



## wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 04:40 pm GMT

PDB ID : 6SKF  
EMDB ID : EMD-10223  
Title : Cryo-EM Structure of T. kodakarensis 70S ribosome  
Authors : Matzov, D.; Sas-Chen, A.; Thomas, J.M.; Santangelo, T.; Meier, J.L.; Schwartz, S.; Shalev-Benami, M.  
Deposited on : 2019-08-15  
Resolution : 2.95 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

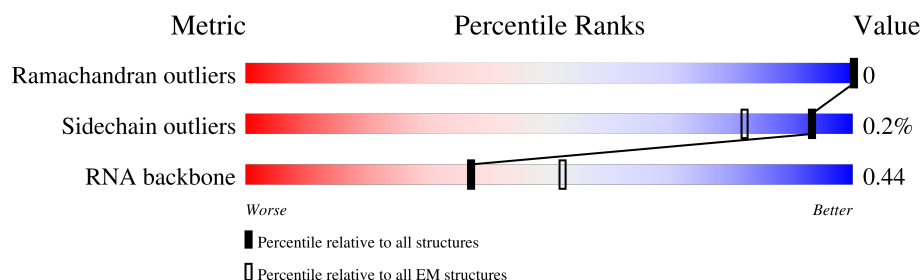
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.95 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	Aa	1498	<div> <div>8%</div> <div>72%</div> <div>24%</div> <div>••</div> </div>
2	Ab	201	<div> <div>25%</div> <div>98%</div> <div>•</div> </div>
3	Ac	209	<div> <div>71%</div> <div>93%</div> <div>7%</div> </div>
4	Ad	200	<div> <div>29%</div> <div>95%</div> <div>5%</div> </div>
5	Ae	180	<div> <div>16%</div> <div>97%</div> <div>•</div> </div>
6	Af	243	<div> <div>15%</div> <div>99%</div> <div>•</div> </div>
7	Ag	235	<div> <div>14%</div> <div>95%</div> <div>5%</div> </div>
8	Ah	125	<div> <div>58%</div> <div>98%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
9	Ai	215	34% 100%
10	Aj	130	10% 99%
11	Ak	130	21% 96%
12	Al	135	44% 99%
13	Am	102	76% 98%
14	An	140	26% 89%
15	Ao	147	14% 97%
16	Ap	149	28% 91%
17	Aq	151	20% 98%
18	Ar	56	43% 96%
19	As	114	18% 95%
20	At	67	90% 96%
21	Au	133	41% 86%
22	Av	150	27% 99%
23	Aw	98	22% 97%
24	Ax	65	34% 94%
25	Ay	70	39% 91%
26	Az	62	21% 89%
27	BA	3037	9% 60% 33%
28	BB	126	20% 73% 25%
29	BC	239	7% 99%
30	BD	346	7% 99%
31	BE	255	100%
32	BF	183	81% 91%
33	BG	184	12% 99%

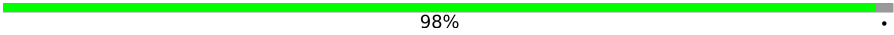
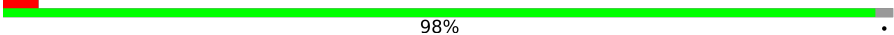

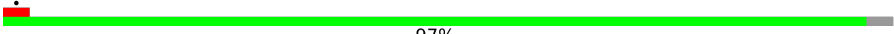

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Mol	Chain	Length	Quality of chain
34	BH	123	<div>36%</div> <div>98%</div> <div>98%</div>
34	BI	123	<div>98%</div> <div>98%</div> <div>98%</div>
35	BJ	182	<div>10%</div> <div>92%</div> <div>8%</div>
36	BK	142	<div>100%</div> <div>100%</div> <div>100%</div>
37	BL	141	<div>10%</div> <div>99%</div> <div>99%</div>
38	BM	83	<div>25%</div> <div>96%</div> <div>96%</div>
38	BN	83	<div>33%</div> <div>96%</div> <div>96%</div>
39	BO	148	<div>29%</div> <div>99%</div> <div>99%</div>
40	BP	194	<div>99%</div> <div>99%</div> <div>99%</div>
41	BQ	201	<div>33%</div> <div>82%</div> <div>18%</div>
42	BR	121	<div>98%</div> <div>98%</div> <div>98%</div>
43	BS	150	<div>8%</div> <div>97%</div> <div>97%</div>
44	BT	77	<div>19%</div> <div>96%</div> <div>96%</div>
45	BU	98	<div>98%</div> <div>98%</div> <div>98%</div>
46	BV	156	<div>97%</div> <div>97%</div> <div>97%</div>
47	BW	86	<div>13%</div> <div>99%</div> <div>99%</div>
48	BX	121	<div>7%</div> <div>99%</div> <div>99%</div>
49	BY	67	<div>93%</div> <div>93%</div> <div>7%</div>
50	BZ	66	<div>27%</div> <div>89%</div> <div>9%</div>
51	Ba	155	<div>5%</div> <div>99%</div> <div>99%</div>
52	Bb	102	<div>16%</div> <div>94%</div> <div>6%</div>
53	Bc	90	<div>12%</div> <div>99%</div> <div>99%</div>
54	Bd	125	<div>6%</div> <div>99%</div> <div>99%</div>
55	Be	90	<div>7%</div> <div>98%</div> <div>98%</div>
56	Bg	86	<div>5%</div> <div>97%</div> <div>97%</div>

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Mol	Chain	Length	Quality of chain
57	Bh	63	 98%.
58	Bi	51	 98%.
59	Bj	51	 8%92%8%.
60	Bk	37	 97%.
61	Bl	94	 6%98%..

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 161921 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	1463	Total	C	N	O	P	0	0
			31591	14101	5837	10190	1463		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	196	Total	C	N	O	S	0	0
			1580	1021	272	284	3		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ac	195	Total	C	N	O	S	0	0
			1524	973	277	271	3		

- Molecule 4 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ad	190	Total	C	N	O	S	0	0
			1550	997	277	273	3		

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ae	174	Total	C	N	O	S	0	0
			1454	912	287	253	2		

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Af	241	Total	C	N	O	S	0	0
			1945	1256	348	336	5		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ag	223	Total	C	N	O	S	0	0
			1753	1107	327	312	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ah	123	Total	C	N	O	S	0	0
			952	599	179	172	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ai	214	Total	C	N	O	S	0	0
			1715	1087	317	303	8		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Aj	129	Total	C	N	O	S	0	0
			1020	662	176	180	2		

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Ak	125	Total	C	N	O	0	0
			982	615	198	169		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Al	133	Total	C	N	O	S	0	0
			1054	656	205	188	5		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Am	100	Total	C	N	O	S	0	0
			803	498	154	148	3		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	An	127	Total	C	N	O	S	0	0
			950	586	190	171	3		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ao	143	Total	C	N	O	S	0	0
			1122	712	216	192	2		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ap	135	Total	C	N	O	S	0	0
			1090	691	214	181	4		

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Aq	149	Total	C	N	O	S	0	0
			1217	776	233	206	2		

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ar	54	Total	C	N	O	S	0	0
			447	284	92	65	6		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	As	108	Total	C	N	O	S	0	0
			879	560	164	152	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	At	64	Total	C	N	O	S	0	0
			538	338	103	95	2		

- Molecule 21 is a protein called 30S ribosomal protein S19.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	Au	116	Total	C	N	O	S	0	0
			952	608	175	163	6		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Av	149	Total	C	N	O		0	0
			1216	788	215	213			

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Aw	95	Total	C	N	O	S	0	0
			777	497	131	146	3		

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ax	61	Total	C	N	O	S	0	0
			461	294	83	79	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ax	64	GLU	LEU	conflict	UNP Q5JE50

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ay	64	Total	C	N	O		0	0
			499	307	99	93			

- Molecule 26 is a protein called Predicted zinc-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Az	55	Total	C	N	O	S	0	0
			426	269	74	75	8		

- Molecule 27 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	BA	2929	Total	C	N	O	P	S	0	0
			63265	28239	11728	20367	2929	2		

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BB	125	Total	C	N	O	P	0	0
			2678	1191	492	870	125		

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BC	237	Total	C	N	O	S	0	0
			1820	1150	356	311	3		

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BD	344	Total	C	N	O	S	0	0
			2746	1765	505	469	7		

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BE	255	Total	C	N	O	S	0	0
			2026	1286	389	347	4		

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BF	169	Total	C	N	O	S	0	0
			1313	821	252	233	7		

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BG	183	Total	C	N	O	S	0	0
			1463	942	253	266	2		

- Molecule 34 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BH	121	Total	C	N	O	S	0	0
			928	591	154	180	3		
34	BI	121	Total	C	N	O	S	0	0
			928	591	154	180	3		

- Molecule 35 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BJ	168	Total	C	N	O	S	0	0
			1378	877	258	236	7		

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	142	Total	C	N	O	S	0	0
			1146	731	213	198	4		

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	140	Total	C	N	O	S	0	0
			1055	658	214	180	3		

- Molecule 38 is a protein called 50S ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	81	Total	C	N	O	S	0	0
			610	382	119	108	1		
38	BN	81	Total	C	N	O	S	0	0
			610	382	119	108	1		

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BO	148	Total	C	N	O	S	0	0
			1165	742	222	198	3		

- Molecule 40 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BP	193	Total	C	N	O	S	0	0
			1582	1010	316	250	6		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BQ	164	Total	C	N	O	S	0	0
			1314	841	243	228	2		

- Molecule 42 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BR	120	Total	C	N	O	S	0	0
			959	601	187	169	2		

- Molecule 43 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BS	146	Total	C	N	O	S	0	0
			1200	753	246	194	7		

- Molecule 44 is a protein called 50S ribosomal protein L18Ae.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	BT	74	Total	C	N	O	0	0
			624	399	113	112		

- Molecule 45 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BU	96	Total	C	N	O	S	0	0
			784	502	158	123	1		

- Molecule 46 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	154	Total	C	N	O	S	0	0
			1234	777	242	211	4		

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	85	Total	C	N	O	S	0	0
			683	438	119	123	3		

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BX	120	Total	C	N	O	S	0	0
			991	628	188	170	5		

- Molecule 49 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	62	Total	C	N	O	S	0	0
			524	334	99	85	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BZ	60	Total	C	N	O	S	0	0
			506	314	98	90	4		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ba	154	Total	C	N	O	S	0	0
			1242	788	235	214	5		

- Molecule 52 is a protein called 50S ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bb	96	Total	C	N	O	S	0	0
			730	473	123	133	1		

- Molecule 53 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Bc	89	Total	C	N	O	0	0
			721	463	140	118		

- Molecule 54 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bd	124	Total	C	N	O	S	0	0
			1022	650	208	162	2		

- Molecule 55 is a protein called 50S ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Be	89	Total	C	N	O	S	0	0
			728	454	155	110	9		

- Molecule 56 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bg	84	Total	C	N	O	S	0	0
			630	392	132	101	5		

- Molecule 57 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Bh	62	Total	C	N	O	S	0	0
			512	314	118	75	5		

- Molecule 58 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bi	50	Total	C	N	O	S	0	0
			432	276	97	59			

- Molecule 59 is a protein called 50S ribosomal protein L40e.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bj	47	Total	C	N	O	S	0	0
			373	233	79	56	5		

- Molecule 60 is a protein called LSU ribosomal protein L41E.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bk	36	Total	C	N	O	S	0	0
			345	218	86	39	2		

- Molecule 61 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bl	93	Total	C	N	O	S	0	0
			778	494	160	119	5		

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	Ag	1	Total 1	Zn 1	0
62	Ar	1	Total 1	Zn 1	0
62	As	1	Total 1	Zn 1	0
62	Ax	1	Total 1	Zn 1	0
62	Az	2	Total 2	Zn 2	0
62	BY	1	Total 1	Zn 1	0
62	Be	1	Total 1	Zn 1	0
62	Bg	1	Total 1	Zn 1	0
62	Bh	1	Total 1	Zn 1	0
62	Bj	1	Total 1	Zn 1	0
62	Bl	1	Total 1	Zn 1	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		AltConf
63	Aa	714	Total 714	O 714	0
63	Ab	8	Total 8	O 8	0
63	Ac	10	Total 10	O 10	0
63	Ad	4	Total 4	O 4	0
63	Ae	13	Total 13	O 13	0
63	Af	14	Total 14	O 14	0
63	Ag	14	Total 14	O 14	0
63	Ah	2	Total 2	O 2	0
63	Ai	13	Total 13	O 13	0

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Mol	Chain	Residues	Atoms		AltConf
63	Aj	12	Total 12	O 12	0
63	Ak	8	Total 8	O 8	0
63	Al	7	Total 7	O 7	0
63	Am	2	Total 2	O 2	0
63	An	8	Total 8	O 8	0
63	Ao	10	Total 10	O 10	0
63	Ap	11	Total 11	O 11	0
63	Aq	10	Total 10	O 10	0
63	Ar	2	Total 2	O 2	0
63	As	6	Total 6	O 6	0
63	At	1	Total 1	O 1	0
63	Au	4	Total 4	O 4	0
63	Av	13	Total 13	O 13	0
63	Aw	1	Total 1	O 1	0
63	Ax	3	Total 3	O 3	0
63	Ay	4	Total 4	O 4	0
63	Az	4	Total 4	O 4	0
63	BA	1226	Total 1226	O 1226	0
63	BB	19	Total 19	O 19	0
63	BC	19	Total 19	O 19	0
63	BD	24	Total 24	O 24	0

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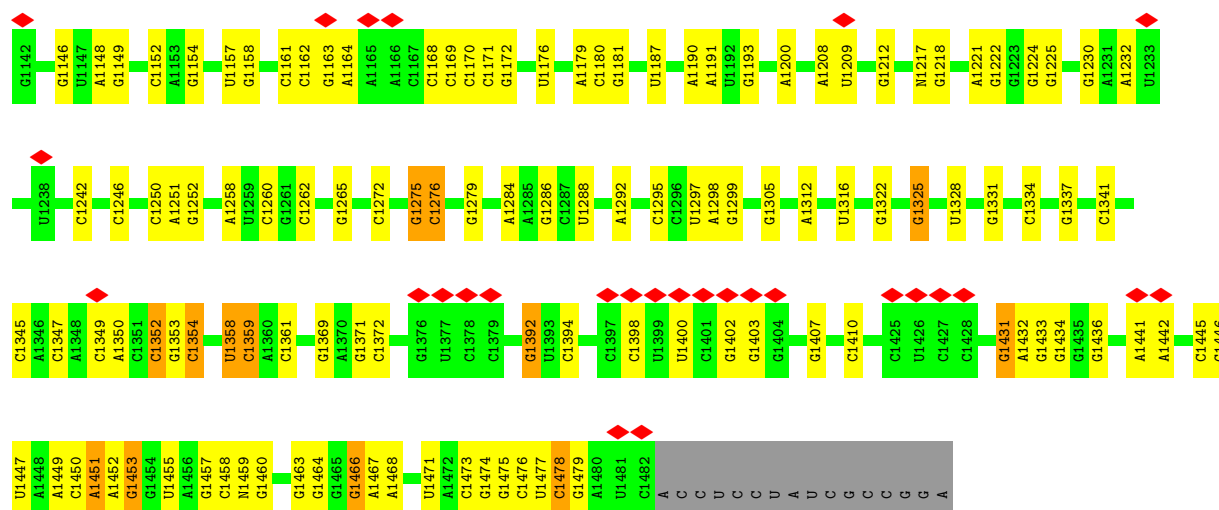
Mol	Chain	Residues	Atoms		AltConf
63	BE	11	Total 11	O 11	0
63	BG	6	Total 6	O 6	0
63	BJ	11	Total 11	O 11	0
63	BK	11	Total 11	O 11	0
63	BL	4	Total 4	O 4	0
63	BM	2	Total 2	O 2	0
63	BN	4	Total 4	O 4	0
63	BO	10	Total 10	O 10	0
63	BP	18	Total 18	O 18	0
63	BQ	7	Total 7	O 7	0
63	BR	8	Total 8	O 8	0
63	BS	7	Total 7	O 7	0
63	BT	3	Total 3	O 3	0
63	BU	7	Total 7	O 7	0
63	BV	7	Total 7	O 7	0
63	BW	4	Total 4	O 4	0
63	BX	6	Total 6	O 6	0
63	BY	3	Total 3	O 3	0
63	BZ	1	Total 1	O 1	0
63	Ba	10	Total 10	O 10	0
63	Bb	1	Total 1	O 1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
63	Bc	3	Total 3	O 3	0
63	Bd	5	Total 5	O 5	0
63	Be	3	Total 3	O 3	0
63	Bg	3	Total 3	O 3	0
63	Bh	11	Total 11	O 11	0
63	Bi	2	Total 2	O 2	0
63	Bj	2	Total 2	O 2	0
63	Bk	3	Total 3	O 3	0
63	Bl	8	Total 8	O 8	0

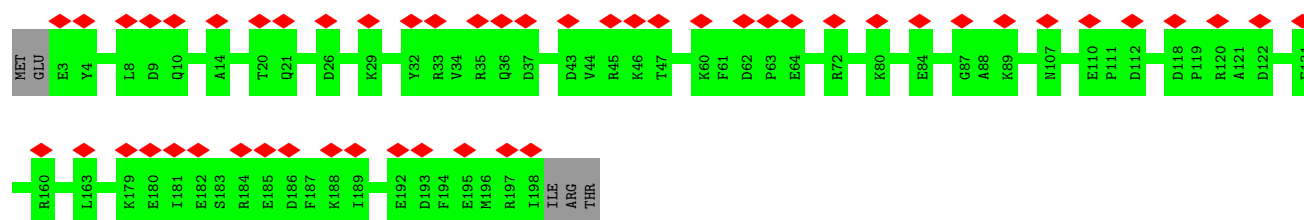




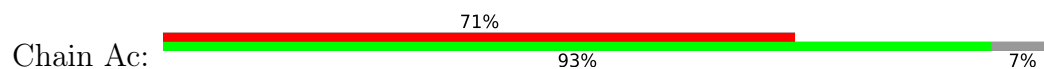
• Molecule 2: 30S ribosomal protein S2



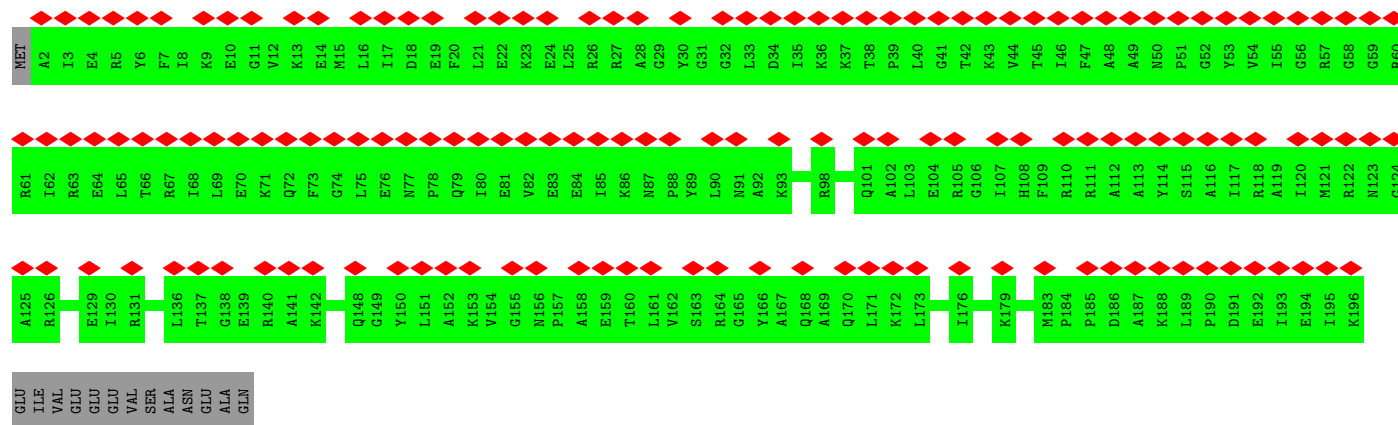
Chain Ab:



