wwPDB EM Validation Summary Report (i)

Nov 10, 2024 – 01:26 am GMT

PDB ID	:	8OVE
EMDB ID	:	EMD-17212
Title	:	CRYO-EM STRUCTURE OF TRYPANOSOMA BRUCEI PROCYCLIC FORM 80S RIBOSOME : TB11CS6H1 snoRNA mutant
Authors	:	Rajan, K.S.; Yonath, A.
Deposited on	:	2023-04-25
Resolution	:	2.60 Å(reported)
Based on initial models	:	4V8M, 8A3W

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

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

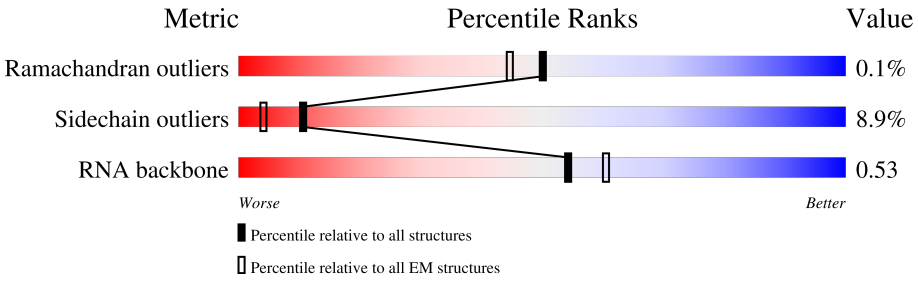
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AA	2280	57% 23% • 19%
2	AB	19	58% 42%
3	BA	1920	65% 17% • 18%
4	BB	1536	55% 17% • 28%
5	BC	209	61% 15% 23%
6	BD	119	86% 14%
7	BE	216	64% 12% • 23%
8	BP	189	• 72% 9% 19%

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Mol	Chain	Length	Quality of chain
9	BQ	221	87% 5% 8%
10	BR	166	88% 10%
11	BS	179	94% 5%
12	BT	260	70% 26%
13	BU	159	89% 6% 5%
14	BW	139	89% 7%
15	BY	125	49% 50%
16	BX	164	66% 5% 29%
17	BZ	143	75% 9% 16%
18	Bp	82	79% 12% 9%
19	Bq	51	88% 10%
20	Br	374	93% 5%
21	Bt	106	88% 8%
22	Bw	257	86% 11%
23	Bx	276	79% 5% 16%
24	Bl	149	92% 5%
25	Bu	308	74% 22%
26	By	189	86% 9% 5%
27	A0	256	78% 7% 15%
28	A2	190	90% 6%
29	A5	220	77% 8% 15%
30	AD	172	44% 7% 49%
31	A8	57	89% 7%
32	AE	174	79% 9% 13%
33	AG	151	88% 5% 7%

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Mol	Chain	Length	Quality of chain
34	AI	152	61% 9% 30%
35	AH	144	89% 5% 6%
36	AJ	130	91% 8%
37	AL	142	77% 8% 14%
38	AM	153	76% 10% 13%
39	AO	167	84% 5% 11%
40	AP	266	74% 9% 17%
41	AS	143	93% 5%
42	AU	113	58% 37%
43	AX	214	87% 10%
44	AZ	103	48% 8% 45%
45	A3	250	84% 8% 8%
46	AT	137	82% 7% 11%
47	A1	273	86% 9% 5%
48	AC	277	70% 5% 25%
49	Bc	146	92% 7%
50	Bz	34	82% 15%
51	Bo	93	91%
52	Bn	84	92% 5%
53	Bm	109	78% 12% 10%
54	Bk	127	92% 5%
55	Bj	170	64% 5% 32%
56	Bi	132	95% 5%
57	Bg	105	86% 12%
58	Bd	71	92% 6%

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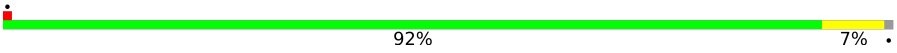
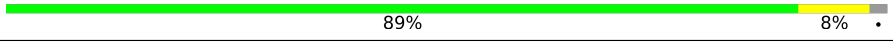
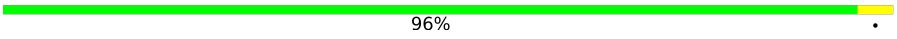
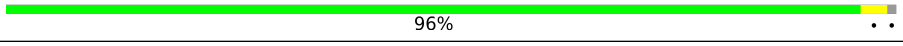
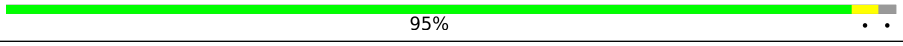
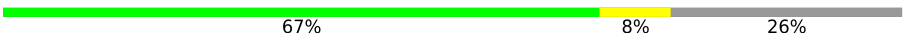
Mol	Chain	Length	Quality of chain
59	Bb	145	
60	Ba	133	
61	BO	222	
62	BN	218	
63	BL	194	
64	BK	213	
65	BI	193	
66	Be	260	
67	AK	149	
68	A6	190	
69	Bf	429	
70	AY	66	
71	Bv	192	
72	Bh	188	
73	BF	78	
74	BG	183	
75	BH	136	
76	Bs	128	
77	BV	130	
78	Az	279	
79	AQ	117	
80	AR	194	
81	AV	111	
82	AW	86	
83	A4	202	

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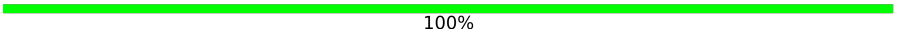
Mol	Chain	Length	Quality of chain
84	A7	318	
85	A	4	

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 203289 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 SSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1836	39217	17534	7038	12809	1836	0	0

- Molecule 2 is a RNA chain called E-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	AB	19	404	181	76	129	18	0	0

- Molecule 3 is a RNA chain called LUS_alpha rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	BA	1579	33850	15122	6138	11010	1580	1	0

- Molecule 4 is a RNA chain called LSUb rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	BB	1109	23703	10602	4238	7754	1109	0	0

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	BC	160	3407	1527	605	1116	159	0	0

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	BD	119	2533	1131	449	835	118	0	0

- Molecule 7 is a RNA chain called SrRNA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BE	166	Total	C	N	O	P	0	0
			3526	1575	620	1165	166		

- Molecule 8 is a protein called 40S ribosomal protein L14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BP	154	Total	C	N	O	S	0	0
			1252	793	242	213	4		

- Molecule 9 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BQ	203	Total	C	N	O	S	0	0
			1716	1077	370	264	5		

- Molecule 10 is a protein called 60S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BR	150	Total	C	N	O	S	0	0
			1209	761	239	201	8		

- Molecule 11 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BS	178	Total	C	N	O	S	0	0
			1465	926	289	243	7		

- Molecule 12 is a protein called 60S ribosomal protein L19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BT	192	Total	C	N	O	S	0	0
			1570	962	345	255	8		

- Molecule 13 is a protein called 60S ribosomal protein L21E, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BU	151	Total	C	N	O	S	0	0
			1197	757	238	196	6		

- Molecule 14 is a protein called 60S ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BW	129	Total	C	N	O	S	0	0
			979	621	185	168	5		

- Molecule 15 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BY	62	Total	C	N	O	S	0	0
			531	347	103	77	4		

- Molecule 16 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BX	117	Total	C	N	O	S	0	0
			955	608	178	167	2		

- Molecule 17 is a protein called 60S ribosomal protein L26, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BZ	120	Total	C	N	O	S	0	0
			971	601	204	161	5		

- Molecule 18 is a protein called 60S ribosomal protein L38, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Bp	75	Total	C	N	O	S	0	0
			609	383	121	101	4		

- Molecule 19 is a protein called 60S ribosomal protein L39, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	Bq	50	Total	C	N	O	0	0
			457	297	98	62		

- Molecule 20 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Br	366	Total	C	N	O	S	0	0
			2871	1796	571	487	17		

- Molecule 21 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Bt	97	Total	C	N	O	S	0	0
			801	507	159	130	5		

- Molecule 22 is a protein called 60S ribosomal protein L7, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Bw	230	Total	C	N	O	S	0	0
			1872	1190	362	312	8		

- Molecule 23 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Bx	232	Total	C	N	O	S	0	0
			1847	1160	363	318	6		

- Molecule 24 is a protein called 60S ribosomal protein L35A, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Bl	144	Total	C	N	O	S	0	0
			1163	728	239	193	3		

- Molecule 25 is a protein called 60S ribosomal protein L5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Bu	240	Total	C	N	O	S	0	0
			1910	1203	366	336	5		

- Molecule 26 is a protein called 60S ribosomal protein L9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	By	180	Total	C	N	O	S	0	0
			1473	934	274	261	4		

- Molecule 27 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A0	218	Total	C	N	O	S	0	0
			1775	1121	334	312	8		

- Molecule 28 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A2	183	Total	C	N	O	S	0	0
			1464	915	282	262	5		

- Molecule 29 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A5	186	Total	C	N	O	S	0	0
			1457	920	287	248	2		

- Molecule 30 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AD	87	Total	C	N	O	S	0	0
			720	472	124	120	4		

- Molecule 31 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A8	53	Total	C	N	O	S	0	0
			439	270	92	72	5		

- Molecule 32 is a protein called 40S ribosomal proteins S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AE	152	Total	C	N	O	S	0	0
			1234	772	251	206	5		

- Molecule 33 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AG	141	Total	C	N	O	S	0	0
			1148	724	227	190	7		

- Molecule 34 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AI	106	Total	C	N	O	S	0	0
			856	548	161	144	3		

- Molecule 35 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AH	135	Total	C	N	O	S	0	0
			1004	616	194	185	9		

- Molecule 36 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AJ	129	Total	C	N	O	S	0	0
			1018	645	191	174	8		

- Molecule 37 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AL	122	Total	C	N	O	S	0	0
			945	600	184	156	5		

- Molecule 38 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	AM	133	Total	C	N	O	S	0	0
			1081	679	211	187	4		

- Molecule 39 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AO	149	Total	C	N	O	S	0	0
			1186	750	235	193	8		

- Molecule 40 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AP	220	Total	C	N	O	S	0	0
			1703	1086	303	305	9		

- Molecule 41 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AS	140	Total	C	N	O	S	0	0
			1096	696	213	185	2		

- Molecule 42 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AU	71	Total	C	N	O	S	0	1
			551	351	100	95	5		

- Molecule 43 is a protein called 40S ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AX	208	Total	C	N	O	S	0	0
			1652	1036	310	294	12		

- Molecule 44 is a protein called 40S ribosomal protein S33, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AZ	57	Total	C	N	O	S	0	0
			438	265	90	79	4		

- Molecule 45 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	A3	230	Total	C	N	O	S	0	0
			1808	1125	367	312	4		

- Molecule 46 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AT	122	Total	C	N	O	S	0	0
			980	623	192	162	3		

- Molecule 47 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	A1	260	Total	C	N	O	S	0	0
			2048	1298	386	355	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AC	208	Total	C	N	O	S	0	0
			1648	1049	297	291	11		

- Molecule 49 is a protein called 60S ribosomal protein L28, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bc	144	Total	C	N	O	S	0	0
			1162	723	234	197	8		

- Molecule 50 is a protein called Ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bz	33	Total	C	N	O	S	0	0
			294	178	76	38	2		

- Molecule 51 is a protein called 60S ribosomal protein L37a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bo	89	Total	C	N	O	S	0	0
			699	434	144	115	6		

- Molecule 52 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bn	80	Total	C	N	O	S	0	0
			676	410	157	103	6		

- Molecule 53 is a protein called Ribosomal protein L36, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Bm	98	Total	C	N	O	S	0	0
			786	493	164	127	2		

- Molecule 54 is a protein called 60S ribosomal protein L35, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bk	123	Total	C	N	O	S	0	0
			1018	639	218	158	3		

- Molecule 55 is a protein called 60S ribosomal protein L34, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Bj	116	Total	C	N	O	S	0	0
			959	593	214	148	4		

- Molecule 56 is a protein called 60S ribosomal protein L32, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bi	131	Total	C	N	O	S	0	0
			1075	678	217	176	4		

- Molecule 57 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Bg	92	Total	C	N	O	S	0	0
			708	441	128	134	5		

- Molecule 58 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bd	69	Total	C	N	O	S	0	0
			561	343	126	91	1		

- Molecule 59 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bb	144	Total	C	N	O	S	0	0
			1137	717	228	186	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Ba	130	Total	C	N	O	S	0	0
			1077	684	220	170	3		

- Molecule 61 is a protein called 60S ribosomal protein L13a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BO	221	Total	C	N	O	S	0	0
			1801	1141	364	289	7		

- Molecule 62 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BN	210	Total	C	N	O	S	0	0
			1722	1074	358	284	6		

- Molecule 63 is a protein called 60S ribosomal protein L11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BL	156	Total	C	N	O	S	0	0
			1246	785	231	223	7		

- Molecule 64 is a protein called 60S ribosomal protein L10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BK	194	Total	C	N	O	S	0	0
			1584	1000	314	259	11		

- Molecule 65 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BI	191	Total	C	N	O	S	0	0
			1517	950	313	246	8		

- Molecule 66 is a protein called 60S ribosomal protein L2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Be	254	Total	C	N	O	S	1	0
			1902	1185	390	314	13		

- Molecule 67 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AK	142	Total	C	N	O	S	0	0
			1143	731	215	194	3		

- Molecule 68 is a protein called Probable 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	A6	178	Total	C	N	O	S	0	0
			1460	920	290	242	8		

- Molecule 69 is a protein called Ribosomal protein L3, mitochondrial, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bf	400	Total	C	N	O	S	0	0
			3211	2023	633	542	13		

- Molecule 70 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AY	59	Total	C	N	O	S	0	0
			471	296	97	77	1		

- Molecule 71 is a protein called 60S ribosomal protein L6, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bv	143	Total	C	N	O	S	0	0
			1101	699	202	197	3		

- Molecule 72 is a protein called 60S ribosomal subunit protein L31, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bh	147	Total	C	N	O	S	0	0
			1188	749	242	193	4		

- Molecule 73 is a RNA chain called SrRNA 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	BF	69	Total	C	N	O	P	0	0
			1444	646	239	490	69		

- Molecule 74 is a RNA chain called SrRNA 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	BG	183	Total	C	N	O	P	0	0
			3919	1746	708	1282	183		

- Molecule 75 is a RNA chain called SrRNA 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	BH	118	Total	C	N	O	P	0	0
			2520	1123	453	826	118		

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bs	50	Total	C	N	O	S	0	0
			394	247	80	60	7		

- Molecule 77 is a protein called 60S ribosomal protein L22, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	BV	122	Total	C	N	O	S	0	0
			973	626	176	168	3		

- Molecule 78 is a protein called RNA-binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	Az	43	Total	C	N	O	0	0
			340	210	68	62		

- Molecule 79 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AQ	100	Total	C	N	O	S	0	0
			800	501	152	144	3		

- Molecule 80 is a protein called 40S ribosomal protein S21, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AR	88	Total	C	N	O	S	0	0
			656	408	117	128	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	88	LYS	GLY	conflict	UNP Q385B8

- Molecule 81 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AV	103	Total	C	N	O	S	0	0
			830	512	175	135	8		

- Molecule 82 is a protein called 40S ribosomal protein S27, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	AW	85	Total	C	N	O	S	0	0
			660	411	124	116	9		

- Molecule 83 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	A4	198	Total	C	N	O	S	0	0
			1596	1020	305	266	5		

- Molecule 84 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	A7	303	Total	C	N	O	S	0	0
			2326	1457	412	445	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A7	28	THR	ALA	conflict	UNP P69103
A7	283	SER	LYS	conflict	UNP P69103

- Molecule 85 is a protein called HIS-THR-CYS-THR.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	A	4	Total	C	N	O	S	0	0
			30	17	6	6	1		

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	AA	52	Total	Mg	0
			52	52	
86	BA	47	Total	Mg	0
			47	47	
86	BB	39	Total	Mg	0
			39	39	
86	BE	3	Total	Mg	0
			3	3	
86	BR	1	Total	Mg	0
			1	1	
86	BW	1	Total	Mg	0
			1	1	
86	A0	1	Total	Mg	0
			1	1	
86	A5	1	Total	Mg	0
			1	1	
86	A3	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
86	Bf	1	Total Mg 1 1	0
86	BG	2	Total Mg 2 2	0

- Molecule 87 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
87	AA	26	Total K 26 26	0
87	BA	2	Total K 2 2	0
87	BB	8	Total K 8 8	0
87	AG	1	Total K 1 1	0
87	AP	1	Total K 1 1	0
87	Be	1	Total K 1 1	0
87	BG	1	Total K 1 1	0
87	AV	1	Total K 1 1	0

- Molecule 88 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
88	AA	26	Total Na 26 26	0
88	BA	11	Total Na 11 11	0
88	BB	10	Total Na 10 10	0
88	BC	1	Total Na 1 1	0
88	BD	1	Total Na 1 1	0
88	Bi	1	Total Na 1 1	0
88	Be	1	Total Na 1 1	0

- Molecule 89 is water.

