Full wwPDB EM Validation Report ⓘ

Sep 3, 2024 – 04:15 PM EDT

PDB ID	:	9BH5
EMDB ID	:	EMD-44533
Title	:	High-resolution C. elegans 80S ribosome structure - class 1
Authors	:	Sehgal, E.; Serrao, V.H.B.; Arribere, J.
Deposited on	:	2024-04-19
Resolution	:	2.63 Å(reported)
Based on initial model	:	.

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

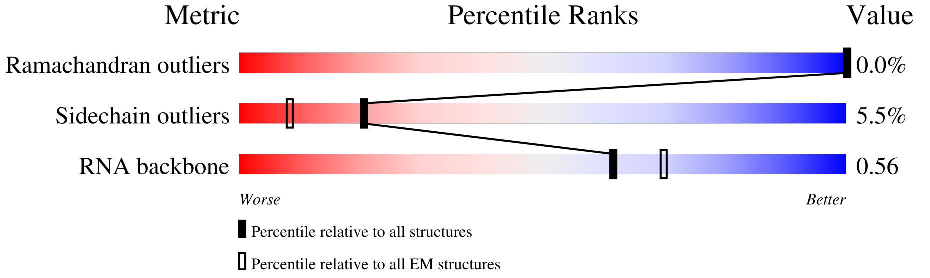
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance ⓘ

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

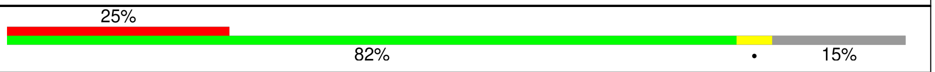
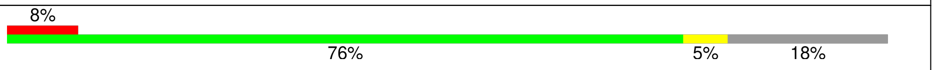
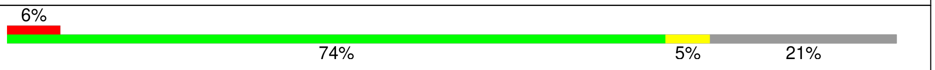
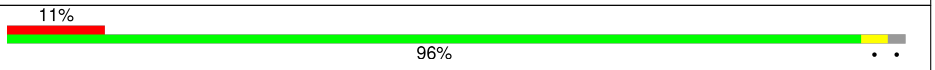
The reported resolution of this entry is 2.63 Å.

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 >=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 <=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	AD	247	
2	AB	257	
3	AC	272	
4	AE	259	
5	A7	119	
6	A8	153	
7	B2	1754	
8	A5	3510	

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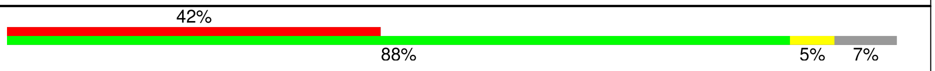
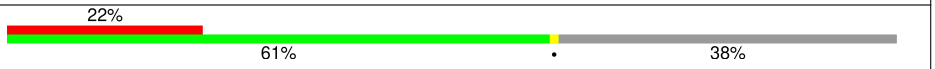
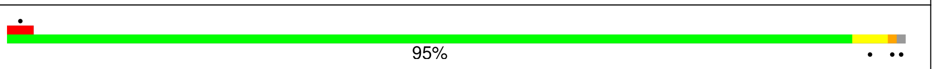
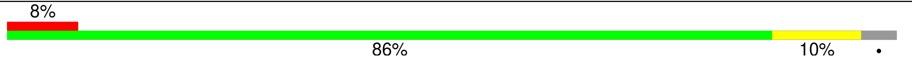
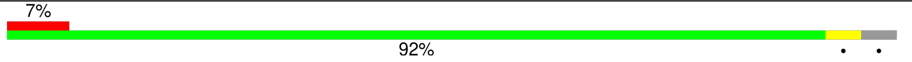
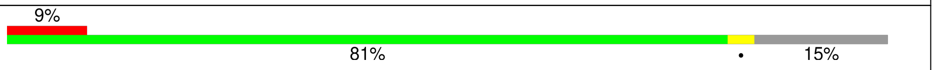
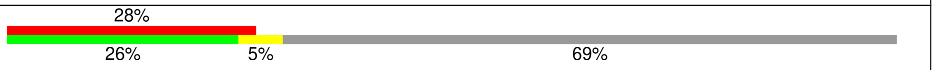
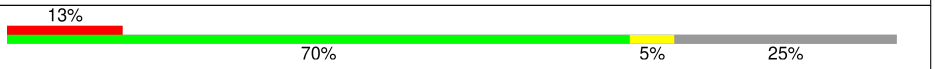
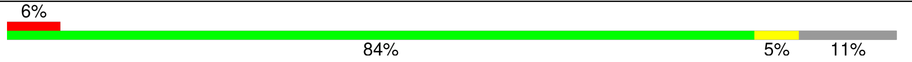
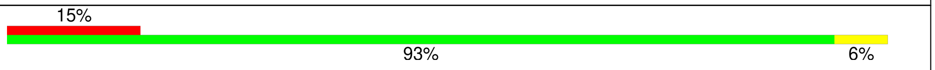
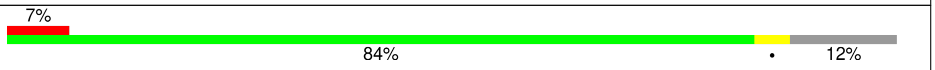
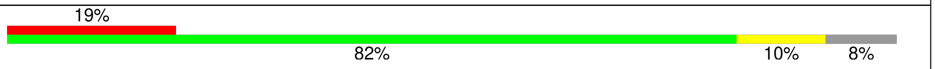
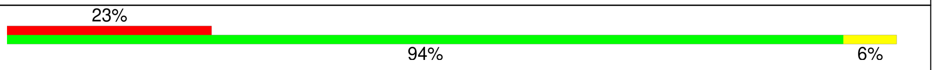
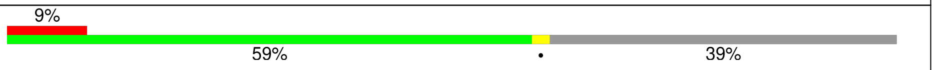
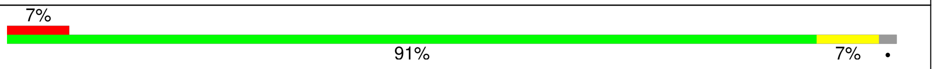
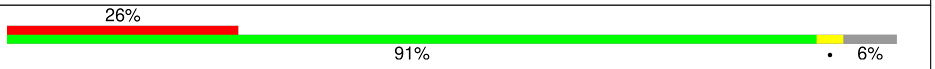
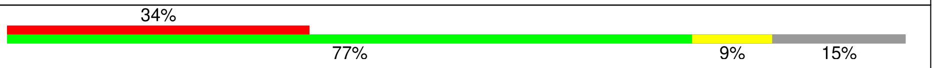
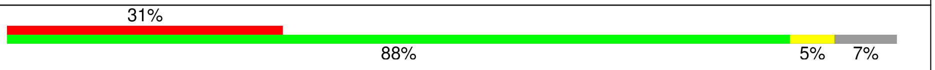
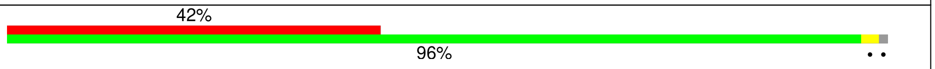
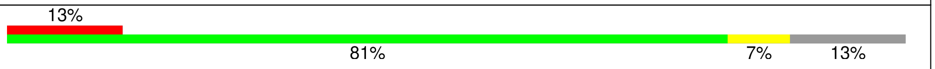
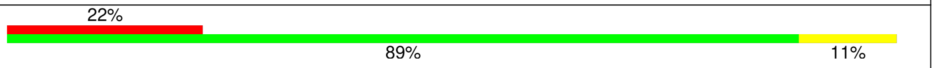
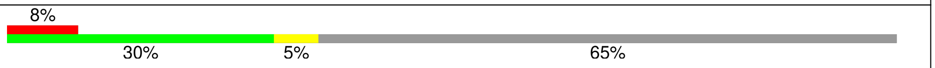
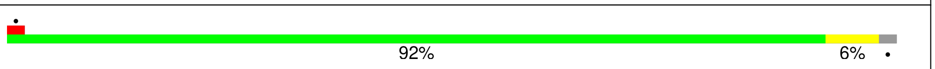
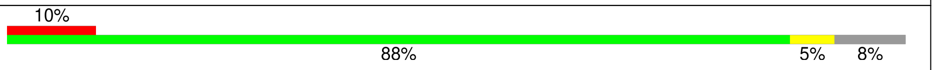
Mol	Chain	Length	Quality of chain
9	AR	130	
10	AK	149	
11	AW	130	
12	AS	154	
13	AT	146	
14	Aa	117	
15	Af	163	
16	AA	276	
17	AO	152	
18	AI	208	
19	AF	210	
20	AM	140	
21	AV	88	
22	AN	151	
23	AZ	117	
24	Ad	56	
25	AY	131	
26	AU	117	
27	AG	246	
28	Ab	83	
29	AP	151	
30	Ac	65	
31	Ae	130	
32	AX	143	
33	AL	155	

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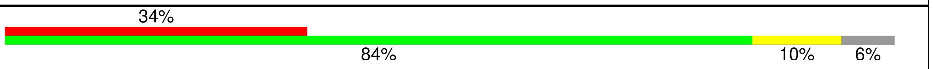
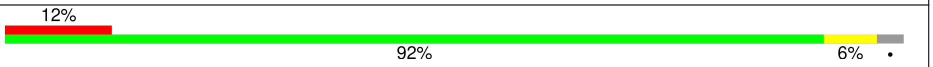
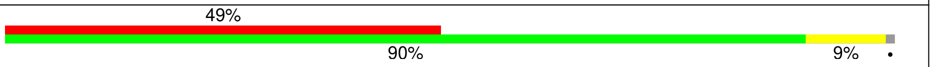
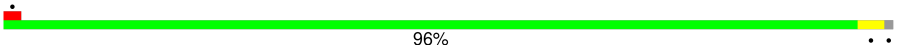
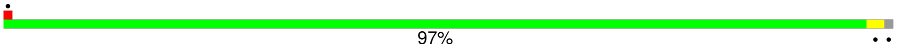
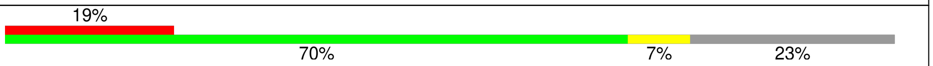
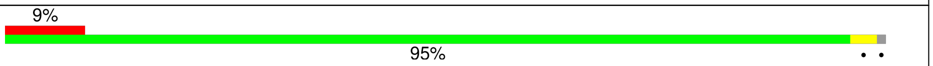
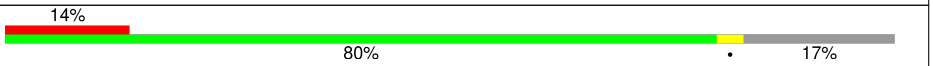
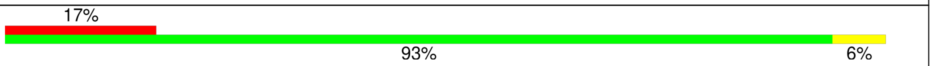
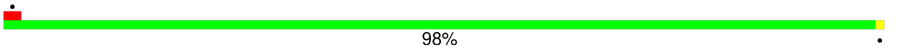
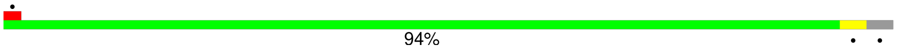
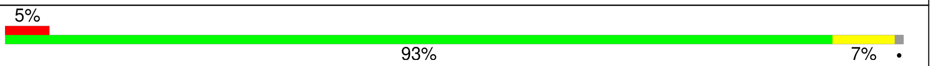
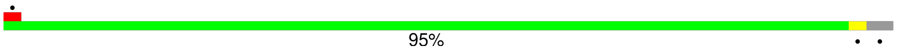
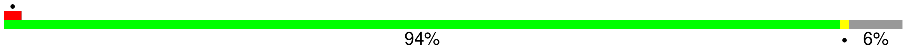
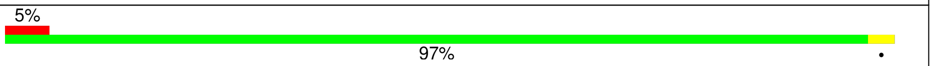
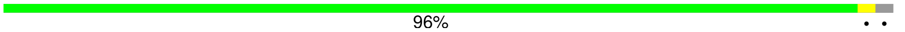
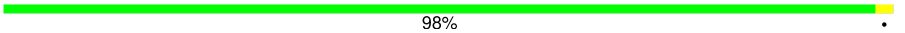
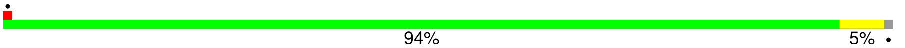
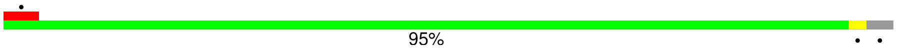
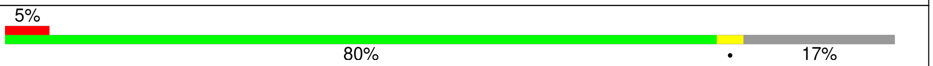
Mol	Chain	Length	Quality of chain
34	AJ	189	
35	AQ	144	
36	AH	194	
37	CF	244	
38	CS	180	
39	CV	140	
40	CB	401	
41	CU	130	
42	CL	207	
43	CA	260	
44	CG	265	
45	CI	214	
46	CO	202	
47	CC	345	
48	Ch	123	
49	CE	217	
50	Co	105	
51	Cf	124	
52	Ci	104	
53	Cl	51	
54	CN	204	
55	Ca	145	
56	Cp	91	
57	CM	135	
58	Cc	115	

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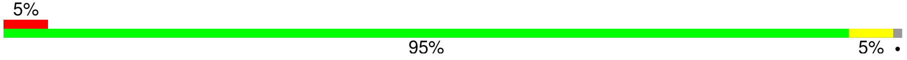
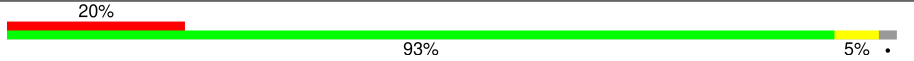
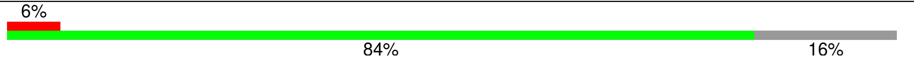
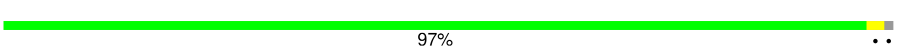
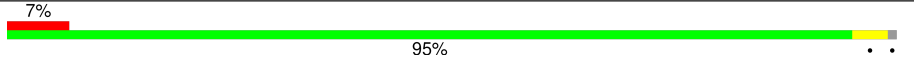
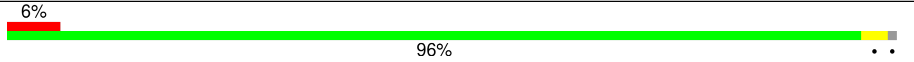
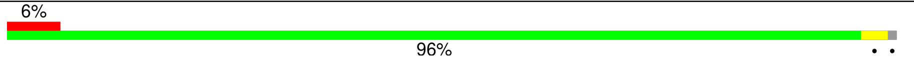
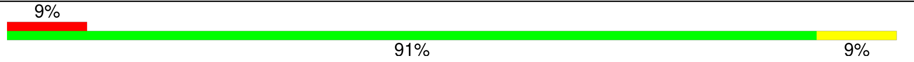
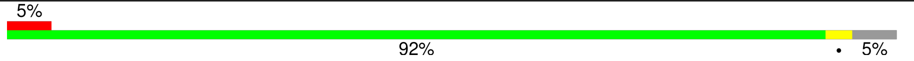
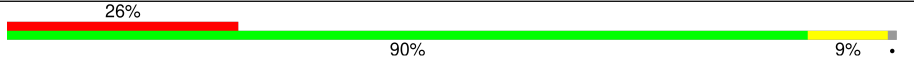
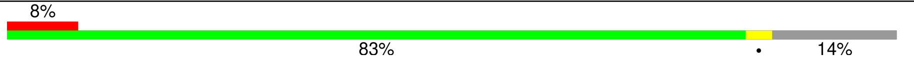
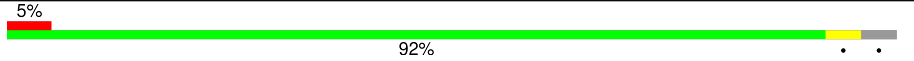
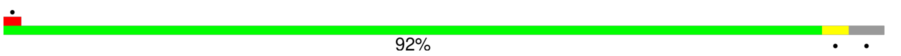
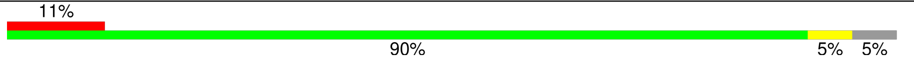
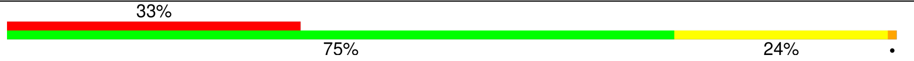
Mol	Chain	Length	Quality of chain
59	CH	189	
60	CY	142	
61	CR	198	
62	Cb	62	
63	CQ	188	
64	CT	161	
65	CD	293	
66	CZ	136	
67	CP	187	
68	Cn	22	
69	Cg	110	
70	Ck	70	
71	Cm	128	
72	Cd	122	
73	Ce	134	
74	CW	159	
75	Cj	92	
76	CJ	196	
77	CX	146	
78	DA	76	
78	DB	76	
79	DC	10	

2 Entry composition (i)

There are 81 unique types of molecules in this entry. The entry contains 332725 atoms, of which 142393 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 Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	AD	211	3343	1029	1706	308	291	9	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	AB	210	3453	1071	1769	298	307	8	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	AC	215	3389	1062	1735	293	292	7	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	AE	255	4120	1277	2107	382	347	7	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
5	A7	119	3810	1131	1281	447	833	118	0	0

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	A8	146	4679	1390	1568	551	1025	145	0	0

- Molecule 7 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	B2	1476	Total 47369	C 14078	H 15858	N 5637	O 10320	P 1476	0	0

- Molecule 8 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	A5	3022	Total 96979	C 28814	H 32467	N 11522	O 21154	P 3022	0	0

- Molecule 9 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AR	121	Total 1985	C 604	H 1009	N 183	O 184	S 5	0	0

- Molecule 10 is a protein called Plectin/S10 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AK	93	Total 1555	C 509	H 786	N 124	O 135	S 1	0	0

- Molecule 11 is a protein called Ribosomal Protein, Small subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AW	129	Total 2110	C 654	H 1082	N 193	O 177	S 4	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AS	148	Total 2453	C 754	H 1248	N 237	O 209	S 5	0	0

- Molecule 13 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AT	140	Total 2260	C 704	H 1149	N 213	O 193	S 1	0	0

- Molecule 14 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Aa	99	Total 1631	C 496	H 828	N 172	O 129	S 6	0	0

- Molecule 15 is a protein called Ubiquitin-like protein 1-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Af	50	Total 789	C 246	H 392	N 77	O 69	S 5	0	0

- Molecule 16 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AA	207	Total 3264	C 1035	H 1652	N 281	O 289	S 7	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AO	135	Total 2063	C 624	H 1049	N 200	O 185	S 5	0	0

- Molecule 18 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AI	207	Total 3391	C 1044	H 1723	N 326	O 296	S 2	0	0

- Molecule 19 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AF	185	Total 2969	C 914	H 1515	N 275	O 259	S 6	0	0

- Molecule 20 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AM	117	Total 1808	C 565	H 904	N 162	O 170	S 7	0	0

- Molecule 21 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
21	AV	81	1239	378	622	114	120	5	0	0

- Molecule 22 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	AN	151	2514	769	1297	236	206	6	0	0

- Molecule 23 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
23	AZ	71	1165	363	601	100	99	2	0	0

- Molecule 24 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
24	Ad	55	895	284	443	93	71	4	0	0

- Molecule 25 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
25	AY	123	2085	637	1093	188	165	2	0	0

- Molecule 26 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
26	AU	100	1650	500	854	154	138	4	0	0

- Molecule 27 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
27	AG	228	3791	1159	1954	350	321	7	0	0

- Molecule 28 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
28	Ab	82	1305	404	663	119	111	8	0	0

- Molecule 29 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
29	AP	132	2186	681	1132	194	173	6	0	0

- Molecule 30 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
30	Ac	65	1069	314	549	106	98	2	0	0

- Molecule 31 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
31	Ae	45	752	219	388	84	61	0	0

- Molecule 32 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
32	AX	140	2242	691	1150	212	186	3	0	0

- Molecule 33 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
33	AL	143	2380	736	1222	223	194	5	0	0

- Molecule 34 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
34	AJ	177	3060	936	1592	288	243	1	0	0

- Molecule 35 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
35	AQ	140	2305	715	1181	215	193	1	0	0

- Molecule 36 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
36	AH	192	3187	993	1643	280	271	0	0

- Molecule 37 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
37	CF	213	3534	1119	1791	320	302	2	0	0

- Molecule 38 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	CS	179	2976	936	1506	278	250	6	0	0

- Molecule 39 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	CV	128	1991	614	1020	182	169	6	0	0

- Molecule 40 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	CB	395	6478	2016	3300	605	547	10	0	0

- Molecule 41 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	CU	100	1692	532	868	147	144	1	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	CL	204	3388	1025	1740	338	283	2	0	0

- Molecule 43 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	CA	249	3875	1178	1980	391	321	5	0	0

- Molecule 44 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	CG	221	3680	1123	1892	354	309	2	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	CI	213	3485	1083	1756	343	290	13	0	0

- Molecule 46 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	CO	201	3328	1031	1714	314	264	5	0	0

- Molecule 47 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	CC	335	5420	1675	2769	521	449	6	0	0

- Molecule 48 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	Ch	122	2094	618	1105	201	169	1	0	0

- Molecule 49 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	CE	139	Total 2311	C 727	H 1195	N 203	O 185	S 1	0	0

- Molecule 50 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	Co	102	Total 1739	C 522	H 902	N 174	O 135	S 6	0	0

- Molecule 51 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Cf	117	Total 1901	C 594	H 971	N 183	O 153	0	0

- Molecule 52 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	Ci	104	Total 1754	C 521	H 918	N 176	O 137	S 2	0	0

- Molecule 53 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	Cl	50	Total 922	C 276	H 487	N 93	O 63	S 3	0	0

- Molecule 54 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	CN	203	Total 3463	C 1068	H 1763	N 358	O 272	S 2	0	0

- Molecule 55 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	Ca	144	Total 2299	C 717	H 1163	N 232	O 183	S 4	0	0

- Molecule 56 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
56	Cp	88	1404	425	726	134	113	6	0	0

- Molecule 57 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
57	CM	132	2204	668	1151	205	178	2	0	0

- Molecule 58 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
58	Cc	96	1497	464	762	129	137	5	0	0

- Molecule 59 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
59	CH	188	3081	954	1577	278	266	6	0	0

- Molecule 60 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
60	CY	132	2181	651	1131	219	176	4	0	0

- Molecule 61 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
61	CR	194	3384	1012	1746	349	274	3	0	0

- Molecule 62 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
62	Cb	52	892	268	460	94	69	1	0	0

- Molecule 63 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
63	CQ	187	3023	918	1550	299	255	1	0	0

- Molecule 64 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
64	CT	160	2621	806	1338	256	218	3	0	0

- Molecule 65 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
65	CD	289	4701	1468	2373	430	428	2	0	0

- Molecule 66 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
66	CZ	135	2301	716	1199	200	184	2	0	0

- Molecule 67 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
67	CP	154	2506	780	1257	249	215	5	0	0

- Molecule 68 is a protein called eL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
68	Cn	22	461	128	252	54	25	2	0	0

- Molecule 69 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
69	Cg	104	1759	526	922	170	139	2	0	0

- Molecule 70 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
70	Ck	69	1181	359	622	100	99	1	0	0

- Molecule 71 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
71	Cm	51	874	258	456	86	69	5	0	0

- Molecule 72 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
72	Cd	105	1770	544	903	169	151	3	0	0

- Molecule 73 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
73	Ce	128	2160	652	1119	216	169	4	0	0

- Molecule 74 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
74	CW	88	1447	442	745	140	118	2	0	0

- Molecule 75 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
75	Cj	88	1433	431	727	154	117	4	0	0

- Molecule 76 is a protein called Large ribosomal subunit protein uL5B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
76	CJ	186	3062	952	1555	281	269	5	0	0

- Molecule 77 is a protein called Large ribosomal subunit protein uL23B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
77	CX	119	1958	606	1004	181	166	1	0	0

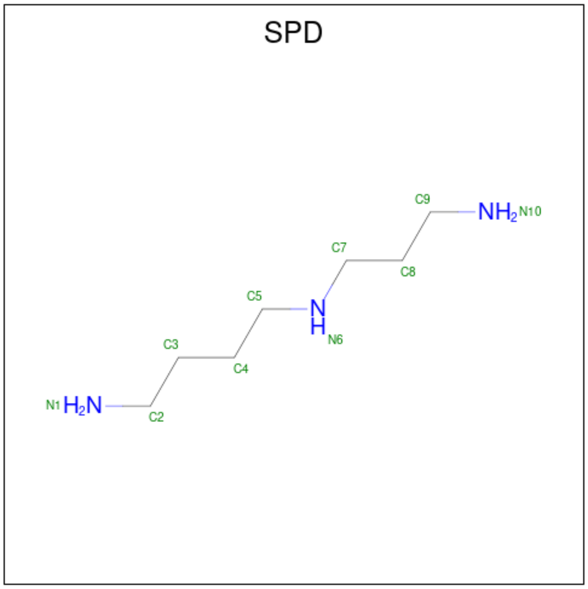
- Molecule 78 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
78	DA	76	2448	725	821	294	532	76	0	0
			Total	C	H	N	O	P		
78	DB	76	2448	725	821	294	532	76	0	0

- Molecule 79 is a RNA chain called mRNA.

