



## Full wwPDB EM Validation Report ⓘ

Apr 21, 2025 – 03:18 PM EDT

PDB ID : 9AZS / pdb\_00009azs  
EMDB ID : EMD-44021  
Title : In situ human Post-eEF1A-AT-P-E state 80S ribosome  
Authors : Wei, Z.; Yong, X.  
Deposited on : 2024-03-11  
Resolution : 2.80 Å(reported)

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

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

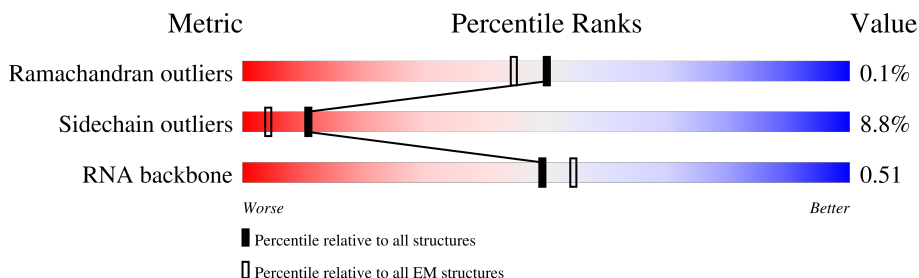
EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 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 2.80 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	LR	187	<div> <div>8%</div> <div>90%</div> <div>9%</div> </div>
2	SE	262	<div> <div>94%</div> <div>6%</div> </div>
3	SI	206	<div> <div>10%</div> <div>92%</div> <div>8%</div> </div>
4	SL	153	<div> <div>8%</div> <div>88%</div> <div>12%</div> </div>
5	SX	141	<div> <div>91%</div> <div>9%</div> </div>
6	SG	237	<div> <div>18%</div> <div>87%</div> <div>13%</div> </div>
7	SJ	185	<div> <div>6%</div> <div>95%</div> <div>5%</div> </div>
8	SY	131	<div> <div>9%</div> <div>87%</div> <div>13%</div> </div>


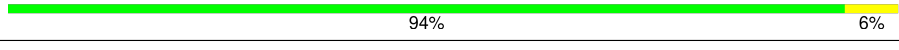
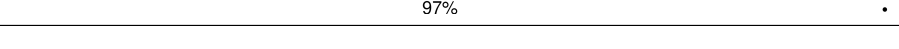
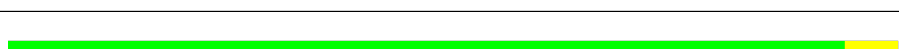
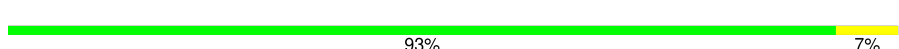
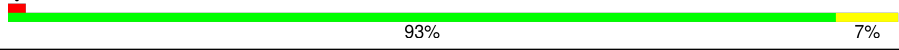

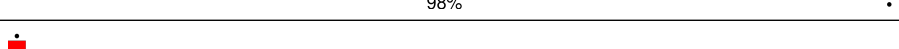
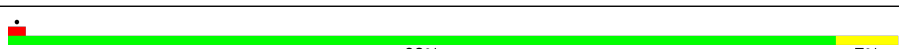
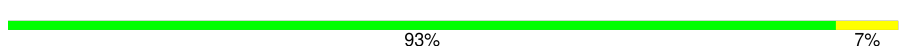
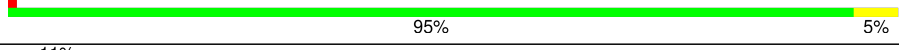
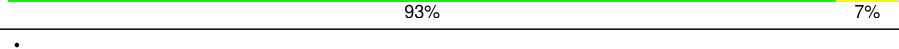
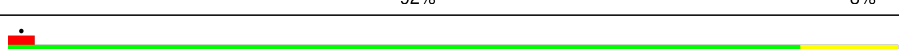
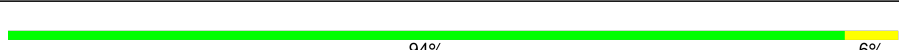
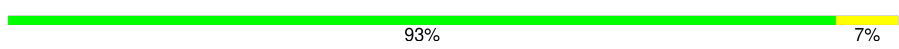
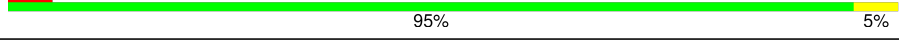
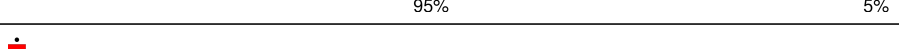


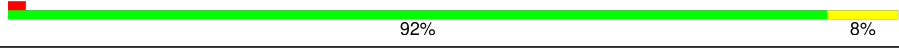
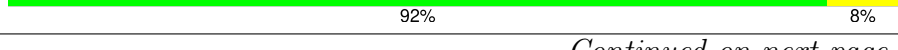



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Mol	Chain	Length	Quality of chain
9	Se	58	
10	SA	221	
11	SB	214	
12	SH	186	
13	SV	83	
14	Sa	102	
15	SC	222	
16	SN	150	
17	SO	140	
18	SW	129	
19	Sb	83	
20	L5	3740	
21	L7	120	
22	L8	156	
23	LA	248	
24	LB	402	
25	LC	368	
26	LD	293	
27	LE	236	
28	LF	225	
29	LG	241	
30	LH	190	
31	LI	202	
32	LJ	176	
33	LL	210	

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Mol	Chain	Length	Quality of chain
34	LM	139	
35	LN	203	
36	LO	201	
37	LP	153	
38	LQ	187	
39	LS	175	
40	LT	159	
41	LU	101	
42	LV	131	
43	LX	120	
44	LY	134	
45	LZ	135	
46	La	147	
47	Lb	109	
48	Lc	98	
49	Ld	107	
50	Le	128	
51	Lf	109	
52	Lg	114	
53	Lh	122	
54	Li	102	
55	Lj	86	
56	Lk	69	
57	Ll	50	
58	Lm	52	

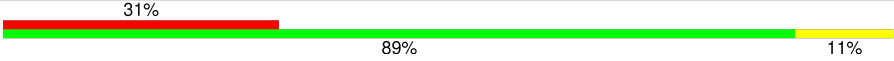

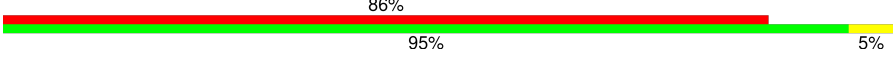
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Mol	Chain	Length	Quality of chain
59	Ln	24	
60	Lo	105	
61	Lp	91	
62	Lr	125	
63	SR	135	
64	SD	227	
65	SF	189	
66	SK	98	
67	SP	121	
68	SQ	144	
69	SS	145	
70	ST	143	
71	SU	104	
72	Sc	64	
73	Sd	55	
74	Sg	313	
75	SM	122	
76	SZ	75	
77	Sf	67	
78	S2	1740	
79	Et	75	
80	Pt	74	
81	Lt	141	
82	Lz	217	
83	Ls	196	

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Mol	Chain	Length	Quality of chain
84	LW	118	
85	AT	76	
86	CF	441	

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 227713 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 2 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 3 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 4 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 5 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 6 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 7 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 8 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 9 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 10 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 11 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 12 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 13 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 14 is a protein called 40S ribosomal protein S26.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 15 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 16 is a protein called 40S ribosomal protein S13.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SO	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

- Molecule 18 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 19 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 20 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L5	3740	Total	C	N	O	P	0	0
			79860	35549	14585	25987	3739		

- Molecule 21 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 22 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

- Molecule 23 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 24 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 25 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 26 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 27 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LE	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 28 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 29 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 30 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 31 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LI	202	Total	C	N	O	S	0	0
			1634	1037	314	269	14		

- Molecule 32 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 33 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 34 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 35 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 36 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 37 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 38 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 39 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 40 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 41 is a protein called Heparin-binding protein HBp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 42 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 43 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 44 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 45 is a protein called 60S ribosomal protein L27.

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

- Molecule 46 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 47 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 48 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 49 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 50 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 51 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 52 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 53 is a protein called 60S ribosomal protein L35.

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

- Molecule 54 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 55 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 56 is a protein called 60S ribosomal protein L38.

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

- Molecule 57 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 58 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 59 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 60 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 61 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 62 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 63 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 64 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 65 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 66 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 67 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SP	121	Total	C	N	O	S	0	0
			985	623	185	170	7		

- Molecule 68 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 69 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 70 is a protein called 40S ribosomal protein S19.



Mol	Chain	Residues	Atoms					AltConf	Trace
70	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 71 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 72 is a protein called 40S ribosomal protein S28.

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

- Molecule 73 is a protein called 40S ribosomal protein S29.

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

- Molecule 74 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 75 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 76 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 77 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 78 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	S2	1740	Total	C	N	O	P	0	0
			36898	16459	6599	12101	1739		

- Molecule 79 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Et	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 80 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Pt	74	Total	C	N	O	P	0	0
			1576	705	286	512	73		

- Molecule 81 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Lt	141	Total	C	N	O	S	0	0
			1046	652	191	199	4		

- Molecule 82 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Lz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Ls	196	Total	C	N	O	S	0	0
			1496	952	259	276	9		

- Molecule 84 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	LW	118	Total	C	N	O	S	0	0
			965	604	199	158	4		

- Molecule 85 is a RNA chain called A/T site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	AT	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 86 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	CF	441	Total	C	N	O	P	S	0	0
			3383	2148	581	636	1	17		

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
87	Sa	1	Total	Zn	0
			1	1	
87	Lg	1	Total	Zn	0
			1	1	
87	Lj	1	Total	Zn	0
			1	1	
87	Lm	1	Total	Zn	0
			1	1	
87	Lo	1	Total	Zn	0
			1	1	
87	Lp	1	Total	Zn	0
			1	1	

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
88	L5	211	Total	Mg	0
			211	211	
88	L7	3	Total	Mg	0
			3	3	
88	L8	4	Total	Mg	0
			4	4	

*Continued on next page...*

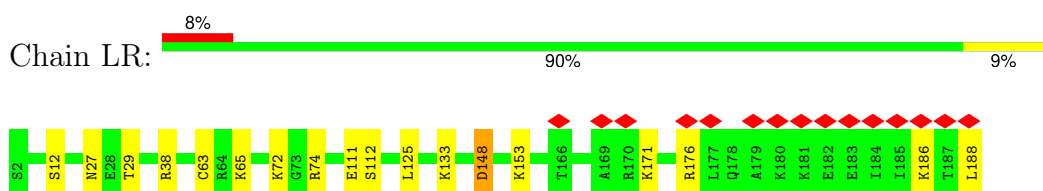
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Mol	Chain	Residues	Atoms		AltConf
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88	LB	1	Total 1	Mg 1	0
88	LI	1	Total 1	Mg 1	0
88	LP	1	Total 1	Mg 1	0
88	LV	1	Total 1	Mg 1	0
88	Le	2	Total 2	Mg 2	0
88	Lg	1	Total 1	Mg 1	0
88	S2	29	Total 29	Mg 29	0

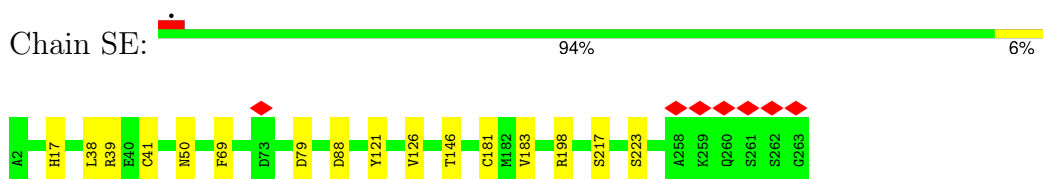
### 3 Residue-property plots [i](#)

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

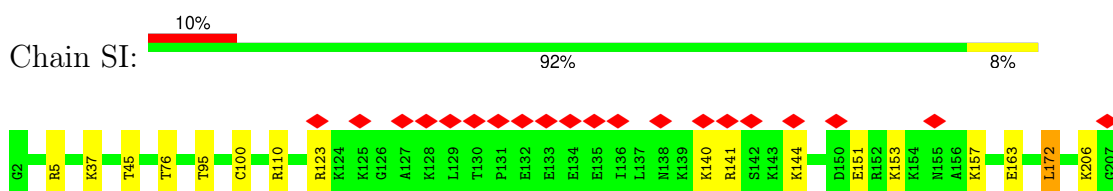
- Molecule 1: 60S ribosomal protein L19



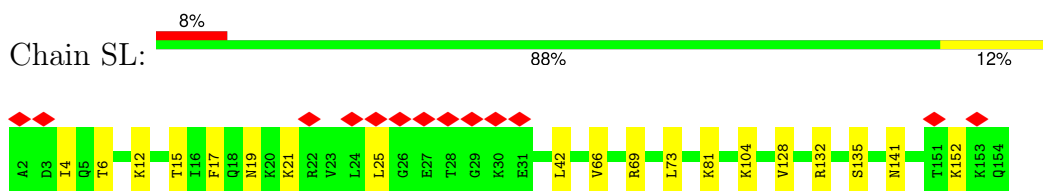
- Molecule 2: Small ribosomal subunit protein eS4, X isoform



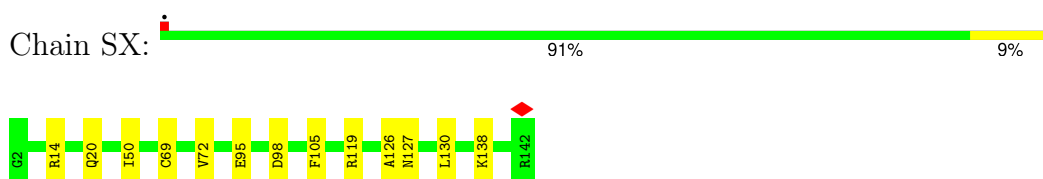
- Molecule 3: 40S ribosomal protein S8



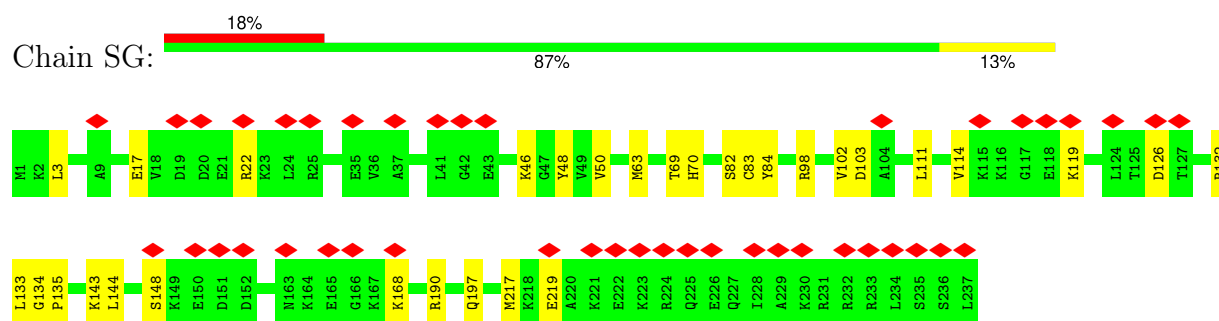
- Molecule 4: 40S ribosomal protein S11



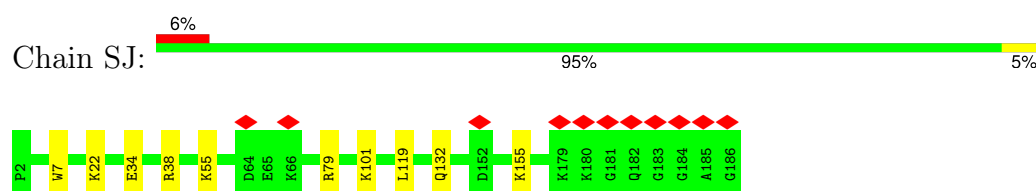
- Molecule 5: 40S ribosomal protein S23



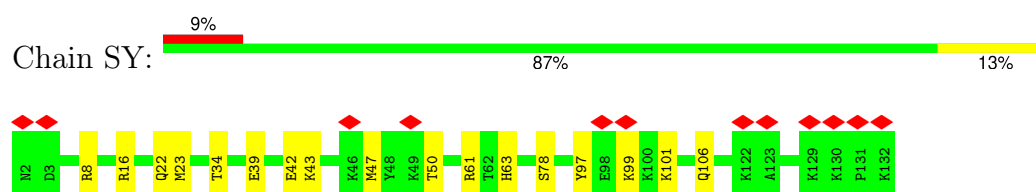
- Molecule 6: 40S ribosomal protein S6



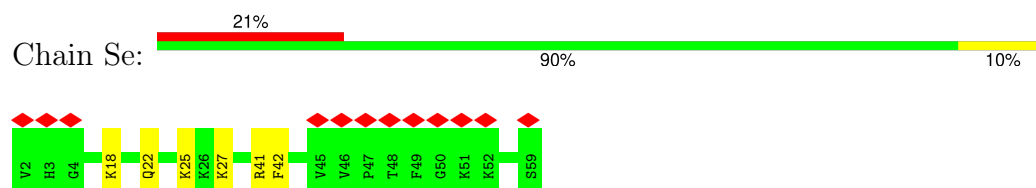
- Molecule 7: 40S ribosomal protein S9



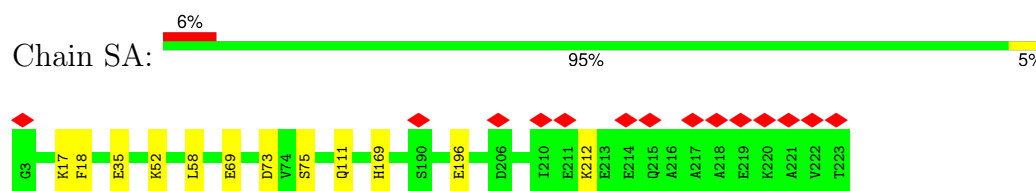
- Molecule 8: 40S ribosomal protein S24



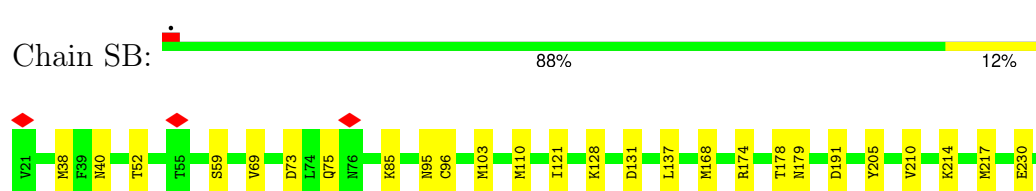
- Molecule 9: Small ribosomal subunit protein eS30



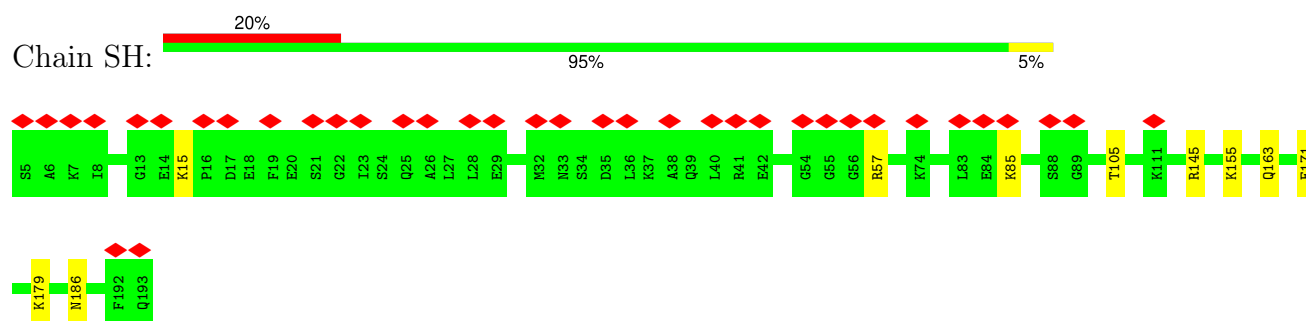
- Molecule 10: 40S ribosomal protein SA



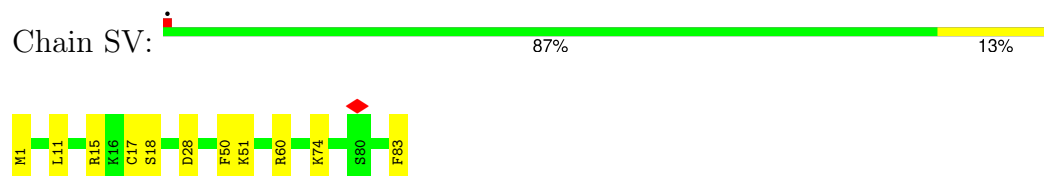
- Molecule 11: 40S ribosomal protein S3a



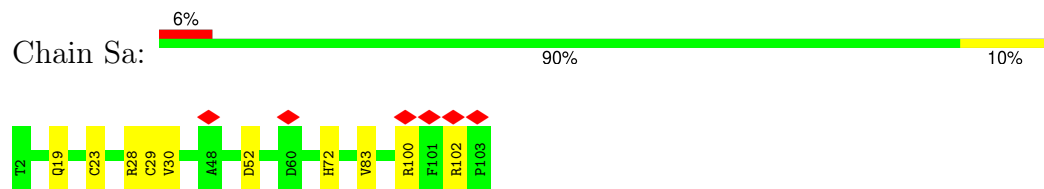
- Molecule 12: 40S ribosomal protein S7



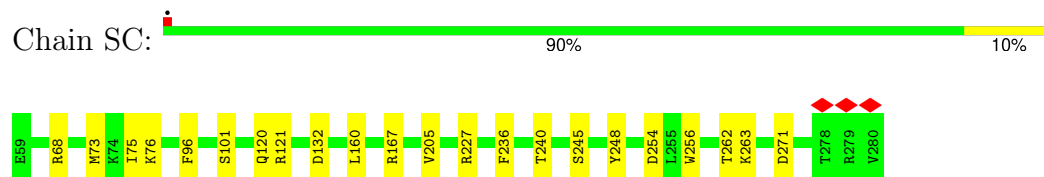
- Molecule 13: 40S ribosomal protein S21



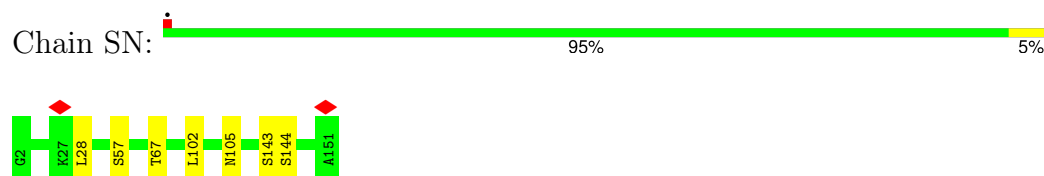
- Molecule 14: 40S ribosomal protein S26