• Molecule 3: 30S ribosomal protein S3



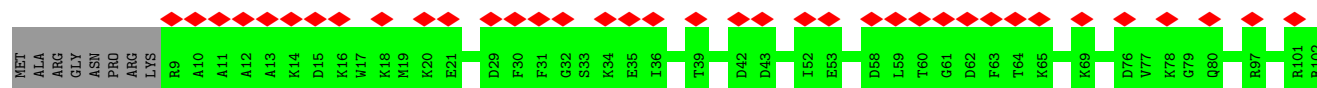
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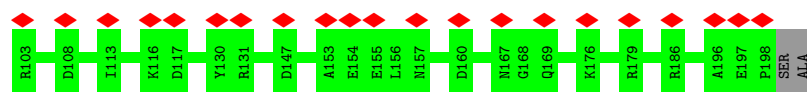


• Molecule 4: 30S ribosomal protein S3Ae

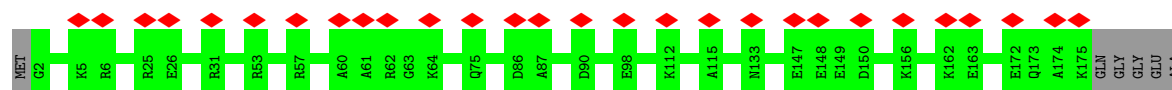


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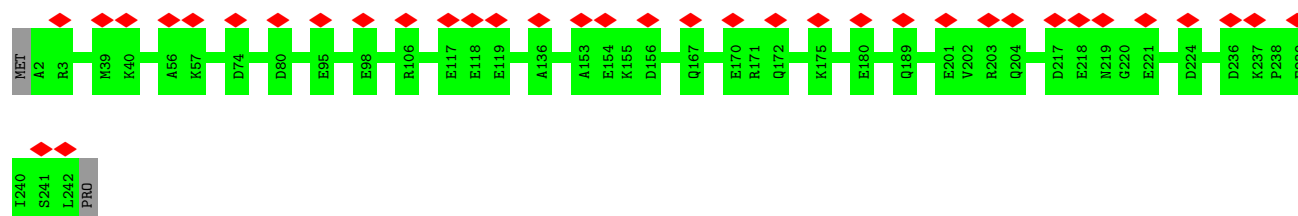




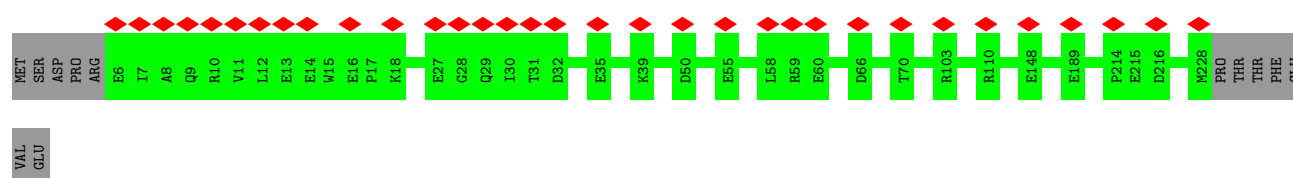
- Molecule 5: 30S ribosomal protein S4



- Molecule 6: 30S ribosomal protein S4e



- Molecule 7: 30S ribosomal protein S5

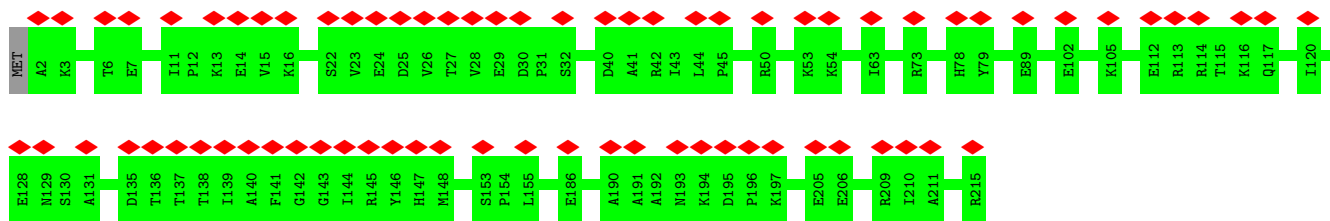


- Molecule 8: 30S ribosomal protein S6e

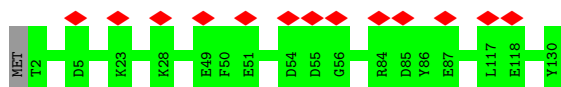


- Molecule 9: 30S ribosomal protein S7

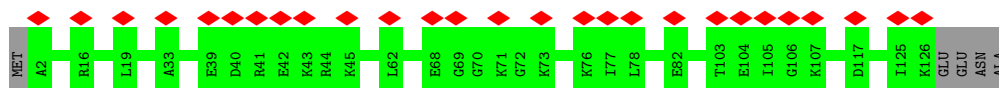




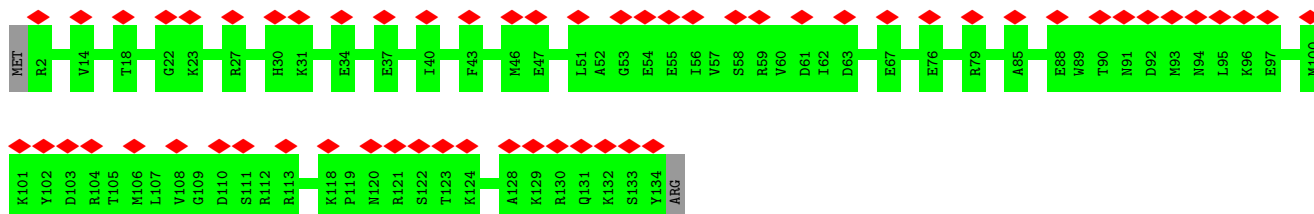
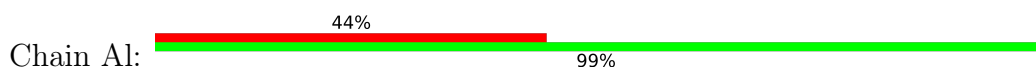
- Molecule 10: 30S ribosomal protein S8



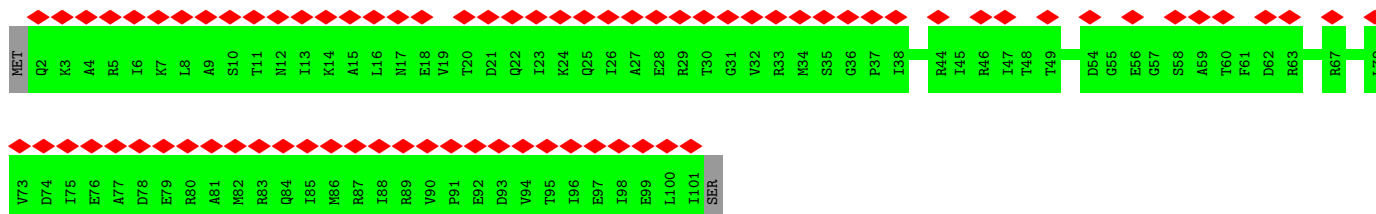
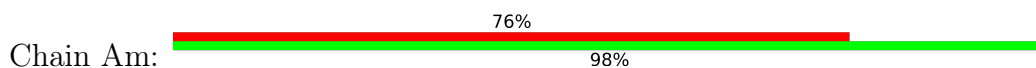
- Molecule 11: 30S ribosomal protein S8e



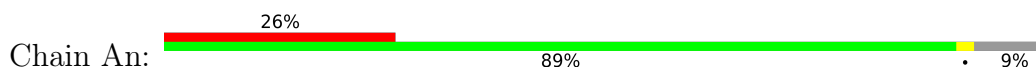
- Molecule 12: 30S ribosomal protein S9

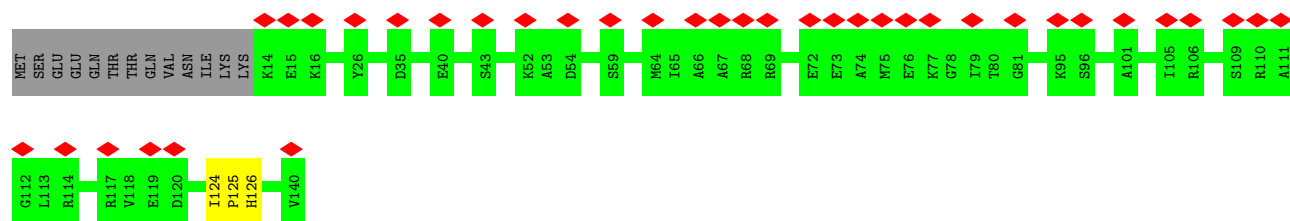


- Molecule 13: 30S ribosomal protein S10

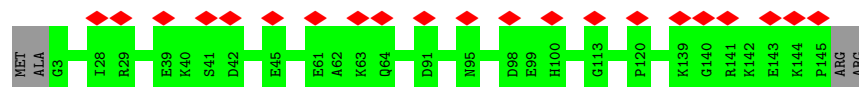


- Molecule 14: 30S ribosomal protein S11

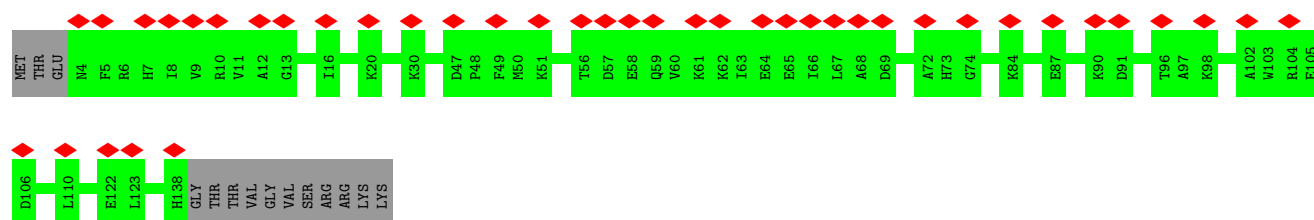
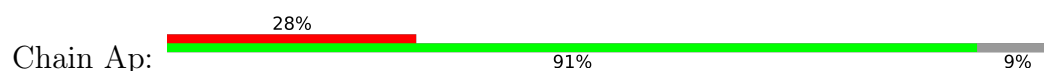




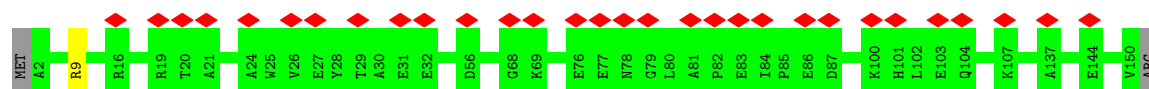
- Molecule 15: 30S ribosomal protein S12



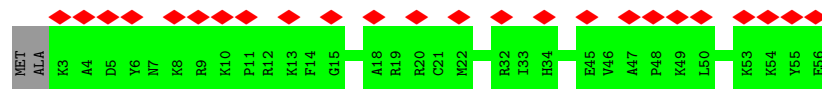
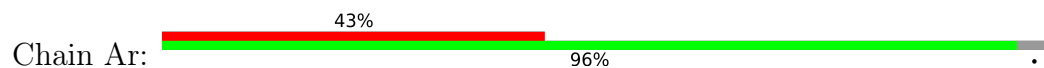
- Molecule 16: 30S ribosomal protein S13



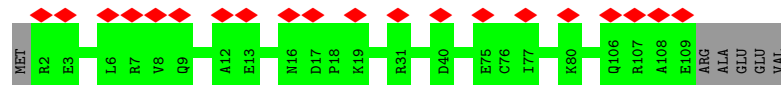
- Molecule 17: 30S ribosomal protein S15



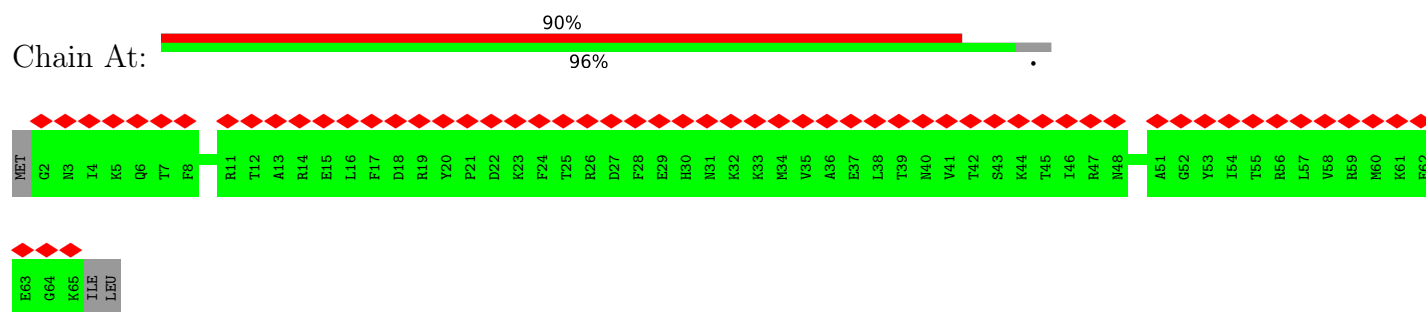
- Molecule 18: 30S ribosomal protein S14 type Z



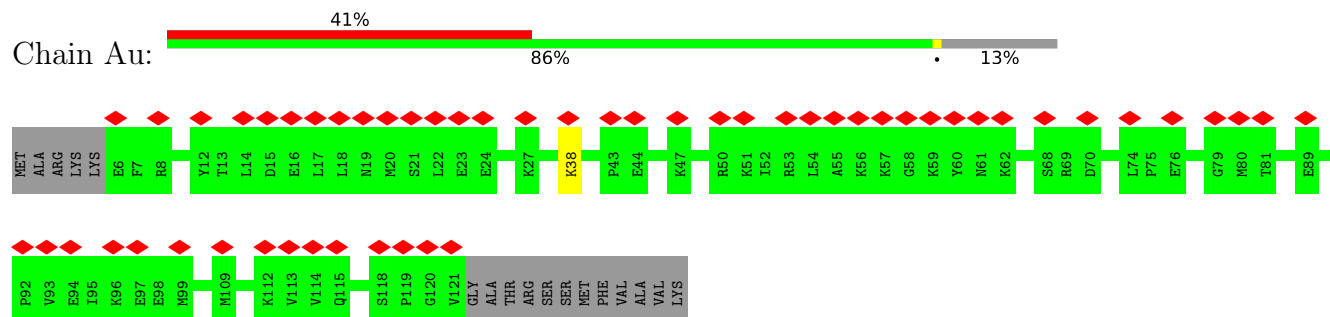
- Molecule 19: 30S ribosomal protein S17



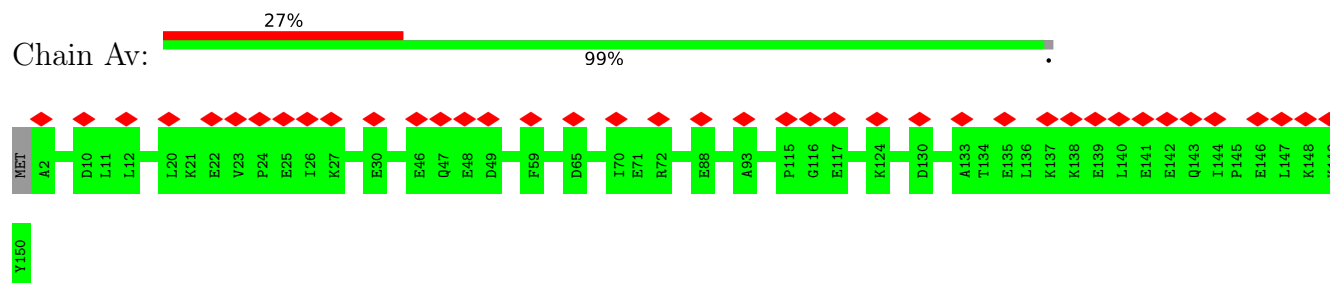
- Molecule 20: 30S ribosomal protein S17e



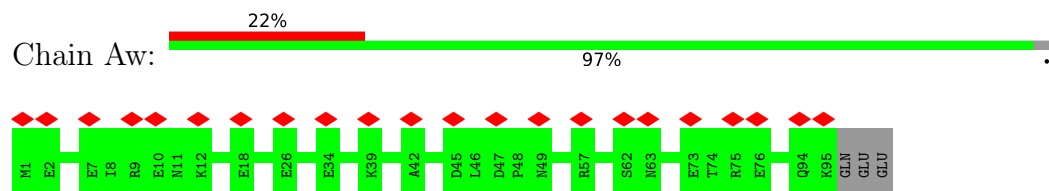
- Molecule 21: 30S ribosomal protein S19



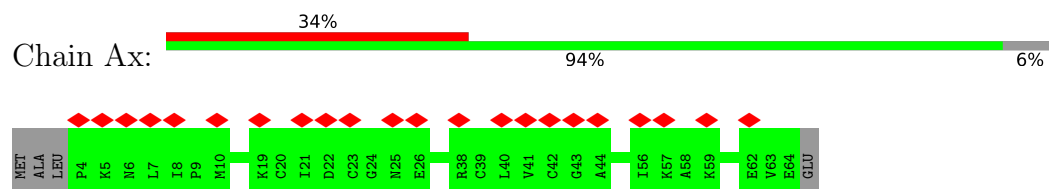
- Molecule 22: 30S ribosomal protein S19e



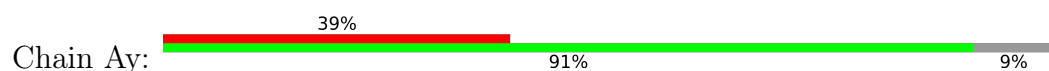
- Molecule 23: 30S ribosomal protein S24e



