



## wwPDB EM Validation Summary Report ⓘ

Aug 27, 2021 – 12:25 am BST

PDB ID : 7O81  
EMDB ID : EMD-12759  
Title : Rabbit 80S ribosome colliding in another ribosome stalled by the SARS-CoV-2 pseudoknot  
Authors : Bhatt, P.R.; Scaiola, A.; Leibundgut, M.A.; Atkins, J.F.; Ban, N.  
Deposited on : 2021-04-14  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

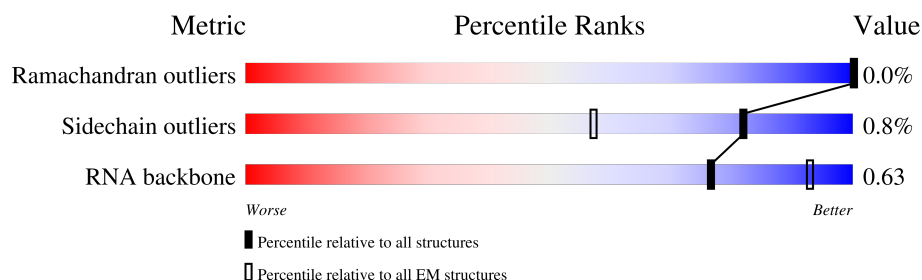
EMDB validation analysis : 0.0.0.dev97  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

# 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 3.10 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A2	1870	<div> <div>6%</div> <div>78%</div> <div>17%</div> <div>5%</div> </div>
2	AA	84	<div> <div>12%</div> <div>98%</div> <div>..</div> </div>
3	AB	69	<div> <div>10%</div> <div>91%</div> <div>9%</div> </div>
4	AC	156	<div> <div>17%</div> <div>47%</div> <div>53%</div> </div>
5	AD	133	<div> <div>33%</div> <div>66%</div> </div>
6	AE	115	<div> <div>7%</div> <div>88%</div> <div>12%</div> </div>
7	AF	317	<div> <div>22%</div> <div>98%</div> <div>..</div> </div>
8	AG	56	<div> <div>98%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	AH	217	
10	AJ	76	
11	AT	75	
12	AU	148	
13	AZ	295	
14	Aa	264	
15	Ab	293	
16	Ac	281	
17	Ad	263	
18	Ae	204	
19	Af	249	
20	Ag	432	
21	Ah	208	
22	Ai	194	
23	Aj	165	
24	Ak	158	
25	Al	132	
26	Am	151	
27	An	151	
28	Ao	145	
29	Ap	172	
30	Aq	135	
31	Ar	152	
32	As	145	
33	At	119	

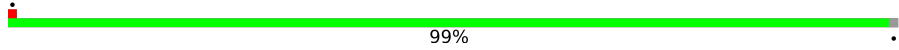
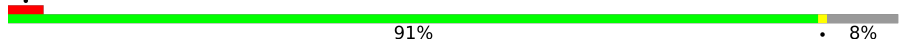
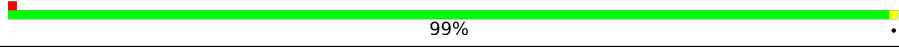
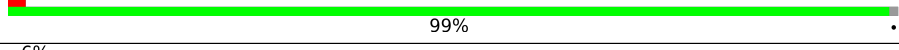

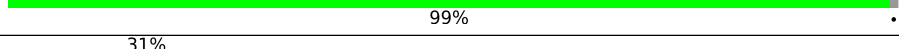
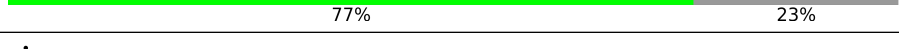
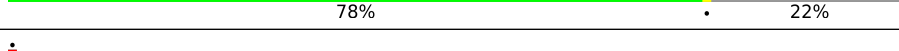
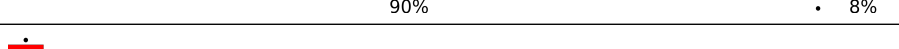
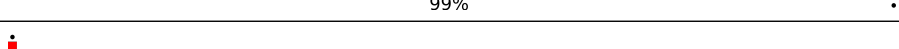
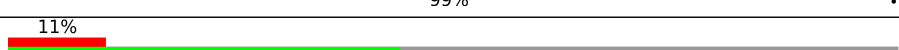

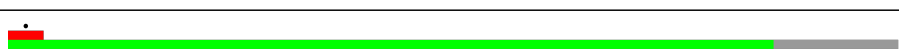
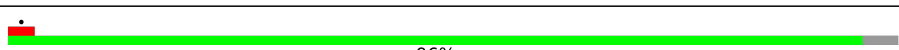
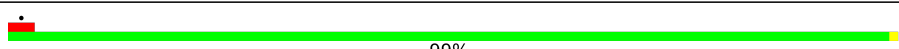

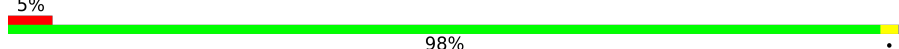
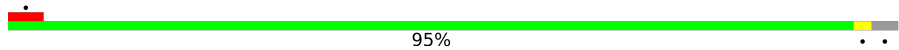

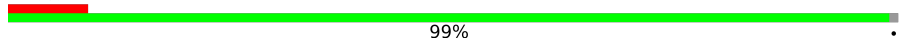
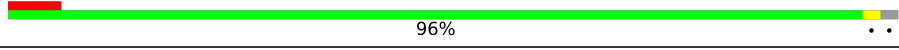

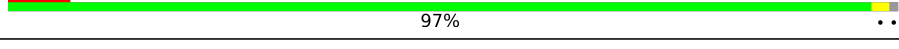
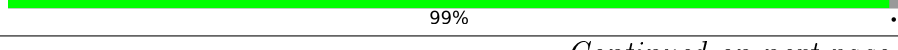

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Mol	Chain	Length	Quality of chain
34	Au	83	
35	Av	130	
36	Aw	143	
37	Ax	130	
38	Ay	124	
39	Az	25	
40	B5	4808	
41	B7	120	
42	B8	158	
43	BA	257	
44	BB	403	
45	BC	413	
46	BD	297	
47	BE	291	
48	BF	247	
49	BG	266	
50	BH	192	
51	BI	214	
52	BJ	178	
53	BK	1071	
54	BL	211	
55	BM	218	
56	BN	204	
57	BO	203	
58	BP	184	

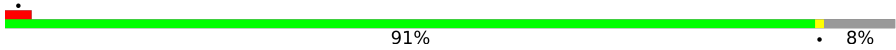

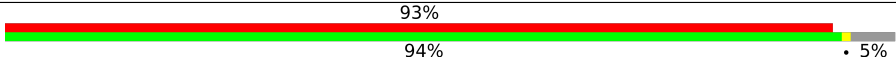
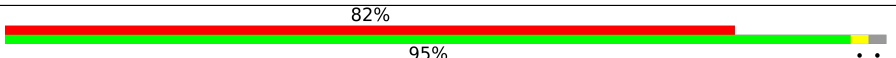
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Mol	Chain	Length	Quality of chain
59	BQ	188	
60	BR	196	
61	BS	176	
62	BT	160	
63	BU	128	
64	BV	140	
65	BW	157	
66	BX	156	
67	BY	145	
68	BZ	136	
69	Ba	148	
70	Bb	245	
71	Bc	115	
72	Bd	125	
73	Be	135	
74	Bf	110	
75	Bg	117	
76	Bh	123	
77	Bi	105	
78	Bj	97	
79	Bk	70	
80	Bl	51	
81	Bm	128	
82	Bo	106	
83	Bp	92	

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Mol	Chain	Length	Quality of chain
84	Br	137	 91% 8%
85	Bs	318	 59% 61% 38%
86	Bt	165	 93% 94% 5%
87	Bv	217	 82% 95%

## 2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 228361 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A2	1770	Total	C	N	O	P	0	0
			37833	16911	6781	12371	1770		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1249	B8N	C	conflict	GB GBCT01000564.1
A2	1338	4AC	C	conflict	GB GBCT01000564.1
A2	1843	4AC	C	conflict	GB GBCT01000564.1

- Molecule 2 is a protein called 40S ribosomal protein S27.

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

- Molecule 3 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AB	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 4 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AC	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 5 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AD	45	Total	C	N	O	S	0	0
			369	228	84	56	1		

- Molecule 6 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AE	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 7 is a protein called RACK1.

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

- Molecule 8 is a protein called uS14.

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

- Molecule 9 is a RNA chain called mRNA containing SARS-CoV-2 sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AH	10	Total	C	N	O	P	0	0
			212	95	39	68	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AH	3466	U	A	conflict	GB NC_045512.2
AH	3468	A	C	conflict	GB NC_045512.2

- Molecule 10 is a RNA chain called A-site Met-tRNA(Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	76	Total	C	N	O	P	0	0
			1622	724	290	532	76		

- Molecule 11 is a RNA chain called P-site tRNA(Pro).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AT	75	Total	C	N	O	P	0	0
			1604	714	284	531	75		

- Molecule 12 is a protein called EDF1.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	AU	110	Total	C	N	O		
			864	529	169	166	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AZ	221	Total	C	N	O	S		
			1743	1107	305	323	8	0	0

- Molecule 14 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Aa	214	Total	C	N	O	S		
			1738	1104	311	309	14	0	0

- Molecule 15 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ab	220	Total	C	N	O	S		
			1706	1105	292	300	9	0	0

- Molecule 16 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ac	225	Total	C	N	O	S		
			1751	1116	315	313	7	0	0

- Molecule 17 is a protein called Ribosomal protein eS4.

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

- Molecule 18 is a protein called Ribosomal protein S5.

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

- Molecule 19 is a protein called 40S ribosomal protein S6.

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

- Molecule 20 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ag	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 21 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 22 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 23 is a protein called Ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Aj	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 24 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ak	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 25 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Al	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 26 is a protein called uS15.

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

- Molecule 27 is a protein called 40S ribosomal protein uS11.

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

- Molecule 28 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ao	128	Total	C	N	O	S	0	0
			1048	665	197	179	7		

- Molecule 29 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ap	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 30 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Aq	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 31 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ar	148	Total	C	N	O	S	0	0
			1217	763	245	208	1		

- Molecule 32 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	As	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 33 is a protein called 40S ribosomal protein uS10.

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

- Molecule 34 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Au	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

- Molecule 35 is a protein called Ribosomal protein S15a.

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

- Molecule 36 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Aw	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 37 is a protein called 40S ribosomal protein S24.

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

- Molecule 38 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ay	73	Total	C	N	O	S	0	0
			579	372	106	100	1		

- Molecule 39 is a protein called 60s ribosomal protein l41.

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

- Molecule 40 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	B5	3764	Total	C	N	O	P	0	0
			80772	36003	14762	26243	3764		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 41 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B7	120	Total	C	N	O	P	0	0
			2570	1141	456	851	122		

- Molecule 42 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	B8	156	Total	C	N	O	P	0	0
			3319	1481	585	1097	156		

- Molecule 43 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BA	253	Total	C	N	O	S	0	0
			1940	1214	396	324	6		

- Molecule 44 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BB	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

- Molecule 45 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BC	362	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

- Molecule 46 is a protein called Ribosomal\_L18\_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BD	294	Total	C	N	O	S	0	0
			2398	1516	439	429	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BD	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 47 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BE	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 48 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BF	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

- Molecule 49 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BG	232	Total	C	N	O	S	0	0
			1868	1191	359	314	4		

- Molecule 50 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BH	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 51 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BI	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

- Molecule 52 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 53 is a protein called Replicase polypeptide 1ab.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BK	39	Total	C	N	O	S	0	0
			290	180	48	55	7		

- Molecule 54 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BL	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 55 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BM	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 56 is a protein called Ribosomal protein L15.

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

- Molecule 57 is a protein called Ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BO	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 58 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BP	159	Total	C	N	O	S	0	0
			1289	809	249	222	9		

- Molecule 59 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BQ	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BR	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 61 is a protein called Ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BS	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

- Molecule 62 is a protein called eL21.

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

- Molecule 63 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BU	99	Total	C	N	O	S	0	0
			806	516	141	147	2		

- Molecule 64 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BV	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 65 is a protein called eL24.



Mol	Chain	Residues	Atoms					AltConf	Trace
65	BW	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 66 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BX	122	Total	C	N	O	S	0	0
			1004	642	190	171	1		

- Molecule 67 is a protein called Ribosomal protein L26.

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

- Molecule 68 is a protein called 60S ribosomal protein L27.

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

- Molecule 69 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ba	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 70 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bb	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 71 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bc	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 72 is a protein called eL31.

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

- Molecule 73 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Be	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 74 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bf	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 75 is a protein called 60S ribosomal protein L34.

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

- Molecule 76 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bh	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 77 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bi	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 78 is a protein called Ribosomal protein L37.

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

- Molecule 79 is a protein called eL38.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bk	24	LYS	ASN	conflict	UNP G1U001

- Molecule 80 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bl	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 81 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bm	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 82 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Bo	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 83 is a protein called eL43.

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

- Molecule 84 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Br	126	Total	C	N	O	S	0	0
			1014	629	209	170	6		

- Molecule 85 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Bs	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 86 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Bt	156	Total	C	N	O	S	0	0
			1178	733	221	220	4		

- Molecule 87 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Bv	212	Total	C	N	O	S	0	0
			1707	1092	308	299	8		

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A2	84	Total	Mg	0
			84	84	
88	B5	250	Total	Mg	0
			250	250	
88	B7	7	Total	Mg	0
			7	7	
88	B8	5	Total	Mg	0
			5	5	
88	BP	1	Total	Mg	0
			1	1	
88	BV	1	Total	Mg	0
			1	1	
88	Ba	1	Total	Mg	0
			1	1	

- Molecule 89 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
89	A2	62	Total	X	0
			62	62	
89	AT	1	Total	X	0
			1	1	
89	An	1	Total	X	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
89	B5	175	Total 175	X 175	0
89	B7	6	Total 6	X 6	0
89	B8	4	Total 4	X 4	0
89	BA	4	Total 4	X 4	0
89	BB	1	Total 1	X 1	0
89	BH	1	Total 1	X 1	0
89	BI	1	Total 1	X 1	0
89	BL	1	Total 1	X 1	0
89	BN	3	Total 3	X 3	0
89	BO	1	Total 1	X 1	0
89	BT	2	Total 2	X 2	0
89	Be	1	Total 1	X 1	0
89	Bf	1	Total 1	X 1	0
89	Bg	1	Total 1	X 1	0

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

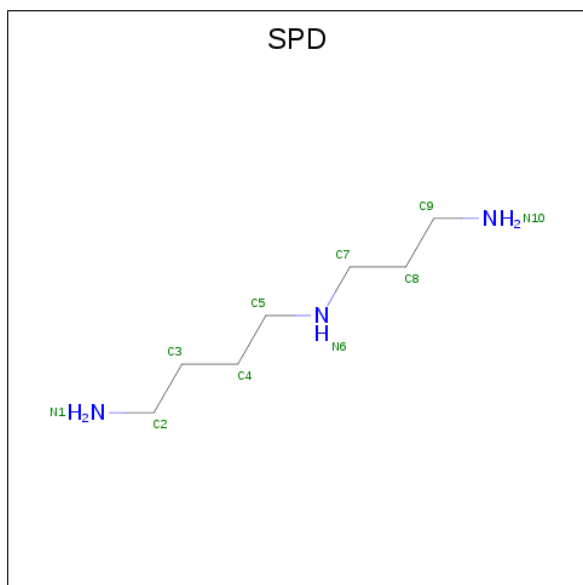
Mol	Chain	Residues	Atoms		AltConf
90	AC	1	Total 1	Zn 1	0
90	AE	1	Total 1	Zn 1	0
90	AG	1	Total 1	Zn 1	0
90	Bg	1	Total 1	Zn 1	0
90	Bj	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
90	Bm	1	Total	Zn	0
			1	1	
90	Bo	1	Total	Zn	0
			1	1	
90	Bp	1	Total	Zn	0
			1	1	

- Molecule 91 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



Mol	Chain	Residues	Atoms			AltConf
91	B5	1	Total	C	N	0
			10	7	3	

- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	A2	391	Total	O	0
			391	391	
92	AE	1	Total	O	0
			1	1	
92	Ab	1	Total	O	0
			1	1	
92	Af	1	Total	O	0
			1	1	
92	Ak	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
92	An	1	Total 1	O 1	0
92	Ap	2	Total 2	O 2	0
92	Ar	1	Total 1	O 1	0
92	As	2	Total 2	O 2	0
92	Aw	5	Total 5	O 5	0
92	B5	1197	Total 1197	O 1197	0
92	B7	35	Total 35	O 35	0
92	B8	35	Total 35	O 35	0
92	BA	4	Total 4	O 4	0
92	BB	3	Total 3	O 3	0
92	BC	3	Total 3	O 3	0
92	BD	1	Total 1	O 1	0
92	BF	2	Total 2	O 2	0
92	BH	1	Total 1	O 1	0
92	BI	1	Total 1	O 1	0
92	BL	1	Total 1	O 1	0
92	BN	2	Total 2	O 2	0
92	BO	1	Total 1	O 1	0
92	BP	3	Total 3	O 3	0
92	BR	5	Total 5	O 5	0
92	BV	3	Total 3	O 3	0

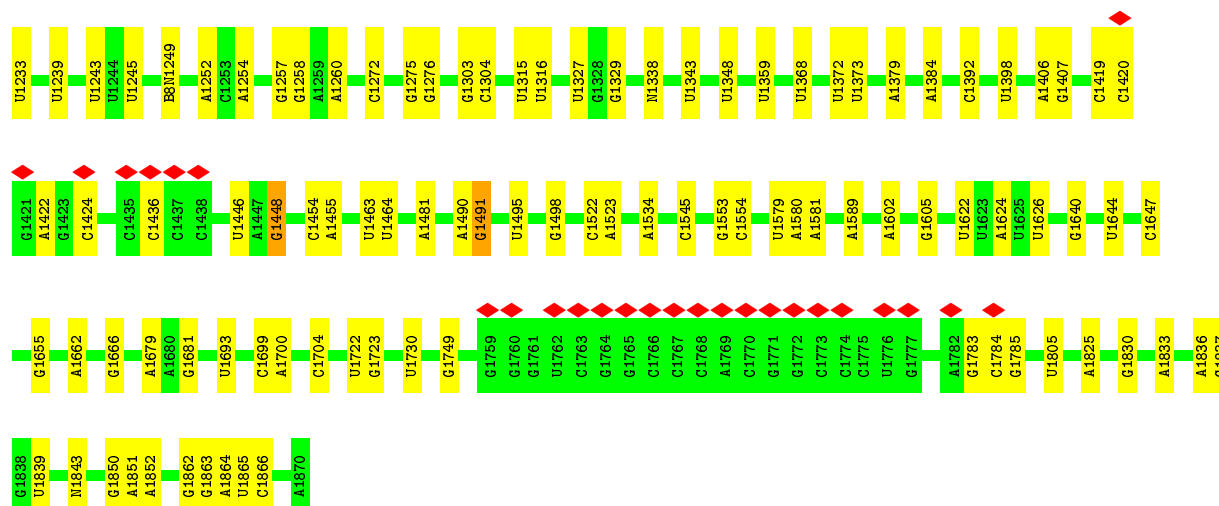
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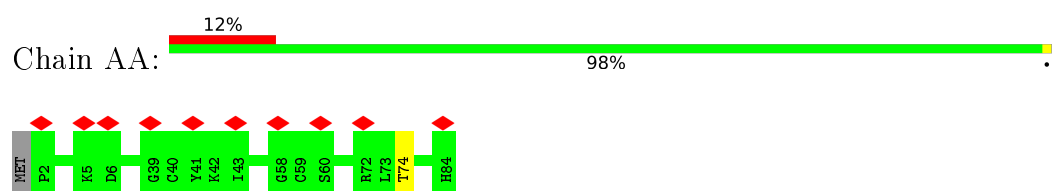
Mol	Chain	Residues	Atoms		AltConf
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92	BY	1	Total 1	O 1	0
92	Ba	7	Total 7	O 7	0
92	Bb	1	Total 1	O 1	0
92	Be	4	Total 4	O 4	0
92	Bg	2	Total 2	O 2	0
92	Bj	3	Total 3	O 3	0
92	Bm	1	Total 1	O 1	0



