



## Full wwPDB EM Validation Report ⓘ

Mar 4, 2025 – 04:05 am GMT

PDB ID : 8Q7Z  
EMDB ID : EMD-18168  
Title : Structure of the G. gallus 80S non-rotated ribosome  
Authors : Nurullina, L.; Jenner, L.; Yusupov, M.  
Deposited on : 2023-08-17  
Resolution : 2.50 Å(reported)  
Based on initial model : 7O7Z

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

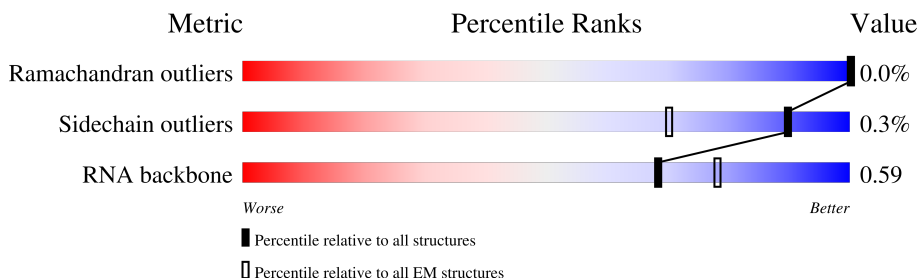
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 Å.

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




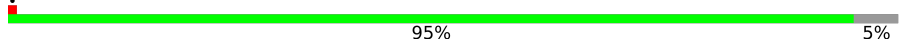

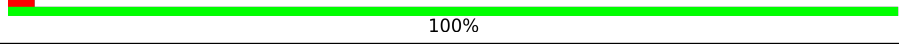
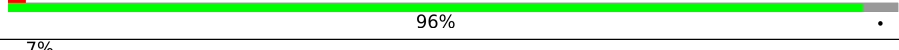
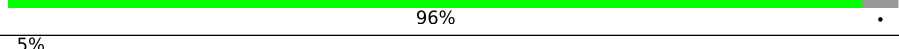
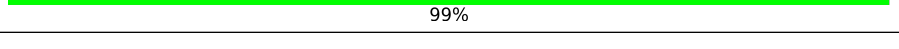
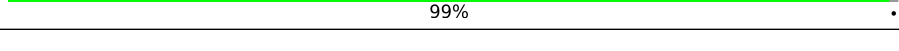
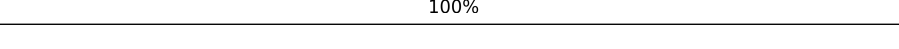
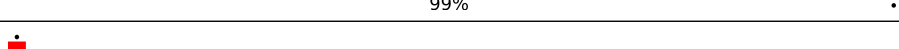
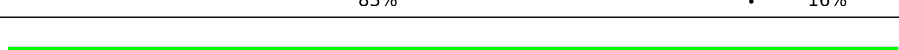
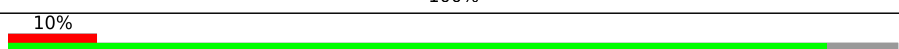
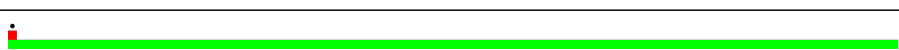
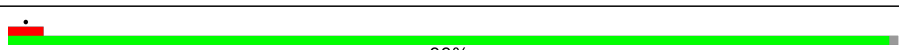
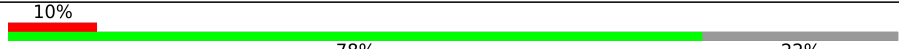
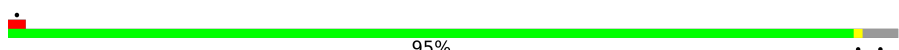


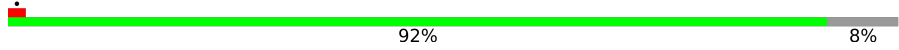
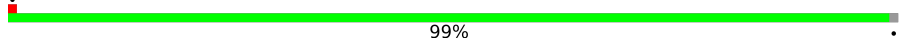
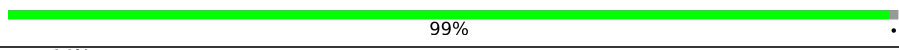
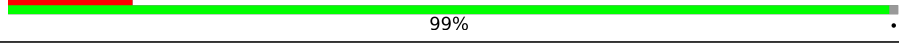



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	B5	4441	<div> <div>8%</div> <div>66%</div> <div>14%</div> <div>20%</div> </div>
2	B8	157	<div> <div>6%</div> <div>88%</div> <div>12%</div> </div>
3	B7	119	<div> <div>93%</div> <div>7%</div> </div>
4	Az	25	<div> <div>100%</div> </div>
5	BA	257	<div> <div>96%</div> <div>.</div> </div>
6	BB	403	<div> <div>99%</div> <div>.</div> </div>
7	BC	421	<div> <div>85%</div> <div>14%</div> </div>
8	BD	297	<div> <div>7%</div> <div>100%</div> </div>

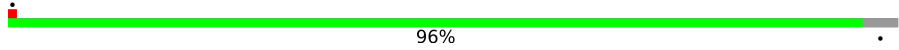
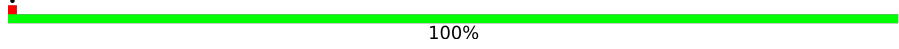
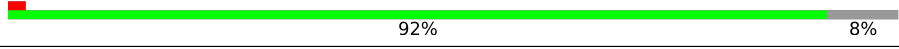
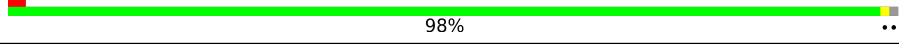
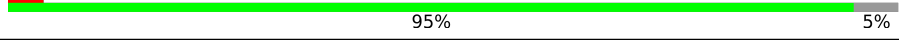

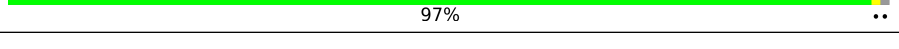
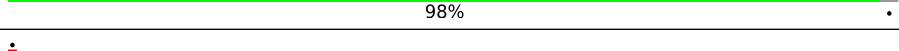
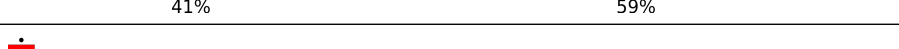
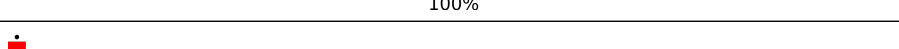
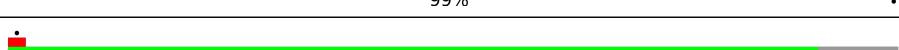
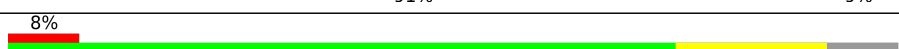
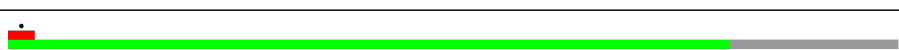
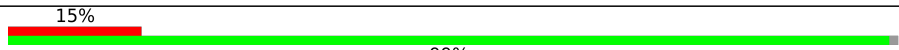
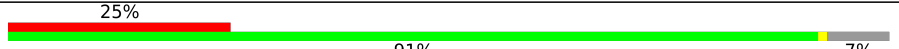

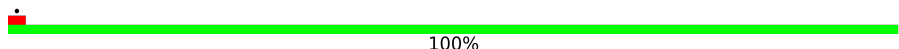



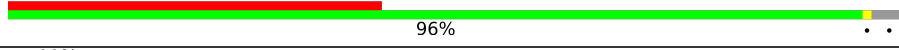
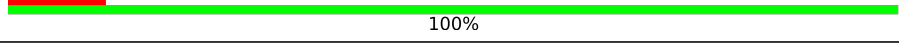
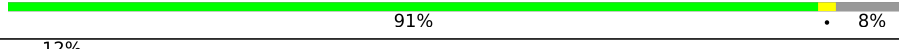
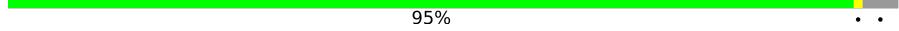

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Mol	Chain	Length	Quality of chain
9	BE	298	
10	BF	246	
11	BG	266	
12	BH	192	
13	BI	214	
14	BJ	178	
15	BL	211	
16	BM	131	
17	BN	204	
18	BO	203	
19	BP	184	
20	BQ	187	
21	BR	196	
22	BS	176	
23	BT	160	
24	BU	128	
25	BV	140	
26	BW	157	
27	BX	155	
28	BY	145	
29	BZ	136	
30	Ba	148	
31	Bb	71	
32	Bc	115	
33	Bd	176	

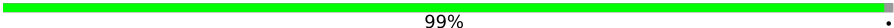



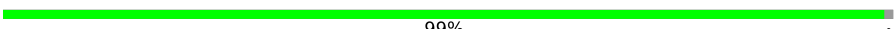
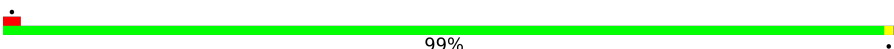
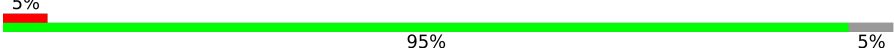

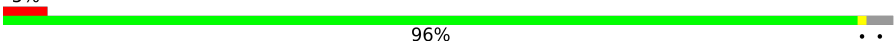

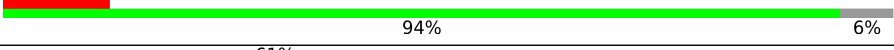
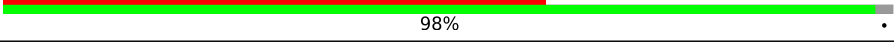


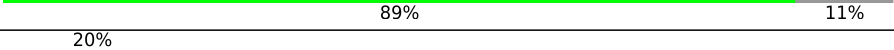
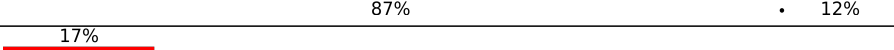
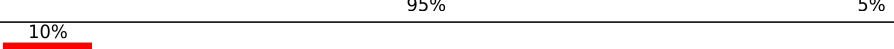
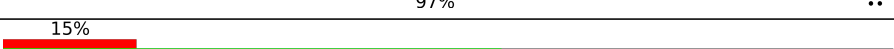




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Mol	Chain	Length	Quality of chain
34	Be	135	
35	Bf	110	
36	Bg	117	
37	Bh	123	
38	Bi	105	
39	Bj	97	
40	Bk	70	
41	Bl	51	
42	Bm	128	
43	Bo	105	
44	Bp	92	
45	Br	138	
46	A2	1823	
47	Aa	264	
48	AA	84	
49	AB	69	
50	Ab	264	
51	Ad	263	
52	AD	133	
53	AE	115	
54	Af	249	
55	Ag	194	
56	Ah	207	
57	Ai	194	
58	Ak	158	

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Mol	Chain	Length	Quality of chain
59	Am	151	
60	An	151	
61	At	119	
62	Au	84	
63	Av	130	
64	Aw	143	
65	Ax	131	
66	AZ	296	
67	Ap	146	
68	AC	156	
69	Ae	204	
70	AF	317	
71	AG	171	
72	Aj	165	
73	Al	132	
74	Ao	145	
75	Ar	152	
76	As	145	
77	Ay	125	
78	Ac	243	
79	V	76	
80	Aq	135	

## 2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 216968 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B5	3562	Total	C	N	O	P	0	0
			76444	34065	13971	24846	3562		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3295	UY1	U	modified residue	GB KT445934.2

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B8	157	Total	C	N	O	P	0	0
			3338	1490	588	1103	157		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B7	119	Total	C	N	O	P	0	0
			2536	1130	449	838	119		

- Molecule 4 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Az	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BA	248	Total	C	N	O	S	0	0
			1898	1191	387	314	6		

- Molecule 6 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BB	398	Total	C	N	O	S	0	0
			3209	2042	603	550	14		

- Molecule 7 is a protein called 60S ribosomal protein L4 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BC	361	Total	C	N	O	S	0	0
			2888	1816	574	484	14		

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BD	296	Total	C	N	O	S	0	0
			2388	1506	437	433	12		

- Molecule 9 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BE	224	Total	C	N	O	S	0	0
			1811	1161	353	295	2		

- Molecule 10 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BF	234	Total	C	N	O	S	0	0
			1939	1245	377	309	8		

- Molecule 11 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BG	210	Total	C	N	O	S	0	0
			1704	1089	326	284	5		

- Molecule 12 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BH	192	Total	C	N	O	S	0	0
			1533	962	288	277	6		

- Molecule 13 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BI	205	Total	C	N	O	S	0	0
			1654	1050	322	268	14		

- Molecule 14 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BJ	170	Total	C	N	O	S	0	0
			1362	861	255	241	5		

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BL	210	Total	C	N	O	S	0	0
			1710	1072	354	279	5		

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BM	130	Total	C	N	O	S	0	0
			1077	688	209	172	8		

- Molecule 17 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BN	203	Total	C	N	O	S	0	0
			1700	1071	359	266	4		

- Molecule 18 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BO	201	Total	C	N	O	S	0	0
			1643	1058	321	259	5		

- Molecule 19 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BP	155	Total	C	N	O	S	0	0
			1259	788	244	218	9		

- Molecule 20 is a protein called Ribosomal protein L18.



Mol	Chain	Residues	Atoms					AltConf	Trace
20	BQ	187	Total	C	N	O	S	0	0
			1503	939	314	245	5		

- Molecule 21 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BR	180	Total	C	N	O	S	0	0
			1503	930	325	238	10		

- Molecule 22 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BS	176	Total	C	N	O	S	0	0
			1464	931	286	236	11		

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BT	159	Total	C	N	O	S	0	0
			1299	825	252	216	6		

- Molecule 24 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BU	100	Total	C	N	O	S	0	0
			817	523	143	149	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BV	134	Total	C	N	O	S	0	0
			993	625	187	176	5		

- Molecule 26 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BW	67	Total	C	N	O	S	0	0
			560	356	107	94	3		

- Molecule 27 is a protein called Ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 28 is a protein called Ribosomal protein L26 like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BY	133	Total	C	N	O	S	0	0
			1106	694	224	185	3		

- Molecule 29 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 30 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ba	147	Total	C	N	O	S	0	0
			1179	748	240	187	4		

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bb	70	Total	C	N	O	S	0	0
			582	360	126	94	2		

- Molecule 32 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bc	95	Total	C	N	O	S	0	0
			738	468	131	133	6		

- Molecule 33 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bd	105	Total	C	N	O	S	0	0
			867	549	168	148	2		

- Molecule 34 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Be	130	Total	C	N	O	S	0	0
			1074	681	219	169	5		

- Molecule 35 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bf	110	Total	C	N	O	S	0	0
			886	559	178	144	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bf	103	VAL	-	insertion	UNP A0A8V0YS49

- Molecule 36 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bg	108	Total	C	N	O	S	0	0
			860	540	178	137	5		

- Molecule 37 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 38 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bi	100	Total	C	N	O	S	0	0
			821	515	173	127	6		

- Molecule 39 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bj	86	Total	C	N	O	S	0	0
			704	432	155	112	5		

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 41 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bl	50	Total	C	N	O	S	0	0
			442	281	96	64	1		

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 43 is a protein called Ribosomal protein L36a like.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bo	105	Total	C	N	O	S	0	0
			861	540	177	138	6		

- Molecule 44 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bp	91	Total	C	N	O	S	0	0
			706	445	134	120	7		

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Br	126	Total	C	N	O	S	0	0
			1025	635	218	169	3		

- Molecule 46 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	A2	1676	Total	C	N	O	P	0	0
			35806	16005	6419	11706	1676		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1206	B8N	U	modified residue	GB KT445934.2
A2	1295	4AC	C	modified residue	GB KT445934.2
A2	1796	4AC	C	modified residue	GB KT445934.2

- Molecule 47 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Aa	213	Total	C	N	O	S	0	0
			1730	1098	309	309	14		

- Molecule 48 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AA	83	Total	C	N	O	S	0	0
			657	410	125	115	7		

- Molecule 49 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AB	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 50 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Ab	219	Total	C	N	O	S	0	0
			1698	1099	291	299	9		

- Molecule 51 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ad	262	Total	C	N	O	S	0	0
			2076	1324	387	357	8		

- Molecule 52 is a protein called Ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AD	57	Total	C	N	O	S	0	0
			452	279	99	73	1		

- Molecule 53 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AE	99	Total	C	N	O	S	0	0
			793	492	165	131	5		

- Molecule 54 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Af	227	Total	C	N	O	S	0	0
			1838	1144	367	320	7		

- Molecule 55 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Ag	187	Total	C	N	O	S	0	0
			1500	956	276	267	1		

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Ah	206	Total	C	N	O	S	0	0
			1685	1059	332	289	5		

- Molecule 57 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ai	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 58 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Ak	152	Total	C	N	O	S	0	0
			1236	784	233	213	6		

- Molecule 59 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Am	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 60 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	An	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	IAS	ASP	modified residue	UNP Q5ZHW8

- Molecule 61 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	At	102	Total	C	N	O	S	0	0
			811	508	154	145	4		

- Molecule 62 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Au	84	Total	C	N	O	S	0	0
			640	394	118	124	4		

- Molecule 63 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Av	129	Total	C	N	O	S	0	0
			1035	659	193	177	6		

- Molecule 64 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Aw	142	Total	C	N	O	S	0	0
			1104	696	220	185	3		

- Molecule 65 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ax	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 66 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AZ	207	Total	C	N	O	S	0	0
			1626	1036	287	295	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	2	ACE	-	acetylation	UNP P50890

- Molecule 67 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ap	141	Total	C	N	O	S	0	0
			1123	715	212	193	3		

- Molecule 68 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AC	74	Total	C	N	O	S	0	0
			611	386	117	101	7		

- Molecule 69 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ae	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 70 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AF	311	Total	C	N	O	S	0	0
			2420	1526	422	460	12		

- Molecule 71 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AG	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 72 is a protein called Ribosomal protein S10.



Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aj	96	Total	C	N	O	S	0	0
			812	532	143	131	6		

- Molecule 73 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Al	118	Total	C	N	O	S	0	0
			916	574	162	172	8		

- Molecule 74 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ao	127	Total	C	N	O	S	0	0
			1044	663	197	177	7		

- Molecule 75 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Ar	144	Total	C	N	O	S	0	0
			1191	748	241	201	1		

- Molecule 76 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	As	143	Total	C	N	O	S	0	0
			1115	698	216	199	2		

- Molecule 77 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ay	70	Total	C	N	O	S	0	0
			555	357	101	96	1		

- Molecule 78 is a protein called DNA-(apurinic or apyrimidinic site) lyase.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ac	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 79 is a RNA chain called Phe tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	V	76	Total	C	N	O	P	0	0
			1628	727	302	524	75		

- Molecule 80 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Aq	134	Total	C	N	O	S	0	0
			1081	678	201	197	5		

- Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	B5	346	Total	Mg	0
			346	346	
81	B8	9	Total	Mg	0
			9	9	
81	B7	11	Total	Mg	0
			11	11	
81	BA	3	Total	Mg	0
			3	3	
81	BH	1	Total	Mg	0
			1	1	
81	BI	2	Total	Mg	0
			2	2	
81	BN	2	Total	Mg	0
			2	2	
81	BP	2	Total	Mg	0
			2	2	
81	BV	1	Total	Mg	0
			1	1	
81	Ba	1	Total	Mg	0
			1	1	
81	Bb	2	Total	Mg	0
			2	2	
81	Be	1	Total	Mg	0
			1	1	
81	Bf	1	Total	Mg	0
			1	1	
81	Bg	1	Total	Mg	0
			1	1	
81	Bj	1	Total	Mg	0
			1	1	
81	Bo	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
81	A2	104	Total 104	Mg 104	0
81	Ak	1	Total 1	Mg 1	0
81	An	3	Total 3	Mg 3	0
81	As	1	Total 1	Mg 1	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	Bg	1	Total 1	Zn 1	0
82	Bj	1	Total 1	Zn 1	0
82	Bm	1	Total 1	Zn 1	0
82	Bo	1	Total 1	Zn 1	0
82	Bp	1	Total 1	Zn 1	0
82	AE	1	Total 1	Zn 1	0
82	AG	1	Total 1	Zn 1	0

- Molecule 83 is water.

