480:A:H2'	7:A:1481:G:O4'	2.17	0.45
7:A:2096:G:O2'	7:A:2098:G:H5'	2.17	0.45
30:a:776:A:H2'	30:a:777:A:O4'	2.17	0.45
33:l:68:VAL:HG21	33:l:110:ILE:HD11	1.99	0.45
46:h:10:MET:HB3	46:h:27:ILE:HG21	1.97	0.45
46:h:11:LEU:HD11	46:h:128:LEU:HD11	1.97	0.45
7:A:760:G:H2'	7:A:761:U:C6	2.51	0.45
9:C:29:PRO:HG2	9:C:34:LEU:HD11	1.99	0.45
7:A:2092:C:O2	7:A:2479:A:N1	2.49	0.44
7:A:1618:A:H2'	7:A:1619:A:C8	2.52	0.44
10:D:17:ALA:HB2	10:D:23:ILE:HD13	1.98	0.44
30:a:682:G:H1'	47:r:69:GLN:HE22	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:31:HIS:HE1	7:A:2421:A:OP2	1.99	0.44
7:A:2055:U:H2'	7:A:2056:G:O4'	2.17	0.44
20:P:100:LEU:HD11	20:P:110:ILE:HD11	2.00	0.44
30:a:511:C:O4'	30:a:558:C:O2'	2.36	0.44
46:h:46:ILE:HG13	46:h:64:LEU:HA	1.99	0.44
18:N:59:ARG:HA	18:N:84:PHE:CZ	2.52	0.44
46:h:25:LEU:HD11	46:h:64:LEU:HB3	1.98	0.44
7:A:210:A:H2'	7:A:211:C:O4'	2.18	0.44
7:A:1710:A:H2'	7:A:1711:G:O4'	2.17	0.44
12:F:79:LEU:HD13	12:F:85:ILE:HG21	2.00	0.44
33:l:86:ASN:HD21	33:l:118:ALA:HB3	1.82	0.44
7:A:614:G:H2'	7:A:2059:A:N7	2.33	0.43
7:A:1377:G:O2'	7:A:1432:A:N1	2.46	0.43
47:r:70:MET:HE2	48:f:89:ILE:HG12	2.00	0.43
30:a:40:G:H4'	30:a:556:A:N6	2.33	0.43
30:a:673:G:H22	30:a:750:G:H1	1.65	0.43
4:3:26:HIS:CD2	4:3:46:LYS:O	2.71	0.43
30:a:271:A:H2'	30:a:272:C:C5	2.53	0.43
33:l:50:VAL:HG21	33:l:89:GLU:HA	2.00	0.43
6:6:36:CYS:SG	6:6:37:SER:N	2.91	0.43
7:A:2009:G:O2'	7:A:2011:U:OP2	2.36	0.43
7:A:6:A:O2'	14:J:136:GLN:NE2	2.52	0.43
7:A:1259:G:OP1	21:Q:22:LYS:NZ	2.41	0.43
15:K:24:VAL:HG13	15:K:33:ALA:HB2	2.00	0.43
30:a:34:A:H2'	30:a:35:A:C8	2.54	0.43
30:a:1238:A:O2'	37:w:31:G:OP1	2.36	0.43
4:3:26:HIS:HD2	4:3:46:LYS:O	2.02	0.43
7:A:1482:G:H2'	7:A:1483:A:O4'	2.19	0.43
7:A:2360:G:O2'	7:A:2365:A:N1	2.43	0.43
30:a:1440:C:H2'	30:a:1441:G:O4'	2.18	0.43
30:a:1123:C:H1'	39:c:177:LEU:HD13	2.01	0.43
30:a:1400:U:H2'	30:a:1401:G:C8	2.54	0.43
7:A:1033:C:O2'	7:A:1046:A:N3	2.46	0.42
7:A:1512:G:H2'	7:A:1513:U:O4'	2.19	0.42
32:k:22:ILE:HA	32:k:85:GLU:O	2.19	0.42
39:c:149:LYS:HE3	39:c:166:TYR:CD2	2.53	0.42
7:A:1411:U:O2'	7:A:2241:A:H8	2.00	0.42
30:a:539:G:H2'	30:a:539:G:N3	2.34	0.42
43:m:33:VAL:HG23	43:m:59:ILE:HG21	2.01	0.42
7:A:1066:A:C2	7:A:1187:U:C2	3.07	0.42
8:B:76:A:C2	8:B:97:A:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:j:92:LEU:HD12	42:j:98:ILE:CD1	2.50	0.42
46:h:100:GLY:O	46:h:101:LEU:HB2	2.20	0.42
30:a:728:C:N3	47:r:68:ARG:NH1	2.67	0.42
7:A:384:A:H2'	7:A:385:G:O4'	2.20	0.42
7:A:444:U:H5''	27:X:32:ASN:HB2	2.02	0.42
7:A:1961:A:H2'	7:A:1962:G:O4'	2.20	0.42
30:a:1324:U:H2'	30:a:1325:G:O4'	2.20	0.42
46:h:17:ALA:HB3	46:h:25:LEU:HD23	2.01	0.42
31:e:36:LEU:HD21	31:e:134:ILE:HD12	2.02	0.42
30:a:1116:G:H5''	39:c:171:THR:HG22	2.02	0.42
7:A:523:G:H4'	7:A:548:A:N1	2.35	0.42
31:e:156:LEU:HA	46:h:73:VAL:HG22	2.01	0.42
32:k:86:VAL:HB	32:k:109:VAL:HG22	2.01	0.42
7:A:576:G:N3	7:A:576:G:H2'	2.35	0.41
46:h:45:PHE:HB3	46:h:66:TYR:HB3	2.01	0.41
39:c:147:GLY:HA3	39:c:171:THR:O	2.20	0.41
7:A:1807:U:H2'	7:A:1813:A:N6	2.35	0.41
21:Q:58:ARG:HA	21:Q:61:TRP:CE3	2.56	0.41
11:E:131:LEU:HD21	11:E:142:ILE:HD12	2.03	0.41
7:A:740:A:O2'	7:A:1392:A:N3	2.45	0.41
7:A:1404:A:OP1	27:X:12:THR:HG21	2.21	0.41
7:A:1249:U:O2'	7:A:1277:A:N1	2.48	0.41
19:O:11:ARG:HD2	19:O:100:TYR:CZ	2.56	0.41
20:P:43:PHE:CE2	20:P:72:ARG:HG3	2.56	0.41
7:A:1366:C:O3'	18:N:108:ARG:NH2	2.48	0.41
15:K:35:ILE:HG21	15:K:103:ALA:HB3	2.03	0.41
14:J:110:LEU:O	14:J:112:LYS:NZ	2.53	0.40
7:A:685:U:H2'	7:A:686:C:C6	2.56	0.40
7:A:1877:A:H2'	7:A:1878:G:O4'	2.20	0.40
12:F:70:ALA:HB2	12:F:79:LEU:HD11	2.02	0.40
30:a:598:U:O2'	46:h:57:GLN:HB3	2.21	0.40
30:a:934:C:O2'	30:a:1512:A:N1	2.54	0.40
31:e:134:ILE:HA	31:e:137:ILE:HG22	2.04	0.40
17:M:54:MET:HE2	17:M:121:ALA:CB	2.50	0.40
30:a:1411:C:H2'	30:a:1412:C:O4'	2.22	0.40
31:e:134:ILE:O	31:e:137:ILE:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	53/59 (90%)	50 (94%)	3 (6%)	0	100	100
2	1	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
3	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
4	3	63/66 (96%)	63 (100%)	0	0	100	100
5	4	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
6	6	44/65 (68%)	39 (89%)	5 (11%)	0	100	100
9	C	271/277 (98%)	263 (97%)	8 (3%)	0	100	100
10	D	205/209 (98%)	200 (98%)	5 (2%)	0	100	100
11	E	204/207 (99%)	200 (98%)	4 (2%)	0	100	100
12	F	176/179 (98%)	167 (95%)	9 (5%)	0	100	100
13	G	173/179 (97%)	162 (94%)	10 (6%)	1 (1%)	21	27
14	J	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
15	K	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
16	L	144/146 (99%)	139 (96%)	4 (3%)	1 (1%)	18	23
17	M	133/144 (92%)	131 (98%)	2 (2%)	0	100	100
18	N	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
19	O	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
20	P	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
21	Q	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
22	R	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
23	S	108/113 (96%)	107 (99%)	1 (1%)	0	100	100
24	T	87/95 (92%)	86 (99%)	1 (1%)	0	100	100
25	U	100/103 (97%)	99 (99%)	1 (1%)	0	100	100
26	W	83/94 (88%)	80 (96%)	3 (4%)	0	100	100
27	X	59/62 (95%)	57 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Y	63/66 (96%)	63 (100%)	0	0	100	100
29	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
31	e	156/166 (94%)	140 (90%)	14 (9%)	2 (1%)	9	10
32	k	113/131 (86%)	95 (84%)	16 (14%)	2 (2%)	6	6
33	l	133/138 (96%)	125 (94%)	8 (6%)	0	100	100
34	o	85/89 (96%)	78 (92%)	7 (8%)	0	100	100
35	q	83/87 (95%)	75 (90%)	8 (10%)	0	100	100
36	t	84/88 (96%)	80 (95%)	4 (5%)	0	100	100
39	c	202/206 (98%)	185 (92%)	17 (8%)	0	100	100
40	g	149/156 (96%)	140 (94%)	9 (6%)	0	100	100
41	i	126/130 (97%)	118 (94%)	8 (6%)	0	100	100
42	j	96/102 (94%)	91 (95%)	5 (5%)	0	100	100
43	m	116/121 (96%)	115 (99%)	1 (1%)	0	100	100
44	n	58/61 (95%)	58 (100%)	0	0	100	100
45	s	81/92 (88%)	77 (95%)	4 (5%)	0	100	100
46	h	120/132 (91%)	95 (79%)	20 (17%)	5 (4%)	2	1
47	r	63/79 (80%)	61 (97%)	2 (3%)	0	100	100
48	f	90/95 (95%)	85 (94%)	5 (6%)	0	100	100
49	7	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	4733/4978 (95%)	4503 (95%)	219 (5%)	11 (0%)	44	55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	e	131	ASN
32	k	34	VAL
46	h	113	LEU
46	h	122	GLN
46	h	44	GLY
46	h	46	ILE
16	L	29	LYS
31	e	149	ARG
32	k	49	ALA
46	h	80	ILE
13	G	127	PRO