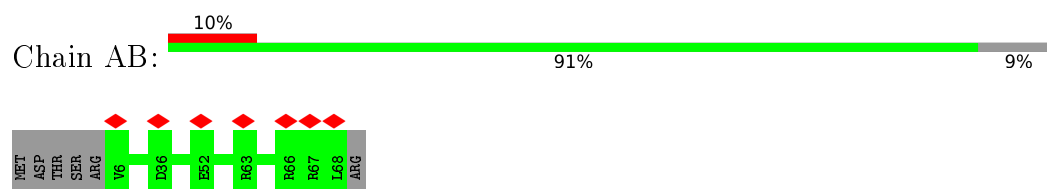




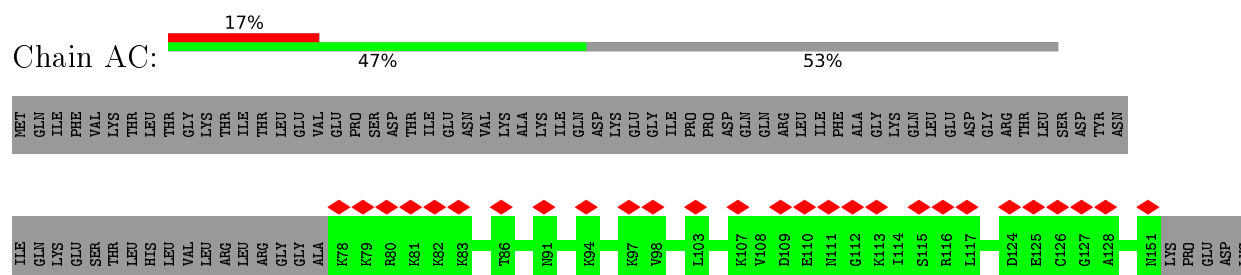
- Molecule 2: 40S ribosomal protein S27



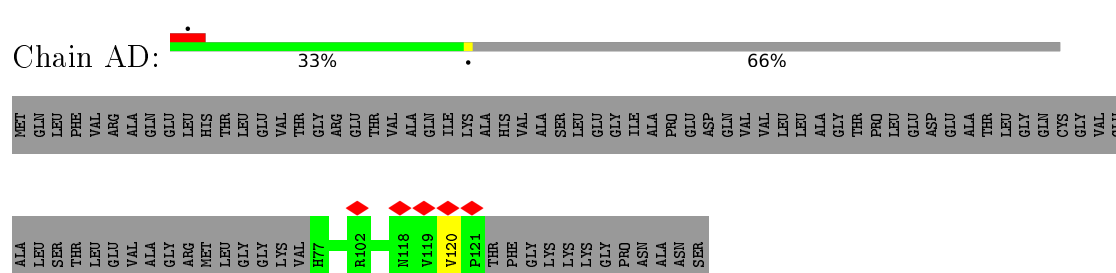
- Molecule 3: Ribosomal protein S28

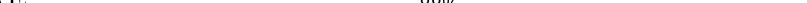


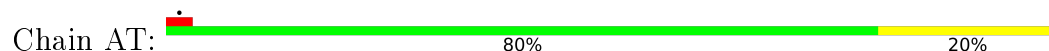
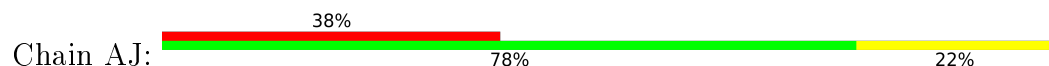
- Molecule 4: Ribosomal protein S27a

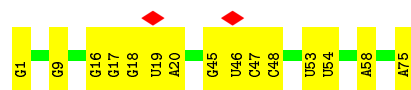


- Molecule 5: 40S ribosomal protein S30

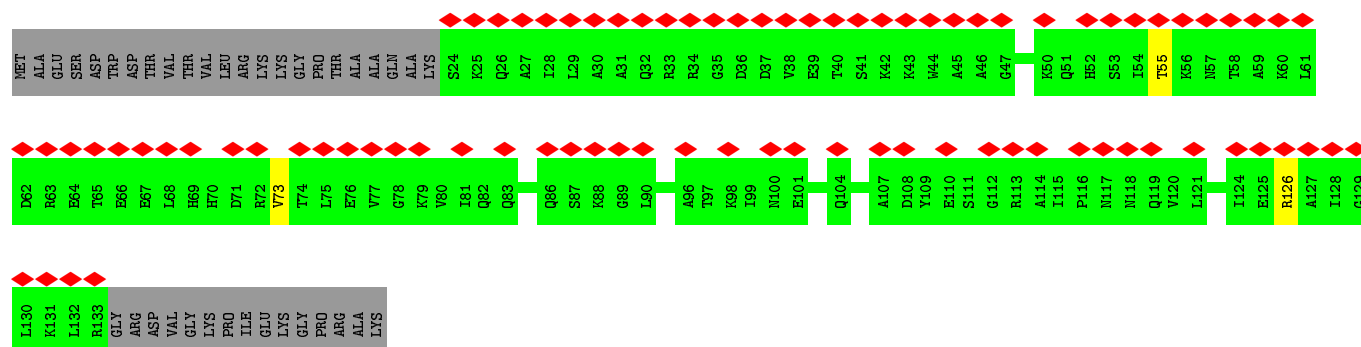
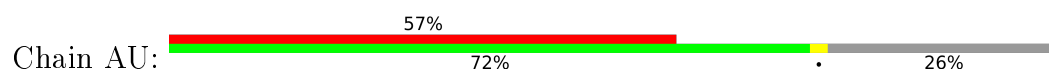


- Chain AE: 

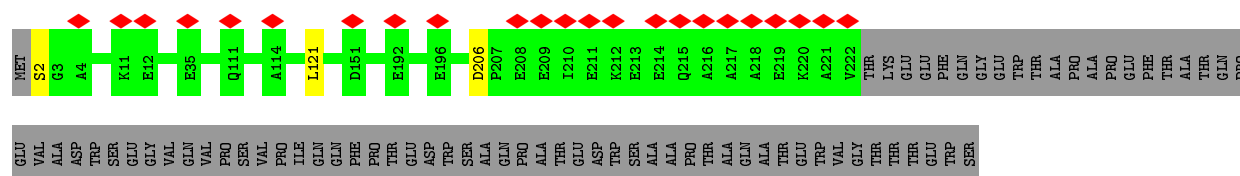
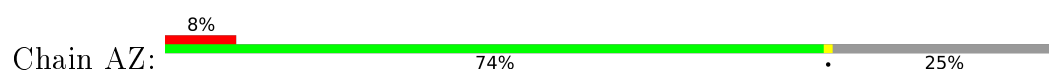




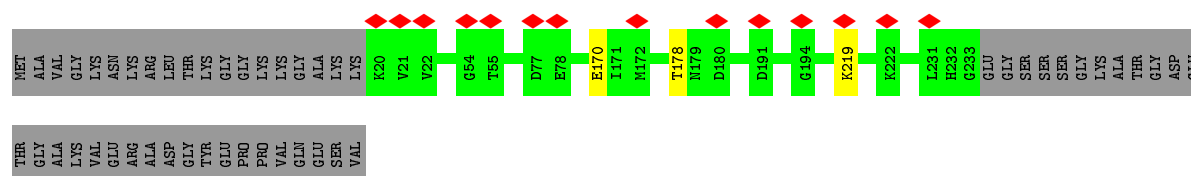
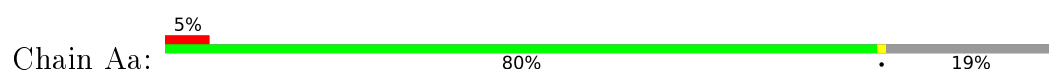
- Molecule 12: EDF1



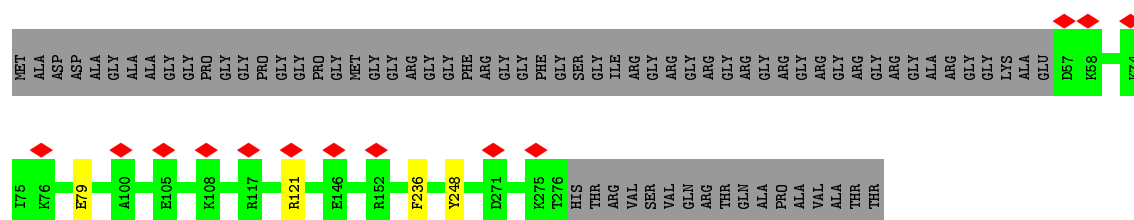
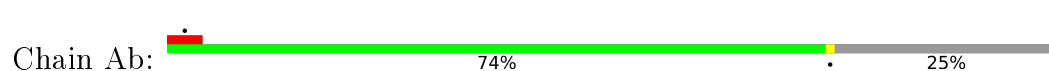
- Molecule 13: 40S ribosomal protein SA



- Molecule 14: 40S ribosomal protein S3a

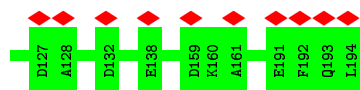


- Molecule 15: Ribosomal protein uS5

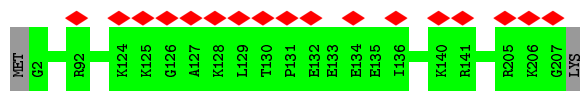


- Molecule 16: 40S ribosomal protein S3

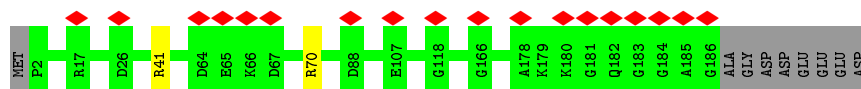




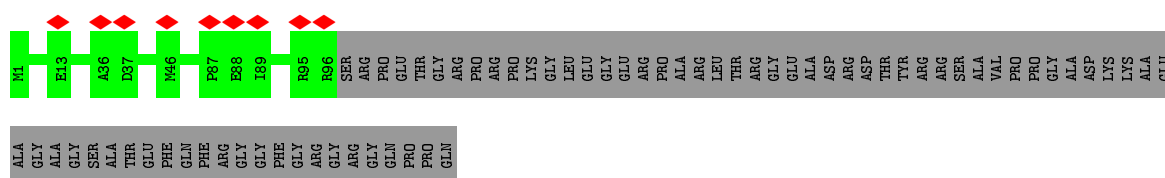
- Molecule 21: 40S ribosomal protein S8



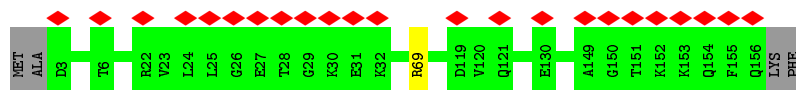
- Molecule 22: Ribosomal protein S9 (Predicted)



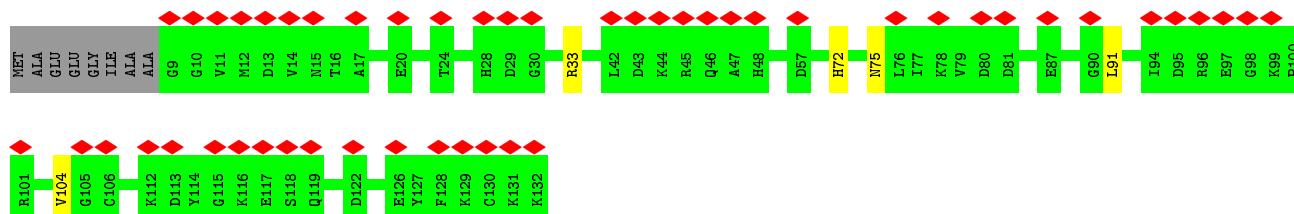
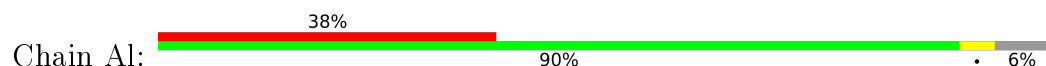
- Molecule 23: Ribosomal protein eS10



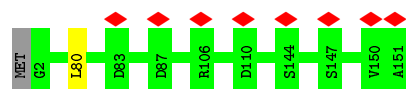
- Molecule 24: 40S ribosomal protein S11



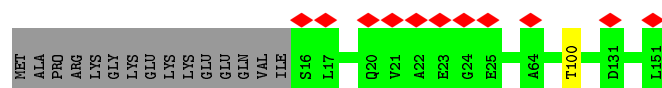
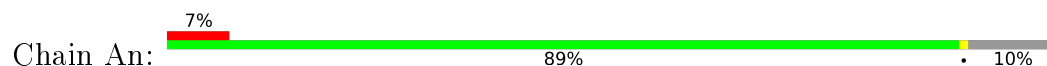
- Molecule 25: 40S ribosomal protein S12



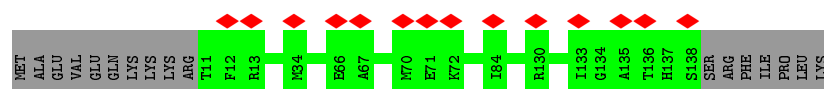
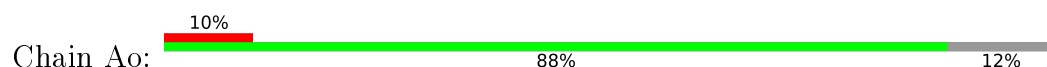
- Molecule 26: uS15



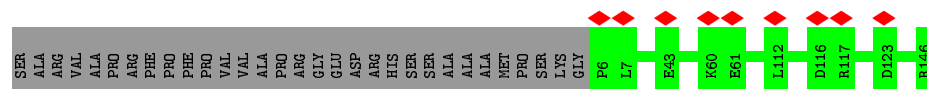
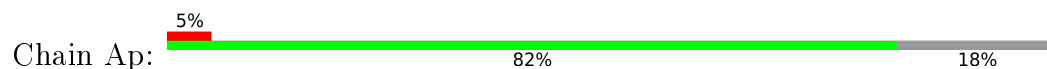
- Molecule 27: 40S ribosomal protein uS11



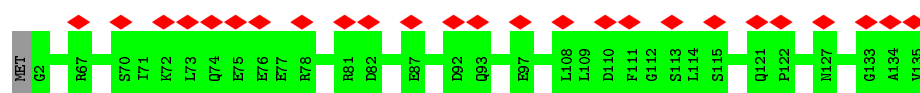
- Molecule 28: 40S ribosomal protein uS19



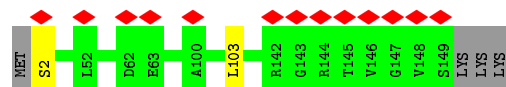
- Molecule 29: uS9



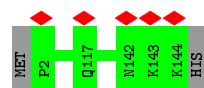
- Molecule 30: 40S ribosomal protein eS17



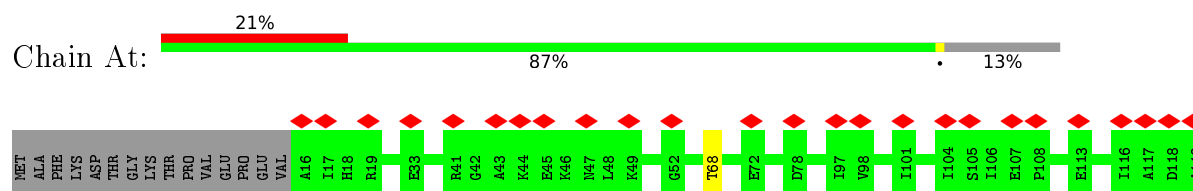
- Molecule 31: 40S ribosomal protein S18



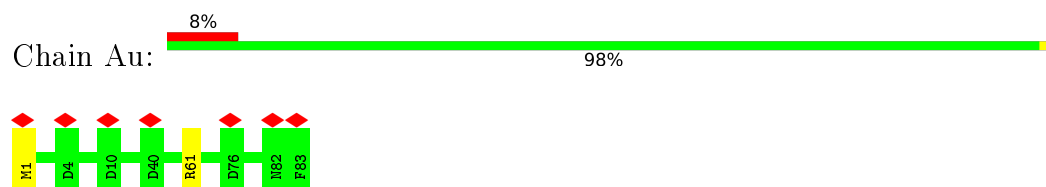
- Molecule 32: Ribosomal protein eS19



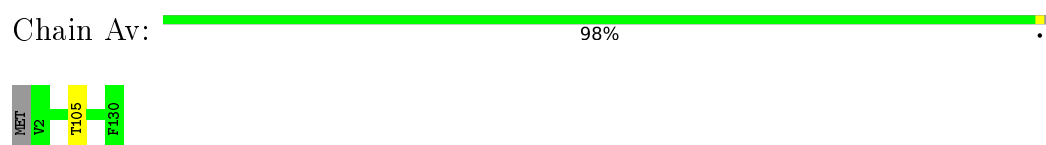
- Molecule 33: 40S ribosomal protein uS10



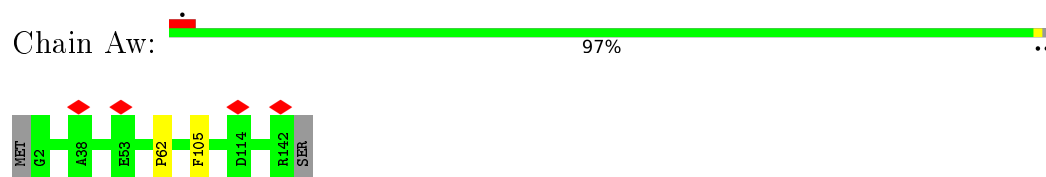
- Molecule 34: Ribosomal protein eS21



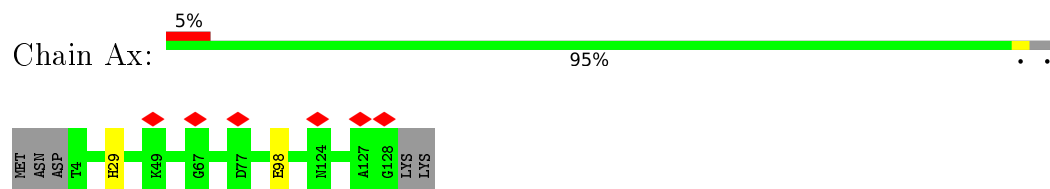
- Molecule 35: Ribosomal protein S15a



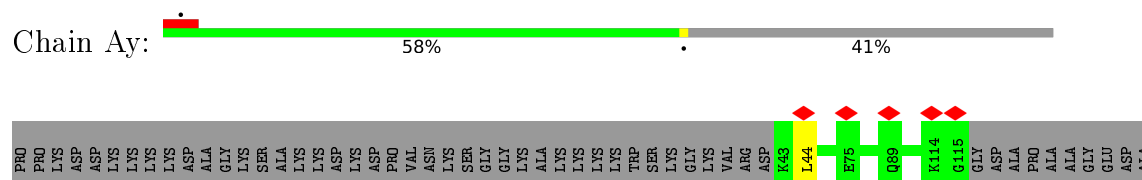
- Molecule 36: 40S ribosomal protein S23