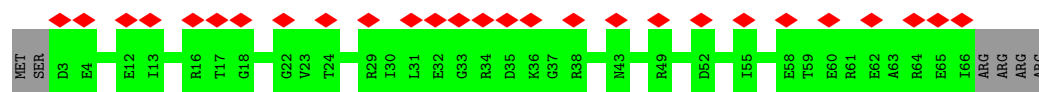
- Molecule 24: 30S ribosomal protein S27e



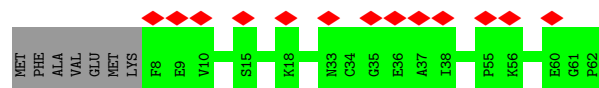
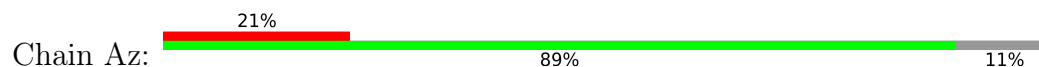
- Molecule 25: 30S ribosomal protein S28e



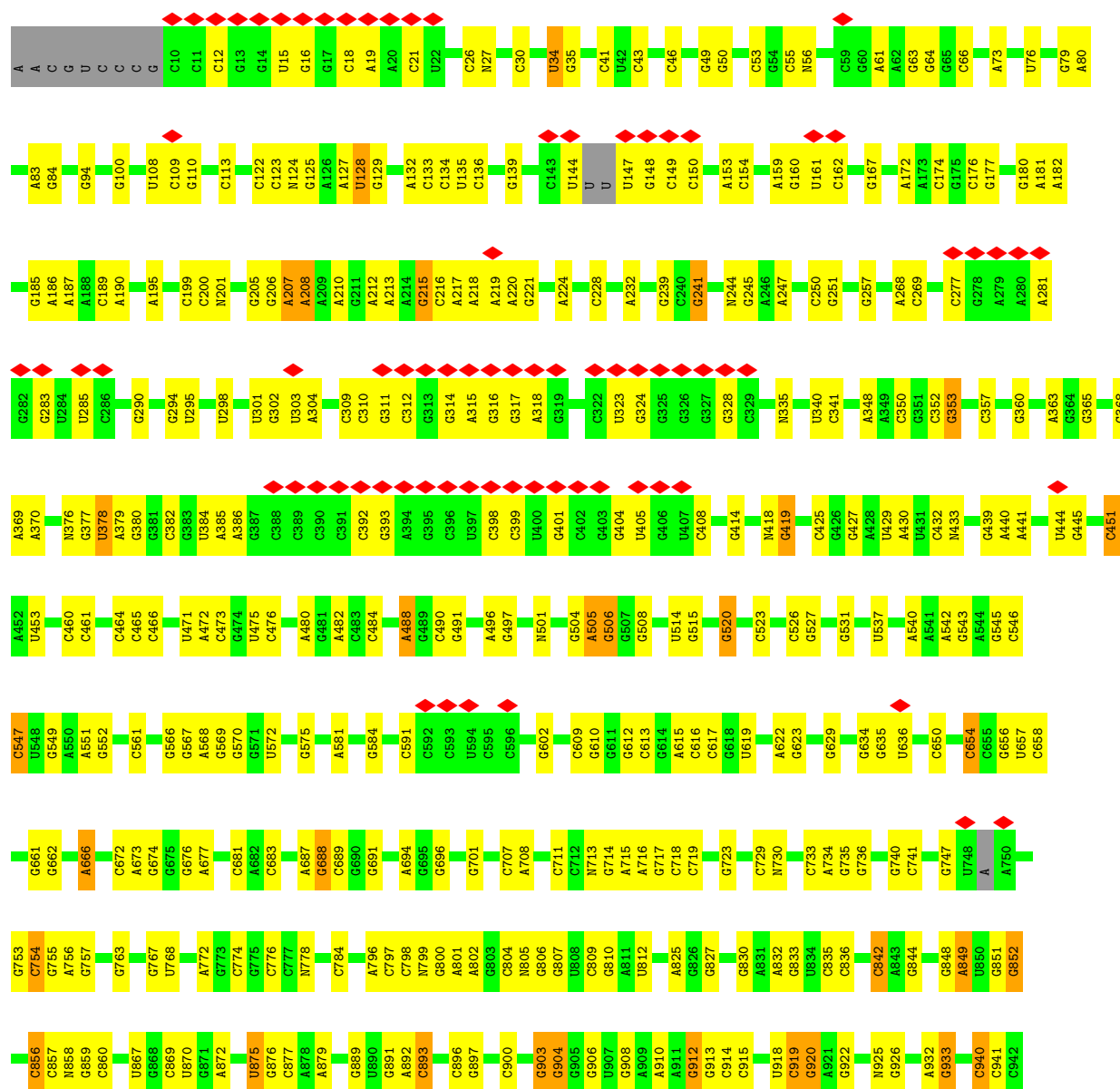




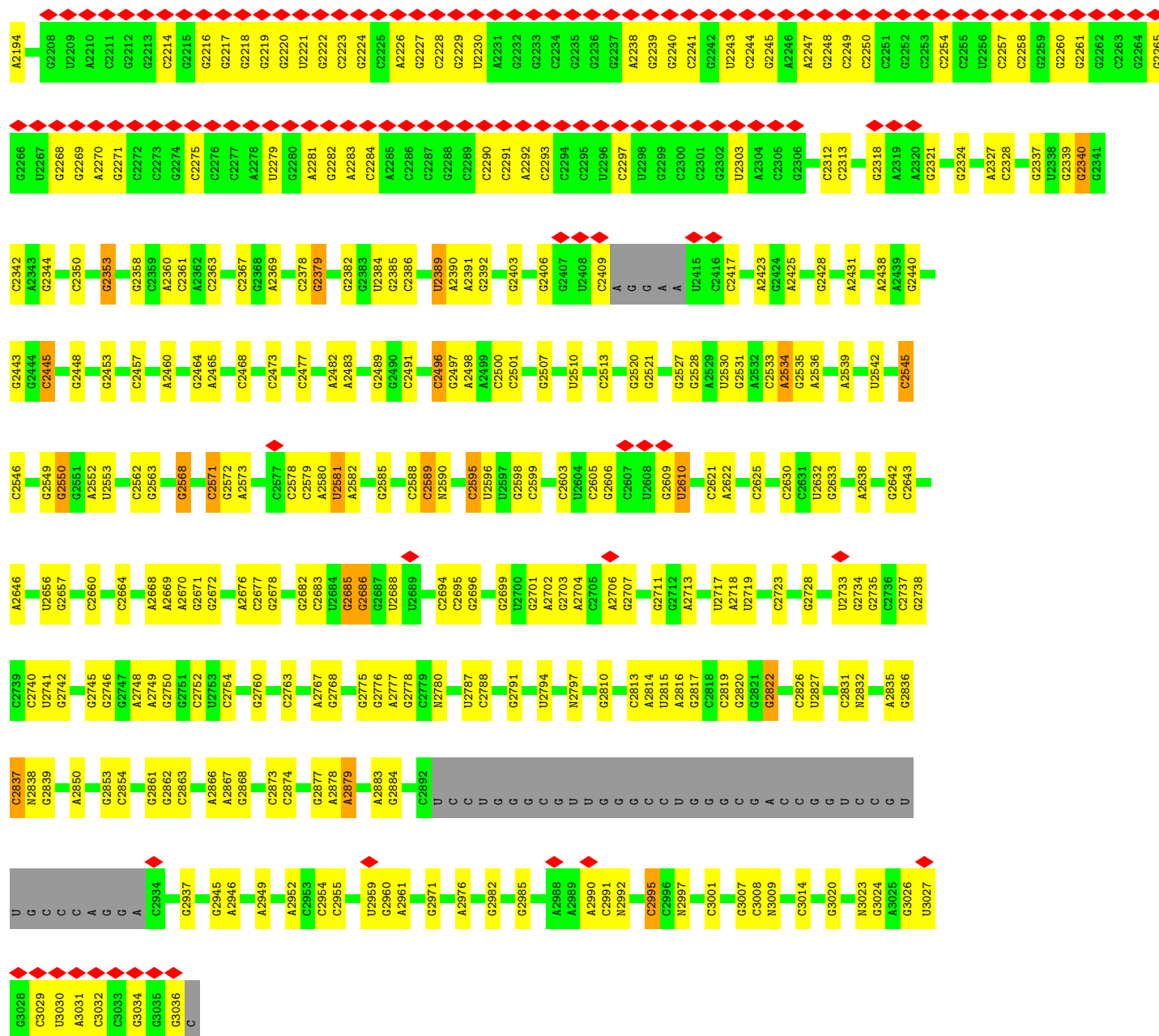
- Molecule 26: Predicted zinc-ribbon RNA-binding protein involved in translation



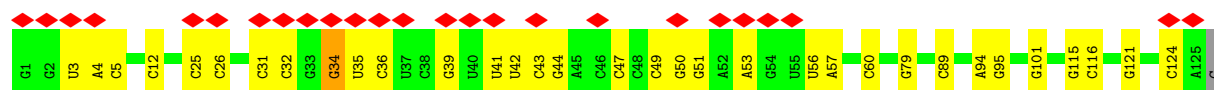
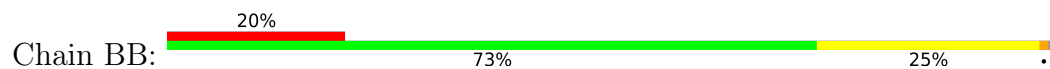
- Molecule 27: 23S rRNA



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G1385	G1388	C1391	C1392	N1396	G1397	G1398	G1399	A1400	G1401	G1404	A1409	U1410	C1414	N1427	N1431	G1432	C1433	N1434	G1435	U1436	A1437	G1438	C1442	G1445	G1446	G1447	U1448	U1449	A1457	U1461	U1462	C1463	C1466	C1469	N1470	U1477	A1478	G1479	U1480	C1485	C1486	U1487									
C1490	C1496	C1502	U1503	C1504	G1514	A1517	G1520	A1521	G1525	A1533	U1534	C1536	N1543	G1547	U1548	U1551	C1556	G1557	G1558	C1559	C1560	G1563	G1564	C1565	G1568	C1571	G1579	A1580	C1581	G1594	A1606	C1607	C1612	U1617	U1624	U1625	U1626														
G1635	A1636	U1638	G1639	N1641	U1646	G1647	G1650	A1651	G1652	C1655	C1656	G1657	U1660	G1661	A1662	A1663	A1664	A1671	U1672	G1673	G1674	C1675	C1679	C1680	G1681	U1682	A1683	A1684	G1685	G1687	G1688	U1691	U1692	C1693	C1696	A1699	U1704	G1705	G1706	A1715	A1716	U1734									
G1741	G1742	A1743	C1744	G1750	G1751	A1752	G1753	A1754	A1755	C1756	C1757	A1761	C1762	A1763	G1764	G1765	U1766	G1767	C1768	C1769	C1770	C1771	U1772	G1773	G1774	G1775	U1776	G1777	C1783	G1784	U1785	G1788	G1789	G1790	G1791	U1792	G1793	U1794	C1795	G1799	G1800	A1801	C1804	C1805	C1806	C1809	N1810	C1818	U1819	C1820	G1821
G1822	C1823	A1824	U1827	G1830	C1831	C1832	G1835	U1836	A1837	C1842	A1848	A1849	G1853	U1854	G1855	G1859	C1860	G1861	U1868	C1875	G1884	G1891	C1892	C1897	C1898	N1899	G1900	A1901	G1902	U1903	G1904	U1905	A1908	G1909	A1913	A1914	A1915	C1916	A1917	C1918	A1919	G1920	C1924								
G1927	C1928	U1929	A1930	G1931	C1932	C1933	N1934	A1937	A1938	G1939	G1940	G1945	U1946	A1947	G1948	G1953	C1954	N1955	G1956	A1957	C1958	G1959	C1960	G1961	C1965	U1969	A1991	A2002	C2007	G2010	U2011	A2012	A2013	A2014	C2015	G2016	G2017	C2018	C2019	G2020	G2021	G2022	A2026	C2027	U2028	A2029	C2033	C2034			
C2035	U2036	C2037	U2038	G2042	G2043	C2047	G2048	A2049	A2050	G2051	G2052	G2053	G2054	G2055	C2060	G2061	G2062	A2067	G2068	C2070	A2073	G2074	C2075	G2076	G2077	A2078	G2080	A2082	G2083	G2084	G2085	G2086	G2087	G2088	A2091	C2099	C2103	G2104	G2105	G2106	C2107	A2026	C2109	G2110	G2111	G2112	C2113				
G2118	G2119	C2120	N2121	G2124	G2125	G2129	C2132	C2133	C2135	C2136	A2137	G2138	G2139	G2140	G2141	G2142	A2143	U2144	A2145	C2148	C2149	U2150	G2151	G2152	C2153	A2154	C2155	N2159	G2160																						

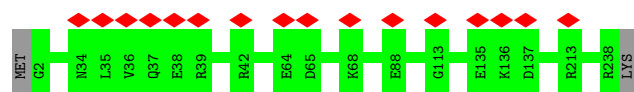


• Molecule 28: 5S rRNA

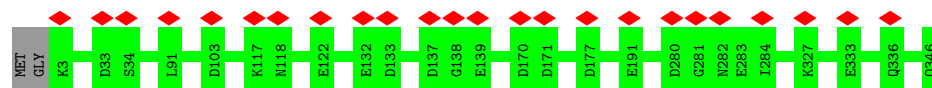


• Molecule 29: 50S ribosomal protein L2

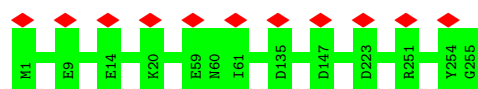




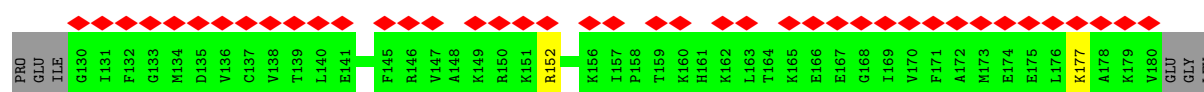
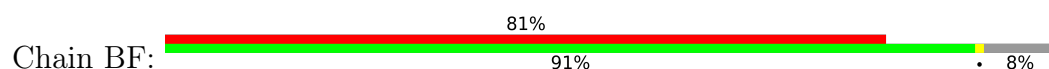
- Molecule 30: 50S ribosomal protein L3



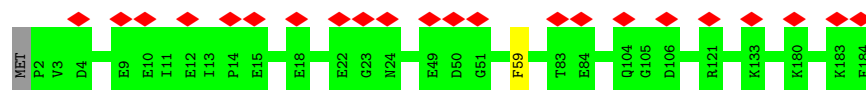
- Molecule 31: 50S ribosomal protein L4



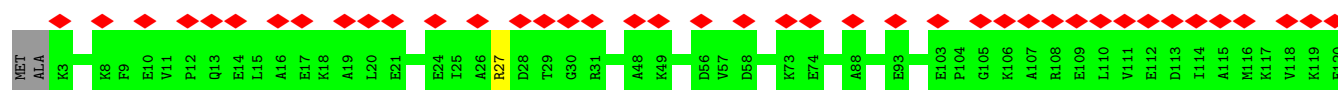
- Molecule 32: 50S ribosomal protein L5



- Molecule 33: 50S ribosomal protein L6



- Molecule 34: 50S ribosomal protein L7Ae

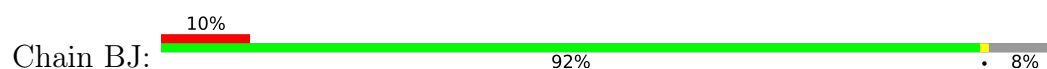




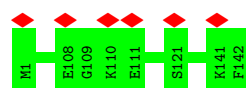
- Molecule 34: 50S ribosomal protein L7Ae



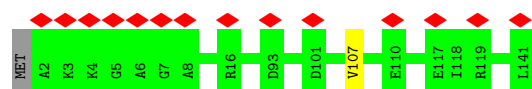
- Molecule 35: 50S ribosomal protein L10e



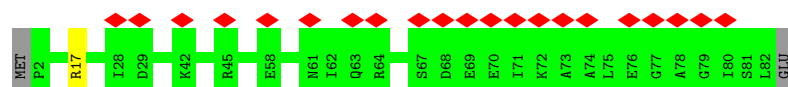
- Molecule 36: 50S ribosomal protein L13



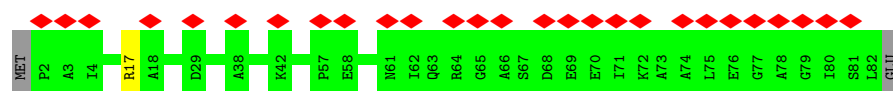
- Molecule 37: 50S ribosomal protein L14



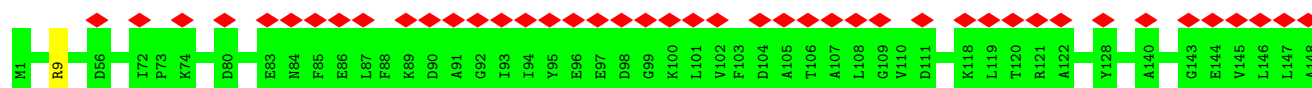
- Molecule 38: 50S ribosomal protein L14e



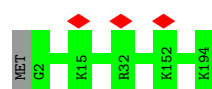
- Molecule 38: 50S ribosomal protein L14e



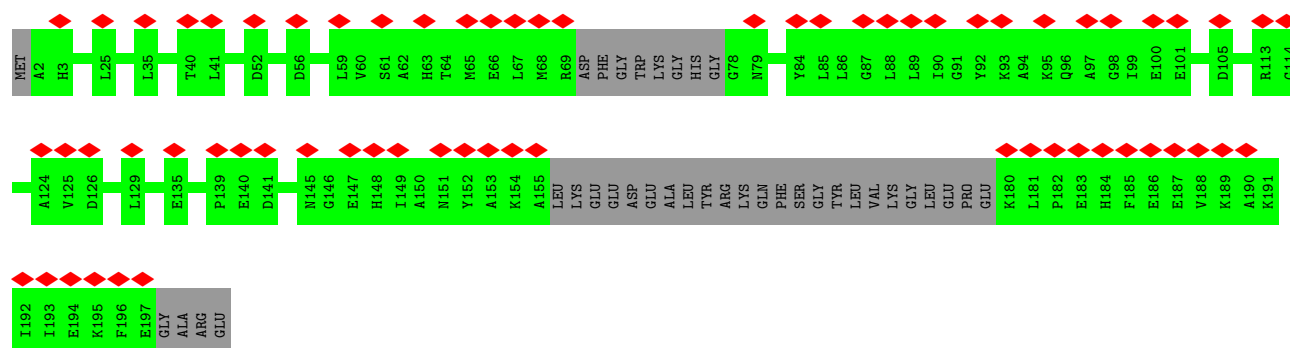
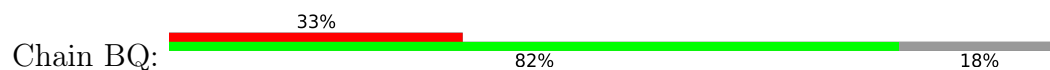
- Molecule 39: 50S ribosomal protein L15