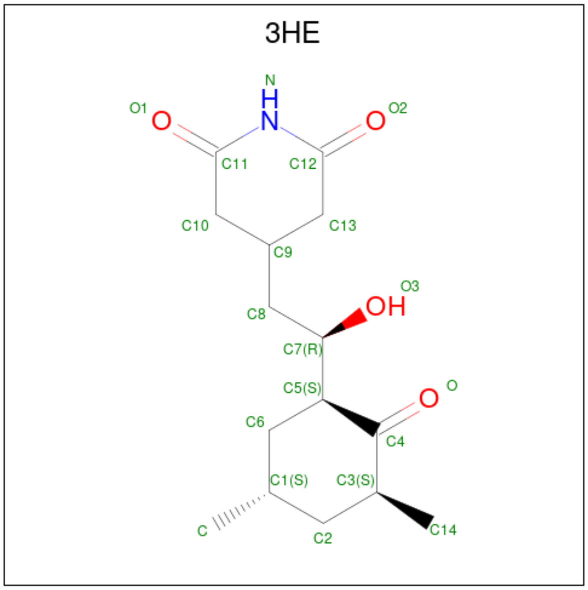
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
79	DC	10	301	90	101	20	80	10	0	0

- Molecule 80 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
80	A5	1	10	7	3	0

- Molecule 81 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: $C_{15}H_{23}NO_4$).



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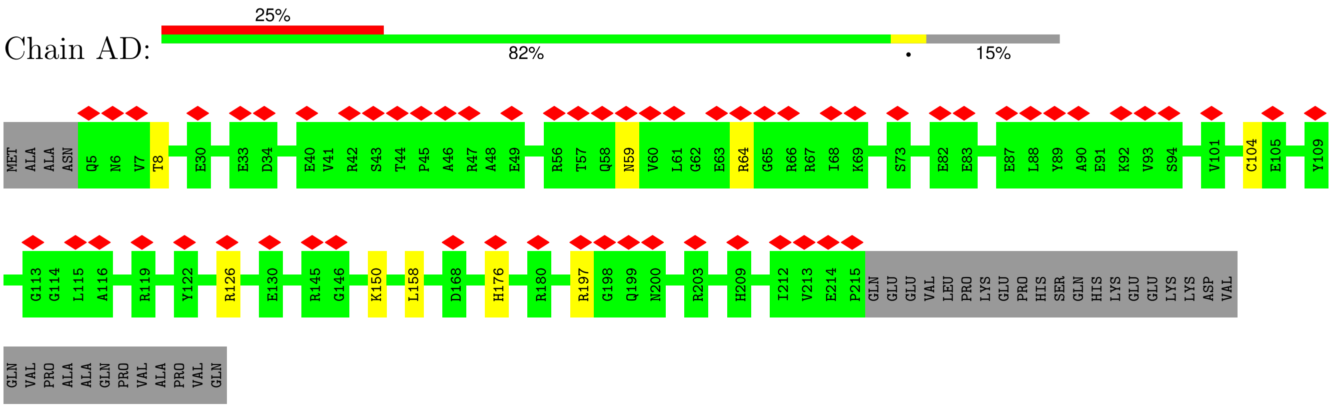
3 Residue-property plots ⓘ

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

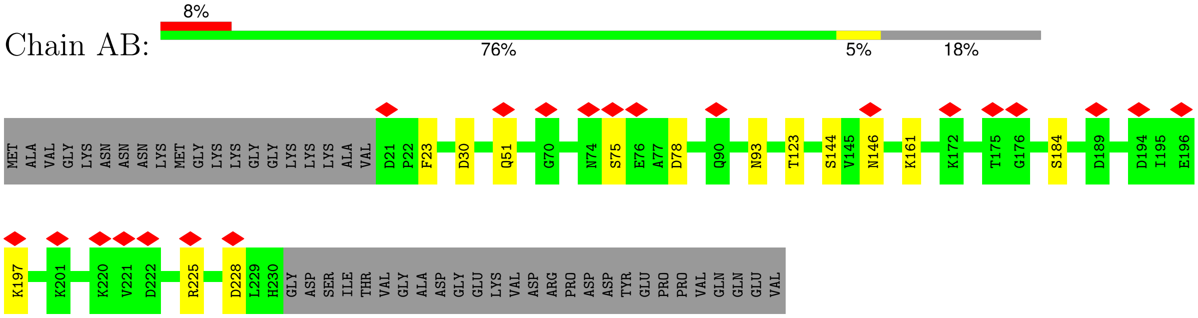
- Molecule 1: Small ribosomal subunit protein uS3

Chain AD:



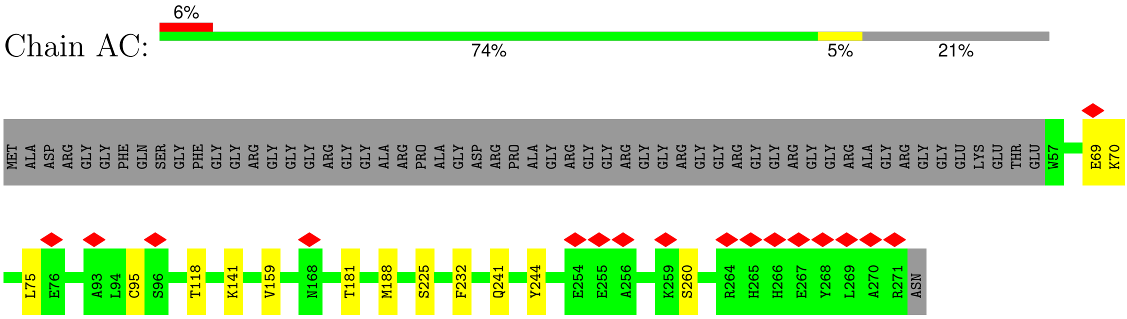
- Molecule 2: Small ribosomal subunit protein eS1

Chain AB:



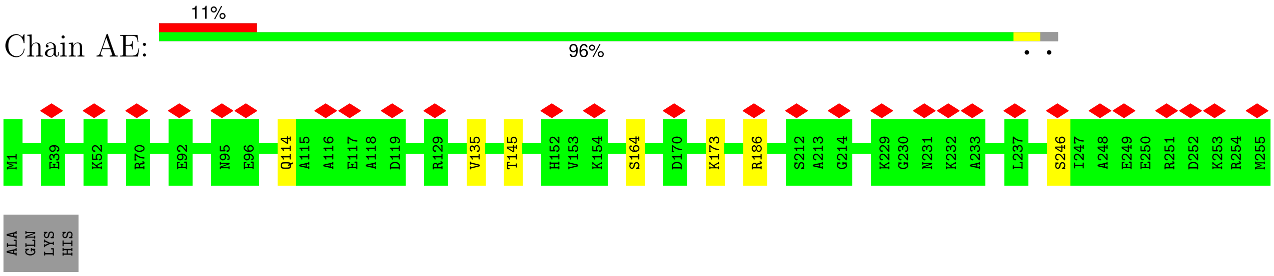
- Molecule 3: Small ribosomal subunit protein uS5

Chain AC:



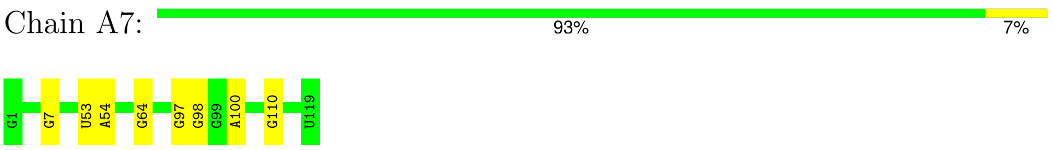
- Molecule 4: Small ribosomal subunit protein eS4

Chain AE:



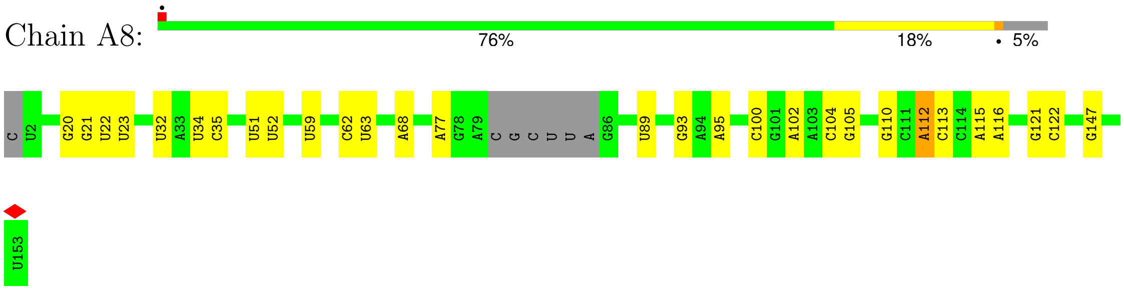
- Molecule 5: 5S rRNA

Chain A7:



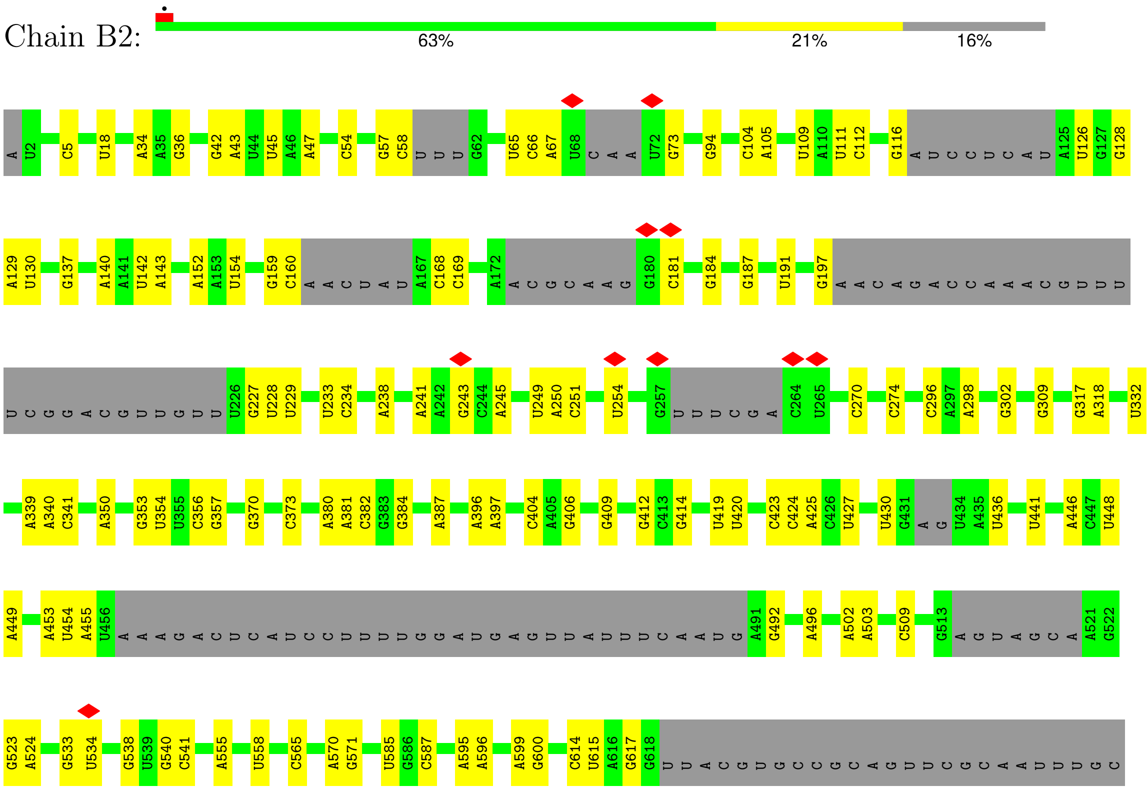
- Molecule 6: 5.8S rRNA

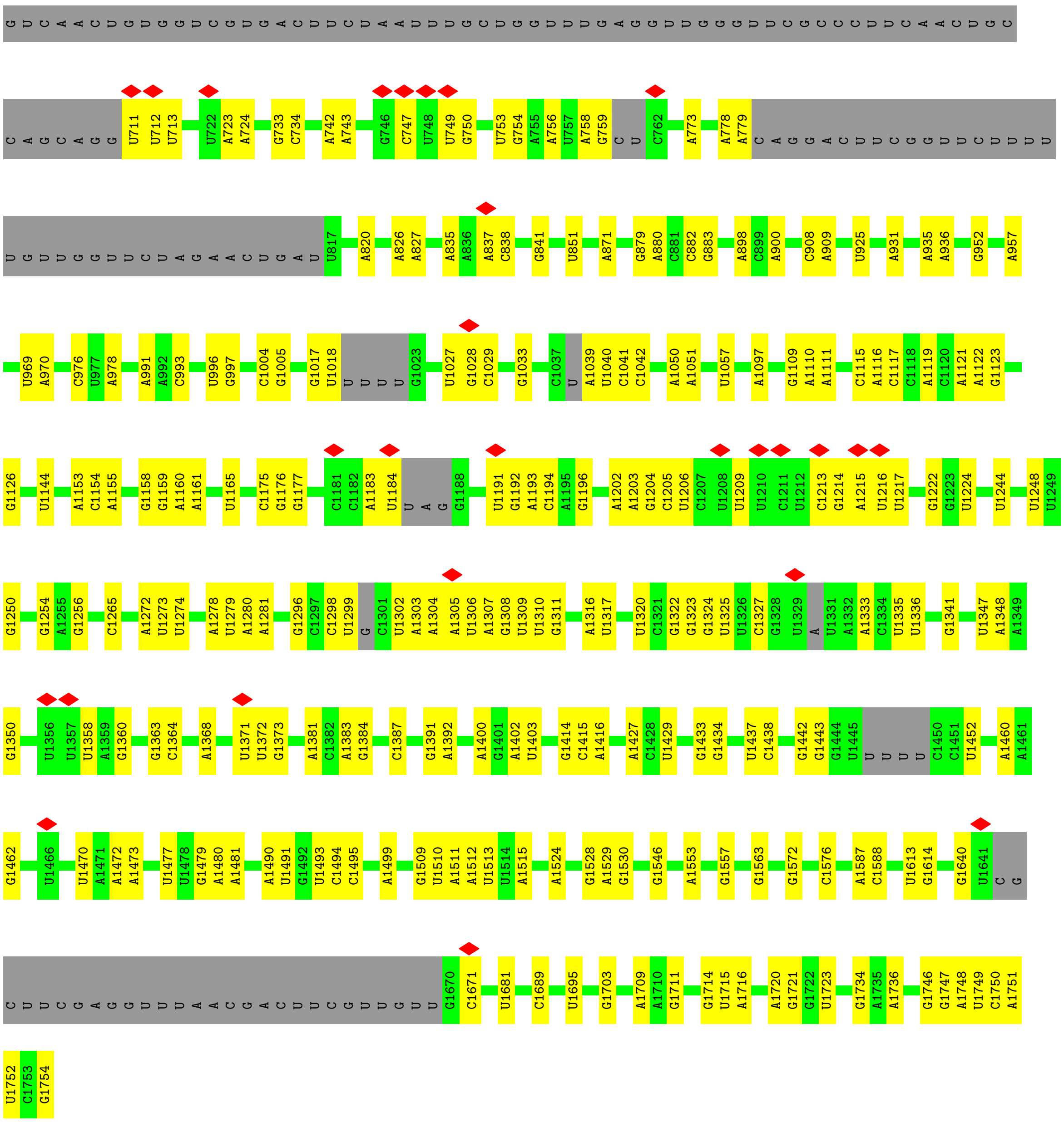
Chain A8:



- Molecule 7: 18S rRNA

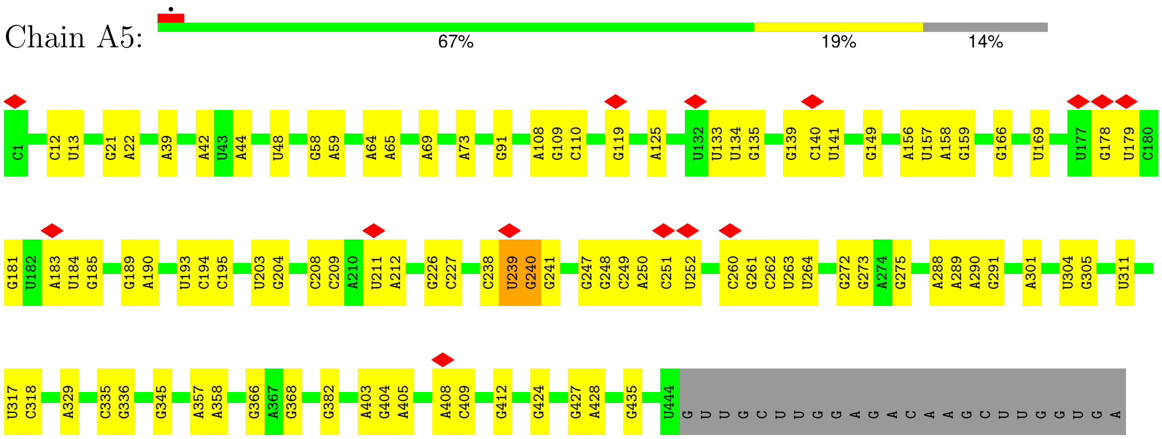
Chain B2:

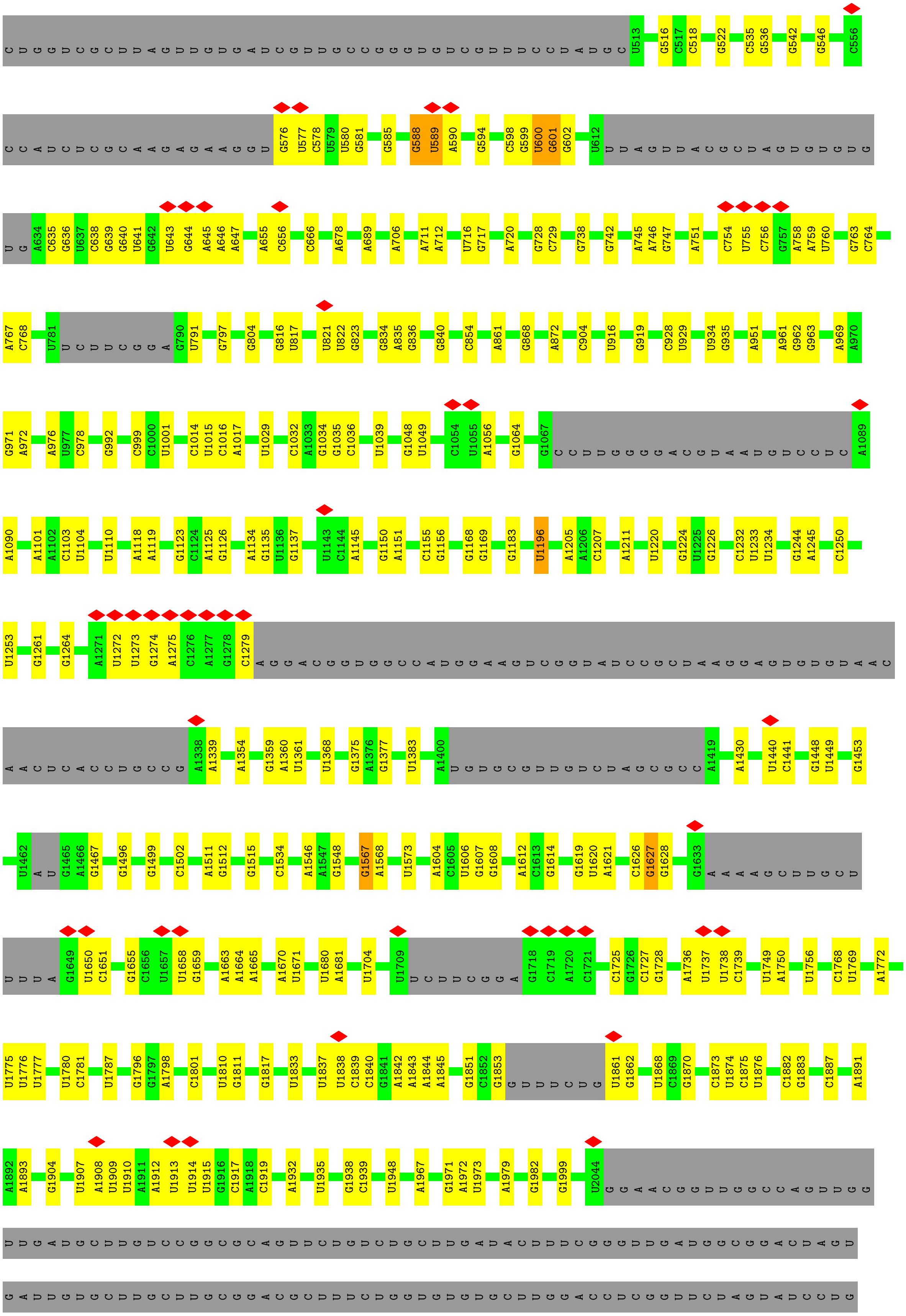




- Molecule 8: 28S rRNA

Chain A5:

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C C A U C U C G G C A A G A G A A G G U G576 U577 C578 U579 U580 G581 G585 G588 U589 A590 G594 C598 G599 U600 G601 G602 U612 U U A G U U A C G C U A G U G U G U G
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A767 C768 U781 U C U U C G G A G790 U791 G797 G804 G816 U817 U821 U822 G823 G834 A835 G836 G840 C854 A861 G868 A872 C904 U916 G919 C928 U929 U934 G935 A951 A961 G962 G963 A969 A970
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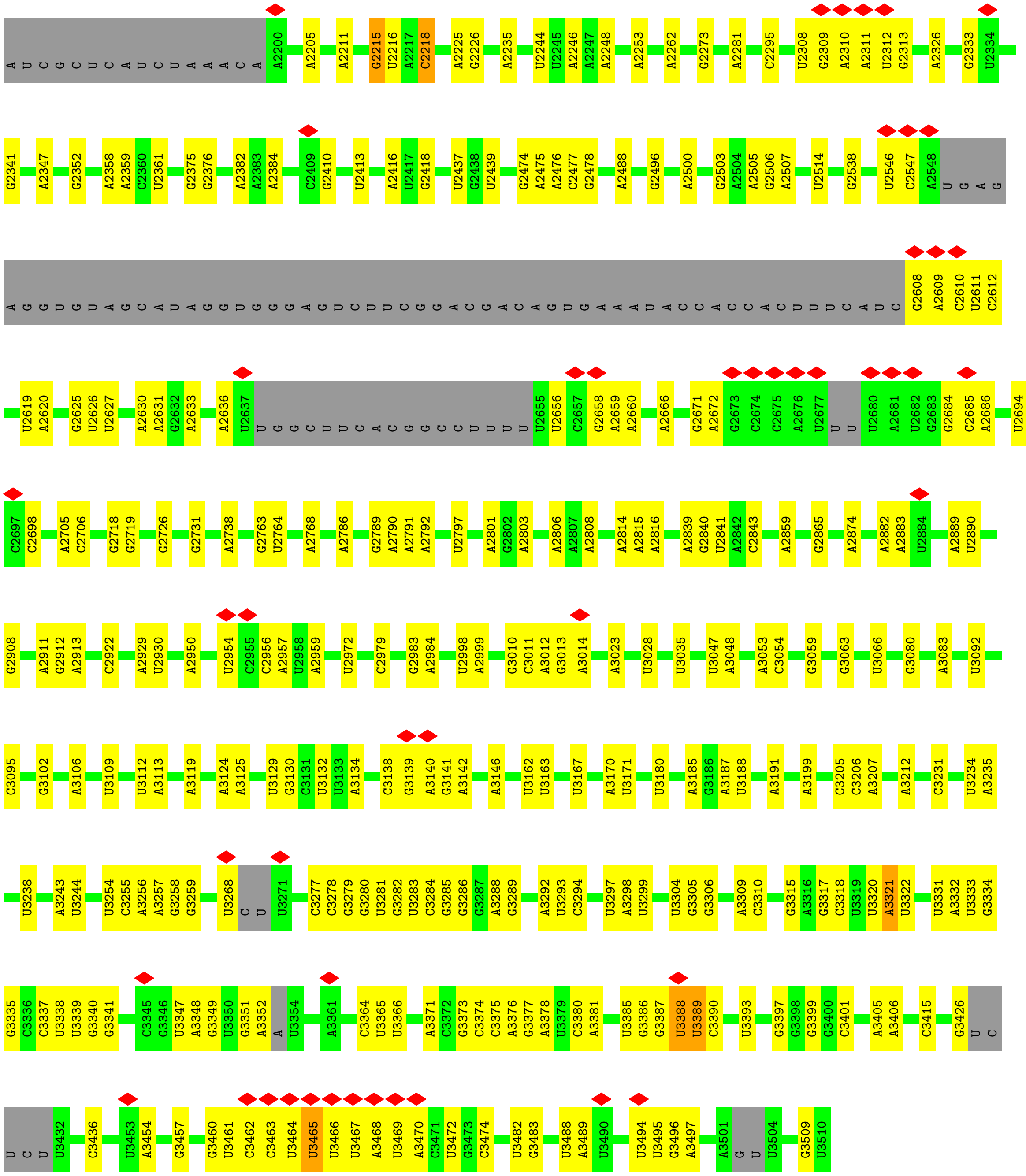
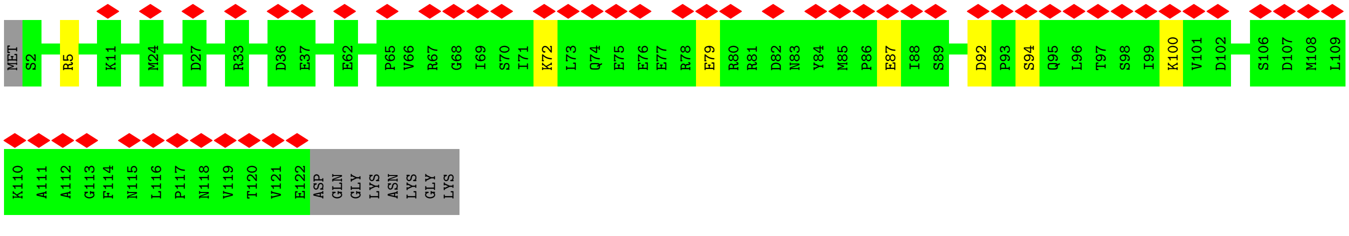