- Molecule 37: 40S ribosomal protein S24



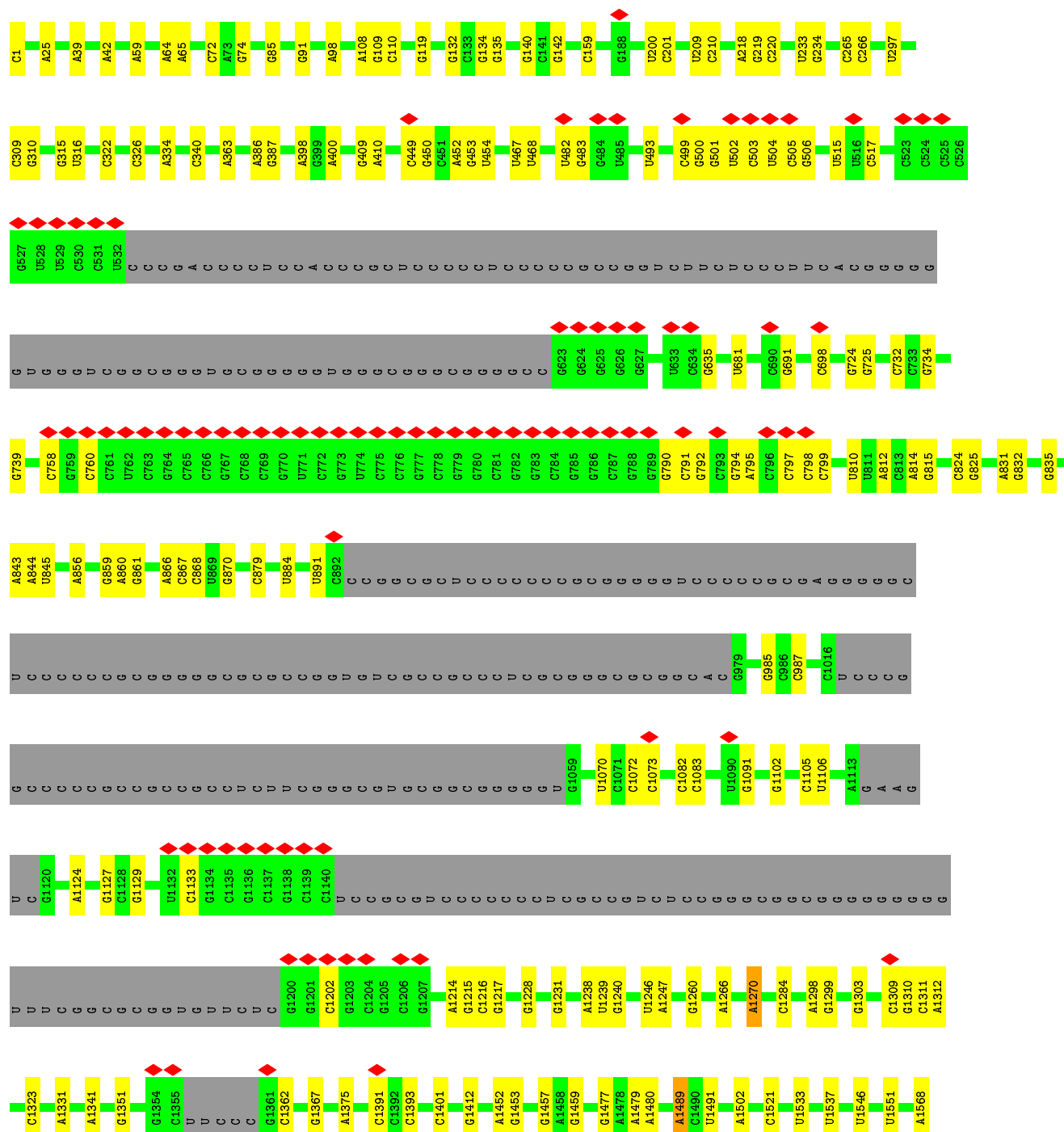
- Molecule 38: 40S ribosomal protein S25



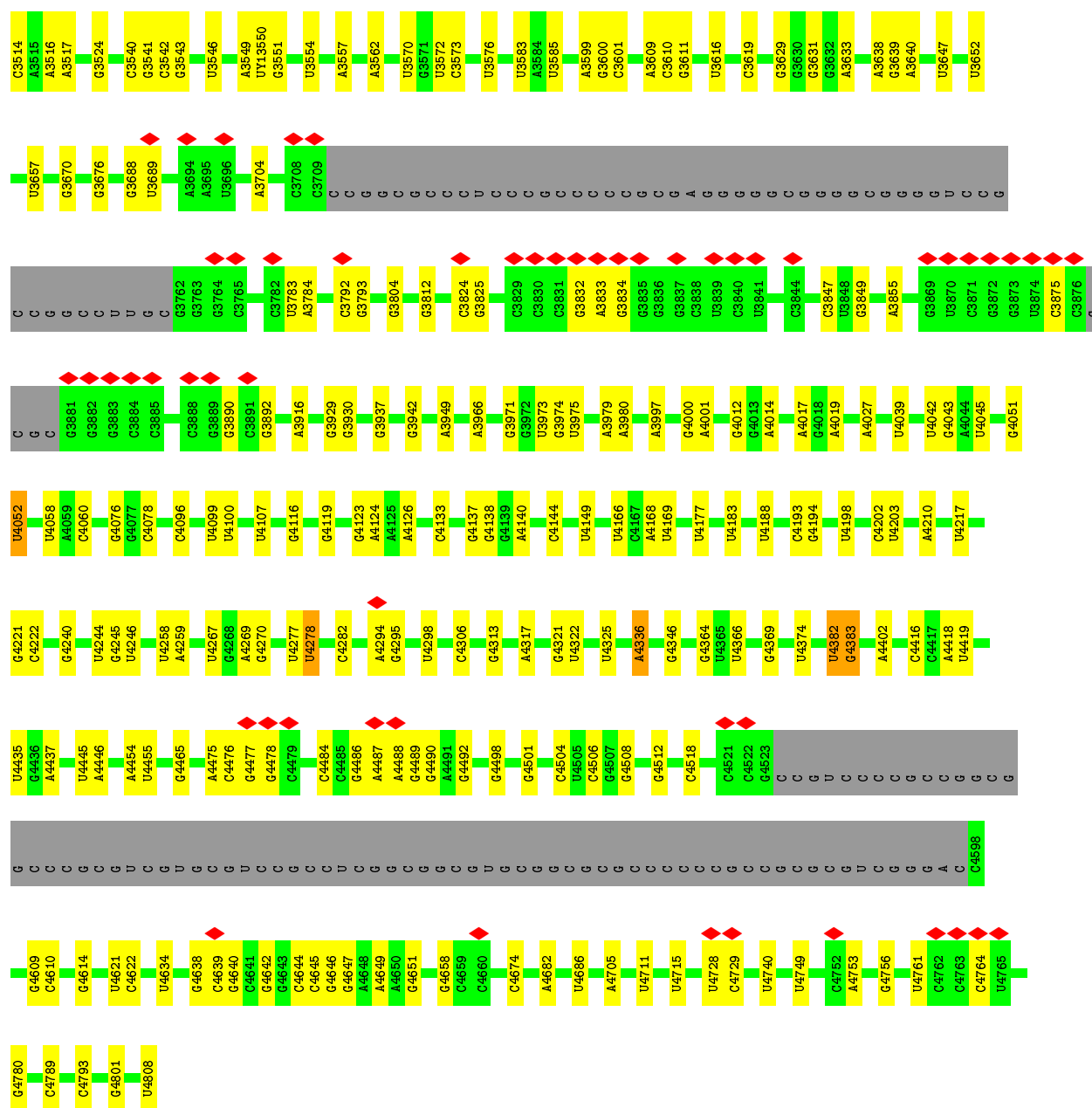
- Molecule 39: 60s ribosomal protein l41











● Molecule 41: 5S rRNA

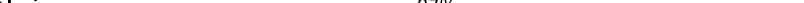


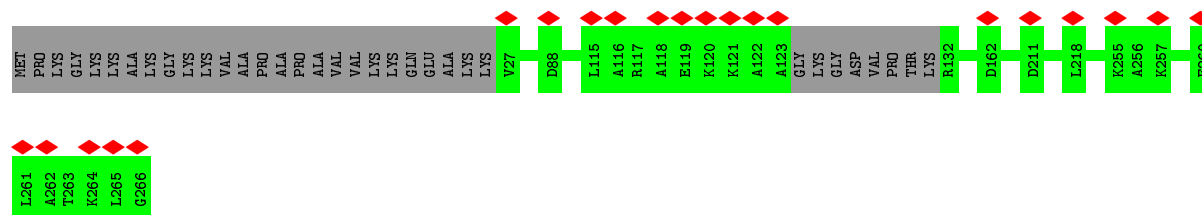
● Molecule 42: 5.8S rRNA



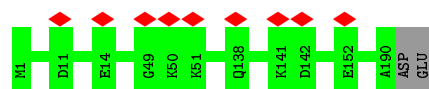


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GLU  
GLY  
ALA  
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ARG  
R22  
K35  
N247

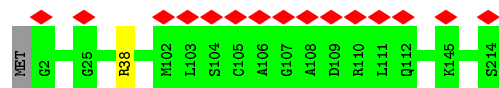
- Chain BG: 



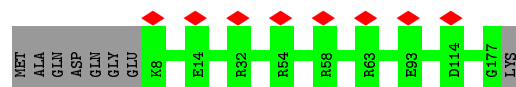
- Chain BH:  5% 99%



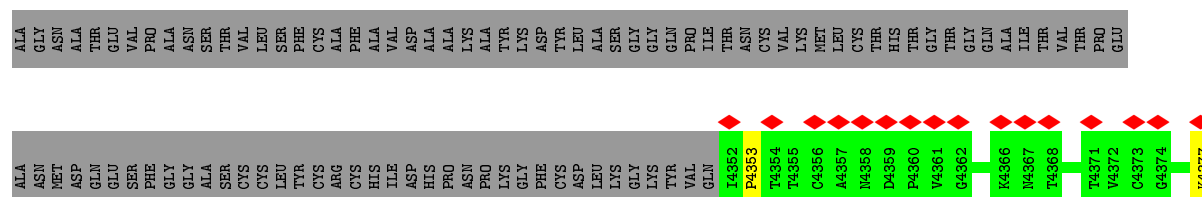
- Chain BI:  7% 99%



- Chain BJ:  96%



- Chain BK:  96%





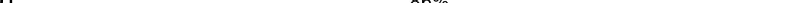
[illegible]

- Chain BN:  100%

**MET**  
**G2**  
**R204**

- Chain BO:  98%

Diagram illustrating the location of the four amino acid substitutions (Q5, D100, R117, and V203) within the protein structure. The substitutions are marked by red diamonds above the corresponding residues.

- Chain BP:  86% 14%

**Met**

V2	M140	E154	Q155	I156	V157	P158	K159	P160	GLU	GLU	GLU	VAL	ALA	GLN	LYS	LYS	LYS	LYS	LYS	LYS	LEU	LYS	GLN	LYS	LEU	MET	ARG	GLU
----	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain BQ: 

Diagram illustrating the protein structure with domains MET, G2, D10, D88, and N188. Red diamonds indicate the positions of the two mutations.

- Chain BR:  91% 8%

Amino Acid	Count (MET)	Color	Red Diamond
S2	1	Green	No
L106	2	Green	Yes
K152	3	Green	Yes
D157	4	Green	Yes
E160	5	Green	Yes
E168	6	Green	Yes
A169	7	Green	Yes
R170	8	Green	Yes
E175	9	Green	Yes
Q178	10	Green	Yes
A179	11	Green	Yes
K180	12	Green	Yes
K181	13	Green	No
GLU	14	Grey	No
GLU	15	Grey	No
ILE	16	Grey	No
ILE	17	Grey	No
LYS	18	Grey	No
THR	19	Grey	No
THR	20	Grey	No
LEU	21	Grey	No
LEU	22	Grey	No
SER	23	Grey	No
SER	24	Grey	No
LYS	25	Grey	No
LYS	26	Grey	No
GLU	27	Grey	No
GLU	28	Grey	No
GLU	29	Grey	No
GLU	30	Grey	No
THR	31	Grey	No
THR	32	Grey	No
LYS	33	Grey	No
LYS	34	Grey	No

- Chain BS: 

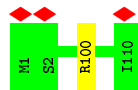




-

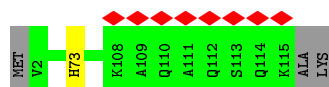
- Molecule 74: eL33

Chain Bf:  99%



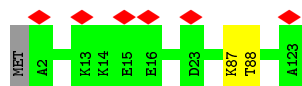
- Molecule 75: 60S ribosomal protein L34

Chain Bg:  97%



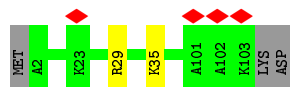
- Molecule 76: uL29

Chain Bh:  98%




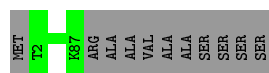
- Molecule 77: 60S ribosomal protein L36

Chain Bi:  95%



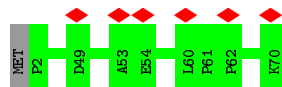
- Molecule 78: Ribosomal protein L37

Chain Bj:  89% 11%



- Molecule 79: eL38

Chain Bk:  99%

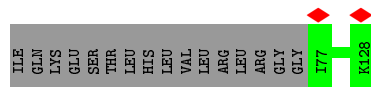
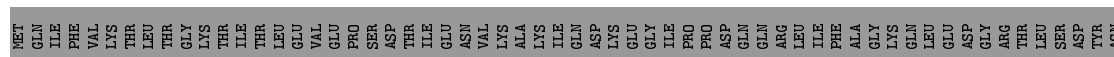


- Molecule 80: eL39

Chain Bl:  96%



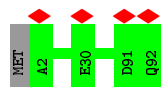
- Molecule 81: 60S ribosomal protein L40



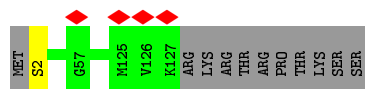
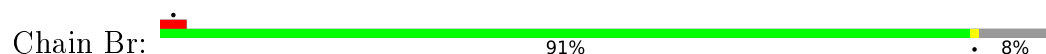
- Molecule 82: eL42



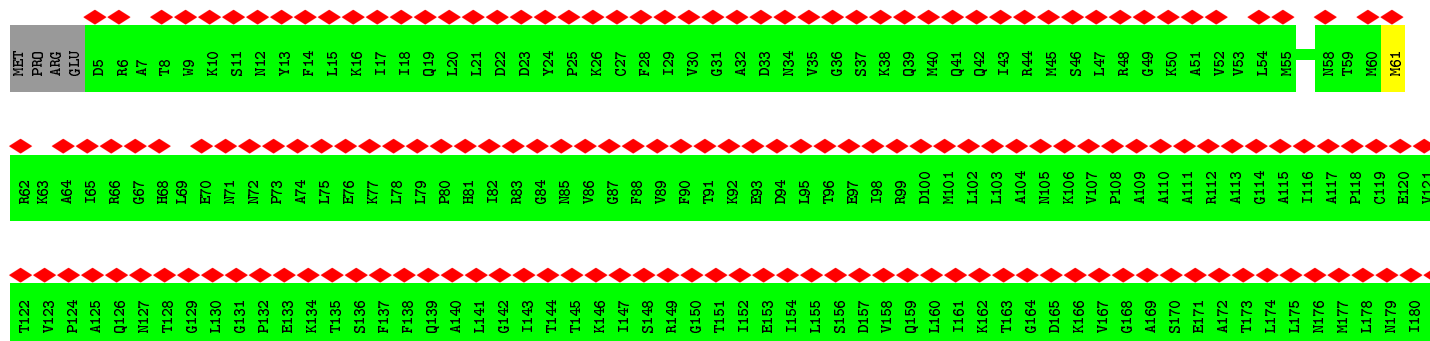
- Molecule 83: eL43

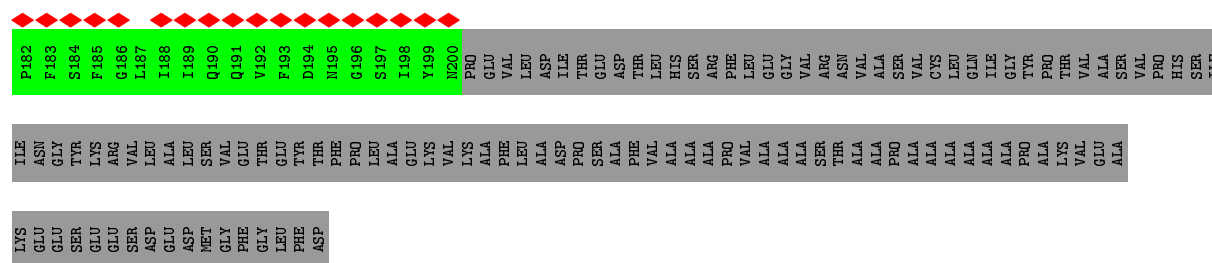


- Molecule 84: Ribosomal protein eL28

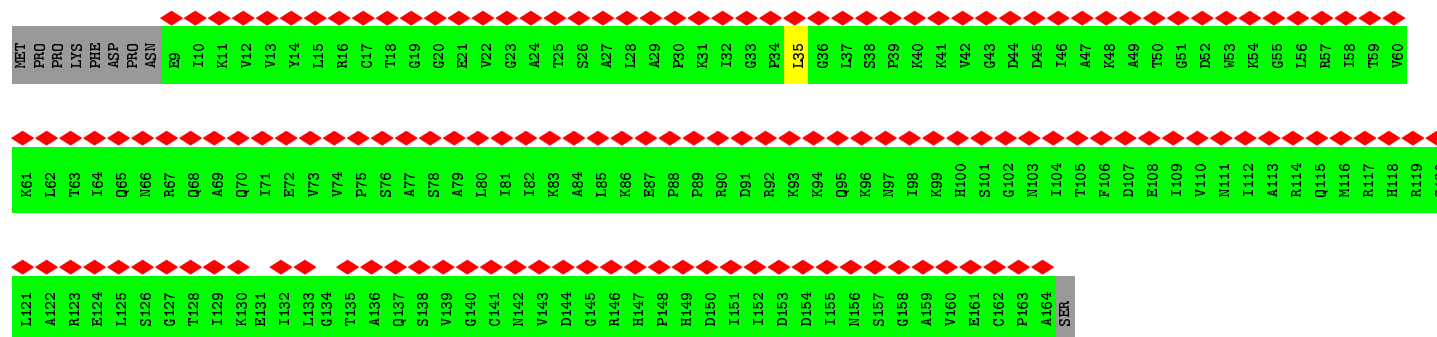


- Molecule 85: 60S acidic ribosomal protein P0

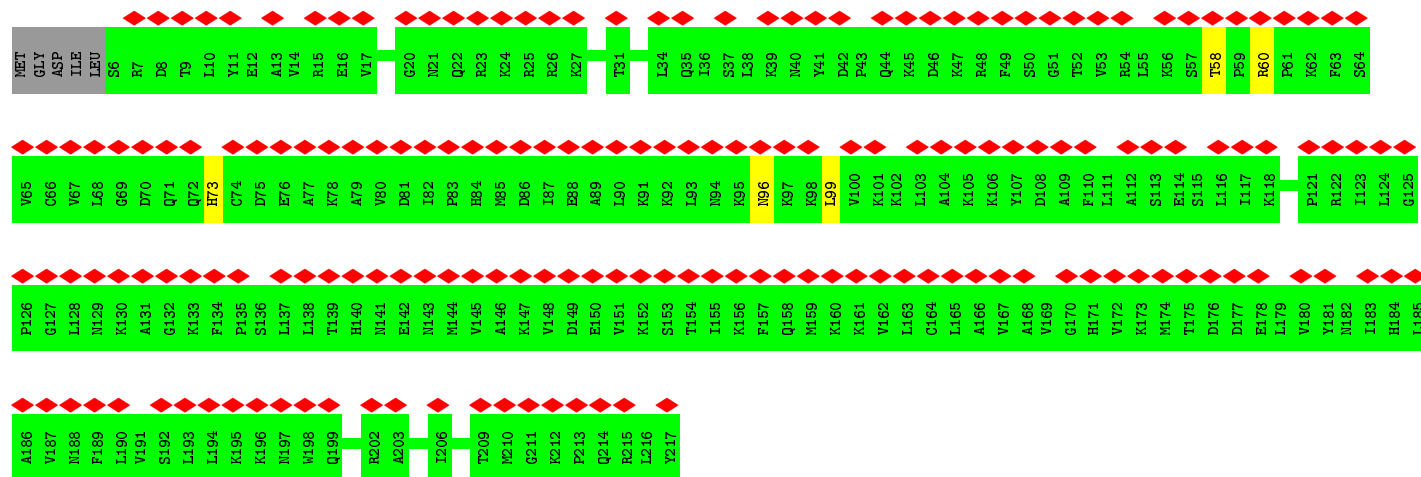
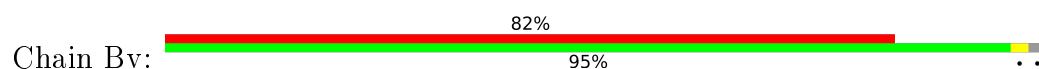