Mol	Chain	Residues	Atoms		AltConf
83	B5	4198	Total 4198	O 4198	0
83	B8	72	Total 72	O 72	0
83	B7	30	Total 30	O 30	0
83	Az	5	Total 5	O 5	0
83	BA	28	Total 28	O 28	0
83	BB	49	Total 49	O 49	0

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Mol	Chain	Residues	Atoms		AltConf
83	BC	45	Total 45	O 45	0
83	BD	22	Total 22	O 22	0
83	BE	11	Total 11	O 11	0
83	BF	24	Total 24	O 24	0
83	BG	15	Total 15	O 15	0
83	BH	15	Total 15	O 15	0
83	BI	13	Total 13	O 13	0
83	BJ	3	Total 3	O 3	0
83	BL	29	Total 29	O 29	0
83	BM	6	Total 6	O 6	0
83	BN	29	Total 29	O 29	0
83	BO	19	Total 19	O 19	0
83	BP	23	Total 23	O 23	0
83	BQ	24	Total 24	O 24	0
83	BR	9	Total 9	O 9	0
83	BS	21	Total 21	O 21	0
83	BT	21	Total 21	O 21	0
83	BU	2	Total 2	O 2	0
83	BV	17	Total 17	O 17	0
83	BW	4	Total 4	O 4	0
83	BX	5	Total 5	O 5	0

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Mol	Chain	Residues	Atoms		AltConf
83	BY	11	Total 11	O 11	0
83	BZ	5	Total 5	O 5	0
83	Ba	23	Total 23	O 23	0
83	Bb	11	Total 11	O 11	0
83	Bc	5	Total 5	O 5	0
83	Bd	9	Total 9	O 9	0
83	Be	17	Total 17	O 17	0
83	Bf	25	Total 25	O 25	0
83	Bg	9	Total 9	O 9	0
83	Bh	3	Total 3	O 3	0
83	Bi	8	Total 8	O 8	0
83	Bj	16	Total 16	O 16	0
83	Bl	5	Total 5	O 5	0
83	Bm	5	Total 5	O 5	0
83	Bo	15	Total 15	O 15	0
83	Bp	12	Total 12	O 12	0
83	Br	16	Total 16	O 16	0
83	A2	832	Total 832	O 832	0
83	Aa	10	Total 10	O 10	0
83	AA	8	Total 8	O 8	0
83	AB	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
83	Ab	11	Total 11	O 11	0
83	Ad	10	Total 10	O 10	0
83	AD	2	Total 2	O 2	0
83	AE	9	Total 9	O 9	0
83	Af	1	Total 1	O 1	0
83	Ah	7	Total 7	O 7	0
83	Ai	7	Total 7	O 7	0
83	Ak	10	Total 10	O 10	0
83	Am	4	Total 4	O 4	0
83	An	7	Total 7	O 7	0
83	At	3	Total 3	O 3	0
83	Au	2	Total 2	O 2	0
83	Av	10	Total 10	O 10	0
83	Aw	8	Total 8	O 8	0
83	Ax	4	Total 4	O 4	0
83	AZ	3	Total 3	O 3	0
83	Ap	1	Total 1	O 1	0
83	Ae	2	Total 2	O 2	0
83	AG	2	Total 2	O 2	0
83	Ar	1	Total 1	O 1	0
83	Ay	4	Total 4	O 4	0

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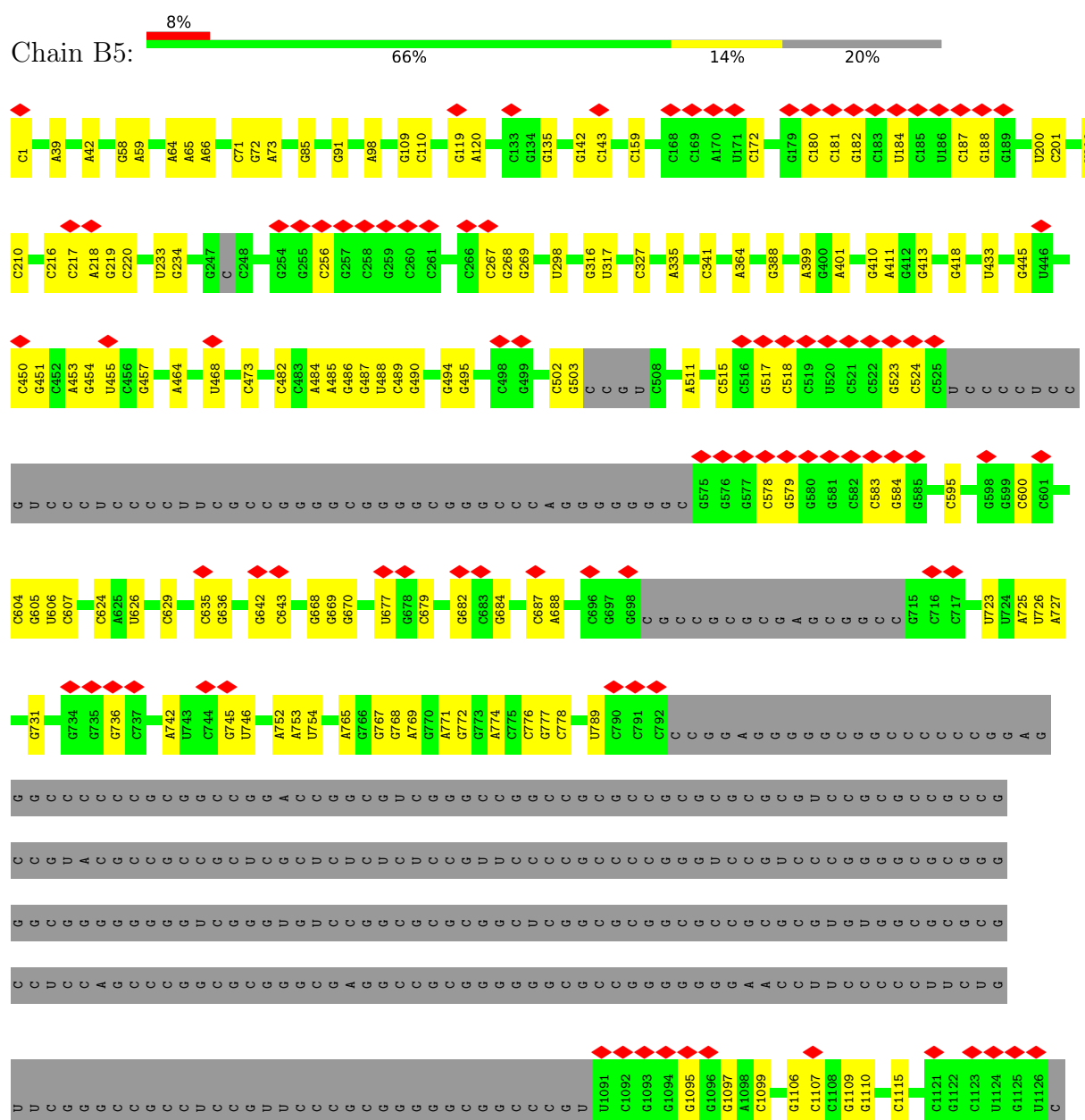
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Mol	Chain	Residues	Atoms		AltConf
83	V	9	Total	O	0
			9	9	
83	Aq	4	Total	O	0
			4	4	

### 3 Residue-property plots

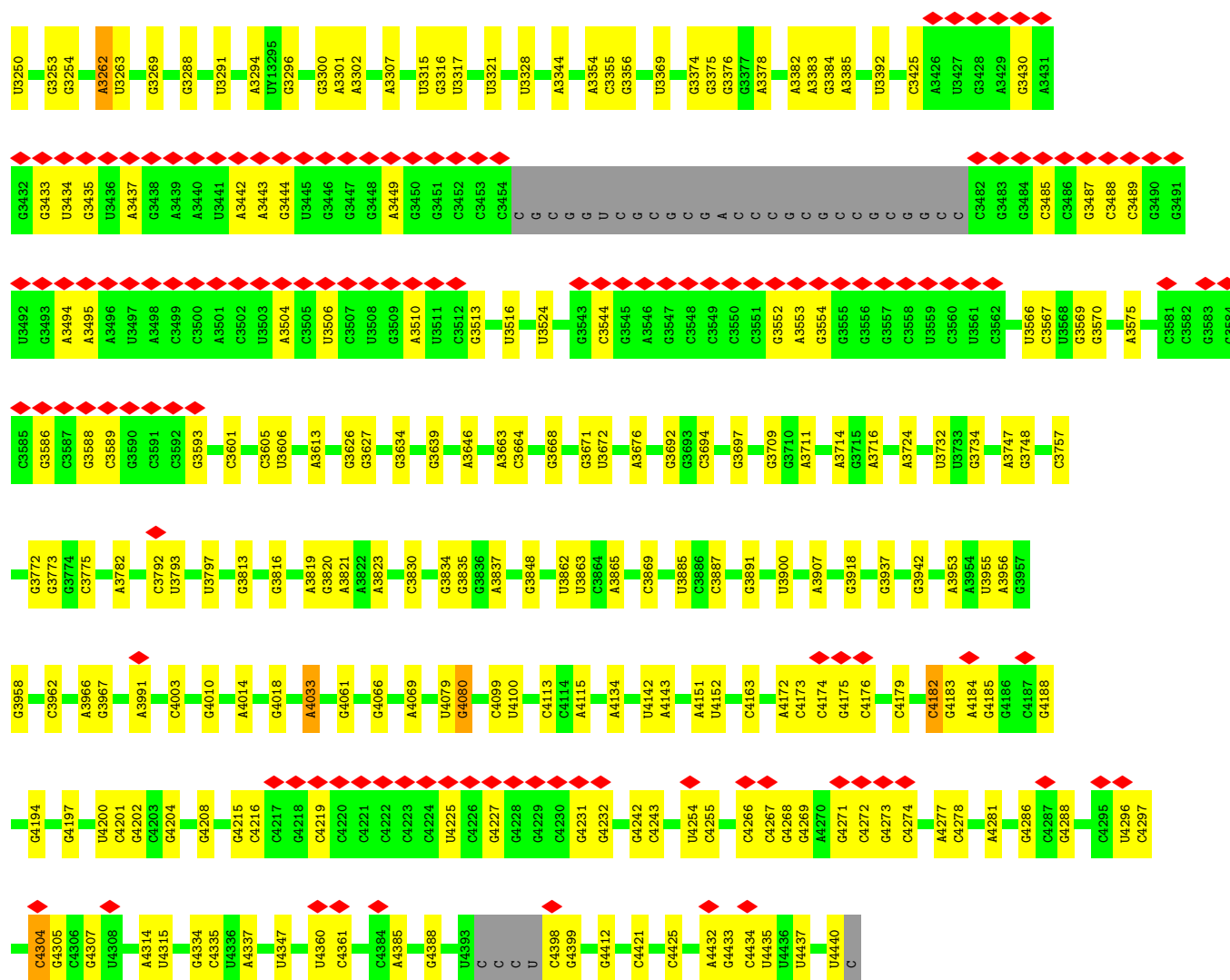
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 28S rRNA

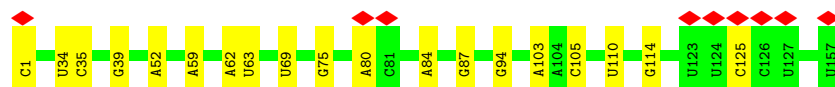








- Molecule 2: 5.8S rRNA



- Molecule 3: 5S rRNA



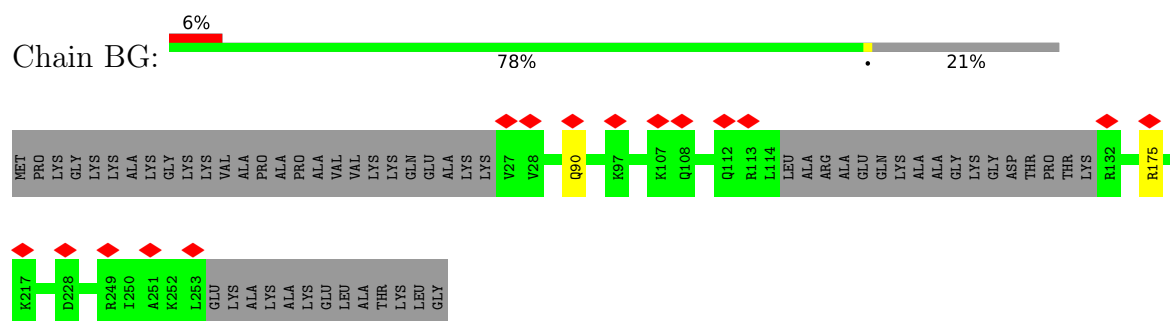
- Molecule 4: 60S ribosomal protein L41



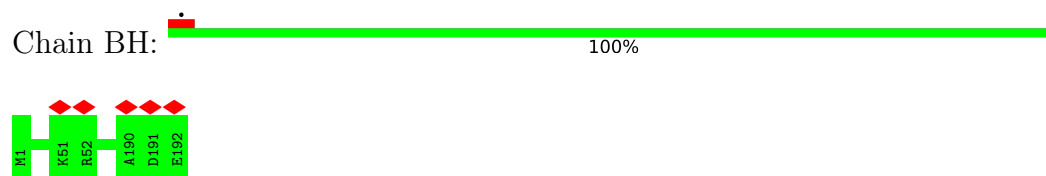
There are no outlier residues recorded for this chain.

- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| MET | ALA | ASP | LYS | GLU | ALA | LYS | LYS | VAL | PRO | SER | SER | VAL | P13 | E14 | L17 | N246 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|

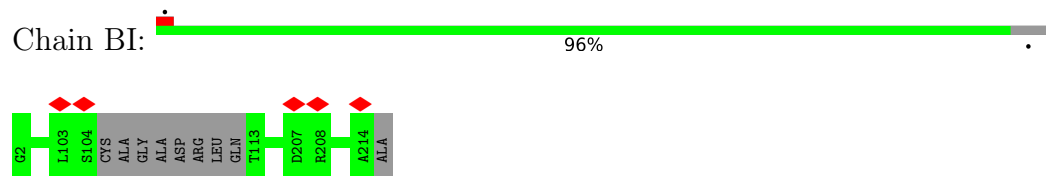
- Molecule 11: Large ribosomal subunit protein eL8



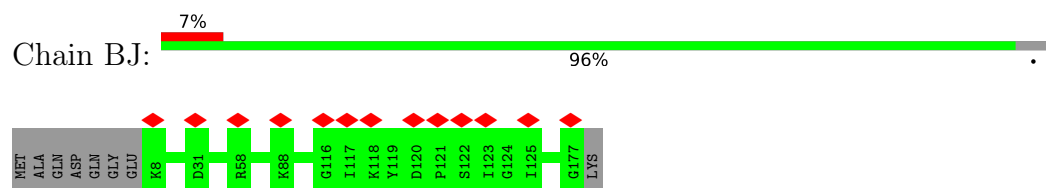
- Molecule 12: 60S ribosomal protein L9



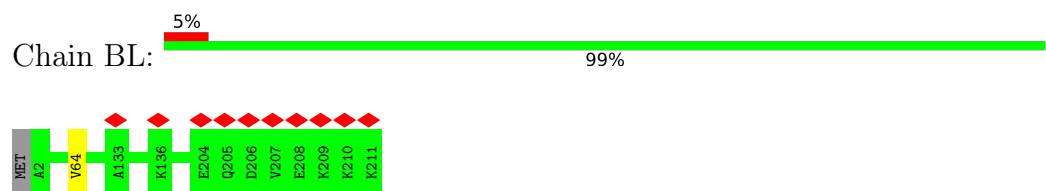
- Molecule 13: Large ribosomal subunit protein uL16



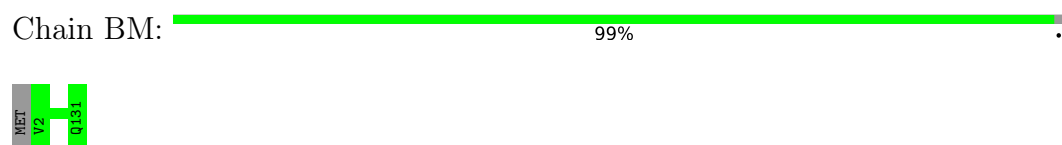
- Molecule 14: 60S ribosomal protein L11



- Molecule 15: Large ribosomal subunit protein eL13



- Molecule 16: 60S ribosomal protein L14



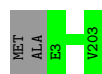
- Molecule 17: Ribosomal protein L15

Chain BN:  100%




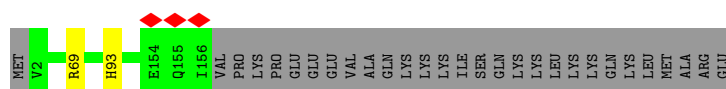
- Molecule 18: Ribosomal protein uL13

Chain BO:  99%



- Molecule 19: 60S ribosomal protein L17

Chain BP:  83% 16%



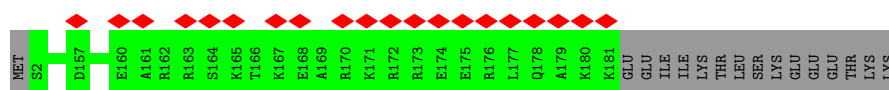
- Molecule 20: Ribosomal protein L18

Chain BQ:  100%

There are no outlier residues recorded for this chain.

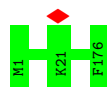
- Molecule 21: Ribosomal protein L19

Chain BR:  10% 92% 8%



- Molecule 22: 60S ribosomal protein L18a

Chain BS:  100%



- Molecule 23: 60S ribosomal protein L21

Chain BT:  99%

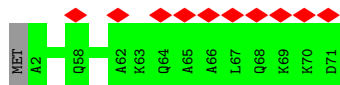


- Molecule 24: Large ribosomal subunit protein eL22

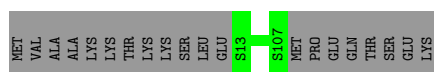
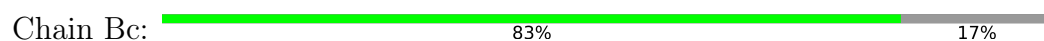




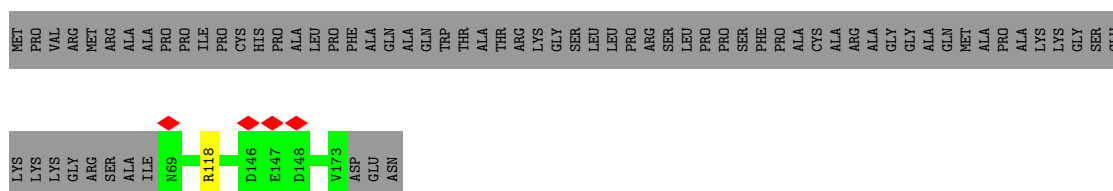
- Molecule 31: 60S ribosomal protein L29



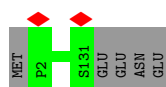
- Molecule 32: Large ribosomal subunit protein eL30



- Molecule 33: 60S ribosomal protein L31



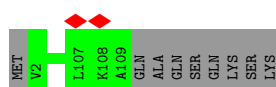
- Molecule 34: Ribosomal protein L32



- Molecule 35: 60S ribosomal protein L35a

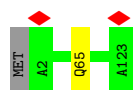


- Molecule 36: 60S ribosomal protein L34



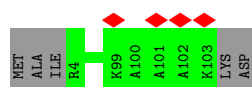
- Molecule 37: Large ribosomal subunit protein uL29

Chain Bh:  98%




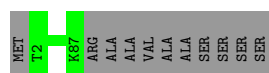
- Molecule 38: Large ribosomal subunit protein eL36

Chain Bi:  95%



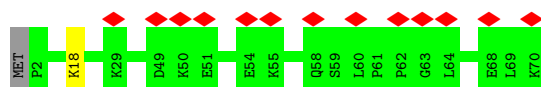
- Molecule 39: Ribosomal protein L37

Chain Bj:  89%



- Molecule 40: 60S ribosomal protein L38

Chain Bk:  19%




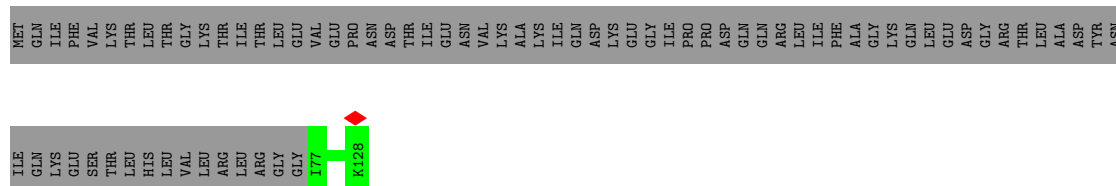
- Molecule 41: Large ribosomal subunit protein eL39