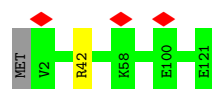
- Molecule 40: 50S ribosomal protein L15e



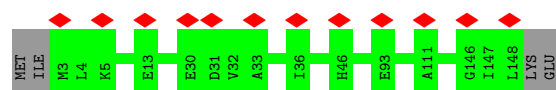
- Molecule 41: 50S ribosomal protein L18



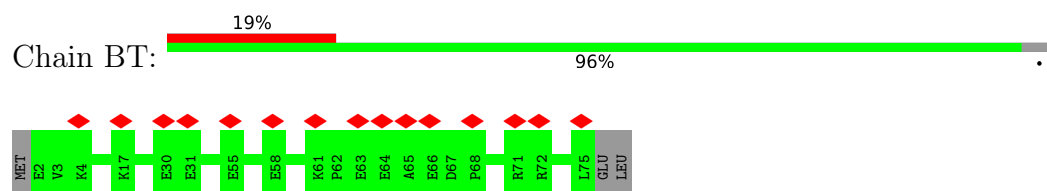
- Molecule 42: 50S ribosomal protein L18e



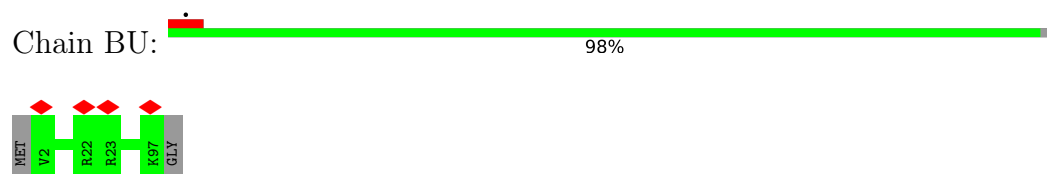
- Molecule 43: 50S ribosomal protein L19e



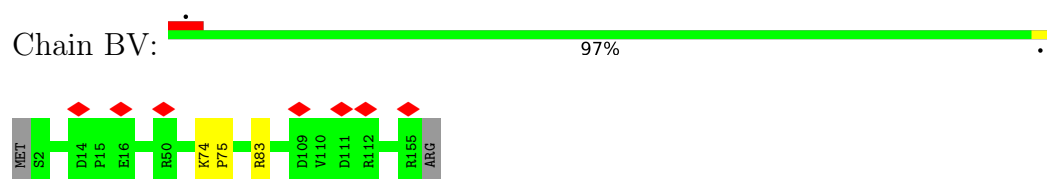
- Molecule 44: 50S ribosomal protein L18Ae



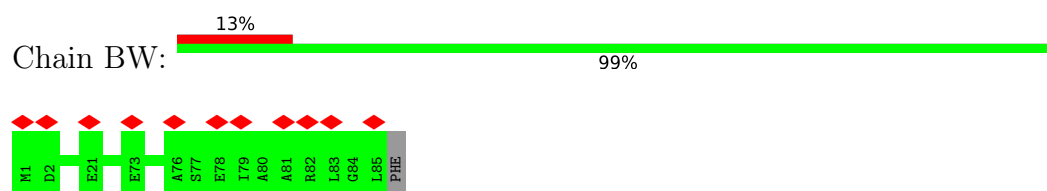
- Molecule 45: 50S ribosomal protein L21e



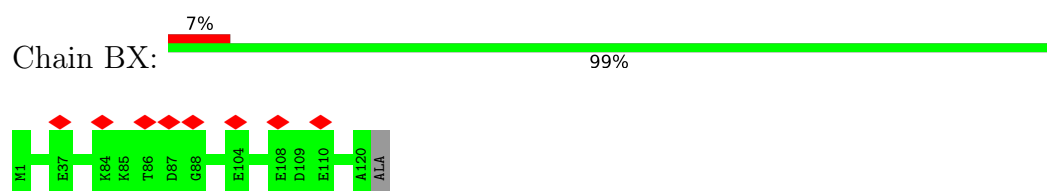
- Molecule 46: 50S ribosomal protein L22



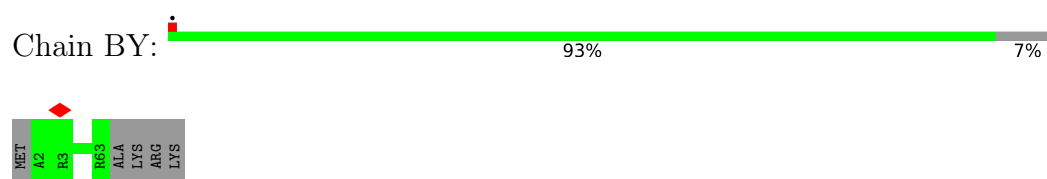
- Molecule 47: 50S ribosomal protein L23



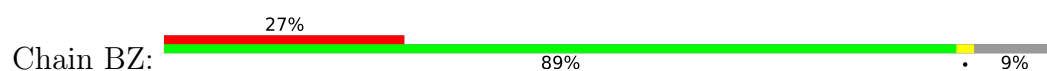
- Molecule 48: 50S ribosomal protein L24



- Molecule 49: 50S ribosomal protein L24e

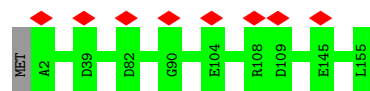


- Molecule 50: 50S ribosomal protein L29





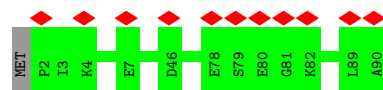
- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L30e



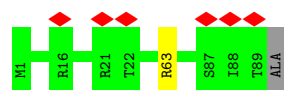
- Molecule 53: 50S ribosomal protein L31e



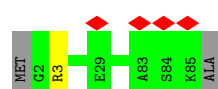
- Molecule 54: 50S ribosomal protein L32e



- Molecule 55: 50S ribosomal protein L34e



- Molecule 56: 50S ribosomal protein L37Ae



- Molecule 57: 50S ribosomal protein L37e

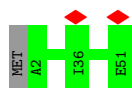


Chain Bh:  98% .




- Molecule 58: 50S ribosomal protein L39e

Chain Bi:  98% .



- Molecule 59: 50S ribosomal protein L40e

Chain Bj:  8% 92% 8%



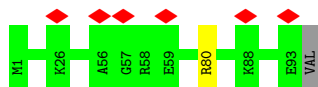
- Molecule 60: LSU ribosomal protein L41E

Chain Bk:  97% .



- Molecule 61: 50S ribosomal protein L44e

Chain Bl:  6% 98% ..



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53737	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 ( $e^-/\text{\AA}^2$ )	34	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	29000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.441	Depositor
Minimum map value	-0.245	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, B8T, OMU, LV2, 5MC, LHH, MA6, A2M, 4SU, OMG, 4AC, 6MZ, 2MG, 5MU, OMC

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	Aa	1.19	25/33361 (0.1%)	1.15	100/52003 (0.2%)
2	Ab	0.39	0/1611	0.47	0/2179
3	Ac	0.33	0/1546	0.50	0/2075
4	Ad	0.38	0/1578	0.51	0/2119
5	Ae	0.40	0/1477	0.52	0/1980
6	Af	0.45	0/1991	0.49	0/2688
7	Ag	0.30	0/1779	0.47	0/2396
8	Ah	0.36	0/968	0.51	0/1300
9	Ai	0.37	0/1748	0.48	0/2347
10	Aj	0.43	0/1039	0.51	0/1397
11	Ak	0.42	0/991	0.53	0/1322
12	Al	0.34	0/1068	0.53	0/1430
13	Am	0.31	0/810	0.49	0/1087
14	An	0.61	2/968 (0.2%)	0.58	1/1304 (0.1%)
15	Ao	0.44	0/1139	0.50	0/1518
16	Ap	0.36	0/1113	0.49	0/1500
17	Aq	0.39	0/1241	0.47	0/1667
18	Ar	0.35	0/457	0.48	0/602
19	As	0.29	0/899	0.47	0/1214
20	At	0.30	0/545	0.48	0/725
21	Au	0.37	0/970	0.49	0/1295
22	Av	0.40	0/1249	0.48	0/1687
23	Aw	0.41	0/790	0.50	0/1063
24	Ax	0.26	0/469	0.49	0/633
25	Ay	0.37	0/501	0.52	0/672
26	Az	0.28	0/440	0.44	0/599
27	BA	1.58	139/66981 (0.2%)	1.39	489/104453 (0.5%)
28	BB	1.06	0/2993	1.17	14/4668 (0.3%)
29	BC	0.69	0/1860	0.66	0/2511
30	BD	0.65	0/2815	0.62	0/3795
31	BE	0.63	0/2066	0.61	0/2785
32	BF	0.48	0/1330	0.60	0/1778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	BG	0.56	0/1490	0.57	0/2006
34	BH	0.46	0/941	0.53	0/1272
34	BI	0.33	0/941	0.50	0/1272
35	BJ	0.61	0/1407	0.63	1/1891 (0.1%)
36	BK	0.67	0/1165	0.68	0/1558
37	BL	0.65	1/1067 (0.1%)	0.62	0/1435
38	BM	0.50	0/614	0.58	0/824
38	BN	0.47	0/614	0.56	0/824
39	BO	0.55	0/1187	0.62	0/1583
40	BP	0.73	0/1621	0.61	0/2163
41	BQ	0.47	0/1342	0.54	0/1804
42	BR	0.58	0/971	0.59	0/1301
43	BS	0.59	0/1216	0.59	0/1607
44	BT	0.58	0/636	0.57	0/852
45	BU	0.62	0/806	0.58	0/1080
46	BV	0.73	2/1259 (0.2%)	0.65	1/1688 (0.1%)
47	BW	0.56	0/690	0.56	0/925
48	BX	0.58	0/1007	0.59	0/1344
49	BY	0.63	0/538	0.54	0/716
50	BZ	0.47	0/506	0.57	0/668
51	Ba	0.61	0/1259	0.63	0/1680
52	Bb	0.47	0/742	0.53	0/1001
53	Bc	0.60	0/736	0.53	0/990
54	Bd	0.66	0/1044	0.60	0/1394
55	Be	0.60	0/746	0.66	0/997
56	Bg	0.63	0/640	0.65	0/855
57	Bh	0.77	0/524	0.66	0/692
58	Bi	0.69	0/441	0.60	0/588
59	Bj	0.55	0/381	0.55	0/505
60	Bk	0.54	0/351	0.67	0/454
61	Bl	0.61	0/796	0.61	0/1056
All	All	1.19	169/166471 (0.1%)	1.11	606/245817 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	An	0	1

The worst 5 of 169 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	BV	75	PRO	N-CA	13.70	1.70	1.47
14	An	125	PRO	N-CA	13.65	1.70	1.47
1	Aa	1463	G	N1-C2	-6.60	1.32	1.37
1	Aa	763	G	N1-C2	-6.49	1.32	1.37
1	Aa	1445	C	C4-C5	-6.41	1.37	1.43

The worst 5 of 606 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BB	31	C	N1-C2-O2	9.66	124.69	118.90
27	BA	2136	C	C2-N1-C1'	8.97	128.67	118.80
27	BA	2187	U	N3-C4-O4	8.57	125.40	119.40
1	Aa	1369	G	N1-C2-N2	-8.51	108.54	116.20
27	BA	1450	C	C2-N1-C1'	8.49	128.14	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	An	126	HIS	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ab	194/201 (96%)	181 (93%)	13 (7%)	0	100	100
3	Ac	193/209 (92%)	181 (94%)	12 (6%)	0	100	100
4	Ad	188/200 (94%)	172 (92%)	16 (8%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ae	172/180 (96%)	162 (94%)	10 (6%)	0	100	100
6	Af	239/243 (98%)	222 (93%)	17 (7%)	0	100	100
7	Ag	221/235 (94%)	207 (94%)	14 (6%)	0	100	100
8	Ah	121/125 (97%)	109 (90%)	12 (10%)	0	100	100
9	Ai	212/215 (99%)	200 (94%)	12 (6%)	0	100	100
10	Aj	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
11	Ak	123/130 (95%)	114 (93%)	9 (7%)	0	100	100
12	Al	131/135 (97%)	123 (94%)	8 (6%)	0	100	100
13	Am	98/102 (96%)	90 (92%)	8 (8%)	0	100	100
14	An	125/140 (89%)	120 (96%)	5 (4%)	0	100	100
15	Ao	141/147 (96%)	137 (97%)	4 (3%)	0	100	100
16	Ap	133/149 (89%)	114 (86%)	19 (14%)	0	100	100
17	Aq	147/151 (97%)	141 (96%)	6 (4%)	0	100	100
18	Ar	52/56 (93%)	47 (90%)	5 (10%)	0	100	100
19	As	106/114 (93%)	100 (94%)	6 (6%)	0	100	100
20	At	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
21	Au	114/133 (86%)	108 (95%)	6 (5%)	0	100	100
22	Av	147/150 (98%)	134 (91%)	13 (9%)	0	100	100
23	Aw	93/98 (95%)	89 (96%)	4 (4%)	0	100	100
24	Ax	59/65 (91%)	57 (97%)	2 (3%)	0	100	100
25	Ay	62/70 (89%)	55 (89%)	7 (11%)	0	100	100
26	Az	53/62 (86%)	47 (89%)	6 (11%)	0	100	100
29	BC	235/239 (98%)	209 (89%)	26 (11%)	0	100	100
30	BD	342/346 (99%)	311 (91%)	31 (9%)	0	100	100
31	BE	253/255 (99%)	232 (92%)	21 (8%)	0	100	100
32	BF	165/183 (90%)	136 (82%)	29 (18%)	0	100	100
33	BG	181/184 (98%)	168 (93%)	13 (7%)	0	100	100
34	BH	119/123 (97%)	111 (93%)	8 (7%)	0	100	100
34	BI	119/123 (97%)	106 (89%)	13 (11%)	0	100	100
35	BJ	164/182 (90%)	149 (91%)	15 (9%)	0	100	100
36	BK	140/142 (99%)	132 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BL	138/141 (98%)	128 (93%)	10 (7%)	0	100	100
38	BM	79/83 (95%)	72 (91%)	7 (9%)	0	100	100
38	BN	79/83 (95%)	69 (87%)	10 (13%)	0	100	100
39	BO	146/148 (99%)	129 (88%)	17 (12%)	0	100	100
40	BP	191/194 (98%)	178 (93%)	13 (7%)	0	100	100
41	BQ	158/201 (79%)	144 (91%)	14 (9%)	0	100	100
42	BR	118/121 (98%)	106 (90%)	12 (10%)	0	100	100
43	BS	144/150 (96%)	128 (89%)	16 (11%)	0	100	100
44	BT	72/77 (94%)	68 (94%)	4 (6%)	0	100	100
45	BU	94/98 (96%)	88 (94%)	6 (6%)	0	100	100
46	BV	152/156 (97%)	143 (94%)	9 (6%)	0	100	100
47	BW	83/86 (96%)	71 (86%)	12 (14%)	0	100	100
48	BX	118/121 (98%)	111 (94%)	7 (6%)	0	100	100
49	BY	60/67 (90%)	59 (98%)	1 (2%)	0	100	100
50	BZ	56/66 (85%)	54 (96%)	2 (4%)	0	100	100
51	Ba	152/155 (98%)	142 (93%)	10 (7%)	0	100	100
52	Bb	94/102 (92%)	86 (92%)	8 (8%)	0	100	100
53	Bc	87/90 (97%)	84 (97%)	3 (3%)	0	100	100
54	Bd	122/125 (98%)	113 (93%)	9 (7%)	0	100	100
55	Be	87/90 (97%)	77 (88%)	10 (12%)	0	100	100
56	Bg	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
57	Bh	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
58	Bi	48/51 (94%)	43 (90%)	5 (10%)	0	100	100
59	Bj	45/51 (88%)	39 (87%)	6 (13%)	0	100	100
60	Bk	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
61	Bl	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
All	All	7621/8020 (95%)	7028 (92%)	593 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 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	Ab	170/175 (97%)	170 (100%)	0	100	100
3	Ac	154/168 (92%)	154 (100%)	0	100	100
4	Ad	162/169 (96%)	162 (100%)	0	100	100
5	Ae	153/156 (98%)	153 (100%)	0	100	100
6	Af	210/212 (99%)	210 (100%)	0	100	100
7	Ag	185/197 (94%)	185 (100%)	0	100	100
8	Ah	104/105 (99%)	104 (100%)	0	100	100
9	Ai	183/184 (100%)	183 (100%)	0	100	100
10	Aj	106/107 (99%)	106 (100%)	0	100	100
11	Ak	101/105 (96%)	101 (100%)	0	100	100
12	Al	110/112 (98%)	110 (100%)	0	100	100
13	Am	89/91 (98%)	89 (100%)	0	100	100
14	An	94/108 (87%)	94 (100%)	0	100	100
15	Ao	117/120 (98%)	117 (100%)	0	100	100
16	Ap	111/123 (90%)	111 (100%)	0	100	100
17	Aq	129/131 (98%)	128 (99%)	1 (1%)	81	92
18	Ar	45/46 (98%)	45 (100%)	0	100	100
19	As	96/101 (95%)	96 (100%)	0	100	100
20	At	58/61 (95%)	58 (100%)	0	100	100
21	Au	104/117 (89%)	103 (99%)	1 (1%)	76	90
22	Av	125/126 (99%)	125 (100%)	0	100	100
23	Aw	85/88 (97%)	85 (100%)	0	100	100
24	Ax	53/56 (95%)	53 (100%)	0	100	100
25	Ay	53/59 (90%)	53 (100%)	0	100	100
26	Az	49/55 (89%)	49 (100%)	0	100	100
29	BC	185/187 (99%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BD	288/289 (100%)	288 (100%)	0	100	100
31	BE	212/212 (100%)	212 (100%)	0	100	100
32	BF	130/155 (84%)	128 (98%)	2 (2%)	65	85
33	BG	158/159 (99%)	157 (99%)	1 (1%)	86	94
34	BH	99/100 (99%)	98 (99%)	1 (1%)	76	90
34	BI	99/100 (99%)	99 (100%)	0	100	100
35	BJ	144/153 (94%)	144 (100%)	0	100	100
36	BK	120/120 (100%)	120 (100%)	0	100	100
37	BL	104/105 (99%)	104 (100%)	0	100	100
38	BM	63/65 (97%)	62 (98%)	1 (2%)	62	84
38	BN	63/65 (97%)	62 (98%)	1 (2%)	62	84
39	BO	116/116 (100%)	115 (99%)	1 (1%)	78	91
40	BP	161/162 (99%)	161 (100%)	0	100	100
41	BQ	138/167 (83%)	138 (100%)	0	100	100
42	BR	101/102 (99%)	100 (99%)	1 (1%)	76	90
43	BS	120/124 (97%)	120 (100%)	0	100	100
44	BT	69/72 (96%)	69 (100%)	0	100	100
45	BU	84/85 (99%)	84 (100%)	0	100	100
46	BV	129/131 (98%)	128 (99%)	1 (1%)	81	92
47	BW	75/76 (99%)	75 (100%)	0	100	100
48	BX	109/109 (100%)	109 (100%)	0	100	100
49	BY	54/58 (93%)	54 (100%)	0	100	100
50	BZ	57/61 (93%)	56 (98%)	1 (2%)	59	82
51	Ba	132/133 (99%)	132 (100%)	0	100	100
52	Bb	76/80 (95%)	76 (100%)	0	100	100
53	Bc	75/76 (99%)	75 (100%)	0	100	100
54	Bd	106/107 (99%)	106 (100%)	0	100	100
55	Be	80/80 (100%)	79 (99%)	1 (1%)	69	87
56	Bg	62/63 (98%)	61 (98%)	1 (2%)	62	84
57	Bh	50/51 (98%)	50 (100%)	0	100	100
58	Bi	45/46 (98%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	Bj	36/38 (95%)	36 (100%)	0	100	100
60	Bk	34/35 (97%)	34 (100%)	0	100	100
61	Bl	83/84 (99%)	82 (99%)	1 (1%)	71	88
All	All	6503/6738 (96%)	6488 (100%)	15 (0%)	93	98