• Molecule 86: Ribosomal protein L12



• Molecule 87: Ribosomal protein uL1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19009	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	56604	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.676	Depositor
Minimum map value	-1.120	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.109	Depositor
Recommended contour level	0.4	Depositor
Map size ( $\text{\AA}$ )	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AME, OMC, AYA, 5MC, G7M, ZN, A2M, B8N, UY1, 6MZ, SAC, HIC, AAC, V5N, MG, MA6, 4AC, 1MA, NMM, 5MU, MLZ, OMG, UR3, PSU, OMU, HY3, SPD, M3L, UNX, GTP

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	A2	0.17	1/40342 (0.0%)	0.68	8/62877 (0.0%)
2	AA	0.24	0/665	0.45	0/891
3	AB	0.23	0/497	0.57	0/666
4	AC	0.25	0/622	0.48	0/822
5	AD	0.23	0/372	0.55	0/489
6	AE	0.24	0/828	0.53	0/1109
7	AF	0.23	0/2493	0.46	0/3394
8	AG	0.24	0/470	0.51	0/623
9	AH	0.15	0/236	0.66	0/365
10	AJ	0.28	1/1767 (0.1%)	0.65	0/2751
11	AT	0.29	1/1746 (0.1%)	0.65	0/2720
12	AU	0.24	0/871	0.46	0/1166
13	AZ	0.24	0/1771	0.46	0/2406
14	Aa	0.23	0/1765	0.45	0/2361
15	Ab	0.24	0/1742	0.45	0/2354
16	Ac	0.24	0/1779	0.49	0/2395
17	Ad	0.24	0/2118	0.49	0/2849
18	Ae	0.23	0/1531	0.47	0/2059
19	Af	0.24	0/1946	0.52	0/2590
20	Ag	0.24	0/1552	0.47	0/2079
21	Ah	0.24	0/1715	0.51	0/2287
22	Ai	0.23	0/1550	0.53	0/2069
23	Aj	0.24	0/834	0.42	0/1125
24	Ak	0.25	0/1284	0.51	0/1717
25	Al	0.23	0/968	0.42	0/1296
26	Am	0.23	0/1232	0.47	0/1656
27	An	0.24	0/1029	0.52	0/1380
28	Ao	0.24	0/1069	0.48	0/1429
29	Ap	0.24	0/1142	0.49	0/1528
30	Aq	0.24	0/1094	0.48	0/1469
31	Ar	0.23	0/1226	0.52	0/1643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	As	0.24	0/1119	0.46	0/1498
33	At	0.23	0/831	0.51	0/1115
34	Au	0.25	0/636	0.47	0/852
35	Av	0.24	0/1051	0.48	0/1406
36	Aw	0.24	0/1107	0.49	0/1475
37	Ax	0.24	0/1032	0.50	0/1371
38	Ay	0.23	0/585	0.46	0/785
39	Az	0.22	0/240	0.65	0/305
40	B5	0.18	3/87403 (0.0%)	0.67	14/136359 (0.0%)
41	B7	0.16	0/2835	0.65	0/4418
42	B8	0.24	1/3635 (0.0%)	0.66	0/5661
43	BA	0.25	0/1965	0.53	0/2633
44	BB	0.24	0/3261	0.49	0/4364
45	BC	0.24	0/2932	0.50	0/3939
46	BD	0.24	0/2437	0.47	0/3264
47	BE	0.24	0/1998	0.49	0/2673
48	BF	0.24	0/1922	0.48	0/2563
49	BG	0.24	0/1899	0.47	0/2555
50	BH	0.24	0/1535	0.49	0/2063
51	BI	0.24	0/1756	0.50	0/2346
52	BJ	0.24	0/1385	0.50	0/1852
53	BK	0.52	1/296 (0.3%)	0.49	0/402
54	BL	0.24	0/1733	0.53	0/2316
55	BM	0.24	0/1158	0.49	0/1547
56	BN	0.24	0/1746	0.54	0/2338
57	BO	0.24	0/1662	0.48	0/2222
58	BP	0.23	0/1317	0.48	0/1768
59	BQ	0.24	0/1539	0.56	0/2054
60	BR	0.23	0/1524	0.52	0/2013
61	BS	0.25	0/1497	0.52	0/2008
62	BT	0.25	0/1326	0.49	0/1770
63	BU	0.24	0/820	0.45	0/1100
64	BV	0.25	0/1048	0.52	0/1402
65	BW	0.24	0/1006	0.50	0/1334
66	BX	0.24	0/1022	0.47	0/1371
67	BY	0.23	0/1132	0.52	0/1504
68	BZ	0.25	0/1130	0.48	0/1507
69	Ba	0.24	0/1179	0.50	0/1572
70	Bb	0.23	0/884	0.50	0/1169
71	Bc	0.23	0/847	0.44	0/1134
72	Bd	0.24	0/903	0.52	0/1216
73	Be	0.23	0/1088	0.51	0/1451
74	Bf	0.25	0/903	0.53	0/1208

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	Bg	0.24	0/916	0.53	0/1220
76	Bh	0.23	0/1021	0.49	0/1348
77	Bi	0.23	0/841	0.52	0/1112
78	Bj	0.24	0/720	0.56	0/952
79	Bk	0.24	0/575	0.44	0/761
80	Bl	0.23	0/459	0.51	0/608
81	Bm	0.23	0/426	0.50	0/564
82	Bo	0.25	0/866	0.50	0/1141
83	Bp	0.24	0/718	0.49	0/953
84	Br	0.23	0/1020	0.53	0/1366
85	Bs	0.24	0/1530	0.45	0/2064
86	Bt	0.23	0/1193	0.47	0/1609
87	Bv	0.24	0/1735	0.45	0/2328
All	All	0.21	8/237600 (0.0%)	0.61	22/348494 (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
82	Bo	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B5	4761	U	C4-O4	12.87	1.33	1.23
11	AT	1	G	OP3-P	-10.62	1.48	1.61
42	B8	1	C	OP3-P	-10.61	1.48	1.61
40	B5	1	C	OP3-P	-10.57	1.48	1.61
1	A2	1	U	OP3-P	-10.52	1.48	1.61

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	4761	U	N3-C4-C5	12.14	121.89	114.60
40	B5	4761	U	C2-N3-C4	-11.53	120.08	127.00
40	B5	4761	U	C5-C4-O4	-9.57	120.16	125.90
1	A2	1454	C	C2-N1-C1'	8.64	128.30	118.80
40	B5	2312	C	C2-N1-C1'	8.47	128.12	118.80

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
82	Bo	53	MLZ	Mainchain

## 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	
2	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
3	AB	61/69 (88%)	61 (100%)	0	0	100	100
4	AC	72/156 (46%)	70 (97%)	2 (3%)	0	100	100
5	AD	43/133 (32%)	43 (100%)	0	0	100	100
6	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
7	AF	311/317 (98%)	301 (97%)	10 (3%)	0	100	100
8	AG	53/56 (95%)	53 (100%)	0	0	100	100
12	AU	108/148 (73%)	107 (99%)	1 (1%)	0	100	100
13	AZ	219/295 (74%)	215 (98%)	4 (2%)	0	100	100
14	Aa	212/264 (80%)	206 (97%)	6 (3%)	0	100	100
15	Ab	218/293 (74%)	216 (99%)	2 (1%)	0	100	100
16	Ac	223/281 (79%)	221 (99%)	1 (0%)	1 (0%)	34	69
17	Ad	260/263 (99%)	254 (98%)	6 (2%)	0	100	100
18	Ae	189/204 (93%)	185 (98%)	4 (2%)	0	100	100
19	Af	235/249 (94%)	235 (100%)	0	0	100	100
20	Ag	188/432 (44%)	186 (99%)	2 (1%)	0	100	100
21	Ah	204/208 (98%)	201 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	Ai	183/194 (94%)	178 (97%)	5 (3%)	0	100	100
23	Aj	94/165 (57%)	93 (99%)	1 (1%)	0	100	100
24	Ak	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
25	Al	122/132 (92%)	121 (99%)	1 (1%)	0	100	100
26	Am	148/151 (98%)	148 (100%)	0	0	100	100
27	An	134/151 (89%)	133 (99%)	1 (1%)	0	100	100
28	Ao	126/145 (87%)	123 (98%)	3 (2%)	0	100	100
29	Ap	139/172 (81%)	134 (96%)	5 (4%)	0	100	100
30	Aq	132/135 (98%)	132 (100%)	0	0	100	100
31	Ar	146/152 (96%)	142 (97%)	4 (3%)	0	100	100
32	As	140/145 (97%)	140 (100%)	0	0	100	100
33	At	102/119 (86%)	99 (97%)	3 (3%)	0	100	100
34	Au	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
35	Av	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
36	Aw	136/143 (95%)	136 (100%)	0	0	100	100
37	Ax	123/130 (95%)	123 (100%)	0	0	100	100
38	Ay	71/124 (57%)	69 (97%)	2 (3%)	0	100	100
39	Az	23/25 (92%)	23 (100%)	0	0	100	100
43	BA	250/257 (97%)	241 (96%)	9 (4%)	0	100	100
44	BB	395/403 (98%)	393 (100%)	2 (0%)	0	100	100
45	BC	360/413 (87%)	356 (99%)	4 (1%)	0	100	100
46	BD	291/297 (98%)	288 (99%)	3 (1%)	0	100	100
47	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
48	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
49	BG	228/266 (86%)	226 (99%)	2 (1%)	0	100	100
50	BH	188/192 (98%)	188 (100%)	0	0	100	100
51	BI	211/214 (99%)	209 (99%)	2 (1%)	0	100	100
52	BJ	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
53	BK	37/1071 (4%)	32 (86%)	4 (11%)	1 (3%)	5	25
54	BL	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
55	BM	136/218 (62%)	133 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	BN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
57	BO	197/203 (97%)	196 (100%)	1 (0%)	0	100	100
58	BP	157/184 (85%)	154 (98%)	3 (2%)	0	100	100
59	BQ	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
60	BR	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
61	BS	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
62	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
63	BU	97/128 (76%)	95 (98%)	2 (2%)	0	100	100
64	BV	137/140 (98%)	137 (100%)	0	0	100	100
65	BW	119/157 (76%)	117 (98%)	2 (2%)	0	100	100
66	BX	120/156 (77%)	119 (99%)	1 (1%)	0	100	100
67	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
68	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
69	Ba	144/148 (97%)	140 (97%)	4 (3%)	0	100	100
70	Bb	103/245 (42%)	98 (95%)	5 (5%)	0	100	100
71	Bc	106/115 (92%)	106 (100%)	0	0	100	100
72	Bd	105/125 (84%)	103 (98%)	2 (2%)	0	100	100
73	Be	128/135 (95%)	128 (100%)	0	0	100	100
74	Bf	108/110 (98%)	108 (100%)	0	0	100	100
75	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
76	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
77	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
78	Bj	84/97 (87%)	84 (100%)	0	0	100	100
79	Bk	67/70 (96%)	67 (100%)	0	0	100	100
80	Bl	48/51 (94%)	48 (100%)	0	0	100	100
81	Bm	49/128 (38%)	49 (100%)	0	0	100	100
82	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
83	Bp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
84	Br	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
85	Bs	194/318 (61%)	187 (96%)	7 (4%)	0	100	100
86	Bt	154/165 (93%)	152 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	Bv	210/217 (97%)	204 (97%)	6 (3%)	0	100	100
All	All	12024/15056 (80%)	11846 (98%)	176 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Ac	211	VAL
53	BK	4388	GLU

### 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	
2	AA	75/76 (99%)	74 (99%)	1 (1%)	69	87
3	AB	56/62 (90%)	56 (100%)	0	100	100
4	AC	67/140 (48%)	67 (100%)	0	100	100
5	AD	38/106 (36%)	37 (97%)	1 (3%)	46	74
6	AE	88/98 (90%)	88 (100%)	0	100	100
7	AF	272/275 (99%)	269 (99%)	3 (1%)	73	89
8	AG	48/49 (98%)	48 (100%)	0	100	100
12	AU	92/121 (76%)	89 (97%)	3 (3%)	38	69
13	AZ	182/243 (75%)	180 (99%)	2 (1%)	73	89
14	Aa	195/231 (84%)	192 (98%)	3 (2%)	65	85
15	Ab	185/223 (83%)	181 (98%)	4 (2%)	52	78
16	Ac	189/232 (82%)	187 (99%)	2 (1%)	73	89
17	Ad	224/225 (100%)	223 (100%)	1 (0%)	91	96
18	Ae	161/170 (95%)	161 (100%)	0	100	100
19	Af	207/218 (95%)	206 (100%)	1 (0%)	88	94
20	Ag	170/360 (47%)	168 (99%)	2 (1%)	71	88
21	Ah	178/180 (99%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	Ai	161/168 (96%)	159 (99%)	2 (1%)	71	88
23	Aj	87/136 (64%)	87 (100%)	0	100	100
24	Ak	139/142 (98%)	138 (99%)	1 (1%)	84	93
25	Al	104/108 (96%)	99 (95%)	5 (5%)	25	58
26	Am	130/131 (99%)	129 (99%)	1 (1%)	81	92
27	An	106/119 (89%)	105 (99%)	1 (1%)	78	91
28	Ao	114/130 (88%)	114 (100%)	0	100	100
29	Ap	117/140 (84%)	117 (100%)	0	100	100
30	Aq	120/121 (99%)	120 (100%)	0	100	100
31	Ar	127/131 (97%)	126 (99%)	1 (1%)	81	92
32	As	112/114 (98%)	112 (100%)	0	100	100
33	At	94/107 (88%)	93 (99%)	1 (1%)	73	89
34	Au	67/67 (100%)	66 (98%)	1 (2%)	65	85
35	Av	112/113 (99%)	111 (99%)	1 (1%)	78	91
36	Aw	112/114 (98%)	111 (99%)	1 (1%)	78	91
37	Ax	107/112 (96%)	105 (98%)	2 (2%)	57	81
38	Ay	64/102 (63%)	63 (98%)	1 (2%)	62	84
39	Az	24/24 (100%)	24 (100%)	0	100	100
43	BA	194/198 (98%)	193 (100%)	1 (0%)	88	94
44	BB	344/347 (99%)	343 (100%)	1 (0%)	92	96
45	BC	302/337 (90%)	301 (100%)	1 (0%)	92	96
46	BD	247/250 (99%)	247 (100%)	0	100	100
47	BE	216/251 (86%)	214 (99%)	2 (1%)	78	91
48	BF	197/215 (92%)	197 (100%)	0	100	100
49	BG	198/223 (89%)	198 (100%)	0	100	100
50	BH	169/171 (99%)	169 (100%)	0	100	100
51	BI	180/181 (99%)	179 (99%)	1 (1%)	86	94
52	BJ	143/149 (96%)	143 (100%)	0	100	100
53	BK	34/936 (4%)	31 (91%)	3 (9%)	10	36
54	BL	175/176 (99%)	170 (97%)	5 (3%)	42	72
55	BM	117/161 (73%)	116 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	BN	171/172 (99%)	171 (100%)	0	100	100
57	BO	171/173 (99%)	170 (99%)	1 (1%)	86	94
58	BP	140/163 (86%)	139 (99%)	1 (1%)	84	93
59	BQ	164/165 (99%)	164 (100%)	0	100	100
60	BR	159/175 (91%)	158 (99%)	1 (1%)	86	94
61	BS	154/154 (100%)	153 (99%)	1 (1%)	86	94
62	BT	139/140 (99%)	139 (100%)	0	100	100
63	BU	88/113 (78%)	88 (100%)	0	100	100
64	BV	106/107 (99%)	106 (100%)	0	100	100
65	BW	100/126 (79%)	100 (100%)	0	100	100
66	BX	110/134 (82%)	109 (99%)	1 (1%)	78	91
67	BY	124/135 (92%)	121 (98%)	3 (2%)	49	76
68	BZ	117/118 (99%)	116 (99%)	1 (1%)	78	91
69	Ba	118/119 (99%)	118 (100%)	0	100	100
70	Bb	87/183 (48%)	87 (100%)	0	100	100
71	Bc	92/98 (94%)	92 (100%)	0	100	100
72	Bd	98/110 (89%)	98 (100%)	0	100	100
73	Be	116/121 (96%)	116 (100%)	0	100	100
74	Bf	89/89 (100%)	88 (99%)	1 (1%)	73	89
75	Bg	98/100 (98%)	97 (99%)	1 (1%)	76	90
76	Bh	109/110 (99%)	107 (98%)	2 (2%)	59	82
77	Bi	86/89 (97%)	84 (98%)	2 (2%)	50	77
78	Bj	73/80 (91%)	73 (100%)	0	100	100
79	Bk	64/65 (98%)	64 (100%)	0	100	100
80	Bl	47/48 (98%)	46 (98%)	1 (2%)	53	79
81	Bm	47/115 (41%)	47 (100%)	0	100	100
82	Bo	92/93 (99%)	91 (99%)	1 (1%)	73	89
83	Bp	74/75 (99%)	74 (100%)	0	100	100
84	Br	109/120 (91%)	109 (100%)	0	100	100
85	Bs	164/258 (64%)	163 (99%)	1 (1%)	86	94
86	Bt	128/137 (93%)	127 (99%)	1 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
87	Bv	191/195 (98%)	186 (97%)	5 (3%)	46	74
All	All	10465/12763 (82%)	10385 (99%)	80 (1%)	82	92

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
58	BP	140	MET
80	Bl	47	THR
61	BS	6	THR
74	Bf	100	ARG
87	Bv	58	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
51	BI	163	GLN
63	BU	38	ASN
52	BJ	112	HIS
60	BR	39	GLN
67	BY	14	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1758/1870 (94%)	241 (13%)	2 (0%)
10	AJ	75/76 (98%)	14 (18%)	0
11	AT	74/75 (98%)	12 (16%)	0
40	B5	3750/4808 (77%)	475 (12%)	2 (0%)
41	B7	118/120 (98%)	8 (6%)	0
42	B8	155/158 (98%)	15 (9%)	0
9	AH	9/217 (4%)	1 (11%)	0
All	All	5939/7324 (81%)	766 (12%)	4 (0%)