Chain Bl:  98%



- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain Bm:  41%

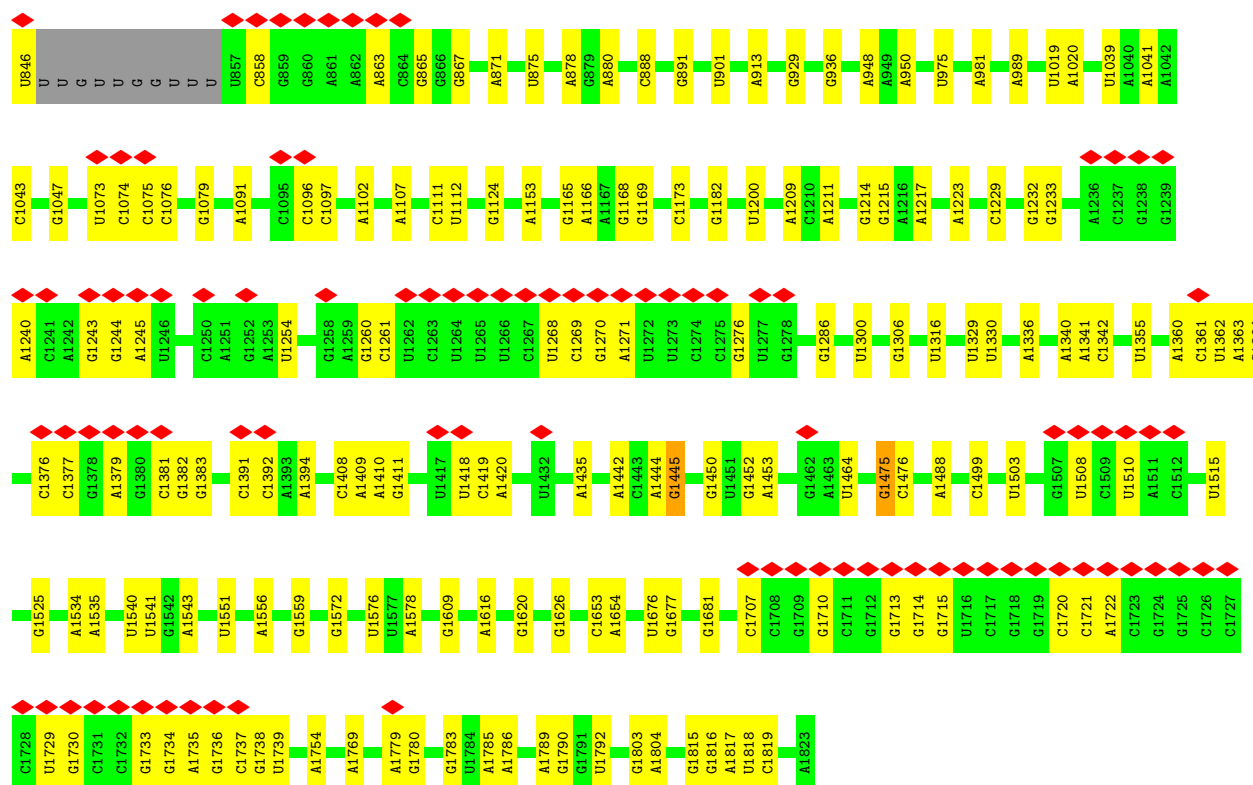


- Molecule 43: Ribosomal protein L36a like

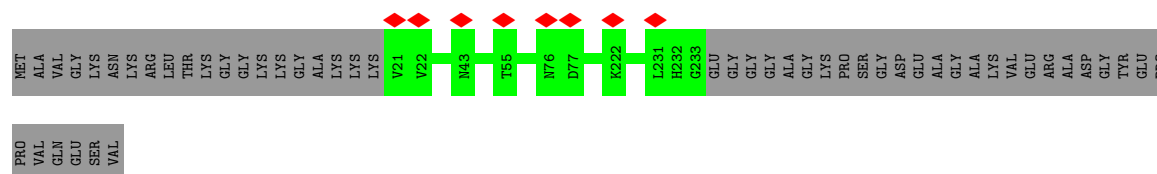
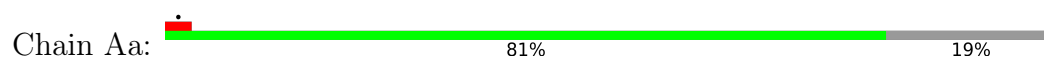
Chain Bo:  100%



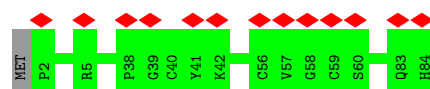




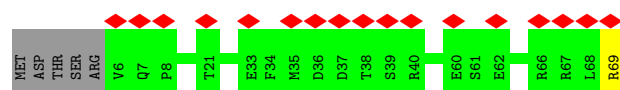
- Molecule 47: Small ribosomal subunit protein eS1




- Molecule 48: 40S ribosomal protein S27

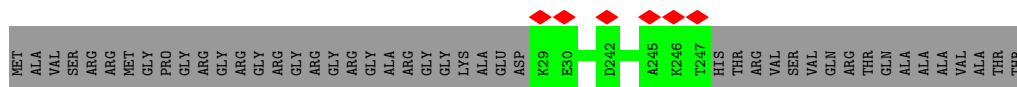


- Molecule 49: 40S ribosomal protein S28



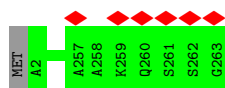
- Molecule 50: 40S ribosomal protein S2

Chain Ab:  83% 17%




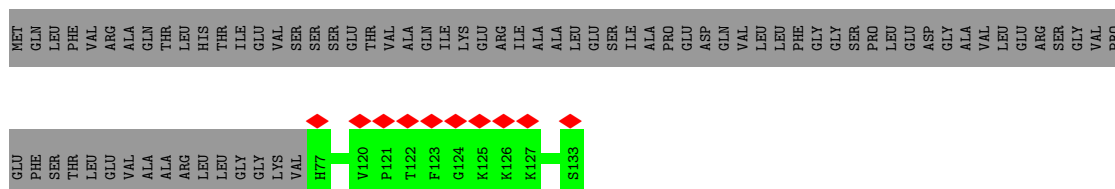
- Molecule 51: Small ribosomal subunit protein eS4

Chain Ad:  100%




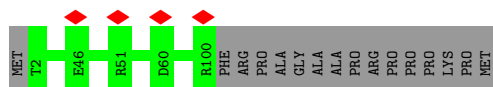
- Molecule 52: Ribosomal protein eS30

Chain AD:  8% 43% 57%




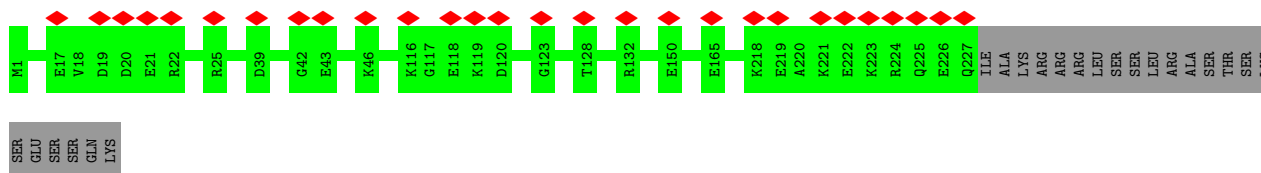
- Molecule 53: 40S ribosomal protein S26

Chain AE:  86% 14%




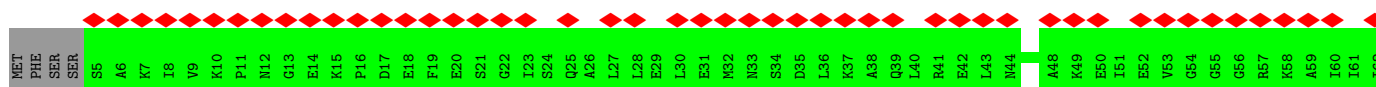
- Molecule 54: Small ribosomal subunit protein eS6

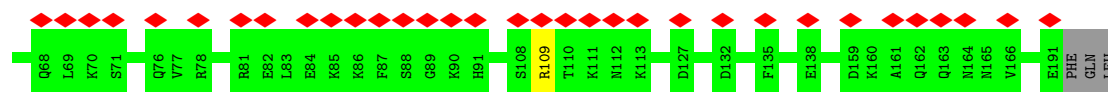
Chain Af:  11% 91% 9%



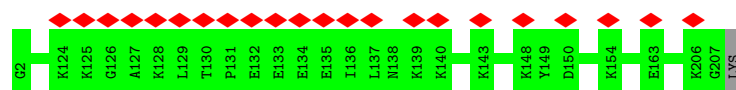
- Molecule 55: 40S ribosomal protein S7

Chain Ag:  42% 96% 2%

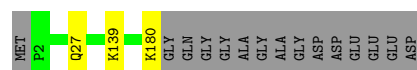




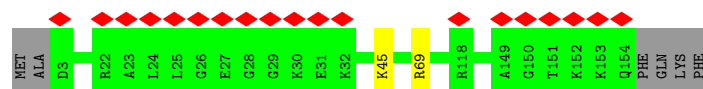
- Molecule 56: 40S ribosomal protein S8



- Molecule 57: 40S ribosomal protein S9



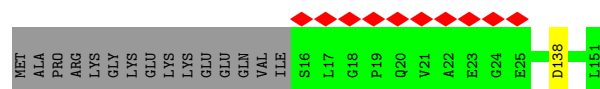
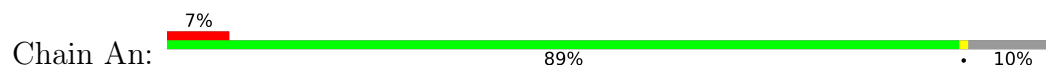
- Molecule 58: 40S ribosomal protein S11



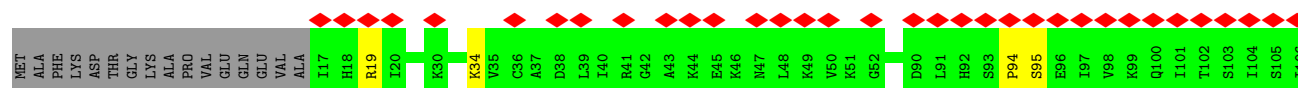
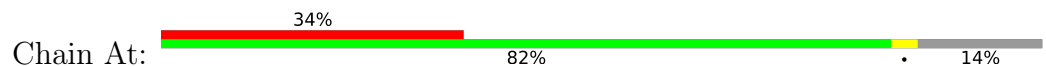
- Molecule 59: Small ribosomal subunit protein uS15

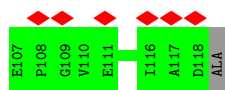


- Molecule 60: Ribosomal protein S14

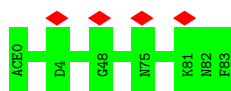


- Molecule 61: 40S ribosomal protein S20





- Molecule 62: Small ribosomal subunit protein eS21



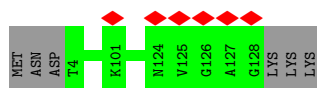
- Molecule 63: 40S ribosomal protein S15a



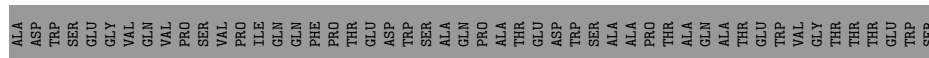
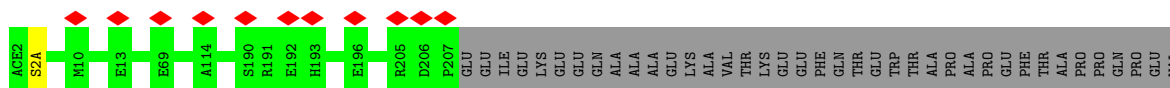
- Molecule 64: Small ribosomal subunit protein uS12



- Molecule 65: 40S ribosomal protein S24



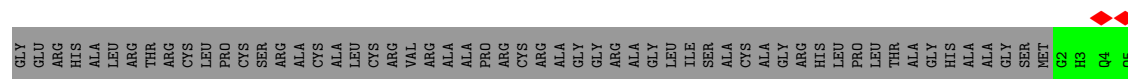
- Molecule 66: Small ribosomal subunit protein uS2



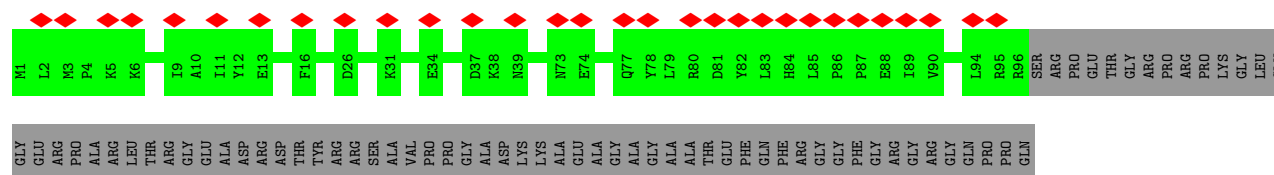
- Molecule 67: Ribosomal protein S16



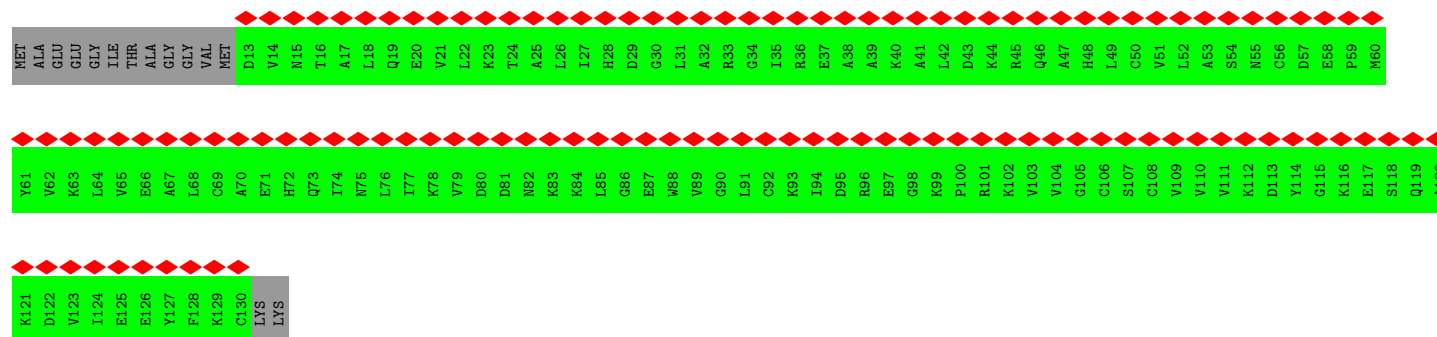
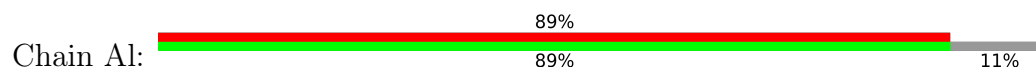




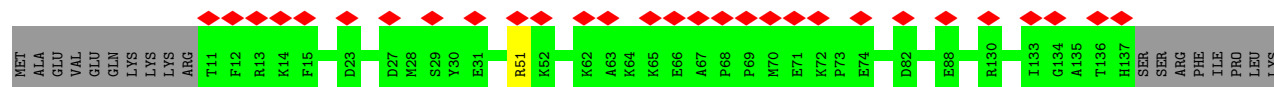
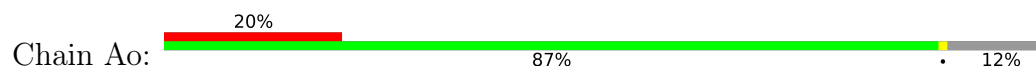
• Molecule 72: Ribosomal protein S10



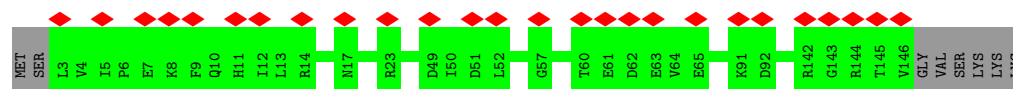
• Molecule 73: Small ribosomal subunit protein eS12



• Molecule 74: Small ribosomal subunit protein uS19



• Molecule 75: 40S ribosomal protein S18



• Molecule 76: 40S ribosomal protein S19







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122598	Depositor
Resolution determination method	FSC 3 SIGMA CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.826	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	465.74, 465.74, 465.74	wwPDB
Map dimensions	580, 580, 580	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.803, 0.803, 0.803	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, B8N, 1MA, UR3, OMG, OMU, OMC, A2M, NMM, ZN, MG, 4AC, 5MC, IAS, HIC, UY1, MLZ, 6MZ, ACE, MA6

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	B5	0.25	1/83215 (0.0%)	0.79	20/129832 (0.0%)
2	B8	0.29	1/3656 (0.0%)	0.74	0/5693
3	B7	0.24	0/2832	0.78	0/4413
4	Az	0.24	0/240	0.72	0/305
5	BA	0.27	0/1937	0.57	0/2597
6	BB	0.26	0/3264	0.52	0/4363
7	BC	0.25	0/2942	0.54	0/3950
8	BD	0.26	0/2431	0.50	0/3255
9	BE	0.25	0/1845	0.53	0/2466
10	BF	0.26	0/1975	0.54	0/2634
11	BG	0.25	0/1736	0.51	0/2342
12	BH	0.26	0/1552	0.54	0/2086
13	BI	0.26	0/1694	0.53	0/2264
14	BJ	0.26	0/1385	0.55	0/1852
15	BL	0.25	0/1742	0.56	0/2324
16	BM	0.26	0/1097	0.53	0/1460
17	BN	0.25	0/1745	0.57	0/2337
18	BO	0.26	0/1675	0.53	0/2239
19	BP	0.25	0/1285	0.53	0/1723
20	BQ	0.26	0/1527	0.60	0/2038
21	BR	0.26	0/1519	0.57	0/2007
22	BS	0.26	0/1503	0.56	0/2016
23	BT	0.26	0/1327	0.51	0/1771
24	BU	0.26	0/831	0.51	0/1115
25	BV	0.27	0/1007	0.53	0/1350
26	BW	0.26	0/573	0.53	0/763
27	BX	0.25	0/993	0.51	0/1334
28	BY	0.25	0/1123	0.57	0/1493
29	BZ	0.26	0/1130	0.51	0/1507
30	Ba	0.25	0/1209	0.53	0/1615
31	Bb	0.24	0/593	0.49	0/782

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Bc	0.26	0/748	0.49	0/1004
33	Bd	0.25	0/882	0.56	0/1187
34	Be	0.24	0/1093	0.54	0/1457
35	Bf	0.27	0/905	0.57	0/1211
36	Bg	0.25	0/870	0.58	0/1159
37	Bh	0.28	0/1023	0.52	0/1351
38	Bi	0.25	0/832	0.56	0/1100
39	Bj	0.26	0/718	0.59	0/948
40	Bk	0.25	0/575	0.50	0/761
41	Bl	0.23	0/452	0.54	0/596
42	Bm	0.24	0/435	0.56	0/575
43	Bo	0.26	0/864	0.54	0/1139
44	Bp	0.25	0/716	0.53	0/950
45	Br	0.24	0/1042	0.59	0/1398
46	A2	0.22	1/39049 (0.0%)	0.78	4/60848 (0.0%)
47	Aa	0.25	0/1757	0.51	0/2352
48	AA	0.23	0/670	0.51	0/897
49	AB	0.24	0/508	0.61	0/680
50	Ab	0.25	0/1734	0.48	0/2342
51	Ad	0.25	0/2118	0.52	0/2848
52	AD	0.24	0/458	0.54	0/602
53	AE	0.25	0/806	0.56	0/1080
54	Af	0.25	0/1861	0.55	0/2481
55	Ag	0.24	0/1522	0.53	0/2039
56	Ah	0.25	0/1715	0.56	0/2289
57	Ai	0.25	0/1520	0.56	0/2030
58	Ak	0.26	0/1257	0.55	0/1680
59	Am	0.25	0/1232	0.50	0/1656
60	An	0.26	0/1020	0.57	0/1366
61	At	0.23	0/821	0.57	0/1103
62	Au	0.26	0/644	0.51	0/863
63	Av	0.25	0/1052	0.53	0/1408
64	Aw	0.29	0/1122	0.56	0/1498
65	Ax	0.26	0/1032	0.54	0/1371
66	AZ	0.26	0/1661	0.52	0/2259
67	Ap	0.25	0/1141	0.53	0/1527
68	AC	0.26	0/623	0.54	0/823
69	Ae	0.24	0/1531	0.54	0/2059
70	AF	0.24	0/2477	0.53	0/3372
71	AG	0.28	0/470	0.55	0/623
72	Aj	0.25	0/836	0.49	0/1128
73	Al	0.26	0/926	0.56	0/1244
74	Ao	0.25	0/1065	0.54	0/1424