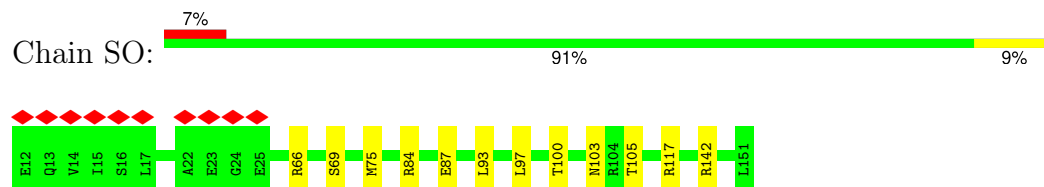
- Molecule 15: 40S ribosomal protein S2



- Molecule 16: 40S ribosomal protein S13



- Molecule 17: Small ribosomal subunit protein uS11

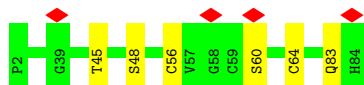


- Molecule 18: 40S ribosomal protein S15a

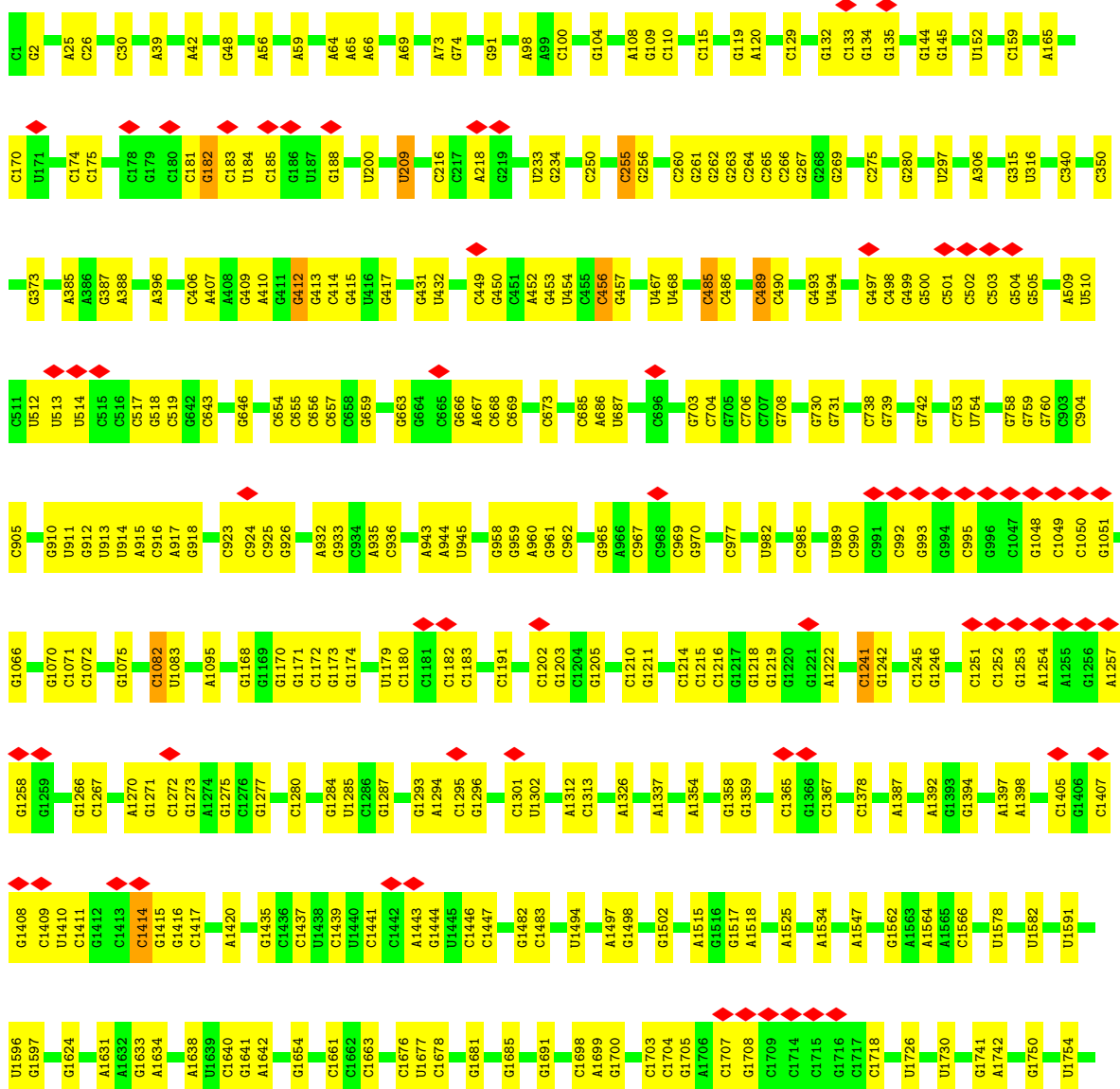
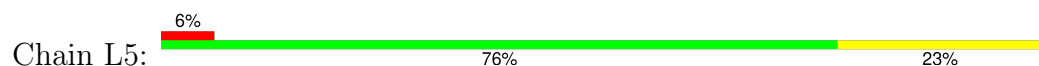




- Molecule 19: Small ribosomal subunit protein eS27

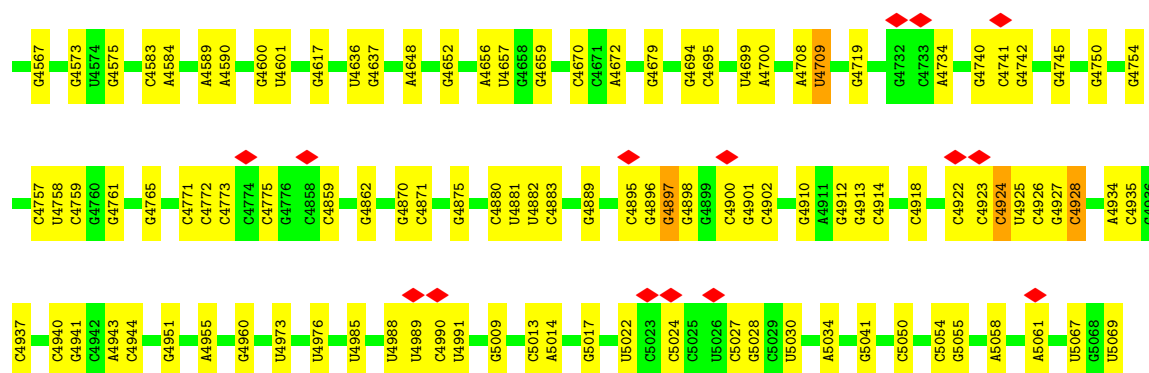


- Molecule 20: 28S rRNA





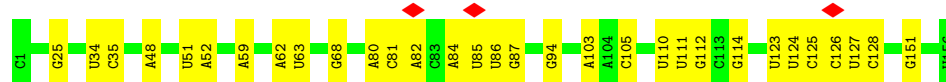
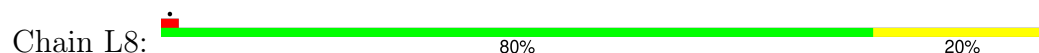




• Molecule 21: 5S rRNA



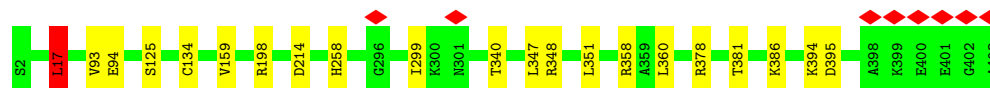
• Molecule 22: 5.8S rRNA



• Molecule 23: 60S ribosomal protein L8



• Molecule 24: Large ribosomal subunit protein uL3



• Molecule 25: 60S ribosomal protein L4





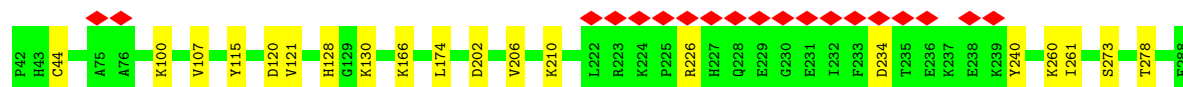
- Molecule 26: Large ribosomal subunit protein uL18

Chain LD: 93% 7%



- Molecule 27: 60S ribosomal protein L6

Chain LE: 8% 92% 8%



- Molecule 28: 60S ribosomal protein L7

Chain LF: 96% .



- Molecule 29: 60S ribosomal protein L7a

Chain LG: 10% 93% 7%



- Molecule 30: 60S ribosomal protein L9

Chain LH: 92% 8%

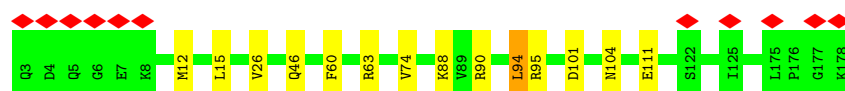
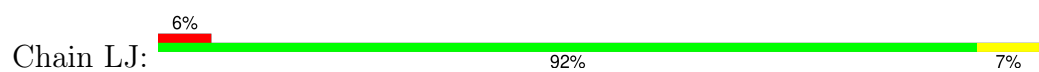


- Molecule 31: 60S ribosomal protein L10-like

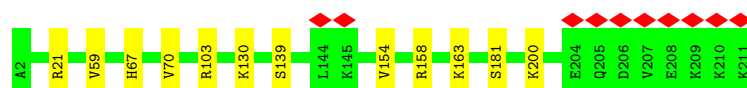
Chain LI: 94% 6%



- Molecule 32: 60S ribosomal protein L11



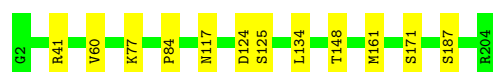
- Molecule 33: Large ribosomal subunit protein eL13



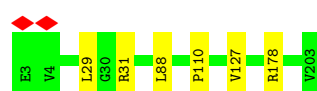
- Molecule 34: 60S ribosomal protein L14



- Molecule 35: 60S ribosomal protein L15



- Molecule 36: 60S ribosomal protein L13a



- Molecule 37: 60S ribosomal protein L17



- Molecule 38: 60S ribosomal protein L18



- Molecule 39: 60S ribosomal protein L18a

Chain LS:  93% 7%




- Molecule 40: 60S ribosomal protein L21

Chain LT:  93% 7%



- Molecule 41: Heparin-binding protein HBp15

Chain LU:  84% 16%




- Molecule 42: 60S ribosomal protein L23

Chain LV:  98%



- Molecule 43: 60S ribosomal protein L23a

Chain LX:  91% 9%



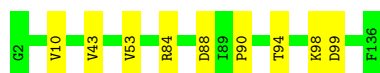
- Molecule 44: 60S ribosomal protein L26

Chain LY:  93% 7%



- Molecule 45: 60S ribosomal protein L27

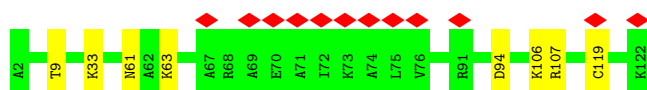
Chain LZ:  93% 7%



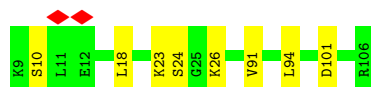
- Molecule 46: 60S ribosomal protein L27a



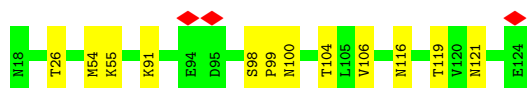
- Molecule 47: 60S ribosomal protein L29



- Molecule 48: 60S ribosomal protein L30



- Molecule 49: 60S ribosomal protein L31



- Molecule 50: 60S ribosomal protein L32



- Molecule 51: 60S ribosomal protein L35a



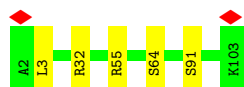
- Molecule 52: 60S ribosomal protein L34



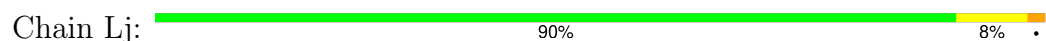
- Molecule 53: 60S ribosomal protein L35



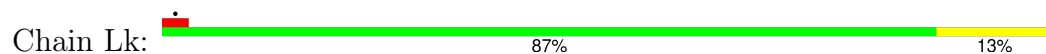
- Molecule 54: 60S ribosomal protein L36



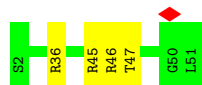
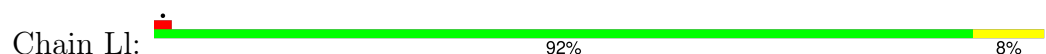
- Molecule 55: 60S ribosomal protein L37



- Molecule 56: 60S ribosomal protein L38




- Molecule 57: 60S ribosomal protein L39



- Molecule 58: Large ribosomal subunit protein eL40



- Molecule 59: 60S ribosomal protein L41

Chain Ln:  83% 17%



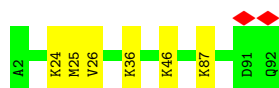
- Molecule 60: 60S ribosomal protein L36a

Chain Lo:  95% 5%




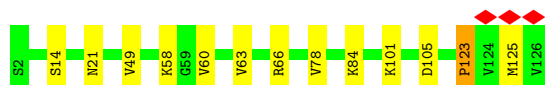
- Molecule 61: 60S ribosomal protein L37a

Chain Lp:  93% 7%



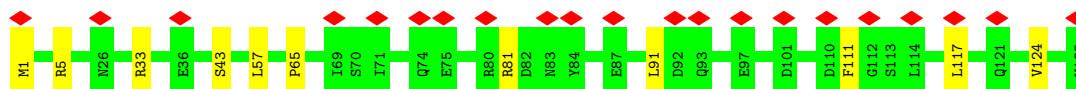
- Molecule 62: 60S ribosomal protein L28

Chain Lr:  90% 10%



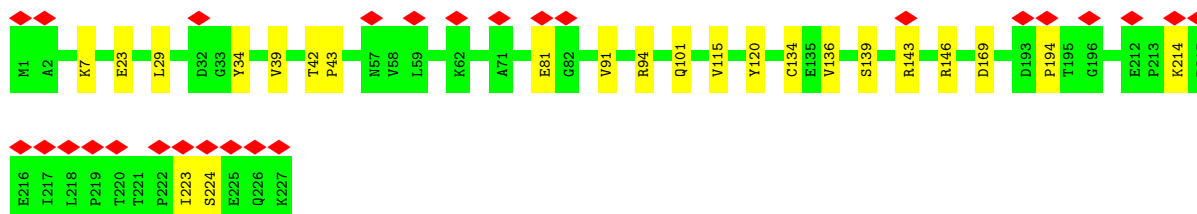
- Molecule 63: 40S ribosomal protein S17

Chain SR:  16% 92% 8%



- Molecule 64: Small ribosomal subunit protein uS3

Chain SD:  12% 90% 10%




- Molecule 65: 40S ribosomal protein S5

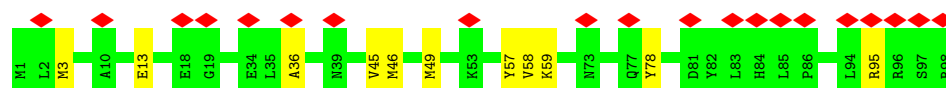


Chain SF:  90% 10%



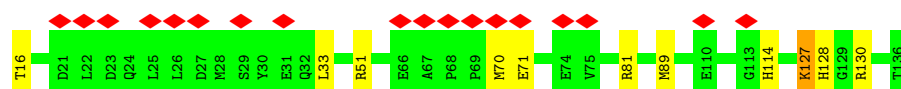
- Molecule 66: 40S ribosomal protein S10

Chain SK:  20% 89% 11%




- Molecule 67: Small ribosomal subunit protein uS19

Chain SP:  15% 91% 8%



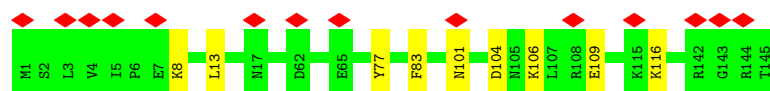
- Molecule 68: Small ribosomal subunit protein uS9

Chain SQ:  6% 86% 14%




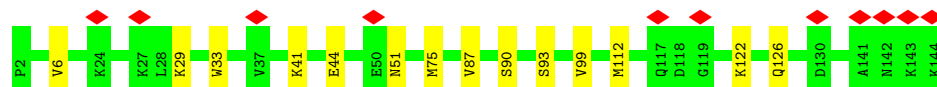
- Molecule 69: 40S ribosomal protein S18

Chain SS:  10% 94% 6%



- Molecule 70: 40S ribosomal protein S19

Chain ST:  8% 90% 10%

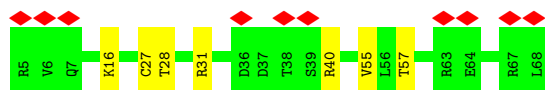


- Molecule 71: 40S ribosomal protein S20

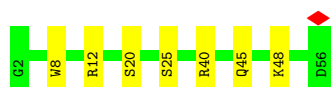
Chain SU:  18% 92% 8%



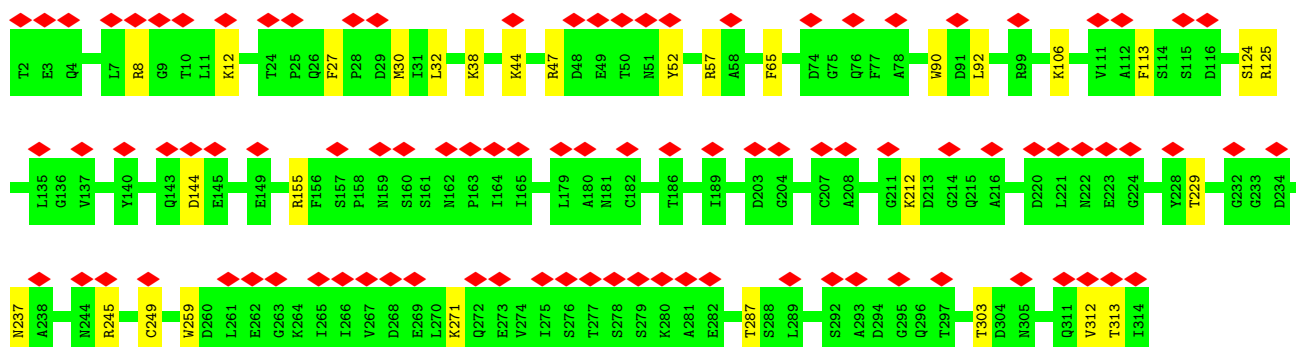
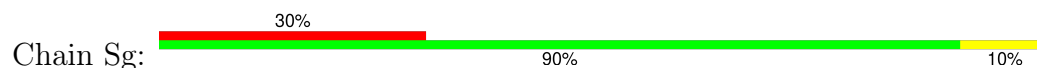
- Molecule 72: 40S ribosomal protein S28



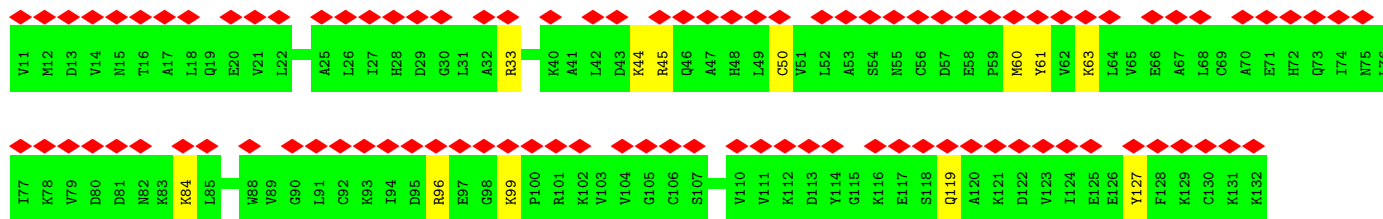
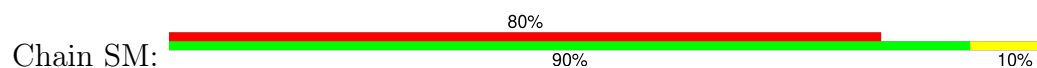
- Molecule 73: 40S ribosomal protein S29



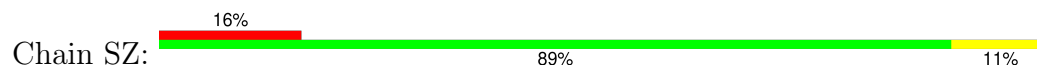
- Molecule 74: Receptor of activated protein C kinase 1



- Molecule 75: Small ribosomal subunit protein eS12

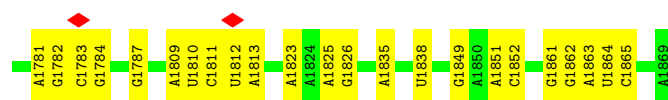


- Molecule 76: Small ribosomal subunit protein eS25



- Molecule 77: Ubiquitin-40S ribosomal protein S27a

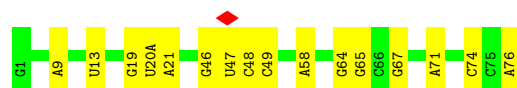
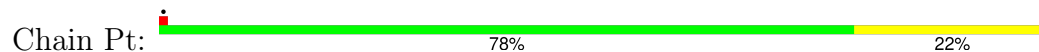




• Molecule 79: E site tRNA



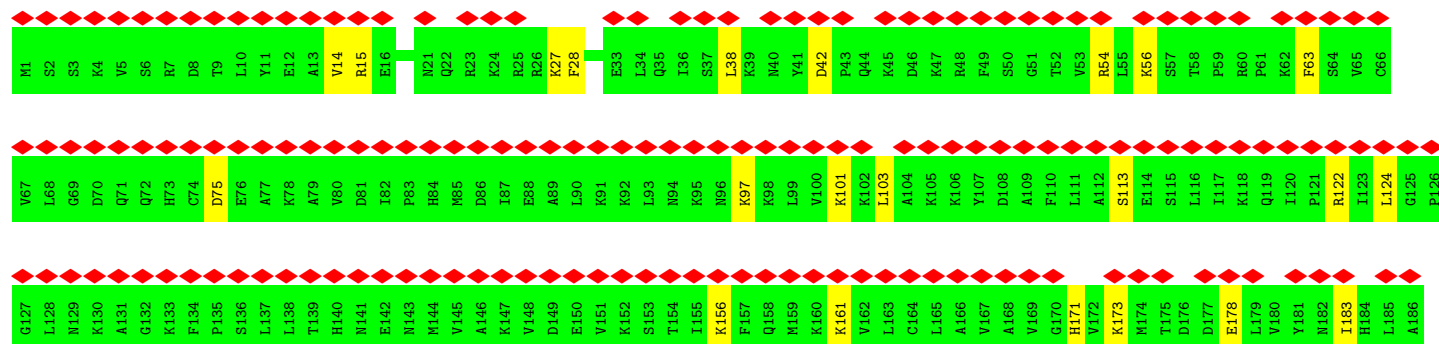
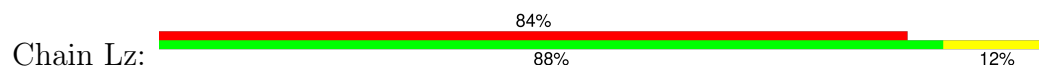
• Molecule 80: P site tRNA

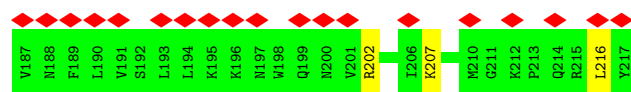


• Molecule 81: 60S ribosomal protein L12



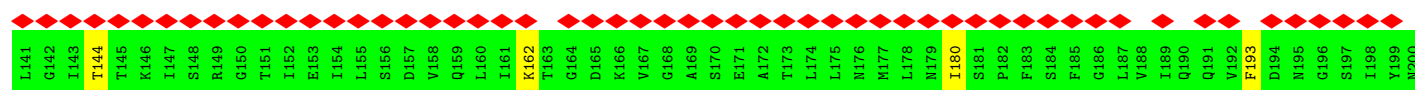
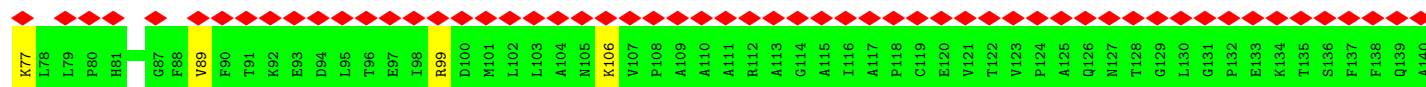
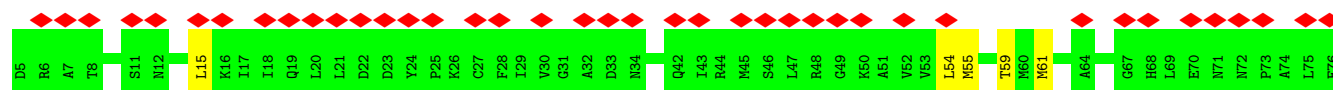
• Molecule 82: 60S ribosomal protein L10a





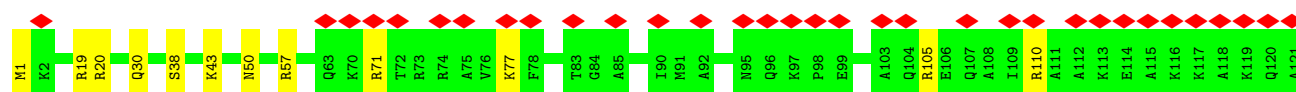
- Molecule 83: 60S acidic ribosomal protein P0