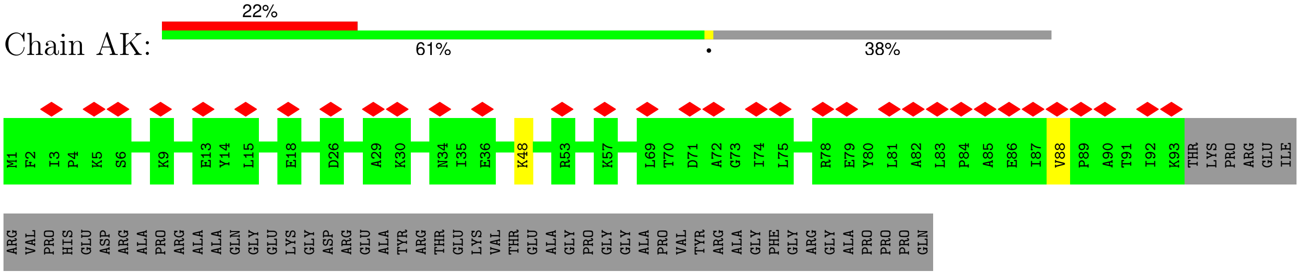
- Molecule 9: Small ribosomal subunit protein eS17

Chain AR:



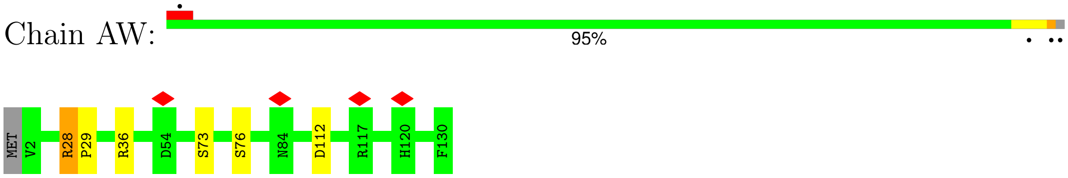
- Molecule 10: Plectin/S10 N-terminal domain-containing protein

Chain AK:



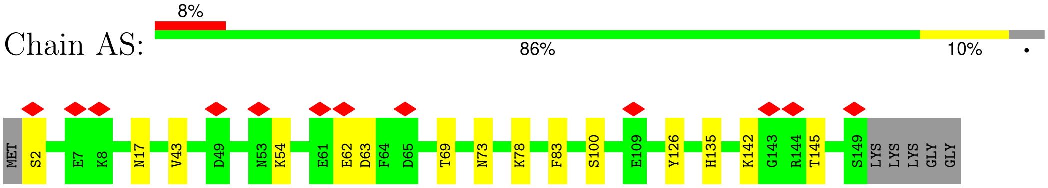
- Molecule 11: Ribosomal Protein, Small subunit

Chain AW:



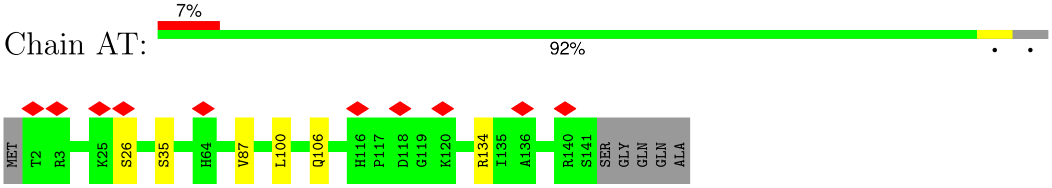
- Molecule 12: Small ribosomal subunit protein uS13

Chain AS:



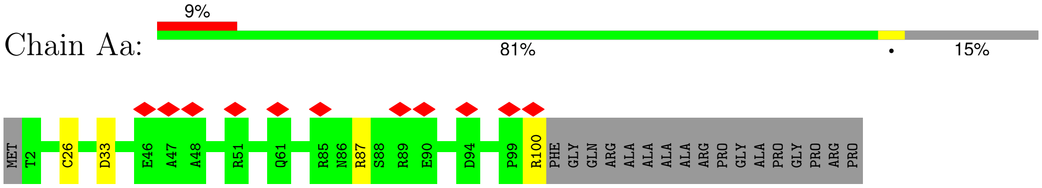
- Molecule 13: Small ribosomal subunit protein eS19

Chain AT:



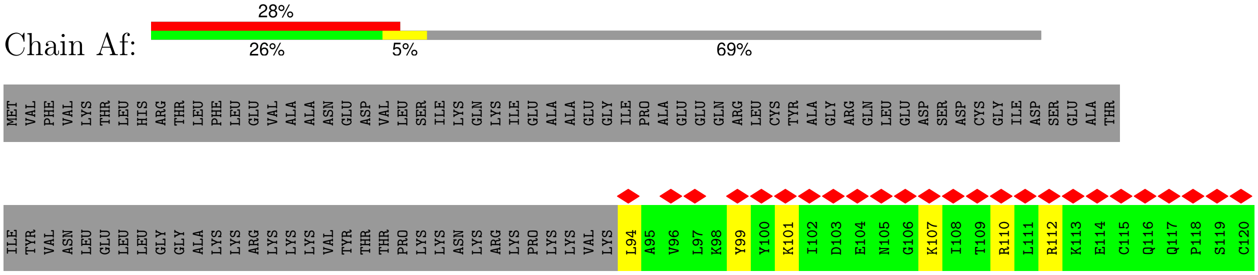
- Molecule 14: Small ribosomal subunit protein eS26

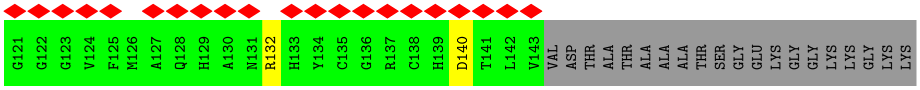
Chain Aa:



- Molecule 15: Ubiquitin-like protein 1-ribosomal protein eS31 fusion protein

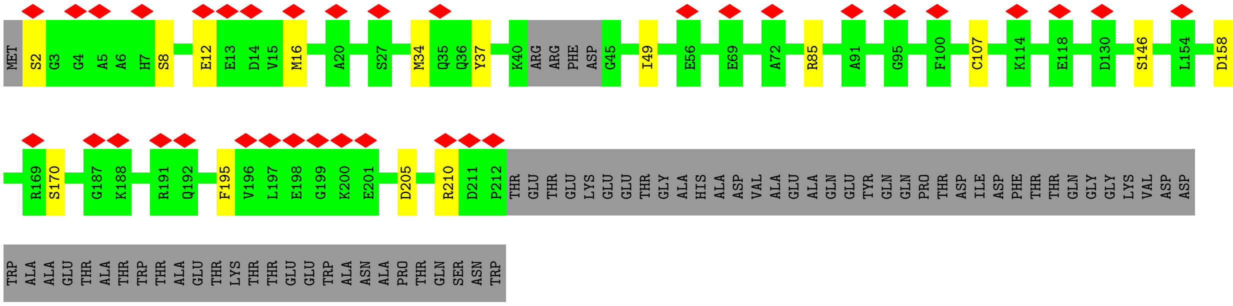
Chain Af:





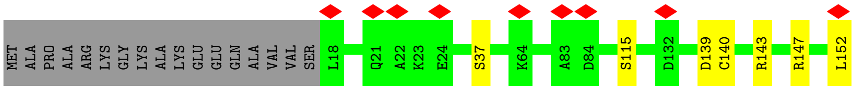
- Molecule 16: Small ribosomal subunit protein uS2

Chain AA:



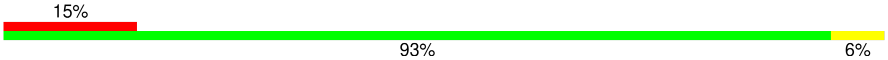
- Molecule 17: Small ribosomal subunit protein uS11

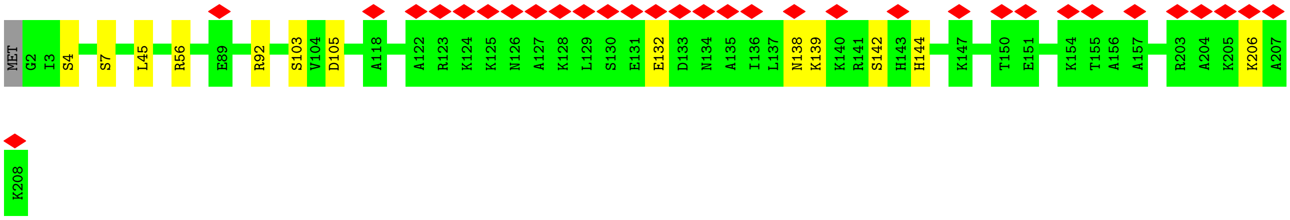
Chain AO:



- Molecule 18: Small ribosomal subunit protein eS8

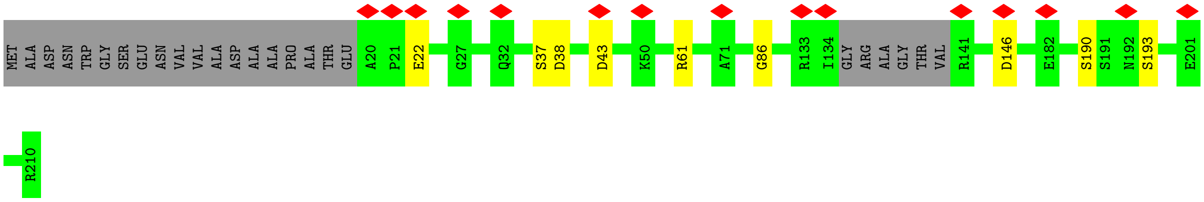
Chain AI:





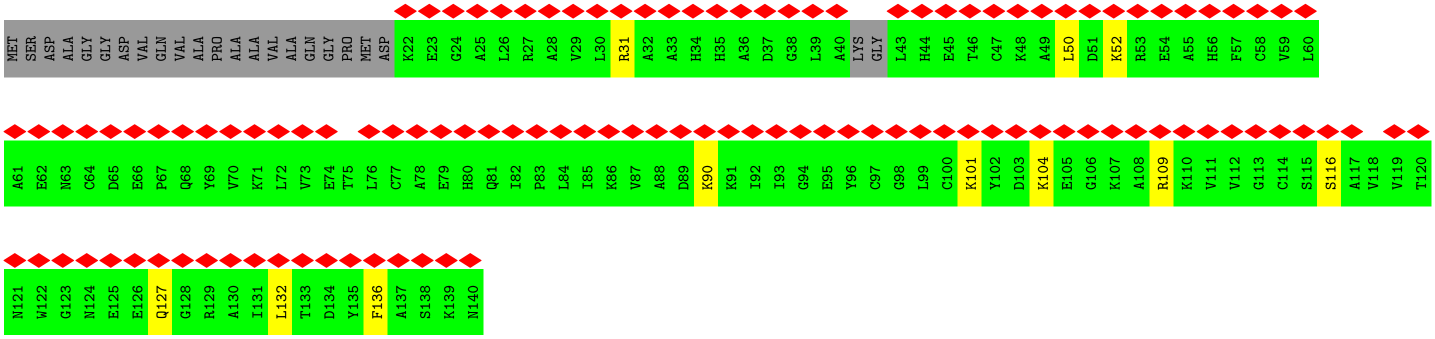
- Molecule 19: Small ribosomal subunit protein uS7

Chain AF:



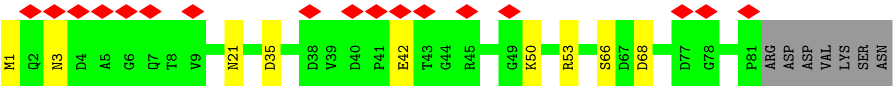
- Molecule 20: Small ribosomal subunit protein eS12

Chain AM:



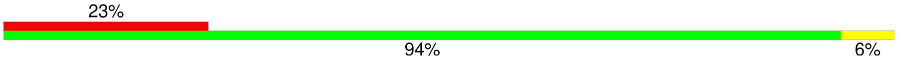
- Molecule 21: Small ribosomal subunit protein eS21

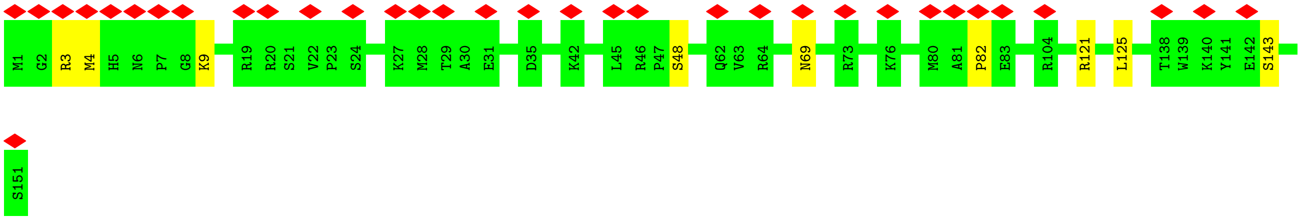
Chain AV:



- Molecule 22: Small ribosomal subunit protein uS15

Chain AN:



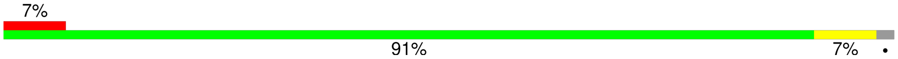


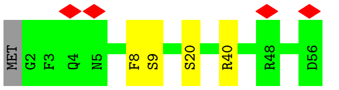
- Molecule 23: Small ribosomal subunit protein eS25

Chain AZ:

- Molecule 24: Small ribosomal subunit protein uS14

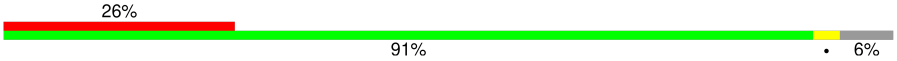
Chain Ad:

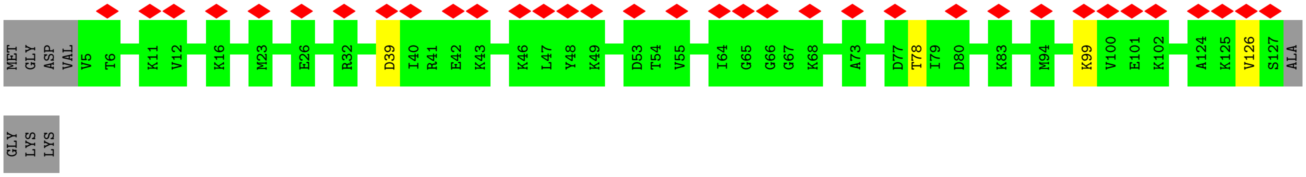




- Molecule 25: Small ribosomal subunit protein eS24

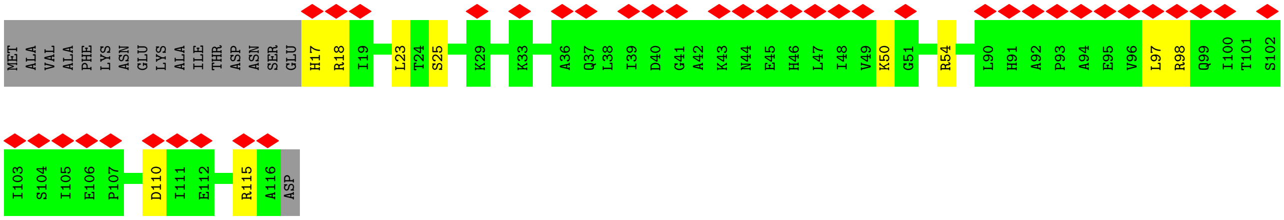
Chain AY:





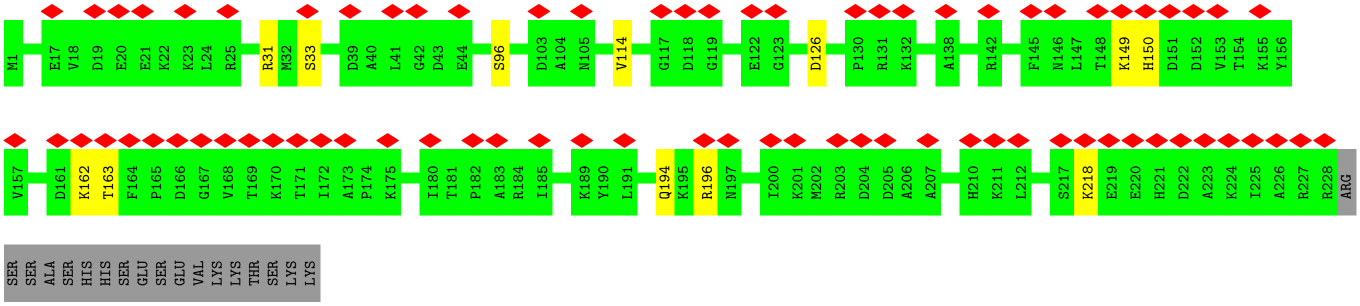
- Molecule 26: Small ribosomal subunit protein uS10

Chain AU:



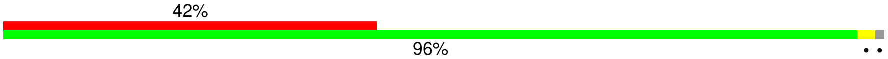
- Molecule 27: Small ribosomal subunit protein eS6

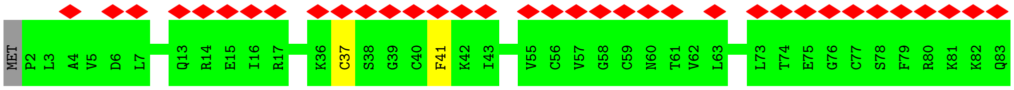
Chain AG:



- Molecule 28: Small ribosomal subunit protein eS27

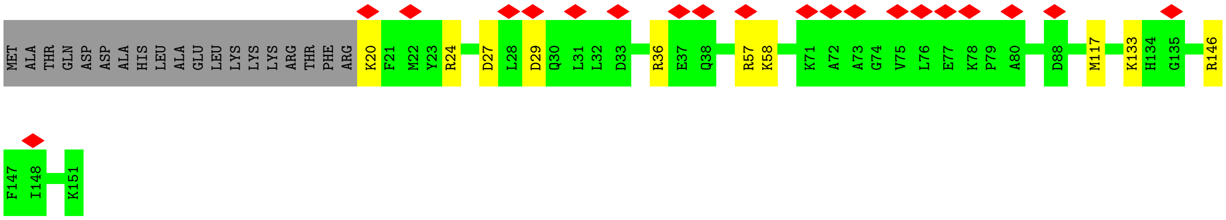
Chain Ab:



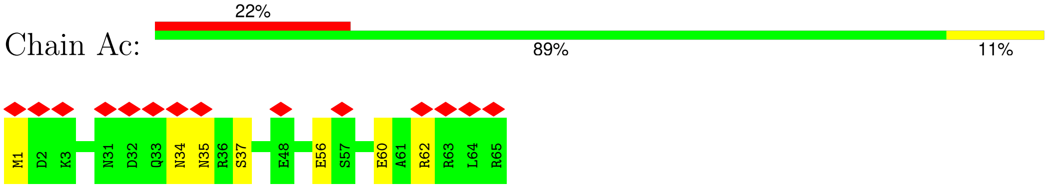


- Molecule 29: Small ribosomal subunit protein uS19

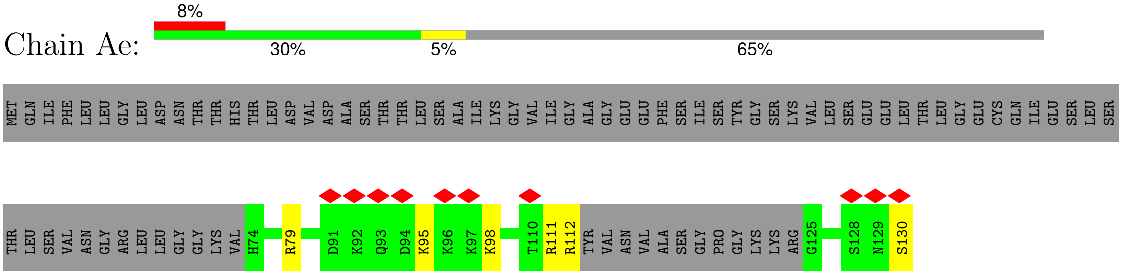
Chain AP:



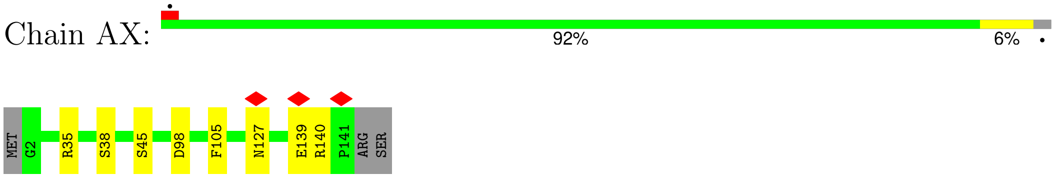
- Molecule 30: Small ribosomal subunit protein eS28



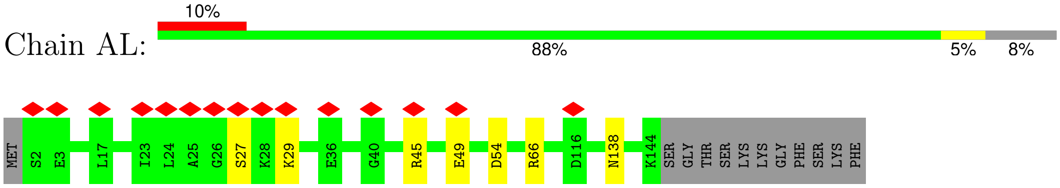
- Molecule 31: Ubiquitin-like domain-containing protein



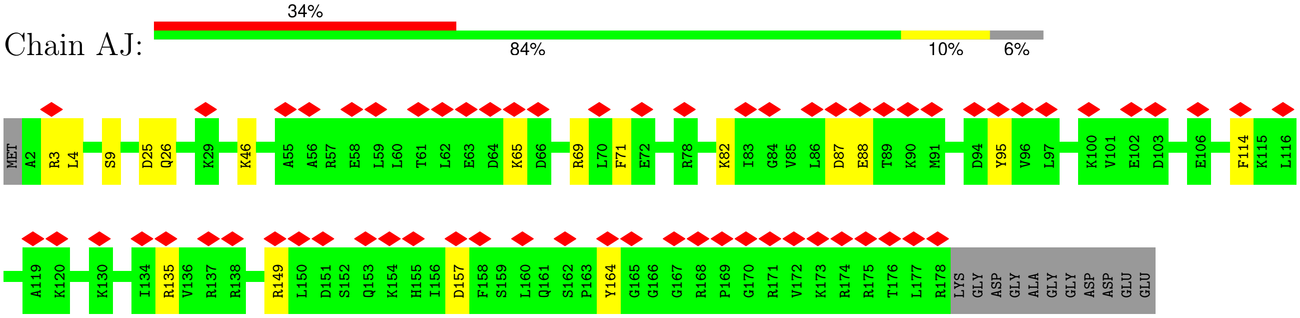
- Molecule 32: Small ribosomal subunit protein uS12



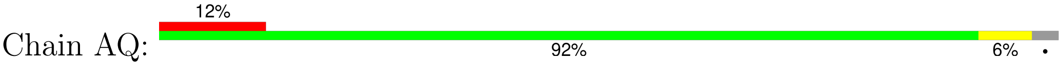
- Molecule 33: Small ribosomal subunit protein uS17

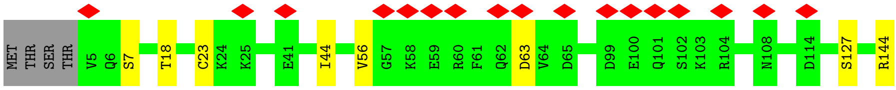


- Molecule 34: Small ribosomal subunit protein uS4



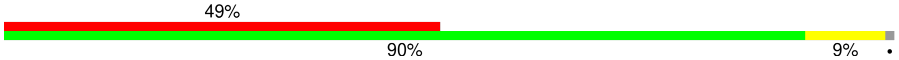
- Molecule 35: Small ribosomal subunit protein uS9

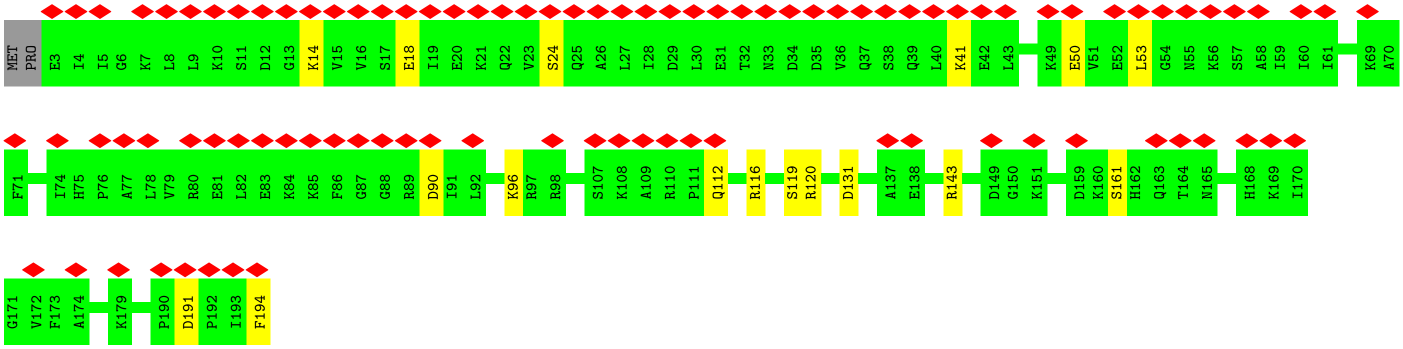




- Molecule 36: Small ribosomal subunit protein eS7

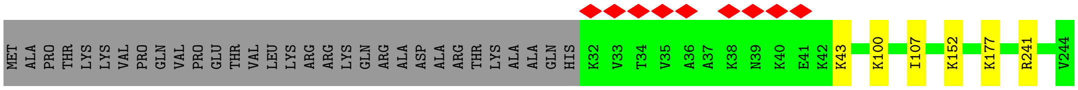
Chain AH:





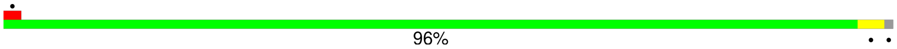
- Molecule 37: Large ribosomal subunit protein uL30