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	Ar	0.25	0/1209	0.58	0/1620
76	As	0.27	0/1120	0.54	0/1499
77	Ay	0.30	0/561	0.56	0/755
78	Ac	0.26	0/1780	0.53	0/2396
79	V	0.21	0/1822	0.82	2/2841 (0.1%)
80	Aq	0.24	0/1095	0.53	0/1469
All	All	0.25	3/222953 (0.0%)	0.70	26/327234 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A2	1	U	OP3-P	-10.73	1.48	1.61
1	B5	1	C	OP3-P	-10.60	1.48	1.61
2	B8	1	C	OP3-P	-10.59	1.48	1.61

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B5	4398	C	C2-N1-C1'	6.90	126.39	118.80
1	B5	2158	U	C2-N1-C1'	6.63	125.66	117.70
1	B5	4398	C	N1-C2-O2	6.52	122.81	118.90
79	V	40	C	C2-N1-C1'	6.48	125.92	118.80
1	B5	1931	C	N1-C2-O2	6.03	122.52	118.90
46	A2	286	C	C2-N1-C1'	5.83	125.22	118.80
1	B5	418	G	O4'-C1'-N9	5.63	112.70	108.20
1	B5	2158	U	N1-C2-O2	5.60	126.72	122.80
46	A2	829	U	C2-N1-C1'	5.56	124.37	117.70
1	B5	2376	C	C2-N1-C1'	5.40	124.74	118.80
1	B5	1931	C	N3-C2-O2	-5.38	118.14	121.90
1	B5	1360	C	N1-C2-O2	5.32	122.09	118.90
1	B5	1685	C	C2-N1-C1'	5.30	124.63	118.80
46	A2	1475	G	C4-N9-C1'	5.29	133.37	126.50
1	B5	180	C	N1-C2-O2	5.28	122.07	118.90
1	B5	4398	C	N3-C2-O2	-5.23	118.24	121.90
46	A2	286	C	N1-C2-O2	5.23	122.04	118.90
1	B5	2376	C	N1-C2-O2	5.22	122.03	118.90
1	B5	3862	U	N1-C2-O2	5.21	126.45	122.80
1	B5	4182	C	C2-N1-C1'	5.12	124.43	118.80
1	B5	2000	G	P-O3'-C3'	5.10	125.82	119.70
1	B5	2000	G	OP2-P-O3'	5.04	116.29	105.20
79	V	40	C	C6-N1-C1'	-5.04	114.75	120.80
1	B5	180	C	N3-C2-O2	-5.03	118.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B5	1360	C	C2-N1-C1'	5.02	124.32	118.80
1	B5	4304	C	OP1-P-O3'	5.01	116.22	105.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Az	23/25 (92%)	23 (100%)	0	0	100	100
5	BA	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
6	BB	395/403 (98%)	388 (98%)	7 (2%)	0	100	100
7	BC	359/421 (85%)	353 (98%)	6 (2%)	0	100	100
8	BD	294/297 (99%)	284 (97%)	10 (3%)	0	100	100
9	BE	218/298 (73%)	215 (99%)	3 (1%)	0	100	100
10	BF	232/246 (94%)	225 (97%)	7 (3%)	0	100	100
11	BG	206/266 (77%)	201 (98%)	5 (2%)	0	100	100
12	BH	190/192 (99%)	190 (100%)	0	0	100	100
13	BI	201/214 (94%)	197 (98%)	4 (2%)	0	100	100
14	BJ	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
15	BL	208/211 (99%)	202 (97%)	5 (2%)	1 (0%)	25	44
16	BM	128/131 (98%)	126 (98%)	2 (2%)	0	100	100
17	BN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	BO	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
19	BP	153/184 (83%)	151 (99%)	2 (1%)	0	100	100
20	BQ	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
21	BR	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
22	BS	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
23	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
24	BU	98/128 (77%)	94 (96%)	4 (4%)	0	100	100
25	BV	132/140 (94%)	131 (99%)	1 (1%)	0	100	100
26	BW	65/157 (41%)	65 (100%)	0	0	100	100
27	BX	117/155 (76%)	113 (97%)	4 (3%)	0	100	100
28	BY	131/145 (90%)	129 (98%)	2 (2%)	0	100	100
29	BZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
30	Ba	145/148 (98%)	142 (98%)	3 (2%)	0	100	100
31	Bb	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
32	Bc	93/115 (81%)	93 (100%)	0	0	100	100
33	Bd	103/176 (58%)	101 (98%)	2 (2%)	0	100	100
34	Be	128/135 (95%)	126 (98%)	2 (2%)	0	100	100
35	Bf	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
36	Bg	106/117 (91%)	105 (99%)	1 (1%)	0	100	100
37	Bh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
38	Bi	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
39	Bj	84/97 (87%)	84 (100%)	0	0	100	100
40	Bk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
41	Bl	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
42	Bm	50/128 (39%)	50 (100%)	0	0	100	100
43	Bo	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
44	Bp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	Br	124/138 (90%)	121 (98%)	3 (2%)	0	100	100
47	Aa	211/264 (80%)	207 (98%)	4 (2%)	0	100	100
48	AA	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
49	AB	62/69 (90%)	59 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	Ab	217/264 (82%)	215 (99%)	2 (1%)	0	100	100
51	Ad	260/263 (99%)	254 (98%)	6 (2%)	0	100	100
52	AD	55/133 (41%)	53 (96%)	2 (4%)	0	100	100
53	AE	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
54	Af	225/249 (90%)	224 (100%)	1 (0%)	0	100	100
55	Ag	185/194 (95%)	175 (95%)	10 (5%)	0	100	100
56	Ah	204/207 (99%)	193 (95%)	11 (5%)	0	100	100
57	Ai	177/194 (91%)	173 (98%)	3 (2%)	1 (1%)	22	39
58	Ak	150/158 (95%)	147 (98%)	3 (2%)	0	100	100
59	Am	148/151 (98%)	148 (100%)	0	0	100	100
60	An	132/151 (87%)	122 (92%)	10 (8%)	0	100	100
61	At	100/119 (84%)	85 (85%)	13 (13%)	2 (2%)	6	11
62	Au	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
63	Av	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
64	Aw	140/143 (98%)	134 (96%)	6 (4%)	0	100	100
65	Ax	123/131 (94%)	123 (100%)	0	0	100	100
66	AZ	205/296 (69%)	198 (97%)	7 (3%)	0	100	100
67	Ap	139/146 (95%)	128 (92%)	11 (8%)	0	100	100
68	AC	72/156 (46%)	62 (86%)	10 (14%)	0	100	100
69	Ae	189/204 (93%)	179 (95%)	10 (5%)	0	100	100
70	AF	309/317 (98%)	288 (93%)	21 (7%)	0	100	100
71	AG	53/171 (31%)	52 (98%)	1 (2%)	0	100	100
72	Aj	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
73	Al	116/132 (88%)	102 (88%)	14 (12%)	0	100	100
74	Ao	125/145 (86%)	118 (94%)	7 (6%)	0	100	100
75	Ar	142/152 (93%)	131 (92%)	11 (8%)	0	100	100
76	As	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
77	Ay	68/125 (54%)	68 (100%)	0	0	100	100
78	Ac	223/243 (92%)	221 (99%)	2 (1%)	0	100	100
80	Aq	132/135 (98%)	122 (92%)	10 (8%)	0	100	100
All	All	11107/12726 (87%)	10791 (97%)	312 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	BL	64	VAL
57	Ai	139	LYS
61	At	95	SER
61	At	94	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	
4	Az	24/24 (100%)	24 (100%)	0	100	100
5	BA	190/199 (96%)	190 (100%)	0	100	100
6	BB	346/349 (99%)	346 (100%)	0	100	100
7	BC	305/338 (90%)	303 (99%)	2 (1%)	81	93
8	BD	248/249 (100%)	248 (100%)	0	100	100
9	BE	195/256 (76%)	194 (100%)	1 (0%)	86	95
10	BF	201/211 (95%)	201 (100%)	0	100	100
11	BG	186/225 (83%)	184 (99%)	2 (1%)	70	87
12	BH	171/171 (100%)	171 (100%)	0	100	100
13	BI	173/178 (97%)	173 (100%)	0	100	100
14	BJ	142/148 (96%)	142 (100%)	0	100	100
15	BL	177/178 (99%)	177 (100%)	0	100	100
16	BM	112/113 (99%)	112 (100%)	0	100	100
17	BN	171/172 (99%)	171 (100%)	0	100	100
18	BO	172/173 (99%)	172 (100%)	0	100	100
19	BP	136/163 (83%)	134 (98%)	2 (2%)	60	82
20	BQ	159/159 (100%)	159 (100%)	0	100	100
21	BR	159/175 (91%)	159 (100%)	0	100	100
22	BS	157/157 (100%)	157 (100%)	0	100	100
23	BT	139/140 (99%)	139 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	BU	90/113 (80%)	90 (100%)	0	100	100
25	BV	102/107 (95%)	101 (99%)	1 (1%)	73	88
26	BW	59/127 (46%)	59 (100%)	0	100	100
27	BX	107/134 (80%)	106 (99%)	1 (1%)	75	90
28	BY	123/135 (91%)	123 (100%)	0	100	100
29	BZ	117/118 (99%)	117 (100%)	0	100	100
30	Ba	121/122 (99%)	121 (100%)	0	100	100
31	Bb	61/62 (98%)	61 (100%)	0	100	100
32	Bc	80/98 (82%)	80 (100%)	0	100	100
33	Bd	95/148 (64%)	94 (99%)	1 (1%)	70	87
34	Be	118/123 (96%)	118 (100%)	0	100	100
35	Bf	89/89 (100%)	89 (100%)	0	100	100
36	Bg	93/101 (92%)	93 (100%)	0	100	100
37	Bh	109/110 (99%)	108 (99%)	1 (1%)	75	90
38	Bi	85/89 (96%)	85 (100%)	0	100	100
39	Bj	73/80 (91%)	73 (100%)	0	100	100
40	Bk	64/65 (98%)	63 (98%)	1 (2%)	58	80
41	Bl	47/48 (98%)	47 (100%)	0	100	100
42	Bm	48/115 (42%)	48 (100%)	0	100	100
43	Bo	92/92 (100%)	92 (100%)	0	100	100
44	Bp	74/75 (99%)	74 (100%)	0	100	100
45	Br	111/118 (94%)	111 (100%)	0	100	100
47	Aa	194/228 (85%)	194 (100%)	0	100	100
48	AA	75/76 (99%)	75 (100%)	0	100	100
49	AB	57/62 (92%)	56 (98%)	1 (2%)	54	78
50	Ab	185/214 (86%)	185 (100%)	0	100	100
51	Ad	223/224 (100%)	223 (100%)	0	100	100
52	AD	46/108 (43%)	46 (100%)	0	100	100
53	AE	87/99 (88%)	87 (100%)	0	100	100
54	Af	199/219 (91%)	199 (100%)	0	100	100
55	Ag	167/174 (96%)	166 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	Ah	177/178 (99%)	177 (100%)	0	100	100
57	Ai	160/168 (95%)	158 (99%)	2 (1%)	65	85
58	Ak	135/140 (96%)	133 (98%)	2 (2%)	60	82
59	Am	130/131 (99%)	130 (100%)	0	100	100
60	An	105/118 (89%)	105 (100%)	0	100	100
61	At	94/106 (89%)	92 (98%)	2 (2%)	48	74
62	Au	69/69 (100%)	69 (100%)	0	100	100
63	Av	112/113 (99%)	112 (100%)	0	100	100
64	Aw	114/115 (99%)	113 (99%)	1 (1%)	75	90
65	Ax	107/113 (95%)	107 (100%)	0	100	100
66	AZ	172/245 (70%)	171 (99%)	1 (1%)	84	94
67	Ap	116/119 (98%)	115 (99%)	1 (1%)	75	90
68	AC	67/140 (48%)	67 (100%)	0	100	100
69	Ae	161/170 (95%)	161 (100%)	0	100	100
70	AF	270/275 (98%)	270 (100%)	0	100	100
71	AG	48/130 (37%)	48 (100%)	0	100	100
72	Aj	88/136 (65%)	88 (100%)	0	100	100
73	Al	100/109 (92%)	100 (100%)	0	100	100
74	Ao	113/130 (87%)	112 (99%)	1 (1%)	75	90
75	Ar	125/132 (95%)	125 (100%)	0	100	100
76	As	112/114 (98%)	111 (99%)	1 (1%)	75	90
77	Ay	61/102 (60%)	61 (100%)	0	100	100
78	Ac	189/202 (94%)	187 (99%)	2 (1%)	70	87
80	Aq	120/121 (99%)	120 (100%)	0	100	100
All	All	9699/10827 (90%)	9672 (100%)	27 (0%)	90	97

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	BC	188	ARG
7	BC	358	LYS
9	BE	261	LYS
11	BG	90	GLN
11	BG	175	ARG

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Mol	Chain	Res	Type
19	BP	69	ARG
19	BP	93	HIS
25	BV	48	ARG
27	BX	92	ASN
33	Bd	118	ARG
37	Bh	65	GLN
40	Bk	18	LYS
49	AB	69	ARG
55	Ag	109	ARG
57	Ai	27	GLN
57	Ai	180	LYS
58	Ak	45	LYS
58	Ak	69	ARG
61	At	19	ARG
61	At	34	LYS
64	Aw	142	ARG
66	AZ	2(A)	SER
67	Ap	146	ARG
74	Ao	51	ARG
76	As	129	ARG
78	Ac	76	ARG
78	Ac	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
7	BC	119	GLN
15	BL	67	HIS
17	BN	8	GLN
17	BN	182	HIS
18	BO	180	GLN
18	BO	184	ASN
21	BR	40	GLN
28	BY	14	ASN
51	Ad	179	ASN
51	Ad	188	ASN
70	AF	311	GLN
72	Aj	32	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B5	3552/4441 (79%)	559 (15%)	23 (0%)
2	B8	156/157 (99%)	16 (10%)	0
3	B7	118/119 (99%)	8 (6%)	0
46	A2	1664/1823 (91%)	296 (17%)	3 (0%)
79	V	75/76 (98%)	26 (34%)	1 (1%)
All	All	5565/6616 (84%)	905 (16%)	27 (0%)

All (905) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B5	39	A
1	B5	42	A
1	B5	58	G
1	B5	59	A
1	B5	64	A
1	B5	65	A
1	B5	66	A
1	B5	71	C
1	B5	72	G
1	B5	73	A
1	B5	85	G
1	B5	91	G
1	B5	98	A
1	B5	109	G
1	B5	110	C
1	B5	119	G
1	B5	120	A
1	B5	135	G
1	B5	142	G
1	B5	143	C
1	B5	159	C
1	B5	172	C
1	B5	181	C
1	B5	182	G
1	B5	184	U
1	B5	187	C
1	B5	188	G
1	B5	200	U
1	B5	201	C
1	B5	209	U
1	B5	210	C
1	B5	216	C
1	B5	217	C

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Mol	Chain	Res	Type
1	B5	218	A
1	B5	219	G
1	B5	220	C
1	B5	233	U
1	B5	234	G
1	B5	256	C
1	B5	267	C
1	B5	268	G
1	B5	269	G
1	B5	298	U
1	B5	316	G
1	B5	317	U
1	B5	327	C
1	B5	335	A
1	B5	341	C
1	B5	364	A
1	B5	388	G
1	B5	410	G
1	B5	411	A
1	B5	413	G
1	B5	433	U
1	B5	445	G
1	B5	450	C
1	B5	451	G
1	B5	453	A
1	B5	454	G
1	B5	455	U
1	B5	457	G
1	B5	464	A
1	B5	468	U
1	B5	473	C
1	B5	482	C
1	B5	484	A
1	B5	485	A
1	B5	486	G
1	B5	487	G
1	B5	488	U
1	B5	490	G
1	B5	494	G
1	B5	495	G
1	B5	503	G
1	B5	511	A

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Mol	Chain	Res	Type
1	B5	515	C
1	B5	517	G
1	B5	518	C
1	B5	523	G
1	B5	524	C
1	B5	578	C
1	B5	579	G
1	B5	583	C
1	B5	584	G
1	B5	595	C
1	B5	600	C
1	B5	604	C
1	B5	605	G
1	B5	606	U
1	B5	607	C
1	B5	624	C
1	B5	626	U
1	B5	629	C
1	B5	635	C
1	B5	636	G
1	B5	642	G
1	B5	643	C
1	B5	668	G
1	B5	669	G
1	B5	670	G
1	B5	677	U
1	B5	679	C
1	B5	682	G
1	B5	684	G
1	B5	687	C
1	B5	688	A
1	B5	723	U
1	B5	725	A
1	B5	726	U
1	B5	727	A
1	B5	731	G
1	B5	736	G
1	B5	742	A
1	B5	745	G
1	B5	746	U
1	B5	752	A
1	B5	753	A

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Mol	Chain	Res	Type
1	B5	754	U
1	B5	765	A
1	B5	767	G
1	B5	768	G
1	B5	769	A
1	B5	771	A
1	B5	772	G
1	B5	774	A
1	B5	776	C
1	B5	778	C
1	B5	789	U
1	B5	1095	G
1	B5	1097	G
1	B5	1099	C
1	B5	1106	G
1	B5	1107	C
1	B5	1109	G
1	B5	1110	G
1	B5	1115	C
1	B5	1128	C
1	B5	1133	G
1	B5	1135	G
1	B5	1145	G
1	B5	1147	U
1	B5	1148	C
1	B5	1152	G
1	B5	1158	C
1	B5	1162	C
1	B5	1184	C
1	B5	1185	U
1	B5	1187	G
1	B5	1192	A
1	B5	1195	C
1	B5	1197	A
1	B5	1198	G
1	B5	1200	G
1	B5	1201	C
1	B5	1202	G
1	B5	1205	C
1	B5	1209	G
1	B5	1210	U
1	B5	1212	C

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Mol	Chain	Res	Type
1	B5	1221	G
1	B5	1222	U
1	B5	1227	U
1	B5	1238	C
1	B5	1251	A2M
1	B5	1262	A
1	B5	1279	A
1	B5	1280	G
1	B5	1284	G
1	B5	1291	G
1	B5	1310	A
1	B5	1317	G
1	B5	1320	A
1	B5	1339	U
1	B5	1357	C
1	B5	1358	G
1	B5	1359	G
1	B5	1360	C
1	B5	1361	A
1	B5	1362	G
1	B5	1363	G
1	B5	1364	C
1	B5	1366	G
1	B5	1367	G
1	B5	1368	A
1	B5	1369	A
1	B5	1371	G
1	B5	1376	G
1	B5	1380	G
1	B5	1405	U
1	B5	1420	A
1	B5	1421	G
1	B5	1425	G
1	B5	1437	U
1	B5	1448	A
1	B5	1457	A2M
1	B5	1470	A
1	B5	1486	A
1	B5	1489	C
1	B5	1501	U
1	B5	1514	U
1	B5	1519	U

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Mol	Chain	Res	Type
1	B5	1547	G
1	B5	1548	OMG
1	B5	1554	A
1	B5	1556	G
1	B5	1557	A
1	B5	1561	A
1	B5	1563	C
1	B5	1564	G
1	B5	1565	A
1	B5	1577	G
1	B5	1584	C
1	B5	1593	G
1	B5	1599	C
1	B5	1600	PSU
1	B5	1603	G
1	B5	1621	G
1	B5	1623	G
1	B5	1624	G
1	B5	1625	C
1	B5	1626	G
1	B5	1627	G
1	B5	1628	U
1	B5	1631	A
1	B5	1642	G
1	B5	1648	C
1	B5	1663	C
1	B5	1668	G
1	B5	1672	G
1	B5	1673	A
1	B5	1674	A
1	B5	1680	C
1	B5	1695	A
1	B5	1712	A
1	B5	1719	G
1	B5	1723	G
1	B5	1724	C
1	B5	1728	C
1	B5	1741	C
1	B5	1742	G
1	B5	1743	U
1	B5	1745	G
1	B5	1746	A

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Mol	Chain	Res	Type
1	B5	1751	G
1	B5	1752	A
1	B5	1764	G
1	B5	1778	G
1	B5	1791	U
1	B5	1801	A
1	B5	1806	A
1	B5	1827	U
1	B5	1829	C
1	B5	1830	C
1	B5	1831	G
1	B5	1840	C
1	B5	1841	A
1	B5	1849	G
1	B5	1857	G
1	B5	1860	G
1	B5	1868	U
1	B5	1870	G
1	B5	1871	A
1	B5	1874	G
1	B5	1932	C
1	B5	1934	A
1	B5	1935	A
1	B5	1951	A
1	B5	1953	U
1	B5	1955	G
1	B5	1957	U
1	B5	1964	G
1	B5	1965	G
1	B5	1978	A
1	B5	1993	C
1	B5	1994	G
1	B5	2001	C
1	B5	2002	G
1	B5	2006	C
1	B5	2010	G
1	B5	2038	C
1	B5	2049	C
1	B5	2050	G
1	B5	2054	G
1	B5	2062	G
1	B5	2063	G