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	
1	0	49/53 (92%)	48 (98%)	1 (2%)	48	67
2	1	46/47 (98%)	46 (100%)	0	100	100
3	2	39/39 (100%)	39 (100%)	0	100	100
4	3	55/56 (98%)	54 (98%)	1 (2%)	51	70
5	4	35/35 (100%)	35 (100%)	0	100	100
6	6	39/54 (72%)	37 (95%)	2 (5%)	21	32
9	C	221/225 (98%)	219 (99%)	2 (1%)	70	84
10	D	168/170 (99%)	168 (100%)	0	100	100
11	E	169/170 (99%)	169 (100%)	0	100	100
12	F	153/154 (99%)	153 (100%)	0	100	100
13	G	148/151 (98%)	147 (99%)	1 (1%)	76	87
14	J	122/123 (99%)	122 (100%)	0	100	100
15	K	101/101 (100%)	101 (100%)	0	100	100
16	L	110/110 (100%)	110 (100%)	0	100	100
17	M	109/116 (94%)	109 (100%)	0	100	100
18	N	99/100 (99%)	99 (100%)	0	100	100
19	O	93/93 (100%)	93 (100%)	0	100	100
20	P	100/100 (100%)	100 (100%)	0	100	100
21	Q	97/98 (99%)	97 (100%)	0	100	100
22	R	84/84 (100%)	84 (100%)	0	100	100
23	S	91/93 (98%)	91 (100%)	0	100	100
24	T	80/85 (94%)	80 (100%)	0	100	100
25	U	86/87 (99%)	86 (100%)	0	100	100
26	W	65/74 (88%)	65 (100%)	0	100	100
27	X	49/50 (98%)	49 (100%)	0	100	100
28	Y	56/57 (98%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	Z	52/53 (98%)	52 (100%)	0	100	100
31	e	122/130 (94%)	114 (93%)	8 (7%)	15	21
32	k	87/100 (87%)	83 (95%)	4 (5%)	24	36
33	l	114/116 (98%)	109 (96%)	5 (4%)	25	38
34	o	82/83 (99%)	82 (100%)	0	100	100
35	q	78/80 (98%)	76 (97%)	2 (3%)	40	59
36	t	69/70 (99%)	69 (100%)	0	100	100
39	c	167/168 (99%)	167 (100%)	0	100	100
40	g	127/132 (96%)	124 (98%)	3 (2%)	43	62
41	i	101/102 (99%)	101 (100%)	0	100	100
42	j	89/92 (97%)	89 (100%)	0	100	100
43	m	101/104 (97%)	100 (99%)	1 (1%)	68	82
44	n	53/54 (98%)	53 (100%)	0	100	100
45	s	72/81 (89%)	72 (100%)	0	100	100
46	h	102/112 (91%)	92 (90%)	10 (10%)	7	10
47	r	56/64 (88%)	55 (98%)	1 (2%)	51	70
48	f	81/84 (96%)	79 (98%)	2 (2%)	42	60
49	7	6/6 (100%)	6 (100%)	0	100	100
All	All	4023/4156 (97%)	3980 (99%)	43 (1%)	63	81

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	12	LYS
4	3	31	HIS
6	6	36	CYS
6	6	39	CYS
9	C	87	ARG
9	C	262	LYS
13	G	18	THR
31	e	23	LYS
31	e	52	LYS
31	e	133	PRO
31	e	136	MET
31	e	137	ILE
31	e	140	THR

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Mol	Chain	Res	Type
31	e	146	GLU
31	e	148	LYS
32	k	34	VAL
32	k	38	ASP
32	k	44	ILE
32	k	52	LEU
33	l	10	LYS
33	l	50	VAL
33	l	123	ARG
33	l	128	SER
33	l	134	LYS
35	q	8	LYS
35	q	26	VAL
40	g	23	VAL
40	g	43	LEU
40	g	59	MET
43	m	33	VAL
46	h	22	HIS
46	h	25	LEU
46	h	26	GLU
46	h	45	PHE
46	h	66	TYR
46	h	71	GLU
46	h	74	ILE
46	h	110	GLN
46	h	112	VAL
46	h	128	LEU
47	r	53	ASN
48	f	14	ILE
48	f	52	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	40	HIS
1	0	50	ASN
2	1	4	ASN
4	3	26	HIS
4	3	31	HIS
4	3	35	ASN
4	3	60	GLN
9	C	86	ASN

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Mol	Chain	Res	Type
9	C	163	GLN
10	D	95	GLN
10	D	128	GLN
11	E	8	ASN
11	E	46	GLN
12	F	27	GLN
12	F	46	ASN
12	F	161	ASN
13	G	129	GLN
14	J	59	ASN
14	J	136	GLN
15	K	34	ASN
16	L	17	ASN
16	L	83	ASN
18	N	27	ASN
18	N	72	ASN
20	P	2	GLN
21	Q	37	GLN
22	R	101	ASN
23	S	73	GLN
24	T	58	ASN
27	X	17	ASN
27	X	23	ASN
28	Y	16	GLN
29	Z	59	GLN
32	k	40	HIS
32	k	103	GLN
33	l	5	ASN
33	l	86	ASN
33	l	88	GLN
34	o	51	HIS
36	t	15	ASN
39	c	64	ASN
39	c	133	GLN
40	g	86	GLN
42	j	56	HIS
43	m	101	ASN
43	m	105	ASN
43	m	118	ASN
46	h	57	GLN
46	h	99	ASN
46	h	122	GLN

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Mol	Chain	Res	Type
47	r	21	ASN
47	r	57	GLN
47	r	69	GLN
48	f	66	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	a	1532/1554 (98%)	314 (20%)	0
37	w	76/77 (98%)	13 (17%)	0
37	y	76/77 (98%)	12 (15%)	0
38	8	5/6 (83%)	1 (20%)	0
7	A	2737/2925 (93%)	351 (12%)	82 (2%)
8	B	111/119 (93%)	17 (15%)	5 (4%)
All	All	4537/4758 (95%)	708 (15%)	87 (1%)

All (708) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	12	A
7	A	13	A
7	A	34	U
7	A	45	G
7	A	46	C
7	A	60	G
7	A	63	G
7	A	71	A
7	A	74	U
7	A	75	G
7	A	93	C
7	A	118	A
7	A	119	U
7	A	163	U
7	A	164	U
7	A	166	A
7	A	175	G
7	A	176	A
7	A	177	G
7	A	183	A
7	A	184	G
7	A	185	A

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Mol	Chain	Res	Type
7	A	199	A
7	A	202	A
7	A	203	U
7	A	216	A
7	A	219	A
7	A	224	A
7	A	225	A
7	A	226	A
7	A	232	U
7	A	233	G
7	A	236	A
7	A	248	G
7	A	251	G
7	A	258	A
7	A	268	A
7	A	275	A
7	A	284	C
7	A	285	U
7	A	288	C
7	A	300	G
7	A	301	U
7	A	302	A
7	A	308	C
7	A	309	U
7	A	310	C
7	A	334	G
7	A	345	A
7	A	346	G
7	A	355	A
7	A	373	A
7	A	374	A
7	A	407	A
7	A	408	G
7	A	410	G
7	A	418	A
7	A	419	G
7	A	433	G
7	A	458	G
7	A	459	A
7	A	471	G
7	A	487	G
7	A	491	C

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Mol	Chain	Res	Type
7	A	498	U
7	A	503	C
7	A	504	A
7	A	528	G
7	A	551	A
7	A	554	U
7	A	555	C
7	A	556	C
7	A	568	G
7	A	576	G
7	A	577	U
7	A	578	A
7	A	579	G
7	A	584	A
7	A	591	U
7	A	595	G
7	A	600	A
7	A	607	G
7	A	615	U
7	A	616	A
7	A	617	G
7	A	619	A
7	A	630	A
7	A	631	G
7	A	647	A
7	A	658	A
7	A	659	A
7	A	673	A
7	A	680	G
7	A	683	A
7	A	691	U
7	A	692	A
7	A	700	U
7	A	701	G
7	A	732	A
7	A	733	U
7	A	761	U
7	A	762	A
7	A	764	C
7	A	777	C
7	A	793	U
7	A	794	U