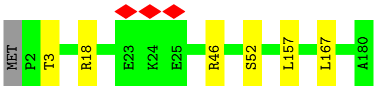
Chain CF:



- Molecule 38: Large ribosomal subunit protein eL20

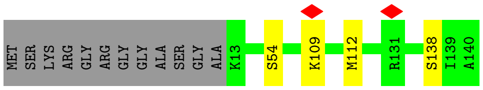
Chain CS:





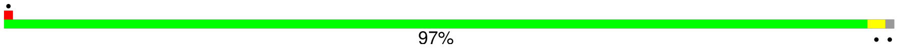
- Molecule 39: Large ribosomal subunit protein uL14

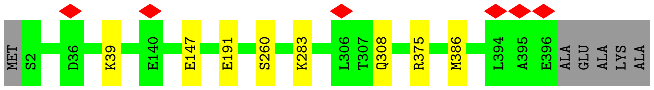
Chain CV:



- Molecule 40: Large ribosomal subunit protein uL3

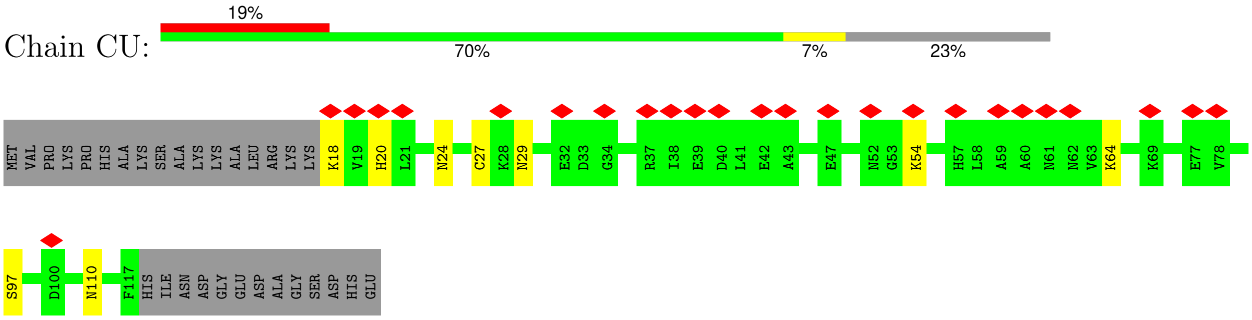
Chain CB:





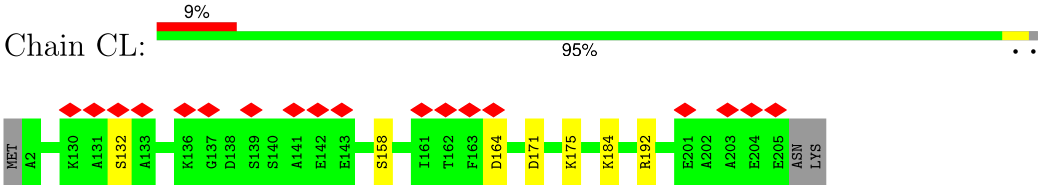
- Molecule 41: Large ribosomal subunit protein eL22

Chain CU:



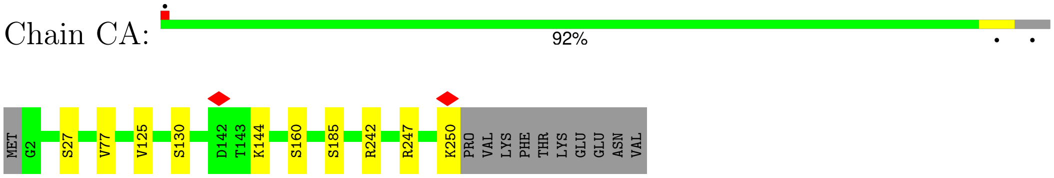
- Molecule 42: Large ribosomal subunit protein eL13

Chain CL:



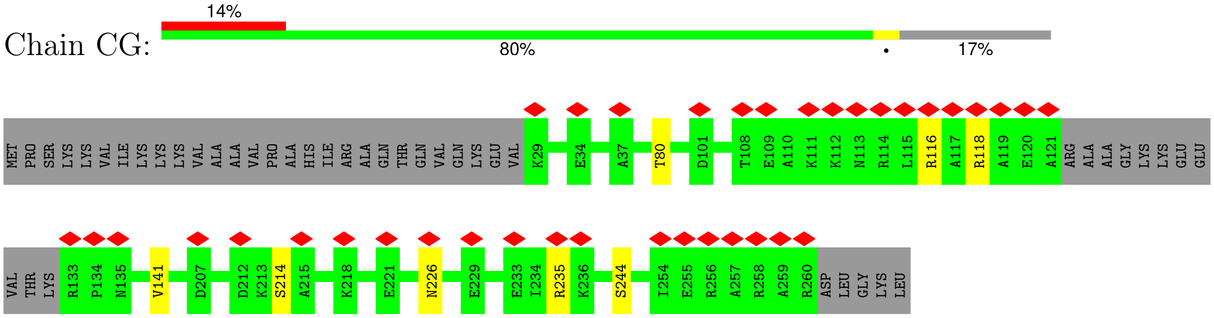
- Molecule 43: Large ribosomal subunit protein uL2

Chain CA:



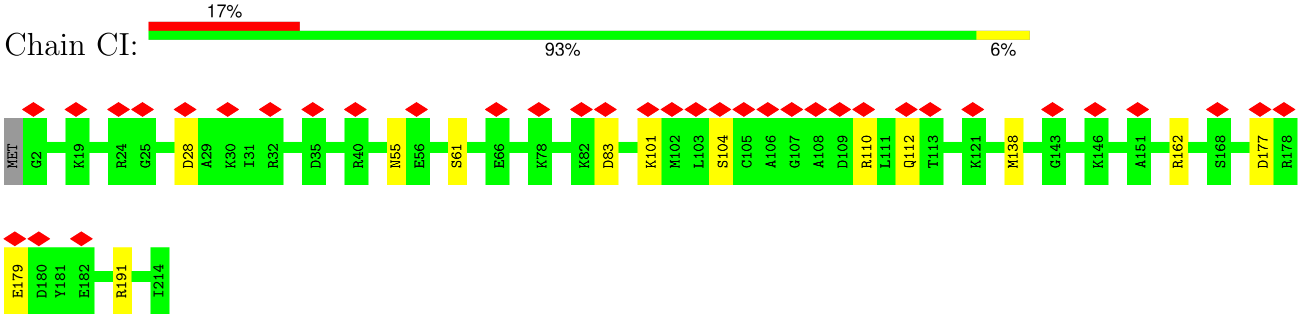
- Molecule 44: Large ribosomal subunit protein eL8

Chain CG:



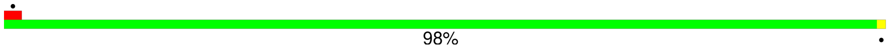
- Molecule 45: Large ribosomal subunit protein uL16

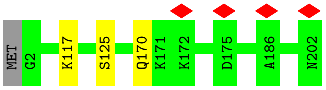
Chain CI:



- Molecule 46: Large ribosomal subunit protein uL13

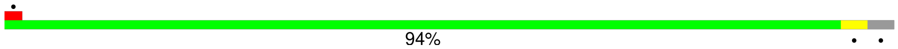
Chain CO:

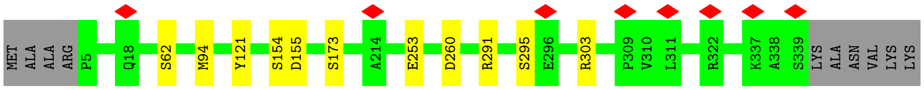




- Molecule 47: Large ribosomal subunit protein uL4

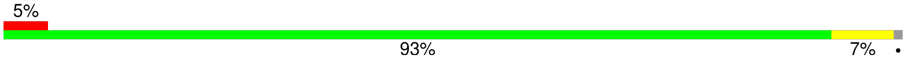
Chain CC:

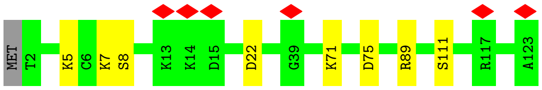




- Molecule 48: Large ribosomal subunit protein uL29

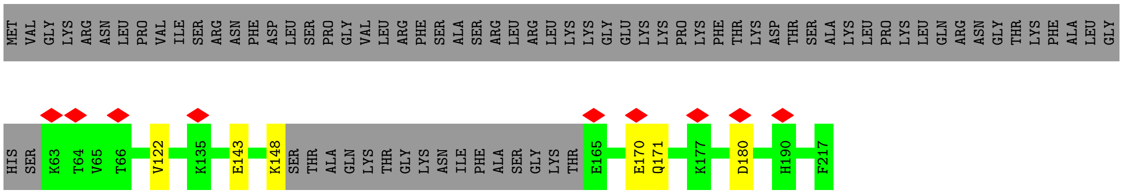
Chain Ch:





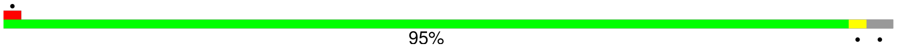
- Molecule 49: Large ribosomal subunit protein eL6

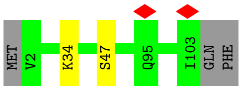
Chain CE:



- Molecule 50: Large ribosomal subunit protein eL42

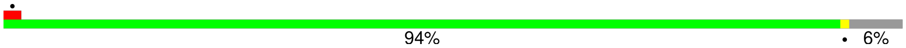
Chain Co:

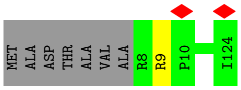




- Molecule 51: Large ribosomal subunit protein eL33

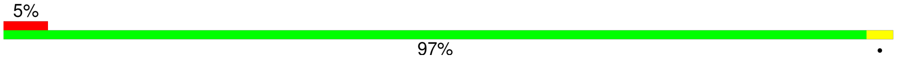
Chain Cf:

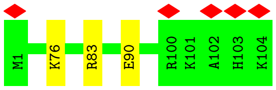




- Molecule 52: Large ribosomal subunit protein eL36

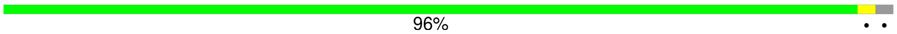
Chain Ci:

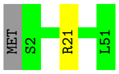




- Molecule 53: Large ribosomal subunit protein eL39

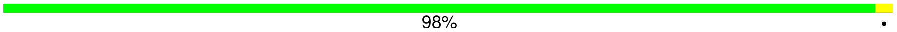
Chain Cl:

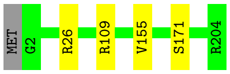




- Molecule 54: Large ribosomal subunit protein eL15

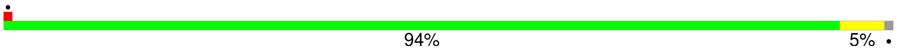
Chain CN:

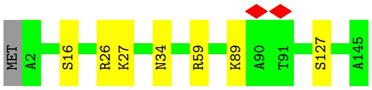




- Molecule 55: Large ribosomal subunit protein uL15

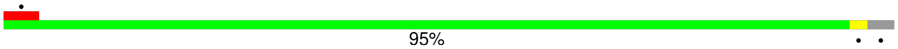
Chain Ca:

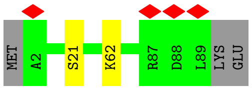




- Molecule 56: Large ribosomal subunit protein eL43

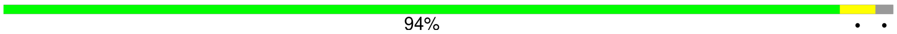
Chain Cp:

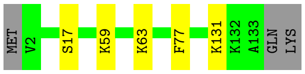




- Molecule 57: Large ribosomal subunit protein eL14

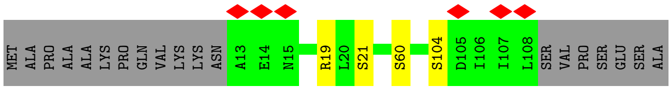
Chain CM:





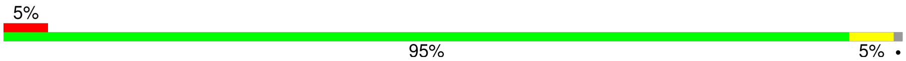
- Molecule 58: Large ribosomal subunit protein eL30

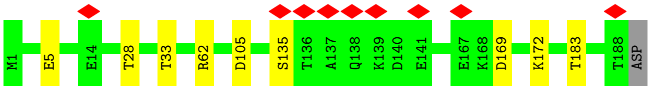
Chain Cc:



- Molecule 59: Large ribosomal subunit protein uL6

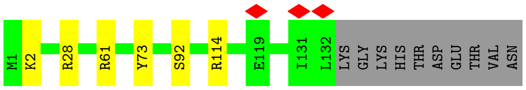
Chain CH:





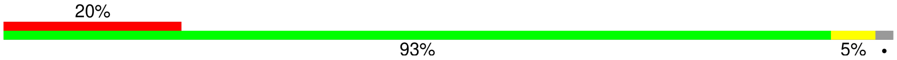
- Molecule 60: Large ribosomal subunit protein uL24

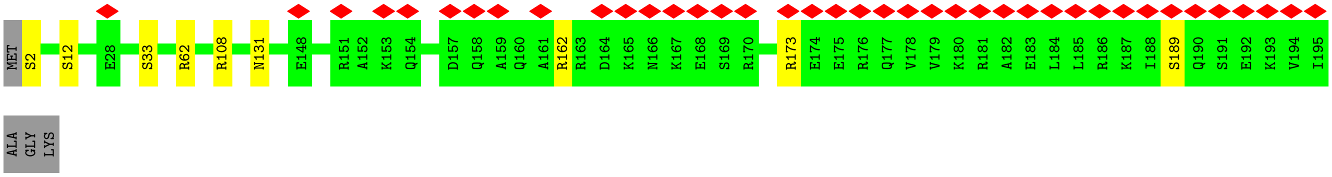
Chain CY:



- Molecule 61: Large ribosomal subunit protein eL19

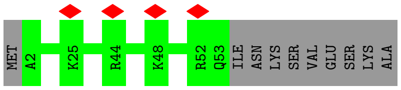
Chain CR:





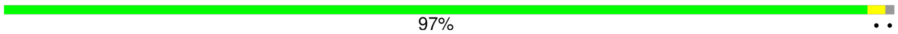
- Molecule 62: 60S ribosomal protein L29

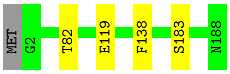
Chain Cb:



- Molecule 63: Large ribosomal subunit protein eL18

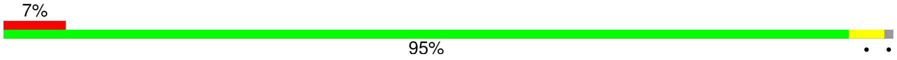
Chain CQ:

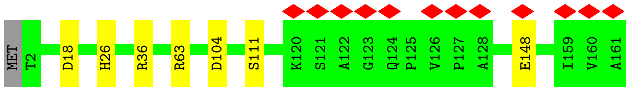




- Molecule 64: Large ribosomal subunit protein eL21

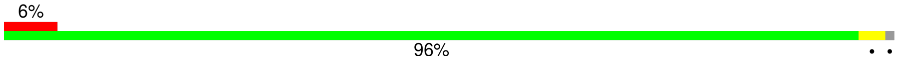
Chain CT:

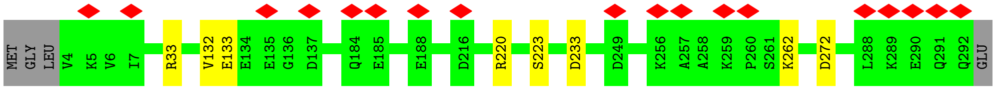




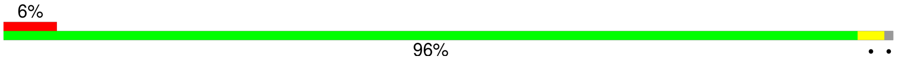
- Molecule 65: Large ribosomal subunit protein uL18

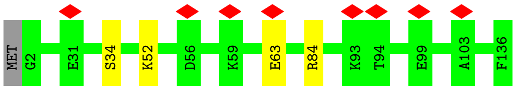
Chain CD:





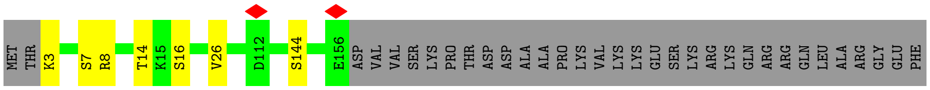
- Molecule 66: Large ribosomal subunit protein eL27

Chain CZ:


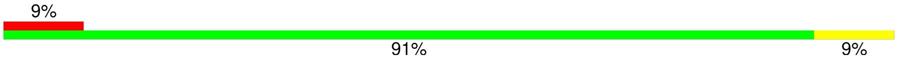


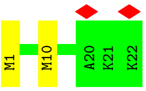
- Molecule 67: Large ribosomal subunit protein uL22

Chain CP:

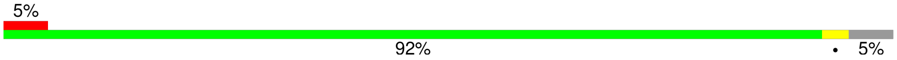



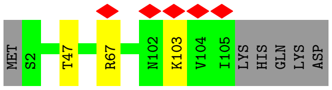
- Molecule 68: eL41

Chain Cn:




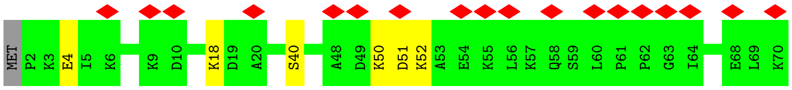
- Molecule 69: Large ribosomal subunit protein eL34

Chain Cg:




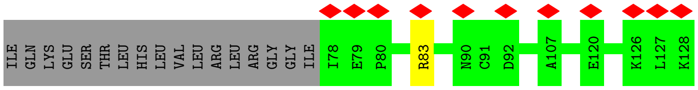
- Molecule 70: Large ribosomal subunit protein eL38

Chain Ck:

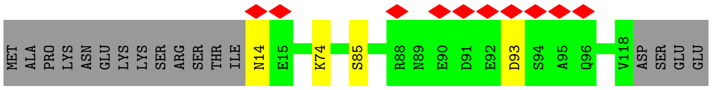
- Molecule 71: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Cm:

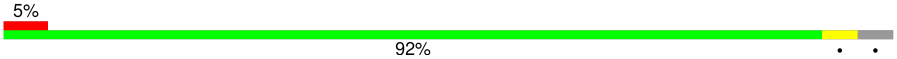
- Molecule 72: Large ribosomal subunit protein eL31

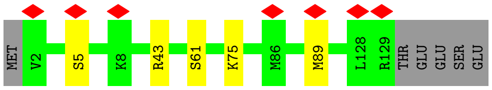
Chain Cd:



- Molecule 73: Large ribosomal subunit protein eL32

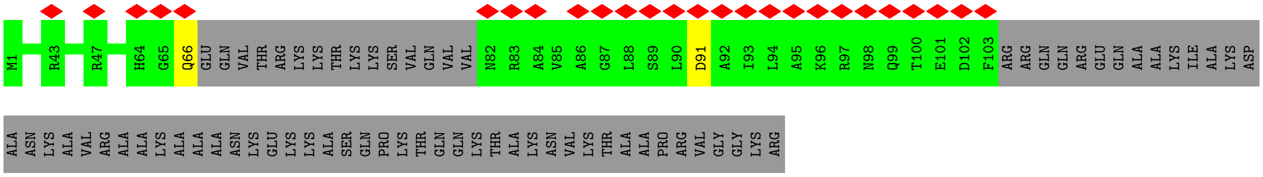
Chain Ce:





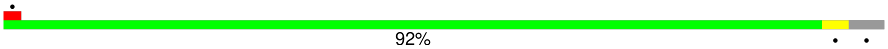
- Molecule 74: Large ribosomal subunit protein eL24

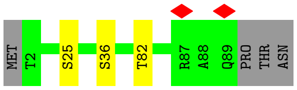
Chain CW:



- Molecule 75: Ribosomal protein L37

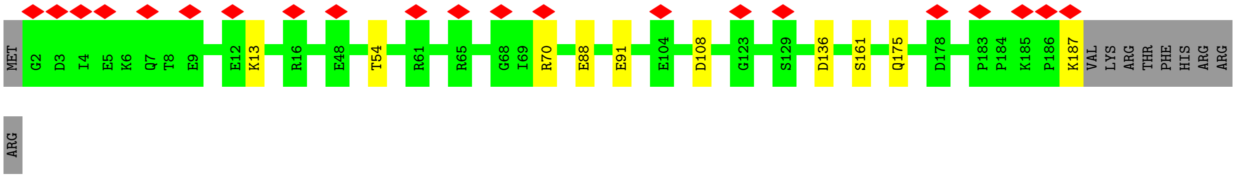
Chain Cj:





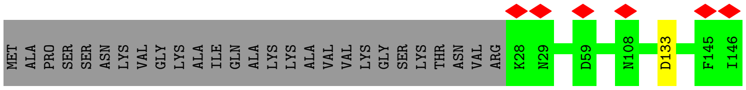
- Molecule 76: Large ribosomal subunit protein uL5B

Chain CJ:



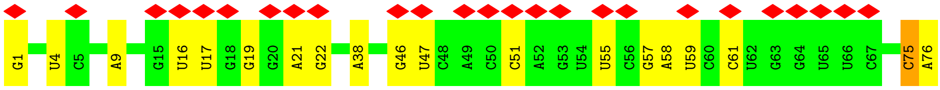
- Molecule 77: Large ribosomal subunit protein uL23B

Chain CX:



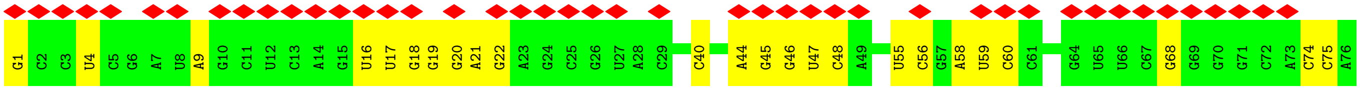
- Molecule 78: tRNA

Chain DA:



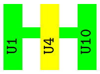
- Molecule 78: tRNA

Chain DB:



- Molecule 79: mRNA

Chain DC:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98135	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40.94	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.866	Depositor
Minimum map value	-1.111	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.182	Depositor
Map size (Å)	441.99997, 441.99997, 441.99997	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, 3HE

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	AD	0.30	0/1659	0.55	0/2226
2	AB	0.30	0/1710	0.51	0/2294
3	AC	0.32	0/1689	0.51	0/2289
4	AE	0.32	0/2053	0.56	0/2767
5	A7	0.65	0/2826	0.74	0/4402
6	A8	0.67	0/3477	0.78	1/5416 (0.0%)
7	B2	0.62	0/35235	0.76	3/54872 (0.0%)
8	A5	0.82	12/72151 (0.0%)	0.86	37/112424 (0.0%)
9	AR	0.29	0/988	0.58	0/1328
10	AK	0.31	0/790	0.50	0/1072
11	AW	0.32	0/1043	0.57	0/1399
12	AS	0.30	0/1225	0.56	0/1641
13	AT	0.30	0/1135	0.52	0/1524
14	Aa	0.33	0/819	0.60	0/1097
15	Af	0.27	0/404	0.55	0/540
16	AA	0.31	0/1645	0.50	0/2230
17	AO	0.31	0/1027	0.59	0/1377
18	AI	0.32	0/1698	0.56	0/2277
19	AF	0.29	0/1475	0.53	0/1986
20	AM	0.26	0/917	0.54	0/1231
21	AV	0.30	0/625	0.57	0/842
22	AN	0.36	0/1240	0.61	1/1658 (0.1%)
23	AZ	0.30	0/572	0.52	0/770
24	Ad	0.35	0/464	0.62	0/615
25	AY	0.31	0/1008	0.56	0/1344
26	AU	0.29	0/808	0.57	0/1090
27	AG	0.30	0/1863	0.55	0/2483
28	Ab	0.28	0/655	0.53	0/880
29	AP	0.31	0/1074	0.54	0/1436
30	Ac	0.28	0/521	0.62	0/695
31	Ae	0.30	0/367	0.66	0/480
32	AX	0.33	0/1112	0.53	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	AL	0.36	0/1182	0.57	0/1591
34	AJ	0.30	0/1490	0.61	0/1991
35	AQ	0.33	0/1143	0.57	0/1529
36	AH	0.29	0/1572	0.52	0/2114
37	CF	0.37	0/1782	0.52	0/2402
38	CS	0.38	0/1505	0.56	0/2026
39	CV	0.36	0/985	0.56	0/1319
40	CB	0.35	0/3247	0.55	0/4355
41	CU	0.34	0/838	0.51	0/1126
42	CL	0.32	0/1673	0.57	0/2235
43	CA	0.37	0/1932	0.59	0/2593
44	CG	0.31	0/1816	0.55	0/2443
45	CI	0.29	0/1767	0.59	0/2362
46	CO	0.36	0/1645	0.53	0/2198
47	CC	0.34	0/2706	0.55	0/3649
48	Ch	0.30	0/995	0.56	0/1318
49	CE	0.33	0/1140	0.51	0/1530
50	Co	0.36	0/850	0.56	0/1118
51	Cf	0.38	0/953	0.59	0/1283
52	Ci	0.31	0/845	0.56	0/1119
53	Cl	0.32	0/443	0.58	0/582
54	CN	0.39	0/1741	0.60	0/2328
55	Ca	0.37	0/1166	0.52	0/1561
56	Cp	0.39	0/687	0.60	0/915
57	CM	0.32	0/1062	0.55	0/1418
58	Cc	0.35	0/744	0.49	0/1004
59	CH	0.33	0/1528	0.57	0/2058
60	CY	0.30	0/1065	0.59	0/1421
61	CR	0.33	0/1658	0.59	0/2201
62	Cb	0.29	0/439	0.53	0/578
63	CQ	0.35	0/1498	0.58	0/2012
64	CT	0.36	0/1308	0.58	0/1755
65	CD	0.35	0/2368	0.53	0/3179
66	CZ	0.35	0/1123	0.52	0/1497
67	CP	0.35	0/1277	0.55	0/1717
68	Cn	0.30	0/210	0.71	0/266
69	Cg	0.38	0/847	0.60	0/1136
70	Ck	0.32	0/565	0.51	0/748
71	Cm	0.29	0/423	0.56	0/557
72	Cd	0.36	0/881	0.56	0/1184
73	Ce	0.35	0/1057	0.59	0/1407
74	CW	0.32	0/712	0.57	0/949
75	Cj	0.37	0/720	0.63	0/956