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Mol	Chain	Res	Type
1	B5	2065	G
1	B5	2097	G
1	B5	2100	OMC
1	B5	2109	A
1	B5	2144	A
1	B5	2151	G
1	B5	2159	C
1	B5	2170	G
1	B5	2174	U
1	B5	2235	G
1	B5	2237	C
1	B5	2238	C
1	B5	2239	U
1	B5	2241	C
1	B5	2255	G
1	B5	2256	A
1	B5	2260	A
1	B5	2262	A
1	B5	2263	G
1	B5	2278	A
1	B5	2286	A
1	B5	2294	C
1	B5	2295	G
1	B5	2303	C
1	B5	2304	G
1	B5	2314	A
1	B5	2319	C
1	B5	2322	A
1	B5	2336	A
1	B5	2387	G
1	B5	2396	C
1	B5	2402	C
1	B5	2409	A
1	B5	2418	C
1	B5	2436	C
1	B5	2443	G
1	B5	2444	A
1	B5	2445	A
1	B5	2457	U
1	B5	2458	C
1	B5	2459	C
1	B5	2460	G

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Mol	Chain	Res	Type
1	B5	2484	G
1	B5	2492	A
1	B5	2512	U
1	B5	2518	U
1	B5	2537	U
1	B5	2539	U
1	B5	2547	A
1	B5	2552	U
1	B5	2555	A
1	B5	2563	C
1	B5	2575	U
1	B5	2576	G
1	B5	2577	U
1	B5	2578	U
1	B5	2604	G
1	B5	2651	G
1	B5	3074	G
1	B5	3095	C
1	B5	3103	G
1	B5	3112	A
1	B5	3121	U
1	B5	3125	A
1	B5	3139	A
1	B5	3173	C
1	B5	3188	A
1	B5	3189	A
1	B5	3190	U
1	B5	3191	G
1	B5	3194	A
1	B5	3212	G
1	B5	3230	G
1	B5	3237	A
1	B5	3246	C
1	B5	3250	U
1	B5	3253	G
1	B5	3254	G
1	B5	3262	A2M
1	B5	3263	U
1	B5	3288	G
1	B5	3291	U
1	B5	3294	A
1	B5	3296	G

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Mol	Chain	Res	Type
1	B5	3300	G
1	B5	3301	A
1	B5	3315	U
1	B5	3316	G
1	B5	3317	U
1	B5	3321	U
1	B5	3328	U
1	B5	3354	A
1	B5	3355	C
1	B5	3356	G
1	B5	3369	U
1	B5	3374	G
1	B5	3375	G
1	B5	3378	A
1	B5	3382	A
1	B5	3383	A
1	B5	3384	G
1	B5	3385	A
1	B5	3392	U
1	B5	3425	C
1	B5	3430	G
1	B5	3433	G
1	B5	3434	U
1	B5	3435	G
1	B5	3437	A
1	B5	3442	A
1	B5	3443	A
1	B5	3444	G
1	B5	3449	A
1	B5	3485	C
1	B5	3487	G
1	B5	3488	C
1	B5	3489	C
1	B5	3494	A
1	B5	3495	A
1	B5	3504	A
1	B5	3506	U
1	B5	3510	A
1	B5	3513	G
1	B5	3516	U
1	B5	3524	U
1	B5	3544	C

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Mol	Chain	Res	Type
1	B5	3552	G
1	B5	3553	A
1	B5	3554	G
1	B5	3566	U
1	B5	3567	C
1	B5	3569	G
1	B5	3570	G
1	B5	3575	A
1	B5	3586	G
1	B5	3588	G
1	B5	3589	C
1	B5	3593	G
1	B5	3601	C
1	B5	3605	C
1	B5	3606	U
1	B5	3613	A
1	B5	3626	G
1	B5	3627	G
1	B5	3634	G
1	B5	3646	A
1	B5	3664	C
1	B5	3668	G
1	B5	3672	U
1	B5	3676	A
1	B5	3692	G
1	B5	3694	C
1	B5	3697	G
1	B5	3709	G
1	B5	3711	A
1	B5	3714	A
1	B5	3716	A
1	B5	3724	A
1	B5	3732	U
1	B5	3734	G
1	B5	3747	A
1	B5	3748	G
1	B5	3757	C
1	B5	3772	G
1	B5	3773	G
1	B5	3775	C
1	B5	3782	A
1	B5	3792	C

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Mol	Chain	Res	Type
1	B5	3793	U
1	B5	3797	U
1	B5	3816	G
1	B5	3819	A
1	B5	3820	G
1	B5	3821	A
1	B5	3823	A
1	B5	3830	C
1	B5	3834	G
1	B5	3837	A
1	B5	3848	G
1	B5	3863	U
1	B5	3865	A
1	B5	3869	C
1	B5	3887	C
1	B5	3891	G
1	B5	3907	A
1	B5	3918	G
1	B5	3953	A
1	B5	3955	U
1	B5	3956	A
1	B5	3958	G
1	B5	3962	C
1	B5	3967	G
1	B5	3991	A
1	B5	4003	C
1	B5	4010	G
1	B5	4018	G
1	B5	4033	A2M
1	B5	4069	A
1	B5	4079	U
1	B5	4080	OMG
1	B5	4099	C
1	B5	4100	U
1	B5	4113	C
1	B5	4115	A
1	B5	4134	A
1	B5	4143	A
1	B5	4151	A
1	B5	4152	U
1	B5	4163	C
1	B5	4172	A

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Mol	Chain	Res	Type
1	B5	4173	C
1	B5	4174	C
1	B5	4175	G
1	B5	4176	C
1	B5	4179	C
1	B5	4182	C
1	B5	4183	G
1	B5	4184	A
1	B5	4185	G
1	B5	4188	G
1	B5	4194	G
1	B5	4197	G
1	B5	4200	U
1	B5	4201	C
1	B5	4202	G
1	B5	4204	G
1	B5	4208	G
1	B5	4215	G
1	B5	4216	C
1	B5	4219	C
1	B5	4225	U
1	B5	4227	G
1	B5	4232	G
1	B5	4242	G
1	B5	4243	C
1	B5	4254	U
1	B5	4255	C
1	B5	4266	C
1	B5	4267	C
1	B5	4268	G
1	B5	4269	G
1	B5	4271	G
1	B5	4272	C
1	B5	4273	G
1	B5	4274	C
1	B5	4277	A
1	B5	4278	C
1	B5	4281	A
1	B5	4286	G
1	B5	4288	G
1	B5	4296	U
1	B5	4297	C

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Mol	Chain	Res	Type
1	B5	4305	G
1	B5	4307	G
1	B5	4314	A
1	B5	4315	U
1	B5	4334	G
1	B5	4335	C
1	B5	4337	A
1	B5	4347	U
1	B5	4360	U
1	B5	4361	C
1	B5	4385	A
1	B5	4388	G
1	B5	4399	G
1	B5	4412	G
1	B5	4421	C
1	B5	4425	C
1	B5	4432	A
1	B5	4433	G
1	B5	4434	C
1	B5	4435	U
1	B5	4437	U
1	B5	4440	U
2	B8	34	U
2	B8	35	C
2	B8	39	G
2	B8	52	A
2	B8	59	A
2	B8	62	A
2	B8	63	U
2	B8	80	A
2	B8	84	A
2	B8	87	G
2	B8	94	G
2	B8	103	A
2	B8	105	C
2	B8	110	U
2	B8	114	G
2	B8	125	C
3	B7	7	G
3	B7	33	U
3	B7	41	G
3	B7	50	A

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Mol	Chain	Res	Type
3	B7	53	U
3	B7	54	A
3	B7	64	G
3	B7	110	G
46	A2	2	A
46	A2	3	C
46	A2	23	G
46	A2	25	A
46	A2	33	G
46	A2	41	G
46	A2	44	U
46	A2	46	A
46	A2	56	G
46	A2	59	U
46	A2	67	C
46	A2	68	A
46	A2	71	G
46	A2	74	G
46	A2	76	U
46	A2	77	A
46	A2	79	A
46	A2	103	A
46	A2	113	G
46	A2	114	G
46	A2	116	OMU
46	A2	126	G
46	A2	128	U
46	A2	129	C
46	A2	141	C
46	A2	142	U
46	A2	148	A
46	A2	154	G
46	A2	161	C
46	A2	162	U
46	A2	174	A
46	A2	177	C
46	A2	183	A
46	A2	191	C
46	A2	194	C
46	A2	260	G
46	A2	264	A
46	A2	267	U

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Mol	Chain	Res	Type
46	A2	268	C
46	A2	271	G
46	A2	274	G
46	A2	281	C
46	A2	286	C
46	A2	288	G
46	A2	291	G
46	A2	308	G
46	A2	315	OMU
46	A2	323	C
46	A2	325	A
46	A2	330	C
46	A2	342	C
46	A2	346	G
46	A2	347	C
46	A2	361	C
46	A2	368	A
46	A2	370	C
46	A2	381	G
46	A2	382	G
46	A2	389	OMU
46	A2	390	C
46	A2	399	G
46	A2	409	A
46	A2	410	A
46	A2	411	C
46	A2	425	A
46	A2	432	G
46	A2	433	C
46	A2	434	A
46	A2	435	G
46	A2	443	G
46	A2	448	U
46	A2	453	C
46	A2	461	A
46	A2	468	G
46	A2	469	A
46	A2	477	A
46	A2	497	A
46	A2	508	G
46	A2	511	C
46	A2	516	A

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Mol	Chain	Res	Type
46	A2	520	G
46	A2	524	G
46	A2	525	A
46	A2	529	C
46	A2	531	C
46	A2	537	A
46	A2	544	A
46	A2	548	A
46	A2	550	G
46	A2	552	U
46	A2	556	U
46	A2	565	A
46	A2	567	G
46	A2	569	C
46	A2	570	U
46	A2	575	C
46	A2	578	G
46	A2	582	C
46	A2	589	A
46	A2	592	U
46	A2	604	A
46	A2	605	OMG
46	A2	616	A
46	A2	621	C
46	A2	625	A
46	A2	629	A2M
46	A2	630	A
46	A2	632	A
46	A2	633	A
46	A2	634	G
46	A2	694	C
46	A2	695	C
46	A2	696	C
46	A2	697	A
46	A2	698	G
46	A2	761	U
46	A2	771	A
46	A2	774	PSU
46	A2	781	G
46	A2	782	PSU
46	A2	790	A
46	A2	791	G

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Mol	Chain	Res	Type
46	A2	796	G
46	A2	797	C
46	A2	798	C
46	A2	799	G
46	A2	805	A
46	A2	826	G
46	A2	828	A
46	A2	829	U
46	A2	837	C
46	A2	839	G
46	A2	846	U
46	A2	858	C
46	A2	863	A
46	A2	865	G
46	A2	867	G
46	A2	871	A
46	A2	875	U
46	A2	878	A
46	A2	880	A
46	A2	888	C
46	A2	891	G
46	A2	901	U
46	A2	913	A
46	A2	929	G
46	A2	936	G
46	A2	948	A
46	A2	950	A
46	A2	975	U
46	A2	981	A
46	A2	1019	U
46	A2	1020	A
46	A2	1041	A
46	A2	1043	C
46	A2	1047	G
46	A2	1073	U
46	A2	1074	C
46	A2	1075	C
46	A2	1076	C
46	A2	1079	G
46	A2	1091	A
46	A2	1096	C
46	A2	1097	C

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Mol	Chain	Res	Type
46	A2	1102	A
46	A2	1107	A
46	A2	1111	C
46	A2	1112	U
46	A2	1124	G
46	A2	1153	A
46	A2	1165	G
46	A2	1166	A
46	A2	1168	G
46	A2	1169	G
46	A2	1173	C
46	A2	1182	G
46	A2	1200	U
46	A2	1209	A
46	A2	1211	A
46	A2	1214	G
46	A2	1215	G
46	A2	1217	A
46	A2	1223	A
46	A2	1229	C
46	A2	1232	G
46	A2	1233	G
46	A2	1240	A
46	A2	1243	G
46	A2	1244	G
46	A2	1245	A
46	A2	1254	U
46	A2	1260	G
46	A2	1261	C
46	A2	1268	U
46	A2	1269	C
46	A2	1270	G
46	A2	1271	A
46	A2	1276	G
46	A2	1300	U
46	A2	1306	G
46	A2	1316	U
46	A2	1329	U
46	A2	1330	U
46	A2	1336	A
46	A2	1340	A
46	A2	1342	C

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Mol	Chain	Res	Type
46	A2	1355	U
46	A2	1360	A
46	A2	1361	C
46	A2	1362	U
46	A2	1363	A
46	A2	1364	G
46	A2	1376	C
46	A2	1377	C
46	A2	1379	A
46	A2	1381	C
46	A2	1382	G
46	A2	1383	G
46	A2	1391	C
46	A2	1392	C
46	A2	1394	A
46	A2	1408	C
46	A2	1409	A
46	A2	1410	A
46	A2	1411	G
46	A2	1418	U
46	A2	1419	C
46	A2	1420	A
46	A2	1435	A
46	A2	1442	A
46	A2	1444	A
46	A2	1445	OMG
46	A2	1450	G
46	A2	1452	G
46	A2	1453	A
46	A2	1464	U
46	A2	1475	G
46	A2	1476	C
46	A2	1488	A
46	A2	1499	C
46	A2	1503	U
46	A2	1508	U
46	A2	1510	U
46	A2	1515	U
46	A2	1525	G
46	A2	1534	A
46	A2	1535	A
46	A2	1540	U

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Mol	Chain	Res	Type
46	A2	1541	U
46	A2	1543	A
46	A2	1551	U
46	A2	1556	A
46	A2	1559	G
46	A2	1572	G
46	A2	1576	U
46	A2	1578	A
46	A2	1609	G
46	A2	1616	A
46	A2	1620	G
46	A2	1626	G
46	A2	1653	C
46	A2	1654	A
46	A2	1676	U
46	A2	1677	G
46	A2	1681	G
46	A2	1707	C
46	A2	1710	G
46	A2	1713	G
46	A2	1714	G
46	A2	1715	G
46	A2	1720	C
46	A2	1721	C
46	A2	1722	A
46	A2	1729	U
46	A2	1730	G
46	A2	1734	G
46	A2	1735	A
46	A2	1736	G
46	A2	1737	C
46	A2	1738	G
46	A2	1739	U
46	A2	1754	A
46	A2	1769	A
46	A2	1779	A
46	A2	1780	G
46	A2	1783	G
46	A2	1785	A
46	A2	1789	A
46	A2	1790	G
46	A2	1792	U

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Mol	Chain	Res	Type
46	A2	1803	G
46	A2	1815	G
46	A2	1816	G
46	A2	1817	A
46	A2	1818	U
46	A2	1819	C
79	V	7	A
79	V	8	U
79	V	9	A
79	V	10	G
79	V	16	U
79	V	17	U
79	V	18	G
79	V	20	G
79	V	22	G
79	V	27	G
79	V	31	A
79	V	32	C
79	V	36	A
79	V	37	G
79	V	38	A
79	V	40	C
79	V	41	C
79	V	45	G
79	V	46	G
79	V	47	U
79	V	49	C
79	V	53	G
79	V	59	U
79	V	60	C
79	V	61	C
79	V	76	A

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B5	119	G
1	B5	216	C
1	B5	489	C
1	B5	502	C
1	B5	771	A
1	B5	777	G

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Mol	Chain	Res	Type
1	B5	1197	A
1	B5	1358	G
1	B5	1366	G
1	B5	1513	C
1	B5	1556	G
1	B5	1626	G
1	B5	1993	C
1	B5	2000	G
1	B5	2005	G
1	B5	2061	U
1	B5	3245	U
1	B5	3249	U
1	B5	4142	U
1	B5	4182	C
1	B5	4231	G
1	B5	4304	C
1	B5	4432	A
46	A2	1418	U
46	A2	1733	G
46	A2	1779	A
79	V	8	U