Mol	Chain	Residues	Atoms	AltConf
89	AA	92	Total O 92 92	0
89	BA	78	Total O 78 78	0
89	BB	100	Total O 100 100	0
89	BC	3	Total O 3 3	0
89	BE	3	Total O 3 3	0
89	BQ	2	Total O 2 2	0
89	BT	1	Total O 1 1	0
89	Br	1	Total O 1 1	0
89	A0	1	Total O 1 1	0
89	A8	1	Total O 1 1	0
89	AH	1	Total O 1 1	0
89	AO	1	Total O 1 1	0
89	AS	1	Total O 1 1	0
89	A1	1	Total O 1 1	0
89	Bz	2	Total O 2 2	0
89	Bo	1	Total O 1 1	0
89	Bn	3	Total O 3 3	0
89	Bj	2	Total O 2 2	0
89	Bd	1	Total O 1 1	0
89	Bb	2	Total O 2 2	0
89	BN	1	Total O 1 1	0

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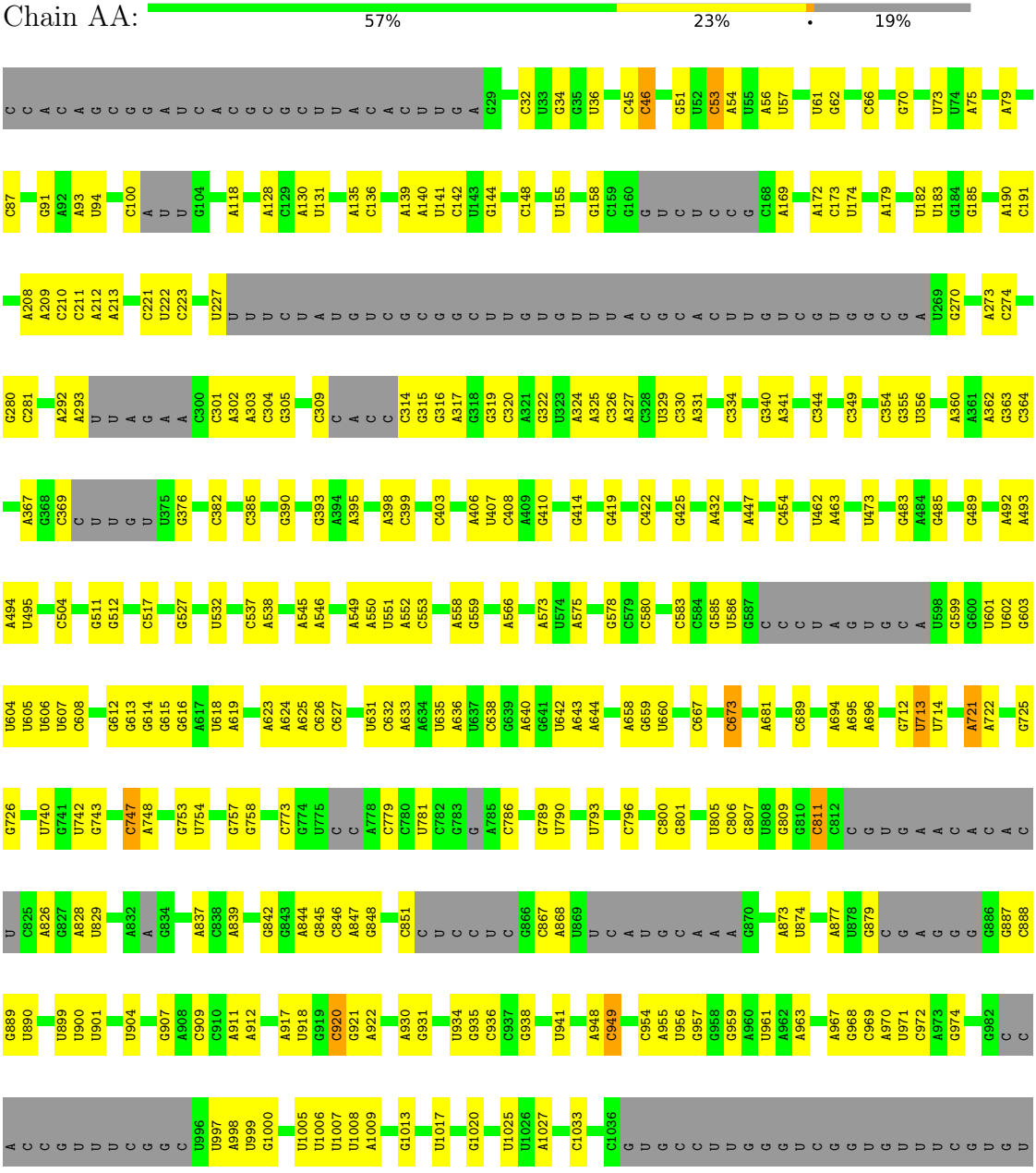
Mol	Chain	Residues	Atoms	AltConf
89	BK	1	Total O 1 1	0
89	BI	1	Total O 1 1	0
89	Be	10	Total O 10 10	0
89	BG	5	Total O 5 5	0
89	BH	2	Total O 2 2	0
89	AV	6	Total O 6 6	0

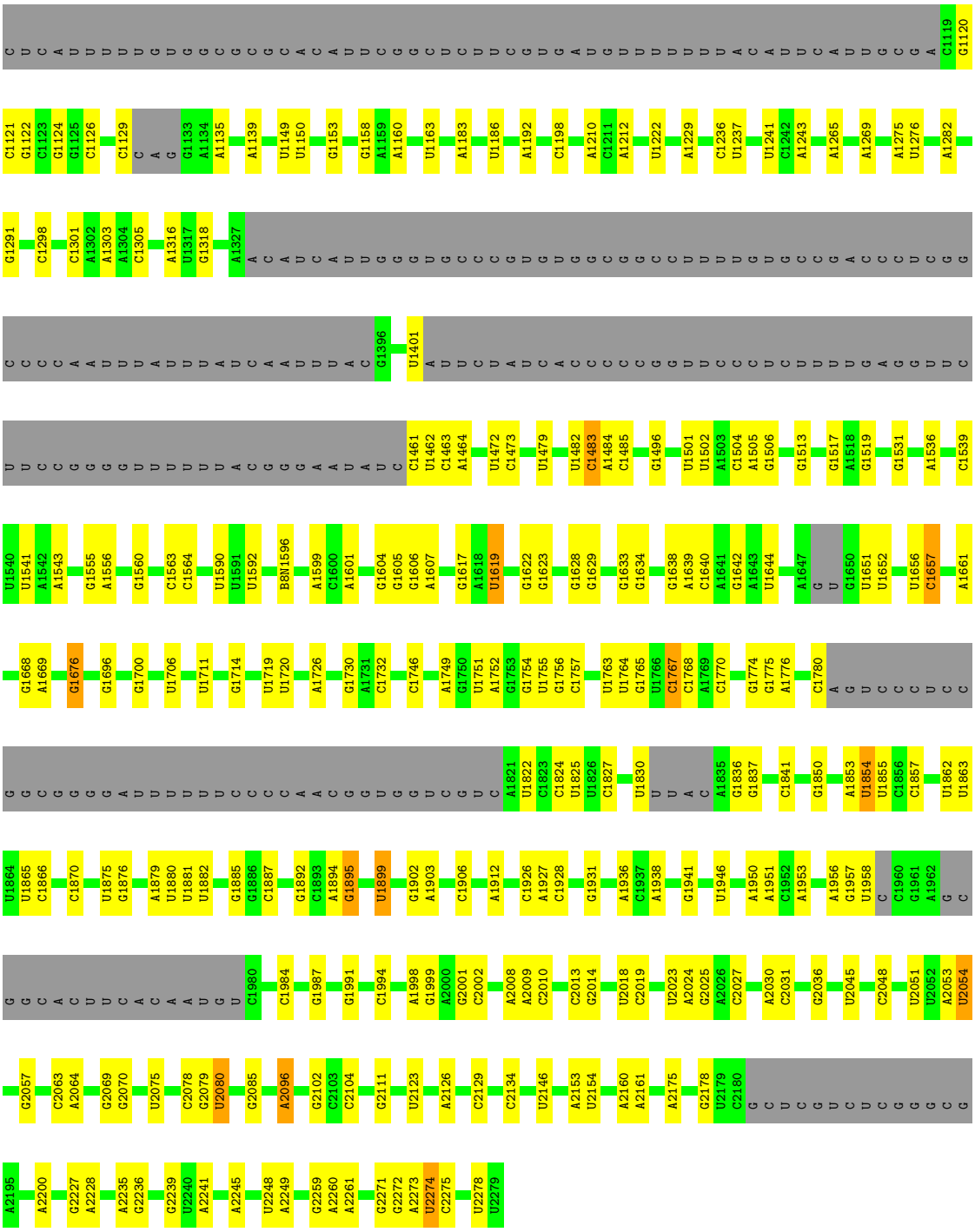
3 Residue-property plots (i)

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

- Molecule 1: SSU rRNA

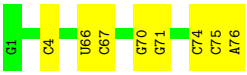
Chain AA:





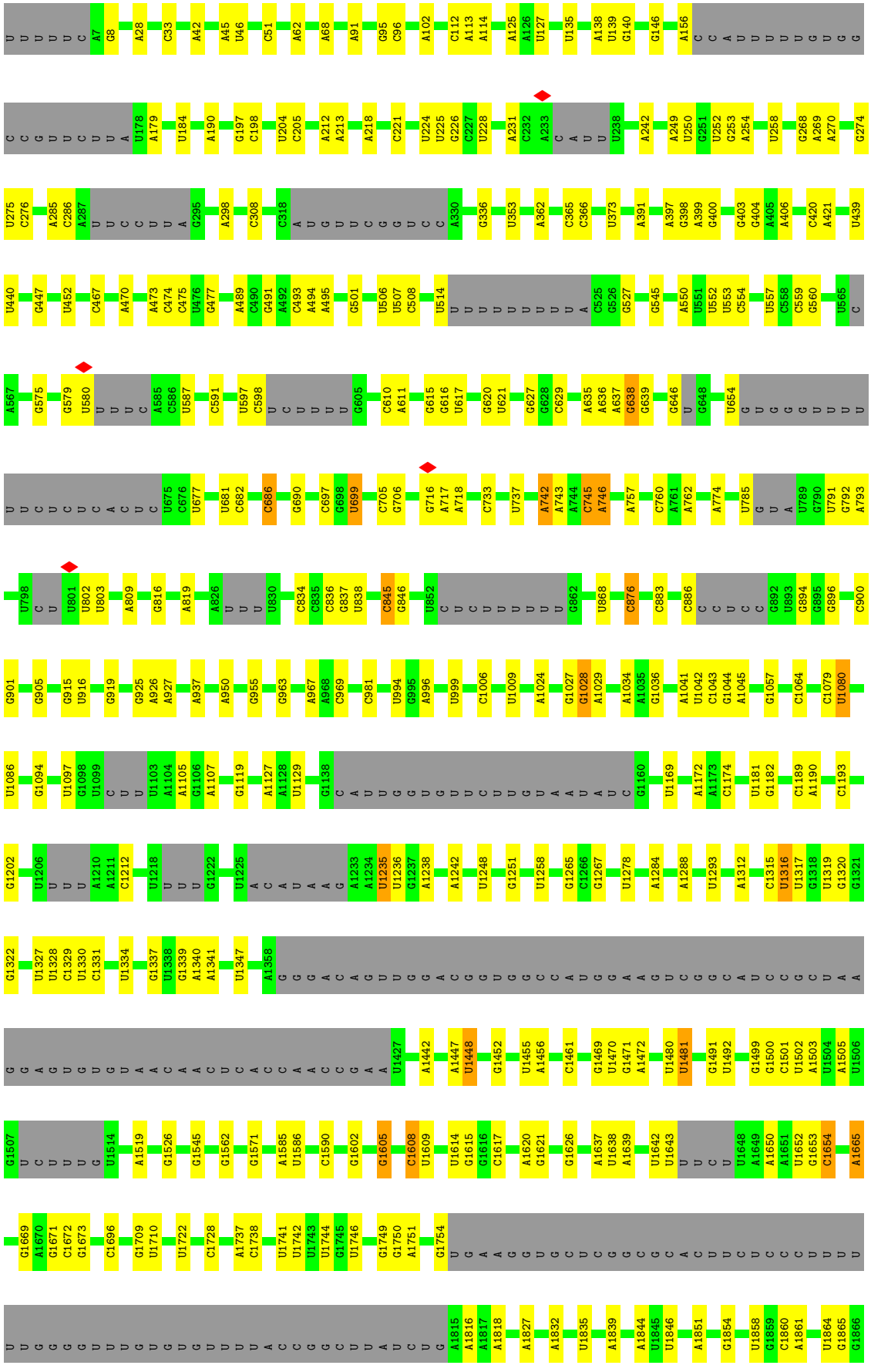
• Molecule 2: E-SITE TRNA

Chain AB:



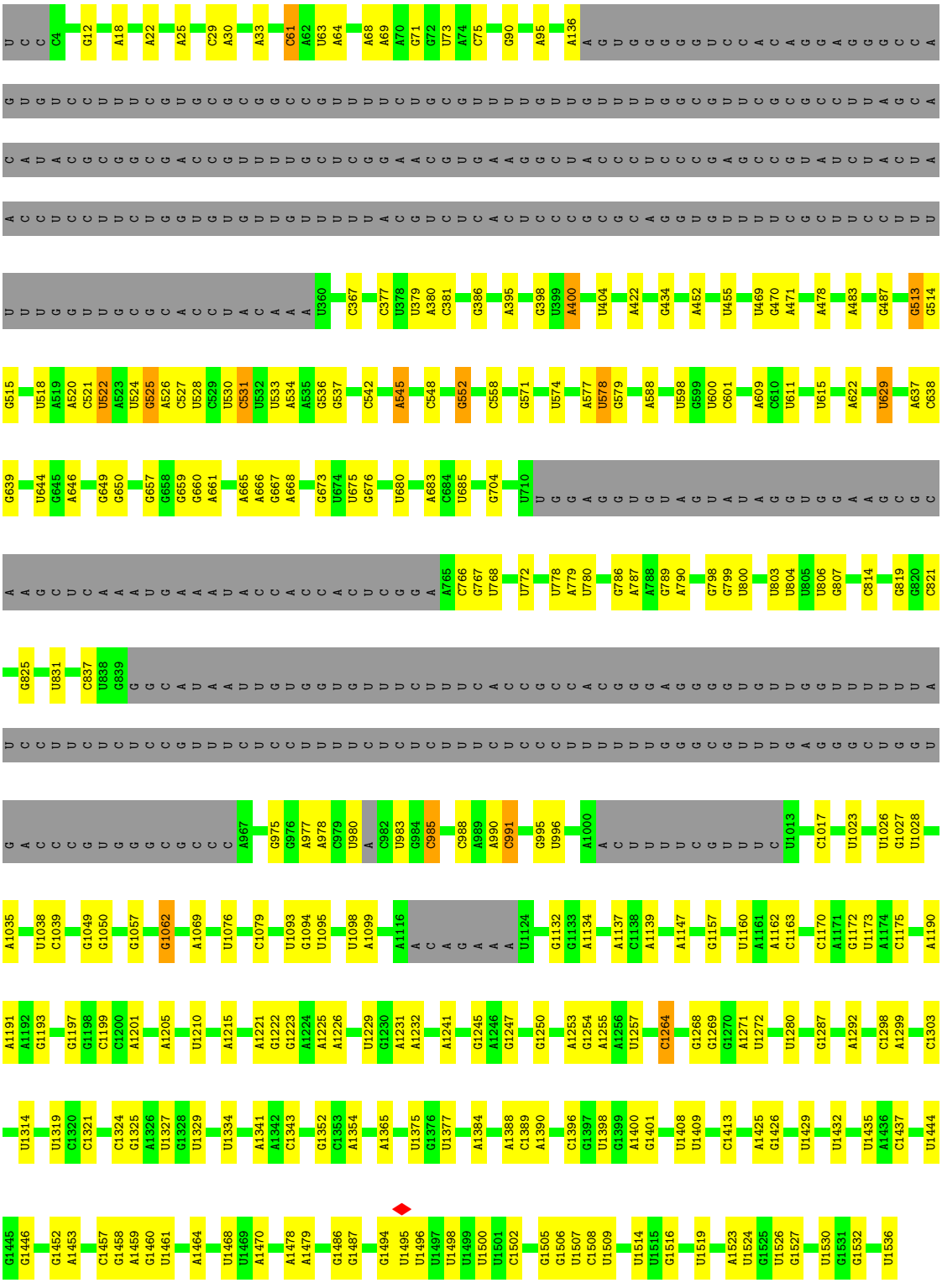
• Molecule 3: LUS_alpha rRNA

Chain BA:



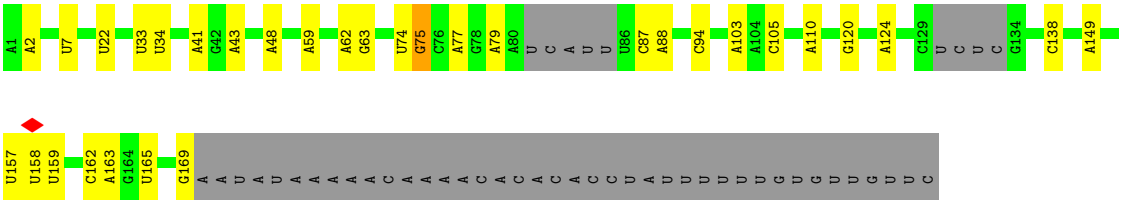
• Molecule 4: LSUb rRNA

Chain BB:



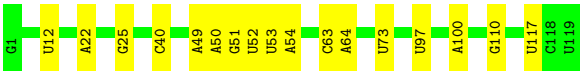
• Molecule 5: 5.8S rRNA

Chain BC:



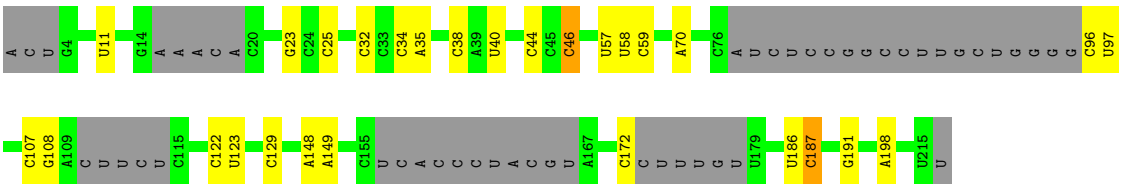
• Molecule 6: 5S rRNA

Chain BD:



• Molecule 7: SrRNA 1

Chain BE:



• Molecule 8: 40S ribosomal protein L14, putative

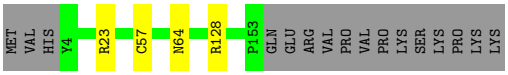
Chain BP:

• Molecule 9: Ribosomal protein L15

Chain BQ:

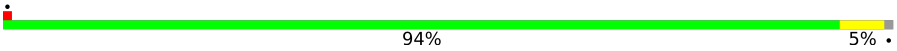
• Molecule 10: 60S ribosomal protein L17, putative

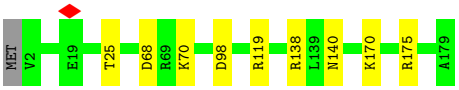
Chain BR:



• Molecule 11: 60S ribosomal protein L18a

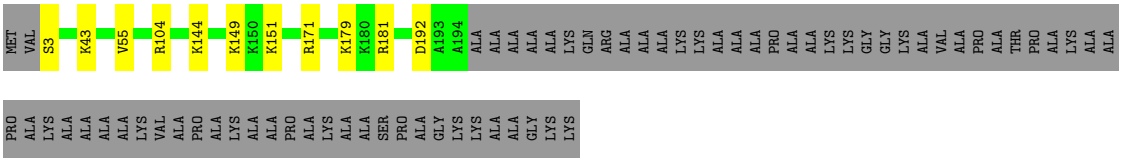
Chain BS:





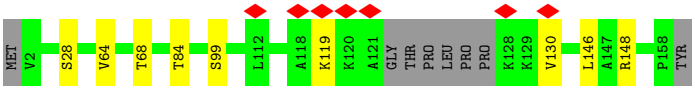
• Molecule 12: 60S ribosomal protein L19, putative

Chain BT:



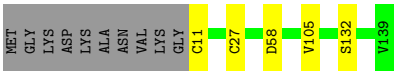
• Molecule 13: 60S ribosomal protein L21E, putative

Chain BU:



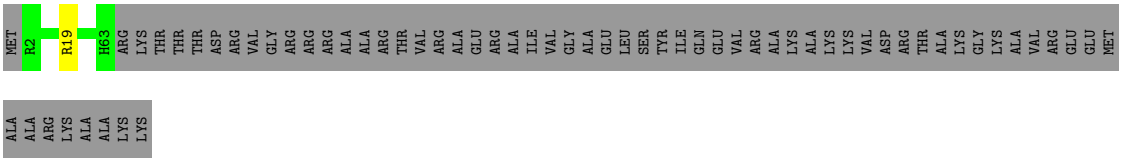
• Molecule 14: 60S ribosomal protein L23, putative

Chain BW:



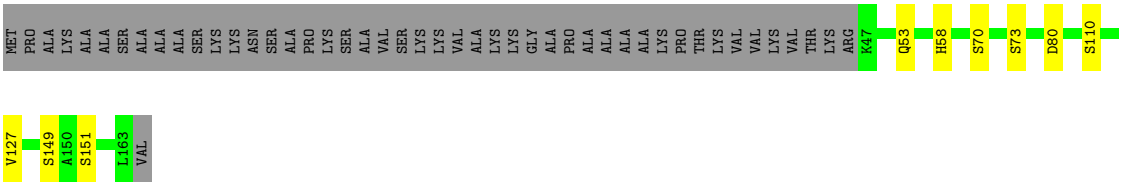
• Molecule 15: Ribosomal protein L24

Chain BY:



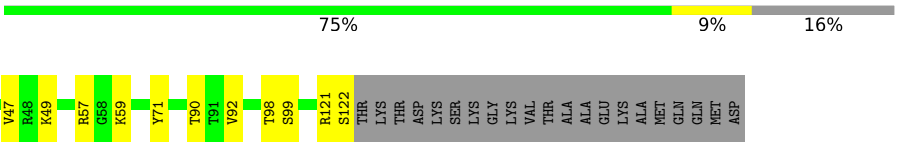
• Molecule 16: 60S ribosomal protein L23a

Chain BX:



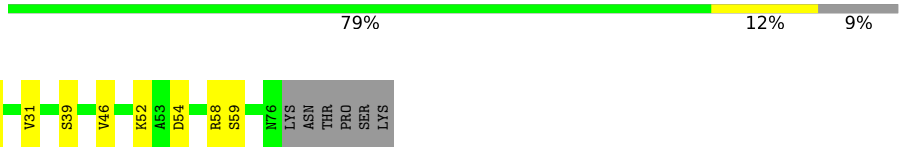
• Molecule 17: 60S ribosomal protein L26, putative

Chain BZ:



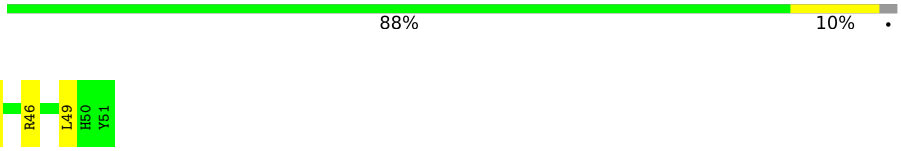
• Molecule 18: 60S ribosomal protein L38, putative

Chain Bp:



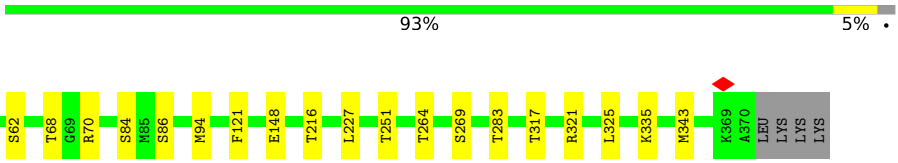
• Molecule 19: 60S ribosomal protein L39, putative

Chain Bq:



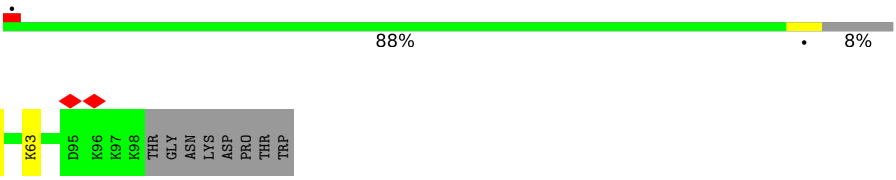
• Molecule 20: 60S ribosomal protein L4

Chain Br:



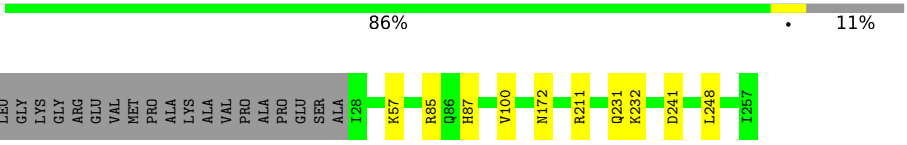
• Molecule 21: 60S ribosomal protein L44

Chain Bt:



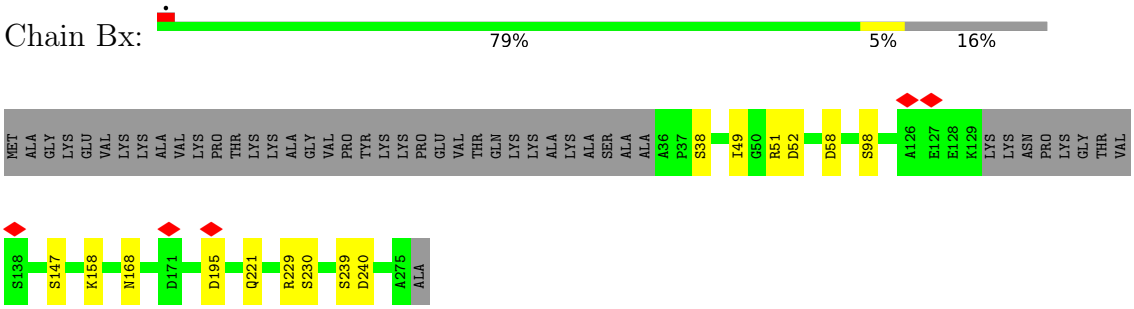
• Molecule 22: 60S ribosomal protein L7, putative

Chain Bw:



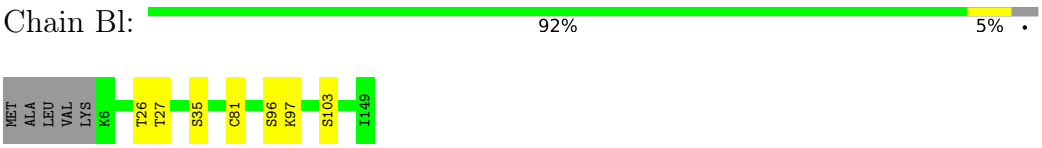
• Molecule 23: 60S ribosomal protein L7a

Chain Bx:



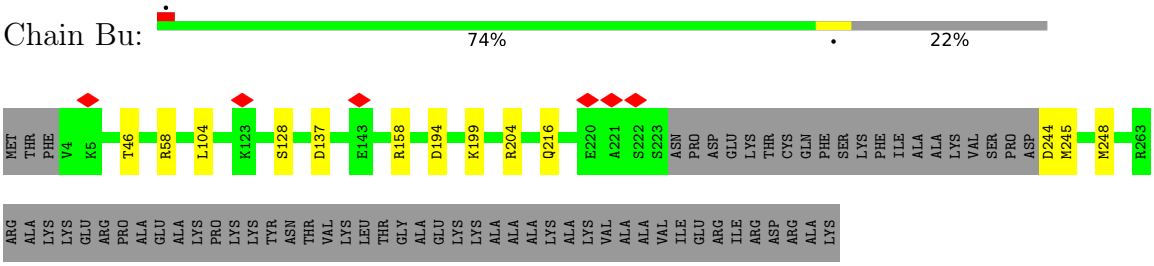
• Molecule 24: 60S ribosomal protein L35A, putative