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	CJ	0.32	0/1533	0.56	0/2052
77	CX	0.33	0/972	0.51	0/1310
78	DA	0.51	1/1819 (0.1%)	0.79	2/2833 (0.1%)
78	DB	0.45	1/1819 (0.1%)	0.75	0/2833
79	DC	0.53	0/218	0.83	0/332
All	All	0.61	14/204224 (0.0%)	0.73	44/299262 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	AW	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A5	3465	U	C2-N3	56.83	1.77	1.37
8	A5	3465	U	N3-C4	48.70	1.82	1.38
8	A5	3465	U	N1-C2	43.86	1.78	1.38
8	A5	3465	U	N1-C6	38.73	1.72	1.38
8	A5	3462	C	C1'-N1	36.82	2.04	1.48
8	A5	3462	C	N1-C6	35.20	1.58	1.37
8	A5	3465	U	C4-C5	29.52	1.70	1.43
8	A5	3465	U	C5-C6	29.23	1.60	1.34
8	A5	3462	C	N1-C2	23.74	1.63	1.40
78	DB	1	G	OP3-P	-10.57	1.48	1.61
78	DA	1	G	OP3-P	-10.55	1.48	1.61
8	A5	3462	C	N3-C4	-7.54	1.28	1.33
8	A5	3462	C	C4-C5	-6.46	1.37	1.43
8	A5	3462	C	C2'-C1'	6.20	1.60	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A5	3462	C	C6-N1-C2	-94.93	82.33	120.30
8	A5	3462	C	C5-C6-N1	42.12	142.06	121.00
8	A5	3462	C	N1-C2-N3	29.02	139.51	119.20
8	A5	3462	C	N3-C4-C5	-23.74	112.41	121.90
8	A5	3462	C	N3-C2-O2	-23.09	105.73	121.90
8	A5	3462	C	C2-N1-C1'	17.11	137.62	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A5	3462	C	C6-N1-C1'	15.99	139.99	120.80
8	A5	600	U	OP1-P-O3'	-12.24	78.28	105.20
8	A5	3462	C	O4'-C1'-N1	11.20	117.16	108.20
8	A5	239	U	OP1-P-O3'	-11.03	80.93	105.20
8	A5	3388	U	OP1-P-O3'	-10.96	81.09	105.20
8	A5	239	U	OP2-P-O3'	-10.81	81.41	105.20
8	A5	588	G	OP1-P-O3'	-10.78	81.48	105.20
8	A5	3462	C	N1-C1'-C2'	10.31	127.41	114.00
8	A5	3388	U	OP2-P-O3'	-9.95	83.32	105.20
8	A5	3465	U	N1-C2-N3	-9.54	109.18	114.90
8	A5	588	G	OP2-P-O3'	-9.53	84.24	105.20
8	A5	601	G	OP1-P-OP2	9.37	133.66	119.60
22	AN	82	PRO	CA-N-CD	-8.58	99.49	111.50
8	A5	600	U	OP2-P-O3'	-8.47	86.56	105.20
7	B2	454	U	N3-C4-O4	-8.46	113.47	119.40
7	B2	454	U	C5-C4-O4	8.34	130.91	125.90
8	A5	240	G	OP1-P-OP2	7.71	131.17	119.60
8	A5	3389	U	OP1-P-OP2	7.29	130.53	119.60
8	A5	3465	U	C6-N1-C2	7.26	125.36	121.00
8	A5	589	U	OP1-P-OP2	7.07	130.20	119.60
8	A5	1567	G	O4'-C1'-N9	7.05	113.84	108.20
8	A5	3462	C	N3-C4-N4	7.01	122.91	118.00
8	A5	3462	C	N1-C2-O2	-6.91	114.75	118.90
78	DA	75	C	C2-N1-C1'	6.57	126.03	118.80
8	A5	3462	C	C4-C5-C6	6.55	120.68	117.40
8	A5	3462	C	C5-C4-N4	6.41	124.69	120.20
78	DA	75	C	N1-C2-O2	6.24	122.65	118.90
8	A5	412	G	O4'-C1'-N9	6.22	113.17	108.20
8	A5	3462	C	C2-N3-C4	6.17	122.99	119.90
8	A5	3465	U	C6-N1-C1'	-5.95	112.87	121.20
8	A5	1680	U	C2-N1-C1'	5.94	124.82	117.70
6	A8	112	A	O4'-C1'-N9	5.92	112.94	108.20
8	A5	2218	C	N3-C2-O2	-5.82	117.82	121.90
8	A5	1627	G	O4'-C1'-N9	5.43	112.54	108.20
8	A5	2215	G	O4'-C1'-N9	5.39	112.51	108.20
7	B2	1429	U	C2-N1-C1'	5.34	124.11	117.70
8	A5	3321	A	P-O3'-C3'	5.08	125.80	119.70
8	A5	1196	U	C5-C4-O4	-5.07	122.86	125.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AW	28	ARG	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	AD	209/247 (85%)	206 (99%)	3 (1%)	0	100	100
2	AB	208/257 (81%)	200 (96%)	8 (4%)	0	100	100
3	AC	213/272 (78%)	207 (97%)	6 (3%)	0	100	100
4	AE	253/259 (98%)	244 (96%)	9 (4%)	0	100	100
9	AR	119/130 (92%)	111 (93%)	8 (7%)	0	100	100
10	AK	91/149 (61%)	88 (97%)	3 (3%)	0	100	100
11	AW	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	16	24
12	AS	146/154 (95%)	143 (98%)	3 (2%)	0	100	100
13	AT	138/146 (94%)	132 (96%)	6 (4%)	0	100	100
14	Aa	97/117 (83%)	94 (97%)	3 (3%)	0	100	100
15	Af	48/163 (29%)	44 (92%)	4 (8%)	0	100	100
16	AA	203/276 (74%)	194 (96%)	9 (4%)	0	100	100
17	AO	133/152 (88%)	129 (97%)	4 (3%)	0	100	100
18	AI	205/208 (99%)	198 (97%)	7 (3%)	0	100	100
19	AF	181/210 (86%)	170 (94%)	10 (6%)	1 (1%)	22	32
20	AM	113/140 (81%)	101 (89%)	12 (11%)	0	100	100
21	AV	79/88 (90%)	77 (98%)	2 (2%)	0	100	100
22	AN	149/151 (99%)	147 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	AZ	69/117 (59%)	68 (99%)	1 (1%)	0	100	100
24	Ad	53/56 (95%)	53 (100%)	0	0	100	100
25	AY	121/131 (92%)	114 (94%)	7 (6%)	0	100	100
26	AU	98/117 (84%)	90 (92%)	8 (8%)	0	100	100
27	AG	226/246 (92%)	221 (98%)	5 (2%)	0	100	100
28	Ab	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
29	AP	130/151 (86%)	124 (95%)	6 (5%)	0	100	100
30	Ac	63/65 (97%)	63 (100%)	0	0	100	100
31	Ae	41/130 (32%)	37 (90%)	4 (10%)	0	100	100
32	AX	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
33	AL	141/155 (91%)	137 (97%)	4 (3%)	0	100	100
34	AJ	175/189 (93%)	168 (96%)	7 (4%)	0	100	100
35	AQ	138/144 (96%)	133 (96%)	5 (4%)	0	100	100
36	AH	190/194 (98%)	177 (93%)	13 (7%)	0	100	100
37	CF	211/244 (86%)	203 (96%)	8 (4%)	0	100	100
38	CS	177/180 (98%)	171 (97%)	6 (3%)	0	100	100
39	CV	126/140 (90%)	126 (100%)	0	0	100	100
40	CB	393/401 (98%)	387 (98%)	6 (2%)	0	100	100
41	CU	98/130 (75%)	95 (97%)	3 (3%)	0	100	100
42	CL	202/207 (98%)	200 (99%)	2 (1%)	0	100	100
43	CA	247/260 (95%)	238 (96%)	9 (4%)	0	100	100
44	CG	217/265 (82%)	214 (99%)	3 (1%)	0	100	100
45	CI	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
46	CO	199/202 (98%)	196 (98%)	3 (2%)	0	100	100
47	CC	333/345 (96%)	320 (96%)	13 (4%)	0	100	100
48	Ch	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
49	CE	135/217 (62%)	127 (94%)	8 (6%)	0	100	100
50	Co	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
51	Cf	115/124 (93%)	112 (97%)	3 (3%)	0	100	100
52	Ci	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
53	Cl	48/51 (94%)	48 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	CN	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
55	Ca	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
56	Cp	86/91 (94%)	84 (98%)	2 (2%)	0	100	100
57	CM	130/135 (96%)	127 (98%)	3 (2%)	0	100	100
58	Cc	94/115 (82%)	93 (99%)	1 (1%)	0	100	100
59	CH	186/189 (98%)	174 (94%)	12 (6%)	0	100	100
60	CY	130/142 (92%)	126 (97%)	4 (3%)	0	100	100
61	CR	192/198 (97%)	191 (100%)	1 (0%)	0	100	100
62	Cb	50/62 (81%)	47 (94%)	3 (6%)	0	100	100
63	CQ	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
64	CT	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
65	CD	287/293 (98%)	279 (97%)	8 (3%)	0	100	100
66	CZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
67	CP	152/187 (81%)	147 (97%)	5 (3%)	0	100	100
68	Cn	20/22 (91%)	19 (95%)	1 (5%)	0	100	100
69	Cg	102/110 (93%)	101 (99%)	1 (1%)	0	100	100
70	Ck	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
71	Cm	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
72	Cd	103/122 (84%)	100 (97%)	3 (3%)	0	100	100
73	Ce	126/134 (94%)	123 (98%)	3 (2%)	0	100	100
74	CW	84/159 (53%)	82 (98%)	2 (2%)	0	100	100
75	Cj	86/92 (94%)	84 (98%)	2 (2%)	0	100	100
76	CJ	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
77	CX	117/146 (80%)	115 (98%)	2 (2%)	0	100	100
All	All	10473/11907 (88%)	10136 (97%)	335 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	AW	29	PRO
19	AF	86	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AD	173/204 (85%)	164 (95%)	9 (5%)	19	32
2	AB	191/228 (84%)	177 (93%)	14 (7%)	11	18
3	AC	175/202 (87%)	161 (92%)	14 (8%)	10	15
4	AE	218/221 (99%)	211 (97%)	7 (3%)	34	52
9	AR	111/118 (94%)	104 (94%)	7 (6%)	15	24
10	AK	82/122 (67%)	80 (98%)	2 (2%)	44	64
11	AW	110/111 (99%)	105 (96%)	5 (4%)	23	37
12	AS	130/134 (97%)	115 (88%)	15 (12%)	4	6
13	AT	116/120 (97%)	110 (95%)	6 (5%)	19	32
14	Aa	84/94 (89%)	80 (95%)	4 (5%)	21	35
15	Af	42/134 (31%)	34 (81%)	8 (19%)	1	1
16	AA	172/228 (75%)	157 (91%)	15 (9%)	8	12
17	AO	103/115 (90%)	96 (93%)	7 (7%)	13	21
18	AI	172/173 (99%)	159 (92%)	13 (8%)	11	17
19	AF	156/172 (91%)	148 (95%)	8 (5%)	20	33
20	AM	94/108 (87%)	83 (88%)	11 (12%)	4	5
21	AV	68/75 (91%)	59 (87%)	9 (13%)	3	3
22	AN	130/130 (100%)	122 (94%)	8 (6%)	15	24
23	AZ	62/98 (63%)	60 (97%)	2 (3%)	34	52
24	Ad	46/47 (98%)	42 (91%)	4 (9%)	8	12
25	AY	107/112 (96%)	103 (96%)	4 (4%)	29	46
26	AU	90/104 (86%)	80 (89%)	10 (11%)	5	7
27	AG	195/212 (92%)	183 (94%)	12 (6%)	15	24
28	Ab	75/76 (99%)	73 (97%)	2 (3%)	40	60
29	AP	112/128 (88%)	102 (91%)	10 (9%)	8	11
30	Ac	58/58 (100%)	51 (88%)	7 (12%)	4	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Ae	37/107 (35%)	31 (84%)	6 (16%)	2	2
32	AX	115/118 (98%)	107 (93%)	8 (7%)	12	20
33	AL	126/136 (93%)	119 (94%)	7 (6%)	17	29
34	AJ	160/167 (96%)	142 (89%)	18 (11%)	4	6
35	AQ	115/119 (97%)	107 (93%)	8 (7%)	12	20
36	AH	170/172 (99%)	153 (90%)	17 (10%)	6	8
37	CF	184/210 (88%)	178 (97%)	6 (3%)	33	51
38	CS	156/157 (99%)	150 (96%)	6 (4%)	28	45
39	CV	101/107 (94%)	97 (96%)	4 (4%)	27	42
40	CB	335/338 (99%)	327 (98%)	8 (2%)	44	64
41	CU	92/116 (79%)	83 (90%)	9 (10%)	6	9
42	CL	167/170 (98%)	160 (96%)	7 (4%)	25	41
43	CA	191/202 (95%)	181 (95%)	10 (5%)	19	32
44	CG	192/228 (84%)	184 (96%)	8 (4%)	25	41
45	CI	179/180 (99%)	166 (93%)	13 (7%)	11	18
46	CO	165/166 (99%)	162 (98%)	3 (2%)	54	73
47	CC	279/286 (98%)	268 (96%)	11 (4%)	27	44
48	Ch	106/107 (99%)	98 (92%)	8 (8%)	11	17
49	CE	122/188 (65%)	116 (95%)	6 (5%)	21	34
50	Co	90/93 (97%)	88 (98%)	2 (2%)	47	67
51	Cf	95/99 (96%)	94 (99%)	1 (1%)	70	83
52	Ci	86/86 (100%)	83 (96%)	3 (4%)	31	48
53	Cl	46/47 (98%)	45 (98%)	1 (2%)	47	67
54	CN	172/173 (99%)	168 (98%)	4 (2%)	45	65
55	Ca	116/117 (99%)	109 (94%)	7 (6%)	16	25
56	Cp	68/71 (96%)	66 (97%)	2 (3%)	37	57
57	CM	111/114 (97%)	106 (96%)	5 (4%)	23	37
58	Cc	80/95 (84%)	76 (95%)	4 (5%)	20	33
59	CH	167/168 (99%)	158 (95%)	9 (5%)	18	31
60	CY	114/123 (93%)	108 (95%)	6 (5%)	19	31
61	CR	172/174 (99%)	163 (95%)	9 (5%)	19	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	Cb	47/56 (84%)	47 (100%)	0	100	100
63	CQ	152/153 (99%)	148 (97%)	4 (3%)	41	61
64	CT	135/136 (99%)	128 (95%)	7 (5%)	19	32
65	CD	239/242 (99%)	231 (97%)	8 (3%)	33	51
66	CZ	119/120 (99%)	115 (97%)	4 (3%)	32	49
67	CP	130/159 (82%)	123 (95%)	7 (5%)	18	31
68	Cn	20/20 (100%)	18 (90%)	2 (10%)	6	8
69	Cg	92/98 (94%)	89 (97%)	3 (3%)	33	51
70	Ck	63/64 (98%)	57 (90%)	6 (10%)	7	10
71	Cm	47/115 (41%)	46 (98%)	1 (2%)	48	69
72	Cd	96/112 (86%)	92 (96%)	4 (4%)	25	41
73	Ce	111/117 (95%)	106 (96%)	5 (4%)	23	37
74	CW	73/128 (57%)	71 (97%)	2 (3%)	40	60
75	Cj	73/77 (95%)	70 (96%)	3 (4%)	26	42
76	CJ	160/170 (94%)	150 (94%)	10 (6%)	15	24
77	CX	103/124 (83%)	102 (99%)	1 (1%)	73	85
All	All	9041/10049 (90%)	8545 (94%)	496 (6%)	20	29

All (496) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AD	8	THR
1	AD	59	ASN
1	AD	64	ARG
1	AD	104	CYS
1	AD	126	ARG
1	AD	150	LYS
1	AD	158	LEU
1	AD	176	HIS
1	AD	197	ARG
2	AB	23	PHE
2	AB	30	ASP
2	AB	51	GLN
2	AB	75	SER
2	AB	78	ASP
2	AB	93	ASN

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Mol	Chain	Res	Type
2	AB	123	THR
2	AB	144	SER
2	AB	146	ASN
2	AB	161	LYS
2	AB	184	SER
2	AB	197	LYS
2	AB	225	ARG
2	AB	228	ASP
3	AC	69	GLU
3	AC	70	LYS
3	AC	75	LEU
3	AC	95	CYS
3	AC	118	THR
3	AC	141	LYS
3	AC	159	VAL
3	AC	181	THR
3	AC	188	MET
3	AC	225	SER
3	AC	232	PHE
3	AC	241	GLN
3	AC	244	TYR
3	AC	260	SER
4	AE	114	GLN
4	AE	135	VAL
4	AE	145	THR
4	AE	164	SER
4	AE	173	LYS
4	AE	186	ARG
4	AE	246	SER
9	AR	5	ARG
9	AR	72	LYS
9	AR	79	GLU
9	AR	87	GLU
9	AR	92	ASP
9	AR	94	SER
9	AR	100	LYS
10	AK	48	LYS
10	AK	88	VAL
11	AW	28	ARG
11	AW	36	ARG
11	AW	73	SER
11	AW	76	SER

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Mol	Chain	Res	Type
11	AW	112	ASP
12	AS	2	SER
12	AS	17	ASN
12	AS	43	VAL
12	AS	54	LYS
12	AS	62	GLU
12	AS	63	ASP
12	AS	69	THR
12	AS	73	ASN
12	AS	78	LYS
12	AS	83	PHE
12	AS	100	SER
12	AS	126	TYR
12	AS	135	HIS
12	AS	142	LYS
12	AS	145	THR
13	AT	26	SER
13	AT	35	SER
13	AT	87	VAL
13	AT	100	LEU
13	AT	106	GLN
13	AT	134	ARG
14	Aa	26	CYS
14	Aa	33	ASP
14	Aa	87	ARG
14	Aa	100	ARG
15	Af	94	LEU
15	Af	99	TYR
15	Af	101	LYS
15	Af	107	LYS
15	Af	110	ARG
15	Af	112	ARG
15	Af	132	ARG
15	Af	140	ASP
16	AA	2	SER
16	AA	8	SER
16	AA	12	GLU
16	AA	16	MET
16	AA	34	MET
16	AA	37	TYR
16	AA	49	ILE
16	AA	85	ARG

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Mol	Chain	Res	Type
16	AA	107	CYS
16	AA	146	SER
16	AA	158	ASP
16	AA	170	SER
16	AA	195	PHE
16	AA	205	ASP
16	AA	210	ARG
17	AO	37	SER
17	AO	115	SER
17	AO	139	ASP
17	AO	140	CYS
17	AO	143	ARG
17	AO	147	ARG
17	AO	152	LEU
18	AI	4	SER
18	AI	7	SER
18	AI	45	LEU
18	AI	56	ARG
18	AI	92	ARG
18	AI	103	SER
18	AI	105	ASP
18	AI	132	GLU
18	AI	138	ASN
18	AI	139	LYS
18	AI	142	SER
18	AI	144	HIS
18	AI	206	LYS
19	AF	22	GLU
19	AF	37	SER
19	AF	38	ASP
19	AF	43	ASP
19	AF	61	ARG
19	AF	146	ASP
19	AF	190	SER
19	AF	193	SER
20	AM	31	ARG
20	AM	50	LEU
20	AM	52	LYS
20	AM	90	LYS
20	AM	101	LYS
20	AM	104	LYS
20	AM	109	ARG

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Mol	Chain	Res	Type
20	AM	116	SER
20	AM	127	GLN
20	AM	132	LEU
20	AM	136	PHE
21	AV	1	MET
21	AV	3	ASN
21	AV	21	ASN
21	AV	35	ASP
21	AV	42	GLU
21	AV	50	LYS
21	AV	53	ARG
21	AV	66	SER
21	AV	68	ASP
22	AN	3	ARG
22	AN	4	MET
22	AN	9	LYS
22	AN	48	SER
22	AN	69	ASN
22	AN	121	ARG
22	AN	125	LEU
22	AN	143	SER
23	AZ	76	ARG
23	AZ	98	HIS
24	Ad	8	PHE
24	Ad	9	SER
24	Ad	20	SER
24	Ad	40	ARG
25	AY	39	ASP
25	AY	78	THR
25	AY	99	LYS
25	AY	126	VAL
26	AU	17	HIS
26	AU	18	ARG
26	AU	23	LEU
26	AU	25	SER
26	AU	50	LYS
26	AU	54	ARG
26	AU	97	LEU
26	AU	98	ARG
26	AU	110	ASP
26	AU	115	ARG
27	AG	31	ARG

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Mol	Chain	Res	Type
27	AG	33	SER
27	AG	96	SER
27	AG	114	VAL
27	AG	126	ASP
27	AG	149	LYS
27	AG	150	HIS
27	AG	162	LYS
27	AG	163	THR
27	AG	194	GLN
27	AG	196	ARG
27	AG	218	LYS
28	Ab	37	CYS
28	Ab	41	PHE
29	AP	20	LYS
29	AP	24	ARG
29	AP	27	ASP
29	AP	29	ASP
29	AP	36	ARG
29	AP	57	ARG
29	AP	58	LYS
29	AP	117	MET
29	AP	133	LYS
29	AP	146	ARG
30	Ac	1	MET
30	Ac	34	ASN
30	Ac	35	ASN
30	Ac	37	SER
30	Ac	56	GLU
30	Ac	60	GLU
30	Ac	62	ARG
31	Ae	79	ARG
31	Ae	95	LYS
31	Ae	98	LYS
31	Ae	111	ARG
31	Ae	112	ARG
31	Ae	130	SER
32	AX	35	ARG
32	AX	38	SER
32	AX	45	SER
32	AX	98	ASP
32	AX	105	PHE
32	AX	127	ASN

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Mol	Chain	Res	Type
32	AX	139	GLU
32	AX	140	ARG
33	AL	27	SER
33	AL	29	LYS
33	AL	45	ARG
33	AL	49	GLU
33	AL	54	ASP
33	AL	66	ARG
33	AL	138	ASN
34	AJ	3	ARG
34	AJ	4	LEU
34	AJ	9	SER
34	AJ	25	ASP
34	AJ	26	GLN
34	AJ	46	LYS
34	AJ	65	LYS
34	AJ	69	ARG
34	AJ	71	PHE
34	AJ	82	LYS
34	AJ	87	ASP
34	AJ	88	GLU
34	AJ	95	TYR
34	AJ	114	PHE
34	AJ	135	ARG
34	AJ	149	ARG
34	AJ	157	ASP
34	AJ	164	TYR
35	AQ	7	SER
35	AQ	18	THR
35	AQ	23	CYS
35	AQ	44	ILE
35	AQ	56	VAL
35	AQ	63	ASP
35	AQ	127	SER
35	AQ	144	ARG
36	AH	14	LYS
36	AH	18	GLU
36	AH	24	SER
36	AH	41	LYS
36	AH	50	GLU
36	AH	53	LEU
36	AH	90	ASP

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Mol	Chain	Res	Type
36	AH	96	LYS
36	AH	112	GLN
36	AH	116	ARG
36	AH	119	SER
36	AH	120	ARG
36	AH	131	ASP
36	AH	143	ARG
36	AH	161	SER
36	AH	191	ASP
36	AH	194	PHE
37	CF	43	LYS
37	CF	100	LYS
37	CF	107	ILE
37	CF	152	LYS
37	CF	177	LYS
37	CF	241	ARG
38	CS	3	THR
38	CS	18	ARG
38	CS	46	ARG
38	CS	52	SER
38	CS	157	LEU
38	CS	167	LEU
39	CV	54	SER
39	CV	109	LYS
39	CV	112	MET
39	CV	138	SER
40	CB	39	LYS
40	CB	147	GLU
40	CB	191	GLU
40	CB	260	SER
40	CB	283	LYS
40	CB	308	GLN
40	CB	375	ARG
40	CB	386	MET
41	CU	18	LYS
41	CU	20	HIS
41	CU	24	ASN
41	CU	27	CYS
41	CU	29	ASN
41	CU	54	LYS
41	CU	64	LYS
41	CU	97	SER

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Mol	Chain	Res	Type
41	CU	110	ASN
42	CL	132	SER
42	CL	158	SER
42	CL	164	ASP
42	CL	171	ASP
42	CL	175	LYS
42	CL	184	LYS
42	CL	192	ARG
43	CA	27	SER
43	CA	77	VAL
43	CA	125	VAL
43	CA	130	SER
43	CA	144	LYS
43	CA	160	SER
43	CA	185	SER
43	CA	242	ARG
43	CA	247	ARG
43	CA	250	LYS
44	CG	80	THR
44	CG	116	ARG
44	CG	118	ARG
44	CG	141	VAL
44	CG	214	SER
44	CG	226	ASN
44	CG	235	ARG
44	CG	244	SER
45	CI	28	ASP
45	CI	55	ASN
45	CI	61	SER
45	CI	83	ASP
45	CI	101	LYS
45	CI	104	SER
45	CI	110	ARG
45	CI	112	GLN
45	CI	138	MET
45	CI	162	ARG
45	CI	177	ASP
45	CI	179	GLU
45	CI	191	ARG
46	CO	117	LYS
46	CO	125	SER
46	CO	170	GLN

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Mol	Chain	Res	Type
47	CC	62	SER
47	CC	94	MET
47	CC	121	TYR
47	CC	154	SER
47	CC	155	ASP
47	CC	173	SER
47	CC	253	GLU
47	CC	260	ASP
47	CC	291	ARG
47	CC	295	SER
47	CC	303	ARG
48	Ch	5	LYS
48	Ch	7	LYS
48	Ch	8	SER
48	Ch	22	ASP
48	Ch	71	LYS
48	Ch	75	ASP
48	Ch	89	ARG
48	Ch	111	SER
49	CE	122	VAL
49	CE	143	GLU
49	CE	148	LYS
49	CE	170	GLU
49	CE	171	GLN
49	CE	180	ASP
50	Co	34	LYS
50	Co	47	SER
51	Cf	9	ARG
52	Ci	76	LYS
52	Ci	83	ARG
52	Ci	90	GLU
53	Cl	21	ARG
54	CN	26	ARG
54	CN	109	ARG
54	CN	155	VAL
54	CN	171	SER
55	Ca	16	SER
55	Ca	26	ARG
55	Ca	27	LYS
55	Ca	34	ASN
55	Ca	59	ARG
55	Ca	89	LYS