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

142 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	$\# Z  > 2$
1	OMG	B5	3639	1	18,26,27	0.93	2 (11%)	19,38,41	0.60	0
1	PSU	B5	1700	1	18,21,22	0.52	0	22,30,33	0.56	0
1	PSU	B5	3995	1	18,21,22	0.48	0	22,30,33	0.60	0
1	PSU	B5	4132	1	18,21,22	0.47	0	22,30,33	0.61	0
1	A2M	B5	3201	1	18,25,26	0.66	0	18,36,39	0.70	1 (5%)
2	OMG	B8	75	2	18,26,27	0.92	1 (5%)	19,38,41	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
46	PSU	A2	1132	81,46	18,21,22	0.48	0	22,30,33	0.58	0
1	UY1	B5	3295	81,1	19,22,23	0.50	0	22,31,34	0.54	0
1	A2M	B5	3262	81,1	18,25,26	0.64	0	18,36,39	0.84	1 (5%)
1	OMC	B5	3364	1	19,22,23	0.31	0	26,31,34	0.47	0
46	PSU	A2	93	46	18,21,22	0.50	0	22,30,33	0.56	0
1	PSU	B5	1769	1	18,21,22	0.49	0	22,30,33	0.57	0
1	OMU	B5	3670	1	19,22,23	0.31	0	26,31,34	0.47	0
1	6MZ	B5	3663	1	18,25,26	0.72	0	16,36,39	0.69	1 (6%)
2	PSU	B8	55	2	18,21,22	0.45	0	22,30,33	0.61	0
1	PSU	B5	3172	81,1	18,21,22	0.49	0	22,30,33	0.60	0
1	OMC	B5	3285	1	19,22,23	0.30	0	26,31,34	0.36	0
1	A2M	B5	3966	81,1	18,25,26	0.66	0	18,36,39	0.94	2 (11%)
1	PSU	B5	3975	1	18,21,22	0.52	0	22,30,33	0.55	0
1	PSU	B5	3755	1	18,21,22	0.48	0	22,30,33	0.58	0
46	PSU	A2	647	46	18,21,22	0.47	0	22,30,33	0.57	0
1	OMC	B5	3318	1	19,22,23	0.28	0	26,31,34	0.41	0
1	A2M	B5	2112	81,1	18,25,26	0.65	0	18,36,39	0.71	1 (5%)
1	OMC	B5	2171	81,1	19,22,23	0.29	0	26,31,34	0.40	0
46	OMU	A2	1284	46	19,22,23	0.24	0	26,31,34	0.47	0
1	UR3	B5	3973	1	19,22,23	0.30	0	26,32,35	0.31	0
1	A2M	B5	3307	1	18,25,26	0.65	0	18,36,39	0.81	1 (5%)
1	OMG	B5	2113	1	18,26,27	0.91	2 (11%)	19,38,41	0.64	0
46	A2M	A2	165	46	18,25,26	0.65	0	18,36,39	0.83	1 (5%)
1	OMU	B5	3941	1	19,22,23	0.30	0	26,31,34	0.47	0
1	A2M	B5	3302	1	18,25,26	0.66	0	18,36,39	0.74	1 (5%)
1	PSU	B5	3885	1	18,21,22	0.52	0	22,30,33	0.62	1 (4%)
76	NMM	As	67	76	9,11,12	1.59	1 (11%)	6,12,14	3.56	2 (33%)
1	PSU	B5	1652	1	18,21,22	0.48	0	22,30,33	0.57	0
1	1MA	B5	1247	81,1	16,25,26	0.82	1 (6%)	18,37,40	0.61	0
1	PSU	B5	3804	1	18,21,22	0.46	0	22,30,33	0.58	0
46	4AC	A2	1295	46	21,24,25	0.33	0	29,34,37	0.41	0
46	A2M	A2	1341	46	18,25,26	0.65	0	18,36,39	0.73	1 (5%)
1	OMU	B5	2586	1	19,22,23	0.32	0	26,31,34	0.55	0
1	PSU	B5	3742	1	18,21,22	0.50	0	22,30,33	0.56	0
1	OMC	B5	3979	1	19,22,23	0.32	0	26,31,34	0.47	0
1	PSU	B5	3846	1	18,21,22	0.49	0	22,30,33	0.58	0
1	A2M	B5	4014	1	18,25,26	0.66	0	18,36,39	0.74	1 (5%)
1	A2M	B5	2536	81,1	18,25,26	0.65	0	18,36,39	0.69	1 (5%)
1	OMG	B5	3835	1	18,26,27	0.90	2 (11%)	19,38,41	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
46	PSU	A2	775	46	18,21,22	0.46	0	22,30,33	0.58	0
1	5MC	B5	3259	81,1	18,22,23	0.29	0	26,32,35	0.43	0
1	A2M	B5	1251	1	18,25,26	0.65	0	18,36,39	0.72	1 (5%)
46	OMU	A2	171	46	19,22,23	0.25	0	26,31,34	0.55	0
1	OMC	B5	1265	1	19,22,23	0.28	0	26,31,34	0.42	0
1	OMG	B5	3104	1	18,26,27	0.93	1 (5%)	19,38,41	0.69	0
46	A2M	A2	629	81,46	18,25,26	0.64	0	18,36,39	0.76	1 (5%)
46	PSU	A2	642	46	18,21,22	0.49	0	22,30,33	0.59	0
46	PSU	A2	774	46	18,21,22	0.47	0	22,30,33	0.60	0
46	OMG	A2	470	81,46	18,26,27	0.93	2 (11%)	19,38,41	0.60	0
1	PSU	B5	4372	81,1	18,21,22	0.50	0	22,30,33	0.58	0
1	OMC	B5	2553	1	19,22,23	0.28	0	26,31,34	0.39	0
46	OMC	A2	173	46	19,22,23	0.29	0	26,31,34	0.45	0
46	MA6	A2	1805	46	18,26,27	0.74	0	19,38,41	0.73	0
1	PSU	B5	4071	1	18,21,22	0.51	0	22,30,33	0.57	0
46	OMG	A2	1445	81,46	18,26,27	0.89	1 (5%)	19,38,41	0.62	0
1	OMG	B5	3942	1	18,26,27	0.92	2 (11%)	19,38,41	0.62	0
1	PSU	B5	4343	1	18,21,22	0.48	0	22,30,33	0.59	0
46	OMU	A2	315	46	19,22,23	0.33	0	26,31,34	0.64	0
1	OMG	B5	3269	1	18,26,27	0.91	2 (11%)	19,38,41	0.58	0
1	OMC	B5	1790	81,1	19,22,23	0.29	0	26,31,34	0.59	0
1	PSU	B5	1606	81,1	18,21,22	0.49	0	22,30,33	0.59	0
1	OMC	B5	2100	1	19,22,23	0.32	0	26,31,34	0.42	0
46	OMG	A2	1286	46	18,26,27	0.90	1 (5%)	19,38,41	0.62	0
46	OMC	A2	1658	46	19,22,23	0.27	0	26,31,34	0.42	0
46	PSU	A2	109	81,46	18,21,22	0.50	0	22,30,33	0.57	0
1	PSU	B5	3874	1	18,21,22	0.47	0	22,30,33	0.60	0
1	OMU	B5	3402	1	19,22,23	0.29	0	26,31,34	0.48	0
1	5MC	B5	3890	1	18,22,23	0.34	0	26,32,35	0.63	0
1	PSU	B5	3736	1	18,21,22	0.49	0	22,30,33	0.55	0
1	PSU	B5	3900	1	18,21,22	0.51	0	22,30,33	0.59	1 (4%)
46	4AC	A2	1796	46	21,24,25	0.30	0	29,34,37	0.30	0
6	HIC	BB	245	6	8,11,12	1.64	1 (12%)	6,14,16	1.00	0
46	A2M	A2	158	46	18,25,26	0.65	0	18,36,39	0.70	1 (5%)
1	OMC	B5	2610	1	19,22,23	0.28	0	26,31,34	0.34	0
2	PSU	B8	69	2,81	18,21,22	0.54	0	22,30,33	0.66	1 (4%)
1	PSU	B5	4022	1	18,21,22	0.49	0	22,30,33	0.57	0
1	PSU	B5	3397	81,1	18,21,22	0.47	0	22,30,33	0.59	0
46	OMG	A2	562	46	18,26,27	0.91	1 (5%)	19,38,41	0.60	0
46	6MZ	A2	1786	81,46	18,25,26	0.72	0	16,36,39	0.82	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
46	PSU	A2	1039	46	18,21,22	0.60	1 (5%)	22,30,33	0.65	0
46	A2M	A2	27	81,46	18,25,26	0.65	0	18,36,39	0.75	1 (5%)
1	PSU	B5	3866	1	18,21,22	0.49	0	22,30,33	0.57	0
46	MA6	A2	1804	46	18,26,27	0.76	1 (5%)	19,38,41	0.66	0
1	OMG	B5	2625	1	18,26,27	0.92	2 (11%)	19,38,41	0.59	0
1	PSU	B5	3114	81,1	18,21,22	0.45	0	22,30,33	0.63	0
1	A2M	B5	401	1	18,25,26	0.66	0	18,36,39	0.71	1 (5%)
1	OMG	B5	3937	1	18,26,27	0.94	2 (11%)	19,38,41	0.63	0
1	OMG	B5	1445	1	18,26,27	0.93	2 (11%)	19,38,41	0.66	0
46	OMG	A2	605	46	18,26,27	0.91	1 (5%)	19,38,41	0.67	0
1	PSU	B5	3796	1	18,21,22	0.47	0	22,30,33	0.58	0
1	OMG	B5	4080	1	18,26,27	0.92	2 (11%)	19,38,41	0.61	0
1	OMU	B5	3749	1	19,22,23	0.30	0	26,31,34	0.45	0
1	OMC	B5	3346	1	19,22,23	0.28	0	26,31,34	0.44	0
1	A2M	B5	3344	1	18,25,26	0.66	0	18,36,39	0.73	1 (5%)
1	PSU	B5	1771	1	18,21,22	0.47	0	22,30,33	0.61	0
1	A2M	B5	399	1	18,25,26	0.65	0	18,36,39	0.73	1 (5%)
1	PSU	B5	3116	1	18,21,22	0.50	0	22,30,33	0.58	0
46	OMU	A2	116	46	19,22,23	0.28	0	26,31,34	0.42	0
1	OMG	B5	3376	81,1	18,26,27	0.95	3 (16%)	19,38,41	0.69	0
1	OMG	B5	4066	1	18,26,27	0.93	2 (11%)	19,38,41	0.68	0
1	OMG	B5	3221	1	18,26,27	0.91	1 (5%)	19,38,41	0.63	0
46	PSU	A2	610	46	18,21,22	0.46	0	22,30,33	0.61	0
46	OMG	A2	644	46	18,26,27	0.94	2 (11%)	19,38,41	0.60	0
43	MLZ	B <sub>o</sub>	53	43	8,9,10	0.73	0	4,9,11	0.64	0
46	OMU	A2	389	46	19,22,23	0.32	0	26,31,34	0.50	0
46	PSU	A2	258	46	18,21,22	0.48	0	22,30,33	0.57	0
1	OMU	B5	4063	1	19,22,23	0.31	0	26,31,34	0.54	0
1	PSU	B5	1600	1	18,21,22	0.66	1 (5%)	22,30,33	0.59	0
1	PSU	B5	3192	1	18,21,22	0.54	0	22,30,33	0.59	1 (4%)
46	A2M	A2	551	46	18,25,26	0.65	0	18,36,39	0.77	1 (5%)
1	PSU	B5	3964	81,1	18,21,22	0.51	0	22,30,33	0.59	0
1	OMG	B5	1241	1	18,26,27	0.98	3 (16%)	19,38,41	0.67	0
1	A2M	B5	1780	81,1	18,25,26	0.66	0	18,36,39	0.90	1 (5%)
60	IAS	An	138	60	6,7,8	1.05	0	6,8,10	1.30	1 (16%)
46	A2M	A2	989	46	18,25,26	0.64	0	18,36,39	0.80	1 (5%)
1	A2M	B5	2564	1	18,25,26	0.65	0	18,36,39	0.71	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	A2M	B5	4033	1	18,25,26	0.66	0	18,36,39	0.75	1 (5%)
1	A2M	B5	1447	1	18,25,26	0.65	0	18,36,39	0.76	1 (5%)
1	A2M	B5	1457	81,1	18,25,26	0.64	0	18,36,39	0.81	1 (5%)
1	PSU	B5	1690	1	18,21,22	0.47	0	22,30,33	0.59	0
1	OMG	B5	3813	1	18,26,27	0.92	2 (11%)	19,38,41	0.61	0
1	OMC	B5	3899	1	19,22,23	0.29	0	26,31,34	0.37	0
46	PSU	A2	782	46	18,21,22	0.60	1 (5%)	22,30,33	0.67	1 (4%)
1	OMG	B5	4061	1	18,26,27	0.90	1 (5%)	19,38,41	0.65	0
46	OMU	A2	121	46	19,22,23	0.29	0	26,31,34	0.46	0
46	A2M	A2	445	46	18,25,26	0.64	0	18,36,39	0.72	1 (5%)
1	OMG	B5	3671	1	18,26,27	0.92	1 (5%)	19,38,41	0.70	0
1	PSU	B5	3739	1	18,21,22	0.47	0	22,30,33	0.62	0
1	OMG	B5	1548	81,1	18,26,27	0.98	2 (11%)	19,38,41	0.63	0
1	OMG	B5	2173	1	18,26,27	0.92	2 (11%)	19,38,41	0.57	0
46	B8N	A2	1206	46	24,29,30	0.58	0	29,42,45	0.64	0
1	A2M	B5	3195	1	18,25,26	0.66	0	18,36,39	0.73	1 (5%)
1	PSU	B5	4019	1	18,21,22	0.48	0	22,30,33	0.58	0
46	A2M	A2	99	81,46	18,25,26	0.65	0	18,36,39	0.77	1 (5%)
1	PSU	B5	4116	1	18,21,22	0.48	0	22,30,33	0.59	0
1	OMC	B5	3178	81,1	19,22,23	0.26	0	26,31,34	0.47	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
1	OMG	B5	3639	1	-	1/5/27/28	0/3/3/3
1	PSU	B5	1700	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3995	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4132	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3201	1	-	1/5/27/28	0/3/3/3
2	OMG	B8	75	2	-	0/5/27/28	0/3/3/3
46	PSU	A2	1132	81,46	-	0/7/25/26	0/2/2/2
1	UY1	B5	3295	81,1	-	2/9/27/28	0/2/2/2
1	A2M	B5	3262	81,1	-	2/5/27/28	0/3/3/3
1	OMC	B5	3364	1	-	0/9/27/28	0/2/2/2
46	PSU	A2	93	46	-	0/7/25/26	0/2/2/2
1	PSU	B5	1769	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	B5	3670	1	-	0/9/27/28	0/2/2/2
1	6MZ	B5	3663	1	-	0/5/27/28	0/3/3/3
2	PSU	B8	55	2	-	0/7/25/26	0/2/2/2
1	PSU	B5	3172	81,1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3285	1	-	0/9/27/28	0/2/2/2
1	A2M	B5	3966	81,1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3975	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3755	1	-	0/7/25/26	0/2/2/2
46	PSU	A2	647	46	-	0/7/25/26	0/2/2/2
1	OMC	B5	3318	1	-	0/9/27/28	0/2/2/2
1	A2M	B5	2112	81,1	-	1/5/27/28	0/3/3/3
1	OMC	B5	2171	81,1	-	3/9/27/28	0/2/2/2
46	OMU	A2	1284	46	-	0/9/27/28	0/2/2/2
1	UR3	B5	3973	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3307	1	-	0/5/27/28	0/3/3/3
1	OMG	B5	2113	1	-	2/5/27/28	0/3/3/3
46	A2M	A2	165	46	-	0/5/27/28	0/3/3/3
1	OMU	B5	3941	1	-	0/9/27/28	0/2/2/2
1	A2M	B5	3302	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3885	1	-	0/7/25/26	0/2/2/2
76	NMM	As	67	76	-	5/9/11/13	-
1	PSU	B5	1652	1	-	0/7/25/26	0/2/2/2
1	1MA	B5	1247	81,1	-	0/3/25/26	0/3/3/3
1	PSU	B5	3804	1	-	0/7/25/26	0/2/2/2
46	4AC	A2	1295	46	-	2/11/29/30	0/2/2/2
46	A2M	A2	1341	46	-	1/5/27/28	0/3/3/3
1	OMU	B5	2586	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	3742	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3979	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	3846	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	4014	1	-	0/5/27/28	0/3/3/3
1	A2M	B5	2536	81,1	-	0/5/27/28	0/3/3/3
1	OMG	B5	3835	1	-	0/5/27/28	0/3/3/3
46	PSU	A2	775	46	-	0/7/25/26	0/2/2/2
1	5MC	B5	3259	81,1	-	0/7/25/26	0/2/2/2
1	A2M	B5	1251	1	-	1/5/27/28	0/3/3/3
46	OMU	A2	171	46	-	0/9/27/28	0/2/2/2
1	OMC	B5	1265	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	3104	1	-	0/5/27/28	0/3/3/3
46	A2M	A2	629	81,46	-	2/5/27/28	0/3/3/3
46	PSU	A2	642	46	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PSU	A2	774	46	-	3/7/25/26	0/2/2/2
46	OMG	A2	470	81,46	-	0/5/27/28	0/3/3/3
1	PSU	B5	4372	81,1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2553	1	-	0/9/27/28	0/2/2/2
46	OMC	A2	173	46	-	0/9/27/28	0/2/2/2
46	MA6	A2	1805	46	-	1/7/29/30	0/3/3/3
1	PSU	B5	4071	1	-	0/7/25/26	0/2/2/2
46	OMG	A2	1445	81,46	-	1/5/27/28	0/3/3/3
1	OMG	B5	3942	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4343	1	-	0/7/25/26	0/2/2/2
46	OMU	A2	315	46	-	2/9/27/28	0/2/2/2
1	OMG	B5	3269	1	-	0/5/27/28	0/3/3/3
1	OMC	B5	1790	81,1	-	0/9/27/28	0/2/2/2
1	PSU	B5	1606	81,1	-	0/7/25/26	0/2/2/2
1	OMC	B5	2100	1	-	3/9/27/28	0/2/2/2
46	OMG	A2	1286	46	-	0/5/27/28	0/3/3/3
46	OMC	A2	1658	46	-	0/9/27/28	0/2/2/2
46	PSU	A2	109	81,46	-	0/7/25/26	0/2/2/2
1	PSU	B5	3874	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	3402	1	-	0/9/27/28	0/2/2/2
1	5MC	B5	3890	1	-	3/7/25/26	0/2/2/2
1	PSU	B5	3736	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3900	1	-	0/7/25/26	0/2/2/2
46	4AC	A2	1796	46	-	0/11/29/30	0/2/2/2
6	HIC	BB	245	6	-	1/5/6/8	0/1/1/1
46	A2M	A2	158	46	-	0/5/27/28	0/3/3/3
1	OMC	B5	2610	1	-	0/9/27/28	0/2/2/2
2	PSU	B8	69	2,81	-	0/7/25/26	0/2/2/2
1	PSU	B5	4022	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3397	81,1	-	0/7/25/26	0/2/2/2
46	OMG	A2	562	46	-	1/5/27/28	0/3/3/3
46	6MZ	A2	1786	81,46	-	0/5/27/28	0/3/3/3
46	PSU	A2	1039	46	-	1/7/25/26	0/2/2/2
46	A2M	A2	27	81,46	-	0/5/27/28	0/3/3/3
1	PSU	B5	3866	1	-	0/7/25/26	0/2/2/2
46	MA6	A2	1804	46	-	0/7/29/30	0/3/3/3
1	OMG	B5	2625	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3114	81,1	-	0/7/25/26	0/2/2/2
1	A2M	B5	401	1	-	0/5/27/28	0/3/3/3
1	OMG	B5	3937	1	-	1/5/27/28	0/3/3/3
1	OMG	B5	1445	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	OMG	A2	605	46	-	3/5/27/28	0/3/3/3
1	PSU	B5	3796	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4080	1	-	0/5/27/28	0/3/3/3
1	OMU	B5	3749	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	3346	1	-	1/9/27/28	0/2/2/2
1	A2M	B5	3344	1	-	1/5/27/28	0/3/3/3
1	PSU	B5	1771	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	399	1	-	1/5/27/28	0/3/3/3
1	PSU	B5	3116	1	-	0/7/25/26	0/2/2/2
46	OMU	A2	116	46	-	2/9/27/28	0/2/2/2
1	OMG	B5	3376	81,1	-	0/5/27/28	0/3/3/3
1	OMG	B5	4066	1	-	0/5/27/28	0/3/3/3
1	OMG	B5	3221	1	-	0/5/27/28	0/3/3/3
46	PSU	A2	610	46	-	0/7/25/26	0/2/2/2
46	OMG	A2	644	46	-	0/5/27/28	0/3/3/3
43	MLZ	Bo	53	43	-	3/7/8/10	-
46	OMU	A2	389	46	-	7/9/27/28	0/2/2/2
46	PSU	A2	258	46	-	0/7/25/26	0/2/2/2
1	OMU	B5	4063	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	1600	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3192	1	-	0/7/25/26	0/2/2/2
46	A2M	A2	551	46	-	0/5/27/28	0/3/3/3
1	PSU	B5	3964	81,1	-	2/7/25/26	0/2/2/2
1	OMG	B5	1241	1	-	0/5/27/28	0/3/3/3
1	A2M	B5	1780	81,1	-	0/5/27/28	0/3/3/3
60	IAS	An	138	60	-	3/7/7/8	-
46	A2M	A2	989	46	-	0/5/27/28	0/3/3/3
1	A2M	B5	2564	1	-	0/5/27/28	0/3/3/3
1	A2M	B5	4033	1	-	1/5/27/28	0/3/3/3
1	A2M	B5	1447	1	-	0/5/27/28	0/3/3/3
1	A2M	B5	1457	81,1	-	2/5/27/28	0/3/3/3
1	PSU	B5	1690	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3813	1	-	1/5/27/28	0/3/3/3
1	OMC	B5	3899	1	-	0/9/27/28	0/2/2/2
46	PSU	A2	782	46	-	0/7/25/26	0/2/2/2
1	OMG	B5	4061	1	-	0/5/27/28	0/3/3/3
46	OMU	A2	121	46	-	0/9/27/28	0/2/2/2
46	A2M	A2	445	46	-	0/5/27/28	0/3/3/3
1	OMG	B5	3671	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3739	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	1548	81,1	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	B5	2173	1	-	0/5/27/28	0/3/3/3
46	B8N	A2	1206	46	-	4/16/34/35	0/2/2/2
1	A2M	B5	3195	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4019	1	-	0/7/25/26	0/2/2/2
46	A2M	A2	99	81,46	-	0/5/27/28	0/3/3/3
1	PSU	B5	4116	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3178	81,1	-	4/9/27/28	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	As	67	NMM	CZ-NH2	4.34	1.44	1.34
6	BB	245	HIC	CD2-CG	3.54	1.41	1.36
1	B5	1548	OMG	C5-C6	-2.44	1.42	1.47
1	B5	1241	OMG	C5-C6	-2.37	1.42	1.47
1	B5	1600	PSU	O4'-C1'	-2.35	1.40	1.43
1	B5	3937	OMG	C5-C6	-2.26	1.42	1.47
46	A2	470	OMG	C5-C6	-2.25	1.42	1.47
1	B5	2173	OMG	C5-C6	-2.24	1.42	1.47
1	B5	2625	OMG	C5-C6	-2.23	1.42	1.47
1	B5	3639	OMG	C5-C6	-2.22	1.42	1.47
46	A2	644	OMG	C5-C6	-2.22	1.42	1.47
1	B5	3671	OMG	C5-C6	-2.21	1.42	1.47
2	B8	75	OMG	C5-C6	-2.21	1.42	1.47
1	B5	3813	OMG	C5-C6	-2.20	1.42	1.47
1	B5	3942	OMG	C5-C6	-2.17	1.43	1.47
46	A2	782	PSU	O4'-C1'	-2.17	1.40	1.43
1	B5	3376	OMG	C5-C6	-2.16	1.43	1.47
46	A2	1039	PSU	O4'-C1'	-2.16	1.40	1.43
46	A2	562	OMG	C5-C6	-2.16	1.43	1.47
1	B5	3269	OMG	C5-C6	-2.15	1.43	1.47
1	B5	1241	OMG	C8-N7	-2.14	1.31	1.35
1	B5	3104	OMG	C5-C6	-2.14	1.43	1.47
1	B5	1548	OMG	C8-N7	-2.14	1.31	1.35
1	B5	3221	OMG	C5-C6	-2.13	1.43	1.47
1	B5	4080	OMG	C5-C6	-2.12	1.43	1.47
1	B5	4061	OMG	C5-C6	-2.11	1.43	1.47
46	A2	605	OMG	C5-C6	-2.11	1.43	1.47
46	A2	1445	OMG	C5-C6	-2.10	1.43	1.47
1	B5	4066	OMG	C5-C6	-2.10	1.43	1.47
1	B5	3639	OMG	C8-N7	-2.09	1.31	1.35
46	A2	1286	OMG	C5-C6	-2.09	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B5	1445	OMG	C5-C6	-2.09	1.43	1.47
1	B5	2113	OMG	C5-C6	-2.08	1.43	1.47
46	A2	470	OMG	C8-N7	-2.07	1.31	1.35
1	B5	2625	OMG	C8-N7	-2.07	1.31	1.35
1	B5	3269	OMG	C8-N7	-2.07	1.31	1.35
1	B5	3937	OMG	C8-N7	-2.06	1.31	1.35
1	B5	3376	OMG	C8-N7	-2.05	1.31	1.35
1	B5	3942	OMG	C8-N7	-2.05	1.31	1.35
1	B5	3376	OMG	C5-C4	-2.05	1.37	1.43
1	B5	4066	OMG	C8-N7	-2.04	1.31	1.35
1	B5	4080	OMG	C8-N7	-2.04	1.31	1.35
1	B5	1445	OMG	C8-N7	-2.03	1.31	1.35
1	B5	1241	OMG	C5-C4	-2.03	1.37	1.43
1	B5	3813	OMG	C8-N7	-2.03	1.31	1.35
46	A2	644	OMG	C8-N7	-2.03	1.31	1.35
1	B5	3835	OMG	C5-C6	-2.02	1.43	1.47
1	B5	2173	OMG	C8-N7	-2.02	1.31	1.35
1	B5	3835	OMG	C8-N7	-2.02	1.31	1.35
1	B5	2113	OMG	C8-N7	-2.02	1.31	1.35
1	B5	1247	1MA	C8-N7	-2.01	1.31	1.35
46	A2	1804	MA6	C8-N7	-2.01	1.31	1.34