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	BN	17	ARG
56	Bg	3	ARG
39	BO	9	ARG
61	Bl	80	ARG
50	BZ	27	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
38	BN	63	GLN
39	BO	25	HIS
53	Bc	16	ASN
43	BS	143	GLN
51	Ba	33	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	1428/1498 (95%)	274 (19%)	0
27	BA	2876/3037 (94%)	668 (23%)	46 (1%)
28	BB	124/126 (98%)	26 (20%)	2 (1%)
All	All	4428/4661 (95%)	968 (21%)	48 (1%)

5 of 968 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Aa	4	C
1	Aa	17	C
1	Aa	33	U
1	Aa	45	U
1	Aa	47	A

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	1928	C
27	BA	2268	G
27	BA	2053	U
27	BA	2173	G
27	BA	2482	A

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

229 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
27	OMG	BA	1106	27	18,26,27	2.11	7 (38%)	19,38,41	1.42	3 (15%)
1	OMC	Aa	825	1	19,22,23	2.62	7 (36%)	26,31,34	0.86	0
27	OMU	BA	34	27	19,22,23	2.62	7 (36%)	26,31,34	1.63	4 (15%)
27	4AC	BA	335	27	21,24,25	3.13	9 (42%)	29,34,37	1.14	3 (10%)
1	OMG	Aa	1026	1	18,26,27	2.25	7 (38%)	19,38,41	1.35	4 (21%)
27	B8T	BA	357	27	19,22,23	0.79	0	26,31,34	0.85	1 (3%)
27	4AC	BA	730	27	21,24,25	3.16	10 (47%)	29,34,37	1.37	5 (17%)
27	5MC	BA	2055	27	18,22,23	3.24	7 (38%)	26,32,35	1.11	1 (3%)
1	OMG	Aa	771	1	18,26,27	2.24	7 (38%)	19,38,41	1.37	4 (21%)
27	4AC	BA	27	27	21,24,25	3.17	10 (47%)	29,34,37	1.35	5 (17%)
27	OMC	BA	250	27	19,22,23	2.66	7 (36%)	26,31,34	1.42	5 (19%)
27	4AC	BA	3023	27	21,24,25	3.17	9 (42%)	29,34,37	1.33	7 (24%)
1	4AC	Aa	827	1	21,24,25	3.18	9 (42%)	29,34,37	1.24	4 (13%)
1	4AC	Aa	41	1	21,24,25	3.26	9 (42%)	29,34,37	1.68	5 (17%)
27	A2M	BA	488	27	18,25,26	4.06	8 (44%)	18,36,39	2.96	4 (22%)
1	4AC	Aa	5	1	21,24,25	3.13	10 (47%)	29,34,37	1.64	5 (17%)
27	OMC	BA	2545	27	19,22,23	2.58	7 (36%)	26,31,34	1.29	2 (7%)
1	4AC	Aa	1459	1	21,24,25	2.56	7 (33%)	29,34,37	1.66	8 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	OMG	BA	833	27	18,26,27	2.27	8 (44%)	19,38,41	1.71	4 (21%)
27	5MU	BA	2384	27	19,22,23	4.63	7 (36%)	28,32,35	3.73	12 (42%)
27	A2M	BA	872	27	18,25,26	4.15	9 (50%)	18,36,39	3.01	4 (22%)
27	4AC	BA	799	27	21,24,25	2.98	10 (47%)	29,34,37	1.33	3 (10%)
27	OMG	BA	2672	27	18,26,27	2.14	6 (33%)	19,38,41	1.74	4 (21%)
1	5MC	Aa	1352	1	18,22,23	3.42	7 (38%)	26,32,35	1.15	3 (11%)
27	OMC	BA	754	27	19,22,23	2.71	7 (36%)	26,31,34	0.99	0
1	OMG	Aa	636	1	18,26,27	2.31	7 (38%)	19,38,41	1.32	3 (15%)
1	4AC	Aa	136	1	21,24,25	3.33	9 (42%)	29,34,37	1.72	5 (17%)
1	OMC	Aa	1361	27,1	19,22,23	2.56	7 (36%)	26,31,34	0.82	0
27	4AC	BA	1641	27	21,24,25	3.13	9 (42%)	29,34,37	1.25	5 (17%)
27	5MC	BA	2075	27	18,22,23	2.86	7 (38%)	26,32,35	1.02	1 (3%)
27	OMC	BA	2630	27	19,22,23	2.48	7 (36%)	26,31,34	1.10	2 (7%)
1	OMG	Aa	994	1	18,26,27	2.43	8 (44%)	19,38,41	1.45	4 (21%)
27	5MU	BA	298	27	19,22,23	4.46	7 (36%)	28,32,35	3.72	10 (35%)
27	OMC	BA	561	27	19,22,23	2.59	7 (36%)	26,31,34	0.94	1 (3%)
27	5MC	BA	1696	27	18,22,23	3.02	7 (38%)	26,32,35	1.07	2 (7%)
1	4AC	Aa	458	1	21,24,25	1.02	1 (4%)	29,34,37	1.19	3 (10%)
27	OMG	BA	2168	27	18,26,27	2.19	7 (38%)	19,38,41	1.54	6 (31%)
27	OMU	BA	657	27	19,22,23	2.56	6 (31%)	26,31,34	1.65	6 (23%)
27	4AC	BA	1955	27	21,24,25	2.89	10 (47%)	29,34,37	1.16	4 (13%)
27	4AC	BA	376	27	21,24,25	3.01	9 (42%)	29,34,37	1.32	5 (17%)
27	OMG	BA	2152	27	18,26,27	2.01	5 (27%)	19,38,41	1.53	4 (21%)
27	4AC	BA	1434	27	21,24,25	2.91	10 (47%)	29,34,37	1.70	6 (20%)
27	OMG	BA	365	27	18,26,27	2.04	7 (38%)	19,38,41	1.44	3 (15%)
27	OMG	BA	1892	27	18,26,27	2.12	7 (38%)	19,38,41	1.37	3 (15%)
27	5MC	BA	1965	27	18,22,23	2.86	7 (38%)	26,32,35	1.15	2 (7%)
27	OMU	BA	1776	27	19,22,23	2.71	7 (36%)	26,31,34	1.79	6 (23%)
27	5MU	BA	572	27	19,22,23	4.45	7 (36%)	28,32,35	3.73	12 (42%)
27	OMC	BA	718	27	19,22,23	2.65	7 (36%)	26,31,34	1.30	4 (15%)
1	LV2	Aa	918	1	20,23,24	0.94	0	26,33,36	0.81	0
1	5MC	Aa	1478	1	18,22,23	3.03	7 (38%)	26,32,35	1.48	6 (23%)
1	4AC	Aa	298	1	21,24,25	3.17	9 (42%)	29,34,37	1.61	5 (17%)
27	OMU	BA	1551	27	19,22,23	2.93	7 (36%)	26,31,34	1.77	5 (19%)
27	OMU	BA	2389	27	19,22,23	1.29	3 (15%)	26,31,34	1.84	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LHH	BA	2955	27	22,25,26	2.39	5 (22%)	29,35,38	2.00	6 (20%)
27	A2M	BA	2702	27	18,25,26	4.02	9 (50%)	18,36,39	2.59	4 (22%)
27	5MU	BA	2688	27	19,22,23	4.44	7 (36%)	28,32,35	3.70	11 (39%)
1	OMG	Aa	246	1	18,26,27	2.14	7 (38%)	19,38,41	1.36	3 (15%)
1	OMU	Aa	52	1	19,22,23	2.82	7 (36%)	26,31,34	1.62	4 (15%)
27	A2M	BA	756	27	18,25,26	4.21	8 (44%)	18,36,39	2.86	4 (22%)
1	OMU	Aa	240	1	19,22,23	2.88	7 (36%)	26,31,34	1.76	4 (15%)
1	6MZ	Aa	1449	1	18,25,26	0.77	0	16,36,39	1.94	3 (18%)
27	4AC	BA	925	27	21,24,25	1.06	1 (4%)	29,34,37	1.55	6 (20%)
1	4AC	Aa	569	1	21,24,25	3.15	9 (42%)	29,34,37	1.40	5 (17%)
27	5MU	BA	537	27	19,22,23	4.44	7 (36%)	28,32,35	3.88	10 (35%)
1	4AC	Aa	525	1	21,24,25	3.00	10 (47%)	29,34,37	1.88	6 (20%)
1	4AC	Aa	847	1	21,24,25	3.09	10 (47%)	29,34,37	1.19	3 (10%)
27	5MC	BA	944	27	18,22,23	2.92	7 (38%)	26,32,35	1.31	3 (11%)
27	OMU	BA	2542	27	19,22,23	2.70	7 (36%)	26,31,34	1.75	5 (19%)
1	4AC	Aa	682	1	21,24,25	3.23	9 (42%)	29,34,37	1.47	5 (17%)
27	OMG	BA	763	27	18,26,27	2.15	7 (38%)	19,38,41	1.47	4 (21%)
1	OMG	Aa	1434	1	18,26,27	2.16	7 (38%)	19,38,41	1.47	3 (15%)
27	OMG	BA	290	27	18,26,27	2.21	8 (44%)	19,38,41	1.64	4 (21%)
27	LHH	BA	526	27	22,25,26	2.41	5 (22%)	29,35,38	1.77	7 (24%)
27	A2M	BA	1400	27	18,25,26	4.07	10 (55%)	18,36,39	2.89	4 (22%)
27	OMC	BA	1750	27	19,22,23	2.54	7 (36%)	26,31,34	1.22	5 (19%)
27	OMU	BA	2610	27	19,22,23	3.04	8 (42%)	26,31,34	1.83	4 (15%)
1	5MC	Aa	1276	1	18,22,23	4.83	16 (88%)	26,32,35	1.16	2 (7%)
27	OMG	BA	64	27	18,26,27	2.01	6 (33%)	19,38,41	1.37	3 (15%)
27	OMG	BA	2745	27	18,26,27	2.16	6 (33%)	19,38,41	1.75	4 (21%)
27	OMU	BA	619	27	19,22,23	2.81	7 (36%)	26,31,34	1.79	6 (23%)
1	LHH	Aa	1020	1	22,25,26	2.56	5 (22%)	29,35,38	1.85	8 (27%)
27	OMC	BA	869	27	19,22,23	2.60	7 (36%)	26,31,34	1.06	2 (7%)
1	5MC	Aa	464	1	18,22,23	3.34	7 (38%)	26,32,35	1.22	2 (7%)
1	OMG	Aa	876	1	18,26,27	2.30	8 (44%)	19,38,41	1.37	4 (21%)
27	OMG	BA	215	27	18,26,27	2.27	7 (38%)	19,38,41	1.91	4 (21%)
1	4AC	Aa	730	1	21,24,25	3.06	10 (47%)	29,34,37	1.68	5 (17%)
27	LHH	BA	617	27	22,25,26	2.53	5 (22%)	29,35,38	1.66	6 (20%)
27	4AC	BA	1357	27	21,24,25	3.02	10 (47%)	29,34,37	1.38	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	4AC	BA	805	27	21,24,25	2.86	10 (47%)	29,34,37	1.40	7 (24%)
1	5MU	Aa	917	1	19,22,23	1.39	4 (21%)	28,32,35	2.22	6 (21%)
27	OMG	BA	2728	27	18,26,27	2.20	6 (33%)	19,38,41	1.58	4 (21%)
1	5MC	Aa	672	1	18,22,23	3.12	7 (38%)	26,32,35	1.20	2 (7%)
1	OMG	Aa	450	1	18,26,27	2.16	7 (38%)	19,38,41	1.30	3 (15%)
27	4AC	BA	418	27	21,24,25	3.20	10 (47%)	29,34,37	1.17	4 (13%)
27	4AC	BA	2780	27	21,24,25	3.13	9 (42%)	29,34,37	1.67	7 (24%)
1	B8T	Aa	1051	1	19,22,23	0.80	0	26,31,34	0.89	1 (3%)
1	MA6	Aa	1468	1	19,26,27	1.34	1 (5%)	18,38,41	3.39	2 (11%)
27	OMG	BA	2019	27	18,26,27	2.41	8 (44%)	19,38,41	1.70	4 (21%)
1	MA6	Aa	1467	1	19,26,27	1.42	3 (15%)	18,38,41	3.19	2 (11%)
1	OMG	Aa	1265	1	18,26,27	2.27	8 (44%)	19,38,41	1.42	3 (15%)
1	5MC	Aa	1004	1	18,22,23	3.24	7 (38%)	26,32,35	1.14	2 (7%)
1	OMG	Aa	138	1	18,26,27	2.27	7 (38%)	19,38,41	1.40	3 (15%)
27	LHH	BA	2457	27	22,25,26	2.52	5 (22%)	29,35,38	2.16	7 (24%)
27	OMG	BA	1398	27	18,26,27	2.09	5 (27%)	19,38,41	1.37	3 (15%)
1	OMG	Aa	498	1	18,26,27	2.23	7 (38%)	19,38,41	1.37	3 (15%)
27	4AC	BA	713	27	21,24,25	3.04	9 (42%)	29,34,37	1.17	2 (6%)
27	4SU	BA	2553	27	18,21,22	3.87	8 (44%)	26,30,33	1.94	5 (19%)
27	4SU	BA	2581	27	18,21,22	4.00	8 (44%)	26,30,33	2.26	5 (19%)
27	OMG	BA	2324	27	18,26,27	2.19	7 (38%)	19,38,41	1.43	3 (15%)
27	4AC	BA	2797	27	21,24,25	2.96	10 (47%)	29,34,37	1.17	3 (10%)
1	OMC	Aa	296	1	19,22,23	2.62	7 (36%)	26,31,34	0.96	1 (3%)
1	OMG	Aa	320	1	18,26,27	2.25	7 (38%)	19,38,41	1.42	3 (15%)
27	4AC	BA	433	27	21,24,25	3.00	9 (42%)	29,34,37	1.23	3 (10%)
1	4AC	Aa	1217	1	21,24,25	3.44	9 (42%)	29,34,37	1.59	6 (20%)
27	OMC	BA	2595	27	19,22,23	2.57	7 (36%)	26,31,34	1.27	3 (11%)
1	A2M	Aa	352	1	18,25,26	0.94	1 (5%)	18,36,39	1.29	2 (11%)
27	4AC	BA	244	27	21,24,25	2.99	10 (47%)	29,34,37	1.21	4 (13%)
27	OMG	BA	2550	27	18,26,27	2.09	6 (33%)	19,38,41	2.06	6 (31%)
1	2MG	Aa	670	1	18,26,27	2.27	7 (38%)	16,38,41	1.24	2 (12%)
27	OMG	BA	2353	27	18,26,27	2.06	6 (33%)	19,38,41	1.46	4 (21%)
27	OMG	BA	2527	27	18,26,27	2.10	6 (33%)	19,38,41	1.38	3 (15%)
27	4AC	BA	1899	27	21,24,25	2.96	10 (47%)	29,34,37	1.26	4 (13%)
27	4AC	BA	2838	27	21,24,25	3.16	9 (42%)	29,34,37	1.30	4 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	5MC	BA	2863	27	18,22,23	3.13	7 (38%)	26,32,35	1.23	4 (15%)
27	OMG	BA	912	27	18,26,27	2.21	7 (38%)	19,38,41	2.02	4 (21%)
27	4AC	BA	124	27	21,24,25	2.91	10 (47%)	29,34,37	1.21	3 (10%)
27	OMG	BA	552	27	18,26,27	2.18	7 (38%)	19,38,41	1.56	5 (26%)
27	4AC	BA	56	27	21,24,25	3.10	9 (42%)	29,34,37	1.35	5 (17%)
1	OMG	Aa	892	1	18,26,27	2.18	7 (38%)	19,38,41	1.35	3 (15%)
1	5MC	Aa	457	1	18,22,23	4.90	15 (83%)	26,32,35	1.12	1 (3%)
27	OMC	BA	2124	27	19,22,23	2.58	7 (36%)	26,31,34	1.08	3 (11%)
1	OMU	Aa	479	1	19,22,23	2.97	8 (42%)	26,31,34	1.69	5 (19%)
1	OMG	Aa	532	1	18,26,27	2.14	7 (38%)	19,38,41	1.37	3 (15%)
27	A2M	BA	1517	27	18,25,26	3.93	7 (38%)	18,36,39	2.89	3 (16%)
1	4AC	Aa	358	1	21,24,25	3.25	9 (42%)	29,34,37	1.60	5 (17%)
27	4AC	BA	2992	27	21,24,25	3.32	10 (47%)	29,34,37	1.39	5 (17%)
1	B8T	Aa	1141	1	19,22,23	0.81	0	26,31,34	0.76	0
27	OMC	BA	2047	27	19,22,23	2.56	7 (36%)	26,31,34	1.06	1 (3%)
1	4AC	Aa	818	1	21,24,25	3.11	10 (47%)	29,34,37	1.57	5 (17%)
1	OMG	Aa	1025	1	18,26,27	2.17	7 (38%)	19,38,41	1.41	3 (15%)
27	4AC	BA	1543	27	21,24,25	3.12	9 (42%)	29,34,37	1.21	4 (13%)
27	5MU	BA	1548	27	19,22,23	4.67	7 (36%)	28,32,35	3.64	10 (35%)
27	OMU	BA	453	27	19,22,23	2.72	7 (36%)	26,31,34	1.82	5 (19%)
27	4AC	BA	858	27	21,24,25	2.97	10 (47%)	29,34,37	1.65	2 (6%)
27	OMG	BA	1953	27	18,26,27	2.21	7 (38%)	19,38,41	1.73	4 (21%)
27	OMC	BA	1820	27	19,22,23	2.58	7 (36%)	26,31,34	1.29	5 (19%)
27	5MU	BA	1085	27	19,22,23	4.18	7 (36%)	28,32,35	4.37	11 (39%)
1	4AC	Aa	373	1	21,24,25	3.15	9 (42%)	29,34,37	1.45	6 (20%)
1	OMG	Aa	1107	1	18,26,27	2.30	8 (44%)	19,38,41	1.43	4 (21%)
27	OMG	BA	674	27	18,26,27	1.85	6 (33%)	19,38,41	1.69	7 (36%)
27	4AC	BA	2159	27	21,24,25	2.98	10 (47%)	29,34,37	1.32	5 (17%)
27	OMC	BA	2571	27	19,22,23	2.66	7 (36%)	26,31,34	1.28	4 (15%)
1	B8T	Aa	1262	1	19,22,23	0.78	0	26,31,34	0.93	1 (3%)
27	OMU	BA	2656	27	19,22,23	2.65	7 (36%)	26,31,34	1.67	4 (15%)
1	OMU	Aa	304	1	19,22,23	2.87	7 (36%)	26,31,34	1.71	4 (15%)
1	OMG	Aa	852	1	18,26,27	2.09	5 (27%)	19,38,41	1.32	3 (15%)
27	OMG	BA	800	27	18,26,27	1.97	6 (33%)	19,38,41	1.25	4 (21%)
27	4AC	BA	1810	27	21,24,25	3.05	10 (47%)	29,34,37	1.44	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	A2M	BA	849	27	18,25,26	4.04	8 (44%)	18,36,39	3.29	6 (33%)
27	A2M	BA	879	27	18,25,26	4.12	7 (38%)	18,36,39	2.95	4 (22%)
27	A2M	BA	1265	27	18,25,26	4.19	6 (33%)	18,36,39	3.27	4 (22%)
27	OMU	BA	1340	27	19,22,23	2.65	7 (36%)	26,31,34	1.71	5 (19%)
27	OMG	BA	1525	27	18,26,27	2.23	7 (38%)	19,38,41	1.64	4 (21%)
27	4AC	BA	1305	27	21,24,25	3.31	10 (47%)	29,34,37	1.55	6 (20%)
1	LHH	Aa	229	1	22,25,26	2.50	5 (22%)	29,35,38	1.70	6 (20%)
1	OMU	Aa	1358	1	19,22,23	2.52	7 (36%)	26,31,34	2.31	8 (30%)
27	4AC	BA	1337	27	21,24,25	3.01	10 (47%)	29,34,37	1.18	3 (10%)
27	4AC	BA	1470	27	21,24,25	3.05	9 (42%)	29,34,37	1.55	6 (20%)
27	5MU	BA	875	27	19,22,23	4.58	7 (36%)	28,32,35	3.71	11 (39%)
1	OMG	Aa	1275	1	18,26,27	1.04	1 (5%)	19,38,41	1.08	2 (10%)
1	4AC	Aa	1007	1	21,24,25	1.07	1 (4%)	29,34,37	1.16	4 (13%)
1	4AC	Aa	697	1	21,24,25	3.24	9 (42%)	29,34,37	1.64	6 (20%)
27	OMG	BA	723	27	18,26,27	2.18	8 (44%)	19,38,41	1.82	4 (21%)
27	OMG	BA	2016	27	18,26,27	2.23	6 (33%)	19,38,41	1.59	4 (21%)
27	OMU	BA	1319	27	19,22,23	2.75	7 (36%)	26,31,34	1.70	5 (19%)
1	OMC	Aa	1354	1	19,22,23	2.75	7 (36%)	26,31,34	1.03	2 (7%)
27	OMG	BA	419	27	18,26,27	2.17	5 (27%)	19,38,41	3.64	6 (31%)
27	OMG	BA	2568	27	18,26,27	1.01	1 (5%)	19,38,41	1.06	2 (10%)
27	4AC	BA	1431	27	21,24,25	3.15	10 (47%)	29,34,37	1.41	6 (20%)
1	OMC	Aa	190	1	19,22,23	2.74	7 (36%)	26,31,34	0.89	0
27	A2M	BA	825	27	18,25,26	4.12	9 (50%)	18,36,39	2.85	3 (16%)
27	OMG	BA	2379	27	18,26,27	2.14	5 (27%)	19,38,41	1.82	4 (21%)
1	5MC	Aa	854	1	18,22,23	2.93	7 (38%)	26,32,35	1.46	5 (19%)
27	4AC	BA	201	27	21,24,25	2.89	10 (47%)	29,34,37	1.65	6 (20%)
27	A2M	BA	932	27	18,25,26	4.18	8 (44%)	18,36,39	2.67	4 (22%)
1	5MC	Aa	1476	1	18,22,23	4.81	15 (83%)	26,32,35	1.20	2 (7%)
27	A2M	BA	212	27	18,25,26	0.89	1 (5%)	18,36,39	1.44	3 (16%)
27	4AC	BA	1396	27	21,24,25	3.07	10 (47%)	29,34,37	1.45	6 (20%)
27	OMG	BA	1940	27	18,26,27	2.05	6 (33%)	19,38,41	1.26	3 (15%)
27	OMC	BA	2018	27	19,22,23	2.36	7 (36%)	26,31,34	1.07	3 (11%)
27	OMG	BA	1799	27	18,26,27	2.33	8 (44%)	19,38,41	1.64	5 (26%)
27	5MC	BA	2035	27	18,22,23	4.78	15 (83%)	26,32,35	1.19	2 (7%)
27	4AC	BA	2997	27	21,24,25	3.17	9 (42%)	29,34,37	1.22	3 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	Aa	8	1	19,22,23	2.73	7 (36%)	26,31,34	1.85	8 (30%)
27	OMG	BA	2528	27	18,26,27	2.31	6 (33%)	19,38,41	1.97	5 (26%)
1	OMC	Aa	535	1	19,22,23	2.71	7 (36%)	26,31,34	0.93	0
27	OMG	BA	2657	27	18,26,27	2.18	7 (38%)	19,38,41	1.49	3 (15%)
1	OMG	Aa	659	1	18,26,27	2.19	8 (44%)	19,38,41	1.35	4 (21%)
27	OMG	BA	353	27	18,26,27	2.44	8 (44%)	19,38,41	1.90	5 (26%)
27	4AC	BA	778	27	21,24,25	3.14	10 (47%)	29,34,37	1.04	2 (6%)
1	5MC	Aa	942	1	18,22,23	3.37	7 (38%)	26,32,35	1.04	2 (7%)
27	OMG	BA	575	27	18,26,27	2.15	7 (38%)	19,38,41	1.42	4 (21%)
27	4AC	BA	1375	27	21,24,25	3.10	10 (47%)	29,34,37	1.32	4 (13%)
1	OMG	Aa	913	1	18,26,27	2.40	8 (44%)	19,38,41	2.05	6 (31%)
27	OMG	BA	2010	27	18,26,27	2.13	6 (33%)	19,38,41	1.40	3 (15%)
27	OMC	BA	1790	27	19,22,23	2.51	7 (36%)	26,31,34	1.12	1 (3%)
27	OMG	BA	1558	27	18,26,27	2.13	7 (38%)	19,38,41	1.54	6 (31%)
27	4AC	BA	3009	27	21,24,25	3.09	10 (47%)	29,34,37	1.22	3 (10%)
27	5MC	BA	2070	27	18,22,23	0.95	2 (11%)	26,32,35	1.20	3 (11%)
1	OMG	Aa	446	1	18,26,27	2.20	7 (38%)	19,38,41	1.40	4 (21%)
1	OMC	Aa	752	1	19,22,23	2.69	7 (36%)	26,31,34	0.98	1 (3%)
27	OMG	BA	63	27	18,26,27	2.13	5 (27%)	19,38,41	1.74	5 (26%)
27	4AC	BA	501	27	21,24,25	3.05	9 (42%)	29,34,37	1.32	3 (10%)
1	OMG	Aa	382	1	18,26,27	2.18	7 (38%)	19,38,41	1.44	3 (15%)
27	4AC	BA	2590	27	21,24,25	3.04	10 (47%)	29,34,37	1.20	5 (17%)
27	5MU	BA	1905	27	19,22,23	4.46	7 (36%)	28,32,35	3.81	11 (39%)
27	4AC	BA	2832	27	21,24,25	3.03	10 (47%)	29,34,37	1.29	4 (13%)
27	OMU	BA	1969	27	19,22,23	2.75	7 (36%)	26,31,34	1.73	5 (19%)
1	OMG	Aa	381	1	18,26,27	2.22	8 (44%)	19,38,41	1.44	4 (21%)
27	OMU	BA	768	27	19,22,23	2.74	7 (36%)	26,31,34	1.74	4 (15%)
27	OMG	BA	2521	27	18,26,27	2.18	7 (38%)	19,38,41	1.55	3 (15%)
1	4AC	Aa	501	1	21,24,25	3.24	9 (42%)	29,34,37	1.51	5 (17%)
27	OMU	BA	1480	27	19,22,23	2.72	7 (36%)	26,31,34	1.59	4 (15%)
27	4AC	BA	1934	27	21,24,25	2.98	9 (42%)	29,34,37	1.31	4 (13%)
27	4AC	BA	1427	27	21,24,25	2.99	9 (42%)	29,34,37	1.27	4 (13%)
27	A2M	BA	505	27	18,25,26	4.08	8 (44%)	18,36,39	3.44	6 (33%)
27	5MC	BA	2605	27	18,22,23	3.26	7 (38%)	26,32,35	0.90	1 (3%)
27	4AC	BA	2121	27	21,24,25	2.90	10 (47%)	29,34,37	1.33	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4AC	Aa	605	1	21,24,25	3.30	9 (42%)	29,34,37	1.91	7 (24%)