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Mol	Chain	Res	Type
55	Ca	127	SER
56	Cp	21	SER
56	Cp	62	LYS
57	CM	17	SER
57	CM	59	LYS
57	CM	63	LYS
57	CM	77	PHE
57	CM	131	LYS
58	Cc	19	ARG
58	Cc	21	SER
58	Cc	60	SER
58	Cc	104	SER
59	CH	5	GLU
59	CH	28	THR
59	CH	33	THR
59	CH	62	ARG
59	CH	105	ASP
59	CH	135	SER
59	CH	169	ASP
59	CH	172	LYS
59	CH	183	THR
60	CY	2	LYS
60	CY	28	ARG
60	CY	61	ARG
60	CY	73	TYR
60	CY	92	SER
60	CY	114	ARG
61	CR	2	SER
61	CR	12	SER
61	CR	33	SER
61	CR	62	ARG
61	CR	108	ARG
61	CR	131	ASN
61	CR	162	ARG
61	CR	173	ARG
61	CR	189	SER
63	CQ	82	THR
63	CQ	119	GLU
63	CQ	138	PHE
63	CQ	183	SER
64	CT	18	ASP
64	CT	26	HIS

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Mol	Chain	Res	Type
64	CT	36	ARG
64	CT	63	ARG
64	CT	104	ASP
64	CT	111	SER
64	CT	148	GLU
65	CD	33	ARG
65	CD	132	VAL
65	CD	133	GLU
65	CD	220	ARG
65	CD	223	SER
65	CD	233	ASP
65	CD	262	LYS
65	CD	272	ASP
66	CZ	34	SER
66	CZ	52	LYS
66	CZ	63	GLU
66	CZ	84	ARG
67	CP	3	LYS
67	CP	7	SER
67	CP	8	ARG
67	CP	14	THR
67	CP	16	SER
67	CP	26	VAL
67	CP	144	SER
68	Cn	1	MET
68	Cn	10	MET
69	Cg	47	THR
69	Cg	67	ARG
69	Cg	103	LYS
70	Ck	4	GLU
70	Ck	18	LYS
70	Ck	40	SER
70	Ck	50	LYS
70	Ck	51	ASP
70	Ck	52	LYS
71	Cm	83	ARG
72	Cd	14	ASN
72	Cd	74	LYS
72	Cd	85	SER
72	Cd	93	ASP
73	Ce	5	SER
73	Ce	43	ARG

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Mol	Chain	Res	Type
73	Ce	61	SER
73	Ce	75	LYS
73	Ce	89	MET
74	CW	66	GLN
74	CW	91	ASP
75	Cj	25	SER
75	Cj	36	SER
75	Cj	82	THR
76	CJ	13	LYS
76	CJ	54	THR
76	CJ	70	ARG
76	CJ	88	GLU
76	CJ	91	GLU
76	CJ	108	ASP
76	CJ	136	ASP
76	CJ	161	SER
76	CJ	175	GLN
76	CJ	187	LYS
77	CX	133	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	AD	5	GLN
17	AO	114	GLN
20	AM	44	HIS
20	AM	140	ASN
21	AV	21	ASN
33	AL	18	ASN
34	AJ	155	HIS
37	CF	98	HIS
67	CP	12	ASN
74	CW	82	ASN
77	CX	115	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A7	118/119 (99%)	8 (6%)	0
6	A8	144/153 (94%)	29 (20%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	B2	1456/1754 (83%)	340 (23%)	28 (1%)
78	DA	75/76 (98%)	18 (24%)	0
78	DB	75/76 (98%)	22 (29%)	1 (1%)
79	DC	8/10 (80%)	1 (12%)	0
8	A5	3004/3510 (85%)	634 (21%)	74 (2%)
All	All	4880/5698 (85%)	1052 (21%)	103 (2%)

All (1052) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A7	7	G
5	A7	53	U
5	A7	54	A
5	A7	64	G
5	A7	97	G
5	A7	98	G
5	A7	100	A
5	A7	110	G
6	A8	20	G
6	A8	21	G
6	A8	22	U
6	A8	23	U
6	A8	32	U
6	A8	34	U
6	A8	35	C
6	A8	51	U
6	A8	52	U
6	A8	59	U
6	A8	62	C
6	A8	63	U
6	A8	68	A
6	A8	77	A
6	A8	89	U
6	A8	93	G
6	A8	95	A
6	A8	100	C
6	A8	102	A
6	A8	104	C
6	A8	105	G
6	A8	110	G
6	A8	112	A
6	A8	113	C

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Mol	Chain	Res	Type
6	A8	115	A
6	A8	116	A
6	A8	121	G
6	A8	122	C
6	A8	147	G
7	B2	5	C
7	B2	18	U
7	B2	34	A
7	B2	36	G
7	B2	42	G
7	B2	43	A
7	B2	45	U
7	B2	47	A
7	B2	54	C
7	B2	57	G
7	B2	58	C
7	B2	65	U
7	B2	66	C
7	B2	67	A
7	B2	73	G
7	B2	94	G
7	B2	104	C
7	B2	105	A
7	B2	109	U
7	B2	111	U
7	B2	112	C
7	B2	116	G
7	B2	126	U
7	B2	128	G
7	B2	129	A
7	B2	130	U
7	B2	137	G
7	B2	140	A
7	B2	142	U
7	B2	143	A
7	B2	152	A
7	B2	154	U
7	B2	160	C
7	B2	168	C
7	B2	169	C
7	B2	181	C
7	B2	184	G

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Mol	Chain	Res	Type
7	B2	187	G
7	B2	191	U
7	B2	197	G
7	B2	227	G
7	B2	229	U
7	B2	233	U
7	B2	234	C
7	B2	238	A
7	B2	241	A
7	B2	243	G
7	B2	245	A
7	B2	249	U
7	B2	250	A
7	B2	251	C
7	B2	254	U
7	B2	270	C
7	B2	274	C
7	B2	296	C
7	B2	298	A
7	B2	302	G
7	B2	309	G
7	B2	317	G
7	B2	318	A
7	B2	332	U
7	B2	339	A
7	B2	340	A
7	B2	341	C
7	B2	350	A
7	B2	354	U
7	B2	357	G
7	B2	370	G
7	B2	373	C
7	B2	380	A
7	B2	381	A
7	B2	382	C
7	B2	384	G
7	B2	387	A
7	B2	396	A
7	B2	397	A
7	B2	404	C
7	B2	406	G
7	B2	409	G

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Mol	Chain	Res	Type
7	B2	412	G
7	B2	414	G
7	B2	419	U
7	B2	420	U
7	B2	423	C
7	B2	424	C
7	B2	425	A
7	B2	427	U
7	B2	430	U
7	B2	436	U
7	B2	441	U
7	B2	446	A
7	B2	449	A
7	B2	453	A
7	B2	455	A
7	B2	492	G
7	B2	496	A
7	B2	502	A
7	B2	503	A
7	B2	509	C
7	B2	523	G
7	B2	524	A
7	B2	533	G
7	B2	534	U
7	B2	538	G
7	B2	540	G
7	B2	541	C
7	B2	555	A
7	B2	558	U
7	B2	565	C
7	B2	570	A
7	B2	571	G
7	B2	585	U
7	B2	587	C
7	B2	595	A
7	B2	596	A
7	B2	599	A
7	B2	600	G
7	B2	614	C
7	B2	615	U
7	B2	617	G
7	B2	712	U

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Mol	Chain	Res	Type
7	B2	713	U
7	B2	723	A
7	B2	724	A
7	B2	733	G
7	B2	734	C
7	B2	742	A
7	B2	743	A
7	B2	747	C
7	B2	749	U
7	B2	750	G
7	B2	753	U
7	B2	754	G
7	B2	756	A
7	B2	758	A
7	B2	759	G
7	B2	773	A
7	B2	778	A
7	B2	779	A
7	B2	820	A
7	B2	826	A
7	B2	827	A
7	B2	835	A
7	B2	837	A
7	B2	838	C
7	B2	841	G
7	B2	851	U
7	B2	871	A
7	B2	879	G
7	B2	880	A
7	B2	882	C
7	B2	883	G
7	B2	898	A
7	B2	900	A
7	B2	909	A
7	B2	925	U
7	B2	931	A
7	B2	935	A
7	B2	936	A
7	B2	952	G
7	B2	957	A
7	B2	969	U
7	B2	970	A

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Mol	Chain	Res	Type
7	B2	976	C
7	B2	978	A
7	B2	991	A
7	B2	993	C
7	B2	996	U
7	B2	997	G
7	B2	1004	C
7	B2	1005	G
7	B2	1017	G
7	B2	1018	U
7	B2	1028	G
7	B2	1029	C
7	B2	1033	G
7	B2	1040	U
7	B2	1042	C
7	B2	1050	A
7	B2	1051	A
7	B2	1057	U
7	B2	1097	A
7	B2	1109	G
7	B2	1110	A
7	B2	1111	A
7	B2	1115	C
7	B2	1116	A
7	B2	1117	C
7	B2	1119	A
7	B2	1122	A
7	B2	1123	G
7	B2	1126	G
7	B2	1144	U
7	B2	1153	A
7	B2	1154	C
7	B2	1155	A
7	B2	1158	G
7	B2	1159	G
7	B2	1160	A
7	B2	1161	A
7	B2	1165	U
7	B2	1175	C
7	B2	1176	G
7	B2	1177	G
7	B2	1184	U

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Mol	Chain	Res	Type
7	B2	1191	U
7	B2	1193	A
7	B2	1194	C
7	B2	1196	G
7	B2	1202	A
7	B2	1203	A
7	B2	1204	G
7	B2	1205	C
7	B2	1206	U
7	B2	1209	U
7	B2	1214	G
7	B2	1215	A
7	B2	1216	U
7	B2	1217	U
7	B2	1222	G
7	B2	1224	U
7	B2	1244	U
7	B2	1248	U
7	B2	1250	G
7	B2	1254	G
7	B2	1256	G
7	B2	1265	C
7	B2	1272	A
7	B2	1273	U
7	B2	1274	U
7	B2	1279	U
7	B2	1280	A
7	B2	1281	A
7	B2	1296	G
7	B2	1298	C
7	B2	1299	U
7	B2	1302	U
7	B2	1303	A
7	B2	1304	A
7	B2	1305	A
7	B2	1306	U
7	B2	1307	A
7	B2	1308	G
7	B2	1310	U
7	B2	1311	G
7	B2	1316	A
7	B2	1317	U

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Mol	Chain	Res	Type
7	B2	1320	U
7	B2	1322	G
7	B2	1323	G
7	B2	1324	G
7	B2	1325	U
7	B2	1327	C
7	B2	1333	A
7	B2	1335	U
7	B2	1336	U
7	B2	1341	G
7	B2	1347	U
7	B2	1348	A
7	B2	1350	G
7	B2	1358	U
7	B2	1360	G
7	B2	1364	C
7	B2	1368	A
7	B2	1371	U
7	B2	1372	U
7	B2	1373	G
7	B2	1381	A
7	B2	1383	A
7	B2	1384	G
7	B2	1387	C
7	B2	1391	G
7	B2	1392	A
7	B2	1400	A
7	B2	1402	A
7	B2	1403	U
7	B2	1414	G
7	B2	1415	C
7	B2	1416	A
7	B2	1427	A
7	B2	1433	G
7	B2	1434	G
7	B2	1438	C
7	B2	1442	G
7	B2	1443	G
7	B2	1452	U
7	B2	1460	A
7	B2	1462	G
7	B2	1470	U

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Mol	Chain	Res	Type
7	B2	1472	A
7	B2	1473	A
7	B2	1477	U
7	B2	1479	G
7	B2	1480	A
7	B2	1481	A
7	B2	1491	U
7	B2	1493	U
7	B2	1494	C
7	B2	1495	C
7	B2	1499	A
7	B2	1510	U
7	B2	1512	A
7	B2	1513	U
7	B2	1515	A
7	B2	1524	A
7	B2	1528	G
7	B2	1529	A
7	B2	1530	G
7	B2	1546	G
7	B2	1553	A
7	B2	1557	G
7	B2	1563	G
7	B2	1572	G
7	B2	1576	C
7	B2	1587	A
7	B2	1588	C
7	B2	1613	U
7	B2	1614	G
7	B2	1640	G
7	B2	1671	C
7	B2	1681	U
7	B2	1689	C
7	B2	1695	U
7	B2	1703	G
7	B2	1709	A
7	B2	1711	G
7	B2	1714	G
7	B2	1716	A
7	B2	1720	A
7	B2	1721	G
7	B2	1723	U

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Mol	Chain	Res	Type
7	B2	1734	G
7	B2	1736	A
7	B2	1746	G
7	B2	1747	G
7	B2	1748	A
7	B2	1749	U
7	B2	1750	C
7	B2	1752	U
7	B2	1754	G
8	A5	12	C
8	A5	13	U
8	A5	22	A
8	A5	39	A
8	A5	42	A
8	A5	44	A
8	A5	48	U
8	A5	58	G
8	A5	59	A
8	A5	64	A
8	A5	65	A
8	A5	69	A
8	A5	73	A
8	A5	91	G
8	A5	108	A
8	A5	109	G
8	A5	110	C
8	A5	119	G
8	A5	125	A
8	A5	133	U
8	A5	134	U
8	A5	135	G
8	A5	139	G
8	A5	140	C
8	A5	141	U
8	A5	149	G
8	A5	156	A
8	A5	157	U
8	A5	158	A
8	A5	159	G
8	A5	166	G
8	A5	169	U
8	A5	178	G

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Mol	Chain	Res	Type
8	A5	179	U
8	A5	181	G
8	A5	183	A
8	A5	184	U
8	A5	185	G
8	A5	189	G
8	A5	190	A
8	A5	193	U
8	A5	194	C
8	A5	195	C
8	A5	203	U
8	A5	204	G
8	A5	208	C
8	A5	209	C
8	A5	211	U
8	A5	212	A
8	A5	226	G
8	A5	227	C
8	A5	238	C
8	A5	239	U
8	A5	240	G
8	A5	241	G
8	A5	247	G
8	A5	248	G
8	A5	249	C
8	A5	250	A
8	A5	252	U
8	A5	260	C
8	A5	261	G
8	A5	262	C
8	A5	263	U
8	A5	264	U
8	A5	272	G
8	A5	273	G
8	A5	275	G
8	A5	289	A
8	A5	290	A
8	A5	291	G
8	A5	301	A
8	A5	304	U
8	A5	305	G
8	A5	311	U

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Mol	Chain	Res	Type
8	A5	317	U
8	A5	318	C
8	A5	329	A
8	A5	335	C
8	A5	336	G
8	A5	345	G
8	A5	357	A
8	A5	358	A
8	A5	366	G
8	A5	368	G
8	A5	382	G
8	A5	404	G
8	A5	405	A
8	A5	408	A
8	A5	409	C
8	A5	424	G
8	A5	427	G
8	A5	428	A
8	A5	435	G
8	A5	516	G
8	A5	518	C
8	A5	522	G
8	A5	535	C
8	A5	536	G
8	A5	542	G
8	A5	546	G
8	A5	577	U
8	A5	578	C
8	A5	581	G
8	A5	585	G
8	A5	588	G
8	A5	590	A
8	A5	594	G
8	A5	598	C
8	A5	599	G
8	A5	600	U
8	A5	601	G
8	A5	602	G
8	A5	635	C
8	A5	636	G
8	A5	638	C
8	A5	639	G

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Mol	Chain	Res	Type
8	A5	640	G
8	A5	641	U
8	A5	643	U
8	A5	644	G
8	A5	645	A
8	A5	646	A
8	A5	647	A
8	A5	655	A
8	A5	656	C
8	A5	666	C
8	A5	678	A
8	A5	689	A
8	A5	706	A
8	A5	711	A
8	A5	712	A
8	A5	716	U
8	A5	717	G
8	A5	720	A
8	A5	728	G
8	A5	729	C
8	A5	738	G
8	A5	742	G
8	A5	745	A
8	A5	746	A
8	A5	747	G
8	A5	751	A
8	A5	755	U
8	A5	756	C
8	A5	758	A
8	A5	759	A
8	A5	760	U
8	A5	763	G
8	A5	764	C
8	A5	767	A
8	A5	768	C
8	A5	791	U
8	A5	797	G
8	A5	804	G
8	A5	816	G
8	A5	817	U
8	A5	821	U
8	A5	822	U

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Mol	Chain	Res	Type
8	A5	823	G
8	A5	834	G
8	A5	835	A
8	A5	836	G
8	A5	840	G
8	A5	854	C
8	A5	861	A
8	A5	868	G
8	A5	872	A
8	A5	904	C
8	A5	916	U
8	A5	919	G
8	A5	929	U
8	A5	934	U
8	A5	935	G
8	A5	951	A
8	A5	961	A
8	A5	962	G
8	A5	963	G
8	A5	969	A
8	A5	971	G
8	A5	972	A
8	A5	976	A
8	A5	978	C
8	A5	992	G
8	A5	999	C
8	A5	1001	U
8	A5	1014	C
8	A5	1015	U
8	A5	1016	C
8	A5	1017	A
8	A5	1029	U
8	A5	1032	C
8	A5	1034	G
8	A5	1036	C
8	A5	1039	U
8	A5	1048	G
8	A5	1049	U
8	A5	1056	A
8	A5	1064	G
8	A5	1090	A
8	A5	1101	A

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Mol	Chain	Res	Type
8	A5	1103	C
8	A5	1104	U
8	A5	1110	U
8	A5	1118	A
8	A5	1119	A
8	A5	1123	G
8	A5	1125	A
8	A5	1126	G
8	A5	1134	A
8	A5	1135	G
8	A5	1137	G
8	A5	1145	A
8	A5	1150	G
8	A5	1151	A
8	A5	1156	G
8	A5	1168	G
8	A5	1169	G
8	A5	1183	G
8	A5	1196	U
8	A5	1205	A
8	A5	1207	C
8	A5	1211	A
8	A5	1220	U
8	A5	1224	G
8	A5	1226	G
8	A5	1232	C
8	A5	1233	U
8	A5	1234	U
8	A5	1244	G
8	A5	1245	A
8	A5	1250	C
8	A5	1253	U
8	A5	1261	G
8	A5	1264	G
8	A5	1272	U
8	A5	1273	U
8	A5	1274	G
8	A5	1275	A
8	A5	1279	C
8	A5	1339	A
8	A5	1354	A
8	A5	1359	G

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Mol	Chain	Res	Type
8	A5	1360	A
8	A5	1361	U
8	A5	1368	U
8	A5	1375	G
8	A5	1377	G
8	A5	1383	U
8	A5	1430	A
8	A5	1440	U
8	A5	1441	C
8	A5	1448	G
8	A5	1449	U
8	A5	1453	G
8	A5	1467	G
8	A5	1496	G
8	A5	1499	G
8	A5	1502	C
8	A5	1511	A
8	A5	1512	G
8	A5	1515	G
8	A5	1534	C
8	A5	1546	A
8	A5	1548	G
8	A5	1567	G
8	A5	1568	A
8	A5	1573	U
8	A5	1604	A
8	A5	1606	U
8	A5	1607	G
8	A5	1608	G
8	A5	1612	A
8	A5	1614	G
8	A5	1619	G
8	A5	1620	U
8	A5	1621	A
8	A5	1626	C
8	A5	1627	G
8	A5	1628	G
8	A5	1650	U
8	A5	1651	C
8	A5	1655	G
8	A5	1658	U
8	A5	1659	G

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Mol	Chain	Res	Type
8	A5	1663	A
8	A5	1664	A
8	A5	1665	A
8	A5	1670	A
8	A5	1671	U
8	A5	1681	A
8	A5	1704	U
8	A5	1725	C
8	A5	1727	C
8	A5	1728	G
8	A5	1736	A
8	A5	1738	U
8	A5	1739	C
8	A5	1749	U
8	A5	1750	A
8	A5	1756	U
8	A5	1768	C
8	A5	1769	U
8	A5	1772	A
8	A5	1775	U
8	A5	1776	U
8	A5	1777	U
8	A5	1780	U
8	A5	1781	C
8	A5	1787	U
8	A5	1796	G
8	A5	1798	A
8	A5	1801	C
8	A5	1810	U
8	A5	1811	G
8	A5	1817	G
8	A5	1833	U
8	A5	1837	U
8	A5	1838	U
8	A5	1839	C
8	A5	1840	C
8	A5	1842	A
8	A5	1843	A
8	A5	1845	A
8	A5	1851	G
8	A5	1853	G
8	A5	1862	G

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Mol	Chain	Res	Type
8	A5	1868	U
8	A5	1870	G
8	A5	1873	C
8	A5	1874	U
8	A5	1875	C
8	A5	1876	U
8	A5	1882	C
8	A5	1883	G
8	A5	1887	C
8	A5	1891	A
8	A5	1893	A
8	A5	1904	G
8	A5	1908	A
8	A5	1910	U
8	A5	1913	U
8	A5	1914	U
8	A5	1915	U
8	A5	1917	C
8	A5	1919	C
8	A5	1932	A
8	A5	1935	U
8	A5	1938	G
8	A5	1939	C
8	A5	1948	U
8	A5	1967	A
8	A5	1971	G
8	A5	1972	A
8	A5	1973	U
8	A5	1979	A
8	A5	1982	G
8	A5	1999	G
8	A5	2205	A
8	A5	2211	A
8	A5	2215	G
8	A5	2216	U
8	A5	2218	C
8	A5	2225	A
8	A5	2226	G
8	A5	2235	A
8	A5	2244	U
8	A5	2246	A
8	A5	2248	A

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Mol	Chain	Res	Type
8	A5	2253	A
8	A5	2262	A
8	A5	2273	G
8	A5	2281	A
8	A5	2295	C
8	A5	2308	U
8	A5	2309	G
8	A5	2310	A
8	A5	2311	A
8	A5	2312	U
8	A5	2313	G
8	A5	2326	A
8	A5	2333	G
8	A5	2341	G
8	A5	2347	A
8	A5	2352	G
8	A5	2358	A
8	A5	2359	A
8	A5	2361	U
8	A5	2375	G
8	A5	2376	G
8	A5	2382	A
8	A5	2384	A
8	A5	2410	G
8	A5	2413	U
8	A5	2416	A
8	A5	2418	G
8	A5	2437	U
8	A5	2439	U
8	A5	2474	G
8	A5	2475	A
8	A5	2476	A
8	A5	2477	C
8	A5	2478	G
8	A5	2488	A
8	A5	2496	G
8	A5	2500	A
8	A5	2503	G
8	A5	2505	A
8	A5	2506	G
8	A5	2507	A
8	A5	2514	U

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Mol	Chain	Res	Type
8	A5	2538	G
8	A5	2546	U
8	A5	2547	C
8	A5	2609	A
8	A5	2610	C
8	A5	2611	U
8	A5	2612	C
8	A5	2619	U
8	A5	2620	A
8	A5	2625	G
8	A5	2626	U
8	A5	2627	U
8	A5	2631	A
8	A5	2633	A
8	A5	2636	A
8	A5	2656	U
8	A5	2658	G
8	A5	2659	A
8	A5	2660	A
8	A5	2666	A
8	A5	2671	G
8	A5	2672	A
8	A5	2684	G
8	A5	2685	C
8	A5	2686	A
8	A5	2694	U
8	A5	2698	C
8	A5	2705	A
8	A5	2706	C
8	A5	2718	G
8	A5	2719	G
8	A5	2726	G
8	A5	2731	G
8	A5	2738	A
8	A5	2763	G
8	A5	2764	U
8	A5	2768	A
8	A5	2786	A
8	A5	2789	G
8	A5	2791	A
8	A5	2792	A
8	A5	2797	U

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Mol	Chain	Res	Type
8	A5	2801	A
8	A5	2803	A
8	A5	2806	A
8	A5	2808	A
8	A5	2814	A
8	A5	2815	A
8	A5	2816	A
8	A5	2839	A
8	A5	2840	G
8	A5	2841	U
8	A5	2843	C
8	A5	2859	A
8	A5	2865	G
8	A5	2874	A
8	A5	2882	A
8	A5	2883	A
8	A5	2889	A
8	A5	2890	U
8	A5	2908	G
8	A5	2911	A
8	A5	2912	G
8	A5	2913	A
8	A5	2922	C
8	A5	2929	A
8	A5	2930	U
8	A5	2950	A
8	A5	2954	U
8	A5	2956	C
8	A5	2957	A
8	A5	2959	A
8	A5	2972	U
8	A5	2979	C
8	A5	2983	G
8	A5	2984	A
8	A5	2998	U
8	A5	2999	A
8	A5	3010	G
8	A5	3011	C
8	A5	3012	A
8	A5	3013	G
8	A5	3014	A
8	A5	3023	A

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Mol	Chain	Res	Type
8	A5	3028	U
8	A5	3035	U
8	A5	3047	U
8	A5	3048	A
8	A5	3053	A
8	A5	3054	C
8	A5	3059	G
8	A5	3063	G
8	A5	3066	U
8	A5	3080	G
8	A5	3083	A
8	A5	3092	U
8	A5	3095	C
8	A5	3102	G
8	A5	3106	A
8	A5	3109	U
8	A5	3112	U
8	A5	3113	A
8	A5	3119	A
8	A5	3124	A
8	A5	3125	A
8	A5	3129	U
8	A5	3130	G
8	A5	3132	U
8	A5	3134	A
8	A5	3138	C
8	A5	3140	A
8	A5	3141	G
8	A5	3142	A
8	A5	3146	A
8	A5	3162	U
8	A5	3163	U
8	A5	3167	U
8	A5	3170	A
8	A5	3171	U
8	A5	3180	U
8	A5	3185	A
8	A5	3187	A
8	A5	3188	U
8	A5	3191	A
8	A5	3199	A
8	A5	3205	C