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	As	67	NMM	NE-CZ-NH2	-7.62	112.49	119.48
76	As	67	NMM	NE-CZ-NH1	4.12	127.97	120.26
46	A2	1786	6MZ	C2-N1-C6	2.44	118.68	116.59
60	An	138	IAS	OD1-CG-CB	-2.40	118.43	125.43
1	B5	3966	A2M	C5-C6-N6	2.35	123.92	120.35
1	B5	3195	A2M	C5-C6-N6	2.34	123.91	120.35
1	B5	2564	A2M	C5-C6-N6	2.34	123.90	120.35
1	B5	3344	A2M	C5-C6-N6	2.33	123.90	120.35
1	B5	401	A2M	C5-C6-N6	2.33	123.89	120.35
46	A2	158	A2M	C5-C6-N6	2.33	123.89	120.35
1	B5	1457	A2M	C5-C6-N6	2.33	123.89	120.35
1	B5	2112	A2M	C5-C6-N6	2.32	123.88	120.35
46	A2	165	A2M	C5-C6-N6	2.32	123.88	120.35
1	B5	4033	A2M	C5-C6-N6	2.32	123.88	120.35
46	A2	1341	A2M	C5-C6-N6	2.32	123.88	120.35
46	A2	99	A2M	C5-C6-N6	2.32	123.87	120.35
46	A2	27	A2M	C5-C6-N6	2.32	123.87	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A2	551	A2M	C5-C6-N6	2.32	123.87	120.35
46	A2	989	A2M	C5-C6-N6	2.32	123.87	120.35
46	A2	445	A2M	C5-C6-N6	2.31	123.86	120.35
1	B5	4014	A2M	C5-C6-N6	2.31	123.86	120.35
1	B5	1251	A2M	C5-C6-N6	2.31	123.86	120.35
1	B5	399	A2M	C5-C6-N6	2.31	123.86	120.35
1	B5	1780	A2M	C5-C6-N6	2.30	123.85	120.35
46	A2	629	A2M	C5-C6-N6	2.29	123.84	120.35
1	B5	3302	A2M	C5-C6-N6	2.29	123.83	120.35
1	B5	1447	A2M	C5-C6-N6	2.29	123.83	120.35
1	B5	3307	A2M	C5-C6-N6	2.29	123.83	120.35
1	B5	3201	A2M	C5-C6-N6	2.29	123.83	120.35
1	B5	3262	A2M	C5-C6-N6	2.26	123.79	120.35
1	B5	2536	A2M	C5-C6-N6	2.25	123.78	120.35
2	B8	69	PSU	O4'-C1'-C2'	2.25	108.31	105.14
46	A2	782	PSU	O4'-C1'-C2'	2.15	108.18	105.14
1	B5	3885	PSU	O4'-C1'-C2'	2.14	108.17	105.14
1	B5	3966	A2M	C2'-C3'-C4'	-2.06	97.52	101.99
1	B5	3900	PSU	O4'-C1'-C2'	2.04	108.02	105.14
1	B5	3663	6MZ	C2-N1-C6	2.03	118.33	116.59
1	B5	3192	PSU	O4'-C1'-C2'	2.02	107.99	105.14

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B5	2171	OMC	C1'-C2'-O2'-CM2
1	B5	3178	OMC	C2'-C1'-N1-C2
1	B5	3178	OMC	C2'-C1'-N1-C6
1	B5	3201	A2M	C1'-C2'-O2'-CM'
1	B5	3639	OMG	C1'-C2'-O2'-CM2
1	B5	4033	A2M	C4'-C5'-O5'-P
6	BB	245	HIC	CA-CB-CG-ND1
43	Bo	53	MLZ	N-CA-CB-CG
43	Bo	53	MLZ	C-CA-CB-CG
46	A2	116	OMU	C3'-C4'-C5'-O5'
46	A2	116	OMU	O4'-C4'-C5'-O5'
46	A2	389	OMU	C3'-C4'-C5'-O5'
46	A2	389	OMU	O4'-C4'-C5'-O5'
46	A2	562	OMG	C1'-C2'-O2'-CM2
46	A2	605	OMG	O4'-C4'-C5'-O5'
46	A2	774	PSU	C2'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
46	A2	774	PSU	C3'-C4'-C5'-O5'
46	A2	1341	A2M	C1'-C2'-O2'-CM'
60	An	138	IAS	N-CA-CB-CG
60	An	138	IAS	C-CA-CB-CG
60	An	138	IAS	CA-CB-CG-OD1
76	As	67	NMM	C-CA-CB-CG
76	As	67	NMM	N-CA-CB-CG
76	As	67	NMM	O-C-CA-CB
46	A2	605	OMG	C3'-C4'-C5'-O5'
46	A2	774	PSU	O4'-C4'-C5'-O5'
46	A2	1206	B8N	N34-C33-C34-O36
76	As	67	NMM	NE-CD-CG-CB
1	B5	2113	OMG	O4'-C4'-C5'-O5'
1	B5	1548	OMG	C3'-C2'-O2'-CM2
46	A2	315	OMU	O4'-C4'-C5'-O5'
1	B5	2113	OMG	C3'-C4'-C5'-O5'
46	A2	389	OMU	C2'-C1'-N1-C6
1	B5	2171	OMC	O4'-C4'-C5'-O5'
46	A2	1206	B8N	N34-C33-C34-O35
46	A2	1295	4AC	O7-C7-N4-C4
46	A2	1295	4AC	CM7-C7-N4-C4
1	B5	1457	A2M	C4'-C5'-O5'-P
46	A2	629	A2M	O4'-C4'-C5'-O5'
1	B5	399	A2M	C1'-C2'-O2'-CM'
1	B5	3890	5MC	O4'-C1'-N1-C6
43	Bo	53	MLZ	CA-CB-CG-CD
46	A2	605	OMG	C4'-C5'-O5'-P
46	A2	1206	B8N	C31-C32-C33-C34
1	B5	3813	OMG	C3'-C2'-O2'-CM2
46	A2	1805	MA6	C4'-C5'-O5'-P
1	B5	3295	UY1	C4'-C5'-O5'-P
1	B5	2171	OMC	C3'-C4'-C5'-O5'
76	As	67	NMM	CA-CB-CG-CD
1	B5	3178	OMC	O4'-C1'-N1-C6
46	A2	1445	OMG	C4'-C5'-O5'-P
46	A2	389	OMU	O4'-C1'-N1-C6
1	B5	3890	5MC	C2'-C1'-N1-C6
1	B5	1251	A2M	C4'-C5'-O5'-P
1	B5	3346	OMC	C3'-C2'-O2'-CM2
1	B5	3178	OMC	O4'-C1'-N1-C2
46	A2	315	OMU	C3'-C4'-C5'-O5'
1	B5	2100	OMC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B5	3890	5MC	O4'-C1'-N1-C2
1	B5	2100	OMC	C2'-C1'-N1-C6
1	B5	3964	PSU	O4'-C1'-C5-C4
1	B5	3295	UY1	O4'-C1'-C5-C4
46	A2	1206	B8N	O4'-C1'-C5-C4
46	A2	389	OMU	O4'-C1'-N1-C2
46	A2	389	OMU	C2'-C1'-N1-C2
1	B5	3262	A2M	C3'-C2'-O2'-CM'
46	A2	629	A2M	C3'-C4'-C5'-O5'
1	B5	3964	PSU	O4'-C1'-C5-C6
1	B5	2100	OMC	C2'-C1'-N1-C2
1	B5	1457	A2M	O4'-C4'-C5'-O5'
1	B5	3262	A2M	O4'-C4'-C5'-O5'
1	B5	3344	A2M	C3'-C4'-C5'-O5'
1	B5	2112	A2M	C3'-C2'-O2'-CM'
1	B5	3937	OMG	C3'-C2'-O2'-CM2
46	A2	389	OMU	C4'-C5'-O5'-P
46	A2	1039	PSU	C4'-C5'-O5'-P

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 501 ligands modelled in this entry, 501 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

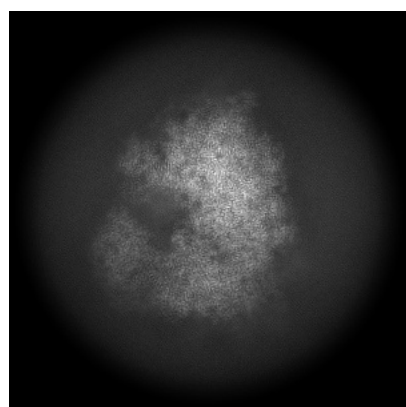
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18168. These allow visual inspection of the internal detail of the map and identification of artifacts.

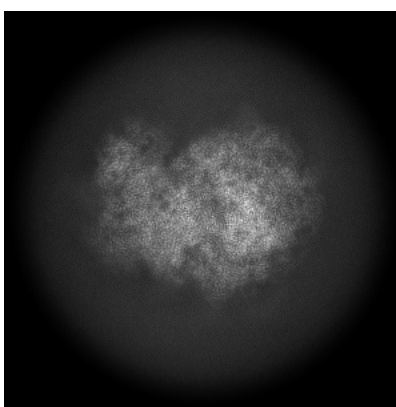
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

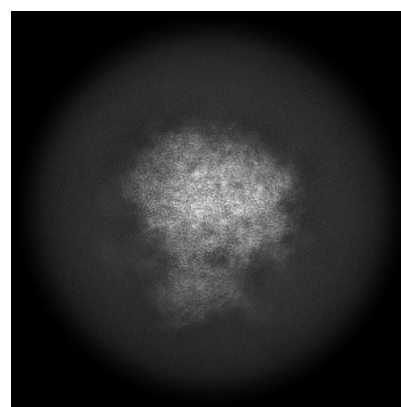
#### 6.1.1 Primary map



X



Y

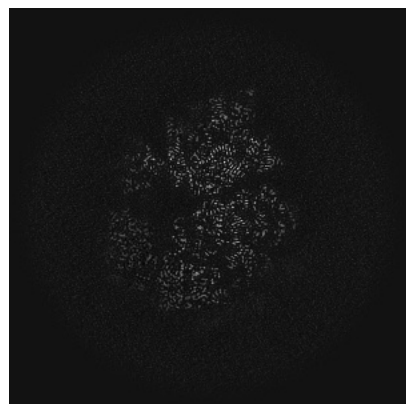


Z

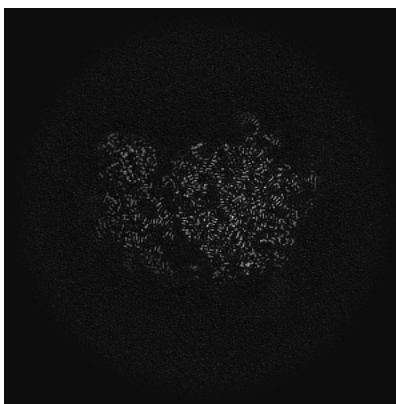
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

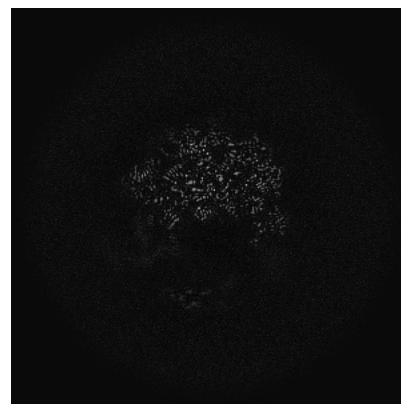
#### 6.2.1 Primary map



X Index: 290



Y Index: 290



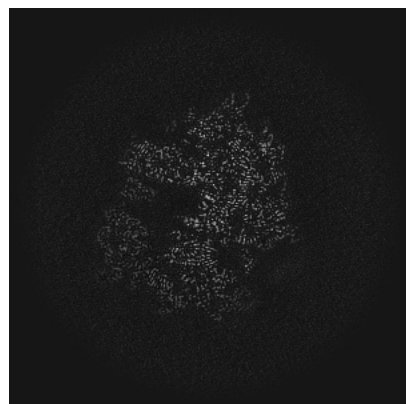
Z Index: 290



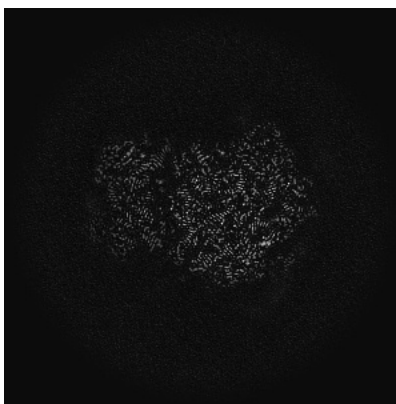
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

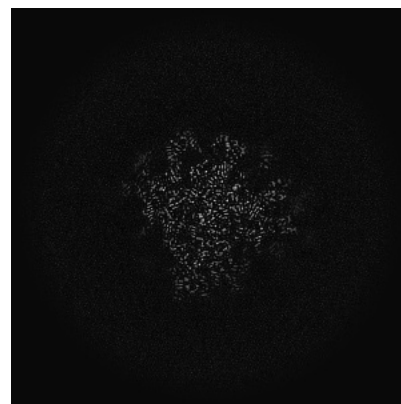
### 6.3.1 Primary map



X Index: 270



Y Index: 300

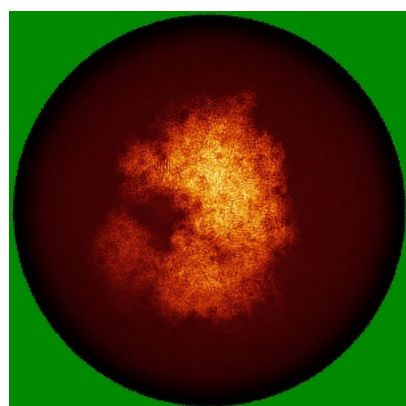


Z Index: 348

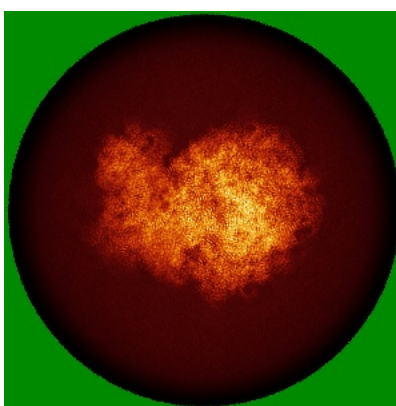
The images above show the largest variance slices of the map in three orthogonal directions.

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

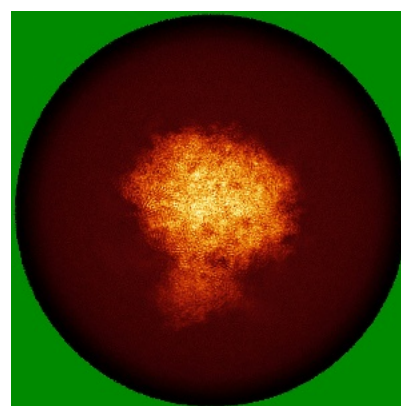
### 6.4.1 Primary map



X



Y

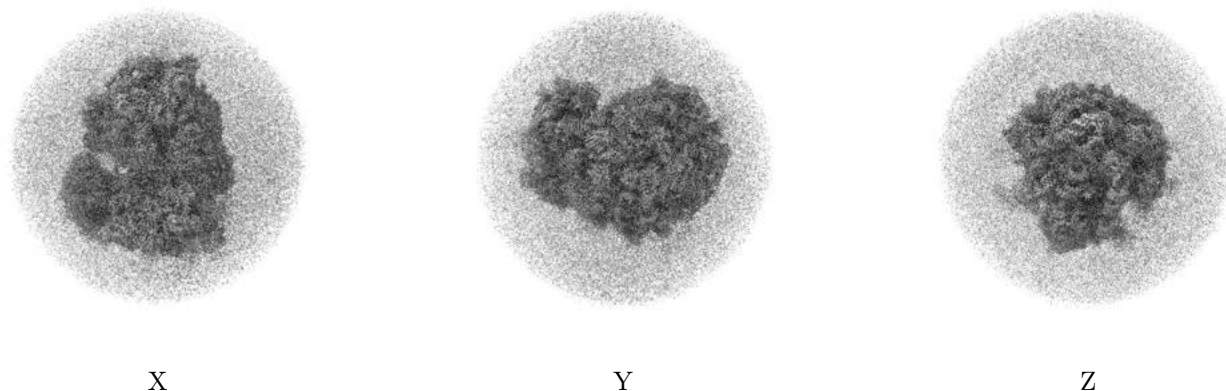


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

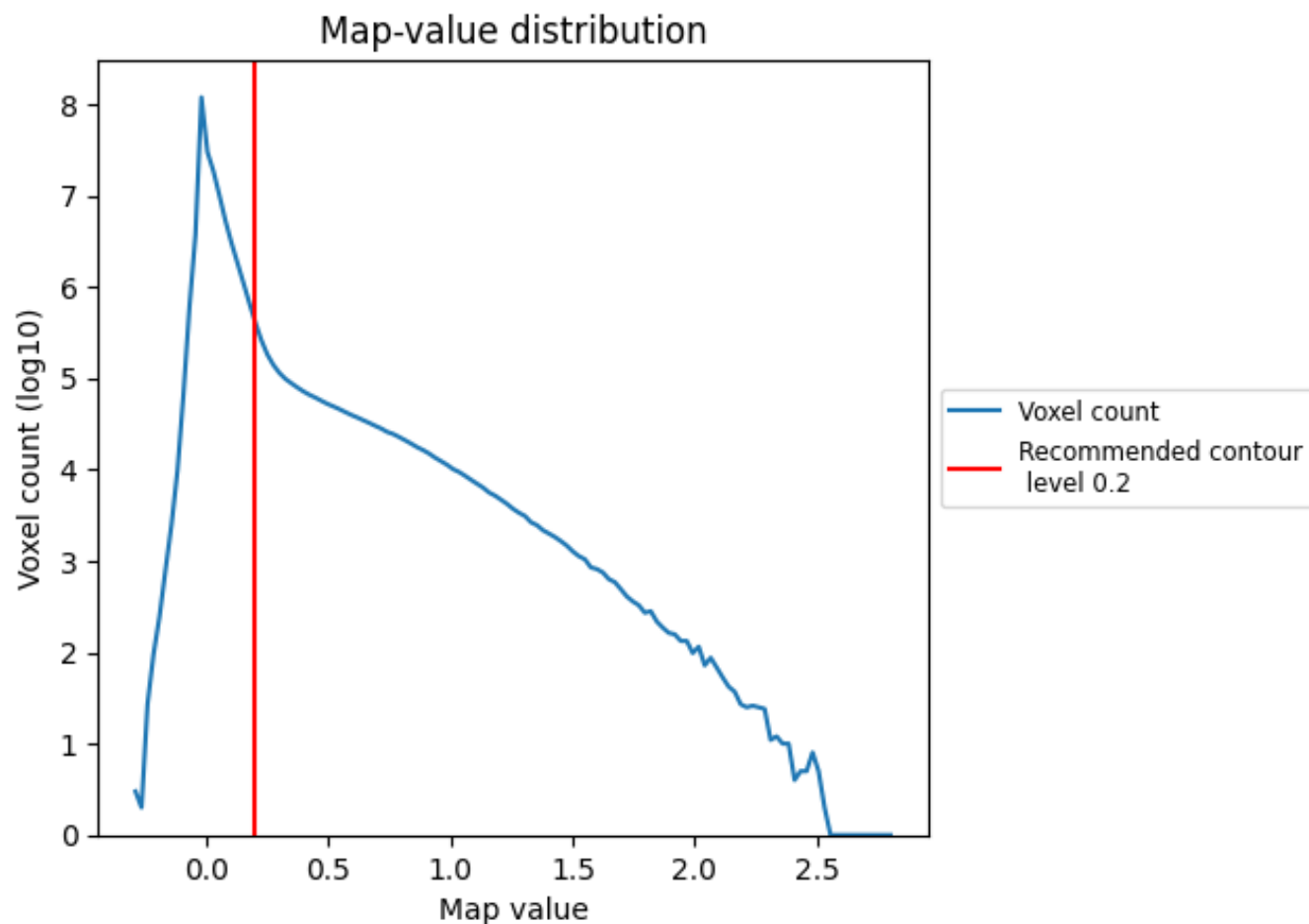
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