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
27	OMG	BA	1106	27	-	0/5/27/28	0/3/3/3
1	OMC	Aa	825	1	-	0/9/27/28	0/2/2/2
27	OMU	BA	34	27	-	1/9/27/28	0/2/2/2
27	4AC	BA	335	27	-	0/11/29/30	0/2/2/2
1	OMG	Aa	1026	1	-	1/5/27/28	0/3/3/3
27	B8T	BA	357	27	-	0/7/27/28	0/2/2/2
27	4AC	BA	730	27	-	0/11/29/30	0/2/2/2
27	5MC	BA	2055	27	-	2/7/25/26	0/2/2/2
1	OMG	Aa	771	1	-	0/5/27/28	0/3/3/3
27	4AC	BA	27	27	-	2/11/29/30	0/2/2/2
27	OMC	BA	250	27	-	0/9/27/28	0/2/2/2
27	4AC	BA	3023	27	-	2/11/29/30	0/2/2/2
1	4AC	Aa	827	1	-	0/11/29/30	0/2/2/2
1	4AC	Aa	41	1	-	2/11/29/30	0/2/2/2
27	A2M	BA	488	27	-	3/5/27/28	0/3/3/3
1	4AC	Aa	5	1	-	4/11/29/30	0/2/2/2
27	OMC	BA	2545	27	-	1/9/27/28	0/2/2/2
1	4AC	Aa	1459	1	-	0/11/29/30	0/2/2/2
27	OMG	BA	833	27	-	0/5/27/28	0/3/3/3
27	5MU	BA	2384	27	-	0/7/25/26	0/2/2/2
27	A2M	BA	872	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	799	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	2672	27	-	0/5/27/28	0/3/3/3
1	5MC	Aa	1352	1	-	2/7/25/26	0/2/2/2
27	OMC	BA	754	27	-	2/9/27/28	0/2/2/2
1	OMG	Aa	636	1	-	2/5/27/28	0/3/3/3
1	4AC	Aa	136	1	-	2/11/29/30	0/2/2/2
1	OMC	Aa	1361	27,1	-	0/9/27/28	0/2/2/2
27	4AC	BA	1641	27	-	2/11/29/30	0/2/2/2
27	5MC	BA	2075	27	-	0/7/25/26	0/2/2/2
27	OMC	BA	2630	27	-	0/9/27/28	0/2/2/2
1	OMG	Aa	994	1	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	5MU	BA	298	27	-	0/7/25/26	0/2/2/2
27	OMC	BA	561	27	-	0/9/27/28	0/2/2/2
27	5MC	BA	1696	27	-	0/7/25/26	0/2/2/2
1	4AC	Aa	458	1	-	6/11/29/30	0/2/2/2
27	OMG	BA	2168	27	-	0/5/27/28	0/3/3/3
27	OMU	BA	657	27	-	1/9/27/28	0/2/2/2
27	4AC	BA	1955	27	-	2/11/29/30	0/2/2/2
27	4AC	BA	376	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	2152	27	-	2/5/27/28	0/3/3/3
27	4AC	BA	1434	27	-	2/11/29/30	0/2/2/2
27	OMG	BA	365	27	-	1/5/27/28	0/3/3/3
27	OMG	BA	1892	27	-	1/5/27/28	0/3/3/3
27	5MC	BA	1965	27	-	0/7/25/26	0/2/2/2
27	OMU	BA	1776	27	-	0/9/27/28	0/2/2/2
27	5MU	BA	572	27	-	0/7/25/26	0/2/2/2
27	OMC	BA	718	27	-	0/9/27/28	0/2/2/2
1	LV2	Aa	918	1	-	0/9/29/30	0/2/2/2
1	5MC	Aa	1478	1	-	3/7/25/26	0/2/2/2
1	4AC	Aa	298	1	-	0/11/29/30	0/2/2/2
27	OMU	BA	1551	27	-	3/9/27/28	0/2/2/2
27	OMU	BA	2389	27	-	2/9/27/28	0/2/2/2
27	LHH	BA	2955	27	-	3/13/31/32	0/2/2/2
27	A2M	BA	2702	27	-	1/5/27/28	0/3/3/3
27	5MU	BA	2688	27	-	0/7/25/26	0/2/2/2
1	OMG	Aa	246	1	-	0/5/27/28	0/3/3/3
1	OMU	Aa	52	1	-	2/9/27/28	0/2/2/2
27	A2M	BA	756	27	-	0/5/27/28	0/3/3/3
1	OMU	Aa	240	1	-	0/9/27/28	0/2/2/2
1	6MZ	Aa	1449	1	-	0/5/27/28	0/3/3/3
27	4AC	BA	925	27	-	2/11/29/30	0/2/2/2
1	4AC	Aa	569	1	-	0/11/29/30	0/2/2/2
27	5MU	BA	537	27	-	0/7/25/26	0/2/2/2
1	4AC	Aa	525	1	-	5/11/29/30	0/2/2/2
1	4AC	Aa	847	1	-	0/11/29/30	0/2/2/2
27	5MC	BA	944	27	-	0/7/25/26	0/2/2/2
27	OMU	BA	2542	27	-	0/9/27/28	0/2/2/2
1	4AC	Aa	682	1	-	0/11/29/30	0/2/2/2
27	OMG	BA	763	27	-	0/5/27/28	0/3/3/3
1	OMG	Aa	1434	1	-	1/5/27/28	0/3/3/3
27	OMG	BA	290	27	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHH	BA	526	27	-	1/13/31/32	0/2/2/2
27	A2M	BA	1400	27	-	1/5/27/28	0/3/3/3
27	OMC	BA	1750	27	-	0/9/27/28	0/2/2/2
27	OMU	BA	2610	27	-	3/9/27/28	0/2/2/2
1	5MC	Aa	1276	1	-	2/7/25/26	0/2/2/2
27	OMG	BA	64	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	2745	27	-	0/5/27/28	0/3/3/3
27	OMU	BA	619	27	-	1/9/27/28	0/2/2/2
1	LHH	Aa	1020	1	-	4/13/31/32	0/2/2/2
27	OMC	BA	869	27	-	2/9/27/28	0/2/2/2
1	5MC	Aa	464	1	-	0/7/25/26	0/2/2/2
1	OMG	Aa	876	1	-	2/5/27/28	0/3/3/3
27	OMG	BA	215	27	-	2/5/27/28	0/3/3/3
1	4AC	Aa	730	1	-	2/11/29/30	0/2/2/2
27	LHH	BA	617	27	-	5/13/31/32	0/2/2/2
27	4AC	BA	1357	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	805	27	-	0/11/29/30	0/2/2/2
1	5MU	Aa	917	1	-	2/7/25/26	0/2/2/2
27	OMG	BA	2728	27	-	0/5/27/28	0/3/3/3
1	5MC	Aa	672	1	-	0/7/25/26	0/2/2/2
1	OMG	Aa	450	1	-	0/5/27/28	0/3/3/3
27	4AC	BA	418	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	2780	27	-	0/11/29/30	0/2/2/2
1	B8T	Aa	1051	1	-	0/7/27/28	0/2/2/2
1	MA6	Aa	1468	1	-	2/7/29/30	0/3/3/3
27	OMG	BA	2019	27	-	2/5/27/28	0/3/3/3
1	MA6	Aa	1467	1	-	0/7/29/30	0/3/3/3
1	OMG	Aa	1265	1	-	0/5/27/28	0/3/3/3
1	5MC	Aa	1004	1	-	2/7/25/26	0/2/2/2
1	OMG	Aa	138	1	-	0/5/27/28	0/3/3/3
27	LHH	BA	2457	27	-	4/13/31/32	0/2/2/2
27	OMG	BA	1398	27	-	0/5/27/28	0/3/3/3
1	OMG	Aa	498	1	-	0/5/27/28	0/3/3/3
27	4AC	BA	713	27	-	0/11/29/30	0/2/2/2
27	4SU	BA	2553	27	-	0/7/25/26	0/2/2/2
27	4SU	BA	2581	27	-	2/7/25/26	0/2/2/2
27	OMG	BA	2324	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	2797	27	-	0/11/29/30	0/2/2/2
1	OMC	Aa	296	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	Aa	320	1	-	0/5/27/28	0/3/3/3
27	4AC	BA	433	27	-	0/11/29/30	0/2/2/2
1	4AC	Aa	1217	1	-	4/11/29/30	0/2/2/2
27	OMC	BA	2595	27	-	2/9/27/28	0/2/2/2
1	A2M	Aa	352	1	-	1/5/27/28	0/3/3/3
27	4AC	BA	244	27	-	1/11/29/30	0/2/2/2
27	OMG	BA	2550	27	-	2/5/27/28	0/3/3/3
1	2MG	Aa	670	1	-	0/5/27/28	0/3/3/3
27	OMG	BA	2353	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	2527	27	-	2/5/27/28	0/3/3/3
27	4AC	BA	1899	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	2838	27	-	2/11/29/30	0/2/2/2
27	5MC	BA	2863	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	912	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	124	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	552	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	56	27	-	0/11/29/30	0/2/2/2
1	OMG	Aa	892	1	-	3/5/27/28	0/3/3/3
1	5MC	Aa	457	1	-	2/7/25/26	0/2/2/2
27	OMC	BA	2124	27	-	0/9/27/28	0/2/2/2
1	OMU	Aa	479	1	-	1/9/27/28	0/2/2/2
1	OMG	Aa	532	1	-	2/5/27/28	0/3/3/3
27	A2M	BA	1517	27	-	1/5/27/28	0/3/3/3
1	4AC	Aa	358	1	-	2/11/29/30	0/2/2/2
27	4AC	BA	2992	27	-	3/11/29/30	0/2/2/2
1	B8T	Aa	1141	1	-	0/7/27/28	0/2/2/2
27	OMC	BA	2047	27	-	0/9/27/28	0/2/2/2
1	4AC	Aa	818	1	-	2/11/29/30	0/2/2/2
1	OMG	Aa	1025	1	-	1/5/27/28	0/3/3/3
27	4AC	BA	1543	27	-	3/11/29/30	0/2/2/2
27	5MU	BA	1548	27	-	2/7/25/26	0/2/2/2
27	OMU	BA	453	27	-	2/9/27/28	0/2/2/2
27	4AC	BA	858	27	-	2/11/29/30	0/2/2/2
27	OMG	BA	1953	27	-	2/5/27/28	0/3/3/3
27	OMC	BA	1820	27	-	0/9/27/28	0/2/2/2
27	5MU	BA	1085	27	-	0/7/25/26	0/2/2/2
1	4AC	Aa	373	1	-	0/11/29/30	0/2/2/2
1	OMG	Aa	1107	1	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMG	BA	674	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	2159	27	-	0/11/29/30	0/2/2/2
27	OMC	BA	2571	27	-	2/9/27/28	0/2/2/2
1	B8T	Aa	1262	1	-	0/7/27/28	0/2/2/2
27	OMU	BA	2656	27	-	0/9/27/28	0/2/2/2
1	OMU	Aa	304	1	-	1/9/27/28	0/2/2/2
1	OMG	Aa	852	1	-	0/5/27/28	0/3/3/3
27	OMG	BA	800	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	1810	27	-	2/11/29/30	0/2/2/2
27	A2M	BA	849	27	-	2/5/27/28	0/3/3/3
27	A2M	BA	879	27	-	0/5/27/28	0/3/3/3
27	A2M	BA	1265	27	-	2/5/27/28	0/3/3/3
27	OMU	BA	1340	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	1525	27	-	2/5/27/28	0/3/3/3
27	4AC	BA	1305	27	-	2/11/29/30	0/2/2/2
1	LHH	Aa	229	1	-	3/13/31/32	0/2/2/2
1	OMU	Aa	1358	1	-	3/9/27/28	0/2/2/2
27	4AC	BA	1337	27	-	2/11/29/30	0/2/2/2
27	4AC	BA	1470	27	-	0/11/29/30	0/2/2/2
27	5MU	BA	875	27	-	2/7/25/26	0/2/2/2
1	OMG	Aa	1275	1	-	1/5/27/28	0/3/3/3
1	4AC	Aa	1007	1	-	2/11/29/30	0/2/2/2
1	4AC	Aa	697	1	-	4/11/29/30	0/2/2/2
27	OMG	BA	723	27	-	1/5/27/28	0/3/3/3
27	OMG	BA	2016	27	-	0/5/27/28	0/3/3/3
27	OMU	BA	1319	27	-	0/9/27/28	0/2/2/2
1	OMC	Aa	1354	1	-	2/9/27/28	0/2/2/2
27	OMG	BA	419	27	-	2/5/27/28	0/3/3/3
27	OMG	BA	2568	27	-	3/5/27/28	0/3/3/3
27	4AC	BA	1431	27	-	0/11/29/30	0/2/2/2
1	OMC	Aa	190	1	-	2/9/27/28	0/2/2/2
27	A2M	BA	825	27	-	0/5/27/28	0/3/3/3
27	OMG	BA	2379	27	-	3/5/27/28	0/3/3/3
1	5MC	Aa	854	1	-	1/7/25/26	0/2/2/2
27	4AC	BA	201	27	-	2/11/29/30	0/2/2/2
27	A2M	BA	932	27	-	0/5/27/28	0/3/3/3
1	5MC	Aa	1476	1	-	0/7/25/26	0/2/2/2
27	A2M	BA	212	27	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	BA	1396	27	-	2/11/29/30	0/2/2/2
27	OMG	BA	1940	27	-	2/5/27/28	0/3/3/3
27	OMC	BA	2018	27	-	2/9/27/28	0/2/2/2
27	OMG	BA	1799	27	-	3/5/27/28	0/3/3/3
27	5MC	BA	2035	27	-	0/7/25/26	0/2/2/2
27	4AC	BA	2997	27	-	0/11/29/30	0/2/2/2
1	OMU	Aa	8	1	-	3/9/27/28	0/2/2/2
27	OMG	BA	2528	27	-	0/5/27/28	0/3/3/3
1	OMC	Aa	535	1	-	0/9/27/28	0/2/2/2
27	OMG	BA	2657	27	-	0/5/27/28	0/3/3/3
1	OMG	Aa	659	1	-	0/5/27/28	0/3/3/3
27	OMG	BA	353	27	-	2/5/27/28	0/3/3/3
27	4AC	BA	778	27	-	0/11/29/30	0/2/2/2
1	5MC	Aa	942	1	-	0/7/25/26	0/2/2/2
27	OMG	BA	575	27	-	2/5/27/28	0/3/3/3
27	4AC	BA	1375	27	-	2/11/29/30	0/2/2/2
1	OMG	Aa	913	1	-	2/5/27/28	0/3/3/3
27	OMG	BA	2010	27	-	0/5/27/28	0/3/3/3
27	OMC	BA	1790	27	-	2/9/27/28	0/2/2/2
27	OMG	BA	1558	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	3009	27	-	2/11/29/30	0/2/2/2
27	5MC	BA	2070	27	-	0/7/25/26	0/2/2/2
1	OMG	Aa	446	1	-	2/5/27/28	0/3/3/3
1	OMC	Aa	752	1	-	0/9/27/28	0/2/2/2
27	OMG	BA	63	27	-	0/5/27/28	0/3/3/3
27	4AC	BA	501	27	-	0/11/29/30	0/2/2/2
1	OMG	Aa	382	1	-	2/5/27/28	0/3/3/3
27	4AC	BA	2590	27	-	0/11/29/30	0/2/2/2
27	5MU	BA	1905	27	-	0/7/25/26	0/2/2/2
27	4AC	BA	2832	27	-	1/11/29/30	0/2/2/2
27	OMU	BA	1969	27	-	0/9/27/28	0/2/2/2
1	OMG	Aa	381	1	-	0/5/27/28	0/3/3/3
27	OMU	BA	768	27	-	0/9/27/28	0/2/2/2
27	OMG	BA	2521	27	-	0/5/27/28	0/3/3/3
1	4AC	Aa	501	1	-	0/11/29/30	0/2/2/2
27	OMU	BA	1480	27	-	2/9/27/28	0/2/2/2
27	4AC	BA	1934	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	1427	27	-	0/11/29/30	0/2/2/2
27	A2M	BA	505	27	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	5MC	BA	2605	27	-	0/7/25/26	0/2/2/2
27	4AC	BA	2121	27	-	0/11/29/30	0/2/2/2
1	4AC	Aa	605	1	-	1/11/29/30	0/2/2/2