Chain Bl:



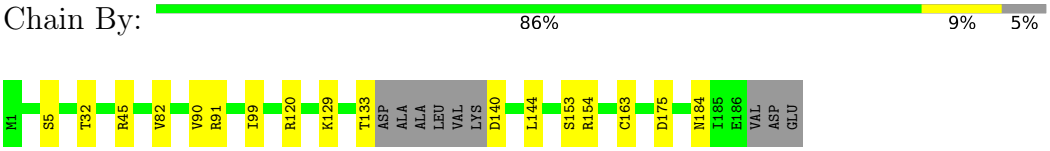
• Molecule 25: 60S ribosomal protein L5, putative

Chain Bu:



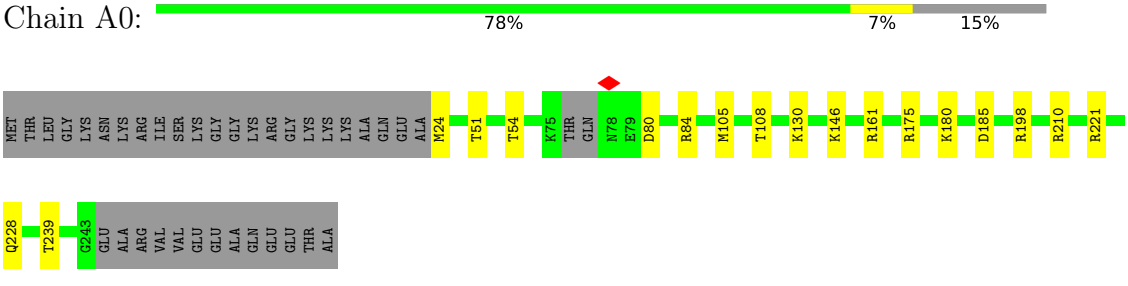
• Molecule 26: 60S ribosomal protein L9, putative

Chain By:



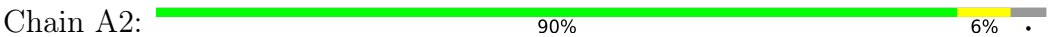
• Molecule 27: 40S ribosomal protein S3a

Chain A0:



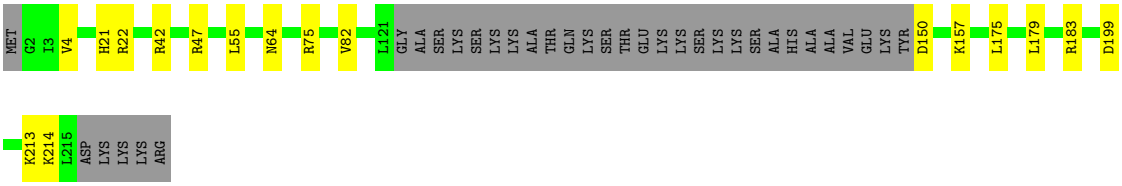
• Molecule 28: 40S ribosomal protein S5, putative

Chain A2:



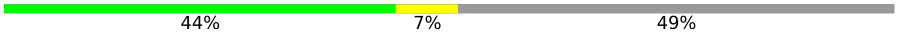
• Molecule 29: 40S ribosomal protein S8

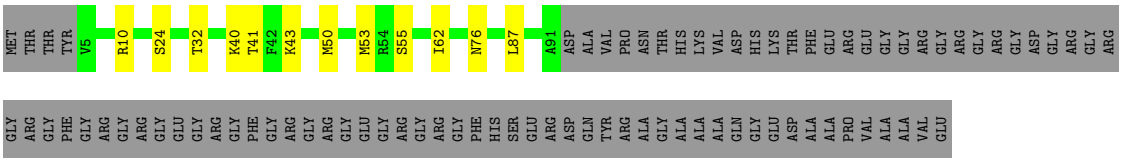
Chain A5:



• Molecule 30: 40S ribosomal protein S10, putative

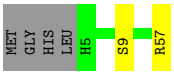
Chain AD:





• Molecule 31: Putative ribosomal protein S29

Chain A8:



• Molecule 32: 40S ribosomal proteins S11, putative

Chain AE:

• Molecule 33: 40S ribosomal protein S13, putative

Chain AG:

• Molecule 34: 40S ribosomal protein S15, putative

Chain AI:

• Molecule 35: 40S ribosomal protein S14

Chain AH:

• Molecule 36: 40S ribosomal protein S15a, putative

Chain AJ:

• Molecule 37: 40S ribosomal protein S17, putative

Chain AL:

• Molecule 38: 40S ribosomal protein S18, putative

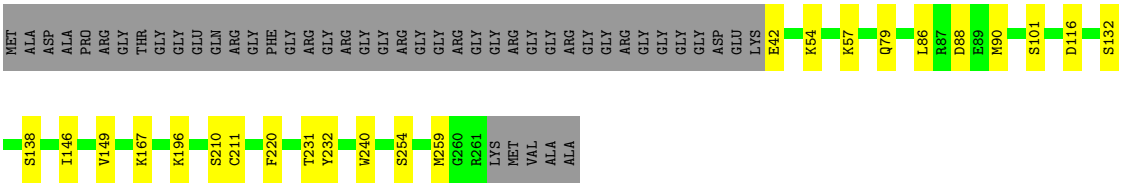
Chain AM:

• Molecule 39: Ribosomal protein S19, putative

Chain AO:

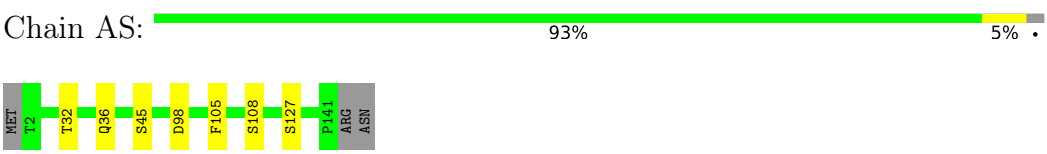
• Molecule 40: 40S ribosomal protein S2, putative

Chain AP:



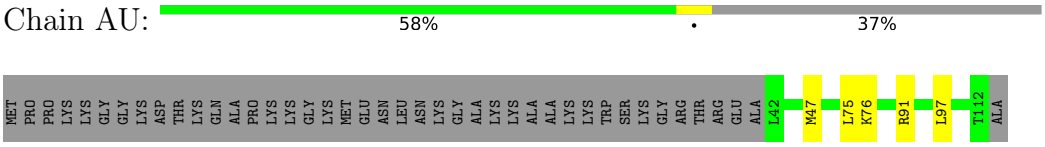
• Molecule 41: 40S ribosomal protein S23, putative

Chain AS:



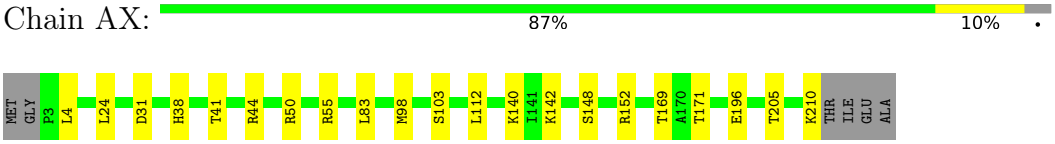
• Molecule 42: 40S ribosomal protein S25

Chain AU:



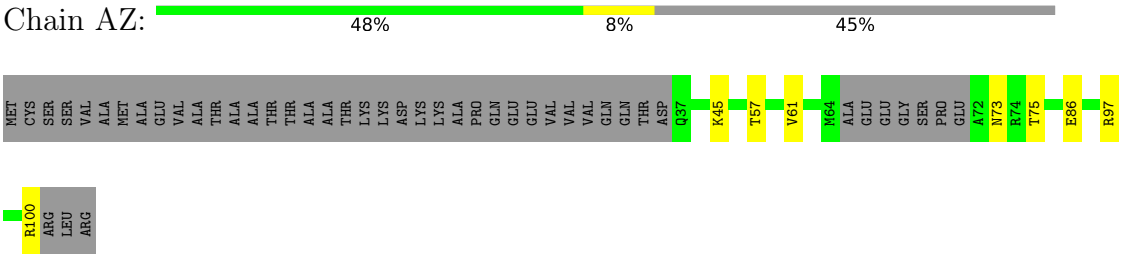
• Molecule 43: 40S ribosomal protein S3, putative

Chain AX:



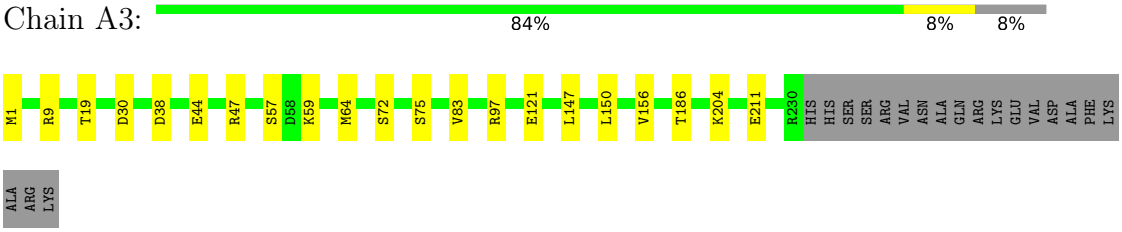
• Molecule 44: 40S ribosomal protein S33, putative

Chain AZ:



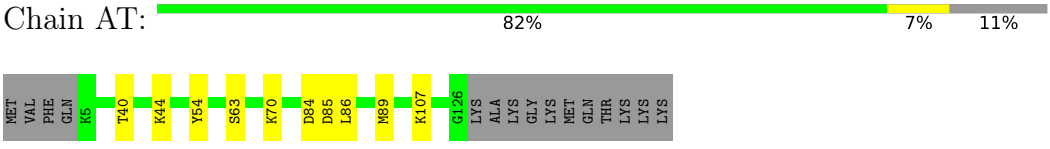
• Molecule 45: 40S ribosomal protein S6

Chain A3:



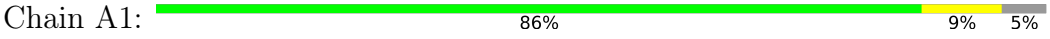
• Molecule 46: 40S ribosomal protein S24

Chain AT:

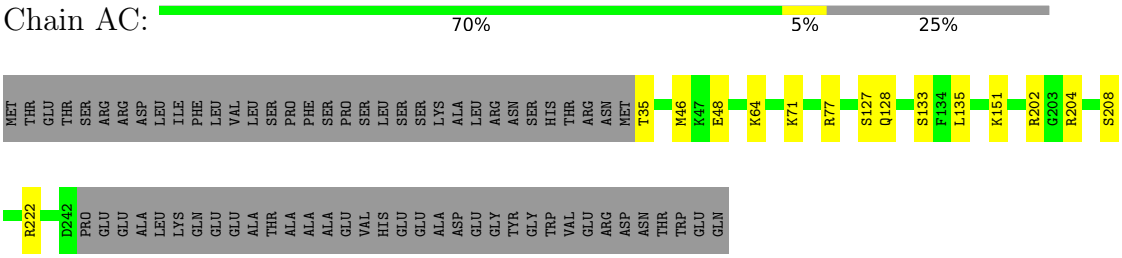


• Molecule 47: 40S ribosomal protein S4

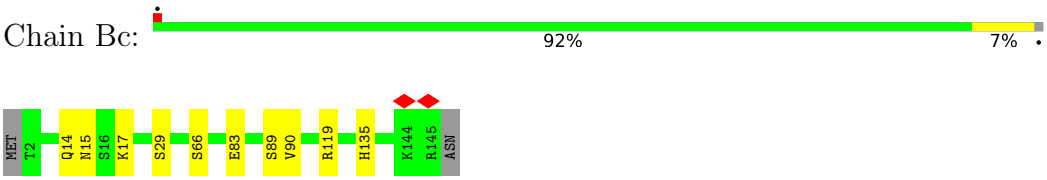
Chain A1:



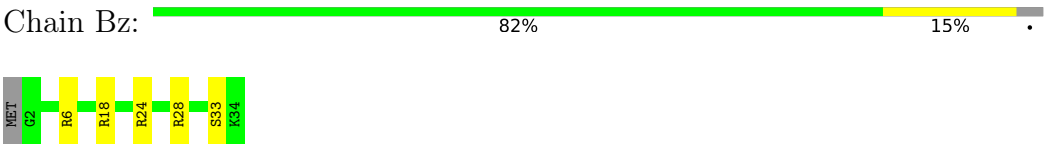
• Molecule 48: 40S ribosomal protein SA



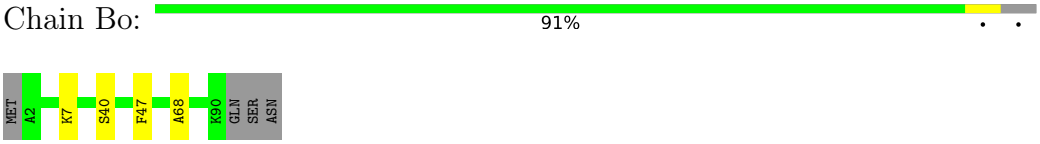
• Molecule 49: 60S ribosomal protein L28, putative



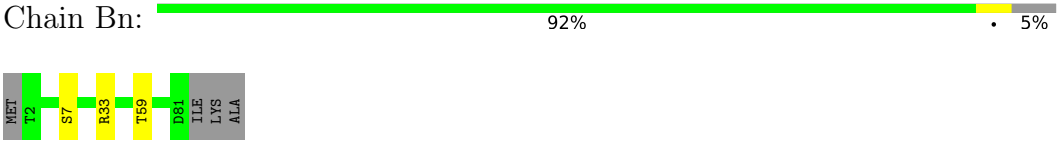
• Molecule 50: Ribosomal protein L41



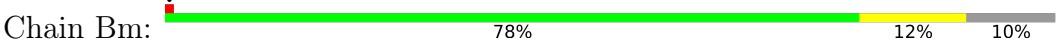
• Molecule 51: 60S ribosomal protein L37a, putative

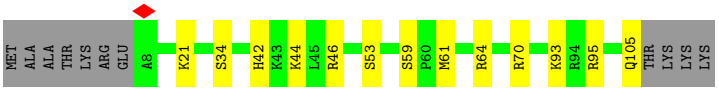


• Molecule 52: Ribosomal protein L37



• Molecule 53: Ribosomal protein L36, putative



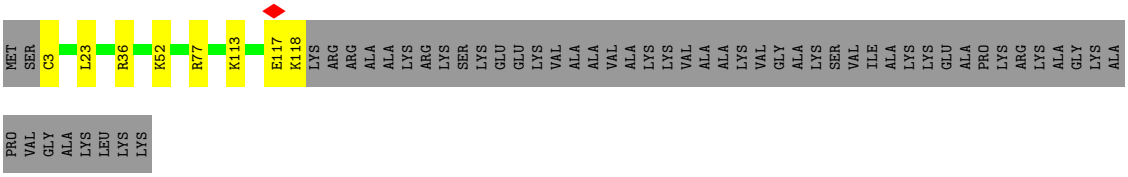


• Molecule 54: 60S ribosomal protein L35, putative

Chain Bk:

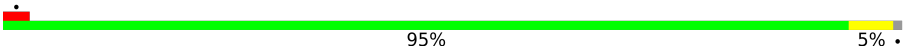
• Molecule 55: 60S ribosomal protein L34, putative

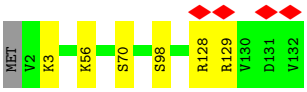
Chain Bj:



• Molecule 56: 60S ribosomal protein L32, putative

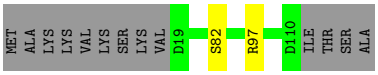
Chain Bi:





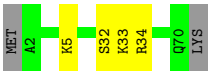
• Molecule 57: 60S ribosomal protein L30

Chain Bg:



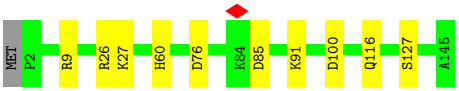
• Molecule 58: 60S ribosomal protein L29

Chain Bd:



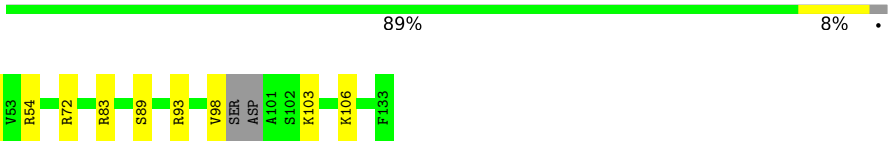
• Molecule 59: 60S ribosomal protein L27a

Chain Bb:



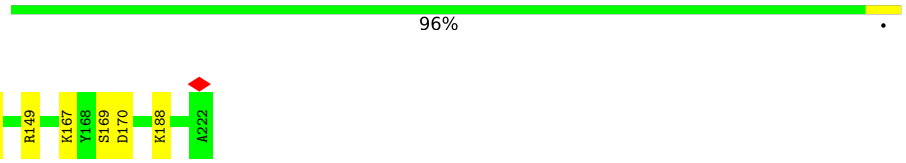
• Molecule 60: 60S ribosomal protein L27

Chain Ba:



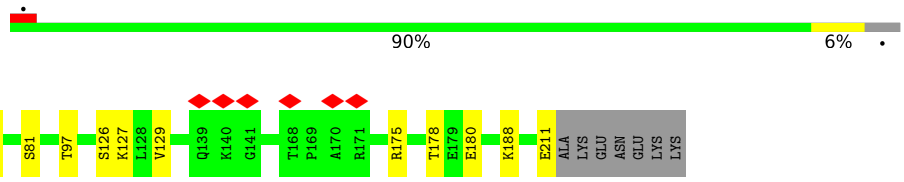
• Molecule 61: 60S ribosomal protein L13a, putative

Chain BO:



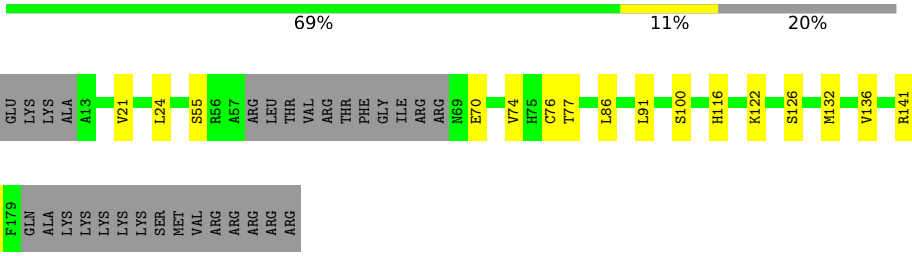
• Molecule 62: 60S ribosomal protein L13

Chain BN:



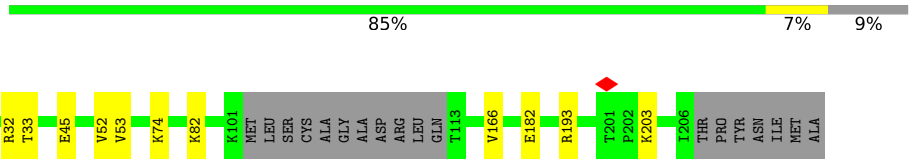
• Molecule 63: 60S ribosomal protein L11, putative

Chain BL:



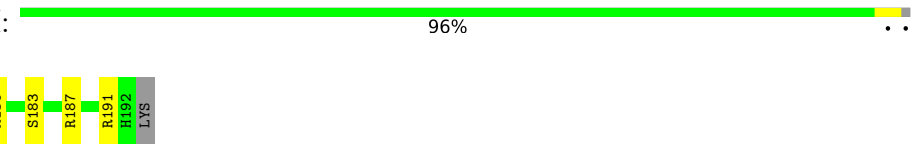
• Molecule 64: 60S ribosomal protein L10, putative

Chain BK:



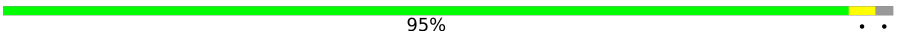
• Molecule 65: 60S ribosomal protein L18

Chain BI:



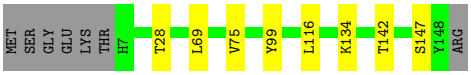
• Molecule 66: 60S ribosomal protein L2, putative

Chain Be:



• Molecule 67: 40S ribosomal protein S16, putative

Chain AK:



• Molecule 68: Probable 40S ribosomal protein S9

Chain A6:

• Molecule 69: Ribosomal protein L3, mitochondrial, putative

Chain Bf:

• Molecule 70: 40S ribosomal protein S30

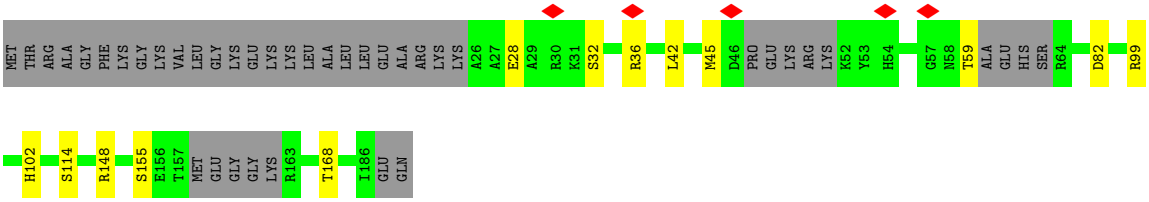
Chain AY:

• Molecule 71: 60S ribosomal protein L6, putative

Chain Bv:

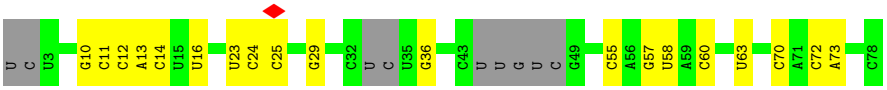
• Molecule 72: 60S ribosomal subunit protein L31, putative

Chain Bh:



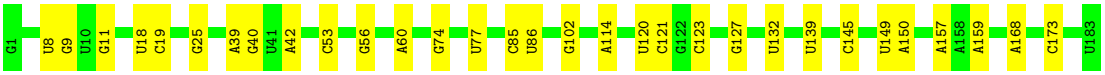
• Molecule 73: SrRNA 6

Chain BF:



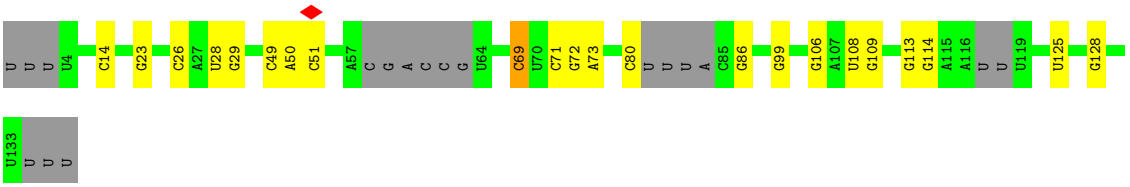
• Molecule 74: SrRNA 2

Chain BG:



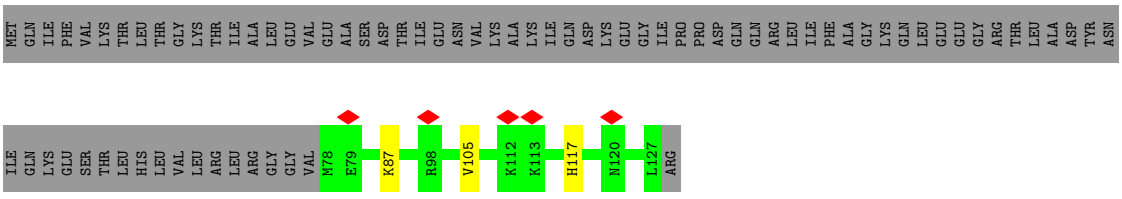
• Molecule 75: SrRNA 4

Chain BH:



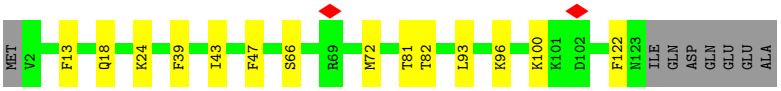
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Bs:



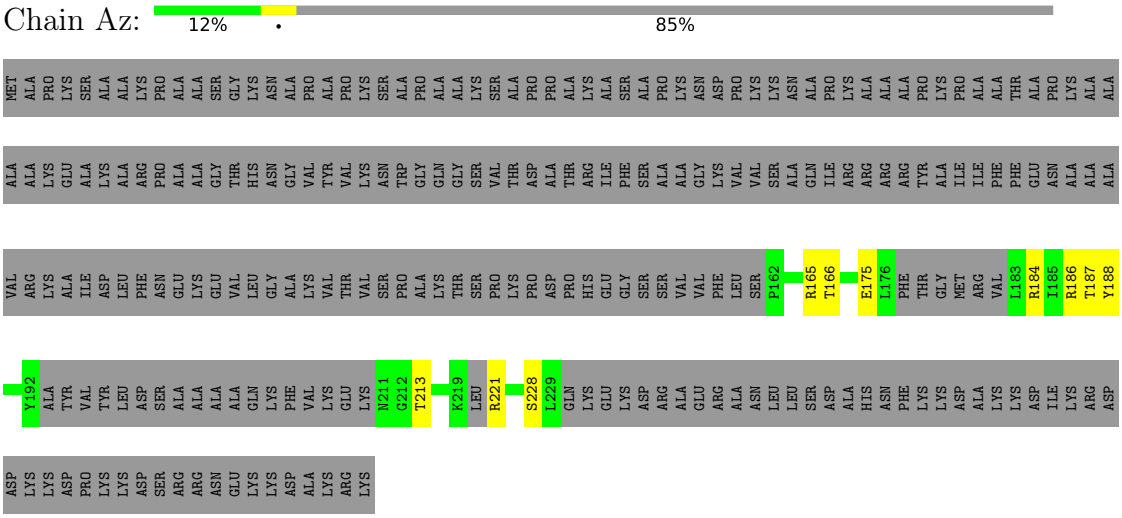
• Molecule 77: 60S ribosomal protein L22, putative

Chain BV:



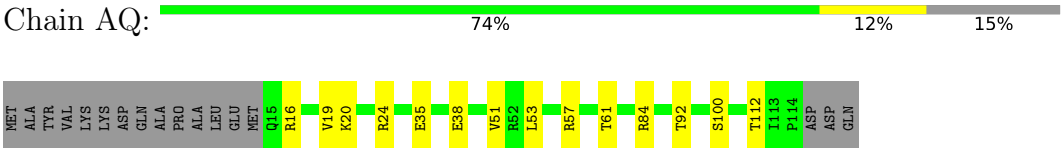
• Molecule 78: RNA-binding protein

Chain Az:



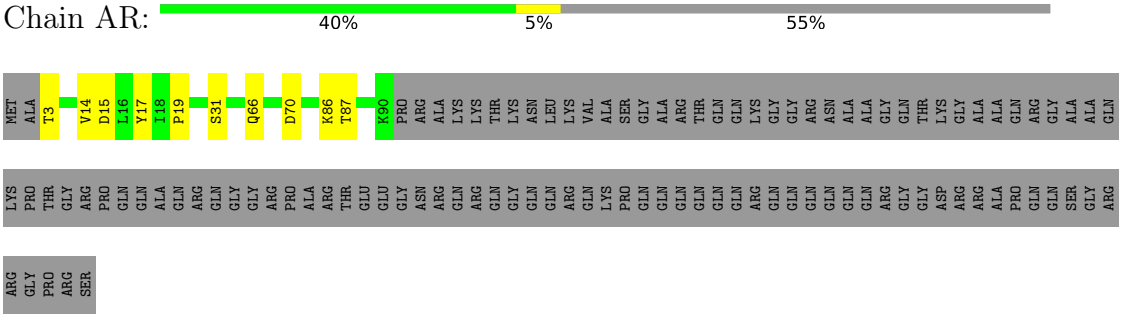
• Molecule 79: Ribosomal protein S10

Chain AQ:



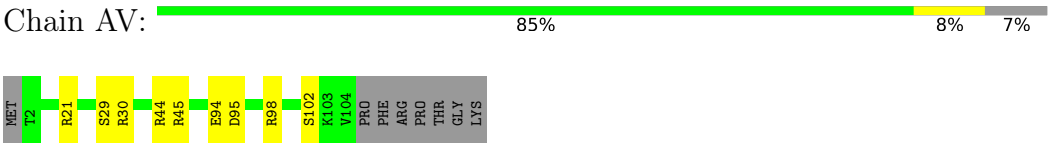
• Molecule 80: 40S ribosomal protein S21, putative

Chain AR:



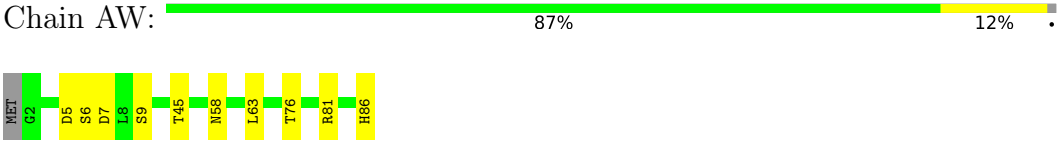
• Molecule 81: 40S ribosomal protein S26

Chain AV:



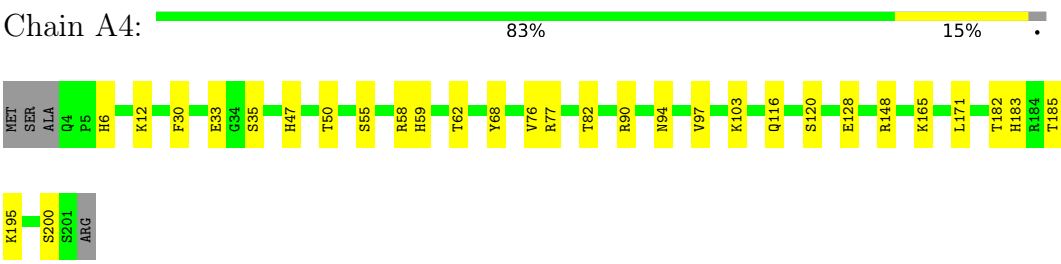
• Molecule 82: 40S ribosomal protein S27, putative