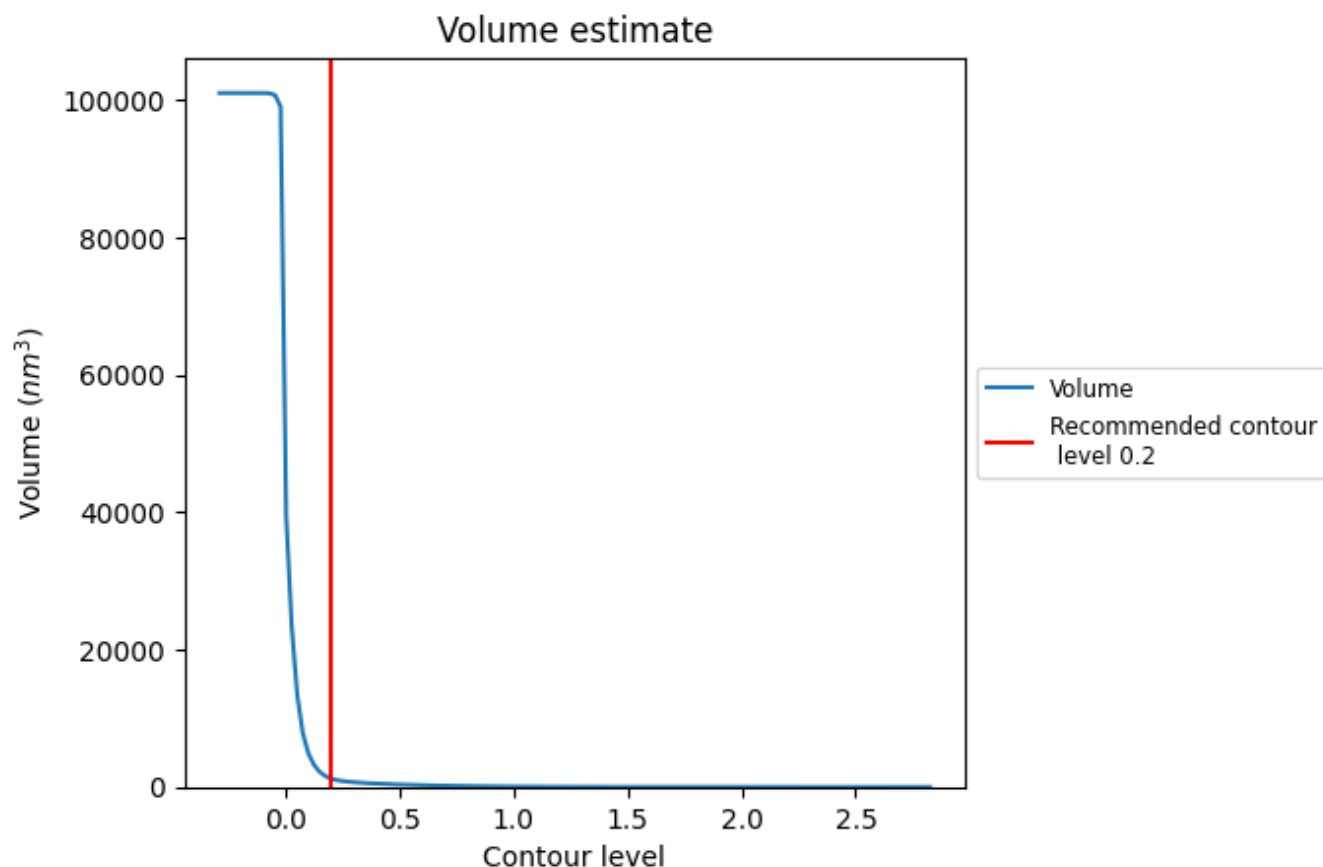
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

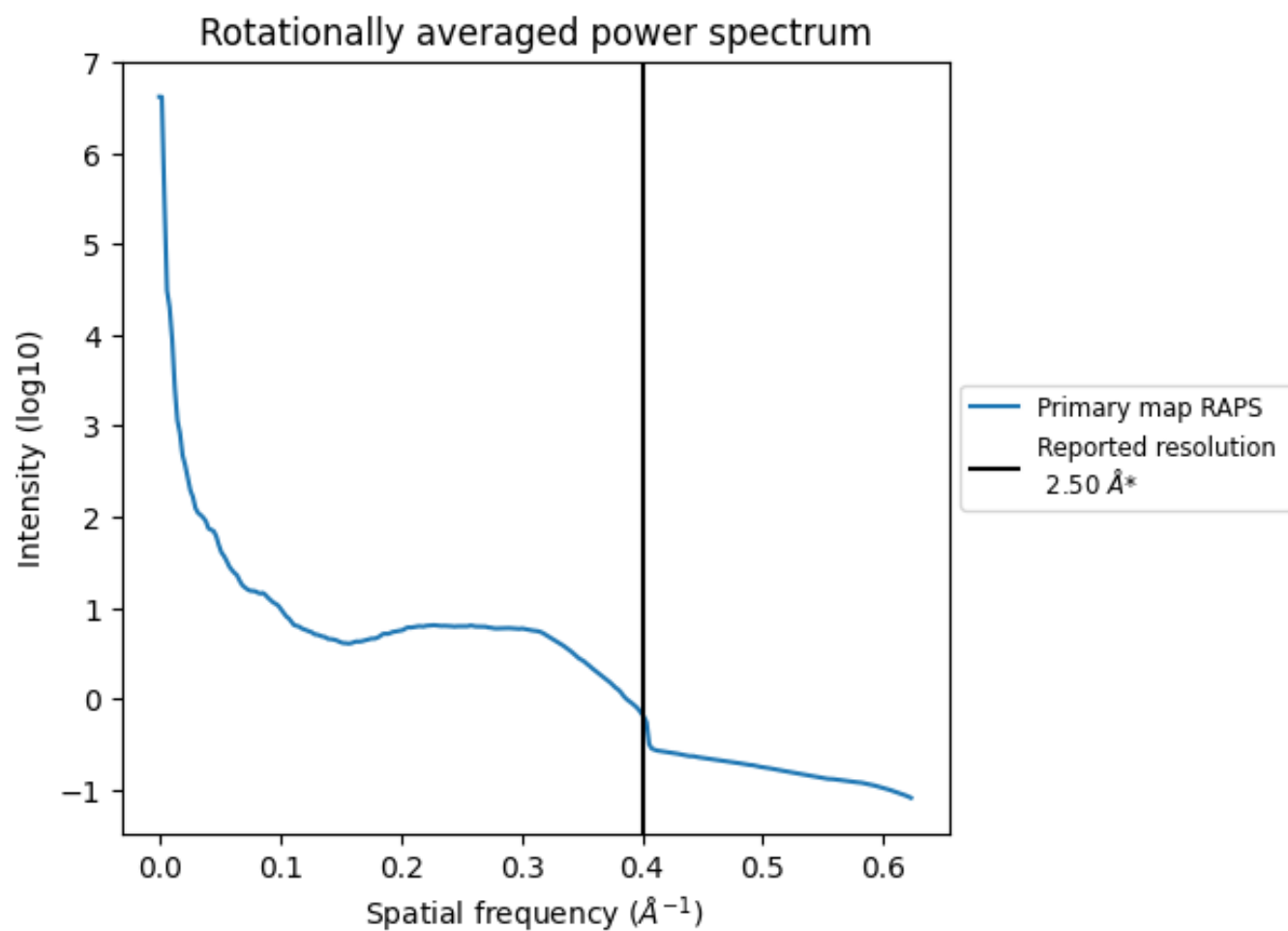
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1226 nm<sup>3</sup>; this corresponds to an approximate mass of 1108 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 0.400 Å<sup>-1</sup>

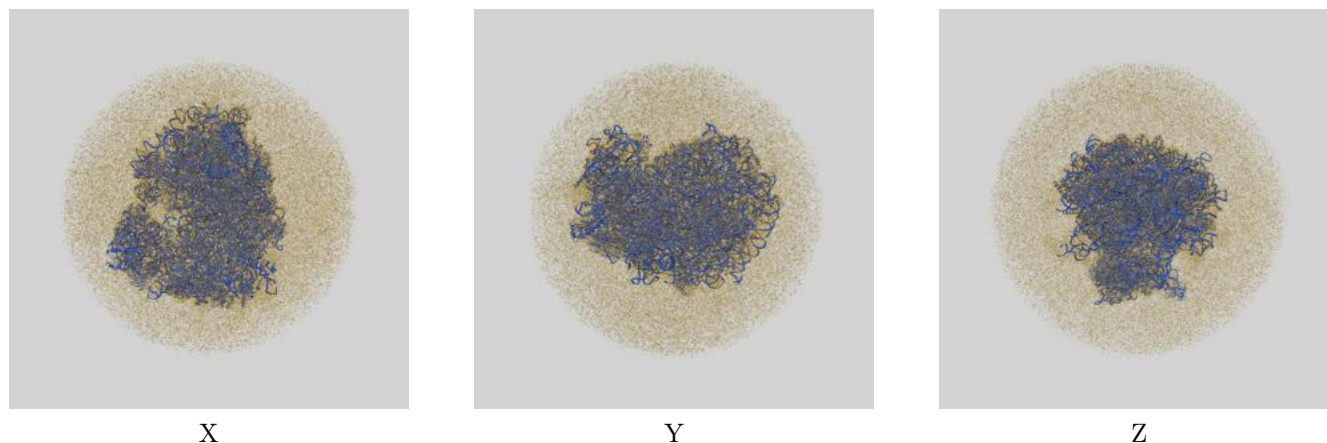
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

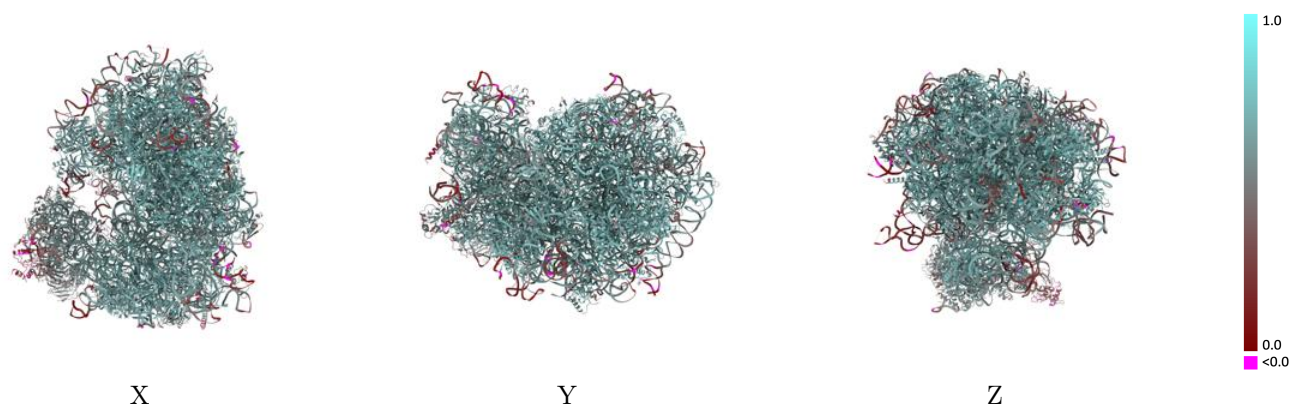
This section contains information regarding the fit between EMDB map EMD-18168 and PDB model 8Q7Z. Per-residue inclusion information can be found in section [3](#) on page [24](#).

### 9.1 Map-model overlay [i](#)



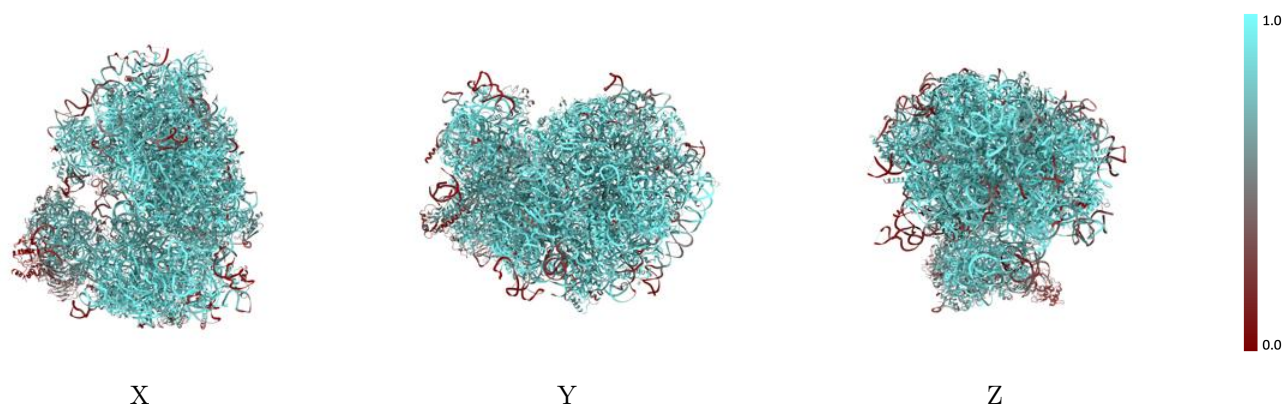
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

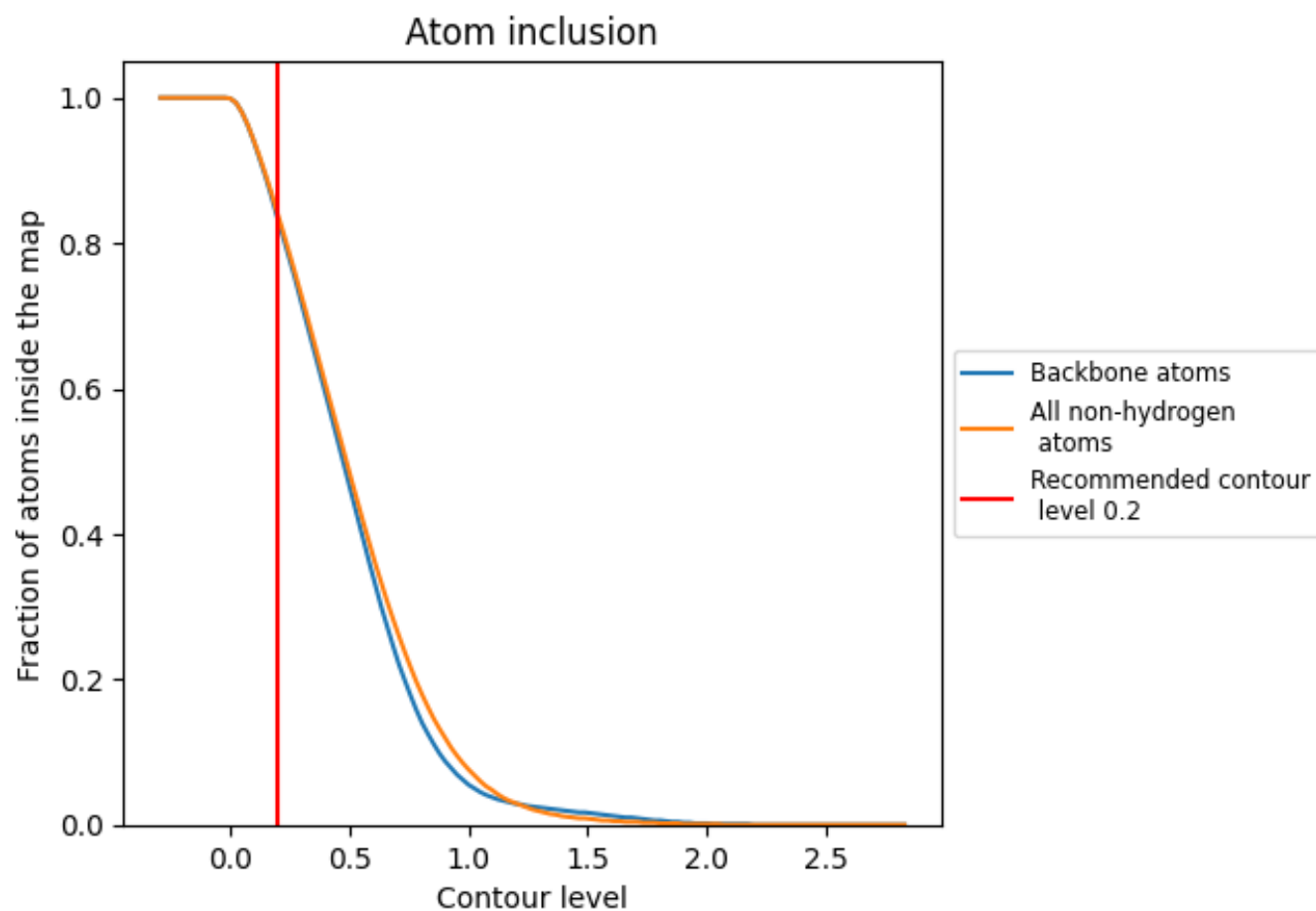
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.2).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.6160
A2	 0.8570	 0.5980
AA	 0.7270	 0.5760
AB	 0.5470	 0.5230
AC	 0.0390	 0.2340
AD	 0.6930	 0.5710
AE	 0.8700	 0.6600
AF	 0.3390	 0.4560
AG	 0.7830	 0.5950
AZ	 0.7970	 0.6150
Aa	 0.8260	 0.6260
Ab	 0.8670	 0.6510
Ac	 0.5510	 0.5170
Ad	 0.9170	 0.6570
Ae	 0.6880	 0.5580
Af	 0.7370	 0.5630
Ag	 0.4980	 0.5000
Ah	 0.8280	 0.6260
Ai	 0.9040	 0.6480
Aj	 0.5370	 0.4940
Ak	 0.8490	 0.6430
Al	 0.0370	 0.1750
Am	 0.8760	 0.6570
An	 0.8480	 0.6360
Ao	 0.6100	 0.5240
Ap	 0.7430	 0.5710
Aq	 0.5090	 0.4910
Ar	 0.6520	 0.5250
As	 0.7210	 0.5640
At	 0.5200	 0.4930
Au	 0.8220	 0.6340
Av	 0.9390	 0.6780
Aw	 0.8880	 0.6570
Ax	 0.8710	 0.6350
Ay	 0.5310	 0.4860











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Chain	Atom inclusion	Q-score
Az	 0.9080	 0.6760
B5	 0.8680	 0.6130
B7	 0.9750	 0.6660
B8	 0.9150	 0.6420
BA	 0.9740	 0.7140
BB	 0.9450	 0.6970
BC	 0.9460	 0.6910
BD	 0.8490	 0.6340
BE	 0.8670	 0.6410
BF	 0.9480	 0.7040
BG	 0.8200	 0.6240
BH	 0.9100	 0.6640
BI	 0.9190	 0.6740
BJ	 0.7960	 0.6130
BL	 0.8780	 0.6500
BM	 0.9390	 0.6820
BN	 0.9880	 0.7210
BO	 0.9470	 0.6880
BP	 0.9440	 0.6960
BQ	 0.9700	 0.7140
BR	 0.8300	 0.6260
BS	 0.9650	 0.7020
BT	 0.9000	 0.6770
BU	 0.6920	 0.5570
BV	 0.9460	 0.7040
BW	 0.8520	 0.6440
BX	 0.9070	 0.6730
BY	 0.9190	 0.6660
BZ	 0.8970	 0.6590
Ba	 0.9750	 0.7190
Bb	 0.8190	 0.6220
Bc	 0.9170	 0.6690
Bd	 0.8960	 0.6670
Be	 0.9630	 0.7080
Bf	 0.9610	 0.7170
Bg	 0.9240	 0.6820
Bh	 0.9020	 0.6650
Bi	 0.8940	 0.6560
Bj	 0.9780	 0.7030
Bk	 0.7090	 0.5970
Bl	 0.9080	 0.6780
Bm	 0.9300	 0.6810

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Chain	Atom inclusion	Q-score
Bo	 0.9070	 0.6850
Bp	 0.9270	 0.6870
Br	 0.9320	 0.6860
V	 0.3470	 0.3090