Chain Ls:



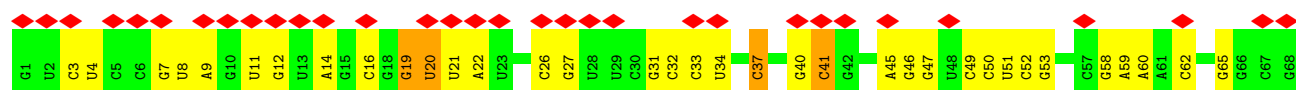
- Molecule 84: 60S ribosomal protein L24

Chain LW:



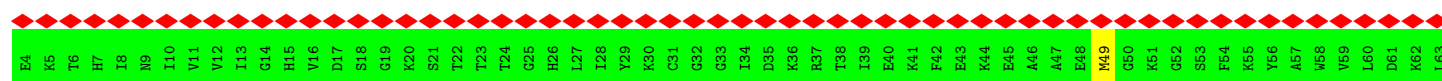
- Molecule 85: A/T site tRNA

Chain AT:



- Molecule 86: Elongation factor 1-alpha 1

Chain CF:



K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	
R322	R323	R324	R325	R326	R327	R328	R329	R330	R331	R332	R333	R334	R335	R336	R337	R338	R339	R340	R341	R342	R343	R344	R345	R346	R347	R348	R349	R350	R351	R352	R353	R354	R355	R356	R357	R358	R359	R360	R361	R362	R363	R364	R365	R366	R367	R368	R369	R370	R371	R372	R373	R374	R375	R376	R377	R378	R379	R380	R381	R382	R383
P245	P246	P249	P250	P253	P262	P263	P264	P265	P266	P267	P271	P272	P273	P274	P275	P276	P277	P278	P279	P280	P281	P282	P283	P284	P285	P286	P287	P288	P289	P290	P291	P294	P295	P296	P297	P298	P299	P300	P301	P302	P303	P304	P305	P306	P307	P308	P309	P313	P314	P319	P320	P321									
E124	E125	E126	E127	E128	E129	E130	E131	E132	E133	E134	E135	E136	E137	E138	E139	E140	E141	E142	E143	E144	E145	E146	E147	E148	E149	E150	E151	E152	E153	E154	E155	E156	E157	E158	E159	E160	E161	E162	E163	E164	E165	E166	E167	E168	E169	E170	E171	E172	E173	E174	E175	E176	E177	E178	E179	E180	E181	E182	E183		
K64	K65	E66	R67	E68	R69	G70	I71	T72	I73	D74	I75	S76	L77	W78	K79	F80	E81	T82	S83	K84	Y85	Y86	Y87	T88	I89	D91	A92	P93	G94	H95	R96	D97	F98	I99	K100	N101	M102	I103	T104	G105	T106	S107	Q108	A109	D110	C111	A112	V113	L114	I115	V116	A117	A118	G119	V120	E122	F123				

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48914	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.535	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0491	Depositor
Map size ( $\text{\AA}$ )	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.068, 1.068, 1.068	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, MG, ZN

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	LR	0.44	0/1582	0.64	1/2091 (0.0%)
2	SE	0.34	0/2118	0.59	0/2849
3	SI	0.39	0/1715	0.63	1/2287 (0.0%)
4	SL	0.43	0/1268	0.63	0/1696
5	SX	0.39	0/1116	0.57	0/1490
6	SG	0.76	3/1946 (0.2%)	0.99	7/2590 (0.3%)
7	SJ	0.34	0/1550	0.60	0/2069
8	SY	0.32	0/1083	0.60	0/1438
9	Se	0.31	0/465	0.59	0/612
10	SA	0.38	0/1778	0.61	0/2416
11	SB	0.38	0/1765	0.57	0/2362
12	SH	0.34	0/1519	0.59	0/2033
13	SV	0.36	0/643	0.61	0/860
14	Sa	0.44	0/836	0.69	0/1121
15	SC	0.40	0/1762	0.61	1/2381 (0.0%)
16	SN	0.39	0/1232	0.59	0/1656
17	SO	0.38	0/1062	0.66	0/1425
18	SW	0.41	0/1051	0.57	0/1406
19	Sb	0.37	0/665	0.57	0/891
20	L5	0.97	0/89312	0.90	91/139287 (0.1%)
21	L7	0.92	0/2861	0.80	0/4459
22	L8	0.98	0/3701	0.84	1/5766 (0.0%)
23	LA	0.56	0/1936	0.66	0/2596
24	LB	0.51	0/3306	0.62	1/4424 (0.0%)
25	LC	0.50	0/2981	0.63	1/4002 (0.0%)
26	LD	0.47	0/2428	0.58	0/3252
27	LE	0.43	0/1942	0.61	0/2606
28	LF	0.52	0/1905	0.63	1/2539 (0.0%)
29	LG	0.54	2/1960 (0.1%)	0.82	4/2637 (0.2%)
30	LH	0.45	0/1537	0.62	1/2066 (0.0%)
31	LI	0.48	0/1673	0.61	0/2233
32	LJ	0.40	0/1433	0.62	1/1915 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	LL	0.46	0/1732	0.61	0/2315
34	LM	0.48	0/1161	0.60	0/1554
35	LN	0.57	0/1746	0.63	1/2338 (0.0%)
36	LO	0.51	0/1682	0.61	0/2250
37	LP	0.52	0/1268	0.59	0/1701
38	LQ	0.54	0/1537	0.68	1/2052 (0.0%)
39	LS	0.55	0/1493	0.59	0/2003
40	LT	0.55	0/1326	0.64	0/1770
41	LU	0.40	0/839	0.59	0/1126
42	LV	0.51	0/993	0.59	0/1332
43	LX	0.47	0/1002	0.59	0/1345
44	LY	0.50	0/1132	0.59	0/1504
45	LZ	0.52	0/1130	0.68	2/1507 (0.1%)
46	La	0.54	0/1191	0.58	0/1591
47	Lb	0.39	0/889	0.60	0/1175
48	Lc	0.48	0/774	0.61	0/1038
49	Ld	0.50	0/903	0.64	0/1216
50	Le	0.58	1/1071 (0.1%)	0.62	0/1429
51	Lf	0.57	0/895	0.66	0/1198
52	Lg	0.53	0/916	0.65	0/1220
53	Lh	0.44	0/1023	0.60	0/1351
54	Li	0.41	0/843	0.61	0/1115
55	Lj	0.61	0/720	0.81	2/952 (0.2%)
56	Lk	0.44	0/575	0.60	0/761
57	Ll	0.50	0/454	0.66	0/599
58	Lm	0.44	0/435	0.57	0/575
59	Ln	0.44	0/231	0.74	0/294
60	Lo	0.50	0/876	0.62	0/1156
61	Lp	0.51	0/718	0.56	0/953
62	Lr	0.60	1/1017 (0.1%)	0.86	4/1364 (0.3%)
63	SR	0.34	0/1105	0.73	3/1484 (0.2%)
64	SD	0.33	0/1793	0.59	0/2414
65	SF	0.34	0/1516	0.60	0/2037
66	SK	0.36	0/851	0.67	0/1147
67	SP	0.32	0/1003	0.64	0/1342
68	SQ	0.34	0/1160	0.67	1/1553 (0.1%)
69	SS	0.32	0/1216	0.60	0/1628
70	ST	0.33	0/1131	0.61	0/1515
71	SU	0.30	0/831	0.58	0/1115
72	Sc	0.33	0/508	0.73	0/680
73	Sd	0.37	0/470	0.60	0/623
74	Sg	0.30	0/2493	0.60	0/3394
75	SM	0.30	0/950	0.60	0/1275

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	SZ	0.32	0/604	0.65	0/810
77	Sf	0.30	0/560	0.66	0/745
78	S2	0.67	0/41242	0.84	50/64255 (0.1%)
79	Et	0.35	0/1778	0.87	0/2767
80	Pt	0.53	0/1761	0.79	0/2741
81	Lt	0.26	0/1058	0.59	0/1430
82	Lz	0.28	0/1769	0.59	0/2371
83	Ls	0.29	0/1519	0.58	0/2052
84	LW	0.44	0/979	0.62	0/1295
85	AT	0.32	0/1805	0.93	5/2809 (0.2%)
86	CF	0.39	3/3442 (0.1%)	0.71	6/4656 (0.1%)
All	All	0.73	10/244247 (0.0%)	0.79	186/358377 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	SX	0	1
12	SH	0	1
23	LA	0	1
24	LB	0	2
32	LJ	0	1
33	LL	0	1
34	LM	0	1
36	LO	0	1
40	LT	0	1
51	Lf	0	2
55	Lj	0	2
65	SF	0	1
67	SP	0	1
68	SQ	0	1
76	SZ	0	1
82	Lz	0	1
All	All	0	19

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	SG	135	PRO	CG-CD	-23.15	0.74	1.50
6	SG	135	PRO	CB-CG	15.88	2.29	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	LG	133	PRO	CB-CG	-10.35	0.98	1.50
86	CF	245	PRO	CB-CG	-10.24	0.98	1.50
62	Lr	123	PRO	CG-CD	-9.44	1.19	1.50
6	SG	135	PRO	N-CD	8.99	1.60	1.47
86	CF	245	PRO	CG-CD	-8.86	1.21	1.50
29	LG	133	PRO	CG-CD	-8.22	1.23	1.50
50	Le	72	SER	CA-CB	-6.34	1.43	1.52
86	CF	419	PRO	CG-CD	-6.05	1.30	1.50

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	SG	135	PRO	CB-CG-CD	-26.51	3.10	106.50
6	SG	135	PRO	CA-N-CD	-19.31	84.47	111.50
29	LG	133	PRO	N-CD-CG	-18.71	75.13	103.20
86	CF	245	PRO	N-CD-CG	-18.44	75.53	103.20
29	LG	133	PRO	CA-CB-CG	-17.37	70.99	104.00
86	CF	245	PRO	CA-CB-CG	-17.00	71.69	104.00
62	Lr	123	PRO	N-CD-CG	-15.38	80.13	103.20
86	CF	245	PRO	CB-CG-CD	13.65	159.72	106.50
29	LG	133	PRO	CB-CG-CD	13.13	157.71	106.50
45	LZ	90	PRO	CA-N-CD	-12.88	93.47	111.50
62	Lr	123	PRO	CA-CB-CG	-11.51	82.13	104.00
55	Lj	39	TYR	C-N-CD	-11.27	95.82	120.60
20	L5	174	C	N3-C2-O2	-10.71	114.40	121.90
6	SG	134	GLY	C-N-CD	10.43	150.30	128.40
78	S2	1629	C	N3-C2-O2	-10.29	114.69	121.90
20	L5	417	G	O4'-C1'-N9	9.86	116.09	108.20
20	L5	456	C	O4'-C1'-N1	9.65	115.92	108.20
20	L5	485	C	C2-N1-C1'	9.43	129.17	118.80
6	SG	135	PRO	CA-CB-CG	-9.37	86.20	104.00
78	S2	1453	C	C2-N1-C1'	9.29	129.02	118.80
63	SR	65	PRO	CA-N-CD	-9.15	98.70	111.50
55	Lj	40	PRO	CA-N-CD	-9.11	98.75	111.50
86	CF	419	PRO	N-CD-CG	-8.99	89.71	103.20
6	SG	135	PRO	N-CA-CB	-8.85	92.68	103.30
78	S2	1694	U	C5-C6-N1	8.73	127.07	122.70
78	S2	1453	C	N1-C2-O2	8.66	124.10	118.90
20	L5	3773	U	N3-C2-O2	-8.63	116.16	122.20
20	L5	1082	C	N3-C2-O2	-8.53	115.93	121.90
78	S2	1811	C	N1-C2-O2	8.27	123.86	118.90
20	L5	1082	C	O4'-C1'-N1	8.26	114.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	S2	1811	C	N3-C2-O2	-7.94	116.34	121.90
20	L5	2710	C	C2-N1-C1'	7.84	127.43	118.80
63	SR	57	LEU	CA-CB-CG	7.73	133.08	115.30
78	S2	356	C	C2-N1-C1'	7.51	127.07	118.80
78	S2	1722	G	N3-C4-N9	7.50	130.50	126.00
20	L5	181	C	N1-C2-O2	7.43	123.36	118.90
20	L5	1378	C	N1-C2-O2	7.41	123.34	118.90
20	L5	4709	U	C2-N1-C1'	7.38	126.55	117.70
86	CF	245	PRO	CA-N-CD	-7.36	101.20	111.50
78	S2	1416	C	N3-C2-O2	-7.36	116.75	121.90
20	L5	1414	C	N3-C2-O2	-7.30	116.79	121.90
20	L5	485	C	C6-N1-C1'	-7.26	112.09	120.80
20	L5	1414	C	N1-C2-O2	7.24	123.24	118.90
20	L5	181	C	C2-N1-C1'	7.20	126.72	118.80
20	L5	490	C	N3-C2-O2	-7.19	116.87	121.90
78	S2	356	C	N1-C2-O2	7.12	123.17	118.90
20	L5	174	C	N1-C2-O2	7.10	123.16	118.90
62	Lr	123	PRO	N-CA-CB	-7.08	94.81	103.30
20	L5	2710	C	N1-C2-O2	7.06	123.13	118.90
20	L5	456	C	N3-C2-O2	-6.99	117.01	121.90
78	S2	1629	C	C6-N1-C2	-6.93	117.53	120.30
20	L5	2255	C	C2-N1-C1'	6.83	126.31	118.80
20	L5	1378	C	C2-N1-C1'	6.83	126.31	118.80
78	S2	1772	C	N3-C2-O2	-6.83	117.12	121.90
20	L5	2255	C	N1-C2-O2	6.82	122.99	118.90
20	L5	129	C	N3-C2-O2	-6.68	117.22	121.90
20	L5	3773	U	N1-C2-O2	6.65	127.45	122.80
29	LG	133	PRO	CA-N-CD	-6.63	102.22	111.50
78	S2	501	C	C2-N1-C1'	6.62	126.08	118.80
28	LF	33	LEU	CA-CB-CG	6.57	130.40	115.30
78	S2	1453	C	N3-C2-O2	-6.56	117.31	121.90
20	L5	181	C	N3-C2-O2	-6.56	117.31	121.90
38	LQ	4	ASP	CB-CG-OD2	6.55	124.20	118.30
78	S2	1453	C	C6-N1-C1'	-6.53	112.96	120.80
20	L5	1252	C	N3-C2-O2	-6.45	117.39	121.90
20	L5	175	C	N3-C2-O2	-6.44	117.39	121.90
78	S2	1772	C	N1-C2-O2	6.41	122.75	118.90
78	S2	1022	U	C2-N1-C1'	6.38	125.35	117.70
78	S2	1424	G	N3-C4-N9	6.35	129.81	126.00
20	L5	3767	C	C2-N1-C1'	6.29	125.72	118.80
20	L5	181	C	C6-N1-C2	-6.25	117.80	120.30
20	L5	4303	C	N3-C2-O2	-6.24	117.53	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L5	100	C	C2-N1-C1'	6.22	125.65	118.80
20	L5	4052	C	C2-N1-C1'	6.19	125.61	118.80
20	L5	1191	C	N3-C2-O2	-6.10	117.63	121.90
85	AT	37	C	N1-C2-O2	6.09	122.55	118.90
20	L5	3641	U	C5-C6-N1	-6.08	119.66	122.70
45	LZ	90	PRO	N-CD-CG	-6.07	94.10	103.20
20	L5	3773	U	O4'-C1'-N1	6.07	113.05	108.20
78	S2	501	C	N1-C2-O2	6.02	122.51	118.90
20	L5	233	U	N3-C2-O2	-6.01	117.99	122.20
78	S2	1722	G	C8-N9-C1'	-5.96	119.25	127.00
20	L5	1378	C	N3-C2-O2	-5.95	117.74	121.90
20	L5	209	U	C2-N1-C1'	5.88	124.76	117.70
20	L5	3761	C	C2-N1-C1'	5.88	125.27	118.80
78	S2	1629	C	N1-C2-O2	5.84	122.41	118.90
20	L5	1597	G	O4'-C1'-N9	5.83	112.86	108.20
20	L5	925	C	N3-C2-O2	-5.81	117.83	121.90
20	L5	485	C	N1-C2-O2	5.81	122.39	118.90
78	S2	1453	C	C6-N1-C2	-5.81	117.98	120.30
20	L5	255	C	N3-C2-O2	-5.79	117.84	121.90
20	L5	4068	U	C2-N1-C1'	5.79	124.65	117.70
20	L5	182	G	N3-C4-N9	-5.78	122.53	126.00
20	L5	2627	C	C2-N1-C1'	5.76	125.13	118.80
78	S2	356	C	C6-N1-C1'	-5.75	113.90	120.80
78	S2	1755	C	N1-C2-O2	5.75	122.35	118.90
20	L5	2710	C	N3-C2-O2	-5.73	117.89	121.90
20	L5	4303	C	C6-N1-C2	-5.72	118.01	120.30
25	LC	2	ALA	C-N-CA	5.70	135.94	121.70
78	S2	1453	C	C5-C6-N1	5.69	123.85	121.00
63	SR	117	LEU	CA-CB-CG	5.69	128.38	115.30
20	L5	4924	C	N3-C2-O2	-5.68	117.92	121.90
20	L5	4928	C	C2-N1-C1'	5.68	125.05	118.80
85	AT	20	U	C2-N1-C1'	5.68	124.51	117.70
20	L5	2257	C	C2-N1-C1'	5.67	125.04	118.80
20	L5	4093	G	O4'-C1'-N9	5.67	112.73	108.20
20	L5	262	G	N1-C6-O6	-5.66	116.51	119.90
78	S2	1694	U	C6-N1-C2	-5.65	117.61	121.00
20	L5	115	C	C2-N1-C1'	5.64	125.01	118.80
20	L5	4709	U	C6-N1-C1'	-5.64	113.31	121.20
78	S2	1722	G	C4-N9-C1'	5.60	133.78	126.50
20	L5	4898	G	C5-C6-O6	5.58	131.95	128.60
20	L5	489	C	N1-C2-O2	5.58	122.25	118.90
20	L5	4281	A	O4'-C1'-N9	5.57	112.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L5	3775	A	C6-C5-N7	-5.55	128.41	132.30
20	L5	2255	C	N3-C2-O2	-5.53	118.03	121.90
86	CF	419	PRO	CA-CB-CG	-5.52	93.51	104.00
20	L5	1251	C	N1-C2-O2	5.48	122.19	118.90
20	L5	1216	C	C2-N1-C1'	5.47	124.81	118.80
78	S2	1424	G	C4-N9-C1'	5.45	133.59	126.50
20	L5	3773	U	C2-N1-C1'	5.43	124.22	117.70
3	SI	172	LEU	CA-CB-CG	5.42	127.76	115.30
20	L5	2710	C	C6-N1-C1'	-5.42	114.30	120.80
85	AT	19	G	O4'-C1'-N9	-5.42	103.87	108.20
78	S2	688	U	P-O3'-C3'	5.41	126.19	119.70
78	S2	1722	G	C6-C5-N7	-5.41	127.15	130.40
85	AT	20	U	N3-C2-O2	-5.40	118.42	122.20
78	S2	427	U	N3-C2-O2	-5.40	118.42	122.20
78	S2	1114	U	O4'-C1'-N1	5.38	112.51	108.20
78	S2	537	C	C2-N1-C1'	5.38	124.72	118.80
20	L5	3775	A	O4'-C1'-N9	5.37	112.50	108.20
85	AT	41	C	N3-C2-O2	-5.35	118.16	121.90
78	S2	118	C	C2-N1-C1'	5.34	124.68	118.80
78	S2	1424	G	C8-N9-C1'	-5.34	120.06	127.00
78	S2	356	C	N3-C2-O2	-5.32	118.17	121.90
20	L5	3761	C	N1-C2-O2	5.31	122.09	118.90
78	S2	293	C	N1-C2-O2	5.31	122.08	118.90
78	S2	1139	C	N3-C2-O2	-5.29	118.20	121.90
20	L5	4758	U	N3-C2-O2	-5.29	118.50	122.20
20	L5	4928	C	N1-C2-O2	5.28	122.07	118.90
20	L5	2257	C	N1-C2-O2	5.28	122.07	118.90
20	L5	263	G	N1-C2-N2	-5.26	111.46	116.20
78	S2	1756	C	N3-C2-O2	-5.26	118.22	121.90
20	L5	2410	C	C2-N1-C1'	5.25	124.58	118.80
78	S2	1306	U	C2-N1-C1'	5.23	123.97	117.70
24	LB	17	LEU	CA-CB-CG	5.22	127.30	115.30
78	S2	325	C	C2-N1-C1'	5.22	124.54	118.80
20	L5	1241	C	C2-N1-C1'	5.21	124.53	118.80
20	L5	4709	U	C5-C4-O4	-5.21	122.77	125.90
20	L5	1252	C	C6-N1-C2	-5.20	118.22	120.30
20	L5	262	G	N1-C2-N2	-5.20	111.52	116.20
6	SG	135	PRO	N-CD-CG	-5.19	95.42	103.20
78	S2	1722	G	N9-C4-C5	-5.19	103.33	105.40
6	SG	144	LEU	CA-CB-CG	5.17	127.20	115.30
20	L5	2018	C	C5-C6-N1	5.17	123.59	121.00
78	S2	1629	C	N1-C2-N3	5.17	122.82	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	LN	134	LEU	CA-CB-CG	5.17	127.19	115.30
20	L5	1241	C	N1-C2-O2	5.16	122.00	118.90
20	L5	4393	G	C8-N9-C4	5.16	108.46	106.40
62	Lr	123	PRO	CA-N-CD	-5.16	104.28	111.50
20	L5	3646	A	N9-C4-C5	-5.15	103.74	105.80
20	L5	2710	C	C6-N1-C2	-5.15	118.24	120.30
20	L5	3761	C	N3-C2-O2	-5.15	118.30	121.90
78	S2	1424	G	C6-C5-N7	-5.13	127.32	130.40
78	S2	632	C	C2-N1-C1'	5.12	124.44	118.80
20	L5	3765	G	C8-N9-C4	-5.12	104.35	106.40
32	LJ	12	MET	CB-CG-SD	5.11	127.73	112.40
78	S2	1694	U	C2-N1-C1'	5.10	123.81	117.70
1	LR	148	ASP	CB-CG-OD1	5.09	122.88	118.30
20	L5	3646	A	C8-N9-C4	5.08	107.83	105.80
20	L5	925	C	N1-C2-O2	5.07	121.94	118.90
20	L5	4897	G	C5-C6-O6	5.07	131.65	128.60
22	L8	51	U	N3-C2-O2	-5.07	118.65	122.20
20	L5	2033	A	P-O3'-C3'	5.07	125.78	119.70
20	L5	263	G	C5-C6-O6	5.06	131.64	128.60
15	SC	132	ASP	CB-CG-OD1	5.06	122.85	118.30
20	L5	4583	C	O4'-C1'-N1	5.04	112.23	108.20
20	L5	412	G	C4-C5-N7	5.04	112.81	110.80
68	SQ	7	LEU	CA-CB-CG	5.04	126.88	115.30
30	LH	17	ASP	CB-CG-OD2	5.03	122.83	118.30
78	S2	1415	C	N1-C2-O2	5.03	121.92	118.90
20	L5	4281	A	C5-N7-C8	-5.03	101.39	103.90
78	S2	1611	G	C5-C6-O6	5.03	131.62	128.60
78	S2	1811	C	N3-C4-C5	5.02	123.91	121.90
78	S2	1520	G	C4-N9-C1'	5.02	133.02	126.50
20	L5	4303	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	LA	13	GLY	Peptide
24	LB	17	LEU	Peptide
24	LB	258	HIS	Peptide
32	LJ	94	LEU	Peptide
33	LL	154	VAL	Peptide
34	LM	87	ALA	Peptide
36	LO	110	PRO	Peptide

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Mol	Chain	Res	Type	Group
40	LT	136	ARG	Peptide
51	Lf	103	VAL	Peptide
51	Lf	106	TYR	Peptide
55	Lj	39	TYR	Peptide
55	Lj	40	PRO	Peptide
82	Lz	183	ILE	Peptide
65	SF	78	MET	Peptide
12	SH	15	LYS	Peptide
67	SP	127	LYS	Peptide
68	SQ	43	GLU	Peptide
5	SX	126	ALA	Peptide
76	SZ	46	ASN	Peptide