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Mol	Chain	Res	Type
7	A	811	A
7	A	812	G
7	A	822	G
7	A	829	A
7	A	831	U
7	A	832	G
7	A	852	G
7	A	859	C
7	A	866	A
7	A	874	U
7	A	875	U
7	A	892	U
7	A	906	G
7	A	913	A
7	A	924	U
7	A	931	C
7	A	940	G
7	A	943	A
7	A	944	C
7	A	947	A
7	A	957	A
7	A	959	C
7	A	964	A
7	A	973	G
7	A	976	U
7	A	987	A
7	A	990	C
7	A	991	A
7	A	992	G
7	A	1005	A
7	A	1007	G
7	A	1020	A
7	A	1029	A
7	A	1042	A
7	A	1051	C
7	A	1058	U
7	A	1059	A
7	A	1068	G
7	A	1072	A
7	A	1079	U
7	A	1084	A
7	A	1093	G

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Mol	Chain	Res	Type
7	A	1099	C
7	A	1153	G
7	A	1154	U
7	A	1155	C
7	A	1156	G
7	A	1157	A
7	A	1158	G
7	A	1174	A
7	A	1178	U
7	A	1179	A
7	A	1180	C
7	A	1181	C
7	A	1185	G
7	A	1188	A
7	A	1189	A
7	A	1199	C
7	A	1246	G
7	A	1247	G
7	A	1278	G
7	A	1293	A
7	A	1296	G
7	A	1311	G
7	A	1312	A
7	A	1315	G
7	A	1339	A
7	A	1340	A
7	A	1341	U
7	A	1342	G
7	A	1346	A
7	A	1389	C
7	A	1391	U
7	A	1404	A
7	A	1418	U
7	A	1423	A
7	A	1435	U
7	A	1450	C
7	A	1457	U
7	A	1458	U
7	A	1459	U
7	A	1460	G
7	A	1461	A
7	A	1465	A

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Mol	Chain	Res	Type
7	A	1473	A
7	A	1474	C
7	A	1489	U
7	A	1490	A
7	A	1499	A
7	A	1507	U
7	A	1514	C
7	A	1525	G
7	A	1526	G
7	A	1528	U
7	A	1529	G
7	A	1531	G
7	A	1536	A
7	A	1539	C
7	A	1542	A
7	A	1543	U
7	A	1544	C
7	A	1557	G
7	A	1558	G
7	A	1595	U
7	A	1607	C
7	A	1608	A
7	A	1617	A
7	A	1626	U
7	A	1632	G
7	A	1653	A
7	A	1654	A
7	A	1691	A
7	A	1692	U
7	A	1693	C
7	A	1719	G
7	A	1752	G
7	A	1758	U
7	A	1759	U
7	A	1779	G
7	A	1791	A
7	A	1792	G
7	A	1793	G
7	A	1802	A
7	A	1811	C
7	A	1820	A
7	A	1829	C

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Mol	Chain	Res	Type
7	A	1830	G
7	A	1845	A
7	A	1858	A
7	A	1877	A
7	A	1887	G
7	A	1899	U
7	A	1900	A
7	A	1902	G
7	A	1935	G
7	A	1943	C
7	A	1947	A
7	A	1948	A
7	A	1958	G
7	A	1959	G
7	A	1966	A
7	A	1967	A
7	A	1984	U
7	A	1992	C
7	A	1996	C
7	A	1999	A
7	A	2000	A
7	A	2001	G
7	A	2011	U
7	A	2020	U
7	A	2022	U
7	A	2026	A
7	A	2052	A
7	A	2060	A
7	A	2061	G
7	A	2062	A
7	A	2072	C
7	A	2084	C
7	A	2085	G
7	A	2089	A
7	A	2090	G
7	A	2098	G
7	A	2122	G
7	A	2126	G
7	A	2128	U
7	A	2131	U
7	A	2132	A
7	A	2218	U

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Mol	Chain	Res	Type
7	A	2227	A
7	A	2232	G
7	A	2233	C
7	A	2240	U
7	A	2254	A
7	A	2267	G
7	A	2268	G
7	A	2297	A
7	A	2312	C
7	A	2315	A
7	A	2316	A
7	A	2318	G
7	A	2334	U
7	A	2337	G
7	A	2341	U
7	A	2348	C
7	A	2349	A
7	A	2350	G
7	A	2351	A
7	A	2354	G
7	A	2356	A
7	A	2363	C
7	A	2364	A
7	A	2376	C
7	A	2379	C
7	A	2408	G
7	A	2412	G
7	A	2414	C
7	A	2431	U
7	A	2435	C
7	A	2436	A
7	A	2453	C
7	A	2454	A
7	A	2458	G
7	A	2459	A
7	A	2464	A
7	A	2470	C
7	A	2476	G
7	A	2477	A
7	A	2505	A
7	A	2531	G
7	A	2534	G

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Mol	Chain	Res	Type
7	A	2547	A
7	A	2558	G
7	A	2559	U
7	A	2583	U
7	A	2595	A
7	A	2596	G
7	A	2602	C
7	A	2631	A
7	A	2632	G
7	A	2638	U
7	A	2642	U
7	A	2690	G
7	A	2692	G
7	A	2718	PSU
7	A	2720	C
7	A	2743	G
7	A	2755	U
7	A	2764	G
7	A	2773	G
7	A	2777	A
7	A	2786	A
7	A	2794	A
7	A	2807	A
7	A	2819	A
7	A	2820	U
7	A	2824	G
7	A	2826	A
7	A	2828	G
7	A	2845	A
7	A	2848	A
7	A	2860	A
7	A	2892	G
7	A	2893	A
7	A	2897	G
7	A	2918	G
8	B	10	G
8	B	12	U
8	B	14	G
8	B	15	C
8	B	23	U
8	B	38	U
8	B	43	A

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Mol	Chain	Res	Type
8	B	49	G
8	B	50	A
8	B	54	U
8	B	55	A
8	B	87	U
8	B	88	C
8	B	97	A
8	B	106	C
8	B	107	G
8	B	108	C
30	a	9	G
30	a	10	A
30	a	11	G
30	a	24	G
30	a	33	G
30	a	34	A
30	a	41	G
30	a	49	C
30	a	50	C
30	a	51	U
30	a	52	A
30	a	53	A
30	a	61	A
30	a	63	G
30	a	68	G
30	a	70	G
30	a	72	A
30	a	76	A
30	a	77	U
30	a	83	C
30	a	84	U
30	a	85	U
30	a	87	C
30	a	89	C
30	a	90	C
30	a	93	G
30	a	95	U
30	a	99	A
30	a	113	G
30	a	114	A
30	a	119	C
30	a	123	U

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Mol	Chain	Res	Type
30	a	127	U
30	a	128	A
30	a	130	C
30	a	133	G
30	a	143	C
30	a	144	U
30	a	145	G
30	a	146	G
30	a	158	G
30	a	159	A
30	a	160	A
30	a	161	A
30	a	162	C
30	a	168	C
30	a	172	U
30	a	173	A
30	a	180	G
30	a	181	G
30	a	188	G
30	a	189	A
30	a	192	C
30	a	194	C
30	a	195	A
30	a	197	G
30	a	209	A
30	a	213	G
30	a	218	U
30	a	219	U
30	a	222	G
30	a	224	U
30	a	231	U
30	a	234	A
30	a	248	C
30	a	253	U
30	a	255	G
30	a	259	G
30	a	272	C
30	a	274	G
30	a	275	C
30	a	281	A
30	a	283	G
30	a	297	G

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Mol	Chain	Res	Type
30	a	313	G
30	a	314	A
30	a	329	A
30	a	332	G
30	a	335	A
30	a	336	C
30	a	337	A
30	a	338	C
30	a	340	G
30	a	347	C
30	a	353	C
30	a	355	G
30	a	359	G
30	a	360	C
30	a	362	G
30	a	374	C
30	a	375	U
30	a	376	U
30	a	377	C
30	a	380	C
30	a	385	G
30	a	391	A
30	a	405	A
30	a	406	C
30	a	410	G
30	a	411	C
30	a	412	G
30	a	414	G
30	a	419	A
30	a	421	G
30	a	422	A
30	a	429	U
30	a	430	C
30	a	431	G
30	a	432	G
30	a	435	C
30	a	436	G
30	a	437	U
30	a	441	G
30	a	442	C
30	a	444	C
30	a	445	U

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Mol	Chain	Res	Type
30	a	450	U
30	a	451	U
30	a	456	A
30	a	461	C
30	a	463	A
30	a	465	U
30	a	467	C
30	a	470	U
30	a	471	U
30	a	474	A
30	a	475	A
30	a	477	A
30	a	479	G
30	a	483	G
30	a	485	A
30	a	493	G
30	a	494	G
30	a	497	C
30	a	503	C
30	a	504	A
30	a	505	G
30	a	507	A
30	a	508	A
30	a	509	G
30	a	510	C
30	a	514	G
30	a	519	A
30	a	520	C
30	a	521	U
30	a	525	U
30	a	526	G
30	a	527	C
30	a	530	G
30	a	536	G
30	a	539	G
30	a	540	U
30	a	541	A
30	a	542	A
30	a	544	A
30	a	546	G
30	a	551	U
30	a	552	G

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Mol	Chain	Res	Type
30	a	553	G
30	a	556	A
30	a	558	C
30	a	568	A
30	a	569	A
30	a	570	U
30	a	571	U
30	a	581	A
30	a	582	A
30	a	585	G
30	a	586	G
30	a	596	G
30	a	597	G
30	a	621	C
30	a	624	C
30	a	630	A
30	a	631	A
30	a	632	C
30	a	633	C
30	a	637	G
30	a	641	G
30	a	642	U
30	a	643	C
30	a	651	A
30	a	659	A
30	a	674	A
30	a	675	G
30	a	709	G
30	a	711	A
30	a	712	G
30	a	727	A
30	a	730	A
30	a	732	U
30	a	733	G
30	a	758	A
30	a	762	A
30	a	764	G
30	a	786	A
30	a	803	A
30	a	824	A
30	a	826	C
30	a	845	G