5 of 766 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	3	C
1	A2	4	C

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Mol	Chain	Res	Type
1	A2	26	U
1	A2	33	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	745	G
1	A2	871	A
40	B5	4294	A
40	B5	4445	U

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

227 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	PSU	B5	1799	40	17,21,22	1.61	2 (11%)	20,30,33	3.12	6 (30%)
1	PSU	A2	610	1	17,21,22	1.59	3 (17%)	20,30,33	3.11	6 (30%)
1	PSU	A2	36	1	17,21,22	1.57	2 (11%)	20,30,33	3.07	6 (30%)
1	PSU	A2	1175	1	17,21,22	1.60	2 (11%)	20,30,33	3.13	6 (30%)
40	A2M	B5	2206	88,40	18,25,26	1.01	1 (5%)	18,36,39	1.21	2 (11%)
40	OMC	B5	2208	40	15,22,23	0.69	0	17,31,34	1.29	2 (11%)
42	OMG	B8	75	42	18,26,27	1.23	2 (11%)	20,38,41	2.15	6 (30%)
40	PSU	B5	3490	40	17,21,22	1.58	2 (11%)	20,30,33	3.09	6 (30%)
43	V5N	BA	216	43	4,11,12	0.78	0	5,14,16	1.55	1 (20%)
40	PSU	B5	4039	40	17,21,22	1.58	2 (11%)	20,30,33	3.13	6 (30%)
40	5MC	B5	4193	40	15,22,23	1.31	1 (6%)	19,32,35	1.45	3 (15%)
1	A2M	A2	1032	1	18,25,26	1.02	1 (5%)	18,36,39	1.19	2 (11%)
1	A2M	A2	485	1	18,25,26	1.01	1 (5%)	18,36,39	1.26	2 (11%)
1	OMC	A2	1392	1	15,22,23	0.66	0	17,31,34	1.35	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	A2M	B5	1479	40	18,25,26	1.02	1 (5%)	18,36,39	1.25	2 (11%)
40	PSU	B5	4169	40	17,21,22	1.62	3 (17%)	20,30,33	3.10	6 (30%)
1	PSU	A2	815	1	17,21,22	1.60	3 (17%)	20,30,33	3.07	6 (30%)
40	A2M	B5	400	40	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
40	OMU	B5	3657	40	14,22,23	0.80	1 (7%)	14,31,34	0.81	0
1	OMG	A2	684	1	18,26,27	1.20	2 (11%)	20,38,41	2.16	6 (30%)
40	OMC	B5	3433	40	15,22,23	0.68	0	17,31,34	1.28	2 (11%)
40	OMG	B5	3676	40	18,26,27	1.24	2 (11%)	20,38,41	2.15	6 (30%)
84	SAC	Br	2	84	7,8,9	0.53	0	8,9,11	0.85	1 (12%)
40	PSU	B5	3427	40	17,21,22	1.57	3 (17%)	20,30,33	3.08	6 (30%)
40	OMU	B5	4052	40	14,22,23	0.80	1 (7%)	14,31,34	0.79	0
40	OMC	B5	4202	40	15,22,23	0.68	0	17,31,34	1.32	2 (11%)
1	OMG	A2	510	88,1	18,26,27	1.20	2 (11%)	20,38,41	2.16	6 (30%)
40	A2M	B5	2244	40	18,25,26	1.00	1 (5%)	18,36,39	1.21	2 (11%)
1	4AC	A2	1338	1	18,24,25	0.84	1 (5%)	20,34,37	1.67	3 (15%)
34	AME	Au	1	34	9,10,11	0.49	0	9,11,13	0.87	1 (11%)
40	PSU	B5	4045	40	17,21,22	1.62	2 (11%)	20,30,33	3.07	6 (30%)
40	OMG	B5	2207	40	18,26,27	1.21	2 (11%)	20,38,41	2.18	6 (30%)
40	OMG	B5	1580	40	18,26,27	1.21	2 (11%)	20,38,41	2.16	6 (30%)
40	1MA	B5	1266	88,40	15,25,26	1.51	3 (20%)	15,37,40	1.36	2 (13%)
1	OMG	A2	1448	1	18,26,27	1.24	2 (11%)	20,38,41	2.17	6 (30%)
1	OMU	A2	429	1	14,22,23	0.75	0	14,31,34	0.81	0
40	PSU	B5	1638	40	17,21,22	1.61	2 (11%)	20,30,33	3.12	6 (30%)
40	PSU	B5	1721	40	17,21,22	1.58	2 (11%)	20,30,33	3.10	6 (30%)
1	PSU	A2	652	1	17,21,22	1.61	2 (11%)	20,30,33	3.11	6 (30%)
1	A2M	A2	99	88,1	18,25,26	1.04	1 (5%)	18,36,39	1.22	2 (11%)
40	OMU	B5	2258	40	14,22,23	0.75	0	14,31,34	0.77	0
40	OMC	B5	3601	40	15,22,23	0.66	0	17,31,34	1.36	2 (11%)
1	A2M	A2	27	88,1	18,25,26	1.00	1 (5%)	18,36,39	1.19	2 (11%)
1	PSU	A2	816	1	17,21,22	1.55	2 (11%)	20,30,33	3.10	6 (30%)
1	PSU	A2	650	1	17,21,22	1.59	2 (11%)	20,30,33	3.07	6 (30%)
40	A2M	B5	1270	40	18,25,26	0.98	1 (5%)	18,36,39	1.23	2 (11%)
40	A2M	B5	1489	88,40	18,25,26	0.99	1 (5%)	18,36,39	1.34	2 (11%)
40	OMC	B5	2194	88,40	15,22,23	0.67	0	17,31,34	1.38	2 (11%)
40	A2M	B5	4269	88,40	18,25,26	1.03	1 (5%)	18,36,39	1.24	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	OMU	B5	4366	40	14,22,23	0.81	1 (7%)	14,31,34	0.82	0
40	OMG	B5	4138	40	18,26,27	1.19	2 (11%)	20,38,41	2.12	6 (30%)
1	OMU	A2	628	1	14,22,23	0.78	1 (7%)	14,31,34	0.80	0
1	PSU	A2	864	1	17,21,22	1.61	3 (17%)	20,30,33	3.09	6 (30%)
40	PSU	B5	1720	40	17,21,22	1.62	3 (17%)	20,30,33	3.09	6 (30%)
1	G7M	A2	1640	1,11	20,26,27	2.81	4 (20%)	20,39,42	2.08	5 (25%)
40	OMC	B5	2704	40	15,22,23	0.67	0	17,31,34	1.32	2 (11%)
1	OMU	A2	1289	1	14,22,23	0.77	0	14,31,34	0.77	0
40	OMC	B5	3540	40	15,22,23	0.68	0	17,31,34	1.31	2 (11%)
1	PSU	A2	1626	1	17,21,22	1.58	3 (17%)	20,30,33	3.09	6 (30%)
40	PSU	B5	4177	40	17,21,22	1.60	2 (11%)	20,30,33	3.10	6 (30%)
11	5MU	AT	53	11	15,22,23	1.06	1 (6%)	16,32,35	1.86	2 (12%)
40	PSU	B5	3462	40	17,21,22	1.57	2 (11%)	20,30,33	3.10	6 (30%)
1	PSU	A2	1348	1	17,21,22	1.58	2 (11%)	20,30,33	3.07	6 (30%)
1	A2M	A2	159	1	18,25,26	1.01	1 (5%)	18,36,39	1.27	2 (11%)
1	A2M	A2	1679	1	18,25,26	1.01	1 (5%)	18,36,39	1.27	2 (11%)
40	PSU	B5	4322	40	17,21,22	1.58	2 (11%)	20,30,33	3.08	6 (30%)
1	PSU	A2	210	1	17,21,22	1.58	2 (11%)	20,30,33	3.12	6 (30%)
1	OMG	A2	868	1	18,26,27	1.24	2 (11%)	20,38,41	2.15	6 (30%)
40	PSU	B5	4278	40	17,21,22	1.60	2 (11%)	20,30,33	3.07	6 (30%)
40	OMG	B5	1260	40	18,26,27	1.20	2 (11%)	20,38,41	2.21	6 (30%)
1	PSU	A2	119	1	17,21,22	1.60	2 (11%)	20,30,33	3.08	6 (30%)
1	OMG	A2	437	1	18,26,27	1.23	2 (11%)	20,38,41	2.17	6 (30%)
11	PSU	AT	54	11	17,21,22	1.53	3 (17%)	20,30,33	3.11	6 (30%)
1	A2M	A2	1384	1	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
40	PSU	B5	1718	40	17,21,22	1.58	2 (11%)	20,30,33	3.09	6 (30%)
40	PSU	B5	4382	40	17,21,22	1.54	2 (11%)	20,30,33	3.13	7 (35%)
40	PSU	B5	3500	40	17,21,22	1.58	2 (11%)	20,30,33	3.08	6 (30%)
40	PSU	B5	4058	40	17,21,22	1.58	2 (11%)	20,30,33	3.09	6 (30%)
40	PSU	B5	3502	40	17,21,22	1.57	2 (11%)	20,30,33	3.08	6 (30%)
40	PSU	B5	3576	40	17,21,22	1.63	2 (11%)	20,30,33	3.14	6 (30%)
40	OMC	B5	1820	88,40	15,22,23	0.67	0	17,31,34	1.33	2 (11%)
40	OMU	B5	2680	40	14,22,23	0.81	1 (7%)	14,31,34	0.78	0
40	OMG	B5	4116	40	18,26,27	1.20	2 (11%)	20,38,41	2.16	6 (30%)
40	OMG	B5	4240	40	18,26,27	1.22	2 (11%)	20,38,41	2.17	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	PSU	B5	4711	40	17,21,22	1.58	2 (11%)	20,30,33	3.08	6 (30%)
42	PSU	B8	69	42	17,21,22	1.56	3 (17%)	20,30,33	3.05	7 (35%)
1	OMC	A2	518	1	15,22,23	0.66	0	17,31,34	1.36	2 (11%)
45	AYA	BC	2	45	6,7,8	0.71	0	5,8,10	0.43	0
40	A2M	B5	3456	40	18,25,26	1.04	1 (5%)	18,36,39	1.22	2 (11%)
40	PSU	B5	4749	40	17,21,22	1.57	2 (11%)	20,30,33	3.09	6 (30%)
40	OMU	B5	3973	40	14,22,23	0.80	1 (7%)	14,31,34	0.76	0
10	5MU	AJ	54	10	15,22,23	1.07	1 (6%)	16,32,35	1.87	2 (12%)
40	6MZ	B5	3966	40	18,25,26	0.88	1 (5%)	16,36,39	2.01	4 (25%)
40	PSU	B5	1801	40	17,21,22	1.60	2 (11%)	20,30,33	3.13	6 (30%)
1	PSU	A2	34	1	17,21,22	1.59	2 (11%)	20,30,33	3.08	6 (30%)
40	OMG	B5	2719	40	18,26,27	1.18	2 (11%)	20,38,41	2.15	6 (30%)
1	PSU	A2	1005	1	17,21,22	1.58	2 (11%)	20,30,33	3.10	6 (30%)
40	OMG	B5	3359	40	18,26,27	1.20	2 (11%)	20,38,41	2.18	6 (30%)
40	PSU	B5	3616	40	17,21,22	1.59	3 (17%)	20,30,33	3.04	6 (30%)
40	A2M	B5	1810	88,40	18,25,26	1.03	1 (5%)	18,36,39	1.25	2 (11%)
1	PSU	A2	1082	1	17,21,22	1.52	3 (17%)	20,30,33	3.08	5 (25%)
1	OMG	A2	645	1	18,26,27	1.21	2 (11%)	20,38,41	2.15	6 (30%)
1	PSU	A2	1178	1	17,21,22	1.60	3 (17%)	20,30,33	3.10	6 (30%)
40	OMG	B5	3476	40	18,26,27	1.21	2 (11%)	20,38,41	2.16	6 (30%)
31	SAC	Ar	2	31	7,8,9	0.53	0	8,9,11	0.87	1 (12%)
36	HY3	Aw	62	36	6,8,9	2.14	1 (16%)	5,10,12	1.08	1 (20%)
40	PSU	B5	3554	40	17,21,22	1.62	3 (17%)	20,30,33	3.07	6 (30%)
1	OMU	A2	355	1	14,22,23	0.81	1 (7%)	14,31,34	0.82	0
40	PSU	B5	4203	40	17,21,22	1.57	2 (11%)	20,30,33	3.07	6 (30%)
1	PSU	A2	109	1	17,21,22	1.57	2 (11%)	20,30,33	3.08	6 (30%)
1	PSU	A2	573	1	17,21,22	1.59	3 (17%)	20,30,33	3.08	6 (30%)
40	PSU	B5	2351	40	17,21,22	1.58	2 (11%)	20,30,33	3.07	6 (30%)
44	HIC	BB	245	44	8,11,12	0.87	0	6,14,16	0.84	0
40	OMG	B5	3974	40	18,26,27	1.20	2 (11%)	20,38,41	2.19	6 (30%)
1	MA6	A2	1851	1	19,26,27	0.93	1 (5%)	18,38,41	1.59	3 (16%)
40	A2M	B5	398	40	18,25,26	1.02	1 (5%)	18,36,39	1.25	2 (11%)
40	OMG	B5	4245	10,40	18,26,27	1.20	2 (11%)	20,38,41	2.17	6 (30%)
40	A2M	B5	2630	88,40	18,25,26	0.99	1 (5%)	18,36,39	1.39	3 (16%)
40	PSU	B5	3466	40	17,21,22	1.57	3 (17%)	20,30,33	3.07	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	PSU	B5	2475	40	17,21,22	1.57	2 (11%)	20,30,33	3.10	6 (30%)
40	A2M	B5	3562	40	18,25,26	1.03	1 (5%)	18,36,39	1.20	2 (11%)
40	A2M	B5	4317	40	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
69	V5N	Ba	39	69	4,11,12	0.76	0	5,14,16	1.54	1 (20%)
40	5MC	B5	3514	88,40	15,22,23	1.29	1 (6%)	19,32,35	1.32	3 (15%)
40	A2M	B5	3599	40	18,25,26	0.99	1 (5%)	18,36,39	1.19	2 (11%)
1	PSU	A2	867	1	17,21,22	1.58	2 (11%)	20,30,33	3.11	6 (30%)
40	PSU	B5	4107	40	17,21,22	1.60	2 (11%)	20,30,33	3.12	6 (30%)
40	PSU	B5	4099	40	17,21,22	1.55	2 (11%)	20,30,33	3.06	6 (30%)
1	A2M	A2	591	1	18,25,26	1.05	1 (5%)	18,36,39	1.23	2 (11%)
1	A2M	A2	669	88,1	18,25,26	0.98	1 (5%)	18,36,39	1.35	2 (11%)
1	OMC	A2	463	1	15,22,23	0.68	0	17,31,34	1.39	2 (11%)
1	OMG	A2	602	1	18,26,27	1.19	2 (11%)	20,38,41	2.14	6 (30%)
1	PSU	A2	1047	1	17,21,22	1.60	3 (17%)	20,30,33	3.06	6 (30%)
1	A2M	A2	166	1	18,25,26	1.06	1 (5%)	18,36,39	1.28	2 (11%)
40	PSU	B5	1632	40	17,21,22	1.53	3 (17%)	20,30,33	3.09	6 (30%)
82	MLZ	B <sub>o</sub>	53	82	8,9,10	0.49	0	4,9,11	0.08	0
40	PSU	B5	1683	40	17,21,22	1.58	2 (11%)	20,30,33	3.12	6 (30%)
40	UR3	B5	4276	40	14,22,23	0.71	0	15,32,35	0.65	0
1	PSU	A2	1239	1	17,21,22	1.59	3 (17%)	20,30,33	3.11	6 (30%)
42	PSU	B8	55	42	17,21,22	1.58	2 (11%)	20,30,33	3.09	6 (30%)
1	PSU	A2	1046	1	17,21,22	1.59	2 (11%)	20,30,33	3.10	6 (30%)
1	OMU	A2	116	1	14,22,23	0.78	1 (7%)	14,31,34	0.76	0
40	OMC	B5	2667	40	15,22,23	0.67	0	17,31,34	1.34	2 (11%)
40	A2M	B5	2658	88,40	18,25,26	1.02	1 (5%)	18,36,39	1.20	2 (11%)
40	PSU	B5	3652	88,40	17,21,22	1.59	3 (17%)	20,30,33	3.07	6 (30%)
40	PSU	B5	3494	40	17,21,22	1.60	2 (11%)	20,30,33	3.10	6 (30%)
40	A2M	B5	4336	40	18,25,26	1.03	1 (5%)	18,36,39	1.21	2 (11%)
40	PSU	B5	1491	40	17,21,22	1.62	2 (11%)	20,30,33	3.10	6 (30%)
1	PSU	A2	1644	88,1	17,21,22	1.59	3 (17%)	20,30,33	3.09	6 (30%)
40	PSU	B5	4166	40	17,21,22	1.50	2 (11%)	20,30,33	3.21	6 (30%)
32	NMM	As	67	32	9,11,12	0.59	0	6,12,14	0.40	0
40	PSU	B5	3447	40	17,21,22	1.60	3 (17%)	20,30,33	3.07	6 (30%)
40	OMC	B5	1284	40	15,22,23	0.68	0	17,31,34	1.31	2 (11%)
1	PSU	A2	1245	1	17,21,22	1.60	3 (17%)	20,30,33	3.09	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	OMG	B5	4364	40	18,26,27	1.22	2 (11%)	20,38,41	2.16	6 (30%)
70	MLZ	Bb	5	70	8,9,10	0.49	0	4,9,11	0.11	0
1	PSU	A2	1693	1	17,21,22	1.58	2 (11%)	20,30,33	3.07	6 (30%)
40	PSU	B5	3496	40	17,21,22	1.60	3 (17%)	20,30,33	3.05	6 (30%)
1	OMG	A2	1491	88,1	18,26,27	1.21	2 (11%)	20,38,41	2.14	6 (30%)
40	OMC	B5	3573	40	15,22,23	0.68	0	17,31,34	1.36	2 (11%)
1	OMU	A2	172	1	14,22,23	0.79	1 (7%)	14,31,34	0.82	0
40	PSU	B5	4325	40	17,21,22	1.60	2 (11%)	20,30,33	3.10	6 (30%)
40	PSU	B5	4740	40	17,21,22	1.57	2 (11%)	20,30,33	3.08	6 (30%)
40	A2M	B5	3450	40	18,25,26	1.02	1 (5%)	18,36,39	1.19	2 (11%)
1	6MZ	A2	1833	88,1	18,25,26	0.94	1 (5%)	16,36,39	1.77	3 (18%)
40	OMG	B5	3942	40	18,26,27	1.20	2 (11%)	20,38,41	2.13	6 (30%)
40	PSU	B5	3369	40	17,21,22	1.63	2 (11%)	20,30,33	3.08	6 (30%)
1	PSU	A2	967	1	17,21,22	1.56	3 (17%)	20,30,33	3.08	6 (30%)
1	PSU	A2	1233	1	17,21,22	1.60	2 (11%)	20,30,33	3.11	6 (30%)
1	B8N	A2	1249	1	17,29,30	1.72	3 (17%)	21,42,45	1.12	2 (9%)
40	UY1	B5	3550	40	18,22,23	1.24	1 (5%)	20,31,34	3.10	6 (30%)
1	PSU	A2	105	1	17,21,22	1.60	2 (11%)	20,30,33	3.11	6 (30%)
1	PSU	A2	1446	1	17,21,22	1.56	3 (17%)	20,30,33	3.04	7 (35%)
40	OMU	B5	4244	40	14,22,23	0.78	1 (7%)	14,31,34	0.78	0
40	A2M	B5	3492	40	18,25,26	1.01	1 (5%)	18,36,39	1.34	2 (11%)
40	PSU	B5	4267	88,40	17,21,22	1.61	3 (17%)	20,30,33	3.07	7 (35%)
40	PSU	B5	4042	40	17,21,22	1.57	2 (11%)	20,30,33	3.11	6 (30%)
1	PSU	A2	1057	1	17,21,22	1.60	3 (17%)	20,30,33	3.06	6 (30%)
1	OMG	A2	1329	1	18,26,27	1.22	2 (11%)	20,38,41	2.15	6 (30%)
13	SAC	AZ	2	13	7,8,9	0.52	0	8,9,11	0.87	1 (12%)
40	PSU	B5	1537	40	17,21,22	1.60	3 (17%)	20,30,33	3.10	6 (30%)
1	OMU	A2	1327	1	14,22,23	0.79	1 (7%)	14,31,34	0.82	0
1	OMC	A2	1704	1	15,22,23	0.68	0	17,31,34	1.41	2 (11%)
40	OMG	B5	3524	40	18,26,27	1.20	2 (11%)	20,38,41	2.13	6 (30%)
1	PSU	A2	802	1	17,21,22	1.59	2 (11%)	20,30,33	3.11	6 (30%)
1	OMU	A2	1805	1	14,22,23	0.79	1 (7%)	14,31,34	0.82	0
40	OMG	B5	3631	40	18,26,27	1.19	2 (11%)	20,38,41	2.18	6 (30%)
1	PSU	A2	687	1	17,21,22	1.60	2 (11%)	20,30,33	3.13	6 (30%)
1	MA6	A2	1852	1	19,26,27	1.04	2 (10%)	18,38,41	1.53	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	A2	93	1	17,21,22	1.57	2 (11%)	20,30,33	3.09	6 (30%)
1	A2M	A2	513	1	18,25,26	1.01	1 (5%)	18,36,39	1.19	2 (11%)
1	A2M	A2	469	1	18,25,26	1.05	1 (5%)	18,36,39	1.23	2 (11%)
1	PSU	A2	823	1	17,21,22	1.56	3 (17%)	20,30,33	3.08	6 (30%)
1	A2M	A2	577	1	18,25,26	1.01	1 (5%)	18,36,39	1.18	2 (11%)
1	PSU	A2	682	1	17,21,22	1.61	2 (11%)	20,30,33	3.09	6 (30%)
1	OMU	A2	1443	88,1	14,22,23	0.77	0	14,31,34	0.81	0
40	OMG	B5	4383	40	18,26,27	1.22	2 (11%)	20,38,41	2.17	6 (30%)
1	4AC	A2	1843	1	18,24,25	0.92	1 (5%)	20,34,37	1.94	3 (15%)
1	OMU	A2	121	1	14,22,23	0.81	1 (7%)	14,31,34	0.79	0
10	PSU	AJ	55	10	17,21,22	1.60	2 (11%)	20,30,33	3.10	6 (30%)
81	M3L	Bm	98	81	10,11,12	0.84	0	9,14,16	0.53	0
1	PSU	A2	407	1	17,21,22	1.58	3 (17%)	20,30,33	3.10	6 (30%)
40	OMC	B5	3619	40	15,22,23	0.68	0	17,31,34	1.35	2 (11%)
40	A2M	B5	3517	40	18,25,26	0.95	1 (5%)	18,36,39	1.33	2 (11%)
40	PSU	B5	1731	40	17,21,22	1.59	2 (11%)	20,30,33	3.07	6 (30%)
40	OMG	B5	2267	40	18,26,27	1.20	2 (11%)	20,38,41	2.15	6 (30%)
40	PSU	B5	4149	40	17,21,22	1.57	3 (17%)	20,30,33	3.03	5 (25%)
40	PSU	B5	4217	40	17,21,22	1.58	3 (17%)	20,30,33	3.09	6 (30%)
40	PSU	B5	4246	40	17,21,22	1.56	2 (11%)	20,30,33	3.04	5 (25%)
41	GTP	B7	1	41	26,34,34	1.05	1 (3%)	33,54,54	2.10	4 (12%)
1	PSU	A2	1368	1	17,21,22	1.57	2 (11%)	20,30,33	3.09	6 (30%)
40	PSU	B5	3371	40	17,21,22	1.58	3 (17%)	20,30,33	3.10	6 (30%)
1	OMC	A2	174	88,1	15,22,23	0.65	0	17,31,34	1.35	2 (11%)
40	OMC	B5	4282	40	15,22,23	0.70	0	17,31,34	1.36	2 (11%)
40	OMC	B5	2265	88,40	15,22,23	0.67	0	17,31,34	1.36	2 (11%)
40	PSU	B5	4298	40	17,21,22	1.60	2 (11%)	20,30,33	3.11	6 (30%)
40	PSU	B5	4419	40	17,21,22	1.61	2 (11%)	20,30,33	3.09	6 (30%)
40	OMC	B5	2647	40	15,22,23	0.71	0	17,31,34	1.34	2 (11%)
40	PSU	B5	4188	40	17,21,22	1.56	3 (17%)	20,30,33	3.04	7 (35%)
40	PSU	B5	3585	88,40	17,21,22	1.62	2 (11%)	20,30,33	3.08	6 (30%)
40	PSU	B5	4435	40	17,21,22	1.61	2 (11%)	20,30,33	3.11	6 (30%)
40	A2M	B5	3557	40	18,25,26	1.04	1 (5%)	18,36,39	1.21	2 (11%)
40	PSU	B5	3583	40	17,21,22	1.57	2 (11%)	20,30,33	3.06	6 (30%)
1	PSU	A2	218	1	17,21,22	1.56	2 (11%)	20,30,33	3.06	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	OMG	B5	1477	40	18,26,27	1.20	2 (11%)	20,38,41	2.17	6 (30%)
40	OMG	B5	4369	40	18,26,27	1.22	2 (11%)	20,38,41	2.14	6 (30%)
40	PSU	B5	4374	40	17,21,22	1.60	3 (17%)	20,30,33	3.07	6 (30%)