Chain AW:



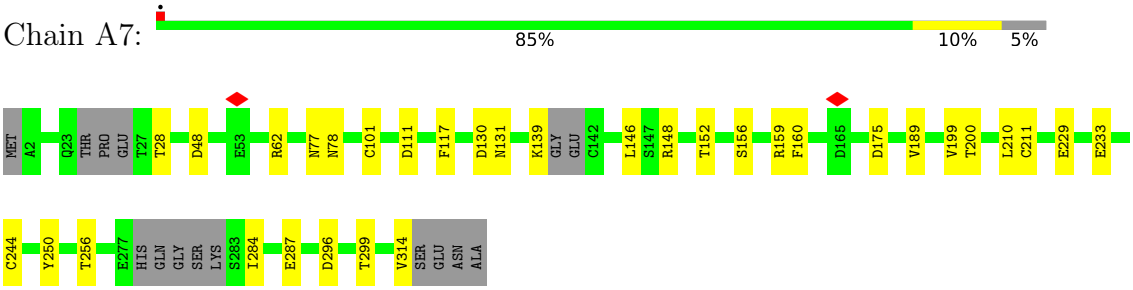
• Molecule 83: 40S ribosomal protein S7

Chain A4:



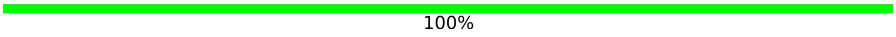
• Molecule 84: Guanine nucleotide-binding protein subunit beta-like protein

Chain A7:



• Molecule 85: HIS-THR-CYS-THR

Chain A:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	552813	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 ($e^-/Å^2$)	1.16	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.301	Depositor
Minimum map value	-0.110	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.01	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: K, PSU, OMG, 7MG, A2M, OMU, OMC, MG, NA, 1MA, MA6, B8N, 5MC

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	0.59	2/43029 (0.0%)	0.90	68/67010 (0.1%)
2	AB	0.32	0/450	0.89	0/698
3	BA	0.46	0/36963	0.84	31/57587 (0.1%)
4	BB	0.49	0/25239	0.87	34/39334 (0.1%)
5	BC	0.41	0/3656	0.78	0/5690
6	BD	0.32	0/2830	0.77	0/4410
7	BE	0.43	0/3933	0.89	7/6113 (0.1%)
8	BP	0.27	0/1271	0.52	0/1704
9	BQ	0.28	0/1755	0.60	1/2346 (0.0%)
10	BR	0.27	0/1233	0.53	0/1654
11	BS	0.27	0/1500	0.54	0/2018
12	BT	0.27	0/1587	0.57	0/2102
13	BU	0.28	0/1221	0.53	0/1638
14	BW	0.29	0/996	0.55	0/1342
15	BY	0.30	0/551	0.59	0/742
16	BX	0.27	0/972	0.52	0/1308
17	BZ	0.26	0/984	0.58	0/1312
18	Bp	0.26	0/617	0.56	0/819
19	Bq	0.25	0/471	0.58	0/626
20	Br	0.27	0/2925	0.55	0/3926
21	Bt	0.29	0/815	0.52	0/1077
22	Bw	0.28	0/1907	0.52	0/2556
23	Bx	0.26	0/1873	0.54	0/2520
24	Bl	0.29	0/1187	0.58	0/1592
25	Bu	0.27	0/1944	0.54	0/2610
26	By	0.24	0/1493	0.52	0/2005
27	A0	0.35	0/1801	0.56	0/2421
28	A2	0.28	0/1486	0.52	0/1997
29	A5	0.29	0/1480	0.56	0/1986
30	AD	0.28	0/740	0.52	0/994
31	A8	0.26	0/445	0.53	0/588
32	AE	0.34	0/1258	0.58	0/1692

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	AG	0.33	0/1170	0.57	0/1567
34	AI	0.33	0/871	0.54	0/1167
35	AH	0.36	0/1019	0.60	0/1367
36	AJ	0.36	0/1035	0.57	0/1386
37	AL	0.26	0/957	0.52	0/1282
38	AM	0.26	0/1098	0.55	0/1470
39	AO	0.27	0/1211	0.54	0/1621
40	AP	0.34	0/1738	0.58	0/2347
41	AS	0.33	0/1117	0.54	0/1495
42	AU	0.31	0/557	0.60	0/745
43	AX	0.27	0/1674	0.54	0/2236
44	AZ	0.33	0/437	0.69	0/581
45	A3	0.29	0/1828	0.62	0/2445
46	AT	0.29	0/995	0.54	0/1323
47	A1	0.30	0/2082	0.57	0/2799
48	AC	0.31	0/1682	0.53	0/2275
49	Bc	0.24	0/1179	0.53	0/1573
50	Bz	0.31	0/298	0.68	0/385
51	Bo	0.31	0/711	0.59	0/946
52	Bn	0.30	0/690	0.65	0/920
53	Bm	0.27	0/796	0.60	0/1057
54	Bk	0.26	0/1026	0.60	0/1355
55	Bj	0.27	0/977	0.59	0/1304
56	Bi	0.29	0/1097	0.55	0/1468
57	Bg	0.29	0/718	0.47	0/969
58	Bd	0.26	0/572	0.54	0/766
59	Bb	0.27	0/1165	0.51	0/1554
60	Ba	0.27	0/1096	0.55	0/1457
61	BO	0.26	0/1832	0.55	0/2446
62	BN	0.27	0/1753	0.55	0/2338
63	BL	0.25	0/1265	0.50	0/1689
64	BK	0.28	0/1616	0.59	0/2165
65	BI	0.26	0/1543	0.56	0/2059
66	Be	0.31	0/1943	0.56	0/2616
67	AK	0.29	0/1164	0.50	0/1565
68	A6	0.30	0/1490	0.56	0/2002
69	Bf	0.28	0/3281	0.57	0/4409
70	AY	0.30	0/477	0.53	0/630
71	Bv	0.27	0/1120	0.52	0/1511
72	Bh	0.25	0/1205	0.54	0/1603
73	BF	0.32	0/1604	0.88	1/2487 (0.0%)
74	BG	0.41	0/4383	0.83	0/6835
75	BH	0.39	0/2813	0.85	3/4377 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Bs	0.23	0/400	0.53	0/531
77	BV	0.27	0/989	0.51	0/1322
78	Az	0.25	0/340	0.58	0/450
79	AQ	0.31	0/809	0.64	0/1091
80	AR	0.30	0/665	0.52	0/905
81	AV	0.41	0/846	0.63	0/1132
82	AW	0.34	0/674	0.54	0/904
83	A4	0.31	0/1628	0.56	0/2201
84	A7	0.27	0/2380	0.51	0/3242
85	A	0.22	0/30	0.50	0/40
All	All	0.43	2/214658 (0.0%)	0.76	145/314827 (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
40	AP	0	1
53	Bm	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1513	G	N9-C4	-5.76	1.33	1.38
1	AA	1513	G	N3-C4	-5.00	1.31	1.35

The worst 5 of 145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BB	528	PSU	P-O3'-C3'	-9.83	107.91	119.70
1	AA	1513	G	N3-C4-N9	-9.28	120.43	126.00
4	BB	515	G	P-O3'-C3'	-8.81	109.12	119.70
1	AA	673	C	C2-N1-C1'	8.70	128.37	118.80
4	BB	531	C	P-O3'-C3'	-8.51	109.49	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	AP	240	TRP	Peptide
53	Bm	21	LYS	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
8	BP	152/189 (80%)	146 (96%)	5 (3%)	1 (1%)	19 38
9	BQ	201/221 (91%)	192 (96%)	9 (4%)	0	100 100
10	BR	148/166 (89%)	145 (98%)	3 (2%)	0	100 100
11	BS	176/179 (98%)	160 (91%)	16 (9%)	0	100 100
12	BT	190/260 (73%)	186 (98%)	4 (2%)	0	100 100
13	BU	147/159 (92%)	135 (92%)	12 (8%)	0	100 100
14	BW	127/139 (91%)	125 (98%)	2 (2%)	0	100 100
15	BY	60/125 (48%)	57 (95%)	3 (5%)	0	100 100
16	BX	115/164 (70%)	113 (98%)	2 (2%)	0	100 100
17	BZ	118/143 (82%)	117 (99%)	1 (1%)	0	100 100
18	Bp	71/82 (87%)	67 (94%)	4 (6%)	0	100 100
19	Bq	48/51 (94%)	44 (92%)	4 (8%)	0	100 100
20	Br	364/374 (97%)	339 (93%)	25 (7%)	0	100 100
21	Bt	95/106 (90%)	87 (92%)	8 (8%)	0	100 100
22	Bw	228/257 (89%)	221 (97%)	7 (3%)	0	100 100
23	Bx	228/276 (83%)	217 (95%)	10 (4%)	1 (0%)	30 52
24	Bl	142/149 (95%)	135 (95%)	7 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Bu	236/308 (77%)	230 (98%)	6 (2%)	0	100	100
26	By	176/189 (93%)	168 (96%)	8 (4%)	0	100	100
27	A0	214/256 (84%)	203 (95%)	10 (5%)	1 (0%)	25	47
28	A2	179/190 (94%)	171 (96%)	8 (4%)	0	100	100
29	A5	182/220 (83%)	171 (94%)	11 (6%)	0	100	100
30	AD	85/172 (49%)	81 (95%)	4 (5%)	0	100	100
31	A8	51/57 (90%)	47 (92%)	3 (6%)	1 (2%)	6	12
32	AE	150/174 (86%)	131 (87%)	19 (13%)	0	100	100
33	AG	139/151 (92%)	129 (93%)	10 (7%)	0	100	100
34	AI	100/152 (66%)	98 (98%)	2 (2%)	0	100	100
35	AH	133/144 (92%)	122 (92%)	11 (8%)	0	100	100
36	AJ	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
37	AL	120/142 (84%)	116 (97%)	4 (3%)	0	100	100
38	AM	131/153 (86%)	116 (88%)	14 (11%)	1 (1%)	16	34
39	AO	147/167 (88%)	141 (96%)	6 (4%)	0	100	100
40	AP	218/266 (82%)	199 (91%)	19 (9%)	0	100	100
41	AS	138/143 (96%)	126 (91%)	12 (9%)	0	100	100
42	AU	69/113 (61%)	68 (99%)	1 (1%)	0	100	100
43	AX	206/214 (96%)	199 (97%)	7 (3%)	0	100	100
44	AZ	53/103 (52%)	50 (94%)	3 (6%)	0	100	100
45	A3	228/250 (91%)	217 (95%)	11 (5%)	0	100	100
46	AT	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
47	A1	258/273 (94%)	239 (93%)	19 (7%)	0	100	100
48	AC	206/277 (74%)	199 (97%)	7 (3%)	0	100	100
49	Bc	142/146 (97%)	133 (94%)	9 (6%)	0	100	100
50	Bz	31/34 (91%)	26 (84%)	5 (16%)	0	100	100
51	Bo	87/93 (94%)	82 (94%)	4 (5%)	1 (1%)	12	26
52	Bn	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
53	Bm	96/109 (88%)	84 (88%)	12 (12%)	0	100	100
54	Bk	121/127 (95%)	113 (93%)	8 (7%)	0	100	100
55	Bj	114/170 (67%)	112 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	Bi	129/132 (98%)	128 (99%)	1 (1%)	0	100	100
57	Bg	90/105 (86%)	89 (99%)	1 (1%)	0	100	100
58	Bd	67/71 (94%)	62 (92%)	5 (8%)	0	100	100
59	Bb	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
60	Ba	126/133 (95%)	121 (96%)	5 (4%)	0	100	100
61	BO	219/222 (99%)	213 (97%)	6 (3%)	0	100	100
62	BN	208/218 (95%)	194 (93%)	14 (7%)	0	100	100
63	BL	152/194 (78%)	145 (95%)	7 (5%)	0	100	100
64	BK	190/213 (89%)	181 (95%)	9 (5%)	0	100	100
65	BI	189/193 (98%)	180 (95%)	9 (5%)	0	100	100
66	Be	253/260 (97%)	247 (98%)	6 (2%)	0	100	100
67	AK	140/149 (94%)	132 (94%)	8 (6%)	0	100	100
68	A6	176/190 (93%)	169 (96%)	7 (4%)	0	100	100
69	Bf	398/429 (93%)	389 (98%)	9 (2%)	0	100	100
70	AY	57/66 (86%)	51 (90%)	6 (10%)	0	100	100
71	Bv	139/192 (72%)	133 (96%)	6 (4%)	0	100	100
72	Bh	139/188 (74%)	135 (97%)	4 (3%)	0	100	100
76	Bs	48/128 (38%)	46 (96%)	2 (4%)	0	100	100
77	BV	120/130 (92%)	116 (97%)	4 (3%)	0	100	100
78	Az	35/279 (12%)	32 (91%)	3 (9%)	0	100	100
79	AQ	98/117 (84%)	96 (98%)	2 (2%)	0	100	100
80	AR	86/194 (44%)	81 (94%)	5 (6%)	0	100	100
81	AV	101/111 (91%)	98 (97%)	3 (3%)	0	100	100
82	AW	83/86 (96%)	76 (92%)	7 (8%)	0	100	100
83	A4	196/202 (97%)	185 (94%)	11 (6%)	0	100	100
84	A7	295/318 (93%)	281 (95%)	14 (5%)	0	100	100
85	A	2/4 (50%)	2 (100%)	0	0	100	100
All	All	10823/12853 (84%)	10283 (95%)	534 (5%)	6 (0%)	50	71

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	Bo	68	ALA

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Mol	Chain	Res	Type
31	A8	9	SER
27	A0	108	THR
8	BP	32	ASP
23	Bx	52	ASP