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Mol	Chain	Res	Type
30	a	849	G
30	a	850	U
30	a	853	C
30	a	856	C
30	a	869	C
30	a	880	U
30	a	924	A
30	a	925	A
30	a	936	G
30	a	941	C
30	a	944	C
30	a	945	A
30	a	970	U
30	a	971	U
30	a	976	G
30	a	978	A
30	a	979	A
30	a	981	G
30	a	985	A
30	a	986	G
30	a	987	A
30	a	994	C
30	a	1002	U
30	a	1003	G
30	a	1010	U
30	a	1014	A
30	a	1016	A
30	a	1030	G
30	a	1033	G
30	a	1035	C
30	a	1036	C
30	a	1039	U
30	a	1040	U
30	a	1041	C
30	a	1042	G
30	a	1044	G
30	a	1046	G
30	a	1049	G
30	a	1050	A
30	a	1051	G
30	a	1056	A
30	a	1058	G

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Mol	Chain	Res	Type
30	a	1063	G
30	a	1065	A
30	a	1074	G
30	a	1075	U
30	a	1096	U
30	a	1099	G
30	a	1104	G
30	a	1105	U
30	a	1111	A
30	a	1134	G
30	a	1136	U
30	a	1140	A
30	a	1148	G
30	a	1149	U
30	a	1155	A
30	a	1168	U
30	a	1176	A
30	a	1177	C
30	a	1178	A
30	a	1193	G
30	a	1205	A
30	a	1206	A
30	a	1220	U
30	a	1221	U
30	a	1222	A
30	a	1223	U
30	a	1236	A
30	a	1237	C
30	a	1247	A
30	a	1257	A
30	a	1266	A
30	a	1267	G
30	a	1269	G
30	a	1289	A
30	a	1290	U
30	a	1291	C
30	a	1296	A
30	a	1307	C
30	a	1309	G
30	a	1311	U
30	a	1314	G
30	a	1328	A

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Mol	Chain	Res	Type
30	a	1329	C
30	a	1331	C
30	a	1344	C
30	a	1345	U
30	a	1347	G
30	a	1355	A
30	a	1373	U
30	a	1389	U
30	a	1390	U
30	a	1406	C
30	a	1407	A
30	a	1415	U
30	a	1427	A
30	a	1449	U
30	a	1451	A
30	a	1455	A
30	a	1459	U
30	a	1462	U
30	a	1464	G
30	a	1497	G
30	a	1502	A
30	a	1504	G
30	a	1513	A
30	a	1515	G
30	a	1516	U
30	a	1527	G
30	a	1529	A
30	a	1530	G
30	a	1539	G
30	a	1540	G
37	y	9	A
37	y	14	A
37	y	18	U
37	y	19	G
37	y	20	G
37	y	21	U
37	y	22	A
37	y	47	G
37	y	48	U
37	y	49	C
37	y	59	A
37	y	75	C

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Mol	Chain	Res	Type
37	w	9	A
37	w	14	A
37	w	18	U
37	w	19	G
37	w	20	G
37	w	21	U
37	w	22	A
37	w	23	G
37	w	47	G
37	w	48	U
37	w	49	C
37	w	59	A
37	w	77	A
38	8	19	C

All (87) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	12	A
7	A	60	G
7	A	67	A
7	A	92	G
7	A	98	U
7	A	172	U
7	A	176	A
7	A	183	A
7	A	184	G
7	A	202	A
7	A	224	A
7	A	299	U
7	A	300	G
7	A	337	A
7	A	389	A
7	A	406	G
7	A	407	A
7	A	410	G
7	A	493	G
7	A	504	A
7	A	549	A
7	A	558	G
7	A	599	G
7	A	615	U

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Mol	Chain	Res	Type
7	A	662	U
7	A	691	U
7	A	727	A
7	A	732	A
7	A	793	U
7	A	811	A
7	A	831	U
7	A	852	G
7	A	855	G
7	A	874	U
7	A	990	C
7	A	1001	U
7	A	1004	U
7	A	1030	G
7	A	1041	C
7	A	1071	G
7	A	1092	A
7	A	1179	A
7	A	1180	C
7	A	1187	U
7	A	1188	A
7	A	1244	A
7	A	1246	G
7	A	1266	A
7	A	1278	G
7	A	1341	U
7	A	1344	C
7	A	1525	G
7	A	1530	G
7	A	1535	U
7	A	1543	U
7	A	1602	U
7	A	1653	A
7	A	1691	A
7	A	1751	U
7	A	1791	A
7	A	1876	A
7	A	1942	A
7	A	1947	A
7	A	2010	A
7	A	2026	A
7	A	2064	G

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Mol	Chain	Res	Type
7	A	2127	U
7	A	2311	G
7	A	2315	A
7	A	2316	A
7	A	2348	C
7	A	2349	A
7	A	2435	C
7	A	2459	A
7	A	2476	G
7	A	2533	U
7	A	2558	G
7	A	2610	G
7	A	2631	A
7	A	2785	U
7	A	2819	A
7	A	2892	G
8	B	37	A
8	B	48	G
8	B	49	G
8	B	85	U
8	B	106	C

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

3 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	$\# Z > 2$
7	2MA	A	2532	52,7,51	22,25,26	0.91	2 (9%)	32,37,40	1.26	3 (9%)
7	OMG	A	2280	52,7,37	23,26,27	0.31	0	32,38,41	0.64	1 (3%)
7	PSU	A	2718	7	18,21,22	0.97	1 (5%)	21,30,33	0.87	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
7	2MA	A	2532	52,7,51	-	2/7/25/26	0/3/3/3
7	OMG	A	2280	52,7,37	-	1/9/27/28	0/3/3/3
7	PSU	A	2718	7	-	1/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2718	PSU	C6-C5	3.56	1.39	1.35
7	A	2532	2MA	C6-N6	-2.29	1.28	1.34
7	A	2532	2MA	C1'-N9	-2.21	1.40	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2532	2MA	CM2-C2-N1	3.52	122.40	117.13
7	A	2532	2MA	C5-C4-N3	-2.68	124.36	127.18
7	A	2532	2MA	C2-N1-C6	2.64	122.16	118.10
7	A	2280	OMG	O2'-C2'-C1'	2.35	113.45	108.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2280	OMG	C1'-C2'-O2'-CM2
7	A	2532	2MA	C4'-C5'-O5'-P
7	A	2532	2MA	O4'-C1'-N9-C8
7	A	2718	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 248 ligands modelled in this entry, 247 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
53	PRO	y	101	37	6,7,8	0.80	0	7,8,10	0.92	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
53	PRO	y	101	37	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	y	101	PRO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

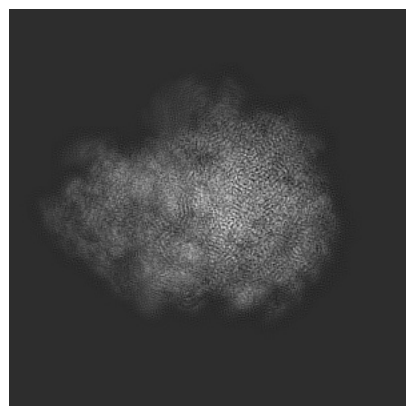
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18332. These allow visual inspection of the internal detail of the map and identification of artifacts.

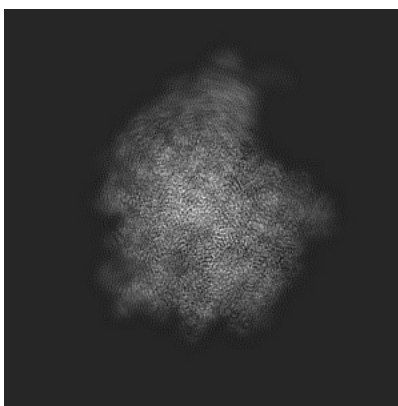
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