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Mol	Chain	Res	Type
8	A5	3206	C
8	A5	3207	A
8	A5	3212	A
8	A5	3231	C
8	A5	3235	A
8	A5	3238	U
8	A5	3243	A
8	A5	3244	U
8	A5	3254	U
8	A5	3255	C
8	A5	3257	A
8	A5	3258	G
8	A5	3259	G
8	A5	3268	U
8	A5	3278	C
8	A5	3279	G
8	A5	3280	G
8	A5	3282	G
8	A5	3284	C
8	A5	3285	G
8	A5	3286	G
8	A5	3288	A
8	A5	3289	G
8	A5	3292	A
8	A5	3293	U
8	A5	3294	C
8	A5	3298	A
8	A5	3299	U
8	A5	3305	G
8	A5	3306	G
8	A5	3310	C
8	A5	3315	G
8	A5	3317	G
8	A5	3318	C
8	A5	3320	U
8	A5	3321	A
8	A5	3322	U
8	A5	3331	U
8	A5	3332	A
8	A5	3333	U
8	A5	3334	G
8	A5	3335	G

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Mol	Chain	Res	Type
8	A5	3337	C
8	A5	3338	U
8	A5	3339	U
8	A5	3341	G
8	A5	3347	U
8	A5	3349	G
8	A5	3351	G
8	A5	3352	A
8	A5	3364	C
8	A5	3366	U
8	A5	3371	A
8	A5	3373	G
8	A5	3375	C
8	A5	3376	A
8	A5	3377	G
8	A5	3378	A
8	A5	3380	C
8	A5	3381	A
8	A5	3385	U
8	A5	3386	G
8	A5	3387	G
8	A5	3388	U
8	A5	3389	U
8	A5	3390	C
8	A5	3393	U
8	A5	3397	G
8	A5	3399	G
8	A5	3401	C
8	A5	3405	A
8	A5	3406	A
8	A5	3415	C
8	A5	3426	G
8	A5	3436	C
8	A5	3454	A
8	A5	3457	G
8	A5	3461	U
8	A5	3463	C
8	A5	3464	U
8	A5	3465	U
8	A5	3466	U
8	A5	3467	U
8	A5	3468	A

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Mol	Chain	Res	Type
8	A5	3469	U
8	A5	3470	A
8	A5	3472	U
8	A5	3474	C
8	A5	3482	U
8	A5	3483	G
8	A5	3488	U
8	A5	3489	A
8	A5	3494	U
8	A5	3495	U
8	A5	3496	G
8	A5	3497	A
8	A5	3509	G
78	DA	4	U
78	DA	9	A
78	DA	16	U
78	DA	17	U
78	DA	19	G
78	DA	21	A
78	DA	22	G
78	DA	38	A
78	DA	46	G
78	DA	47	U
78	DA	51	C
78	DA	55	U
78	DA	57	G
78	DA	58	A
78	DA	59	U
78	DA	61	C
78	DA	75	C
78	DA	76	A
78	DB	4	U
78	DB	9	A
78	DB	16	U
78	DB	17	U
78	DB	18	G
78	DB	19	G
78	DB	20	G
78	DB	21	A
78	DB	22	G
78	DB	40	C
78	DB	44	A

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Mol	Chain	Res	Type
78	DB	45	G
78	DB	46	G
78	DB	47	U
78	DB	48	C
78	DB	55	U
78	DB	56	C
78	DB	59	U
78	DB	60	C
78	DB	68	G
78	DB	74	C
78	DB	75	C
79	DC	4	U

All (103) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	B2	159	G
7	B2	228	U
7	B2	353	G
7	B2	356	C
7	B2	448	U
7	B2	711	U
7	B2	908	C
7	B2	1027	U
7	B2	1039	A
7	B2	1041	C
7	B2	1110	A
7	B2	1121	A
7	B2	1183	A
7	B2	1192	G
7	B2	1213	C
7	B2	1278	A
7	B2	1280	A
7	B2	1305	A
7	B2	1309	U
7	B2	1363	G
7	B2	1371	U
7	B2	1437	U
7	B2	1490	A
7	B2	1509	G
7	B2	1511	A
7	B2	1529	A

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Mol	Chain	Res	Type
7	B2	1715	U
7	B2	1751	A
8	A5	12	C
8	A5	21	G
8	A5	133	U
8	A5	134	U
8	A5	189	G
8	A5	194	C
8	A5	238	C
8	A5	251	C
8	A5	263	U
8	A5	288	A
8	A5	403	A
8	A5	408	A
8	A5	576	G
8	A5	580	U
8	A5	589	U
8	A5	598	C
8	A5	635	C
8	A5	646	A
8	A5	711	A
8	A5	754	C
8	A5	759	A
8	A5	763	G
8	A5	816	G
8	A5	834	G
8	A5	928	C
8	A5	971	G
8	A5	1035	G
8	A5	1118	A
8	A5	1150	G
8	A5	1155	C
8	A5	1650	U
8	A5	1658	U
8	A5	1737	U
8	A5	1749	U
8	A5	1844	A
8	A5	1861	U
8	A5	1875	C
8	A5	1907	U
8	A5	1909	U
8	A5	1912	A

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Mol	Chain	Res	Type
8	A5	2475	A
8	A5	2608	G
8	A5	2609	A
8	A5	2610	C
8	A5	2630	A
8	A5	2658	G
8	A5	2790	A
8	A5	3047	U
8	A5	3139	G
8	A5	3234	U
8	A5	3256	A
8	A5	3257	A
8	A5	3258	G
8	A5	3277	C
8	A5	3281	U
8	A5	3283	U
8	A5	3285	G
8	A5	3297	U
8	A5	3304	U
8	A5	3309	A
8	A5	3320	U
8	A5	3321	A
8	A5	3333	U
8	A5	3334	G
8	A5	3338	U
8	A5	3340	G
8	A5	3348	A
8	A5	3365	U
8	A5	3374	C
8	A5	3375	C
8	A5	3376	A
8	A5	3377	G
8	A5	3389	U
8	A5	3460	G
78	DB	58	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
81	3HE	A5	3602	-	21,21,21	0.51	0	23,30,30	0.96	0
80	SPD	A5	3601	-	9,9,9	0.34	0	8,8,8	0.80	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
81	3HE	A5	3602	-	-	1/8/36/36	0/2/2/2
80	SPD	A5	3601	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

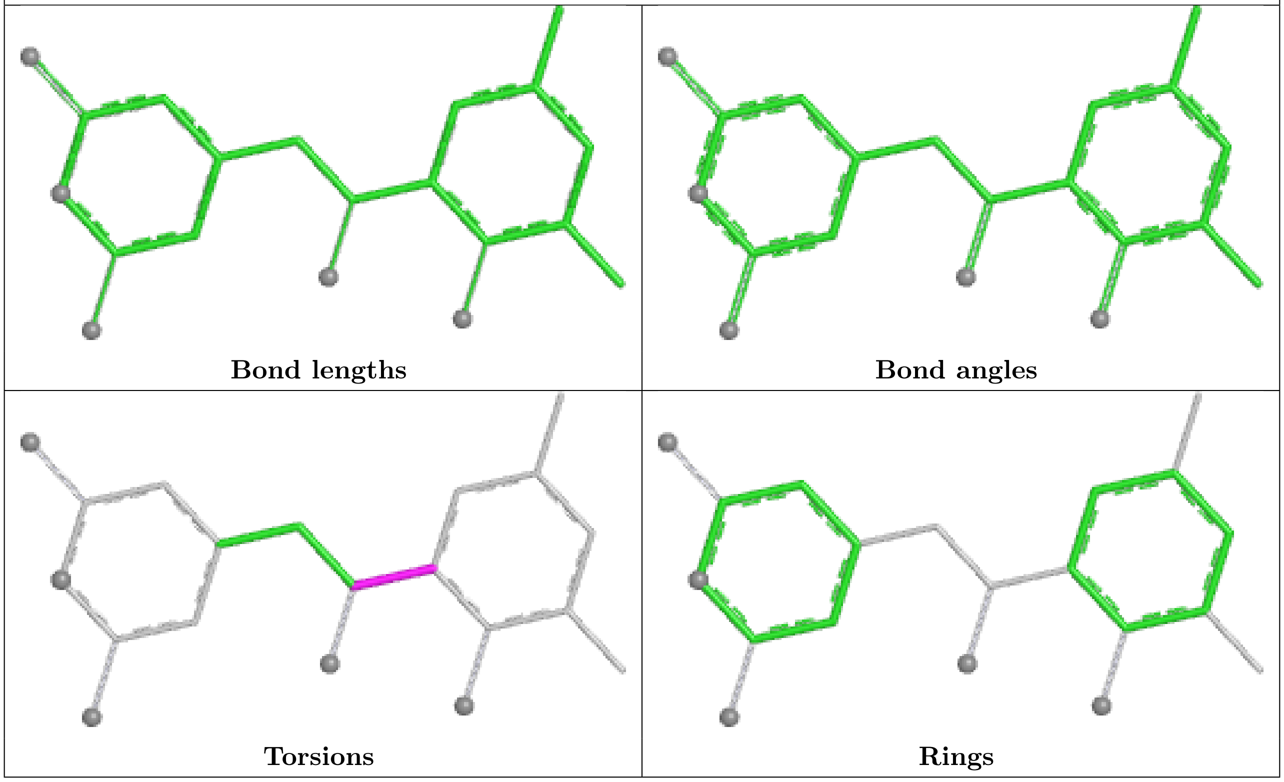
Mol	Chain	Res	Type	Atoms
81	A5	3602	3HE	C6-C5-C7-O3
80	A5	3601	SPD	C4-C5-N6-C7
80	A5	3601	SPD	C8-C7-N6-C5

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand 3HE A5 3602



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	A5	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
7	B2	1
79	DC	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A5	3461:U	O3’	3462:C	P	7.49
1	B2	745:C	O3’	746:G	P	2.82
1	DC	6:U	O3’	7:U	P	2.74

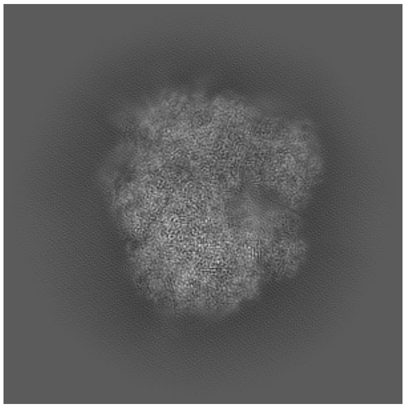
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44533. These allow visual inspection of the internal detail of the map and identification of artifacts.

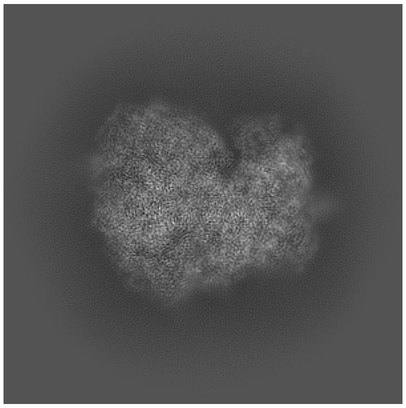
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

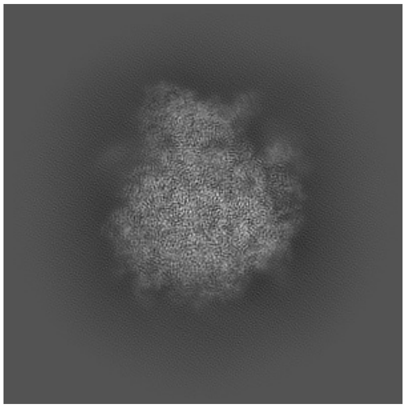
6.1.1 Primary map



X

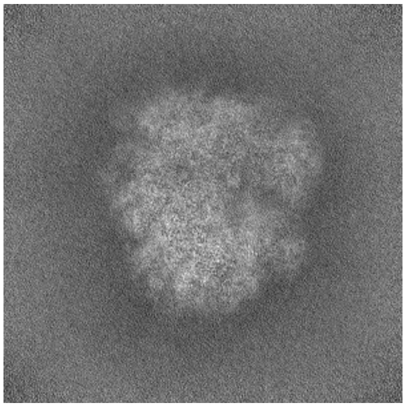


Y

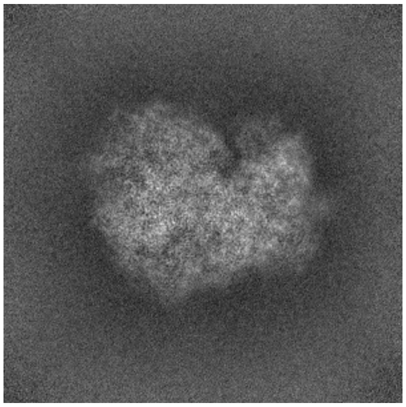


Z

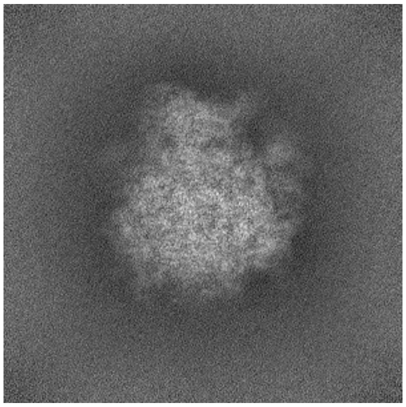
6.1.2 Raw map



X



Y

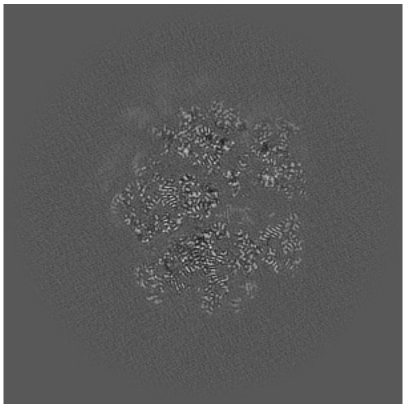


Z

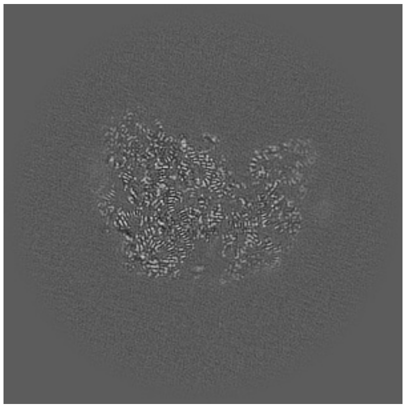
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

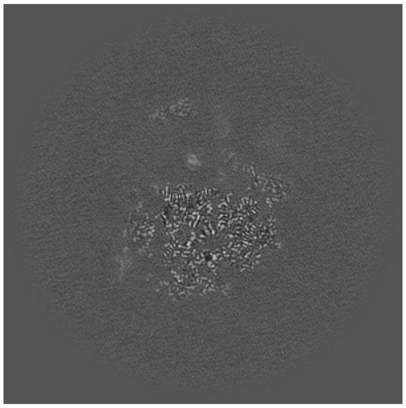
6.2.1 Primary map



X Index: 340

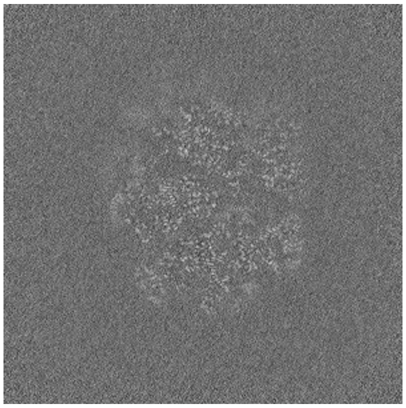


Y Index: 340

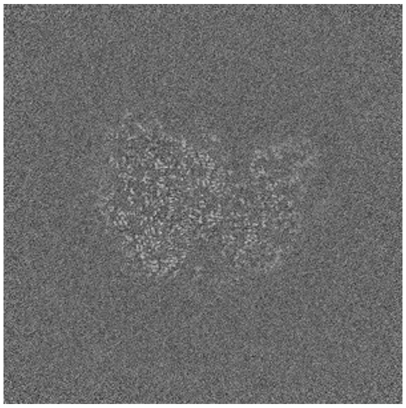


Z Index: 340

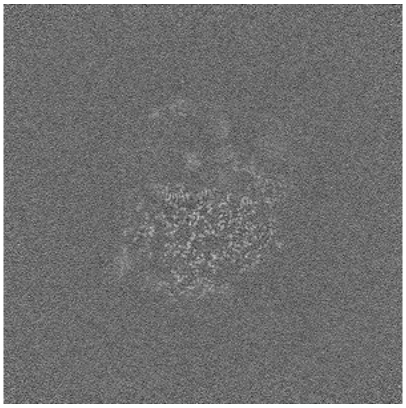
6.2.2 Raw map



X Index: 340



Y Index: 340

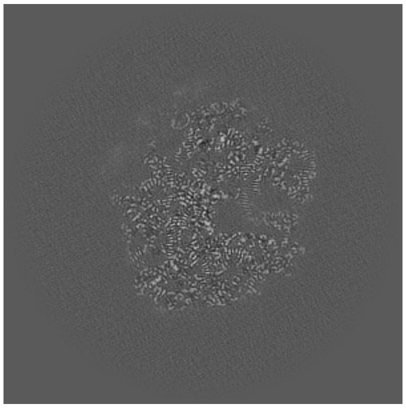


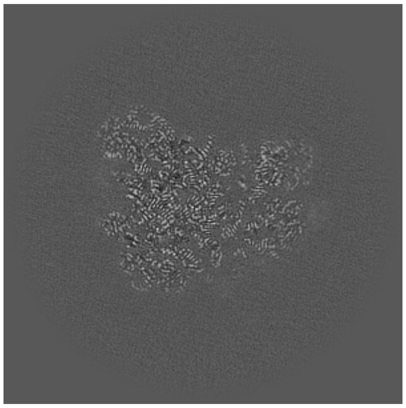
Z Index: 340

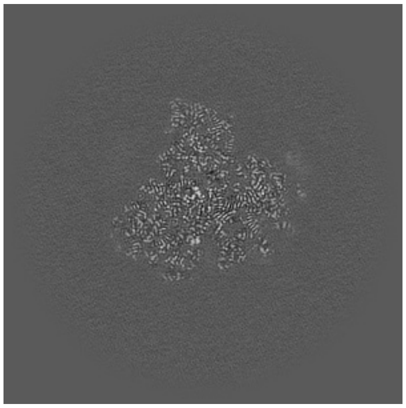
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

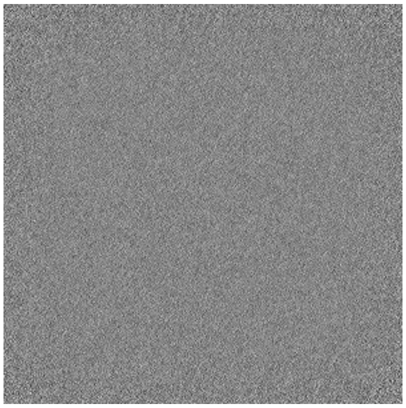
6.3.1 Primary map

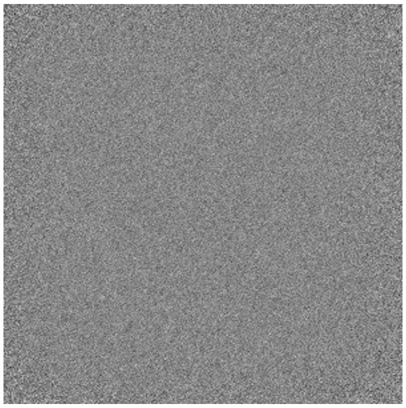

X Index: 318

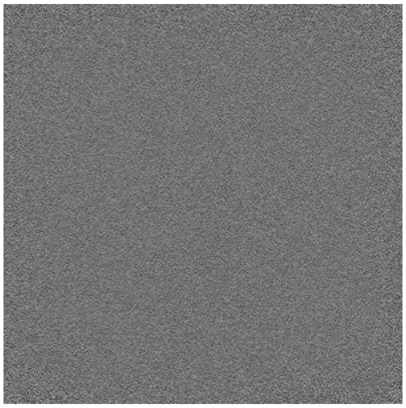

Y Index: 326


Z Index: 266

6.3.2 Raw map


X Index: 0

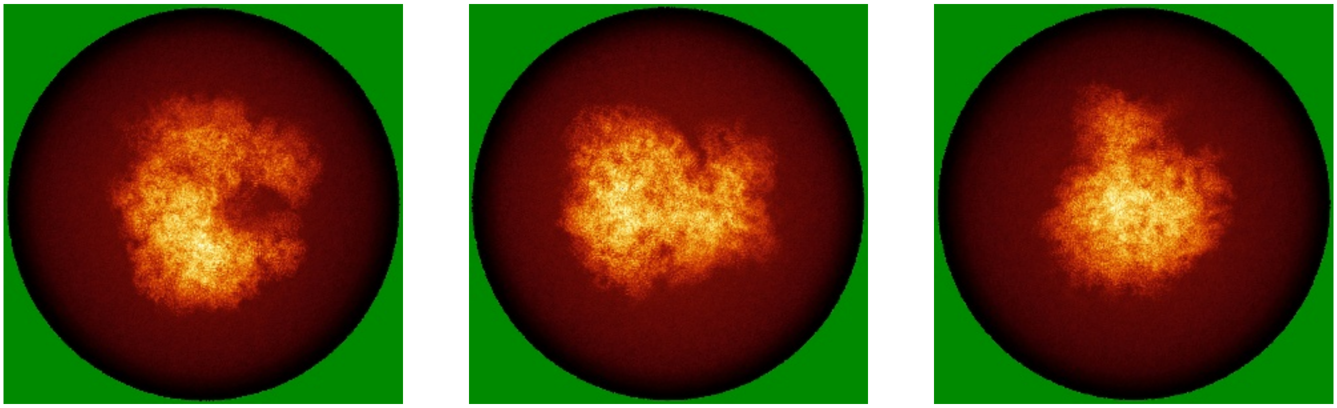

Y Index: 0


Z Index: 679

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

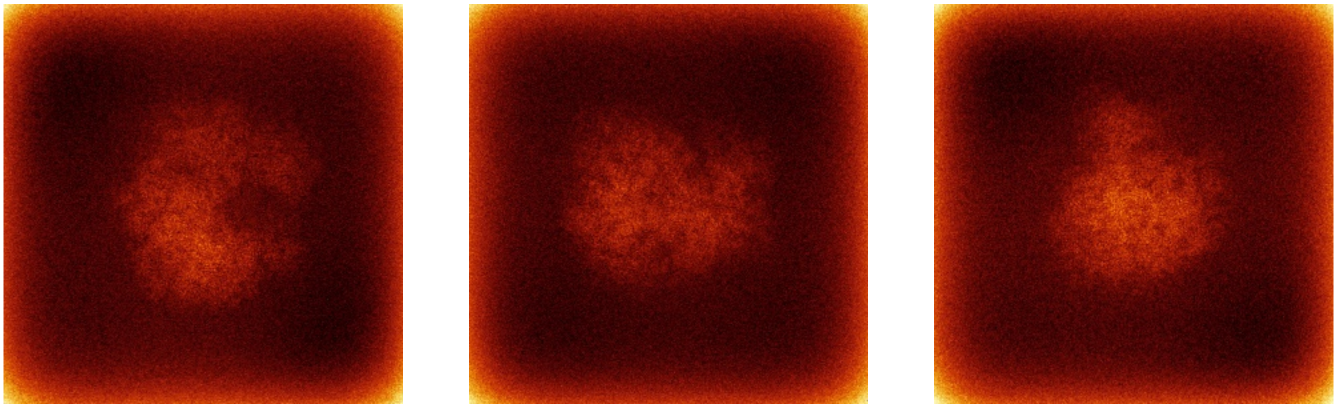
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

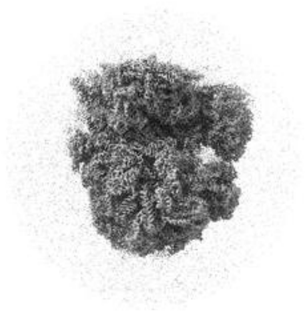


X Y Z

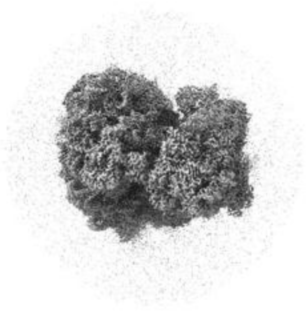
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

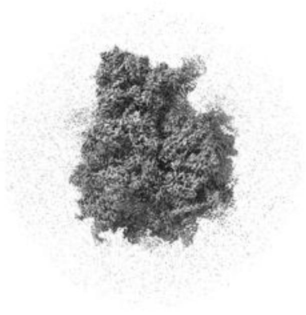
6.5.1 Primary map



X



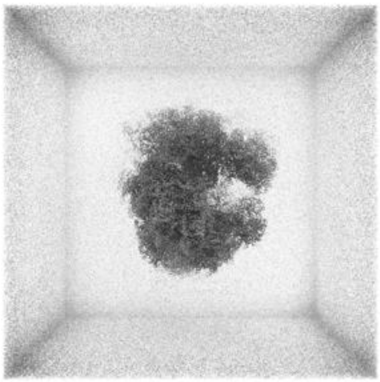
Y



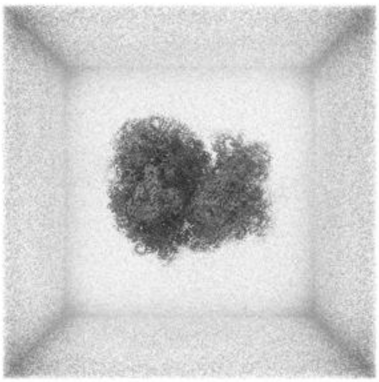
Z

The images above show the 3D surface view of the map at the recommended contour level 0.182. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

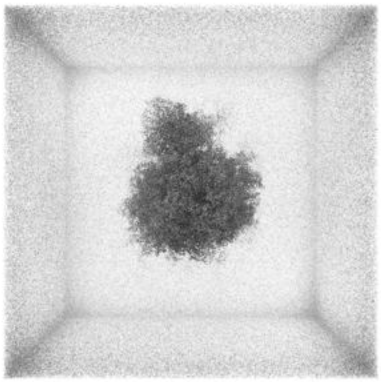
6.5.2 Raw map



X



Y



Z

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.