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
40	PSU	B5	1799	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	610	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2
40	A2M	B5	2206	88,40	-	0/5/27/28	0/3/3/3
40	OMC	B5	2208	40	-	0/7/27/28	0/2/2/2
42	OMG	B8	75	42	-	0/5/27/28	0/3/3/3
40	PSU	B5	3490	40	-	0/7/25/26	0/2/2/2
43	V5N	BA	216	43	-	1/5/10/12	0/1/1/1
40	PSU	B5	4039	40	-	0/7/25/26	0/2/2/2
40	5MC	B5	4193	40	-	2/5/25/26	0/2/2/2
1	A2M	A2	1032	1	-	1/5/27/28	0/3/3/3
1	A2M	A2	485	1	-	0/5/27/28	0/3/3/3
1	OMC	A2	1392	1	-	0/7/27/28	0/2/2/2
40	A2M	B5	1479	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	4169	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	815	1	-	0/7/25/26	0/2/2/2
40	A2M	B5	400	40	-	0/5/27/28	0/3/3/3
40	OMU	B5	3657	40	-	1/7/27/28	0/2/2/2
1	OMG	A2	684	1	-	3/5/27/28	0/3/3/3
40	OMC	B5	3433	40	-	1/7/27/28	0/2/2/2
40	OMG	B5	3676	40	-	1/5/27/28	0/3/3/3
84	SAC	Br	2	84	-	0/7/8/10	-
40	PSU	B5	3427	40	-	0/7/25/26	0/2/2/2
40	OMU	B5	4052	40	-	1/7/27/28	0/2/2/2
40	OMC	B5	4202	40	-	0/7/27/28	0/2/2/2
1	OMG	A2	510	88,1	-	1/5/27/28	0/3/3/3
40	A2M	B5	2244	40	-	0/5/27/28	0/3/3/3
1	4AC	A2	1338	1	-	2/9/29/30	0/2/2/2
34	AME	Au	1	34	-	2/9/10/12	-
40	PSU	B5	4045	40	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMG	B5	2207	40	-	2/5/27/28	0/3/3/3
40	OMG	B5	1580	40	-	0/5/27/28	0/3/3/3
40	1MA	B5	1266	88,40	-	0/3/25/26	0/3/3/3
1	OMG	A2	1448	1	-	3/5/27/28	0/3/3/3
1	OMU	A2	429	1	-	1/7/27/28	0/2/2/2
40	PSU	B5	1638	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	1721	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	99	88,1	-	1/5/27/28	0/3/3/3
40	OMU	B5	2258	40	-	0/7/27/28	0/2/2/2
40	OMC	B5	3601	40	-	0/7/27/28	0/2/2/2
1	A2M	A2	27	88,1	-	2/5/27/28	0/3/3/3
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2
40	A2M	B5	1270	40	-	0/5/27/28	0/3/3/3
40	A2M	B5	1489	88,40	-	2/5/27/28	0/3/3/3
40	OMC	B5	2194	88,40	-	2/7/27/28	0/2/2/2
40	A2M	B5	4269	88,40	-	0/5/27/28	0/3/3/3
40	OMU	B5	4366	40	-	1/7/27/28	0/2/2/2
40	OMG	B5	4138	40	-	0/5/27/28	0/3/3/3
1	OMU	A2	628	1	-	0/7/27/28	0/2/2/2
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	1720	40	-	2/7/25/26	0/2/2/2
1	G7M	A2	1640	1,11	-	0/3/25/26	0/3/3/3
40	OMC	B5	2704	40	-	0/7/27/28	0/2/2/2
1	OMU	A2	1289	1	-	1/7/27/28	0/2/2/2
40	OMC	B5	3540	40	-	0/7/27/28	0/2/2/2
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	4177	40	-	0/7/25/26	0/2/2/2
11	5MU	AT	53	11	-	1/5/25/26	0/2/2/2
40	PSU	B5	3462	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	159	1	-	0/5/27/28	0/3/3/3
1	A2M	A2	1679	1	-	0/5/27/28	0/3/3/3
40	PSU	B5	4322	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	868	1	-	3/5/27/28	0/3/3/3
40	PSU	B5	4278	40	-	3/7/25/26	0/2/2/2
40	OMG	B5	1260	40	-	1/5/27/28	0/3/3/3
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A2	437	1	-	1/5/27/28	0/3/3/3
11	PSU	AT	54	11	-	0/7/25/26	0/2/2/2
1	A2M	A2	1384	1	-	0/5/27/28	0/3/3/3
40	PSU	B5	1718	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4382	40	-	4/7/25/26	0/2/2/2
40	PSU	B5	3500	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4058	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	3502	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	3576	40	-	1/7/25/26	0/2/2/2
40	OMC	B5	1820	88,40	-	1/7/27/28	0/2/2/2
40	OMU	B5	2680	40	-	1/7/27/28	0/2/2/2
40	OMG	B5	4116	40	-	0/5/27/28	0/3/3/3
40	OMG	B5	4240	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	4711	40	-	0/7/25/26	0/2/2/2
42	PSU	B8	69	42	-	0/7/25/26	0/2/2/2
1	OMC	A2	518	1	-	0/7/27/28	0/2/2/2
45	AYA	BC	2	45	-	3/4/6/8	-
40	A2M	B5	3456	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	4749	40	-	0/7/25/26	0/2/2/2
40	OMU	B5	3973	40	-	0/7/27/28	0/2/2/2
10	5MU	AJ	54	10	-	0/5/25/26	0/2/2/2
40	6MZ	B5	3966	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	1801	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2
40	OMG	B5	2719	40	-	0/5/27/28	0/3/3/3
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2
40	OMG	B5	3359	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	3616	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	1810	88,40	-	0/5/27/28	0/3/3/3
1	PSU	A2	1082	1	-	1/7/25/26	0/2/2/2
1	OMG	A2	645	1	-	3/5/27/28	0/3/3/3
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
40	OMG	B5	3476	40	-	1/5/27/28	0/3/3/3
31	SAC	Ar	2	31	-	0/7/8/10	-
36	HY3	Aw	62	36	-	0/1/12/14	0/1/1/1
40	PSU	B5	3554	40	-	0/7/25/26	0/2/2/2
1	OMU	A2	355	1	-	0/7/27/28	0/2/2/2
40	PSU	B5	4203	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	2351	40	-	0/7/25/26	0/2/2/2
44	HIC	BB	245	44	-	1/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMG	B5	3974	40	-	0/5/27/28	0/3/3/3
1	MA6	A2	1851	1	-	0/7/29/30	0/3/3/3
40	A2M	B5	398	40	-	3/5/27/28	0/3/3/3
40	OMG	B5	4245	10,40	-	0/5/27/28	0/3/3/3
40	A2M	B5	2630	88,40	-	1/5/27/28	0/3/3/3
40	PSU	B5	3466	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	2475	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	3562	40	-	0/5/27/28	0/3/3/3
40	A2M	B5	4317	40	-	0/5/27/28	0/3/3/3
69	V5N	Ba	39	69	-	0/5/10/12	0/1/1/1
40	5MC	B5	3514	88,40	-	0/5/25/26	0/2/2/2
40	A2M	B5	3599	40	-	0/5/27/28	0/3/3/3
1	PSU	A2	867	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	4107	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4099	40	-	0/7/25/26	0/2/2/2
1	A2M	A2	591	1	-	1/5/27/28	0/3/3/3
1	A2M	A2	669	88,1	-	2/5/27/28	0/3/3/3
1	OMC	A2	463	1	-	0/7/27/28	0/2/2/2
1	OMG	A2	602	1	-	0/5/27/28	0/3/3/3
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	166	1	-	0/5/27/28	0/3/3/3
40	PSU	B5	1632	40	-	3/7/25/26	0/2/2/2
82	MLZ	Bo	53	82	-	0/7/8/10	-
40	PSU	B5	1683	40	-	0/7/25/26	0/2/2/2
40	UR3	B5	4276	40	-	0/5/25/26	0/2/2/2
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
42	PSU	B8	55	42	-	0/7/25/26	0/2/2/2
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	116	1	-	1/7/27/28	0/2/2/2
40	OMC	B5	2667	40	-	0/7/27/28	0/2/2/2
40	A2M	B5	2658	88,40	-	0/5/27/28	0/3/3/3
40	PSU	B5	3652	88,40	-	0/7/25/26	0/2/2/2
40	PSU	B5	3494	40	-	2/7/25/26	0/2/2/2
40	A2M	B5	4336	40	-	1/5/27/28	0/3/3/3
40	PSU	B5	1491	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	1644	88,1	-	0/7/25/26	0/2/2/2
40	PSU	B5	4166	40	-	2/7/25/26	0/2/2/2
32	NMM	As	67	32	-	0/9/11/13	-
40	PSU	B5	3447	40	-	0/7/25/26	0/2/2/2
40	OMC	B5	1284	40	-	1/7/27/28	0/2/2/2
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMG	B5	4364	40	-	0/5/27/28	0/3/3/3
70	MLZ	Bb	5	70	-	0/7/8/10	-
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	3496	40	-	0/7/25/26	0/2/2/2
1	OMG	A2	1491	88,1	-	1/5/27/28	0/3/3/3
40	OMC	B5	3573	40	-	1/7/27/28	0/2/2/2
1	OMU	A2	172	1	-	0/7/27/28	0/2/2/2
40	PSU	B5	4325	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4740	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	3450	40	-	2/5/27/28	0/3/3/3
1	6MZ	A2	1833	88,1	-	0/5/27/28	0/3/3/3
40	OMG	B5	3942	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	3369	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2
1	B8N	A2	1249	1	-	0/12/34/35	0/2/2/2
40	UY1	B5	3550	40	-	2/9/27/28	0/2/2/2
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
40	OMU	B5	4244	40	-	0/7/27/28	0/2/2/2
40	A2M	B5	3492	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	4267	88,40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4042	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	1329	1	-	0/5/27/28	0/3/3/3
13	SAC	AZ	2	13	-	2/7/8/10	-
40	PSU	B5	1537	40	-	0/7/25/26	0/2/2/2
1	OMU	A2	1327	1	-	0/7/27/28	0/2/2/2
1	OMC	A2	1704	1	-	4/7/27/28	0/2/2/2
40	OMG	B5	3524	40	-	0/5/27/28	0/3/3/3
1	PSU	A2	802	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	1805	1	-	0/7/27/28	0/2/2/2
40	OMG	B5	3631	40	-	1/5/27/28	0/3/3/3
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
1	MA6	A2	1852	1	-	1/7/29/30	0/3/3/3
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	513	1	-	2/5/27/28	0/3/3/3
1	A2M	A2	469	1	-	1/5/27/28	0/3/3/3
1	PSU	A2	823	1	-	1/7/25/26	0/2/2/2
1	A2M	A2	577	1	-	2/5/27/28	0/3/3/3
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	A2	1443	88,1	-	0/7/27/28	0/2/2/2
40	OMG	B5	4383	40	-	0/5/27/28	0/3/3/3
1	4AC	A2	1843	1	-	4/9/29/30	0/2/2/2
1	OMU	A2	121	1	-	0/7/27/28	0/2/2/2
10	PSU	AJ	55	10	-	0/7/25/26	0/2/2/2
81	M3L	Bm	98	81	-	0/9/10/12	-
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
40	OMC	B5	3619	40	-	2/7/27/28	0/2/2/2
40	A2M	B5	3517	40	-	2/5/27/28	0/3/3/3
40	PSU	B5	1731	40	-	0/7/25/26	0/2/2/2
40	OMG	B5	2267	40	-	1/5/27/28	0/3/3/3
40	PSU	B5	4149	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4217	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4246	40	-	1/7/25/26	0/2/2/2
41	GTP	B7	1	41	-	0/18/38/38	0/3/3/3
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
40	PSU	B5	3371	40	-	0/7/25/26	0/2/2/2
1	OMC	A2	174	88,1	-	0/7/27/28	0/2/2/2
40	OMC	B5	4282	40	-	1/7/27/28	0/2/2/2
40	OMC	B5	2265	88,40	-	0/7/27/28	0/2/2/2
40	PSU	B5	4298	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4419	40	-	0/7/25/26	0/2/2/2
40	OMC	B5	2647	40	-	0/7/27/28	0/2/2/2
40	PSU	B5	4188	40	-	0/7/25/26	0/2/2/2
40	PSU	B5	3585	88,40	-	0/7/25/26	0/2/2/2
40	PSU	B5	4435	40	-	0/7/25/26	0/2/2/2
40	A2M	B5	3557	40	-	0/5/27/28	0/3/3/3
40	PSU	B5	3583	40	-	0/7/25/26	0/2/2/2
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
40	OMG	B5	1477	40	-	0/5/27/28	0/3/3/3
40	OMG	B5	4369	40	-	1/5/27/28	0/3/3/3
40	PSU	B5	4374	40	-	0/7/25/26	0/2/2/2

The worst 5 of 361 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1640	G7M	C8-N9	7.38	1.46	1.33
1	A2	1640	G7M	C8-N7	7.14	1.46	1.33
1	A2	1640	G7M	C5-C4	5.92	1.47	1.39
1	A2	1249	B8N	C6-N1	5.55	1.40	1.33
36	Aw	62	HY3	C3-C2	-4.90	1.50	1.55

The worst 5 of 932 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B5	3550	UY1	N1-C2-N3	-10.75	119.88	128.43
41	B7	1	GTP	C5-C6-N1	-8.79	111.41	123.43
40	B5	4166	PSU	N1-C2-N3	-8.74	121.48	128.43
11	AT	54	PSU	N1-C2-N3	-8.50	121.67	128.43
1	A2	1082	PSU	N1-C2-N3	-8.39	121.76	128.43

There are no chirality outliers.