5.3.2 Protein sidechains (i)

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
8	BP	134/158 (85%)	118 (88%)	16 (12%)	4 8
9	BQ	176/193 (91%)	166 (94%)	10 (6%)	17 37
10	BR	128/144 (89%)	124 (97%)	4 (3%)	35 62
11	BS	159/160 (99%)	150 (94%)	9 (6%)	17 37
12	BT	153/198 (77%)	142 (93%)	11 (7%)	12 26
13	BU	125/134 (93%)	116 (93%)	9 (7%)	12 26
14	BW	101/108 (94%)	96 (95%)	5 (5%)	20 43
15	BY	55/102 (54%)	54 (98%)	1 (2%)	54 77
16	BX	104/136 (76%)	95 (91%)	9 (9%)	8 17
17	BZ	105/125 (84%)	92 (88%)	13 (12%)	4 7
18	Bp	70/77 (91%)	60 (86%)	10 (14%)	2 5
19	Bq	46/47 (98%)	41 (89%)	5 (11%)	5 10
20	Br	303/310 (98%)	283 (93%)	20 (7%)	14 30
21	Bt	87/95 (92%)	83 (95%)	4 (5%)	23 46
22	Bw	193/213 (91%)	183 (95%)	10 (5%)	19 41
23	Bx	196/229 (86%)	182 (93%)	14 (7%)	12 26
24	Bl	122/126 (97%)	115 (94%)	7 (6%)	17 37
25	Bu	193/247 (78%)	180 (93%)	13 (7%)	13 29
26	By	165/172 (96%)	148 (90%)	17 (10%)	6 12
27	A0	189/218 (87%)	172 (91%)	17 (9%)	8 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	A2	157/160 (98%)	145 (92%)	12 (8%)	11 23
29	A5	145/180 (81%)	128 (88%)	17 (12%)	4 8
30	AD	76/131 (58%)	64 (84%)	12 (16%)	2 3
31	A8	47/50 (94%)	46 (98%)	1 (2%)	48 73
32	AE	135/156 (86%)	120 (89%)	15 (11%)	5 10
33	AG	124/131 (95%)	116 (94%)	8 (6%)	14 31
34	AI	90/128 (70%)	77 (86%)	13 (14%)	2 5
35	AH	102/112 (91%)	95 (93%)	7 (7%)	13 28
36	AJ	108/109 (99%)	97 (90%)	11 (10%)	6 12
37	AL	96/122 (79%)	84 (88%)	12 (12%)	3 7
38	AM	116/133 (87%)	101 (87%)	15 (13%)	3 6
39	AO	124/137 (90%)	116 (94%)	8 (6%)	14 31
40	AP	182/204 (89%)	160 (88%)	22 (12%)	4 8
41	AS	115/118 (98%)	108 (94%)	7 (6%)	15 34
42	AU	62/94 (66%)	57 (92%)	5 (8%)	9 20
43	AX	176/180 (98%)	155 (88%)	21 (12%)	4 8
44	AZ	48/84 (57%)	40 (83%)	8 (17%)	2 3
45	A3	184/207 (89%)	163 (89%)	21 (11%)	4 9
46	AT	103/116 (89%)	93 (90%)	10 (10%)	6 14
47	A1	219/231 (95%)	194 (89%)	25 (11%)	4 9
48	AC	183/243 (75%)	168 (92%)	15 (8%)	9 20
49	Bc	128/130 (98%)	118 (92%)	10 (8%)	10 22
50	Bz	30/31 (97%)	25 (83%)	5 (17%)	2 3
51	Bo	72/76 (95%)	69 (96%)	3 (4%)	25 50
52	Bn	68/71 (96%)	65 (96%)	3 (4%)	24 48
53	Bm	81/90 (90%)	69 (85%)	12 (15%)	2 4
54	Bk	106/114 (93%)	100 (94%)	6 (6%)	17 37
55	Bj	99/137 (72%)	91 (92%)	8 (8%)	9 20
56	Bi	116/117 (99%)	110 (95%)	6 (5%)	19 41
57	Bg	81/92 (88%)	79 (98%)	2 (2%)	42 68
58	Bd	57/59 (97%)	53 (93%)	4 (7%)	12 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
59	Bb	115/116 (99%)	105 (91%)	10 (9%)	8 17
60	Ba	114/117 (97%)	103 (90%)	11 (10%)	7 14
61	BO	194/195 (100%)	186 (96%)	8 (4%)	26 51
62	BN	181/188 (96%)	168 (93%)	13 (7%)	12 26
63	BL	134/167 (80%)	112 (84%)	22 (16%)	2 3
64	BK	168/185 (91%)	154 (92%)	14 (8%)	9 19
65	BI	163/165 (99%)	157 (96%)	6 (4%)	29 55
66	Be	191/204 (94%)	184 (96%)	7 (4%)	29 55
67	AK	118/124 (95%)	110 (93%)	8 (7%)	13 28
68	A6	157/166 (95%)	139 (88%)	18 (12%)	4 9
69	Bf	341/360 (95%)	324 (95%)	17 (5%)	20 43
70	AY	48/53 (91%)	43 (90%)	5 (10%)	5 11
71	Bv	119/160 (74%)	104 (87%)	15 (13%)	3 7
72	Bh	128/162 (79%)	115 (90%)	13 (10%)	6 12
76	Bs	41/111 (37%)	38 (93%)	3 (7%)	11 25
77	BV	99/116 (85%)	85 (86%)	14 (14%)	3 5
78	Az	36/216 (17%)	26 (72%)	10 (28%)	0 0
79	AQ	90/104 (86%)	76 (84%)	14 (16%)	2 3
80	AR	71/151 (47%)	61 (86%)	10 (14%)	3 5
81	AV	90/97 (93%)	81 (90%)	9 (10%)	6 13
82	AW	74/75 (99%)	64 (86%)	10 (14%)	3 6
83	A4	172/187 (92%)	141 (82%)	31 (18%)	1 2
84	A7	255/268 (95%)	222 (87%)	33 (13%)	3 6
85	A	4/4 (100%)	4 (100%)	0	100 100
All	All	9337/10826 (86%)	8508 (91%)	829 (9%)	10 17

5 of 829 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	AC	135	LEU
63	BL	70	GLU
84	A7	77	ASN
49	Bc	90	VAL
48	AC	133	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
84	A7	46	ASN
81	AV	75	GLN
62	BN	108	ASN
59	Bb	116	GLN
70	AY	60	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1807/2280 (79%)	483 (26%)	19 (1%)
2	AB	17/19 (89%)	8 (47%)	0
3	BA	1553/1920 (80%)	293 (18%)	8 (0%)
4	BB	1102/1536 (71%)	209 (18%)	3 (0%)
5	BC	157/209 (75%)	27 (17%)	0
6	BD	118/119 (99%)	16 (13%)	1 (0%)
7	BE	161/216 (74%)	23 (14%)	2 (1%)
73	BF	66/78 (84%)	18 (27%)	0
74	BG	182/183 (99%)	30 (16%)	1 (0%)
75	BH	114/136 (83%)	21 (18%)	0
All	All	5277/6696 (78%)	1128 (21%)	34 (0%)

5 of 1128 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	32	C
1	AA	34	G
1	AA	45	C
1	AA	46	OMC
1	AA	51	G

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	BB	1272	U
4	BB	1508	C
7	BE	96	C
1	AA	921	G
1	AA	911	A

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

129 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	$\#\|Z\| > 2$
4	PSU	BB	530	4	18,21,22	1.41	3 (16%)	22,30,33	2.10	5 (22%)
1	PSU	AA	131	1	18,21,22	4.37	7 (38%)	22,30,33	1.95	5 (22%)
3	A2M	BA	254	3	18,25,26	3.62	7 (38%)	18,36,39	3.82	4 (22%)
3	PSU	BA	1009	3	18,21,22	4.40	7 (38%)	22,30,33	1.90	5 (22%)
3	A2M	BA	743	4,3	18,25,26	3.61	7 (38%)	18,36,39	3.64	4 (22%)
4	A2M	BB	646	4	18,25,26	3.60	7 (38%)	18,36,39	3.69	4 (22%)
4	A2M	BB	622	4,3	18,25,26	3.60	7 (38%)	18,36,39	3.76	4 (22%)
4	OMU	BB	578	88,4	19,22,23	2.97	8 (42%)	26,31,34	1.82	5 (19%)
3	OMG	BA	1267	3	18,26,27	2.47	8 (44%)	19,38,41	1.65	4 (21%)
4	OMU	BB	73	4	19,22,23	2.99	8 (42%)	26,31,34	1.73	4 (15%)
3	A2M	BA	762	3	18,25,26	3.62	7 (38%)	18,36,39	3.86	4 (22%)
1	PSU	AA	2045	1	18,21,22	4.41	7 (38%)	22,30,33	1.75	5 (22%)
3	PSU	BA	1248	3,86	18,21,22	4.42	7 (38%)	22,30,33	1.73	4 (18%)
4	OMU	BB	1375	4	19,22,23	2.93	8 (42%)	26,31,34	1.79	5 (19%)
5	OMU	BC	7	5,3	19,22,23	2.97	8 (42%)	26,31,34	1.74	4 (15%)
4	A2M	BB	545	4,86	18,25,26	3.69	8 (44%)	18,36,39	3.86	5 (27%)
3	PSU	BA	1169	3	18,21,22	4.46	7 (38%)	22,30,33	1.86	5 (22%)
4	PSU	BB	1334	4	18,21,22	4.38	7 (38%)	22,30,33	1.84	5 (22%)
3	PSU	BA	1614	4,3	18,21,22	4.39	7 (38%)	22,30,33	1.87	5 (22%)
5	A2M	BC	43	5	18,25,26	3.60	7 (38%)	18,36,39	3.74	4 (22%)
3	PSU	BA	1086	3,86	18,21,22	4.41	7 (38%)	22,30,33	1.84	5 (22%)
4	OMC	BB	1175	4	19,22,23	2.92	8 (42%)	26,31,34	0.78	0
5	PSU	BC	74	5	18,21,22	4.47	7 (38%)	22,30,33	1.80	5 (22%)
4	OMG	BB	1062	4	18,26,27	2.51	8 (44%)	19,38,41	1.56	4 (21%)
1	OMG	AA	1517	1	18,26,27	2.47	8 (44%)	19,38,41	1.59	4 (21%)
4	OMC	BB	601	4	19,22,23	2.93	8 (42%)	26,31,34	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMC	AA	46	1	19,22,23	2.84	8 (42%)	26,31,34	0.85	0
3	OMG	BA	1605	3	18,26,27	2.51	8 (44%)	19,38,41	1.61	5 (26%)
5	A2M	BC	163	5,3	18,25,26	3.60	8 (44%)	18,36,39	3.76	4 (22%)
4	OMG	BB	552	4	18,26,27	2.46	8 (44%)	19,38,41	1.52	4 (21%)
4	PSU	BB	644	4	18,21,22	4.39	7 (38%)	22,30,33	1.84	5 (22%)
1	PSU	AA	2146	1	18,21,22	4.30	7 (38%)	22,30,33	1.76	5 (22%)
4	OMC	BB	1413	4	19,22,23	2.86	8 (42%)	26,31,34	0.84	0
1	OMG	AA	1931	1	18,26,27	2.51	8 (44%)	19,38,41	1.63	5 (26%)
3	OMC	BA	760	3	19,22,23	2.92	8 (42%)	26,31,34	0.75	0
1	MA6	AA	2260	1	18,26,27	1.10	1 (5%)	19,38,41	3.31	2 (10%)
1	OMC	AA	2134	1	19,22,23	2.83	8 (42%)	26,31,34	0.75	0
3	OMU	BA	1448	3	19,22,23	2.98	8 (42%)	26,31,34	1.79	5 (19%)
4	PSU	BB	1280	4	18,21,22	4.41	8 (44%)	22,30,33	1.85	6 (27%)
3	A2M	BA	927	3	18,25,26	3.61	7 (38%)	18,36,39	3.65	4 (22%)
4	PSU	BB	522	4	18,21,22	4.47	7 (38%)	22,30,33	1.75	5 (22%)
4	5MC	BB	542	4,86	18,22,23	3.40	7 (38%)	26,32,35	1.04	2 (7%)
3	PSU	BA	1129	3	18,21,22	4.43	7 (38%)	22,30,33	1.83	5 (22%)
3	PSU	BA	1609	3	18,21,22	4.45	7 (38%)	22,30,33	1.84	5 (22%)
1	OMG	AA	1700	1	18,26,27	2.45	8 (44%)	19,38,41	1.66	5 (26%)
4	PSU	BB	611	4	18,21,22	4.37	7 (38%)	22,30,33	1.72	4 (18%)
3	A2M	BA	1665	4,3	18,25,26	3.62	8 (44%)	18,36,39	3.61	4 (22%)
1	A2M	AA	56	86,1	18,25,26	3.63	8 (44%)	18,36,39	3.62	4 (22%)
3	OMG	BA	915	3	18,26,27	2.48	8 (44%)	19,38,41	1.58	4 (21%)
3	OMU	BA	916	3	19,22,23	2.96	8 (42%)	26,31,34	1.74	5 (19%)
3	OMC	BA	1608	3	19,22,23	2.89	8 (42%)	26,31,34	0.78	0
4	PSU	BB	1429	4	18,21,22	4.33	8 (44%)	22,30,33	1.89	5 (22%)
3	A2M	BA	1024	3	18,25,26	3.56	7 (38%)	18,36,39	3.72	4 (22%)
1	OMU	AA	57	1	19,22,23	2.93	8 (42%)	26,31,34	1.75	5 (19%)
1	A2M	AA	2096	1	18,25,26	3.62	7 (38%)	18,36,39	3.89	4 (22%)
4	PSU	BB	1076	4	18,21,22	4.37	7 (38%)	22,30,33	1.92	5 (22%)
4	OMG	BB	1094	4	18,26,27	2.47	8 (44%)	19,38,41	1.63	5 (26%)
1	OMG	AA	1895	86,1	18,26,27	2.47	8 (44%)	19,38,41	1.54	4 (21%)
3	PSU	BA	258	3	18,21,22	4.46	7 (38%)	22,30,33	1.84	5 (22%)
3	OMC	BA	1329	3	19,22,23	3.03	8 (42%)	26,31,34	0.74	0
4	OMU	BB	1093	4	19,22,23	3.00	8 (42%)	26,31,34	1.73	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A2M	BA	996	3	18,25,26	3.61	7 (38%)	18,36,39	3.66	4 (22%)
4	A2M	BB	400	4	18,25,26	3.63	8 (44%)	18,36,39	3.61	5 (27%)
4	A2M	BB	609	4	18,25,26	3.61	7 (38%)	18,36,39	3.60	4 (22%)
1	OMU	AA	2154	1	19,22,23	2.99	8 (42%)	26,31,34	1.87	5 (19%)
1	OMG	AA	1676	88,1	18,26,27	2.54	8 (44%)	19,38,41	1.60	4 (21%)
1	B8N	AA	1596	1	24,29,30	3.03	6 (25%)	29,42,45	1.75	5 (17%)
4	OMG	BB	71	4	18,26,27	2.51	8 (44%)	19,38,41	1.61	4 (21%)
3	OMU	BA	1742	3	19,22,23	2.94	8 (42%)	26,31,34	1.73	4 (15%)
1	A2M	AA	2153	1	18,25,26	3.63	8 (44%)	18,36,39	3.79	4 (22%)
4	OMU	BB	1435	4	19,22,23	2.96	8 (42%)	26,31,34	1.69	4 (15%)
4	A2M	BB	1201	4	18,25,26	3.61	8 (44%)	18,36,39	3.73	4 (22%)
4	PSU	BB	1398	4	18,21,22	4.42	7 (38%)	22,30,33	1.89	6 (27%)
4	OMG	BB	659	4	18,26,27	2.46	8 (44%)	19,38,41	1.59	3 (15%)
1	OMU	AA	1899	1	19,22,23	2.99	8 (42%)	26,31,34	1.76	5 (19%)
4	OMG	BB	1269	4	18,26,27	2.42	8 (44%)	19,38,41	1.52	4 (21%)
4	OMC	BB	1264	4	19,22,23	2.93	8 (42%)	26,31,34	0.85	1 (3%)
3	OMG	BA	1028	3	18,26,27	2.49	8 (44%)	19,38,41	1.55	3 (15%)
1	OMU	AA	2054	1	19,22,23	2.97	8 (42%)	26,31,34	1.72	5 (19%)
4	PSU	BB	1229	4	18,21,22	4.45	7 (38%)	22,30,33	1.88	5 (22%)
4	PSU	BB	528	4	18,21,22	1.49	4 (22%)	22,30,33	2.00	5 (22%)
4	PSU	BB	615	4	18,21,22	4.37	7 (38%)	22,30,33	1.78	5 (22%)
4	OMC	BB	377	4	19,22,23	2.98	8 (42%)	26,31,34	0.71	0
1	OMG	AA	2227	1	18,26,27	2.41	8 (44%)	19,38,41	1.56	4 (21%)
3	OMG	BA	1709	3	18,26,27	2.50	8 (44%)	19,38,41	1.60	5 (26%)
1	OMC	AA	66	1	19,22,23	2.90	8 (42%)	26,31,34	0.77	0
1	PSU	AA	1276	1	18,21,22	4.27	7 (38%)	22,30,33	1.81	5 (22%)
4	PSU	BB	524	4	18,21,22	4.39	7 (38%)	22,30,33	1.75	5 (22%)
4	OMG	BB	1245	4	18,26,27	2.50	8 (44%)	19,38,41	1.57	5 (26%)
4	PSU	BB	1409	4	18,21,22	4.43	7 (38%)	22,30,33	1.76	5 (22%)
4	PSU	BB	1160	4	18,21,22	4.39	7 (38%)	22,30,33	1.88	5 (22%)
5	A2M	BC	41	5	18,25,26	3.61	7 (38%)	18,36,39	3.83	4 (22%)
1	OMU	AA	2123	1	19,22,23	2.87	7 (36%)	26,31,34	1.80	4 (15%)
5	OMG	BC	75	5	18,26,27	2.54	8 (44%)	19,38,41	1.51	4 (21%)
4	A2M	BB	588	3,4,87	18,25,26	3.61	7 (38%)	18,36,39	3.74	5 (27%)
4	A2M	BB	95	4	18,25,26	3.61	8 (44%)	18,36,39	3.64	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OMG	BB	1247	4	18,26,27	2.49	8 (44%)	19,38,41	1.54	4 (21%)
1	7MG	AA	2070	1	22,26,27	4.14	10 (45%)	29,39,42	2.07	9 (31%)
4	OMU	BB	685	4	19,22,23	2.95	8 (42%)	26,31,34	1.77	4 (15%)
1	OMG	AA	1531	1	18,26,27	2.36	8 (44%)	19,38,41	1.57	5 (26%)
4	PSU	BB	629	4	18,21,22	4.40	7 (38%)	22,30,33	1.68	4 (18%)
3	1MA	BA	742	3,86	16,25,26	3.94	4 (25%)	18,37,40	1.79	3 (16%)
4	PSU	BB	1319	4	18,21,22	4.39	7 (38%)	22,30,33	1.87	6 (27%)
3	A2M	BA	1620	4,3,86	18,25,26	3.62	7 (38%)	18,36,39	3.77	4 (22%)
3	PSU	BA	452	3	18,21,22	4.46	7 (38%)	22,30,33	1.79	5 (22%)
1	PSU	AA	61	1	18,21,22	4.42	7 (38%)	22,30,33	1.82	5 (22%)
1	A2M	AA	721	88,86,1	18,25,26	3.70	8 (44%)	18,36,39	3.89	4 (22%)
1	OMU	AA	714	1	19,22,23	2.84	8 (42%)	26,31,34	1.76	4 (15%)
3	OMU	BA	1181	3	19,22,23	2.97	8 (42%)	26,31,34	1.79	5 (19%)
3	A2M	BA	746	3	18,25,26	3.61	7 (38%)	18,36,39	3.89	4 (22%)
4	5MC	BB	1324	4	18,22,23	3.48	7 (38%)	26,32,35	1.21	1 (3%)
4	PSU	BB	518	4	18,21,22	4.46	7 (38%)	22,30,33	1.86	5 (22%)
3	OMG	BA	1621	4,3	18,26,27	2.46	8 (44%)	19,38,41	1.52	4 (21%)
3	OMU	BA	46	3	19,22,23	2.96	8 (42%)	26,31,34	1.79	4 (15%)
3	OMG	BA	925	3	18,26,27	2.48	8 (44%)	19,38,41	1.55	6 (31%)
1	PSU	AA	1619	1	18,21,22	4.49	8 (44%)	22,30,33	1.67	4 (18%)
1	OMU	AA	36	1	19,22,23	2.80	7 (36%)	26,31,34	1.87	5 (19%)
4	PSU	BB	1210	4	18,21,22	4.40	7 (38%)	22,30,33	1.79	5 (22%)
1	OMU	AA	1652	1	19,22,23	3.07	8 (42%)	26,31,34	1.65	4 (15%)
4	A2M	BB	1388	4	18,25,26	3.61	8 (44%)	18,36,39	3.85	4 (22%)
3	PSU	BA	737	3	18,21,22	4.34	7 (38%)	22,30,33	1.86	5 (22%)
3	OMC	BA	1006	3	19,22,23	2.89	8 (42%)	26,31,34	0.76	0
4	PSU	BB	680	4,86	18,21,22	4.37	8 (44%)	22,30,33	1.87	5 (22%)
1	PSU	AA	1592	1	18,21,22	4.39	7 (38%)	22,30,33	1.75	5 (22%)
1	MA6	AA	2261	1	18,26,27	1.17	1 (5%)	19,38,41	3.09	2 (10%)
4	PSU	BB	455	4	18,21,22	4.33	8 (44%)	22,30,33	1.94	5 (22%)
4	OMG	BB	673	4	18,26,27	2.47	8 (44%)	19,38,41	1.60	3 (15%)
3	PSU	BA	1258	3	18,21,22	4.45	7 (38%)	22,30,33	1.83	5 (22%)
4	A2M	BB	1400	4,86	18,25,26	3.61	7 (38%)	18,36,39	3.79	4 (22%)