## 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	
1	LR	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
2	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
3	SI	204/206 (99%)	188 (92%)	16 (8%)	0	100	100
4	SL	151/153 (99%)	138 (91%)	13 (9%)	0	100	100
5	SX	139/141 (99%)	127 (91%)	11 (8%)	1 (1%)	19	48
6	SG	235/237 (99%)	218 (93%)	17 (7%)	0	100	100
7	SJ	183/185 (99%)	171 (93%)	12 (7%)	0	100	100
8	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
9	Se	56/58 (97%)	51 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	SA	219/221 (99%)	202 (92%)	17 (8%)	0	100	100
11	SB	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
12	SH	182/186 (98%)	159 (87%)	23 (13%)	0	100	100
13	SV	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
14	Sa	100/102 (98%)	93 (93%)	7 (7%)	0	100	100
15	SC	220/222 (99%)	206 (94%)	14 (6%)	0	100	100
16	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
17	SO	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
18	SW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
19	Sb	81/83 (98%)	68 (84%)	13 (16%)	0	100	100
23	LA	246/248 (99%)	228 (93%)	18 (7%)	0	100	100
24	LB	400/402 (100%)	375 (94%)	25 (6%)	0	100	100
25	LC	366/368 (100%)	341 (93%)	25 (7%)	0	100	100
26	LD	291/293 (99%)	273 (94%)	18 (6%)	0	100	100
27	LE	232/236 (98%)	206 (89%)	26 (11%)	0	100	100
28	LF	223/225 (99%)	212 (95%)	11 (5%)	0	100	100
29	LG	239/241 (99%)	226 (95%)	13 (5%)	0	100	100
30	LH	188/190 (99%)	174 (93%)	14 (7%)	0	100	100
31	LI	198/202 (98%)	181 (91%)	17 (9%)	0	100	100
32	LJ	174/176 (99%)	165 (95%)	9 (5%)	0	100	100
33	LL	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
34	LM	137/139 (99%)	127 (93%)	9 (7%)	1 (1%)	19	48
35	LN	201/203 (99%)	192 (96%)	7 (4%)	2 (1%)	13	39
36	LO	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
37	LP	151/153 (99%)	140 (93%)	11 (7%)	0	100	100
38	LQ	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
39	LS	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
40	LT	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
41	LU	99/101 (98%)	83 (84%)	16 (16%)	0	100	100
42	LV	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
43	LX	118/120 (98%)	115 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	LY	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
45	LZ	133/135 (98%)	122 (92%)	11 (8%)	0	100	100
46	La	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
47	Lb	105/109 (96%)	96 (91%)	9 (9%)	0	100	100
48	Lc	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
49	Ld	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
50	Le	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
51	Lf	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	14	42
52	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
53	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
54	Li	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
55	Lj	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
56	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
57	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
58	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
59	Ln	22/24 (92%)	22 (100%)	0	0	100	100
60	Lo	103/105 (98%)	95 (92%)	8 (8%)	0	100	100
61	Lp	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
62	Lr	123/125 (98%)	115 (94%)	8 (6%)	0	100	100
63	SR	133/135 (98%)	119 (90%)	13 (10%)	1 (1%)	16	44
64	SD	225/227 (99%)	204 (91%)	21 (9%)	0	100	100
65	SF	187/189 (99%)	165 (88%)	22 (12%)	0	100	100
66	SK	96/98 (98%)	84 (88%)	11 (12%)	1 (1%)	13	39
67	SP	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
68	SQ	142/144 (99%)	122 (86%)	20 (14%)	0	100	100
69	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
70	ST	141/143 (99%)	129 (92%)	11 (8%)	1 (1%)	19	48
71	SU	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
72	Sc	62/64 (97%)	52 (84%)	10 (16%)	0	100	100
73	Sd	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
74	Sg	311/313 (99%)	278 (89%)	33 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	SM	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	44
76	SZ	73/75 (97%)	59 (81%)	14 (19%)	0	100	100
77	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
81	Lt	137/141 (97%)	101 (74%)	35 (26%)	1 (1%)	19	48
82	Lz	215/217 (99%)	165 (77%)	50 (23%)	0	100	100
83	Ls	194/196 (99%)	177 (91%)	17 (9%)	0	100	100
84	LW	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
86	CF	438/441 (99%)	416 (95%)	22 (5%)	0	100	100
All	All	12301/12472 (99%)	11371 (92%)	920 (8%)	10 (0%)	50	77

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
63	SR	124	VAL
5	SX	127	ASN
34	LM	88	ALA
35	LN	124	ASP
66	SK	36	ALA
70	ST	41	LYS
75	SM	96	ARG
81	Lt	144	ASP
51	Lf	107	PRO
35	LN	84	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LR	166/166 (100%)	148 (89%)	18 (11%)	5	17
2	SE	224/224 (100%)	208 (93%)	16 (7%)	12	35
3	SI	178/178 (100%)	161 (90%)	17 (10%)	7	22
4	SL	137/137 (100%)	118 (86%)	19 (14%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SX	113/113 (100%)	102 (90%)	11 (10%)	6	21
6	SG	207/207 (100%)	179 (86%)	28 (14%)	3	10
7	SJ	161/161 (100%)	151 (94%)	10 (6%)	15	43
8	SY	113/113 (100%)	96 (85%)	17 (15%)	2	8
9	Se	47/47 (100%)	41 (87%)	6 (13%)	3	12
10	SA	183/183 (100%)	171 (93%)	12 (7%)	14	39
11	SB	195/195 (100%)	169 (87%)	26 (13%)	3	10
12	SH	166/166 (100%)	157 (95%)	9 (5%)	18	48
13	SV	67/67 (100%)	56 (84%)	11 (16%)	2	6
14	Sa	89/89 (100%)	79 (89%)	10 (11%)	5	16
15	SC	188/188 (100%)	167 (89%)	21 (11%)	5	16
16	SN	130/130 (100%)	123 (95%)	7 (5%)	18	48
17	SO	110/110 (100%)	98 (89%)	12 (11%)	5	17
18	SW	112/112 (100%)	101 (90%)	11 (10%)	6	21
19	Sb	75/75 (100%)	69 (92%)	6 (8%)	10	30
23	LA	190/190 (100%)	175 (92%)	15 (8%)	10	30
24	LB	348/348 (100%)	328 (94%)	20 (6%)	17	46
25	LC	306/306 (100%)	281 (92%)	25 (8%)	9	29
26	LD	246/247 (100%)	226 (92%)	20 (8%)	9	29
27	LE	209/209 (100%)	189 (90%)	20 (10%)	7	22
28	LF	194/194 (100%)	185 (95%)	9 (5%)	23	55
29	LG	203/205 (99%)	187 (92%)	16 (8%)	10	30
30	LH	169/169 (100%)	154 (91%)	15 (9%)	8	25
31	LI	172/172 (100%)	159 (92%)	13 (8%)	11	32
32	LJ	148/148 (100%)	135 (91%)	13 (9%)	8	26
33	LL	176/176 (100%)	165 (94%)	11 (6%)	15	42
34	LM	118/118 (100%)	107 (91%)	11 (9%)	7	23
35	LN	171/171 (100%)	162 (95%)	9 (5%)	19	49
36	LO	173/173 (100%)	168 (97%)	5 (3%)	37	71
37	LP	134/134 (100%)	120 (90%)	14 (10%)	5	18
38	LQ	164/164 (100%)	153 (93%)	11 (7%)	13	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	LS	156/156 (100%)	143 (92%)	13 (8%)	9	28
40	LT	139/139 (100%)	129 (93%)	10 (7%)	12	34
41	LU	91/91 (100%)	75 (82%)	16 (18%)	1	5
42	LV	101/101 (100%)	99 (98%)	2 (2%)	50	81
43	LX	108/108 (100%)	97 (90%)	11 (10%)	6	19
44	LY	124/124 (100%)	114 (92%)	10 (8%)	9	29
45	LZ	117/117 (100%)	109 (93%)	8 (7%)	13	38
46	La	120/120 (100%)	112 (93%)	8 (7%)	13	38
47	Lb	88/90 (98%)	80 (91%)	8 (9%)	7	24
48	Lc	83/83 (100%)	75 (90%)	8 (10%)	7	22
49	Ld	98/98 (100%)	86 (88%)	12 (12%)	4	13
50	Le	114/114 (100%)	107 (94%)	7 (6%)	15	43
51	Lf	88/88 (100%)	83 (94%)	5 (6%)	17	46
52	Lg	98/98 (100%)	92 (94%)	6 (6%)	15	43
53	Lh	109/109 (100%)	103 (94%)	6 (6%)	18	47
54	Li	86/86 (100%)	81 (94%)	5 (6%)	17	45
55	Lj	73/73 (100%)	66 (90%)	7 (10%)	7	22
56	Lk	64/64 (100%)	55 (86%)	9 (14%)	3	9
57	Ll	47/47 (100%)	43 (92%)	4 (8%)	8	27
58	Lm	48/48 (100%)	44 (92%)	4 (8%)	9	28
59	Ln	23/23 (100%)	19 (83%)	4 (17%)	1	5
60	Lo	93/93 (100%)	88 (95%)	5 (5%)	18	48
61	Lp	74/74 (100%)	68 (92%)	6 (8%)	9	29
62	Lr	109/109 (100%)	96 (88%)	13 (12%)	4	14
63	SR	122/122 (100%)	115 (94%)	7 (6%)	17	46
64	SD	190/190 (100%)	167 (88%)	23 (12%)	4	13
65	SF	159/159 (100%)	142 (89%)	17 (11%)	5	17
66	SK	89/89 (100%)	79 (89%)	10 (11%)	5	16
67	SP	107/107 (100%)	96 (90%)	11 (10%)	6	19
68	SQ	119/119 (100%)	101 (85%)	18 (15%)	2	8
69	SS	126/126 (100%)	117 (93%)	9 (7%)	12	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	ST	113/113 (100%)	100 (88%)	13 (12%)	4	15
71	SU	94/94 (100%)	86 (92%)	8 (8%)	8	27
72	Sc	57/57 (100%)	50 (88%)	7 (12%)	4	13
73	Sd	48/48 (100%)	41 (85%)	7 (15%)	2	8
74	Sg	272/272 (100%)	242 (89%)	30 (11%)	5	17
75	SM	102/104 (98%)	91 (89%)	11 (11%)	5	17
76	SZ	66/66 (100%)	59 (89%)	7 (11%)	5	18
77	Sf	60/60 (100%)	54 (90%)	6 (10%)	6	20
81	Lt	112/115 (97%)	105 (94%)	7 (6%)	15	42
82	Lz	195/196 (100%)	171 (88%)	24 (12%)	4	13
83	Ls	162/164 (99%)	149 (92%)	13 (8%)	10	30
84	LW	97/97 (100%)	84 (87%)	13 (13%)	3	10
86	CF	365/366 (100%)	346 (95%)	19 (5%)	19	50
All	All	10688/10702 (100%)	9747 (91%)	941 (9%)	11	26

All (941) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	LR	12	SER
1	LR	27	ASN
1	LR	29	THR
1	LR	38	ARG
1	LR	63	CYS
1	LR	65	LYS
1	LR	72	LYS
1	LR	74	ARG
1	LR	111	GLU
1	LR	112	SER
1	LR	125	LEU
1	LR	133	LYS
1	LR	148	ASP
1	LR	153	LYS
1	LR	171	LYS
1	LR	176	ARG
1	LR	186	LYS
1	LR	188	LEU
2	SE	17	HIS

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Mol	Chain	Res	Type
2	SE	38	LEU
2	SE	39	ARG
2	SE	41	CYS
2	SE	50	ASN
2	SE	69	PHE
2	SE	79	ASP
2	SE	88	ASP
2	SE	121	TYR
2	SE	126	VAL
2	SE	146	THR
2	SE	181	CYS
2	SE	183	VAL
2	SE	198	ARG
2	SE	217	SER
2	SE	223	SER
3	SI	5	ARG
3	SI	37	LYS
3	SI	45	THR
3	SI	76	THR
3	SI	95	THR
3	SI	100	CYS
3	SI	110	ARG
3	SI	123	ARG
3	SI	140	LYS
3	SI	141	ARG
3	SI	144	LYS
3	SI	151	GLU
3	SI	153	LYS
3	SI	157	LYS
3	SI	163	GLU
3	SI	172	LEU
3	SI	206	LYS
4	SL	4	ILE
4	SL	6	THR
4	SL	12	LYS
4	SL	15	THR
4	SL	17	PHE
4	SL	19	ASN
4	SL	21	LYS
4	SL	25	LEU
4	SL	42	LEU
4	SL	66	VAL

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Mol	Chain	Res	Type
4	SL	69	ARG
4	SL	73	LEU
4	SL	81	LYS
4	SL	104	LYS
4	SL	128	VAL
4	SL	132	ARG
4	SL	135	SER
4	SL	141	ASN
4	SL	152	LYS
5	SX	14	ARG
5	SX	20	GLN
5	SX	50	ILE
5	SX	69	CYS
5	SX	72	VAL
5	SX	95	GLU
5	SX	98	ASP
5	SX	105	PHE
5	SX	119	ARG
5	SX	130	LEU
5	SX	138	LYS
6	SG	3	LEU
6	SG	17	GLU
6	SG	22	ARG
6	SG	46	LYS
6	SG	48	TYR
6	SG	50	VAL
6	SG	63	MET
6	SG	69	THR
6	SG	70	HIS
6	SG	82	SER
6	SG	83	CYS
6	SG	84	TYR
6	SG	98	ARG
6	SG	102	VAL
6	SG	103	ASP
6	SG	111	LEU
6	SG	114	VAL
6	SG	119	LYS
6	SG	126	ASP
6	SG	132	ARG
6	SG	133	LEU
6	SG	143	LYS

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Mol	Chain	Res	Type
6	SG	148	SER
6	SG	168	LYS
6	SG	190	ARG
6	SG	197	GLN
6	SG	217	MET
6	SG	219	GLU
7	SJ	7	TRP
7	SJ	22	LYS
7	SJ	34	GLU
7	SJ	38	ARG
7	SJ	55	LYS
7	SJ	79	ARG
7	SJ	101	LYS
7	SJ	119	LEU
7	SJ	132	GLN
7	SJ	155	LYS
8	SY	8	ARG
8	SY	16	ARG
8	SY	22	GLN
8	SY	23	MET
8	SY	34	THR
8	SY	39	GLU
8	SY	42	GLU
8	SY	43	LYS
8	SY	47	MET
8	SY	50	THR
8	SY	61	ARG
8	SY	63	HIS
8	SY	78	SER
8	SY	97	TYR
8	SY	99	LYS
8	SY	101	LYS
8	SY	106	GLN
9	Se	18	LYS
9	Se	22	GLN
9	Se	25	LYS
9	Se	27	LYS
9	Se	41	ARG
9	Se	42	PHE
10	SA	17	LYS
10	SA	18	PHE
10	SA	35	GLU

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Mol	Chain	Res	Type
10	SA	52	LYS
10	SA	58	LEU
10	SA	69	GLU
10	SA	73	ASP
10	SA	75	SER
10	SA	111	GLN
10	SA	169	HIS
10	SA	196	GLU
10	SA	212	LYS
11	SB	38	MET
11	SB	40	ASN
11	SB	52	THR
11	SB	59	SER
11	SB	69	VAL
11	SB	73	ASP
11	SB	75	GLN
11	SB	85	LYS
11	SB	95	ASN
11	SB	96	CYS
11	SB	103	MET
11	SB	110	MET
11	SB	121	ILE
11	SB	128	LYS
11	SB	131	ASP
11	SB	137	LEU
11	SB	168	MET
11	SB	174	ARG
11	SB	178	THR
11	SB	179	ASN
11	SB	191	ASP
11	SB	205	TYR
11	SB	210	VAL
11	SB	214	LYS
11	SB	217	MET
11	SB	230	GLU
12	SH	57	ARG
12	SH	85	LYS
12	SH	105	THR
12	SH	145	ARG
12	SH	155	LYS
12	SH	163	GLN
12	SH	171	GLU

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Mol	Chain	Res	Type
12	SH	179	LYS
12	SH	186	ASN
13	SV	1	MET
13	SV	11	LEU
13	SV	15	ARG
13	SV	17	CYS
13	SV	18	SER
13	SV	28	ASP
13	SV	50	PHE
13	SV	51	LYS
13	SV	60	ARG
13	SV	74	LYS
13	SV	83	PHE
14	Sa	19	GLN
14	Sa	23	CYS
14	Sa	28	ARG
14	Sa	29	CYS
14	Sa	30	VAL
14	Sa	52	ASP
14	Sa	72	HIS
14	Sa	83	VAL
14	Sa	100	ARG
14	Sa	102	ARG
15	SC	68	ARG
15	SC	73	MET
15	SC	75	ILE
15	SC	76	LYS
15	SC	96	PHE
15	SC	101	SER
15	SC	120	GLN
15	SC	121	ARG
15	SC	160	LEU
15	SC	167	ARG
15	SC	205	VAL
15	SC	227	ARG
15	SC	236	PHE
15	SC	240	THR
15	SC	245	SER
15	SC	248	TYR
15	SC	254	ASP
15	SC	256	TRP
15	SC	262	THR

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Mol	Chain	Res	Type
15	SC	263	LYS
15	SC	271	ASP
16	SN	28	LEU
16	SN	57	SER
16	SN	67	THR
16	SN	102	LEU
16	SN	105	ASN
16	SN	143	SER
16	SN	144	SER
17	SO	66	ARG
17	SO	69	SER
17	SO	75	MET
17	SO	84	ARG
17	SO	87	GLU
17	SO	93	LEU
17	SO	97	LEU
17	SO	100	THR
17	SO	103	ASN
17	SO	105	THR
17	SO	117	ARG
17	SO	142	ARG
18	SW	4	MET
18	SW	54	ASP
18	SW	57	ARG
18	SW	62	VAL
18	SW	81	VAL
18	SW	85	ASP
18	SW	98	GLN
18	SW	103	VAL
18	SW	106	THR
18	SW	117	ARG
18	SW	130	PHE
19	Sb	45	THR
19	Sb	48	SER
19	Sb	56	CYS
19	Sb	60	SER
19	Sb	64	CYS
19	Sb	83	GLN
23	LA	15	VAL
23	LA	42	LYS
23	LA	45	VAL
23	LA	54	ARG

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Mol	Chain	Res	Type
23	LA	65	ASP
23	LA	101	VAL
23	LA	102	LEU
23	LA	114	CYS
23	LA	135	THR
23	LA	155	LYS
23	LA	159	SER
23	LA	165	VAL
23	LA	198	ARG
23	LA	207	VAL
23	LA	221	LYS
24	LB	17	LEU
24	LB	93	VAL
24	LB	94	GLU
24	LB	125	SER
24	LB	134	CYS
24	LB	159	VAL
24	LB	198	ARG
24	LB	214	ASP
24	LB	299	ILE
24	LB	340	THR
24	LB	347	LEU
24	LB	348	ARG
24	LB	351	LEU
24	LB	358	ARG
24	LB	360	LEU
24	LB	378	ARG
24	LB	381	THR
24	LB	386	LYS
24	LB	394	LYS
24	LB	395	ASP
25	LC	1	MET
25	LC	3	CYS
25	LC	17	SER
25	LC	29	LYS
25	LC	56	GLU
25	LC	63	SER
25	LC	71	ARG
25	LC	85	HIS
25	LC	95	MET
25	LC	114	ARG
25	LC	122	TYR

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Mol	Chain	Res	Type
25	LC	140	LYS
25	LC	181	LYS
25	LC	186	SER
25	LC	188	ARG
25	LC	189	MET
25	LC	205	ARG
25	LC	213	GLU
25	LC	261	ASP
25	LC	266	THR
25	LC	285	ILE
25	LC	287	THR
25	LC	313	VAL
25	LC	348	LYS
25	LC	350	ARG
26	LD	36	LEU
26	LD	46	THR
26	LD	51	MET
26	LD	58	ARG
26	LD	76	CYS
26	LD	86	TYR
26	LD	107	ARG
26	LD	122	GLN
26	LD	136	ASP
26	LD	164	LYS
26	LD	187	SER
26	LD	210	TYR
26	LD	212	MET
26	LD	220	LYS
26	LD	232	THR
26	LD	235	MET
26	LD	256	LYS
26	LD	259	LYS
26	LD	260	GLU
26	LD	293	ARG
27	LE	44	CYS
27	LE	100	LYS
27	LE	107	VAL
27	LE	115	TYR
27	LE	120	ASP
27	LE	121	VAL
27	LE	128	HIS
27	LE	130	LYS

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Mol	Chain	Res	Type
27	LE	166	LYS
27	LE	174	LEU
27	LE	202	ASP
27	LE	206	VAL
27	LE	210	LYS
27	LE	226	ARG
27	LE	234	ASP
27	LE	240	TYR
27	LE	260	LYS
27	LE	261	ILE
27	LE	273	SER
27	LE	278	THR
28	LF	28	LEU
28	LF	32	ARG
28	LF	44	LYS
28	LF	119	ASN
28	LF	164	LYS
28	LF	186	CYS
28	LF	196	THR
28	LF	221	LYS
28	LF	248	ASN
29	LG	43	GLN
29	LG	73	ARG
29	LG	85	GLN
29	LG	88	ASP
29	LG	90	GLN
29	LG	94	GLN
29	LG	97	LYS
29	LG	117	ARG
29	LG	170	LEU
29	LG	192	ARG
29	LG	201	THR
29	LG	205	THR
29	LG	209	SER
29	LG	235	ARG
29	LG	259	LYS
29	LG	261	LEU
30	LH	2	LYS
30	LH	8	GLN
30	LH	10	VAL
30	LH	19	THR
30	LH	44	GLU

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Mol	Chain	Res	Type
30	LH	51	LYS
30	LH	80	MET
30	LH	84	VAL
30	LH	94	SER
30	LH	113	GLU
30	LH	125	ARG
30	LH	126	VAL
30	LH	135	SER
30	LH	142	ASP
30	LH	170	LYS
31	LI	54	SER
31	LI	71	CYS
31	LI	83	ASP
31	LI	101	LYS
31	LI	102	MET
31	LI	123	GLN
31	LI	129	VAL
31	LI	169	LYS
31	LI	179	ASP
31	LI	187	LYS
31	LI	195	CYS
31	LI	203	HIS
31	LI	214	SER
32	LJ	15	LEU
32	LJ	26	VAL
32	LJ	46	GLN
32	LJ	60	PHE
32	LJ	63	ARG
32	LJ	74	VAL
32	LJ	88	LYS
32	LJ	90	ARG
32	LJ	94	LEU
32	LJ	95	ARG
32	LJ	101	ASP
32	LJ	104	ASN
32	LJ	111	GLU
33	LL	21	ARG
33	LL	59	VAL
33	LL	67	HIS
33	LL	70	VAL
33	LL	103	ARG
33	LL	130	LYS

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Mol	Chain	Res	Type
33	LL	139	SER
33	LL	158	ARG
33	LL	163	LYS
33	LL	181	SER
33	LL	200	LYS
34	LM	16	SER
34	LM	31	ILE
34	LM	35	ARG
34	LM	38	VAL
34	LM	50	MET
34	LM	63	LYS
34	LM	104	MET
34	LM	113	MET
34	LM	117	LYS
34	LM	118	MET
34	LM	132	LYS
35	LN	41	ARG
35	LN	60	VAL
35	LN	77	LYS
35	LN	117	ASN
35	LN	125	SER
35	LN	148	THR
35	LN	161	MET
35	LN	171	SER
35	LN	187	SER
36	LO	29	LEU
36	LO	31	ARG
36	LO	88	LEU
36	LO	127	VAL
36	LO	178	ARG
37	LP	17	SER
37	LP	18	ARG
37	LP	23	ARG
37	LP	24	VAL
37	LP	30	ARG
37	LP	57	CYS
37	LP	58	VAL
37	LP	69	ARG
37	LP	75	GLN
37	LP	76	TRP
37	LP	80	GLN
37	LP	96	LYS