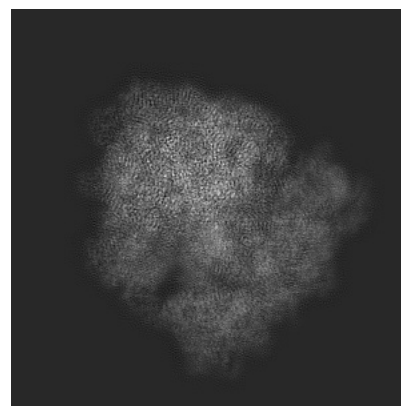
6.1.1 Primary map



X

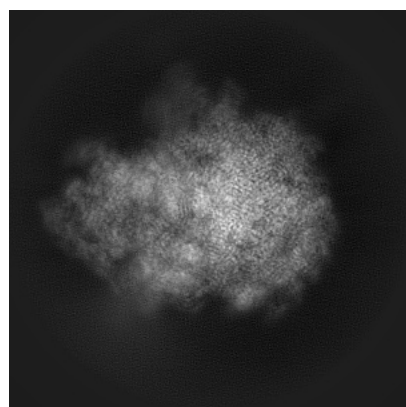


Y

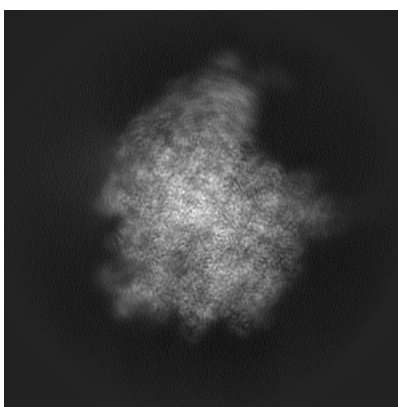


Z

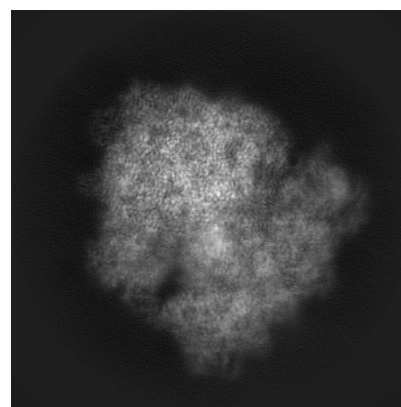
6.1.2 Raw map



X



Y

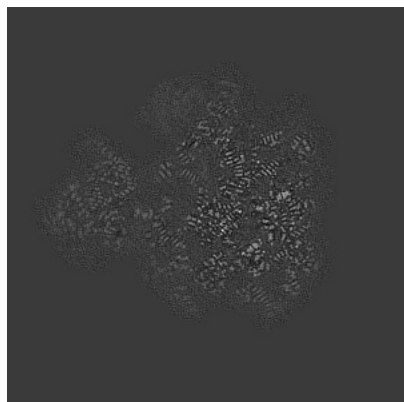


Z

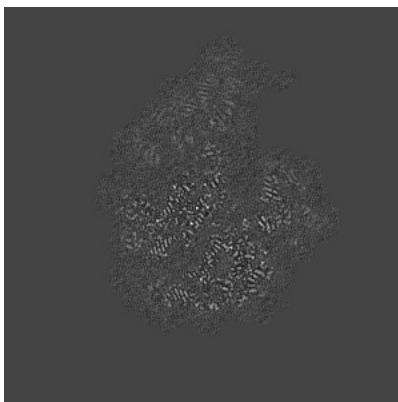
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

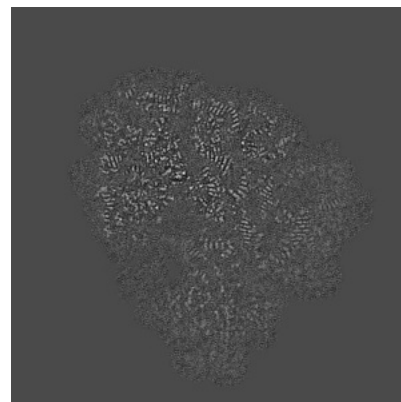
6.2.1 Primary map



X Index: 210

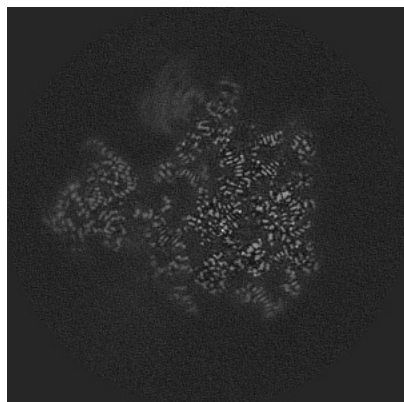


Y Index: 210

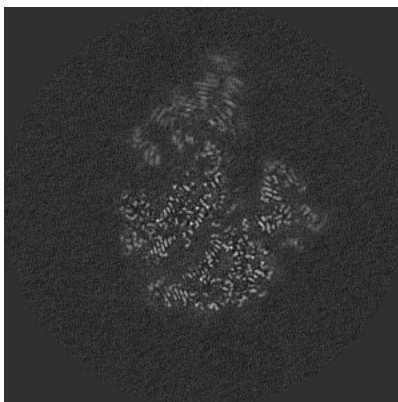


Z Index: 210

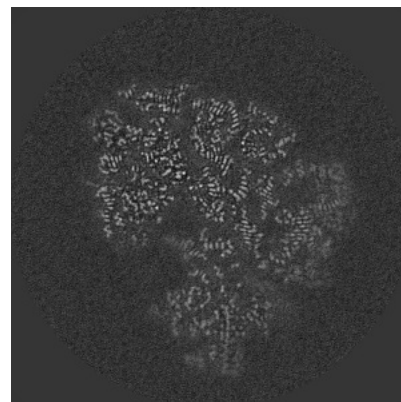
6.2.2 Raw map



X Index: 210



Y Index: 210

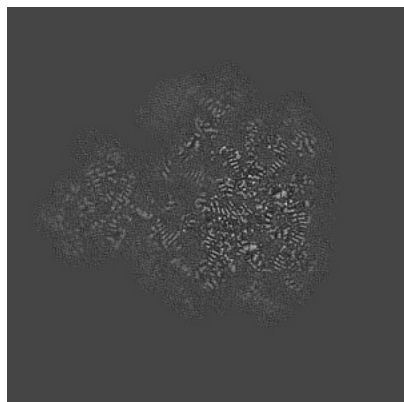


Z Index: 210

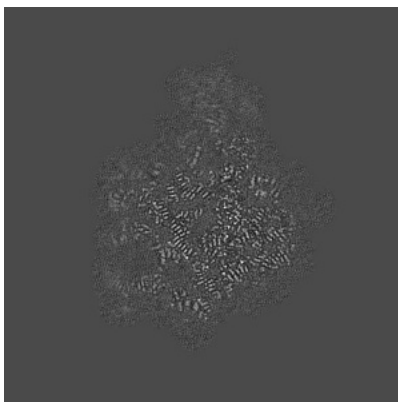
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