The worst 5 of 1672 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	1265	A2M	O4'-C1'	14.99	1.62	1.41
27	BA	756	A2M	O4'-C1'	14.76	1.61	1.41
27	BA	932	A2M	O4'-C1'	14.62	1.61	1.41
27	BA	872	A2M	O4'-C1'	14.38	1.61	1.41
27	BA	879	A2M	O4'-C1'	14.34	1.61	1.41

The worst 5 of 955 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1468	MA6	N1-C6-N6	-13.10	103.27	117.06
27	BA	1905	5MU	C5-C4-N3	12.43	125.92	115.31
27	BA	537	5MU	C5-C4-N3	12.41	125.90	115.31
1	Aa	1467	MA6	N1-C6-N6	-12.33	104.08	117.06
27	BA	1548	5MU	C5-C4-N3	12.23	125.75	115.31

There are no chirality outliers.

5 of 235 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Aa	52	OMU	C3'-C4'-C5'-O5'
1	Aa	52	OMU	O4'-C4'-C5'-O5'
1	Aa	352	A2M	C1'-C2'-O2'-CM'
1	Aa	382	OMG	O4'-C4'-C5'-O5'
1	Aa	446	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

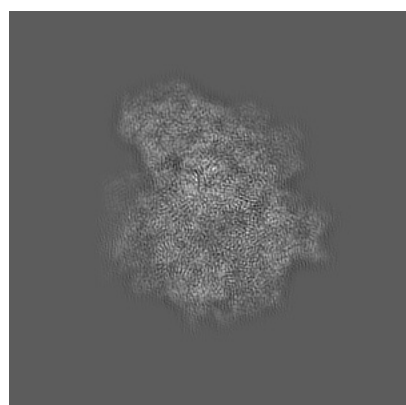
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10223. These allow visual inspection of the internal detail of the map and identification of artifacts.

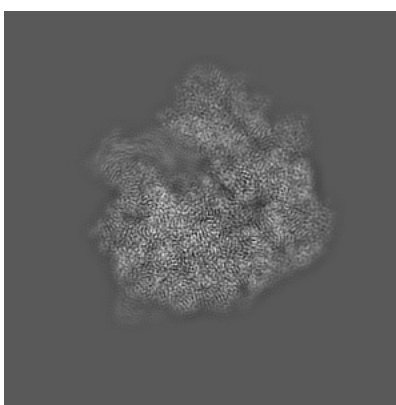
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

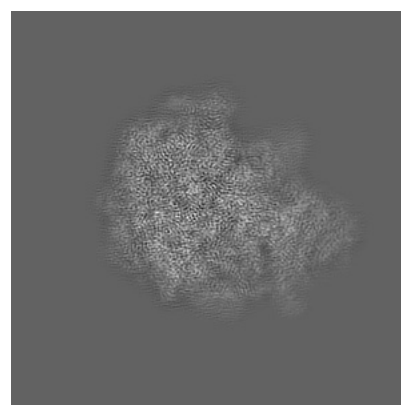
#### 6.1.1 Primary map



X



Y

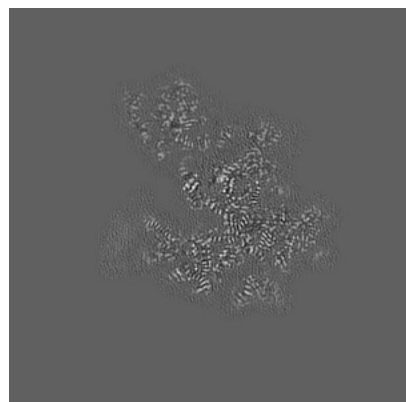


Z

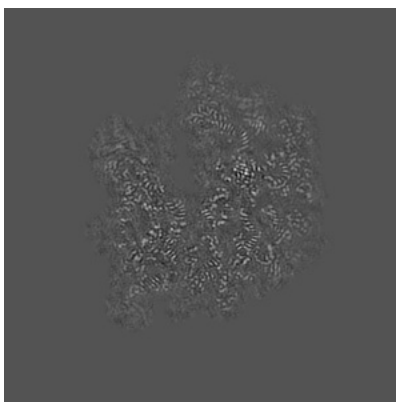
The images above show the map projected in three orthogonal directions.

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

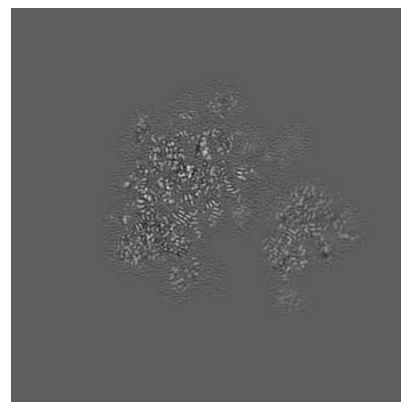
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

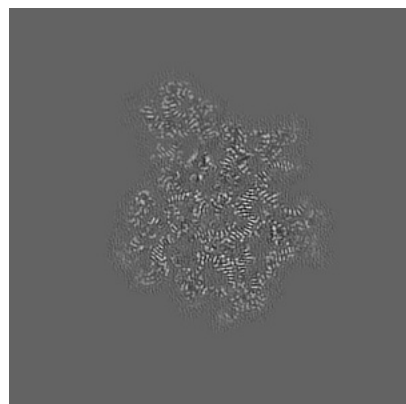


Z Index: 240

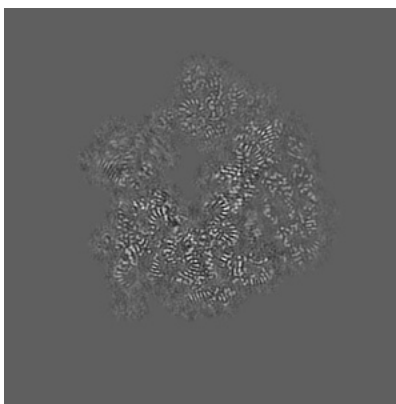
The images above show central slices of the map in three orthogonal directions.

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

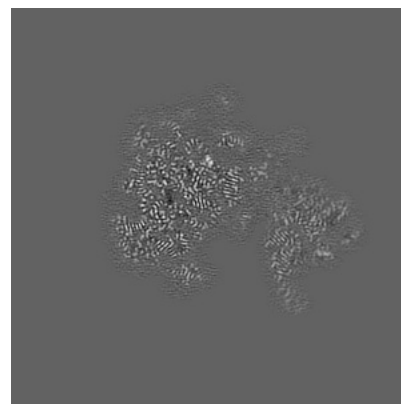
### 6.3.1 Primary map



X Index: 213



Y Index: 224

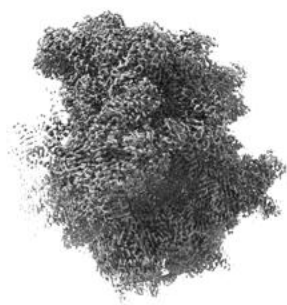


Z Index: 247

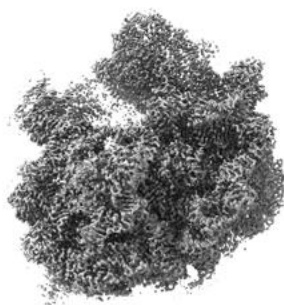
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

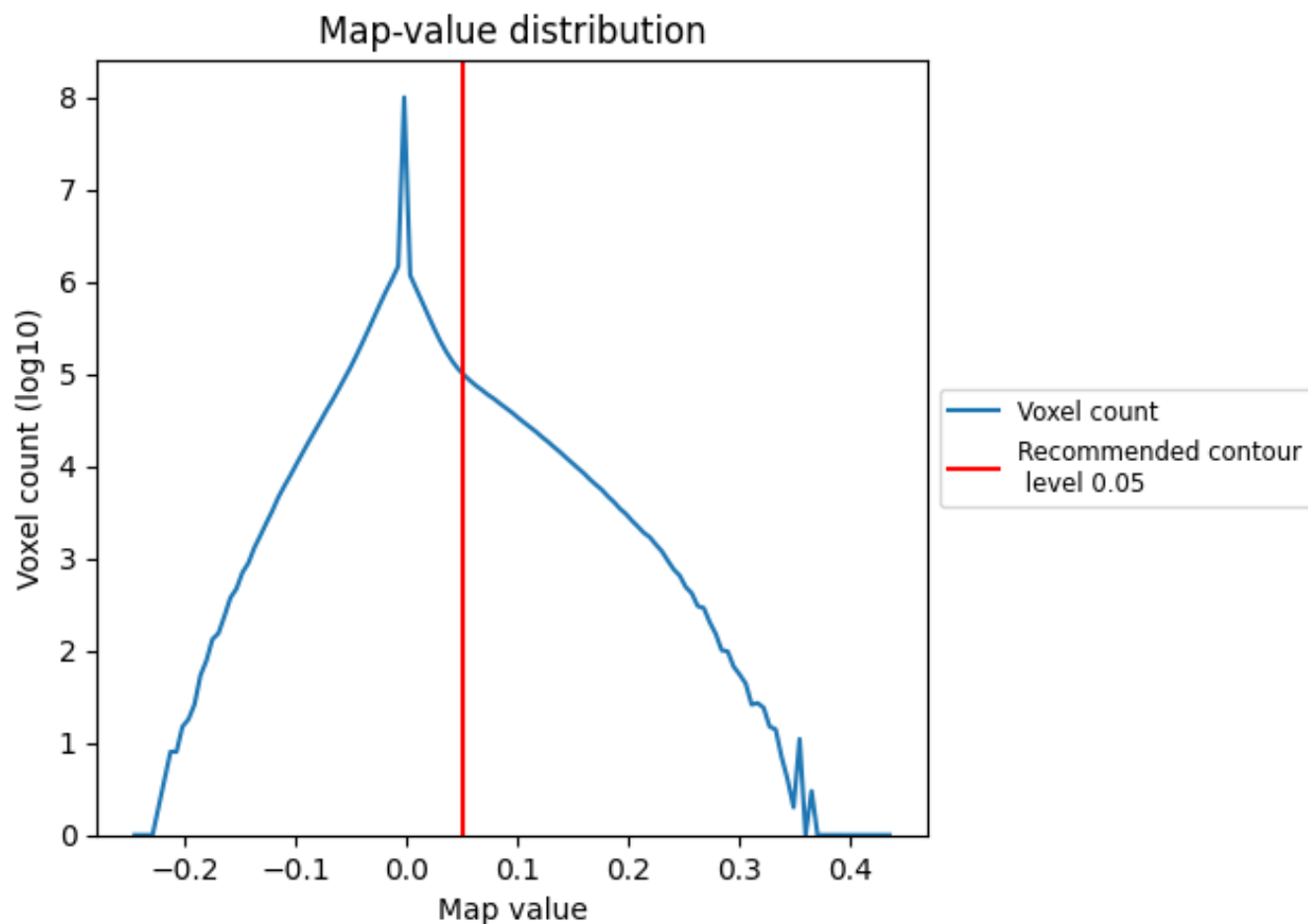
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