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Mol	Chain	Res	Type
37	LP	139	TYR
37	LP	148	MET
38	LQ	3	VAL
38	LQ	28	LEU
38	LQ	62	SER
38	LQ	76	GLU
38	LQ	79	THR
38	LQ	93	GLN
38	LQ	94	GLU
38	LQ	103	LEU
38	LQ	129	ASP
38	LQ	160	HIS
38	LQ	168	ARG
39	LS	21	LYS
39	LS	42	SER
39	LS	48	VAL
39	LS	76	LYS
39	LS	90	THR
39	LS	101	THR
39	LS	111	ARG
39	LS	131	GLU
39	LS	149	LYS
39	LS	154	LEU
39	LS	158	VAL
39	LS	161	ARG
39	LS	169	THR
40	LT	29	THR
40	LT	45	MET
40	LT	48	VAL
40	LT	68	THR
40	LT	83	LYS
40	LT	85	LEU
40	LT	102	ARG
40	LT	104	SER
40	LT	158	PHE
40	LT	159	MET
41	LU	19	LEU
41	LU	22	THR
41	LU	30	GLU
41	LU	34	MET
41	LU	38	ASN
41	LU	39	PHE

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Mol	Chain	Res	Type
41	LU	62	THR
41	LU	68	SER
41	LU	79	SER
41	LU	82	TYR
41	LU	94	ASN
41	LU	95	ASN
41	LU	98	ASP
41	LU	99	TRP
41	LU	110	TYR
41	LU	113	ARG
42	LV	48	ARG
42	LV	112	MET
43	LX	52	LEU
43	LX	63	LYS
43	LX	68	ARG
43	LX	85	SER
43	LX	88	LYS
43	LX	111	GLN
43	LX	116	LEU
43	LX	120	ASP
43	LX	121	VAL
43	LX	147	LEU
43	LX	148	ASP
44	LY	2	LYS
44	LY	28	LYS
44	LY	44	VAL
44	LY	46	SER
44	LY	53	ASP
44	LY	74	TYR
44	LY	88	GLU
44	LY	102	SER
44	LY	120	GLU
44	LY	124	LYS
45	LZ	10	VAL
45	LZ	43	VAL
45	LZ	53	VAL
45	LZ	84	ARG
45	LZ	88	ASP
45	LZ	94	THR
45	LZ	98	LYS
45	LZ	99	ASP
46	La	3	SER

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Mol	Chain	Res	Type
46	La	12	ARG
46	La	61	TYR
46	La	66	ASN
46	La	87	ARG
46	La	102	ASP
46	La	119	LYS
46	La	120	GLN
47	Lb	9	THR
47	Lb	33	LYS
47	Lb	61	ASN
47	Lb	63	LYS
47	Lb	94	ASP
47	Lb	106	LYS
47	Lb	107	ARG
47	Lb	119	CYS
48	Lc	10	SER
48	Lc	18	LEU
48	Lc	23	LYS
48	Lc	24	SER
48	Lc	26	LYS
48	Lc	91	VAL
48	Lc	94	LEU
48	Lc	101	ASP
49	Ld	26	THR
49	Ld	54	MET
49	Ld	55	LYS
49	Ld	91	LYS
49	Ld	98	SER
49	Ld	99	PRO
49	Ld	100	ASN
49	Ld	104	THR
49	Ld	106	VAL
49	Ld	116	ASN
49	Ld	119	THR
49	Ld	121	ASN
50	Le	19	LYS
50	Le	26	ASP
50	Le	33	ARG
50	Le	45	VAL
50	Le	83	LYS
50	Le	102	ASN
50	Le	108	ARG

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Mol	Chain	Res	Type
51	Lf	25	THR
51	Lf	33	VAL
51	Lf	37	ASP
51	Lf	46	ARG
51	Lf	84	VAL
52	Lg	32	TYR
52	Lg	63	VAL
52	Lg	68	SER
52	Lg	73	HIS
52	Lg	105	LYS
52	Lg	106	VAL
53	Lh	29	SER
53	Lh	49	VAL
53	Lh	66	LYS
53	Lh	87	LYS
53	Lh	88	THR
53	Lh	116	LEU
54	Li	3	LEU
54	Li	32	ARG
54	Li	55	ARG
54	Li	64	SER
54	Li	91	SER
55	Lj	2	THR
55	Lj	22	CYS
55	Lj	29	LEU
55	Lj	32	SER
55	Lj	63	ARG
55	Lj	80	GLU
55	Lj	83	THR
56	Lk	16	ARG
56	Lk	18	LYS
56	Lk	21	LYS
56	Lk	29	LYS
56	Lk	32	VAL
56	Lk	39	SER
56	Lk	45	LEU
56	Lk	49	ASP
56	Lk	59	SER
57	Ll	36	ARG
57	Ll	45	ARG
57	Ll	46	ARG
57	Ll	47	THR

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Mol	Chain	Res	Type
58	Lm	81	SER
58	Lm	84	GLN
58	Lm	97	ARG
58	Lm	113	LYS
59	Ln	4	LYS
59	Ln	6	ARG
59	Ln	12	ARG
59	Ln	19	LYS
60	Lo	15	CYS
60	Lo	69	ARG
60	Lo	77	CYS
60	Lo	83	LEU
60	Lo	99	ARG
61	Lp	24	LYS
61	Lp	25	MET
61	Lp	26	VAL
61	Lp	36	LYS
61	Lp	46	LYS
61	Lp	87	LYS
62	Lr	14	SER
62	Lr	21	ASN
62	Lr	49	VAL
62	Lr	58	LYS
62	Lr	60	VAL
62	Lr	63	VAL
62	Lr	66	ARG
62	Lr	78	VAL
62	Lr	84	LYS
62	Lr	101	LYS
62	Lr	105	ASP
62	Lr	123	PRO
62	Lr	125	MET
63	SR	1	MET
63	SR	5	ARG
63	SR	33	ARG
63	SR	43	SER
63	SR	81	ARG
63	SR	91	LEU
63	SR	111	PHE
64	SD	7	LYS
64	SD	23	GLU
64	SD	29	LEU

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Mol	Chain	Res	Type
64	SD	34	TYR
64	SD	39	VAL
64	SD	42	THR
64	SD	43	PRO
64	SD	81	GLU
64	SD	91	VAL
64	SD	94	ARG
64	SD	101	GLN
64	SD	115	VAL
64	SD	120	TYR
64	SD	134	CYS
64	SD	136	VAL
64	SD	139	SER
64	SD	143	ARG
64	SD	146	ARG
64	SD	169	ASP
64	SD	194	PRO
64	SD	214	LYS
64	SD	223	ILE
64	SD	224	SER
65	SF	18	LYS
65	SF	20	PHE
65	SF	22	LYS
65	SF	41	VAL
65	SF	42	LYS
65	SF	77	MET
65	SF	79	HIS
65	SF	83	ASN
65	SF	97	PHE
65	SF	102	LEU
65	SF	127	ARG
65	SF	160	GLU
65	SF	187	SER
65	SF	190	ILE
65	SF	194	ASP
65	SF	201	LYS
65	SF	203	ASN
66	SK	3	MET
66	SK	13	GLU
66	SK	45	VAL
66	SK	46	MET
66	SK	49	MET

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Mol	Chain	Res	Type
66	SK	57	TYR
66	SK	58	VAL
66	SK	59	LYS
66	SK	78	TYR
66	SK	95	ARG
67	SP	16	THR
67	SP	33	LEU
67	SP	51	ARG
67	SP	70	MET
67	SP	71	GLU
67	SP	81	ARG
67	SP	89	MET
67	SP	114	HIS
67	SP	127	LYS
67	SP	128	HIS
67	SP	130	ARG
68	SQ	9	SER
68	SQ	13	PHE
68	SQ	25	CYS
68	SQ	27	ARG
68	SQ	37	ARG
68	SQ	52	LEU
68	SQ	62	ARG
68	SQ	67	ASP
68	SQ	71	ARG
68	SQ	87	SER
68	SQ	95	TYR
68	SQ	105	LYS
68	SQ	115	TYR
68	SQ	117	ARG
68	SQ	126	ARG
68	SQ	127	CYS
68	SQ	129	SER
68	SQ	145	TYR
69	SS	8	LYS
69	SS	13	LEU
69	SS	77	TYR
69	SS	83	PHE
69	SS	101	ASN
69	SS	104	ASP
69	SS	106	LYS
69	SS	109	GLU

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Mol	Chain	Res	Type
69	SS	116	LYS
70	ST	6	VAL
70	ST	29	LYS
70	ST	33	TRP
70	ST	44	GLU
70	ST	51	ASN
70	ST	75	MET
70	ST	87	VAL
70	ST	90	SER
70	ST	93	SER
70	ST	99	VAL
70	ST	112	MET
70	ST	122	LYS
70	ST	126	GLN
71	SU	23	THR
71	SU	36	CYS
71	SU	38	ASP
71	SU	55	ARG
71	SU	62	ARG
71	SU	75	LYS
71	SU	78	ASP
71	SU	88	LEU
72	Sc	16	LYS
72	Sc	27	CYS
72	Sc	28	THR
72	Sc	31	ARG
72	Sc	40	ARG
72	Sc	55	VAL
72	Sc	57	THR
73	Sd	8	TRP
73	Sd	12	ARG
73	Sd	20	SER
73	Sd	25	SER
73	Sd	40	ARG
73	Sd	45	GLN
73	Sd	48	LYS
74	Sg	8	ARG
74	Sg	12	LYS
74	Sg	27	PHE
74	Sg	30	MET
74	Sg	32	LEU
74	Sg	38	LYS

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Mol	Chain	Res	Type
74	Sg	44	LYS
74	Sg	47	ARG
74	Sg	52	TYR
74	Sg	57	ARG
74	Sg	65	PHE
74	Sg	90	TRP
74	Sg	92	LEU
74	Sg	106	LYS
74	Sg	113	PHE
74	Sg	124	SER
74	Sg	125	ARG
74	Sg	144	ASP
74	Sg	155	ARG
74	Sg	212	LYS
74	Sg	229	THR
74	Sg	237	ASN
74	Sg	245	ARG
74	Sg	249	CYS
74	Sg	259	TRP
74	Sg	271	LYS
74	Sg	287	THR
74	Sg	303	THR
74	Sg	312	VAL
74	Sg	313	THR
75	SM	33	ARG
75	SM	44	LYS
75	SM	45	ARG
75	SM	50	CYS
75	SM	60	MET
75	SM	61	TYR
75	SM	63	LYS
75	SM	84	LYS
75	SM	99	LYS
75	SM	119	GLN
75	SM	127	TYR
76	SZ	51	ASP
76	SZ	55	TYR
76	SZ	65	TYR
76	SZ	75	GLU
76	SZ	76	ARG
76	SZ	77	LEU
76	SZ	107	VAL

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Mol	Chain	Res	Type
77	Sf	89	LYS
77	Sf	100	LEU
77	Sf	104	LYS
77	Sf	116	ARG
77	Sf	126	CYS
77	Sf	138	ARG
81	Lt	42	VAL
81	Lt	52	ASP
81	Lt	57	ARG
81	Lt	60	VAL
81	Lt	70	GLN
81	Lt	123	ARG
81	Lt	154	ASP
82	Lz	14	VAL
82	Lz	15	ARG
82	Lz	27	LYS
82	Lz	28	PHE
82	Lz	38	LEU
82	Lz	42	ASP
82	Lz	54	ARG
82	Lz	56	LYS
82	Lz	63	PHE
82	Lz	75	ASP
82	Lz	97	LYS
82	Lz	101	LYS
82	Lz	103	LEU
82	Lz	113	SER
82	Lz	122	ARG
82	Lz	124	LEU
82	Lz	156	LYS
82	Lz	161	LYS
82	Lz	171	HIS
82	Lz	173	LYS
82	Lz	178	GLU
82	Lz	202	ARG
82	Lz	207	LYS
82	Lz	216	LEU
83	Ls	15	LEU
83	Ls	54	LEU
83	Ls	55	MET
83	Ls	59	THR
83	Ls	61	MET

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Mol	Chain	Res	Type
83	Ls	77	LYS
83	Ls	89	VAL
83	Ls	99	ARG
83	Ls	106	LYS
83	Ls	144	THR
83	Ls	162	LYS
83	Ls	180	ILE
83	Ls	193	PHE
84	LW	1	MET
84	LW	19	ARG
84	LW	20	ARG
84	LW	30	GLN
84	LW	38	SER
84	LW	43	LYS
84	LW	50	ASN
84	LW	57	ARG
84	LW	71	ARG
84	LW	77	LYS
84	LW	105	ARG
84	LW	110	ARG
84	LW	124	LYS
86	CF	49	MET
86	CF	78	TRP
86	CF	85	TYR
86	CF	96	ARG
86	CF	97	ASP
86	CF	102	MET
86	CF	135	GLU
86	CF	136	HIS
86	CF	201	MET
86	CF	208	MET
86	CF	215	LYS
86	CF	234	CYS
86	CF	287	THR
86	CF	313	LYS
86	CF	362	ASP
86	CF	376	LYS
86	CF	389	ASP
86	CF	392	LYS
86	CF	393	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	SI	146	GLN
4	SL	19	ASN
6	SG	56	ASN
7	SJ	111	GLN
7	SJ	154	GLN
10	SA	24	HIS
11	SB	75	GLN
12	SH	157	HIS
16	SN	49	GLN
25	LC	317	ASN
25	LC	338	ASN
29	LG	64	GLN
32	LJ	98	ASN
37	LP	118	GLN
37	LP	120	ASN
38	LQ	125	GLN
42	LV	84	GLN
43	LX	73	HIS
50	Le	92	ASN
60	Lo	76	ASN
63	SR	93	GLN
63	SR	118	GLN
65	SF	83	ASN
66	SK	7	ASN
69	SS	85	ASN
72	Sc	26	GLN
74	Sg	14	HIS
74	Sg	26	GLN
76	SZ	45	ASN
83	Ls	41	GLN
84	LW	79	GLN
84	LW	104	GLN
86	CF	367	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	L5	3704/3740 (99%)	865 (23%)	19 (0%)
21	L7	119/120 (99%)	11 (9%)	0
22	L8	155/156 (99%)	30 (19%)	0
78	S2	1715/1740 (98%)	410 (23%)	7 (0%)
79	Et	73/75 (97%)	32 (43%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
80	Pt	72/74 (97%)	16 (22%)	0
85	AT	74/76 (97%)	36 (48%)	3 (4%)
All	All	5912/5981 (98%)	1400 (23%)	29 (0%)

All (1400) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	L5	2	G
20	L5	25	A
20	L5	26	C
20	L5	30	C
20	L5	39	A
20	L5	42	A
20	L5	48	G
20	L5	56	A
20	L5	59	A
20	L5	64	A
20	L5	65	A
20	L5	66	A
20	L5	69	A
20	L5	73	A
20	L5	74	G
20	L5	91	G
20	L5	98	A
20	L5	104	G
20	L5	108	A
20	L5	109	G
20	L5	110	C
20	L5	119	G
20	L5	120	A
20	L5	132	G
20	L5	133	C
20	L5	134	G
20	L5	135	G
20	L5	144	G
20	L5	145	G
20	L5	152	U
20	L5	159	C
20	L5	165	A
20	L5	170	C
20	L5	182	G
20	L5	183	C

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Mol	Chain	Res	Type
20	L5	184	U
20	L5	185	C
20	L5	188	G
20	L5	200	U
20	L5	209	U
20	L5	216	C
20	L5	218	A
20	L5	234	G
20	L5	250	C
20	L5	255	C
20	L5	256	G
20	L5	260	C
20	L5	261	G
20	L5	264	C
20	L5	265	C
20	L5	266	C
20	L5	267	G
20	L5	269	G
20	L5	275	C
20	L5	280	G
20	L5	297	U
20	L5	306	A
20	L5	315	G
20	L5	316	U
20	L5	340	C
20	L5	350	C
20	L5	373	G
20	L5	385	A
20	L5	387	G
20	L5	388	A
20	L5	396	A
20	L5	407	A
20	L5	409	G
20	L5	410	A
20	L5	412	G
20	L5	413	G
20	L5	414	C
20	L5	415	G
20	L5	431	G
20	L5	432	U
20	L5	449	C
20	L5	450	G

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Mol	Chain	Res	Type
20	L5	452	A
20	L5	453	G
20	L5	454	U
20	L5	456	C
20	L5	457	G
20	L5	467	U
20	L5	468	U
20	L5	485	C
20	L5	486	C
20	L5	489	C
20	L5	493	G
20	L5	494	U
20	L5	497	G
20	L5	498	C
20	L5	499	G
20	L5	500	G
20	L5	501	C
20	L5	502	C
20	L5	503	C
20	L5	504	G
20	L5	505	G
20	L5	509	A
20	L5	510	U
20	L5	512	U
20	L5	513	U
20	L5	514	U
20	L5	517	C
20	L5	518	G
20	L5	519	C
20	L5	643	C
20	L5	646	G
20	L5	654	C
20	L5	655	C
20	L5	656	C
20	L5	657	C
20	L5	659	G
20	L5	663	G
20	L5	666	G
20	L5	667	A
20	L5	668	C
20	L5	669	C
20	L5	673	C

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Mol	Chain	Res	Type
20	L5	685	C
20	L5	686	A
20	L5	687	U
20	L5	703	G
20	L5	704	C
20	L5	706	C
20	L5	708	G
20	L5	730	G
20	L5	731	G
20	L5	738	C
20	L5	739	G
20	L5	742	G
20	L5	753	C
20	L5	754	U
20	L5	758	G
20	L5	759	G
20	L5	760	G
20	L5	904	C
20	L5	905	C
20	L5	910	G
20	L5	911	U
20	L5	912	G
20	L5	913	U
20	L5	914	U
20	L5	915	A
20	L5	916	C
20	L5	917	A
20	L5	918	G
20	L5	923	C
20	L5	924	C
20	L5	926	G
20	L5	932	A
20	L5	933	G
20	L5	935	A
20	L5	936	C
20	L5	943	A
20	L5	944	A
20	L5	945	U
20	L5	958	G
20	L5	959	G
20	L5	960	A
20	L5	961	G

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Mol	Chain	Res	Type
20	L5	962	C
20	L5	965	G
20	L5	967	C
20	L5	969	C
20	L5	970	G
20	L5	977	C
20	L5	982	U
20	L5	985	C
20	L5	989	U
20	L5	990	C
20	L5	992	C
20	L5	993	G
20	L5	995	C
20	L5	1048	G
20	L5	1049	C
20	L5	1050	C
20	L5	1051	G
20	L5	1066	G
20	L5	1070	G
20	L5	1071	C
20	L5	1072	C
20	L5	1075	G
20	L5	1082	C
20	L5	1083	U
20	L5	1095	A
20	L5	1168	G
20	L5	1170	G
20	L5	1171	G
20	L5	1172	C
20	L5	1173	G
20	L5	1174	G
20	L5	1179	U
20	L5	1180	C
20	L5	1182	C
20	L5	1183	C
20	L5	1202	C
20	L5	1203	G
20	L5	1205	G
20	L5	1210	C
20	L5	1211	G
20	L5	1214	C
20	L5	1215	C

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Mol	Chain	Res	Type
20	L5	1218	G
20	L5	1219	G
20	L5	1222	A
20	L5	1241	C
20	L5	1242	G
20	L5	1245	C
20	L5	1246	G
20	L5	1253	G
20	L5	1254	A
20	L5	1257	A
20	L5	1258	G
20	L5	1266	G
20	L5	1267	C
20	L5	1270	A
20	L5	1271	G
20	L5	1272	C
20	L5	1273	G
20	L5	1275	G
20	L5	1277	G
20	L5	1280	C
20	L5	1284	G
20	L5	1285	U
20	L5	1287	G
20	L5	1293	G
20	L5	1294	A
20	L5	1295	C
20	L5	1296	G
20	L5	1301	C
20	L5	1302	U
20	L5	1312	A
20	L5	1313	C
20	L5	1326	A
20	L5	1337	A
20	L5	1354	A
20	L5	1358	G
20	L5	1359	G
20	L5	1365	C
20	L5	1367	C
20	L5	1387	A
20	L5	1392	A
20	L5	1394	G
20	L5	1397	A

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Mol	Chain	Res	Type
20	L5	1398	A
20	L5	1405	C
20	L5	1407	C
20	L5	1408	G
20	L5	1409	C
20	L5	1410	U
20	L5	1411	C
20	L5	1414	C
20	L5	1415	G
20	L5	1416	G
20	L5	1417	C
20	L5	1420	A
20	L5	1435	G
20	L5	1437	C
20	L5	1439	C
20	L5	1441	C
20	L5	1443	A
20	L5	1444	G
20	L5	1446	C
20	L5	1447	C
20	L5	1482	G
20	L5	1483	C
20	L5	1494	U
20	L5	1497	A
20	L5	1498	G
20	L5	1502	G
20	L5	1515	A
20	L5	1517	G
20	L5	1518	A
20	L5	1525	A
20	L5	1534	A
20	L5	1547	A
20	L5	1562	G
20	L5	1564	A
20	L5	1566	C
20	L5	1578	U
20	L5	1582	U
20	L5	1591	U
20	L5	1596	U
20	L5	1624	G
20	L5	1631	A
20	L5	1633	G

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Mol	Chain	Res	Type
20	L5	1634	A
20	L5	1638	A
20	L5	1640	C
20	L5	1641	G
20	L5	1642	A
20	L5	1654	G
20	L5	1661	C
20	L5	1663	C
20	L5	1676	C
20	L5	1677	U
20	L5	1678	C
20	L5	1681	G
20	L5	1685	G
20	L5	1691	G
20	L5	1698	C
20	L5	1699	A
20	L5	1700	G
20	L5	1703	C
20	L5	1704	C
20	L5	1705	G
20	L5	1707	C
20	L5	1708	G
20	L5	1718	C
20	L5	1726	U
20	L5	1730	U
20	L5	1741	G
20	L5	1742	A
20	L5	1750	G
20	L5	1754	U
20	L5	1757	U
20	L5	1758	G
20	L5	1760	G
20	L5	1761	G
20	L5	1762	C
20	L5	1763	C
20	L5	1764	G
20	L5	1765	A
20	L5	1766	A
20	L5	1767	A
20	L5	1768	C
20	L5	1769	G
20	L5	1770	A

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Mol	Chain	Res	Type
20	L5	1775	A
20	L5	1787	A
20	L5	1803	G
20	L5	1804	A
20	L5	1806	G
20	L5	1810	G
20	L5	1820	C
20	L5	1821	G
20	L5	1822	U
20	L5	1834	U
20	L5	1836	G
20	L5	1837	A
20	L5	1842	G
20	L5	1843	A
20	L5	1855	G
20	L5	1869	G
20	L5	1882	U
20	L5	1888	A
20	L5	1892	A
20	L5	1893	C
20	L5	1897	A
20	L5	1917	A
20	L5	1918	U
20	L5	1919	G
20	L5	1920	C
20	L5	1921	C
20	L5	1922	G
20	L5	1925	G
20	L5	1931	C
20	L5	1932	A
20	L5	1936	C
20	L5	1940	G
20	L5	1948	G
20	L5	1949	U
20	L5	1961	G
20	L5	1962	A
20	L5	1974	U
20	L5	1975	G
20	L5	1978	C
20	L5	1980	U
20	L5	1981	G
20	L5	1982	G

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Mol	Chain	Res	Type
20	L5	1983	A
20	L5	1984	A
20	L5	1985	G
20	L5	1986	U
20	L5	1991	A
20	L5	1992	U
20	L5	1997	U
20	L5	1998	A
20	L5	1999	A
20	L5	2001	G
20	L5	2002	A
20	L5	2003	G
20	L5	2004	U
20	L5	2011	C
20	L5	2017	A
20	L5	2018	C
20	L5	2024	G
20	L5	2026	A
20	L5	2033	A
20	L5	2034	G
20	L5	2046	G
20	L5	2048	U
20	L5	2055	G
20	L5	2056	G
20	L5	2069	A
20	L5	2084	C
20	L5	2085	G
20	L5	2092	G
20	L5	2093	A
20	L5	2095	A
20	L5	2096	G
20	L5	2097	U
20	L5	2098	G
20	L5	2101	C
20	L5	2103	G
20	L5	2105	A
20	L5	2107	C
20	L5	2108	G
20	L5	2110	C
20	L5	2112	G
20	L5	2250	C
20	L5	2252	G