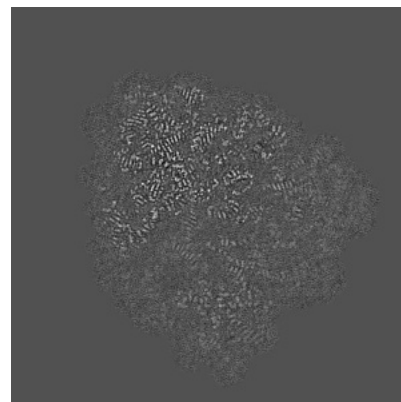
6.3.1 Primary map



X Index: 206

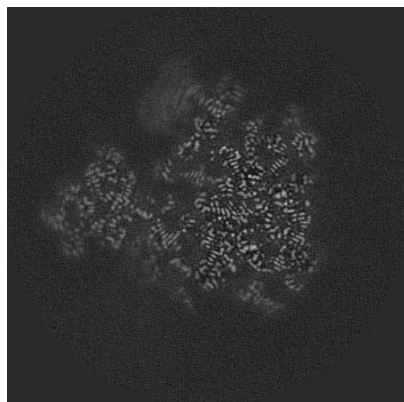


Y Index: 253

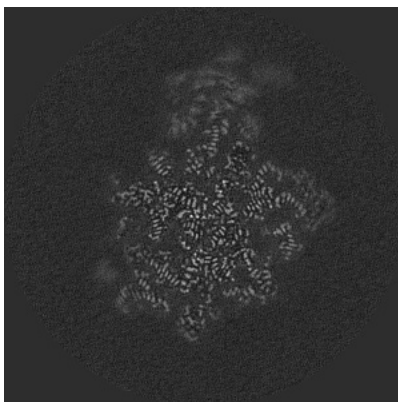


Z Index: 221

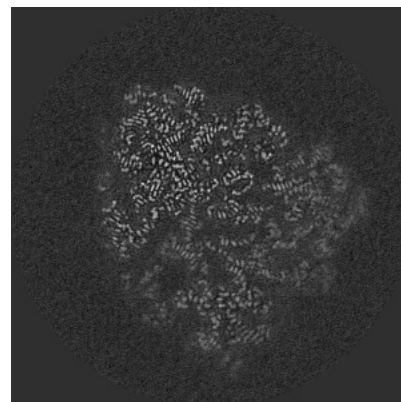
6.3.2 Raw map



X Index: 206



Y Index: 232

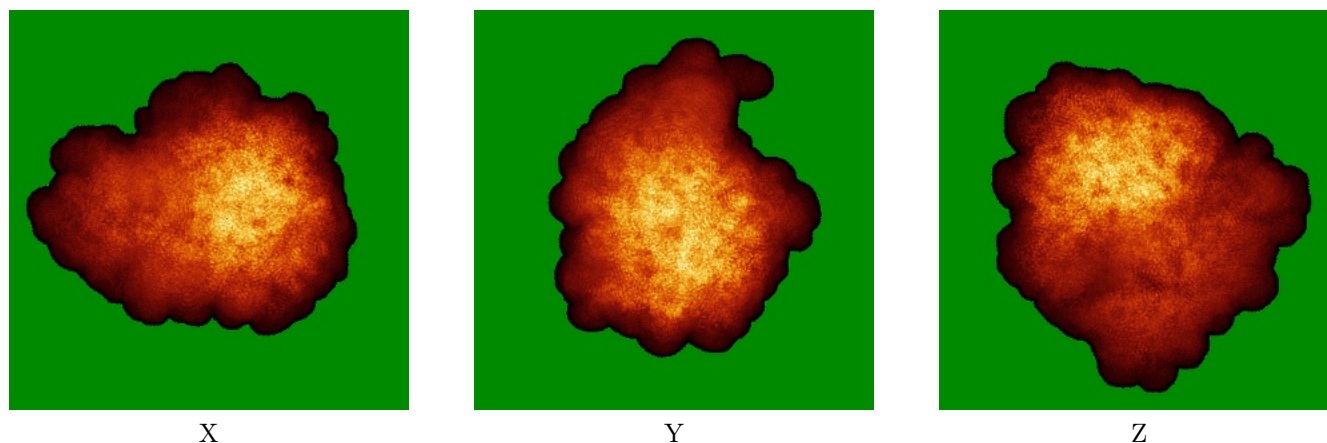


Z Index: 221

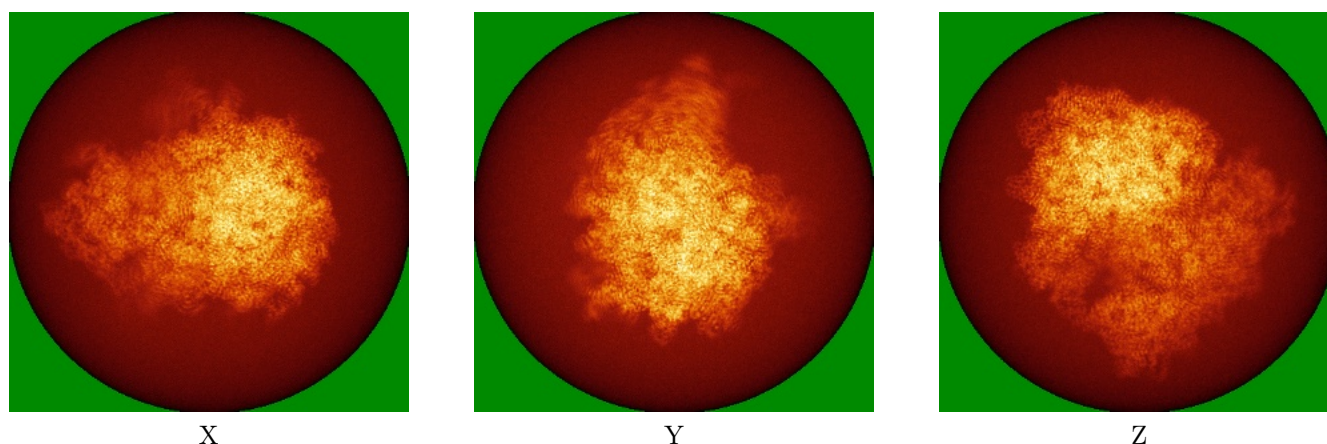
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

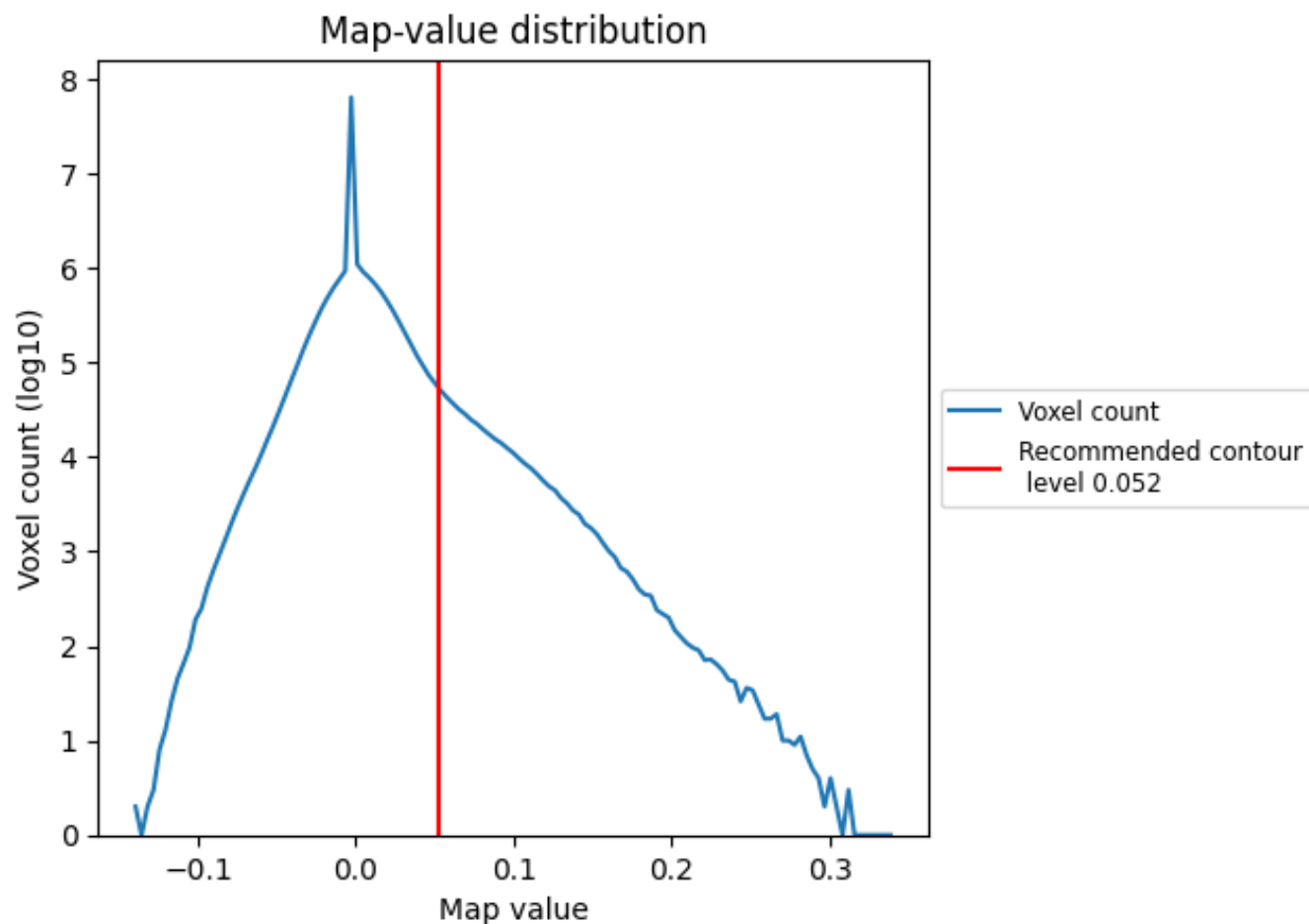
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

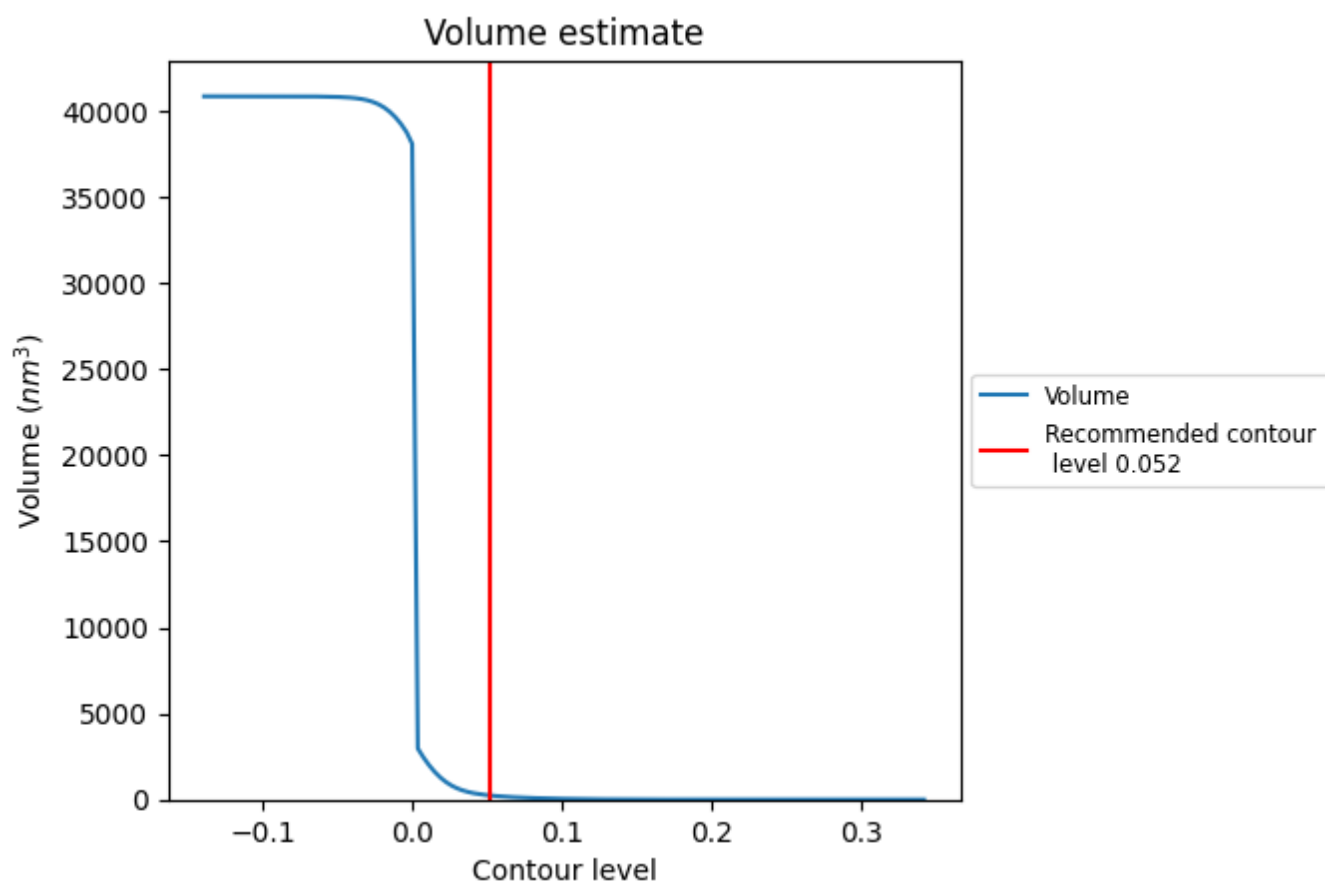
This section contains the results of statistical analysis of the map.