5 of 107 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A2	429	OMU	C2'-C1'-N1-C6
1	A2	645	OMG	O4'-C4'-C5'-O5'
1	A2	669	A2M	O4'-C4'-C5'-O5'
1	A2	684	OMG	C3'-C4'-C5'-O5'
1	A2	1448	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 624 ligands modelled in this entry, 357 are monoatomic and 266 are unknown - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
91	SPD	B5	4901	-	9,9,9	0.15	0	8,8,8	0.16	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
91	SPD	B5	4901	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	1249:B8N	O3'	1250:C	P	3.10

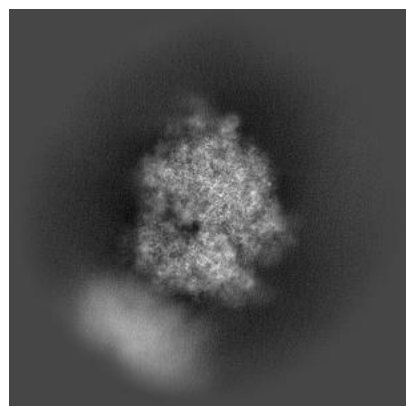
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12759. These allow visual inspection of the internal detail of the map and identification of artifacts.

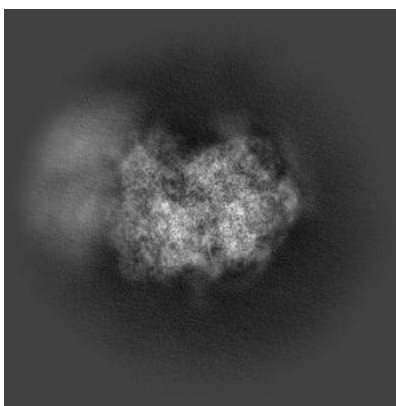
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

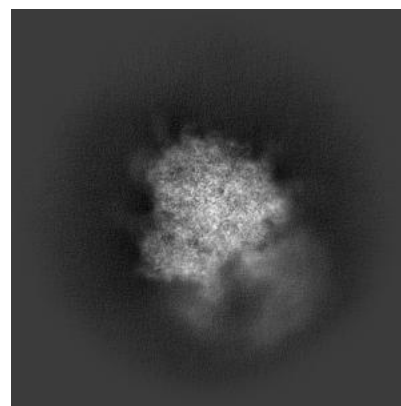
#### 6.1.1 Primary map



X

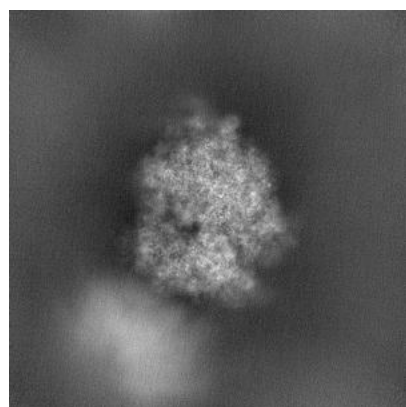


Y

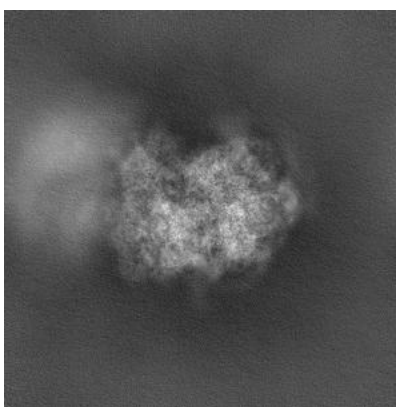


Z

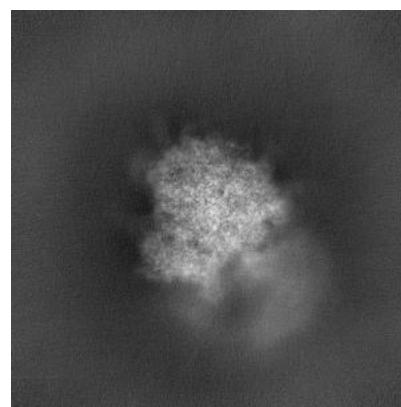
#### 6.1.2 Raw map



X



Y

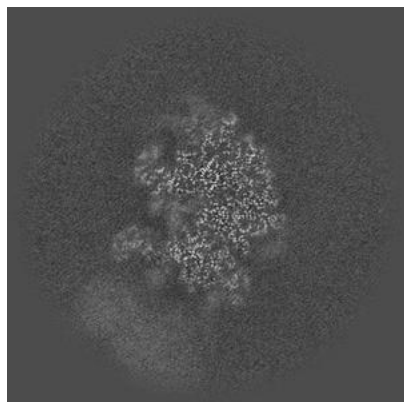


Z

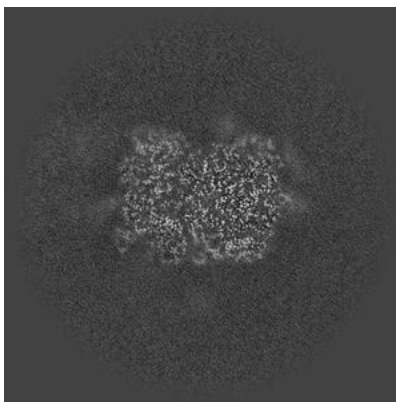
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

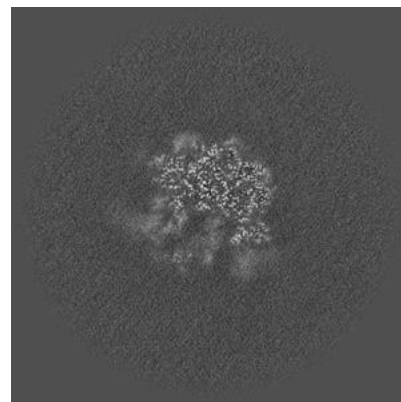
### 6.2.1 Primary map



X Index: 280

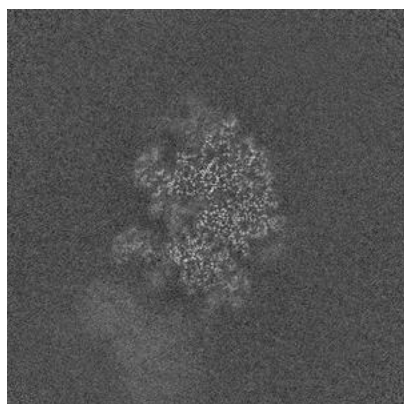


Y Index: 280

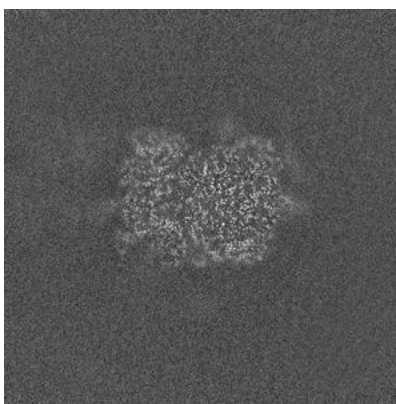


Z Index: 280

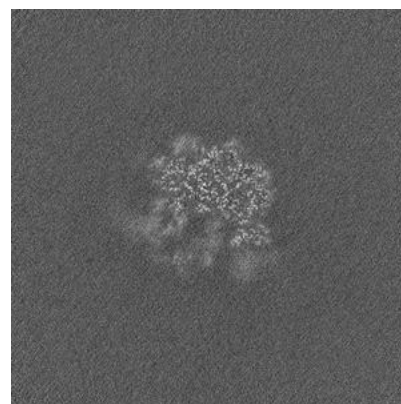
### 6.2.2 Raw map



X Index: 280



Y Index: 280



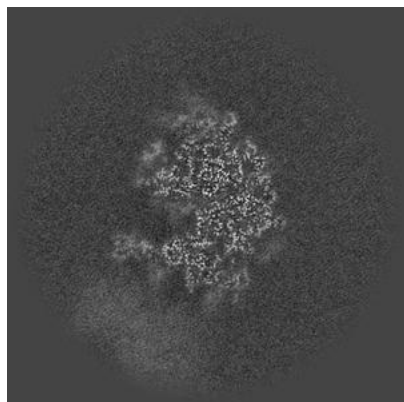
Z Index: 280

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

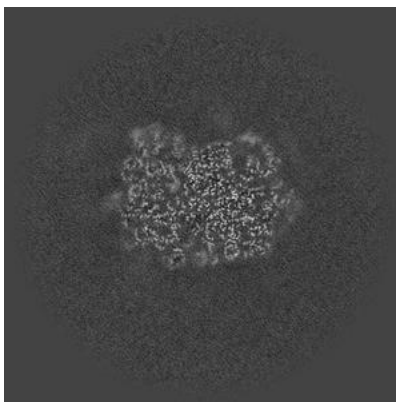


## 6.3 Largest variance slices [i](#)

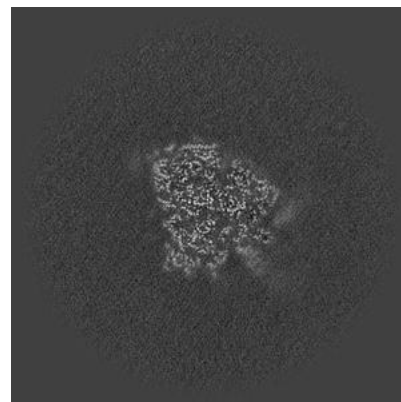
### 6.3.1 Primary map



X Index: 285

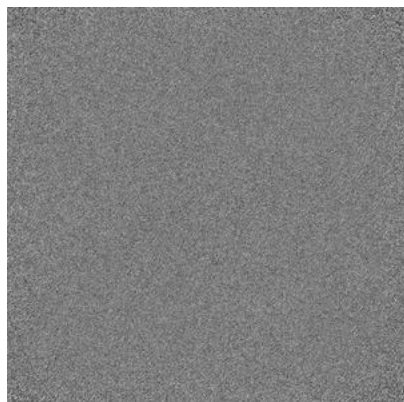


Y Index: 290

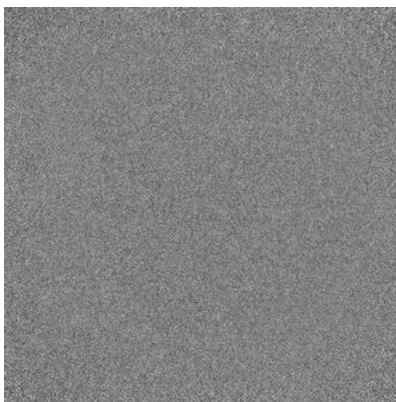


Z Index: 314

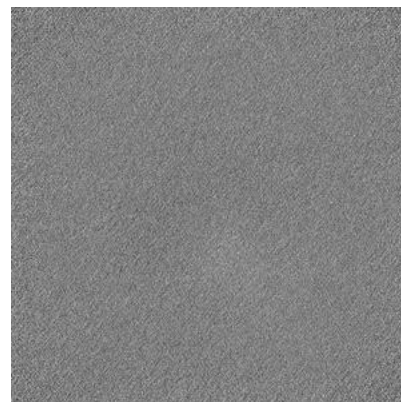
### 6.3.2 Raw map



X Index: 0



Y Index: 0

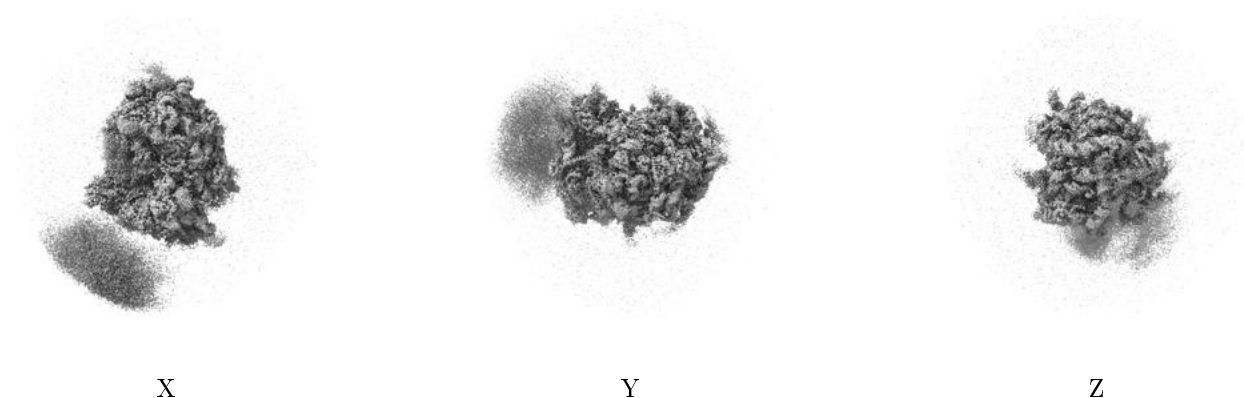


Z Index: 0

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

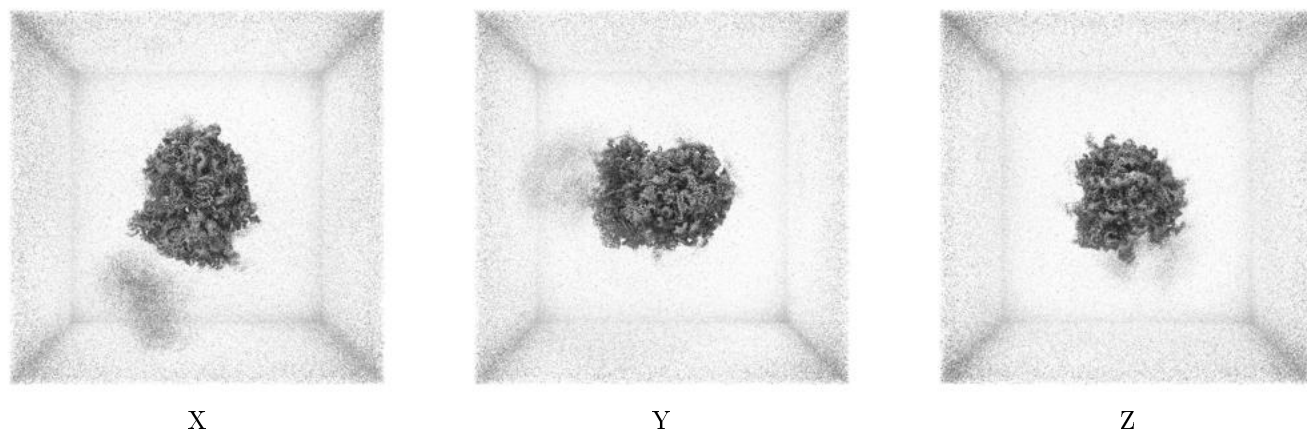
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

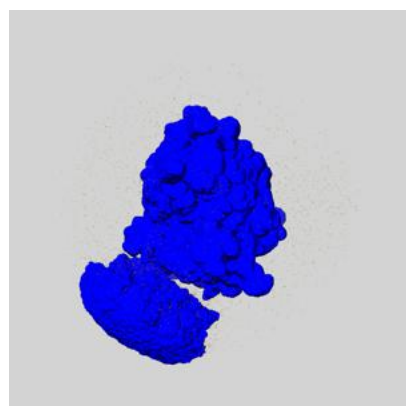
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

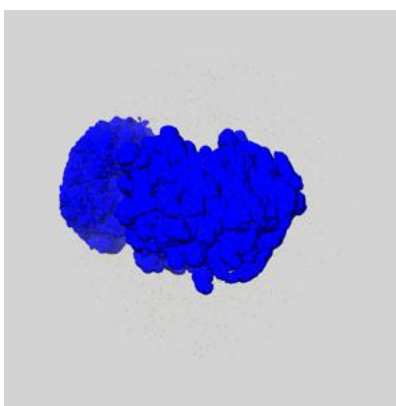
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

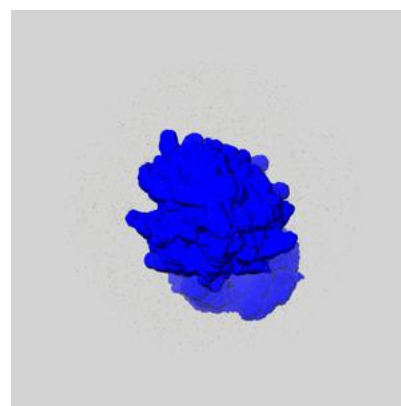
### 6.5.1 emd\_12759\_msk\_1.map [i](#)



X

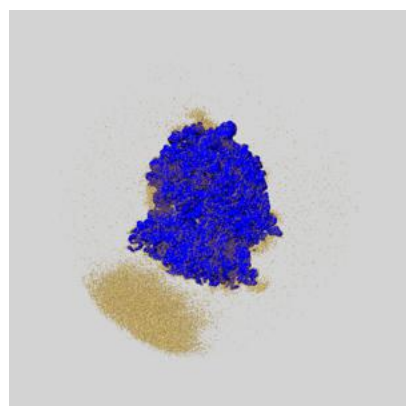


Y

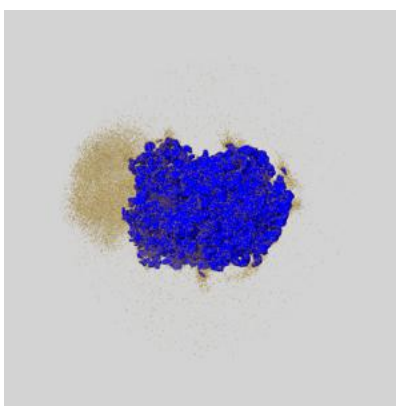


Z

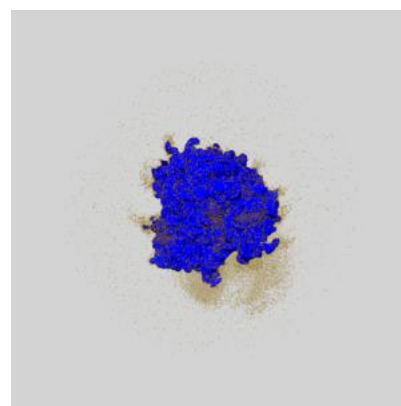
### 6.5.2 emd\_12759\_msk\_2.map [i](#)