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Mol	Chain	Res	Type
20	L5	2253	A
20	L5	2255	C
20	L5	2256	C
20	L5	2257	C
20	L5	2258	C
20	L5	2260	C
20	L5	2261	G
20	L5	2289	C
20	L5	2300	A
20	L5	2301	G
20	L5	2306	G
20	L5	2313	A
20	L5	2331	G
20	L5	2333	G
20	L5	2345	G
20	L5	2348	G
20	L5	2351	C
20	L5	2360	A
20	L5	2381	A
20	L5	2383	C
20	L5	2389	A
20	L5	2395	A
20	L5	2397	G
20	L5	2402	G
20	L5	2417	A
20	L5	2421	G
20	L5	2425	U
20	L5	2441	C
20	L5	2450	G
20	L5	2453	A
20	L5	2464	C
20	L5	2465	C
20	L5	2474	G
20	L5	2475	G
20	L5	2478	C
20	L5	2479	G
20	L5	2484	A
20	L5	2485	U
20	L5	2487	G
20	L5	2488	C
20	L5	2489	C
20	L5	2490	U

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Mol	Chain	Res	Type
20	L5	2491	C
20	L5	2494	U
20	L5	2502	G
20	L5	2503	G
20	L5	2504	C
20	L5	2505	C
20	L5	2506	G
20	L5	2513	A
20	L5	2519	U
20	L5	2520	C
20	L5	2529	A
20	L5	2536	A
20	L5	2537	A
20	L5	2544	G
20	L5	2546	G
20	L5	2547	G
20	L5	2554	U
20	L5	2560	C
20	L5	2565	A
20	L5	2573	A
20	L5	2583	C
20	L5	2586	G
20	L5	2587	A
20	L5	2589	C
20	L5	2618	G
20	L5	2627	C
20	L5	2652	G
20	L5	2653	C
20	L5	2662	G
20	L5	2669	C
20	L5	2676	A
20	L5	2687	U
20	L5	2694	G
20	L5	2695	A
20	L5	2696	A
20	L5	2703	G
20	L5	2707	U
20	L5	2708	U
20	L5	2710	C
20	L5	2711	G
20	L5	2712	G
20	L5	2721	G

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Mol	Chain	Res	Type
20	L5	2724	G
20	L5	2726	G
20	L5	2729	C
20	L5	2739	C
20	L5	2742	G
20	L5	2743	A
20	L5	2746	A
20	L5	2761	U
20	L5	2763	U
20	L5	2764	A
20	L5	2769	U
20	L5	2770	C
20	L5	2787	A
20	L5	2788	U
20	L5	2790	U
20	L5	2806	A
20	L5	2812	A
20	L5	2814	C
20	L5	2826	U
20	L5	2827	G
20	L5	2829	U
20	L5	2838	G
20	L5	2847	G
20	L5	2848	G
20	L5	2855	G
20	L5	2867	C
20	L5	2877	G
20	L5	2892	C
20	L5	2895	A
20	L5	2899	C
20	L5	2900	U
20	L5	2902	G
20	L5	2903	G
20	L5	2904	U
20	L5	2905	C
20	L5	2906	G
20	L5	2908	U
20	L5	3588	C
20	L5	3590	G
20	L5	3591	C
20	L5	3594	C
20	L5	3595	U

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Mol	Chain	Res	Type
20	L5	3596	A
20	L5	3597	G
20	L5	3605	C
20	L5	3615	G
20	L5	3616	U
20	L5	3618	C
20	L5	3626	G
20	L5	3630	A
20	L5	3635	A
20	L5	3644	U
20	L5	3646	A
20	L5	3648	A
20	L5	3662	A
20	L5	3664	G
20	L5	3670	C
20	L5	3673	C
20	L5	3674	G
20	L5	3685	C
20	L5	3711	A
20	L5	3713	U
20	L5	3714	G
20	L5	3726	A
20	L5	3727	A
20	L5	3740	G
20	L5	3748	A
20	L5	3750	G
20	L5	3753	G
20	L5	3756	A
20	L5	3757	G
20	L5	3759	A
20	L5	3760	A
20	L5	3761	C
20	L5	3766	A
20	L5	3773	U
20	L5	3774	A
20	L5	3776	G
20	L5	3777	G
20	L5	3784	A
20	L5	3786	U
20	L5	3788	C
20	L5	3802	U
20	L5	3811	G

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Mol	Chain	Res	Type
20	L5	3812	C
20	L5	3814	U
20	L5	3817	A
20	L5	3818	U
20	L5	3819	G
20	L5	3823	G
20	L5	3838	U
20	L5	3839	G
20	L5	3840	U
20	L5	3841	C
20	L5	3867	A
20	L5	3877	A
20	L5	3878	C
20	L5	3879	G
20	L5	3880	G
20	L5	3885	G
20	L5	3887	C
20	L5	3890	A
20	L5	3897	G
20	L5	3898	G
20	L5	3901	A
20	L5	3906	A
20	L5	3907	G
20	L5	3908	A
20	L5	3915	U
20	L5	3916	G
20	L5	3923	A
20	L5	3930	U
20	L5	3938	G
20	L5	3939	G
20	L5	3942	A
20	L5	3943	A
20	L5	3944	G
20	L5	3946	G
20	L5	3947	A
20	L5	3949	A
20	L5	3951	G
20	L5	3953	G
20	L5	3955	G
20	L5	3956	G
20	L5	3957	U
20	L5	3959	U

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Mol	Chain	Res	Type
20	L5	3960	A
20	L5	3962	A
20	L5	3963	A
20	L5	3964	U
20	L5	3965	A
20	L5	3966	A
20	L5	3968	U
20	L5	3969	G
20	L5	3970	G
20	L5	3973	G
20	L5	3974	G
20	L5	3975	C
20	L5	3976	C
20	L5	3977	C
20	L5	4034	G
20	L5	4037	C
20	L5	4038	C
20	L5	4039	G
20	L5	4041	C
20	L5	4042	G
20	L5	4043	G
20	L5	4046	A
20	L5	4047	A
20	L5	4048	A
20	L5	4049	U
20	L5	4051	C
20	L5	4052	C
20	L5	4053	A
20	L5	4054	C
20	L5	4055	U
20	L5	4057	C
20	L5	4058	U
20	L5	4059	C
20	L5	4060	U
20	L5	4061	G
20	L5	4062	A
20	L5	4063	U
20	L5	4065	G
20	L5	4067	U
20	L5	4068	U
20	L5	4069	U
20	L5	4076	G

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Mol	Chain	Res	Type
20	L5	4084	G
20	L5	4092	G
20	L5	4093	G
20	L5	4097	G
20	L5	4099	G
20	L5	4102	C
20	L5	4104	G
20	L5	4108	G
20	L5	4111	U
20	L5	4114	C
20	L5	4115	G
20	L5	4116	C
20	L5	4117	U
20	L5	4119	C
20	L5	4121	G
20	L5	4122	G
20	L5	4127	A
20	L5	4133	C
20	L5	4134	C
20	L5	4140	C
20	L5	4141	G
20	L5	4142	C
20	L5	4143	G
20	L5	4144	C
20	L5	4146	G
20	L5	4149	C
20	L5	4150	G
20	L5	4160	C
20	L5	4162	C
20	L5	4163	U
20	L5	4170	A
20	L5	4183	G
20	L5	4184	G
20	L5	4191	G
20	L5	4196	G
20	L5	4197	G
20	L5	4203	A
20	L5	4212	A
20	L5	4222	G
20	L5	4225	G
20	L5	4228	G
20	L5	4229	U

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Mol	Chain	Res	Type
20	L5	4232	U
20	L5	4233	A
20	L5	4237	C
20	L5	4249	G
20	L5	4251	A
20	L5	4254	G
20	L5	4255	A
20	L5	4257	A
20	L5	4258	C
20	L5	4265	U
20	L5	4268	A
20	L5	4273	A
20	L5	4281	A
20	L5	4291	G
20	L5	4297	G
20	L5	4304	A
20	L5	4305	G
20	L5	4306	U
20	L5	4314	C
20	L5	4319	C
20	L5	4330	G
20	L5	4332	C
20	L5	4339	A
20	L5	4349	C
20	L5	4354	U
20	L5	4364	G
20	L5	4373	G
20	L5	4376	A
20	L5	4377	G
20	L5	4378	A
20	L5	4380	A
20	L5	4387	C
20	L5	4391	G
20	L5	4394	A
20	L5	4422	A
20	L5	4438	U
20	L5	4448	G
20	L5	4449	A
20	L5	4452	U
20	L5	4453	C
20	L5	4464	A
20	L5	4466	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	L5	4475	G
20	L5	4488	A
20	L5	4500	U
20	L5	4512	U
20	L5	4513	A
20	L5	4515	G
20	L5	4518	A
20	L5	4519	C
20	L5	4524	G
20	L5	4525	C
20	L5	4545	G
20	L5	4548	A
20	L5	4549	G
20	L5	4560	C
20	L5	4567	G
20	L5	4573	G
20	L5	4575	G
20	L5	4584	A
20	L5	4589	A
20	L5	4590	A
20	L5	4600	G
20	L5	4601	U
20	L5	4617	G
20	L5	4636	U
20	L5	4637	G
20	L5	4648	A
20	L5	4652	G
20	L5	4656	A
20	L5	4657	U
20	L5	4659	G
20	L5	4670	C
20	L5	4672	A
20	L5	4679	G
20	L5	4694	G
20	L5	4695	C
20	L5	4700	A
20	L5	4708	A
20	L5	4709	U
20	L5	4719	G
20	L5	4734	A
20	L5	4740	G
20	L5	4741	C

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Mol	Chain	Res	Type
20	L5	4742	G
20	L5	4745	G
20	L5	4750	G
20	L5	4754	G
20	L5	4757	C
20	L5	4759	C
20	L5	4761	G
20	L5	4765	G
20	L5	4771	C
20	L5	4772	C
20	L5	4773	C
20	L5	4775	C
20	L5	4859	C
20	L5	4862	G
20	L5	4870	G
20	L5	4871	C
20	L5	4875	G
20	L5	4880	C
20	L5	4881	U
20	L5	4882	U
20	L5	4883	C
20	L5	4889	G
20	L5	4895	C
20	L5	4896	G
20	L5	4897	G
20	L5	4900	C
20	L5	4901	G
20	L5	4902	C
20	L5	4910	G
20	L5	4912	G
20	L5	4914	C
20	L5	4918	C
20	L5	4922	C
20	L5	4923	C
20	L5	4924	C
20	L5	4925	U
20	L5	4926	C
20	L5	4927	G
20	L5	4928	C
20	L5	4934	A
20	L5	4935	C
20	L5	4937	C

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Mol	Chain	Res	Type
20	L5	4940	C
20	L5	4941	G
20	L5	4943	A
20	L5	4944	C
20	L5	4951	G
20	L5	4955	A
20	L5	4960	G
20	L5	4973	U
20	L5	4976	U
20	L5	4985	U
20	L5	4988	U
20	L5	4989	U
20	L5	4990	C
20	L5	4991	U
20	L5	5009	G
20	L5	5013	C
20	L5	5014	A
20	L5	5017	G
20	L5	5022	U
20	L5	5024	C
20	L5	5027	C
20	L5	5028	G
20	L5	5030	U
20	L5	5034	A
20	L5	5041	G
20	L5	5050	C
20	L5	5054	C
20	L5	5055	G
20	L5	5058	A
20	L5	5061	A
20	L5	5067	U
20	L5	5069	U
21	L7	4	U
21	L7	7	G
21	L7	22	A
21	L7	24	C
21	L7	38	U
21	L7	53	U
21	L7	54	A
21	L7	63	C
21	L7	64	G
21	L7	100	A

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Mol	Chain	Res	Type
21	L7	110	G
22	L8	25	G
22	L8	34	U
22	L8	35	C
22	L8	48	A
22	L8	52	A
22	L8	59	A
22	L8	62	A
22	L8	63	U
22	L8	68	G
22	L8	80	A
22	L8	81	C
22	L8	82	A
22	L8	84	A
22	L8	85	U
22	L8	86	U
22	L8	87	G
22	L8	94	G
22	L8	103	A
22	L8	105	C
22	L8	110	U
22	L8	111	U
22	L8	112	G
22	L8	114	G
22	L8	123	U
22	L8	124	U
22	L8	125	C
22	L8	126	C
22	L8	127	U
22	L8	128	C
22	L8	151	G
78	S2	13	C
78	S2	25	A
78	S2	33	G
78	S2	41	G
78	S2	44	U
78	S2	45	A
78	S2	46	A
78	S2	56	G
78	S2	58	C
78	S2	59	U
78	S2	64	A

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Mol	Chain	Res	Type
78	S2	67	C
78	S2	68	A
78	S2	72	C
78	S2	73	C
78	S2	74	G
78	S2	76	U
78	S2	92	A
78	S2	103	A
78	S2	113	G
78	S2	115	U
78	S2	116	U
78	S2	126	G
78	S2	130	G
78	S2	139	C
78	S2	143	U
78	S2	149	A
78	S2	158	A
78	S2	160	U
78	S2	161	U
78	S2	162	C
78	S2	170	A
78	S2	171	A
78	S2	179	C
78	S2	182	C
78	S2	190	G
78	S2	196	C
78	S2	197	U
78	S2	198	U
78	S2	200	G
78	S2	202	G
78	S2	203	G
78	S2	204	G
78	S2	206	G
78	S2	207	G
78	S2	208	G
78	S2	213	G
78	S2	214	U
78	S2	291	G
78	S2	292	A
78	S2	295	C
78	S2	301	A
78	S2	305	U

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Mol	Chain	Res	Type
78	S2	306	C
78	S2	307	G
78	S2	308	G
78	S2	309	G
78	S2	310	C
78	S2	311	C
78	S2	312	G
78	S2	316	G
78	S2	318	A
78	S2	319	C
78	S2	322	C
78	S2	323	C
78	S2	324	C
78	S2	325	C
78	S2	326	C
78	S2	327	G
78	S2	328	U
78	S2	329	G
78	S2	332	G
78	S2	335	G
78	S2	338	G
78	S2	339	A
78	S2	340	C
78	S2	347	G
78	S2	360	A
78	S2	362	C
78	S2	364	A
78	S2	368	U
78	S2	369	C
78	S2	370	G
78	S2	372	U
78	S2	374	G
78	S2	385	G
78	S2	386	C
78	S2	407	G
78	S2	408	A
78	S2	409	C
78	S2	421	G
78	S2	438	G
78	S2	448	A
78	S2	449	A
78	S2	450	C

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Mol	Chain	Res	Type
78	S2	452	G
78	S2	464	A
78	S2	465	A
78	S2	471	G
78	S2	472	C
78	S2	473	A
78	S2	474	G
78	S2	476	A
78	S2	482	G
78	S2	483	C
78	S2	487	U
78	S2	488	U
78	S2	492	C
78	S2	493	A
78	S2	502	C
78	S2	530	U
78	S2	531	A
78	S2	532	C
78	S2	534	G
78	S2	536	A
78	S2	537	C
78	S2	540	U
78	S2	542	U
78	S2	546	G
78	S2	547	G
78	S2	557	U
78	S2	558	G
78	S2	560	A
78	S2	563	G
78	S2	564	A
78	S2	576	A
78	S2	583	A
78	S2	587	A
78	S2	589	G
78	S2	590	A
78	S2	591	U
78	S2	593	C
78	S2	606	G
78	S2	607	U
78	S2	614	C
78	S2	617	G
78	S2	623	G

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Mol	Chain	Res	Type
78	S2	628	A
78	S2	630	U
78	S2	631	U
78	S2	643	A
78	S2	644	G
78	S2	655	A
78	S2	660	C
78	S2	664	A
78	S2	668	A
78	S2	669	A
78	S2	671	A
78	S2	672	A
78	S2	673	G
78	S2	688	U
78	S2	689	U
78	S2	692	G
78	S2	693	A
78	S2	695	C
78	S2	696	G
78	S2	697	G
78	S2	698	G
78	S2	732	U
78	S2	733	C
78	S2	734	C
78	S2	737	G
78	S2	738	C
78	S2	749	U
78	S2	750	C
78	S2	751	G
78	S2	752	G
78	S2	753	C
78	S2	788	G
78	S2	789	G
78	S2	791	C
78	S2	792	C
78	S2	794	A
78	S2	798	G
78	S2	799	U
78	S2	801	U
78	S2	821	G
78	S2	822	U
78	S2	823	U

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Mol	Chain	Res	Type
78	S2	824	C
78	S2	830	A
78	S2	833	C
78	S2	834	C
78	S2	835	C
78	S2	836	G
78	S2	837	A
78	S2	838	G
78	S2	839	C
78	S2	842	C
78	S2	844	U
78	S2	847	A
78	S2	869	A
78	S2	870	A
78	S2	872	A
78	S2	873	G
78	S2	874	G
78	S2	882	U
78	S2	888	U
78	S2	889	U
78	S2	891	G
78	S2	893	U
78	S2	896	U
78	S2	897	U
78	S2	898	U
78	S2	899	U
78	S2	900	C
78	S2	901	G
78	S2	903	A
78	S2	907	G
78	S2	908	A
78	S2	913	A
78	S2	919	A
78	S2	920	A
78	S2	930	C
78	S2	933	G
78	S2	934	G
78	S2	954	U
78	S2	963	A
78	S2	990	A
78	S2	992	A
78	S2	999	G

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Mol	Chain	Res	Type
78	S2	1001	A
78	S2	1002	U
78	S2	1008	A
78	S2	1017	U
78	S2	1023	A
78	S2	1027	A
78	S2	1033	G
78	S2	1034	A
78	S2	1060	A
78	S2	1061	U
78	S2	1062	A
78	S2	1067	C
78	S2	1083	A
78	S2	1085	C
78	S2	1088	U
78	S2	1108	G
78	S2	1109	C
78	S2	1113	A
78	S2	1114	U
78	S2	1115	U
78	S2	1116	C
78	S2	1121	G
78	S2	1133	A
78	S2	1138	C
78	S2	1148	A
78	S2	1153	C
78	S2	1154	U
78	S2	1161	U
78	S2	1195	A
78	S2	1207	G
78	S2	1208	A
78	S2	1215	C
78	S2	1216	C
78	S2	1217	A
78	S2	1220	A
78	S2	1224	G
78	S2	1227	G
78	S2	1237	C
78	S2	1240	A
78	S2	1242	U
78	S2	1243	U
78	S2	1251	A

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Mol	Chain	Res	Type
78	S2	1253	A
78	S2	1256	G
78	S2	1257	G
78	S2	1259	A
78	S2	1264	C
78	S2	1274	G
78	S2	1275	G
78	S2	1282	A
78	S2	1283	C
78	S2	1284	A
78	S2	1286	G
78	S2	1287	A
78	S2	1294	G
78	S2	1295	A
78	S2	1301	A
78	S2	1302	G
78	S2	1303	C
78	S2	1306	U
78	S2	1308	U
78	S2	1320	G
78	S2	1322	G
78	S2	1342	U
78	S2	1348	G
78	S2	1354	G
78	S2	1355	C
78	S2	1356	G
78	S2	1357	A
78	S2	1371	U
78	S2	1372	U
78	S2	1376	A
78	S2	1378	A
78	S2	1396	A
78	S2	1401	A
78	S2	1402	A
78	S2	1406	G
78	S2	1414	A
78	S2	1415	C
78	S2	1419	C
78	S2	1420	G
78	S2	1421	A
78	S2	1422	G
78	S2	1423	C

*Continued on next page...*

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Mol	Chain	Res	Type
78	S2	1424	G
78	S2	1433	C
78	S2	1434	C
78	S2	1435	C
78	S2	1436	C
78	S2	1437	C
78	S2	1438	A
78	S2	1442	U
78	S2	1449	G
78	S2	1454	A
78	S2	1455	A
78	S2	1463	U
78	S2	1464	C
78	S2	1489	A
78	S2	1490	G
78	S2	1494	U
78	S2	1495	G
78	S2	1497	G
78	S2	1498	A
78	S2	1508	A
78	S2	1520	G
78	S2	1521	C
78	S2	1522	A
78	S2	1533	A
78	S2	1535	U
78	S2	1537	A
78	S2	1544	C
78	S2	1552	G
78	S2	1553	C
78	S2	1556	A
78	S2	1570	G
78	S2	1574	C
78	S2	1575	G
78	S2	1579	A
78	S2	1580	A
78	S2	1581	C
78	S2	1582	C
78	S2	1586	U
78	S2	1587	G
78	S2	1588	A
78	S2	1600	G
78	S2	1601	A

*Continued on next page...*

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Mol	Chain	Res	Type
78	S2	1604	G
78	S2	1606	G
78	S2	1621	U
78	S2	1623	A
78	S2	1629	C
78	S2	1633	A
78	S2	1634	A
78	S2	1637	A
78	S2	1638	G
78	S2	1639	G
78	S2	1640	A
78	S2	1646	C
78	S2	1648	G
78	S2	1654	G
78	S2	1663	A
78	S2	1664	A
78	S2	1665	G
78	S2	1683	C
78	S2	1686	G
78	S2	1693	G
78	S2	1696	C
78	S2	1699	A
78	S2	1715	A
78	S2	1721	U
78	S2	1722	G
78	S2	1743	G
78	S2	1744	G
78	S2	1745	A
78	S2	1748	G
78	S2	1752	C
78	S2	1753	C
78	S2	1754	G
78	S2	1755	C
78	S2	1757	G
78	S2	1758	G
78	S2	1759	G
78	S2	1761	U
78	S2	1771	G
78	S2	1772	C
78	S2	1773	C
78	S2	1774	C
78	S2	1777	G

*Continued on next page...*

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Mol	Chain	Res	Type
78	S2	1782	G
78	S2	1783	C
78	S2	1784	G
78	S2	1787	G
78	S2	1809	A
78	S2	1810	U
78	S2	1812	U
78	S2	1813	A
78	S2	1823	A
78	S2	1825	A
78	S2	1826	G
78	S2	1835	A
78	S2	1838	U
78	S2	1849	G
78	S2	1851	A
78	S2	1852	C
78	S2	1861	G
78	S2	1862	G
78	S2	1863	A
78	S2	1864	U
78	S2	1865	C
79	Et	4	C
79	Et	6	G
79	Et	7	A
79	Et	9	A
79	Et	10	G
79	Et	11	C
79	Et	19	G
79	Et	20	U
79	Et	21	A
79	Et	26	A
79	Et	31	A
79	Et	34	U
79	Et	35	U
79	Et	38	A
79	Et	40	C
79	Et	42	G
79	Et	46	G
79	Et	47	U
79	Et	48	C
79	Et	49	C
79	Et	55	U

*Continued on next page...*

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Mol	Chain	Res	Type
79	Et	58	A
79	Et	59	G
79	Et	60	U
79	Et	61	C
79	Et	66	U
79	Et	67	U
79	Et	69	G
79	Et	70	G
79	Et	71	G
79	Et	73	G
79	Et	76	A
80	Pt	9	A
80	Pt	13	U
80	Pt	19	G
80	Pt	20(A)	U
80	Pt	21	A
80	Pt	46	G
80	Pt	47	U
80	Pt	48	C
80	Pt	49	C
80	Pt	58	A
80	Pt	64	G
80	Pt	65	G
80	Pt	67	G
80	Pt	71	A
80	Pt	74	C
80	Pt	76	A
85	AT	3	C
85	AT	4	U
85	AT	8	U
85	AT	9	A
85	AT	12	G
85	AT	14	A
85	AT	16	C
85	AT	19	G
85	AT	20	U
85	AT	21	U
85	AT	22	A
85	AT	26	C
85	AT	27	G
85	AT	31	G
85	AT	32	C

*Continued on next page...*

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Mol	Chain	Res	Type
85	AT	33	C
85	AT	34	U
85	AT	37	C
85	AT	40	G
85	AT	41	C
85	AT	45	A
85	AT	46	G
85	AT	47	G
85	AT	49	C
85	AT	50	C
85	AT	51	U
85	AT	53	G
85	AT	58	G
85	AT	59	A
85	AT	60	A
85	AT	62	C
85	AT	65	G
85	AT	70	A
85	AT	71	A
85	AT	76	C
85	AT	77	A

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	L5	183	C
20	L5	265	C
20	L5	406	C
20	L5	493	G
20	L5	912	G
20	L5	914	U
20	L5	1082	C
20	L5	1633	G
20	L5	1977	C
20	L5	2033	A
20	L5	2416	G
20	L5	2675	G
20	L5	2760	G
20	L5	2786	C
20	L5	3614	G
20	L5	3673	C
20	L5	4600	G

*Continued on next page...*

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Mol	Chain	Res	Type
20	L5	4699	U
20	L5	4913	G
78	S2	291	G
78	S2	420	G
78	S2	563	G
78	S2	688	U
78	S2	1355	C
78	S2	1434	C
78	S2	1781	A
85	AT	7	G
85	AT	11	U
85	AT	52	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
86	SEP	CF	163	86	8,9,10	1.60	1 (12%)	7,12,14	1.15	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
86	SEP	CF	163	86	-	6/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	CF	163	SEP	P-O1P	3.51	1.61	1.50



There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	CF	163	SEP	C-CA-CB-OG
86	CF	163	SEP	CA-CB-OG-P
86	CF	163	SEP	CB-OG-P-O1P
86	CF	163	SEP	CB-OG-P-O2P
86	CF	163	SEP	CB-OG-P-O3P
86	CF	163	SEP	N-CA-CB-OG

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 261 ligands modelled in this entry, 261 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
20	L5	12
78	S2	6
47	Lb	1
27	LE	1
84	LW	1
12	SH	1
80	Pt	1
31	LI	1
81	Lt	1
79	Et	1
85	AT	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:VAL	N	34.17
1	S2	753:C	O3'	785:C	P	27.02
1	LE	76:ALA	C	88:VAL	N	23.33
1	L5	2910:G	O3'	3584:C	P	20.78
1	S2	698:G	O3'	730:C	P	16.93
1	L5	760:G	O3'	903:C	P	16.55
1	L5	4776:G	O3'	4858:C	P	15.80
1	L5	519:C	O3'	642:G	P	15.63
1	LW	63:GLN	C	70:LYS	N	15.15
1	L5	2112:G	O3'	2249:C	P	13.70
1	L5	996:G	O3'	1047:C	P	13.46
1	S2	739:C	O3'	746:C	P	12.97
1	SH	107:LYS	C	111:LYS	N	11.10
1	L5	1222:A	O3'	1234:G	P	10.50
1	L5	1051:G	O3'	1064:G	P	9.89
1	Pt	15:G	O3'	18:G	P	8.58
1	L5	1100:U	O3'	1167:C	P	7.88
1	S2	225:G	O3'	287:U	P	7.65
1	LI	102:MET	C	114:GLY	N	7.61
1	Lt	87:GLU	C	104:ILE	N	6.97
1	L5	1709:C	O3'	1714:C	P	6.12
1	S2	1693:G	O3'	1694:U	P	5.90
1	Et	16:C	O3'	18:U	P	5.55
1	AT	16:C	O3'	18:G	P	5.21
1	L5	3949:A	O3'	3950:U	P	4.31
1	L5	3985:C	O3'	4018:G	P	3.80
1	S2	1210:G	O3'	1211:G	P	3.04

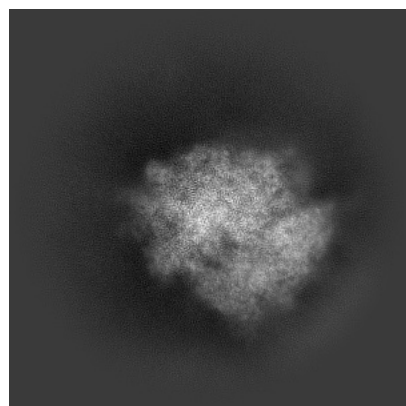
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44021. These allow visual inspection of the internal detail of the map and identification of artifacts.