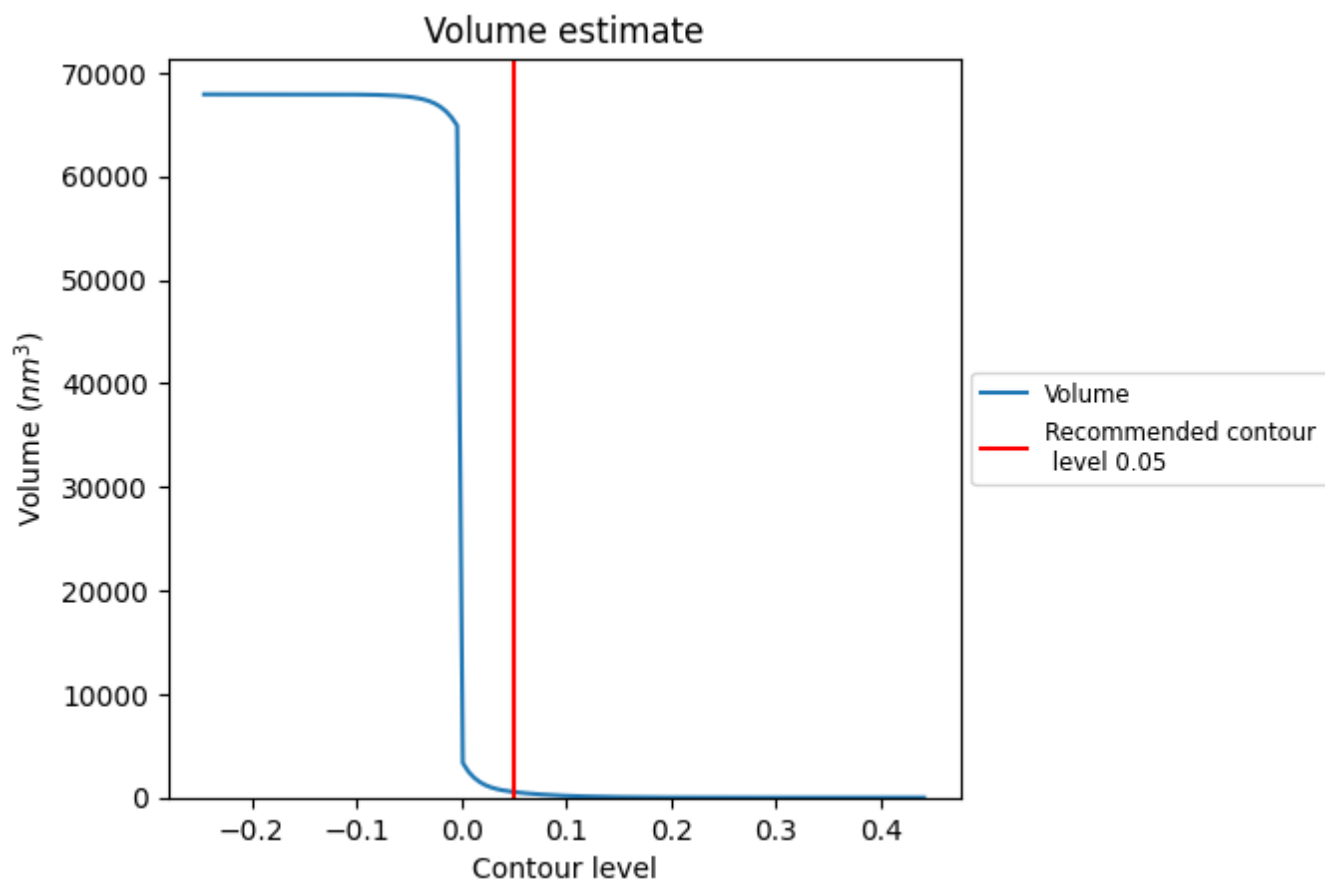
This section contains the results of statistical analysis of the map.

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



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

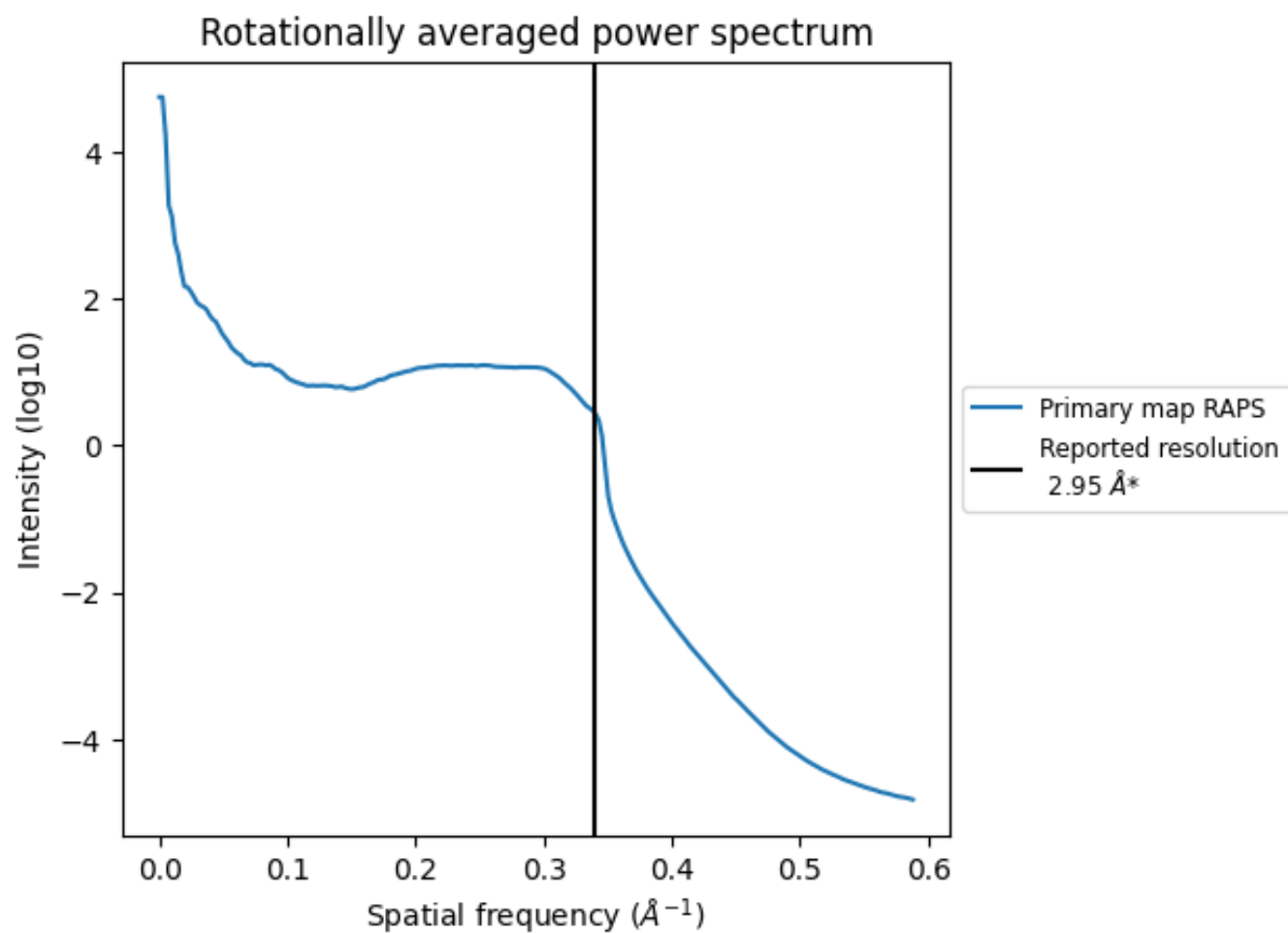
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 541 nm<sup>3</sup>; this corresponds to an approximate mass of 488 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 0.339 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

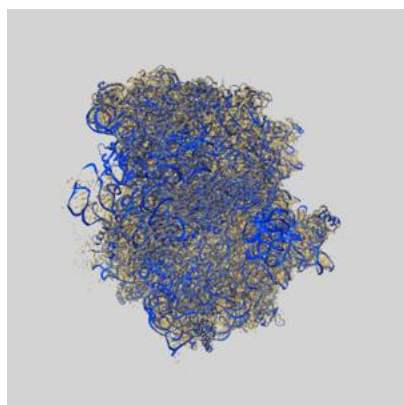
This section was not generated. No FSC curve or half-maps provided.



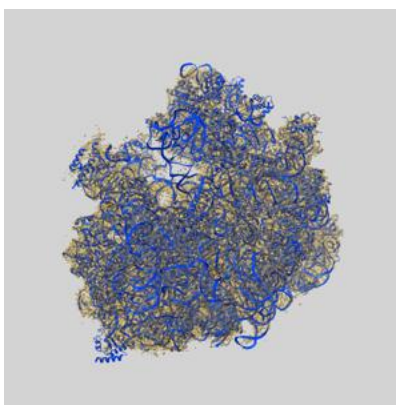
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10223 and PDB model 6SKF. Per-residue inclusion information can be found in section [3](#) on page [19](#).

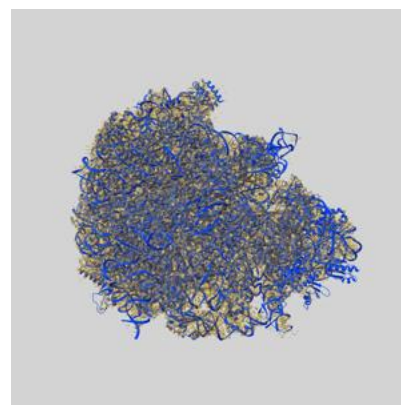
### 9.1 Map-model overlay [i](#)



X



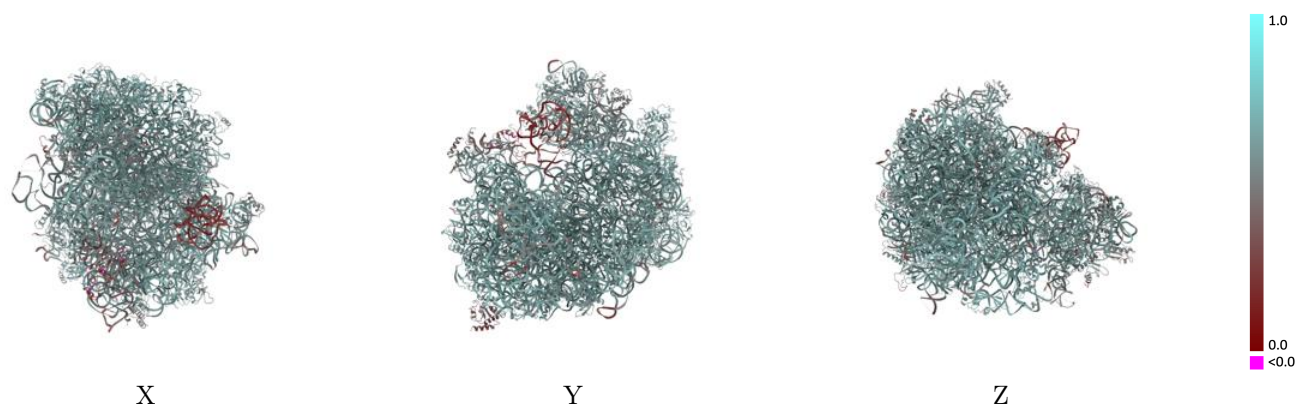
Y



Z

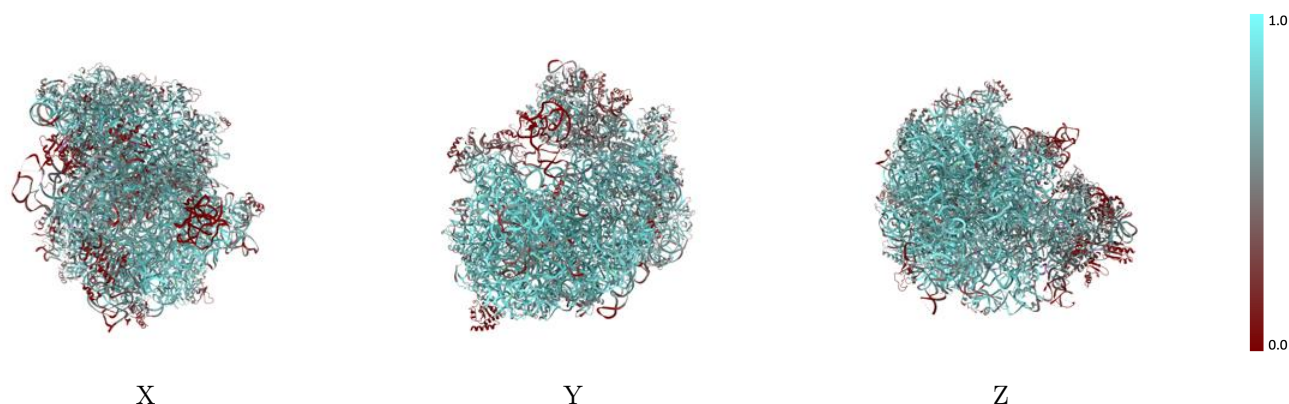
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



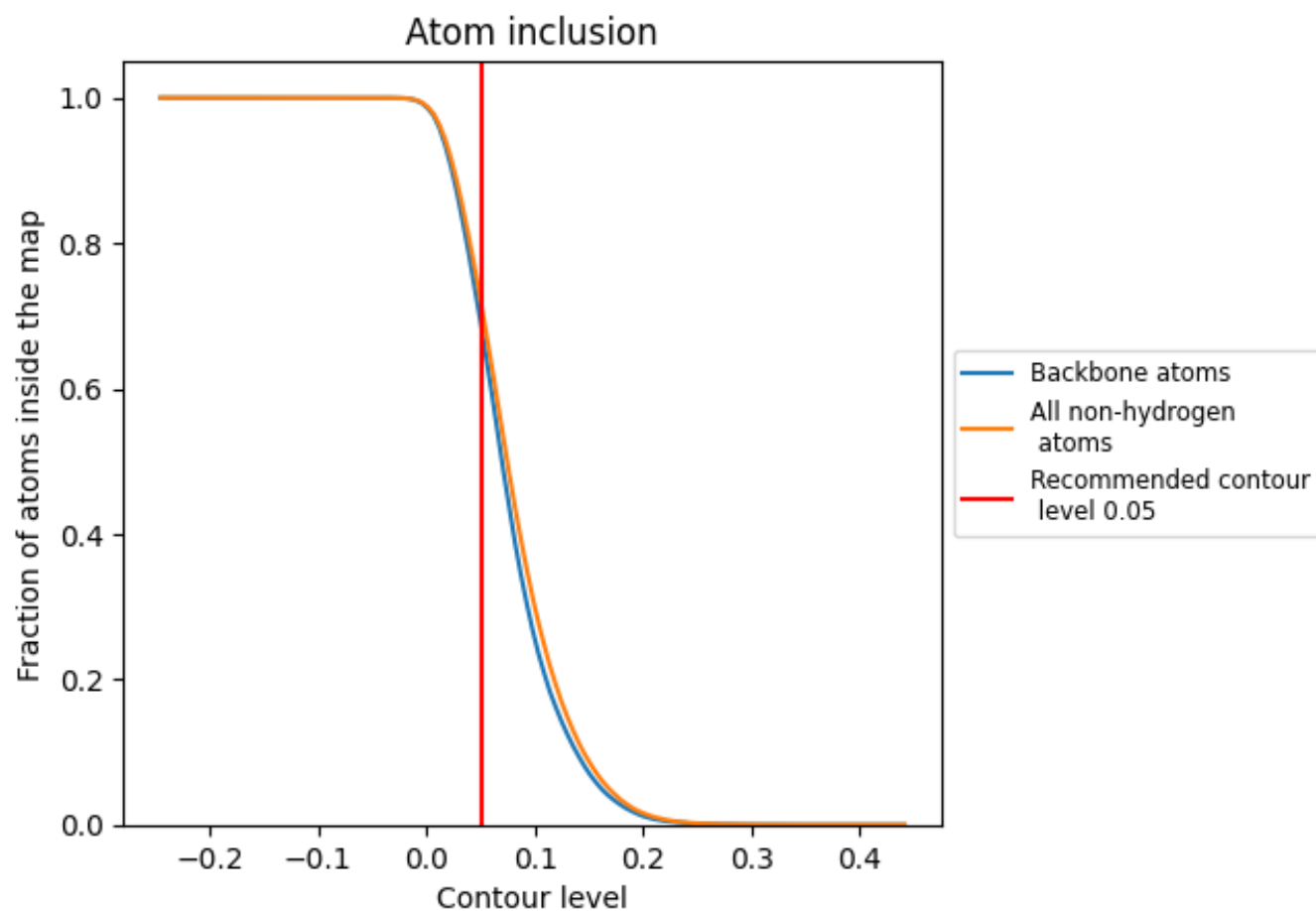
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ



























































The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7215	 0.5970
Aa	 0.7524	 0.6120
Ab	 0.5250	 0.5890
Ac	 0.2443	 0.5210
Ad	 0.5153	 0.5720
Ae	 0.6273	 0.5960
Af	 0.6610	 0.6140
Ag	 0.6510	 0.6090
Ah	 0.3634	 0.5600
Ai	 0.4982	 0.5560
Aj	 0.6690	 0.6090
Ak	 0.6118	 0.5980
Al	 0.4230	 0.5680
Am	 0.2059	 0.5180
An	 0.5507	 0.5760
Ao	 0.5925	 0.6110
Ap	 0.5276	 0.5540
Aq	 0.6230	 0.5870
Ar	 0.4592	 0.5780
As	 0.6273	 0.6170
At	 0.1596	 0.4910
Au	 0.4605	 0.5730
Av	 0.5554	 0.5690
Aw	 0.5728	 0.5920
Ax	 0.5000	 0.5810
Ay	 0.4372	 0.5440
Az	 0.5823	 0.6170
BA	 0.8212	 0.6050
BB	 0.6120	 0.5320
BC	 0.7767	 0.6200
BD	 0.7812	 0.6230
BE	 0.7630	 0.6170
BF	 0.1558	 0.3000
BG	 0.6630	 0.5920
BH	 0.5049	 0.5590



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Chain	Atom inclusion	Q-score
BI	 0.0623	 0.3640
BJ	 0.7314	 0.6020
BK	 0.7457	 0.6140
BL	 0.7414	 0.6150
BM	 0.5943	 0.5770
BN	 0.5421	 0.5580
BO	 0.6002	 0.5700
BP	 0.8302	 0.6350
BQ	 0.4813	 0.5340
BR	 0.7481	 0.6110
BS	 0.7238	 0.5990
BT	 0.6149	 0.5890
BU	 0.8013	 0.6300
BV	 0.7831	 0.6250
BW	 0.6841	 0.5900
BX	 0.7409	 0.6110
BY	 0.8095	 0.6270
BZ	 0.5617	 0.5550
Ba	 0.7606	 0.6100
Bb	 0.6198	 0.5610
Bc	 0.7112	 0.5980
Bd	 0.7668	 0.6230
Be	 0.7388	 0.6080
Bg	 0.7508	 0.6160
Bh	 0.8755	 0.6460
Bi	 0.7913	 0.6290
Bj	 0.7472	 0.6170
Bk	 0.8899	 0.6250
Bl	 0.7299	 0.6170