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.

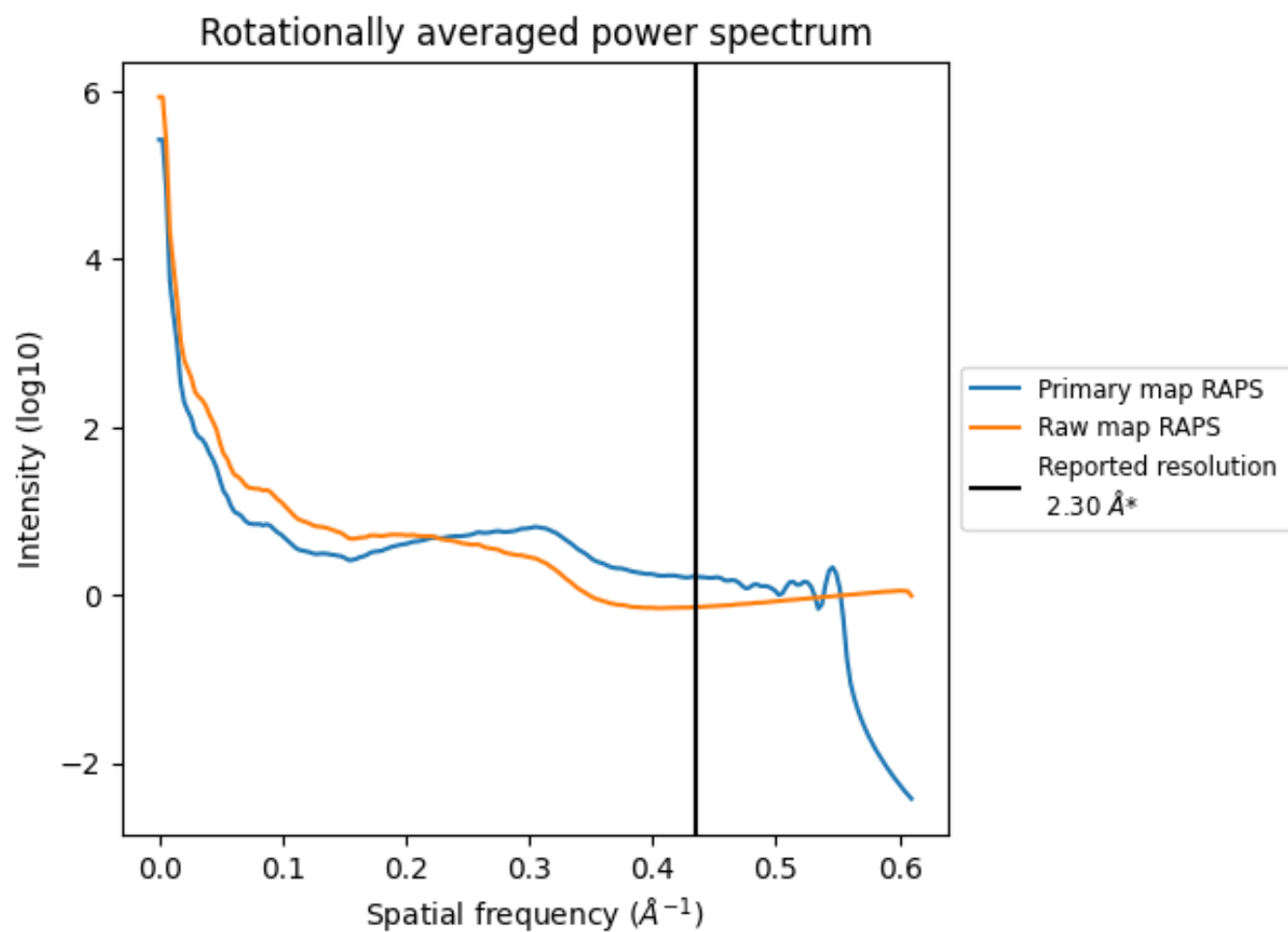
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm³; this corresponds to an approximate mass of 215 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 ⓘ

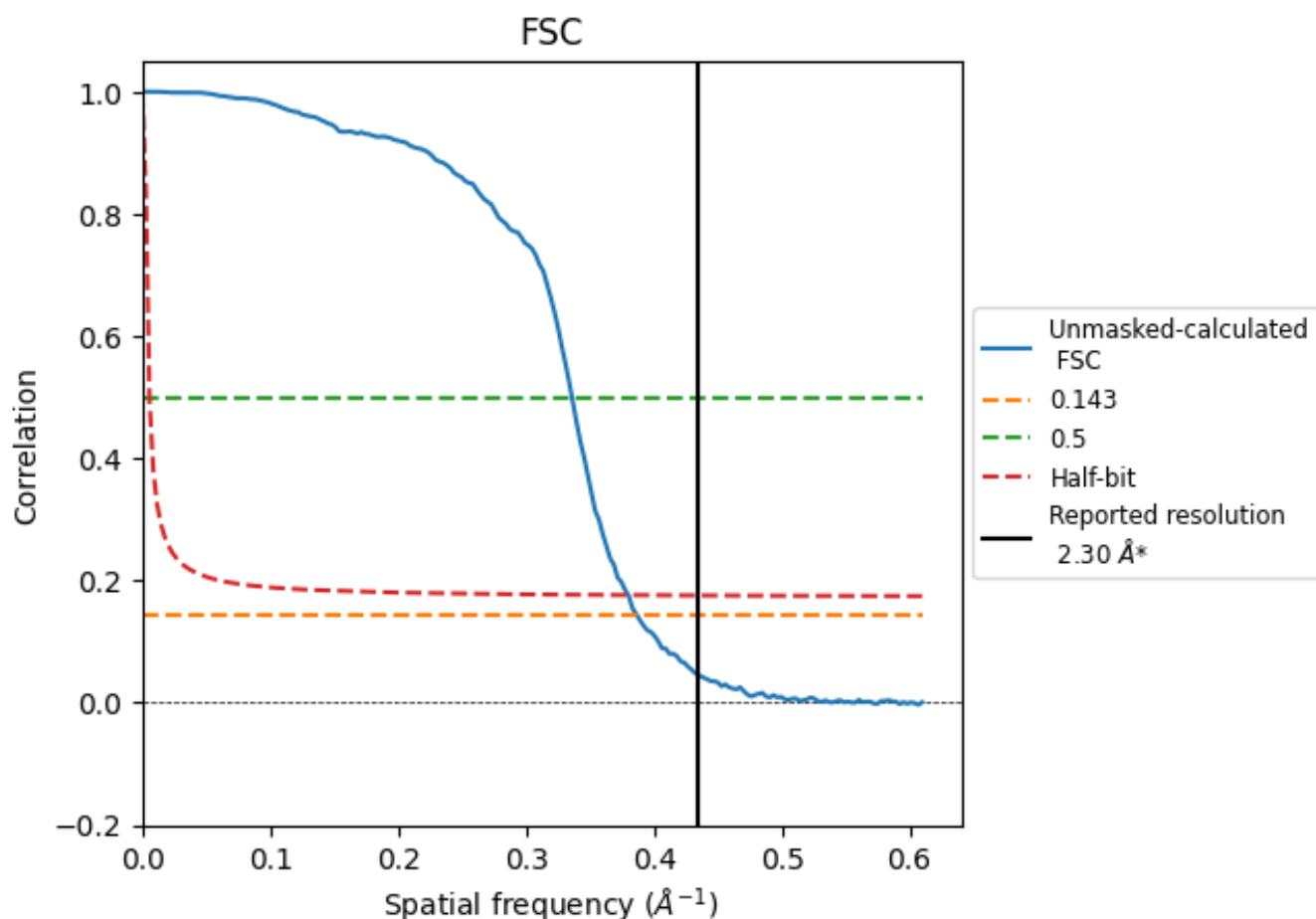


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

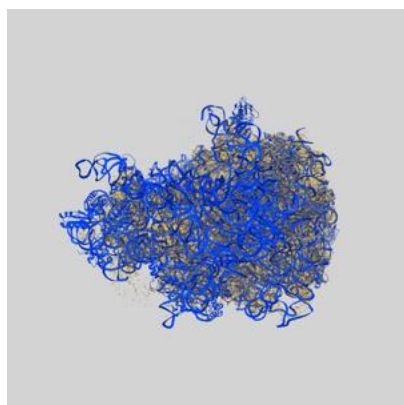
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.59	2.98	2.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.59 differs from the reported value 2.3 by more than 10 %

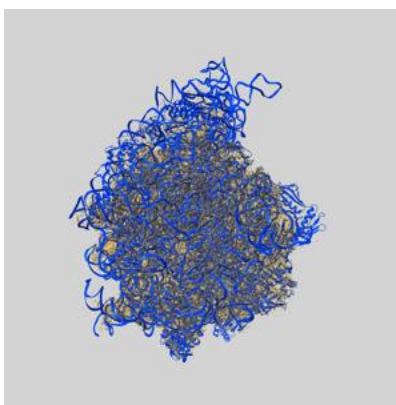
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18332 and PDB model 8QCQ. Per-residue inclusion information can be found in section [3](#) on page [15](#).