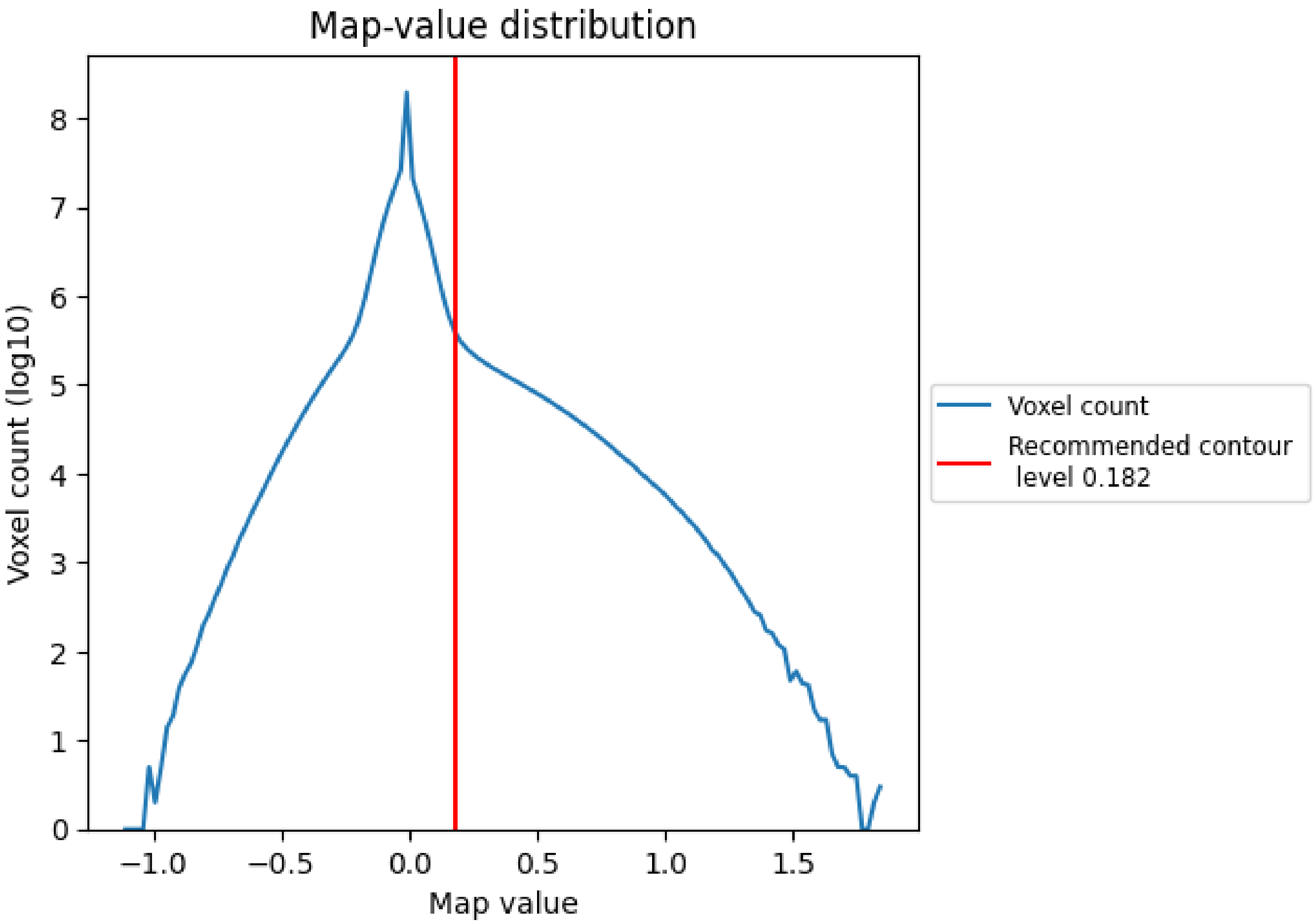
6.6 Mask visualisation

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

7 Map analysis ⓘ

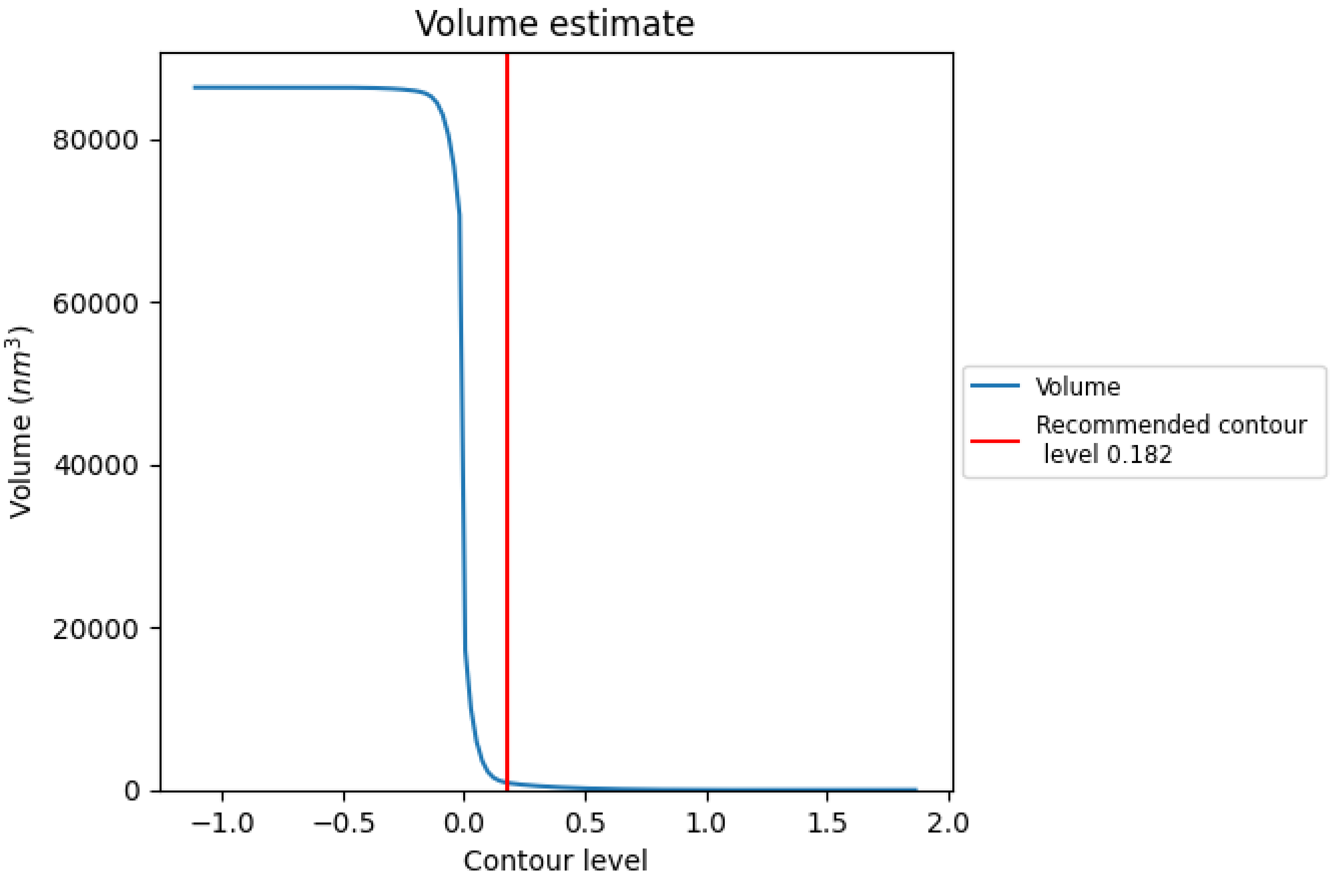
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

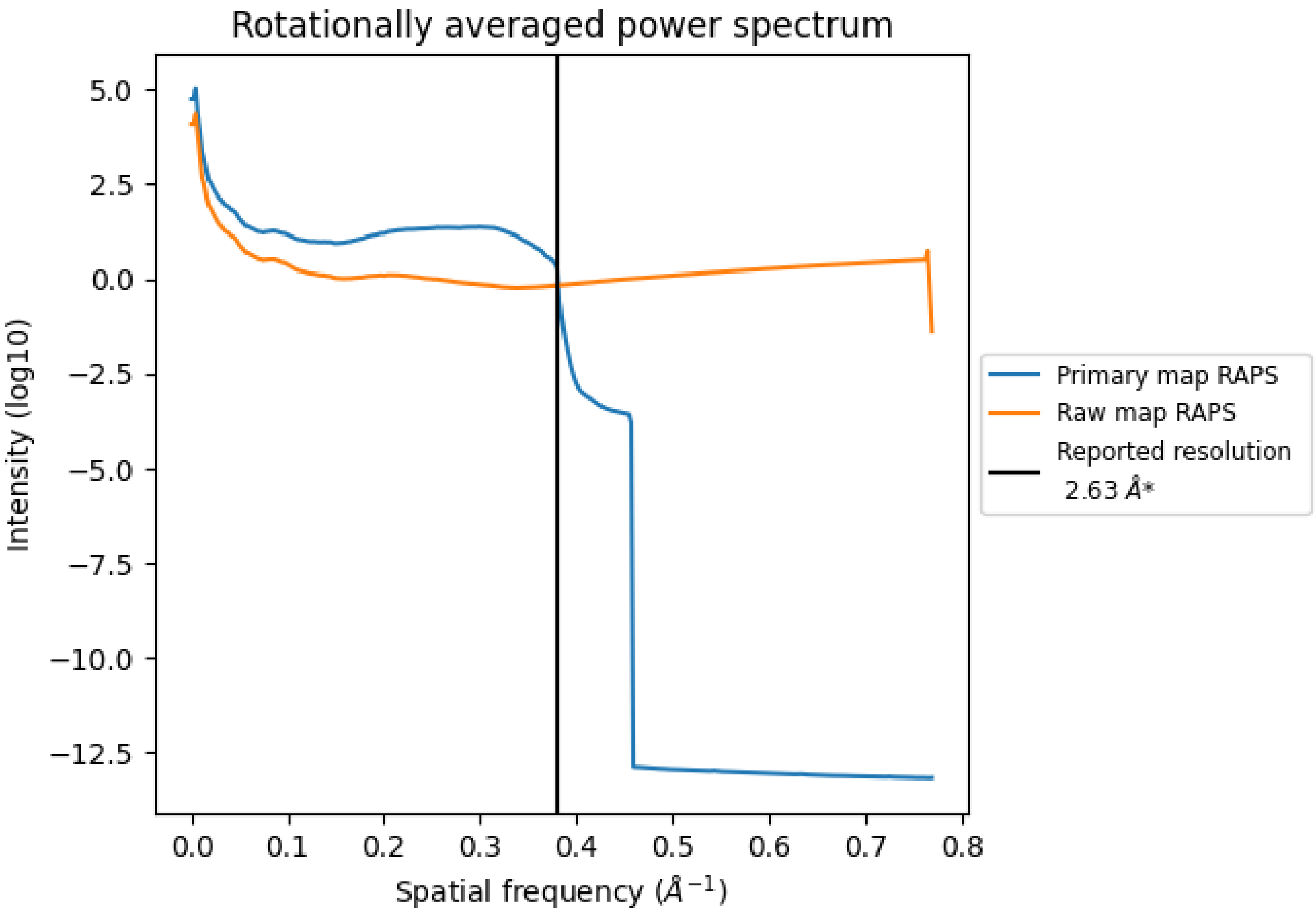
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 874 nm^3; this corresponds to an approximate mass of 789 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 ⓘ

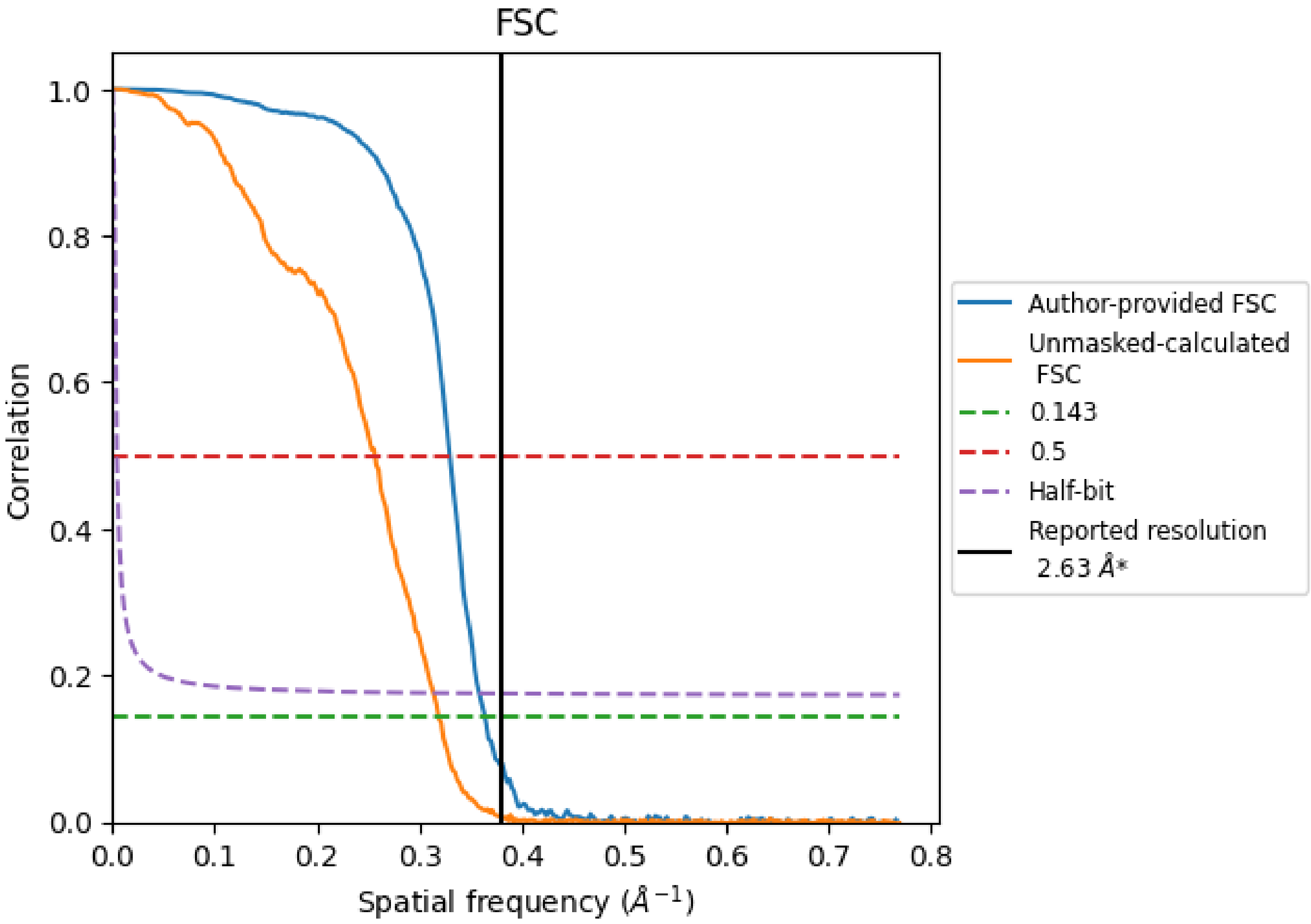


*Reported resolution corresponds to spatial frequency of 0.380 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.380 $Å^{-1}$

8.2 Resolution estimates ⓘ

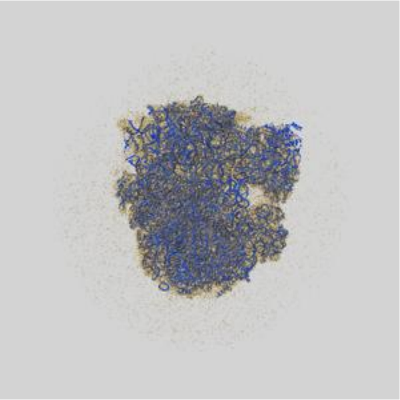
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	2.75	3.03	2.79
Unmasked-calculated*	3.14	3.90	3.19

*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 3.14 differs from the reported value 2.63 by more than 10 %

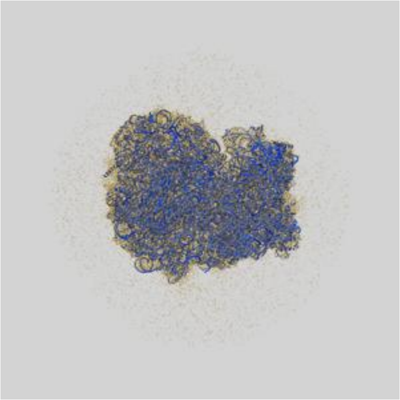
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44533 and PDB model 9BH5. Per-residue inclusion information can be found in section 3 on page 19.

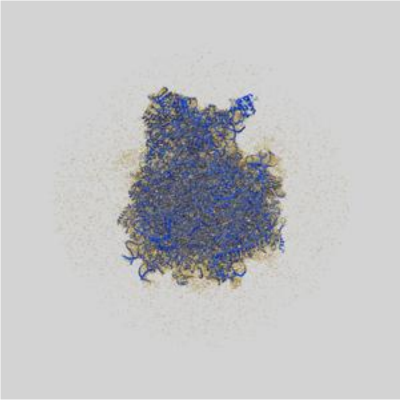
9.1 Map-model overlay



X



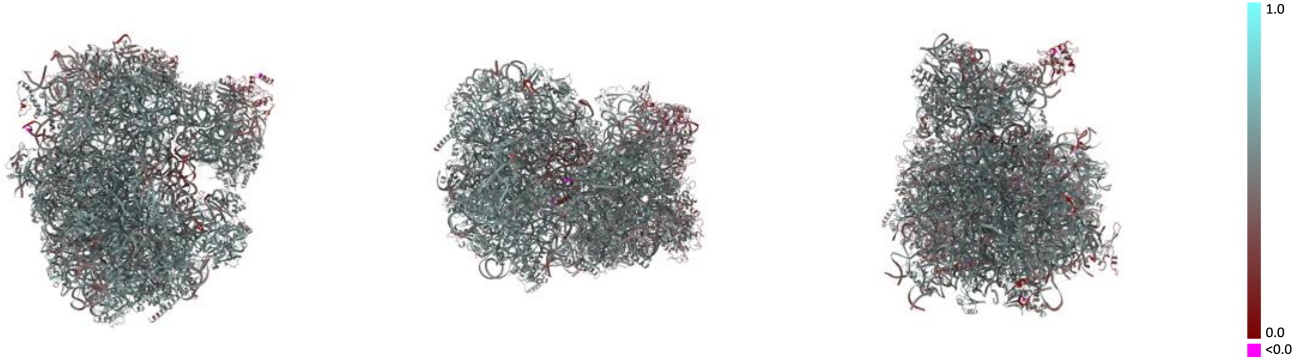
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.182 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.

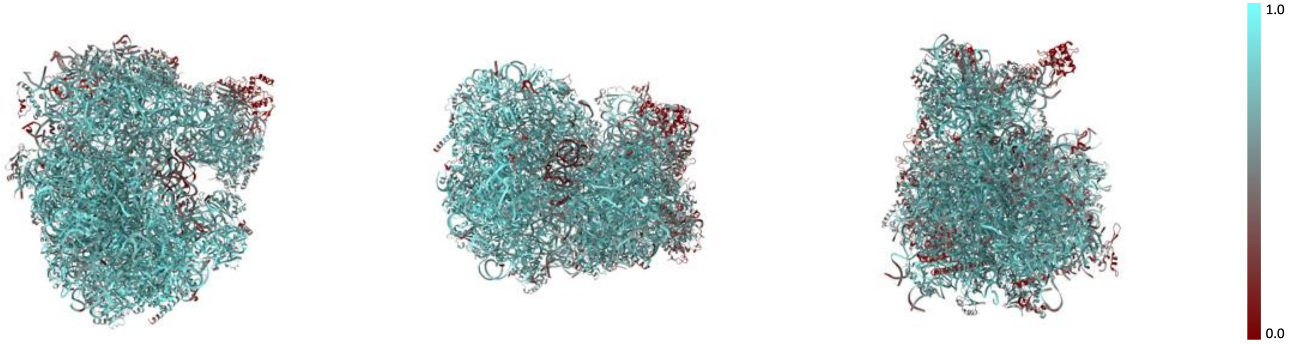
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according 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.

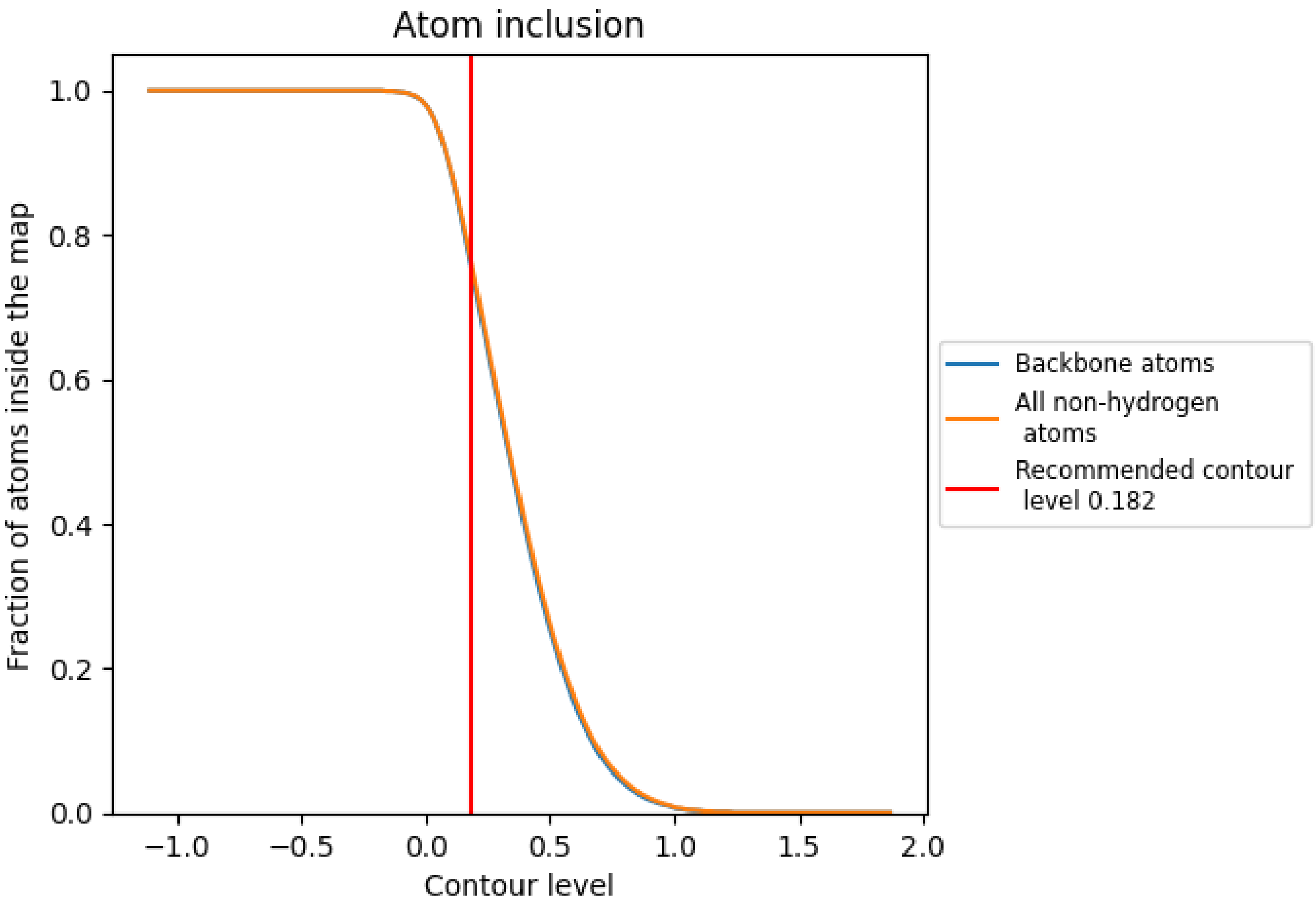
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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 (0.182).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.5170
A5	0.8320	0.5250
A7	0.8770	0.5550
A8	0.8550	0.5490
AA	0.5930	0.4810
AB	0.6720	0.5130
AC	0.7080	0.5050
AD	0.5530	0.4690
AE	0.6650	0.4930
AF	0.6990	0.5180
AG	0.5320	0.4610
AH	0.4250	0.4300
AI	0.6760	0.4980
AJ	0.4940	0.4110
AK	0.4840	0.4600
AL	0.7490	0.5260
AM	0.0600	0.2510
AN	0.5850	0.4850
AO	0.7520	0.5280
AP	0.6540	0.5120
AQ	0.6700	0.5090
AR	0.4630	0.4320
AS	0.6950	0.5170
AT	0.6980	0.5070
AU	0.5100	0.4430
AV	0.5910	0.4640
AW	0.7490	0.5180
AX	0.7870	0.5530
AY	0.5300	0.4550
AZ	0.5670	0.4950
Aa	0.7350	0.5120
Ab	0.4640	0.4510
Ac	0.5900	0.4940
Ad	0.7240	0.5110
Ae	0.6020	0.4780

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Chain	Atom inclusion	Q-score
Af	0.0980	0.2960
B2	0.8070	0.5200
CA	0.8600	0.5500
CB	0.8460	0.5530
CC	0.8070	0.5450
CD	0.7580	0.5450
CE	0.7230	0.5240
CF	0.8240	0.5480
CG	0.6770	0.5070
CH	0.7460	0.5270
CI	0.6500	0.5170
CJ	0.6730	0.5040
CL	0.7600	0.5410
CM	0.8020	0.5460
CN	0.8830	0.5650
CO	0.8310	0.5520
CP	0.8460	0.5530
CQ	0.8650	0.5590
CR	0.6670	0.4970
CS	0.8240	0.5500
CT	0.8020	0.5450
CU	0.6020	0.4950
CV	0.8170	0.5430
CW	0.6000	0.4730
CX	0.7570	0.5310
CY	0.7940	0.5450
CZ	0.7420	0.5200
Ca	0.8680	0.5600
Cb	0.7310	0.5150
Cc	0.7310	0.5160
Cd	0.7890	0.5430
Ce	0.7940	0.5460
Cf	0.8500	0.5560
Cg	0.7830	0.5390
Ch	0.7520	0.5270
Ci	0.7440	0.5360
Cj	0.8670	0.5470
Ck	0.5970	0.5070
Cl	0.8230	0.5540
Cm	0.6060	0.5010
Cn	0.6720	0.4830
Co	0.7980	0.5500

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Chain	Atom inclusion	Q-score
Cp	🟦 0.7870	⬛ 0.5230
DA	⬛ 0.5200	🟫 0.3710
DB	🟫 0.3900	🟫 0.3550
DC	🟦 0.7850	⬛ 0.4680