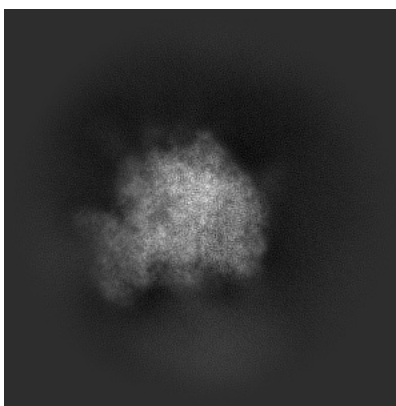
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

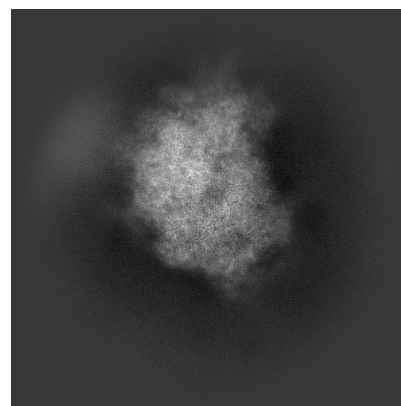
#### 6.1.1 Primary map



X

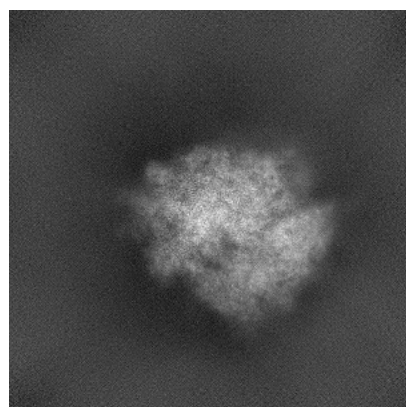


Y

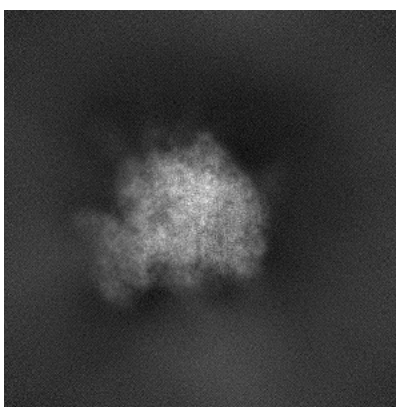


Z

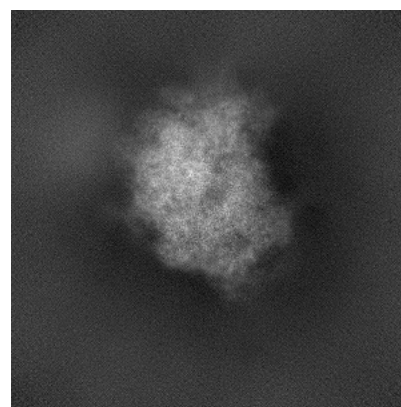
#### 6.1.2 Raw map



X



Y

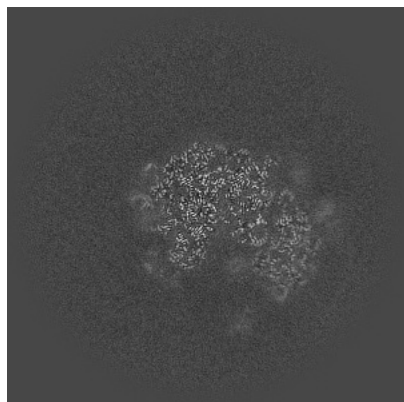


Z

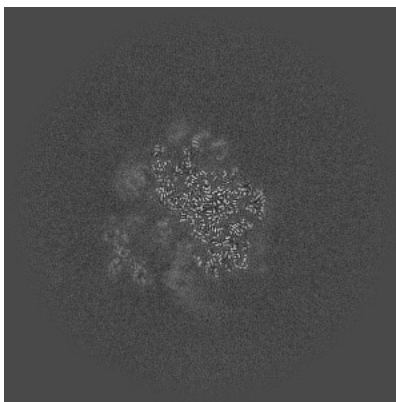
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

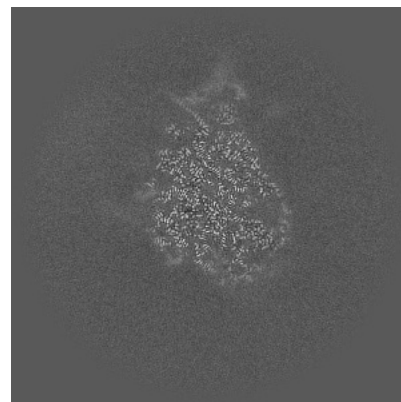
### 6.2.1 Primary map



X Index: 256

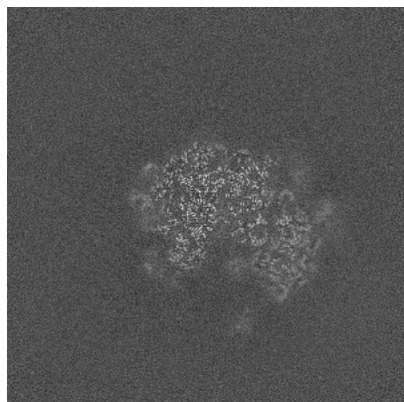


Y Index: 256

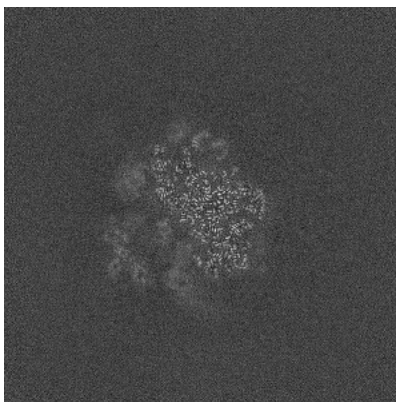


Z Index: 256

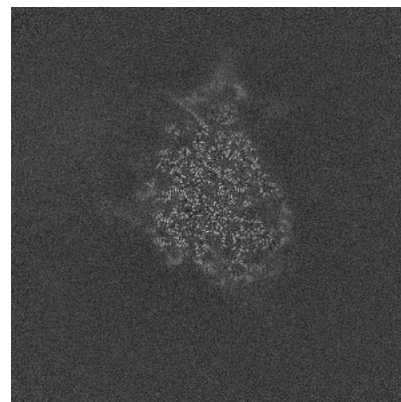
### 6.2.2 Raw map



X Index: 256



Y Index: 256



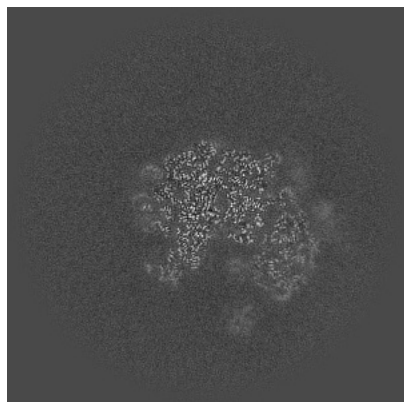
Z Index: 256

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

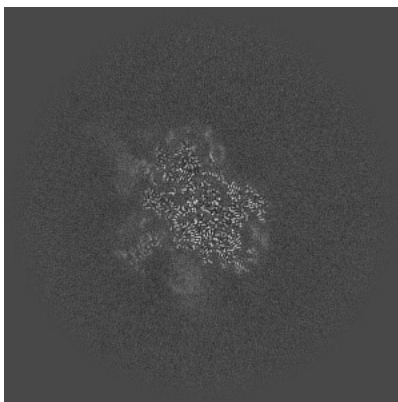


## 6.3 Largest variance slices [i](#)

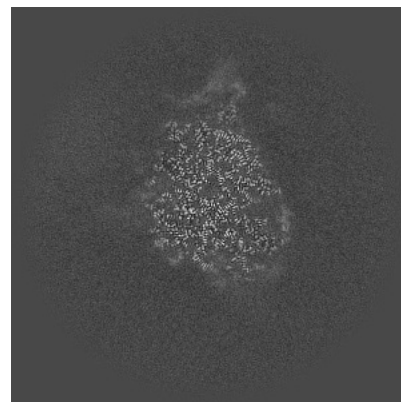
### 6.3.1 Primary map



X Index: 253

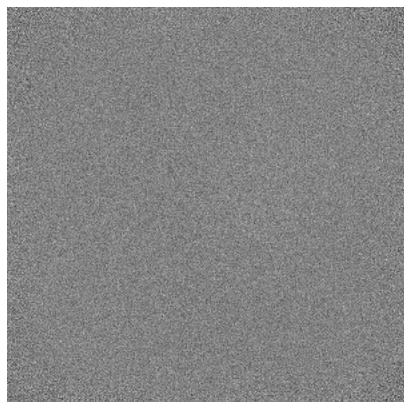


Y Index: 243

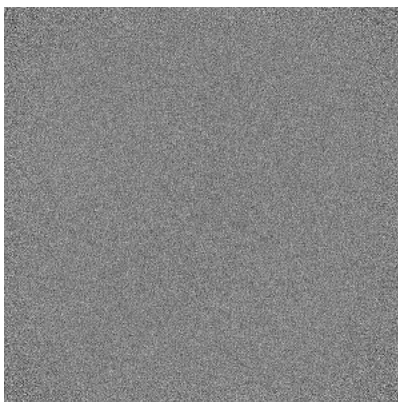


Z Index: 258

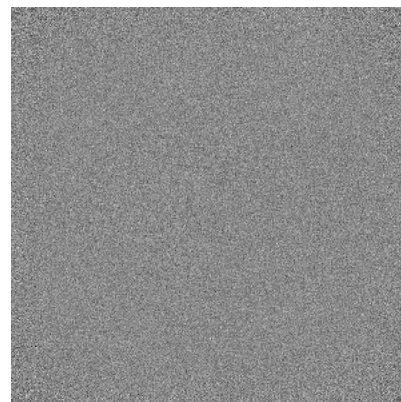
### 6.3.2 Raw map



X Index: 0



Y Index: 0

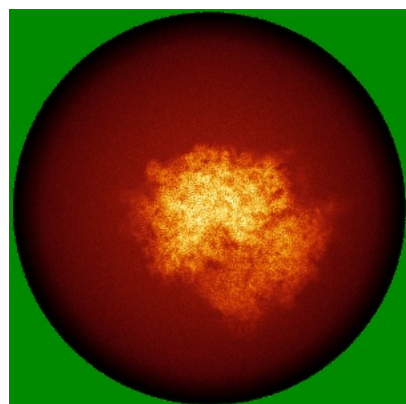


Z Index: 0

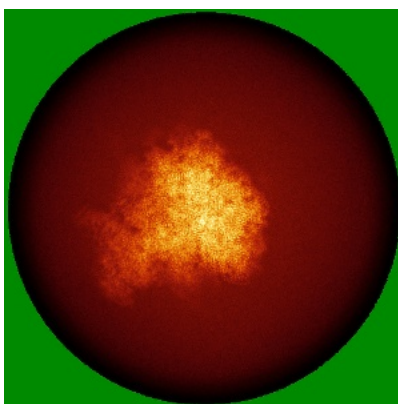
The images above show the largest variance slices of the map in three orthogonal directions.

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

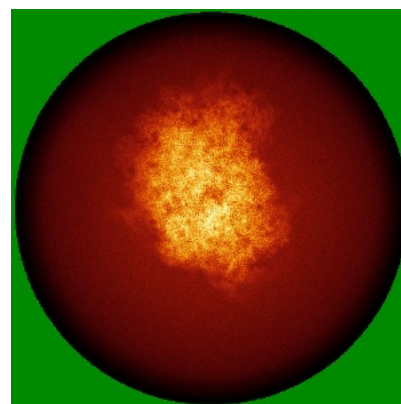
### 6.4.1 Primary map



X

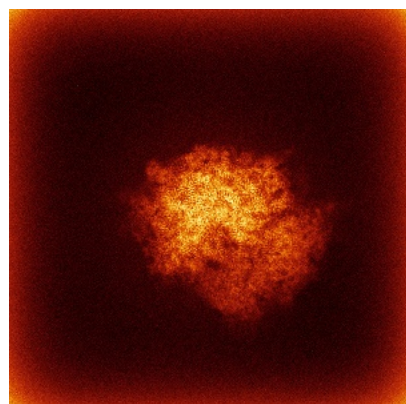


Y

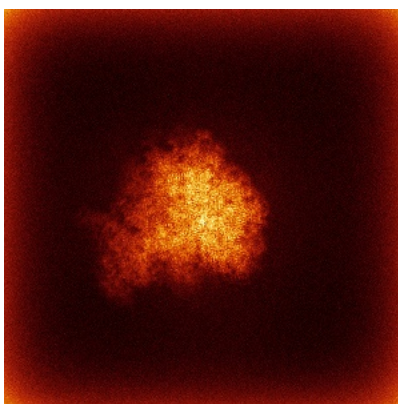


Z

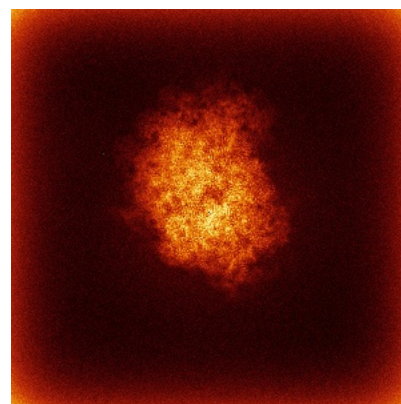
### 6.4.2 Raw map



X



Y

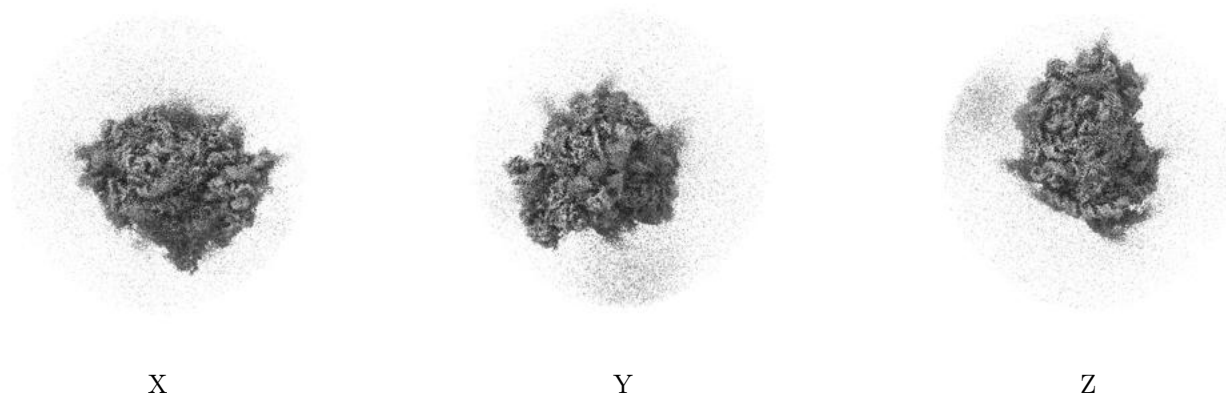


Z

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.

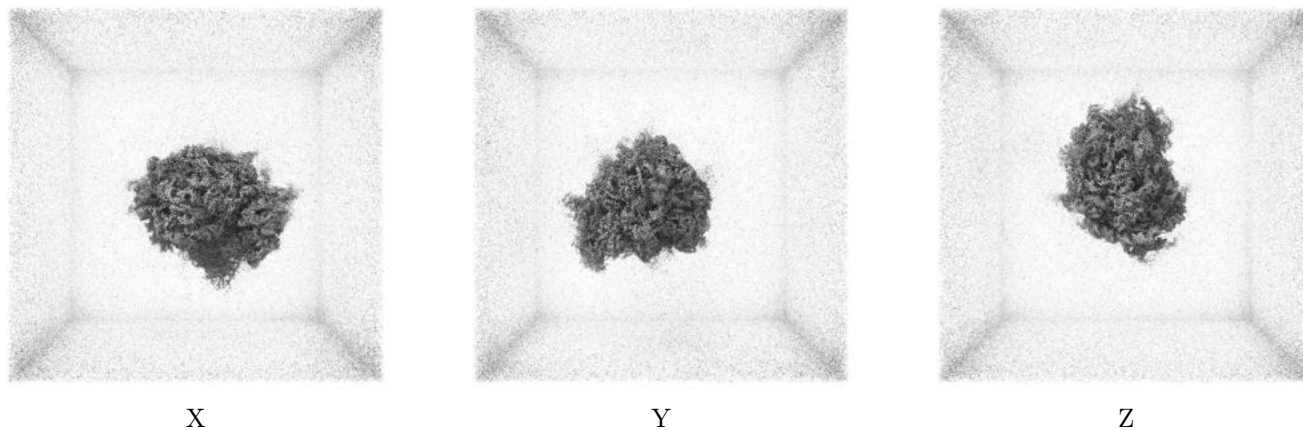
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0491. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

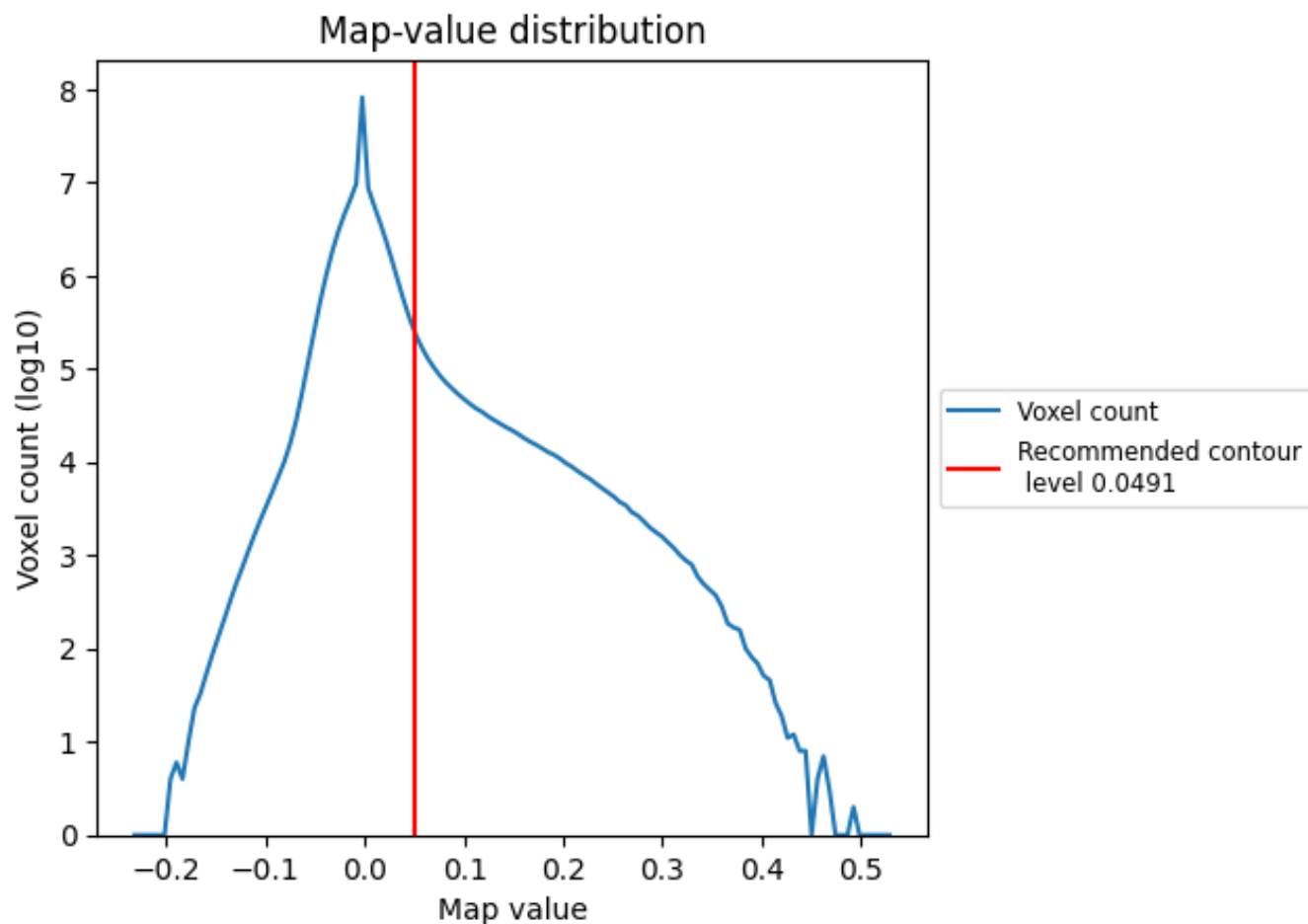
## 6.6 Mask visualisation [i](#)

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.