X



Y

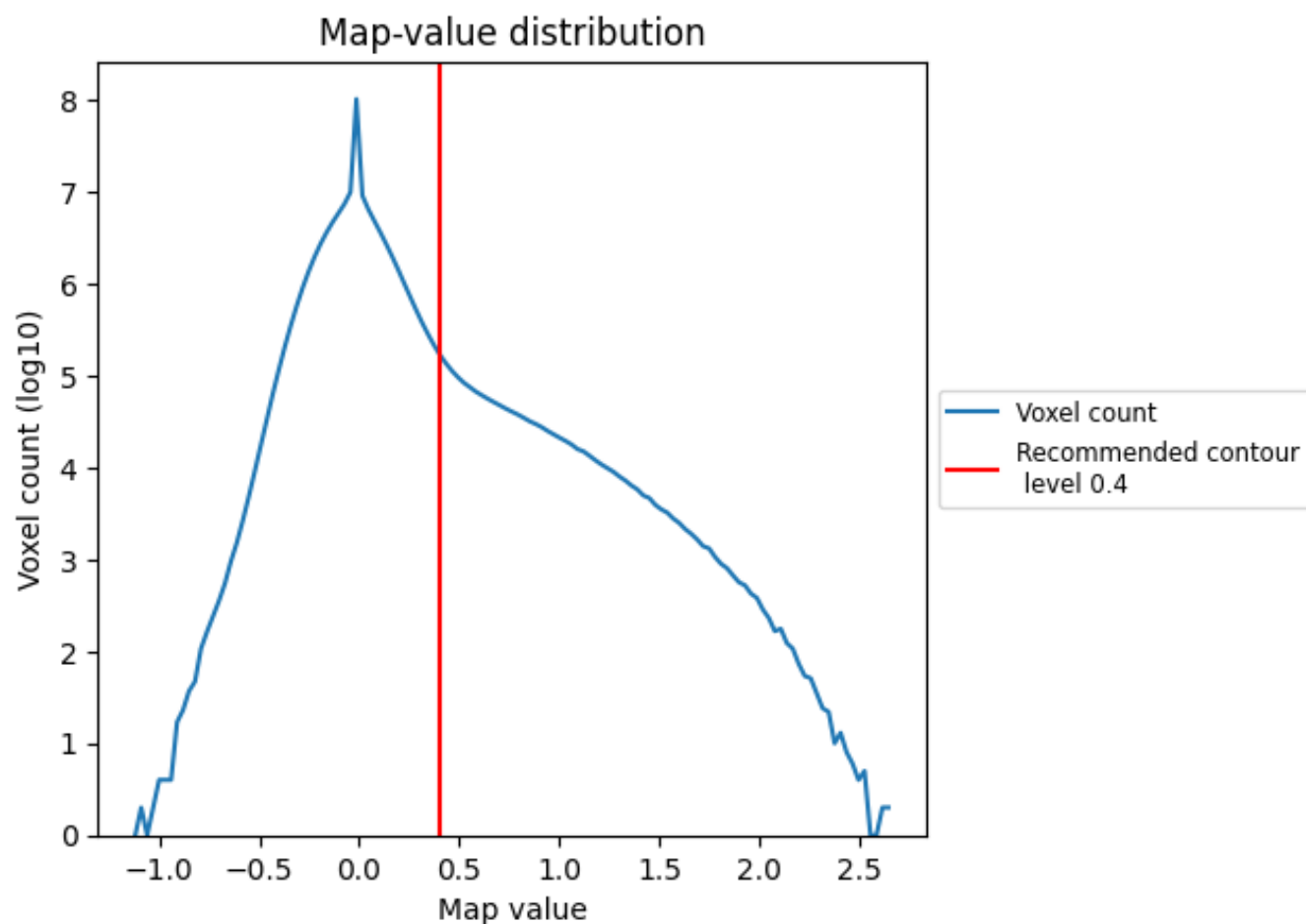


Z

## 7 Map analysis [i](#)

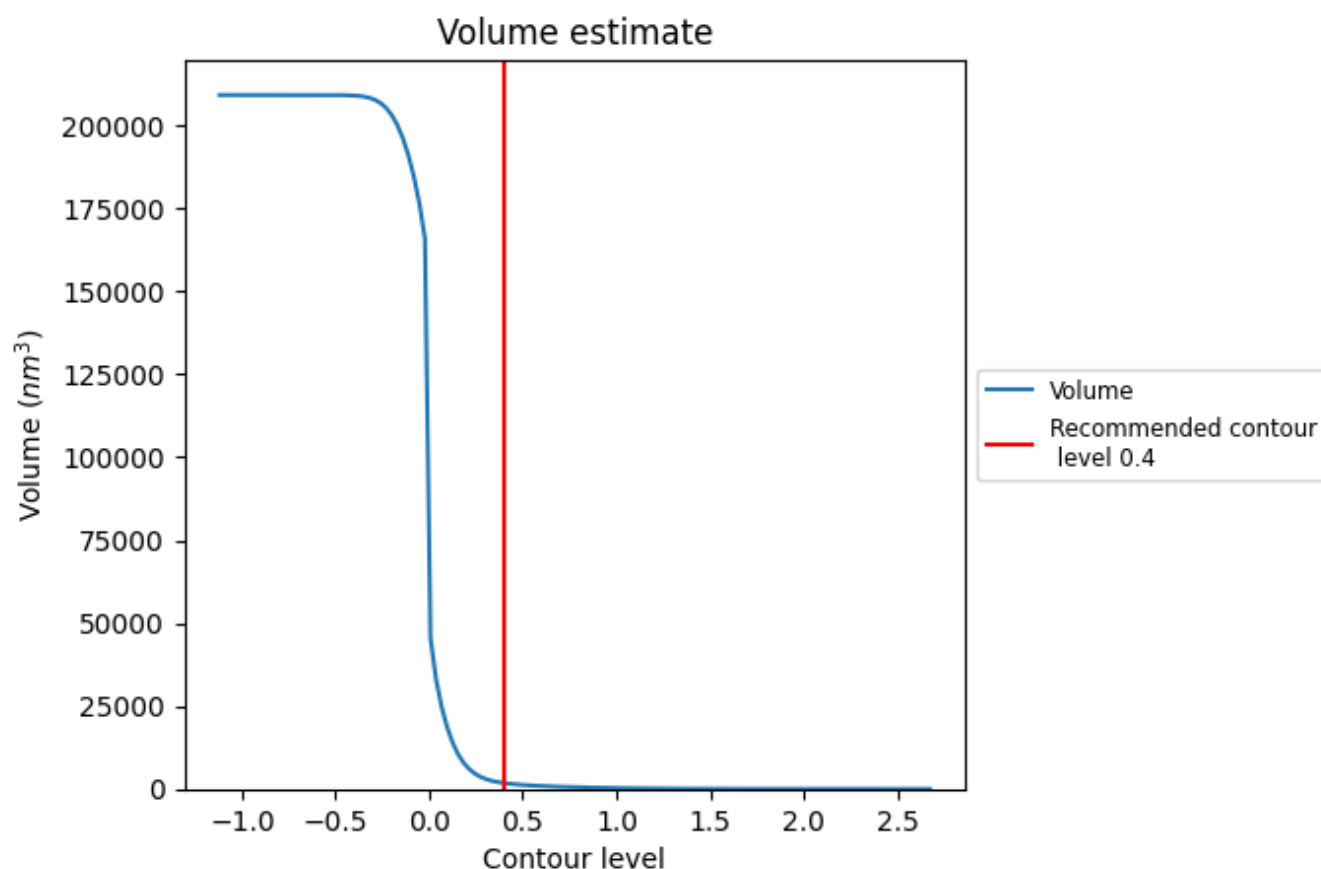
This section contains the results of statistical analysis of the map.

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



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

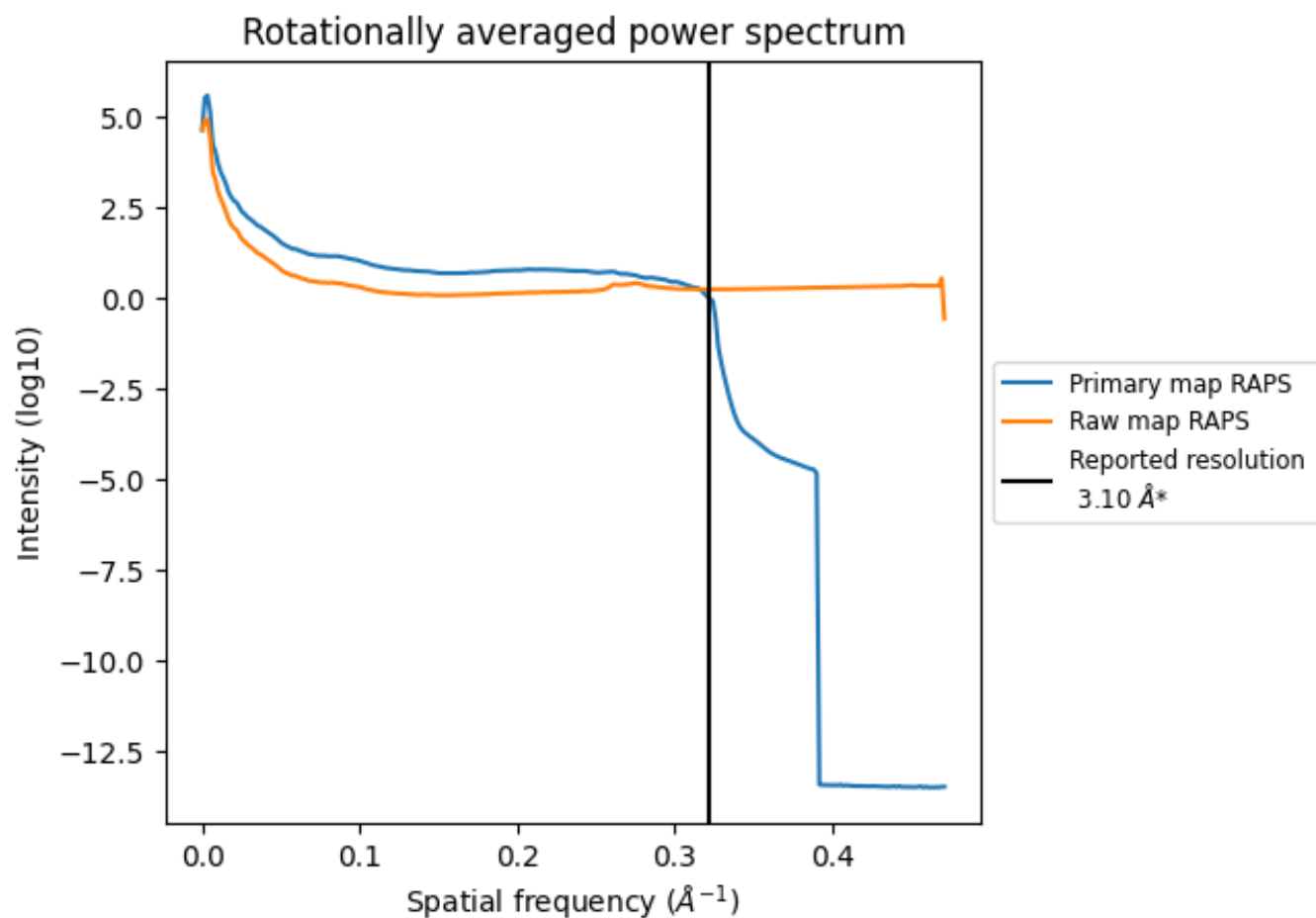
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1771  $\text{nm}^3$ ; this corresponds to an approximate mass of 1600 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 ⓘ

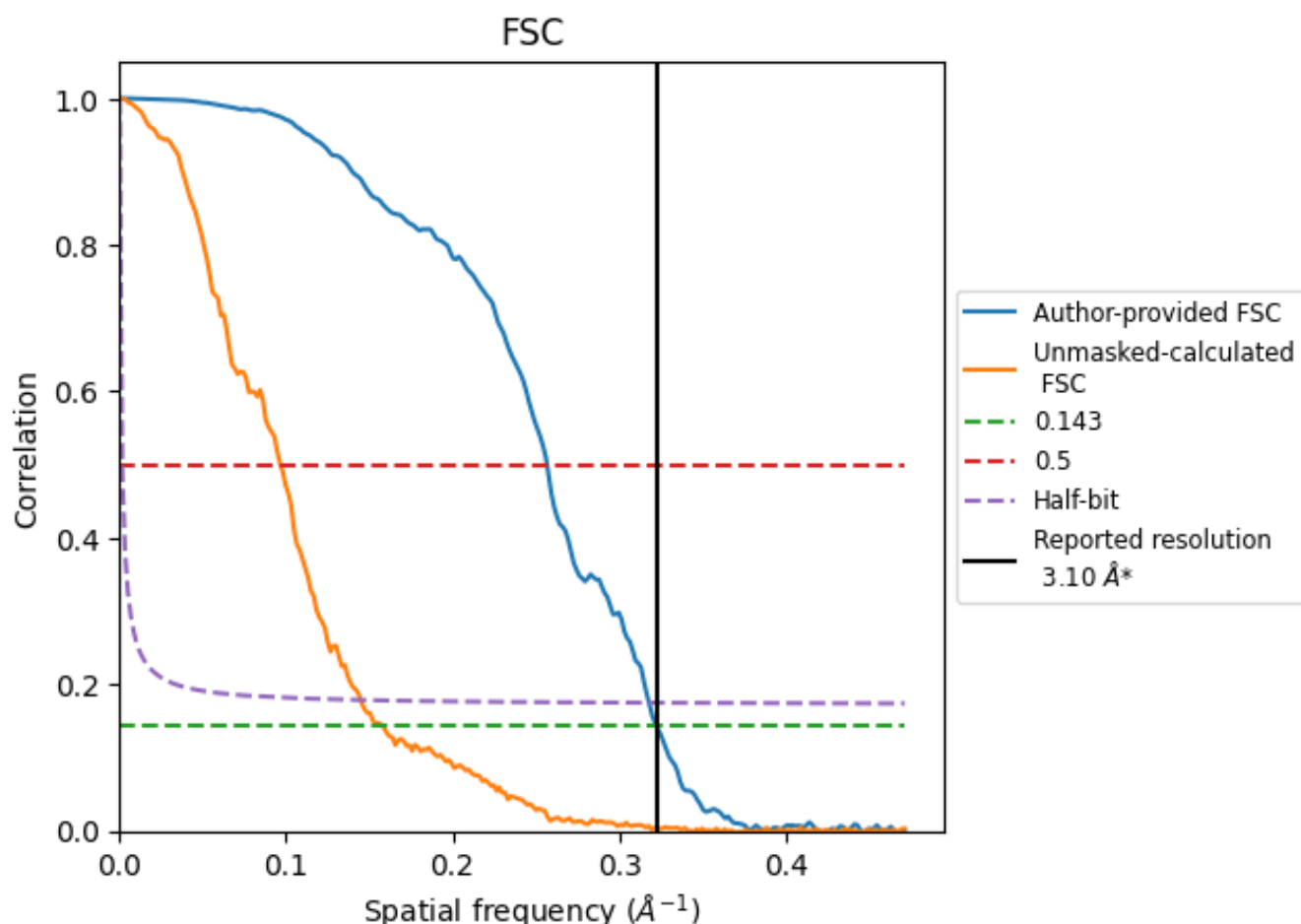


\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.89	3.14
Unmasked-calculated*	6.33	10.34	6.90

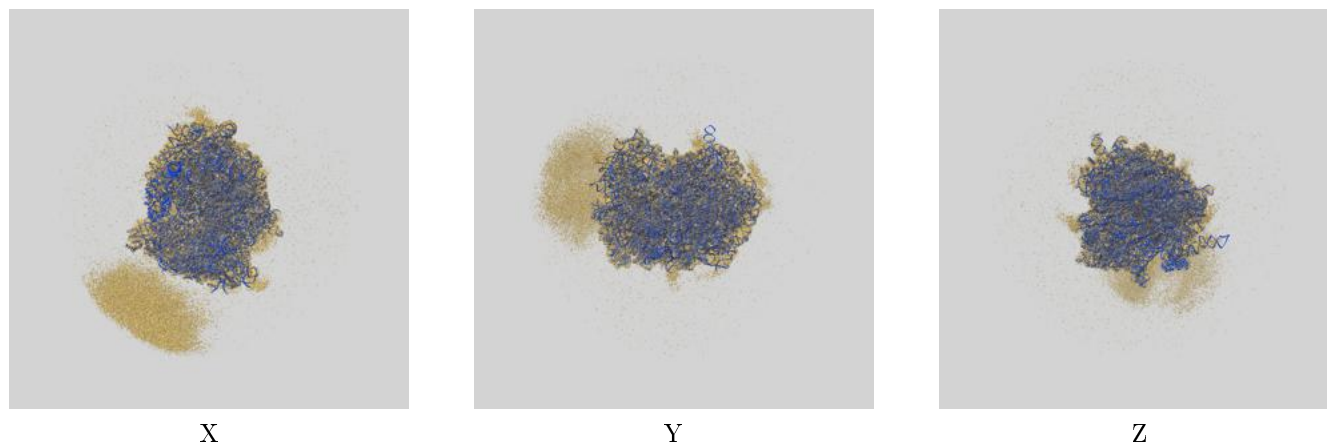
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.33 differs from the reported value 3.1 by more than 10 %



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

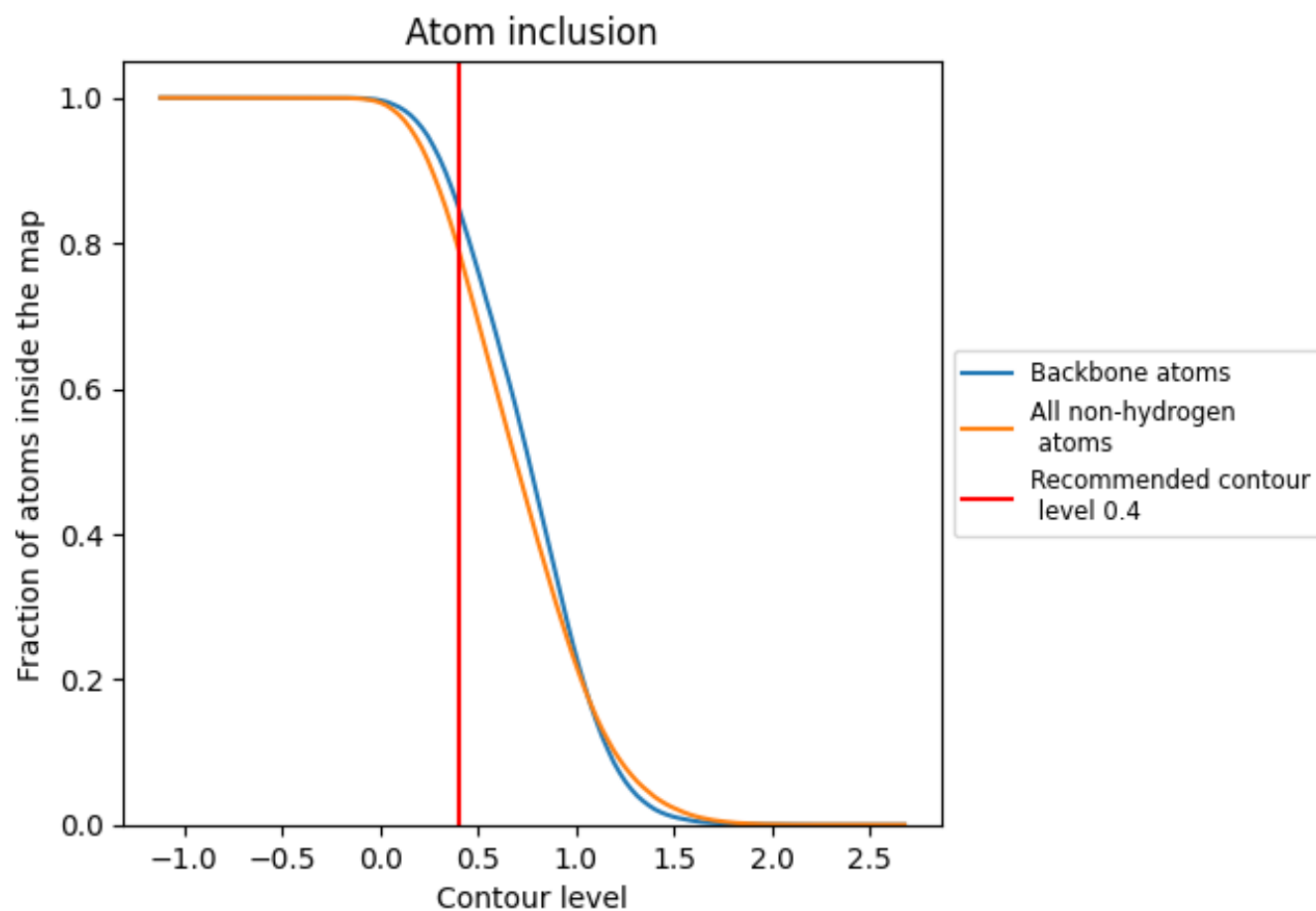
This section contains information regarding the fit between EMDB map EMD-12759 and PDB model 7O81. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.4 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 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.