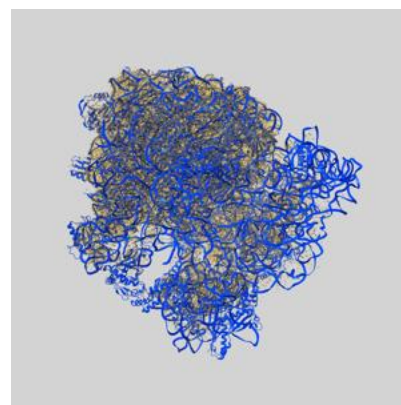
9.1 Map-model overlay [i](#)



X



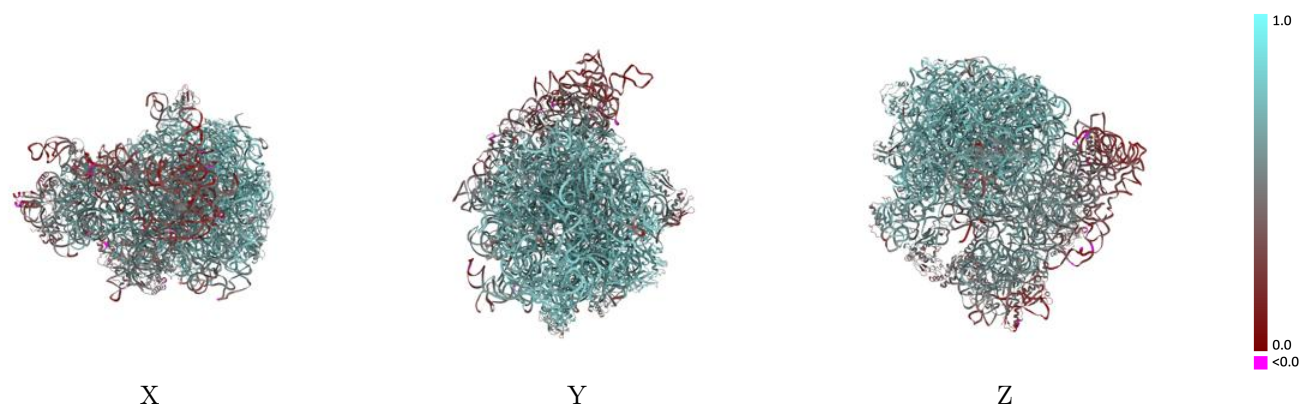
Y



Z

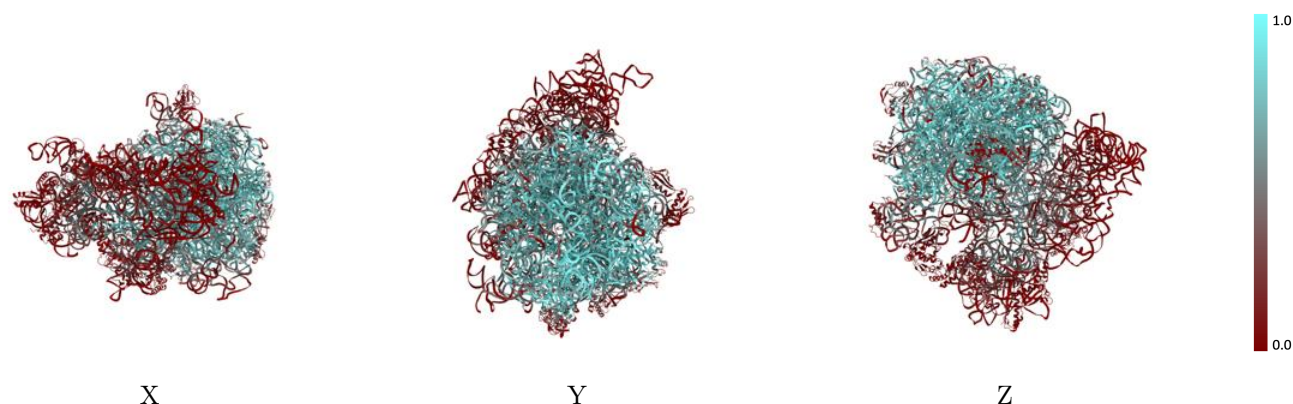
The images above show the 3D surface view of the map at the recommended contour level 0.052 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



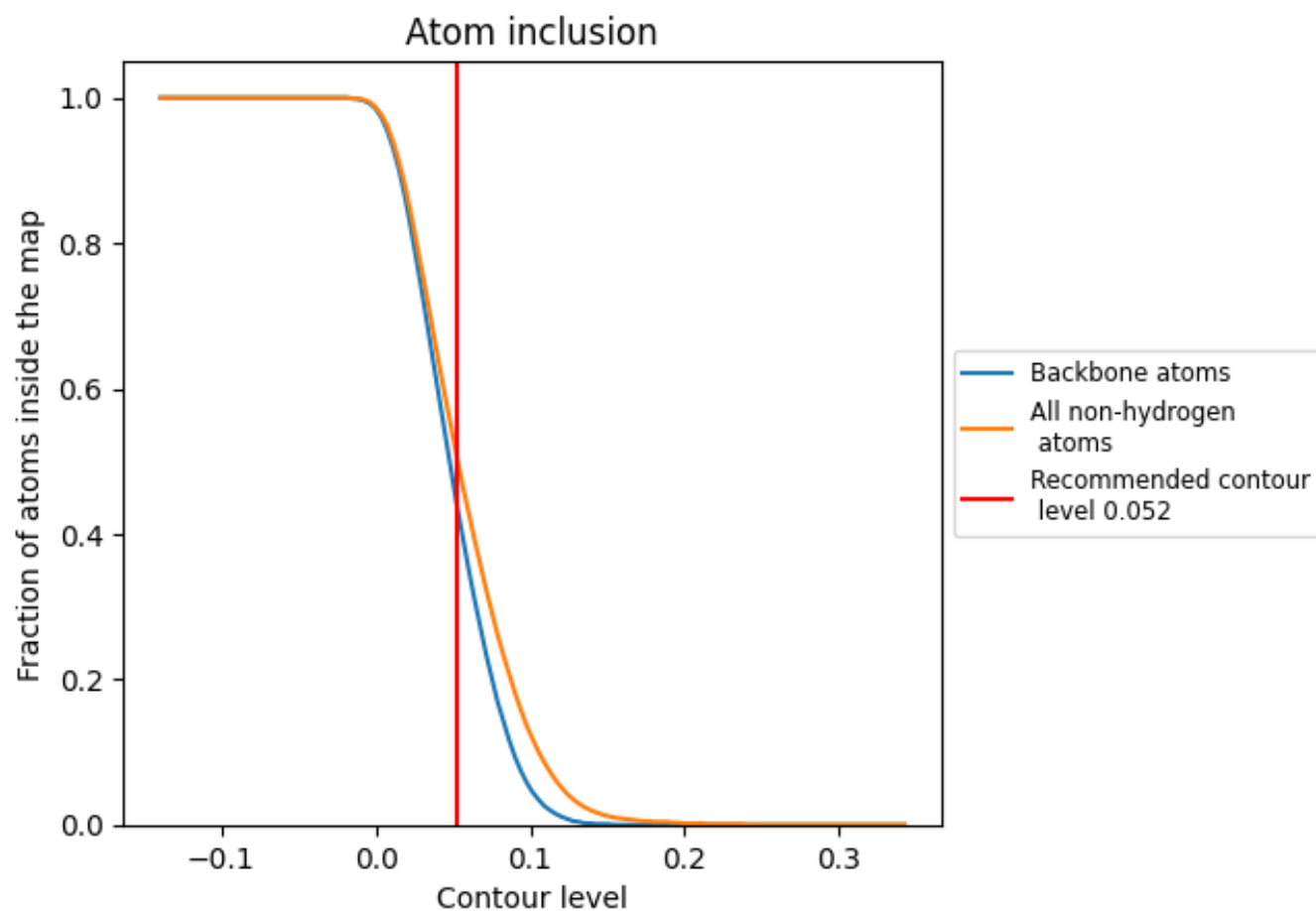
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.052).

9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 51% 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 (0.052) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5110	0.6100
0	0.7220	0.7030
1	0.2310	0.6110
2	0.8900	0.7690
3	0.8190	0.7380
4	0.6400	0.6880
6	0.0140	0.4150
7	0.6980	0.7540
8	0.6670	0.6950
A	0.7460	0.6950
B	0.3720	0.5930
C	0.7190	0.7150
D	0.7220	0.7280
E	0.5750	0.6870
F	0.0490	0.4810
G	0.0850	0.4670
J	0.7340	0.7280
K	0.6980	0.7100
L	0.5780	0.6730
M	0.7080	0.7100
N	0.7540	0.7170
O	0.2020	0.5660
P	0.5950	0.6710
Q	0.7840	0.7390
R	0.5710	0.6890
S	0.7460	0.7230
T	0.4760	0.6400
U	0.3770	0.6040
W	0.7440	0.7180
X	0.4120	0.6100
Y	0.2130	0.5540
Z	0.6320	0.6760
a	0.2780	0.5060
c	0.0850	0.4600
e	0.1180	0.4480



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Chain	Atom inclusion	Q-score
f	 0.0560	 0.4670
g	 0.0320	 0.4210
h	 0.0640	 0.3840
i	 0.0590	 0.4190
j	 0.0860	 0.4040
k	 0.0390	 0.3610
l	 0.1100	 0.5030
m	 0.0570	 0.4470
n	 0.1950	 0.6070
o	 0.1460	 0.4810
q	 0.0130	 0.3100
r	 0.0590	 0.4520
s	 0.0570	 0.4710
t	 0.0160	 0.2970
w	 0.2920	 0.5340
y	 0.3130	 0.5500