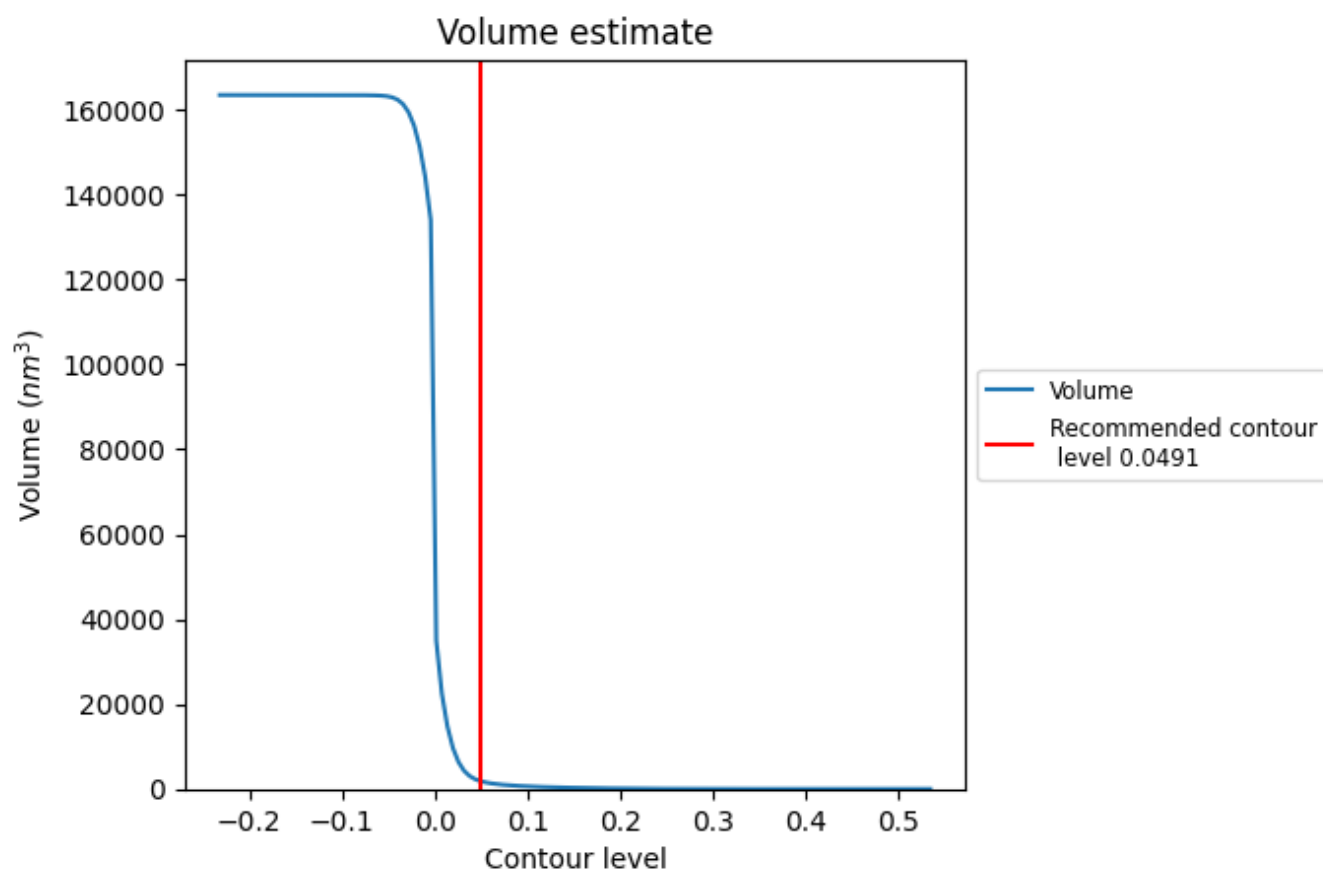
### 7.1 Map-value distribution [i](#)



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.



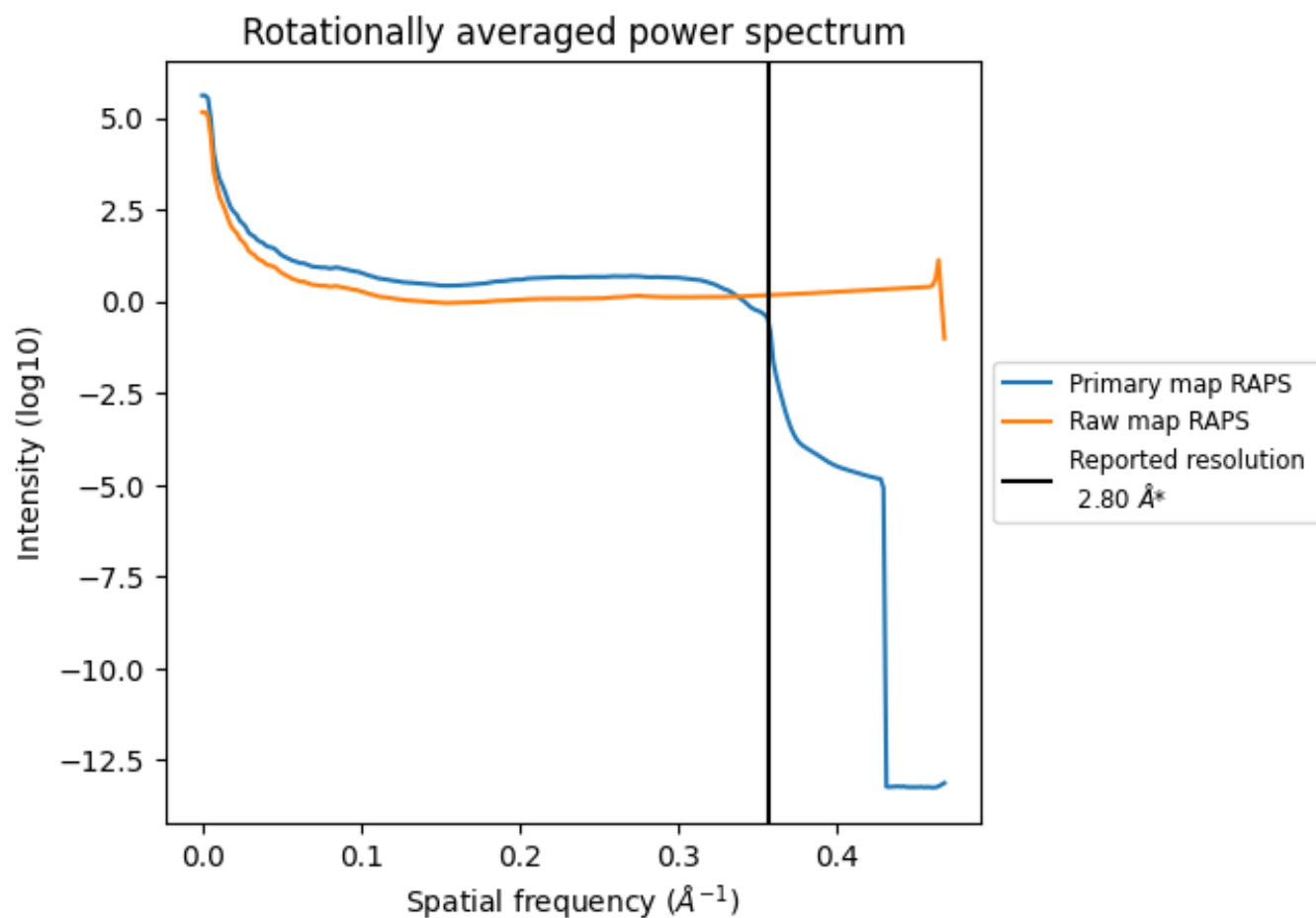
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1858  $\text{nm}^3$ ; this corresponds to an approximate mass of 1678 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 ⓘ

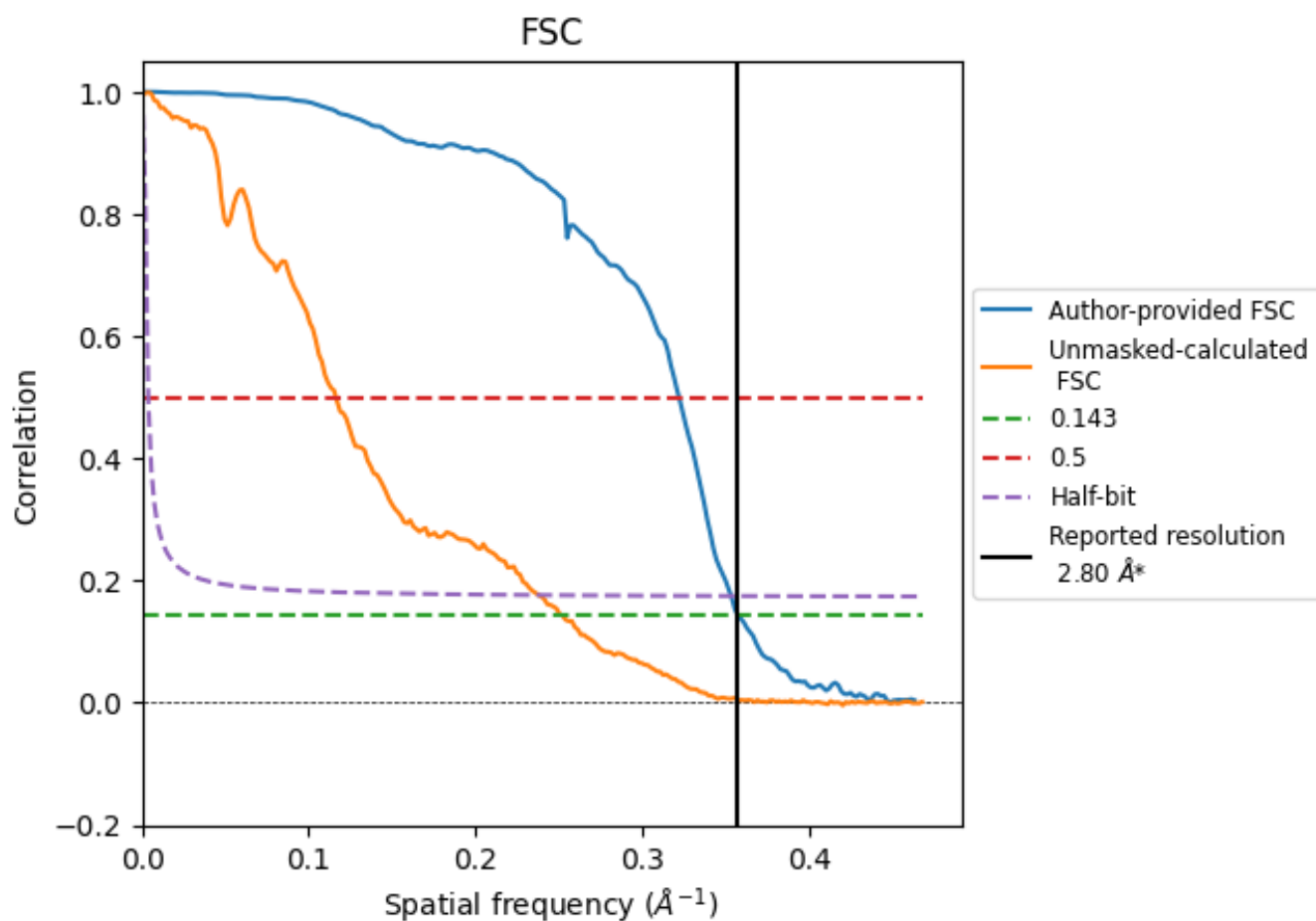


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.357  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

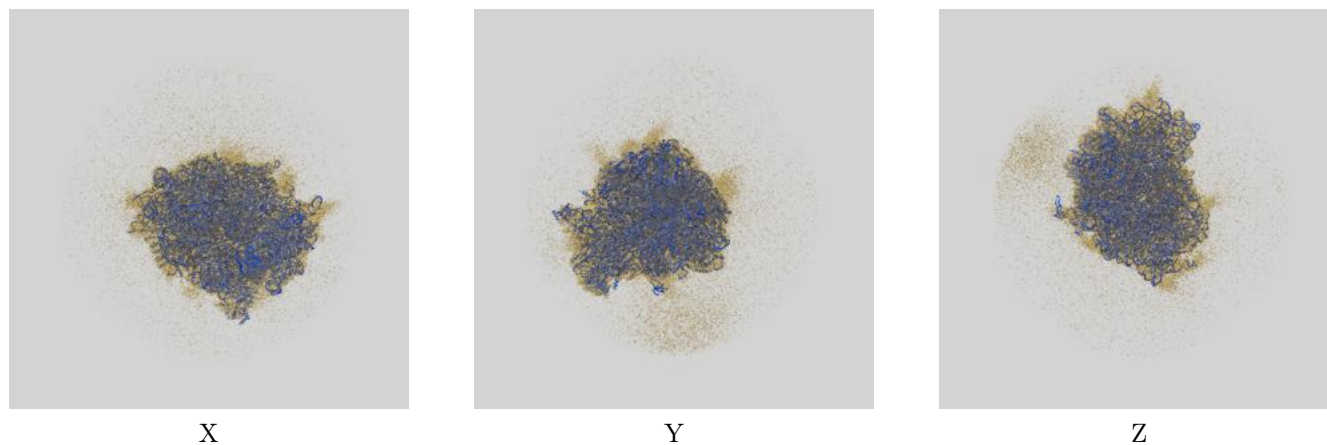
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.10	2.83
Unmasked-calculated*	3.97	8.60	4.20

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.97 differs from the reported value 2.8 by more than 10 %

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

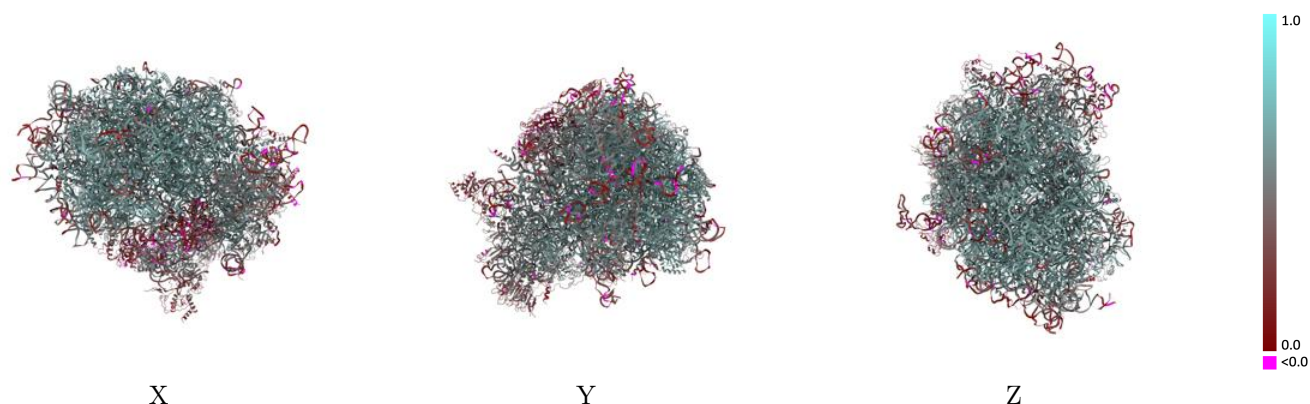
This section contains information regarding the fit between EMDB map EMD-44021 and PDB model 9AZS. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



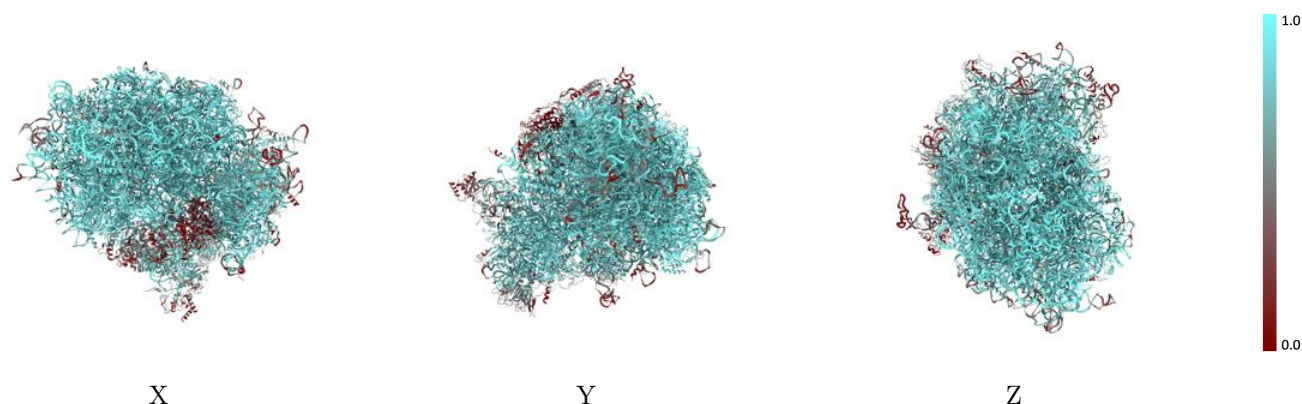
The images above show the 3D surface view of the map at the recommended contour level 0.0491 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



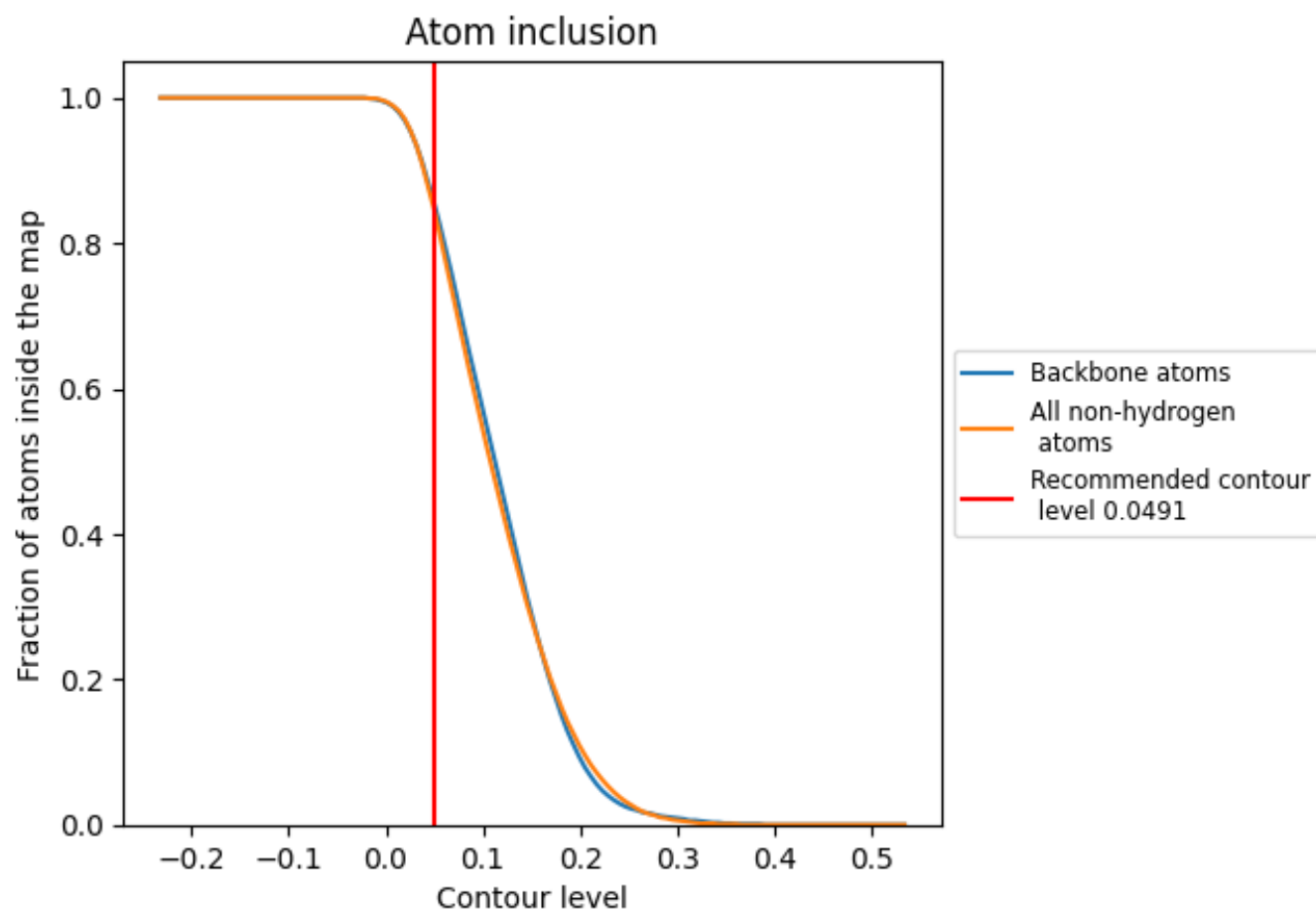
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0491).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.0491) and Q-score for the entire model and for each chain.





















































































Chain	Atom inclusion	Q-score
All	 0.8500	 0.5160
AT	 0.4110	 0.1530
CF	 0.1670	 0.1720
Et	 0.4100	 0.2160
L5	 0.9060	 0.5410
L7	 0.9850	 0.6080
L8	 0.9450	 0.5810
LA	 0.9730	 0.6250
LB	 0.9290	 0.6040
LC	 0.9360	 0.6040
LD	 0.8950	 0.5710
LE	 0.8360	 0.5360
LF	 0.9550	 0.6070
LG	 0.8380	 0.5470
LH	 0.9210	 0.5930
LI	 0.9350	 0.6000
LJ	 0.8190	 0.5180
LL	 0.8900	 0.5790
LM	 0.9190	 0.5810
LN	 0.9880	 0.6340
LO	 0.9490	 0.6120
LP	 0.9440	 0.6190
LQ	 0.9660	 0.6290
LR	 0.8690	 0.5530
LS	 0.9660	 0.6230
LT	 0.9190	 0.5990
LU	 0.8270	 0.5160
LV	 0.9530	 0.6150
LW	 0.6610	 0.4330
LX	 0.9100	 0.5920
LY	 0.9170	 0.5990
LZ	 0.9280	 0.5850
La	 0.9650	 0.6290
Lb	 0.8350	 0.5390
Lc	 0.9250	 0.5860



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Chain	Atom inclusion	Q-score
Ld	 0.9070	 0.5840
Le	 0.9700	 0.6280
Lf	 0.9720	 0.6290
Lg	 0.9160	 0.6000
Lh	 0.9080	 0.5950
Li	 0.9100	 0.5950
Lj	 0.9790	 0.6310
Lk	 0.8470	 0.5540
Ll	 0.9530	 0.6110
Lm	 0.9210	 0.6030
Ln	 0.9710	 0.6240
Lo	 0.9450	 0.6010
Lp	 0.9390	 0.6090
Lr	 0.9420	 0.6060
Ls	 0.2370	 0.1840
Lt	 0.1430	 0.1500
Lz	 0.1850	 0.1430
Pt	 0.9120	 0.4840
S2	 0.8980	 0.4980
SA	 0.7970	 0.5050
SB	 0.8440	 0.5450
SC	 0.8760	 0.5420
SD	 0.7160	 0.4320
SE	 0.8220	 0.4980
SF	 0.7970	 0.4800
SG	 0.6720	 0.4020
SH	 0.6530	 0.4290
SI	 0.8320	 0.5220
SJ	 0.8070	 0.4900
SK	 0.6670	 0.3770
SL	 0.8340	 0.5370
SM	 0.2390	 0.2200
SN	 0.9050	 0.5760
SO	 0.8430	 0.5470
SP	 0.7060	 0.4380
SQ	 0.7500	 0.4640
SR	 0.6910	 0.4300
SS	 0.7070	 0.4540
ST	 0.7360	 0.4510
SU	 0.6670	 0.3900
SV	 0.8470	 0.5260
SW	 0.9330	 0.5750

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Chain	Atom inclusion	Q-score
SX	 0.9000	 0.5640
SY	 0.7080	 0.4220
SZ	 0.6470	 0.4050
Sa	 0.8680	 0.5580
Sb	 0.7980	 0.5070
Sc	 0.6930	 0.4290
Sd	 0.8590	 0.4920
Se	 0.6890	 0.4320
Sf	 0.3430	 0.2160
Sg	 0.5300	 0.3430