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
4	PSU	BB	530	4	-	0/7/25/26	0/2/2/2
1	PSU	AA	131	1	-	0/7/25/26	0/2/2/2
3	A2M	BA	254	3	-	1/5/27/28	0/3/3/3
3	PSU	BA	1009	3	-	0/7/25/26	0/2/2/2
3	A2M	BA	743	4,3	-	1/5/27/28	0/3/3/3
4	A2M	BB	646	4	-	0/5/27/28	0/3/3/3
4	A2M	BB	622	4,3	-	0/5/27/28	0/3/3/3
4	OMU	BB	578	88,4	-	5/9/27/28	0/2/2/2
3	OMG	BA	1267	3	-	0/5/27/28	0/3/3/3
4	OMU	BB	73	4	-	0/9/27/28	0/2/2/2
3	A2M	BA	762	3	-	0/5/27/28	0/3/3/3
1	PSU	AA	2045	1	-	0/7/25/26	0/2/2/2
3	PSU	BA	1248	3,86	-	2/7/25/26	0/2/2/2
4	OMU	BB	1375	4	-	0/9/27/28	0/2/2/2
5	OMU	BC	7	5,3	-	0/9/27/28	0/2/2/2
4	A2M	BB	545	4,86	-	2/5/27/28	0/3/3/3
3	PSU	BA	1169	3	-	0/7/25/26	0/2/2/2
4	PSU	BB	1334	4	-	0/7/25/26	0/2/2/2
3	PSU	BA	1614	4,3	-	2/7/25/26	0/2/2/2
5	A2M	BC	43	5	-	1/5/27/28	0/3/3/3
3	PSU	BA	1086	3,86	-	0/7/25/26	0/2/2/2
4	OMC	BB	1175	4	-	0/9/27/28	0/2/2/2
5	PSU	BC	74	5	-	2/7/25/26	0/2/2/2
4	OMG	BB	1062	4	-	3/5/27/28	0/3/3/3
1	OMG	AA	1517	1	-	0/5/27/28	0/3/3/3
4	OMC	BB	601	4	-	0/9/27/28	0/2/2/2
1	OMC	AA	46	1	-	2/9/27/28	0/2/2/2
3	OMG	BA	1605	3	-	2/5/27/28	0/3/3/3
5	A2M	BC	163	5,3	-	1/5/27/28	0/3/3/3
4	OMG	BB	552	4	-	2/5/27/28	0/3/3/3
4	PSU	BB	644	4	-	0/7/25/26	0/2/2/2
1	PSU	AA	2146	1	-	2/7/25/26	0/2/2/2
4	OMC	BB	1413	4	-	0/9/27/28	0/2/2/2
1	OMG	AA	1931	1	-	0/5/27/28	0/3/3/3
3	OMC	BA	760	3	-	0/9/27/28	0/2/2/2
1	MA6	AA	2260	1	-	0/7/29/30	0/3/3/3
1	OMC	AA	2134	1	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	BA	1448	3	-	2/9/27/28	0/2/2/2
4	PSU	BB	1280	4	-	0/7/25/26	0/2/2/2
3	A2M	BA	927	3	-	0/5/27/28	0/3/3/3
4	PSU	BB	522	4	-	2/7/25/26	0/2/2/2
4	5MC	BB	542	4,86	-	0/7/25/26	0/2/2/2
3	PSU	BA	1129	3	-	0/7/25/26	0/2/2/2
3	PSU	BA	1609	3	-	0/7/25/26	0/2/2/2
1	OMG	AA	1700	1	-	0/5/27/28	0/3/3/3
4	PSU	BB	611	4	-	0/7/25/26	0/2/2/2
3	A2M	BA	1665	4,3	-	3/5/27/28	0/3/3/3
1	A2M	AA	56	86,1	-	0/5/27/28	0/3/3/3
3	OMG	BA	915	3	-	0/5/27/28	0/3/3/3
3	OMU	BA	916	3	-	0/9/27/28	0/2/2/2
3	OMC	BA	1608	3	-	2/9/27/28	0/2/2/2
4	PSU	BB	1429	4	-	0/7/25/26	0/2/2/2
3	A2M	BA	1024	3	-	1/5/27/28	0/3/3/3
1	OMU	AA	57	1	-	1/9/27/28	0/2/2/2
1	A2M	AA	2096	1	-	1/5/27/28	0/3/3/3
4	PSU	BB	1076	4	-	0/7/25/26	0/2/2/2
4	OMG	BB	1094	4	-	0/5/27/28	0/3/3/3
1	OMG	AA	1895	86,1	-	0/5/27/28	0/3/3/3
3	PSU	BA	258	3	-	0/7/25/26	0/2/2/2
3	OMC	BA	1329	3	-	1/9/27/28	0/2/2/2
4	OMU	BB	1093	4	-	0/9/27/28	0/2/2/2
3	A2M	BA	996	3	-	0/5/27/28	0/3/3/3
4	A2M	BB	400	4	-	2/5/27/28	0/3/3/3
4	A2M	BB	609	4	-	1/5/27/28	0/3/3/3
1	OMU	AA	2154	1	-	3/9/27/28	0/2/2/2
1	OMG	AA	1676	88,1	-	2/5/27/28	0/3/3/3
1	B8N	AA	1596	1	-	2/16/34/35	0/2/2/2
4	OMG	BB	71	4	-	0/5/27/28	0/3/3/3
3	OMU	BA	1742	3	-	0/9/27/28	0/2/2/2
1	A2M	AA	2153	1	-	1/5/27/28	0/3/3/3
4	OMU	BB	1435	4	-	0/9/27/28	0/2/2/2
4	A2M	BB	1201	4	-	2/5/27/28	0/3/3/3
4	PSU	BB	1398	4	-	0/7/25/26	0/2/2/2
4	OMG	BB	659	4	-	2/5/27/28	0/3/3/3
1	OMU	AA	1899	1	-	4/9/27/28	0/2/2/2
4	OMG	BB	1269	4	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMC	BB	1264	4	-	2/9/27/28	0/2/2/2
3	OMG	BA	1028	3	-	0/5/27/28	0/3/3/3
1	OMU	AA	2054	1	-	2/9/27/28	0/2/2/2
4	PSU	BB	1229	4	-	0/7/25/26	0/2/2/2
4	PSU	BB	528	4	-	2/7/25/26	0/2/2/2
4	PSU	BB	615	4	-	0/7/25/26	0/2/2/2
4	OMC	BB	377	4	-	0/9/27/28	0/2/2/2
1	OMG	AA	2227	1	-	0/5/27/28	0/3/3/3
3	OMG	BA	1709	3	-	0/5/27/28	0/3/3/3
1	OMC	AA	66	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	1276	1	-	0/7/25/26	0/2/2/2
4	PSU	BB	524	4	-	1/7/25/26	0/2/2/2
4	OMG	BB	1245	4	-	0/5/27/28	0/3/3/3
4	PSU	BB	1409	4	-	0/7/25/26	0/2/2/2
4	PSU	BB	1160	4	-	0/7/25/26	0/2/2/2
5	A2M	BC	41	5	-	0/5/27/28	0/3/3/3
1	OMU	AA	2123	1	-	0/9/27/28	0/2/2/2
5	OMG	BC	75	5	-	2/5/27/28	0/3/3/3
4	A2M	BB	588	3,4,87	-	2/5/27/28	0/3/3/3
4	A2M	BB	95	4	-	1/5/27/28	0/3/3/3
4	OMG	BB	1247	4	-	0/5/27/28	0/3/3/3
1	7MG	AA	2070	1	-	2/7/37/38	0/3/3/3
4	OMU	BB	685	4	-	0/9/27/28	0/2/2/2
1	OMG	AA	1531	1	-	1/5/27/28	0/3/3/3
4	PSU	BB	629	4	-	2/7/25/26	0/2/2/2
3	1MA	BA	742	3,86	-	2/3/25/26	0/3/3/3
4	PSU	BB	1319	4	-	0/7/25/26	0/2/2/2
3	A2M	BA	1620	4,3,86	-	0/5/27/28	0/3/3/3
3	PSU	BA	452	3	-	0/7/25/26	0/2/2/2
1	PSU	AA	61	1	-	2/7/25/26	0/2/2/2
1	A2M	AA	721	88,86,1	-	2/5/27/28	0/3/3/3
1	OMU	AA	714	1	-	0/9/27/28	0/2/2/2
3	OMU	BA	1181	3	-	0/9/27/28	0/2/2/2
3	A2M	BA	746	3	-	0/5/27/28	0/3/3/3
4	5MC	BB	1324	4	-	4/7/25/26	0/2/2/2
4	PSU	BB	518	4	-	0/7/25/26	0/2/2/2
3	OMG	BA	1621	4,3	-	0/5/27/28	0/3/3/3
3	OMU	BA	46	3	-	0/9/27/28	0/2/2/2
3	OMG	BA	925	3	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	1619	1	-	2/7/25/26	0/2/2/2
1	OMU	AA	36	1	-	6/9/27/28	0/2/2/2
4	PSU	BB	1210	4	-	0/7/25/26	0/2/2/2
1	OMU	AA	1652	1	-	1/9/27/28	0/2/2/2
4	A2M	BB	1388	4	-	0/5/27/28	0/3/3/3
3	PSU	BA	737	3	-	4/7/25/26	0/2/2/2
3	OMC	BA	1006	3	-	0/9/27/28	0/2/2/2
4	PSU	BB	680	4,86	-	0/7/25/26	0/2/2/2
1	PSU	AA	1592	1	-	0/7/25/26	0/2/2/2
1	MA6	AA	2261	1	-	0/7/29/30	0/3/3/3
4	PSU	BB	455	4	-	0/7/25/26	0/2/2/2
4	OMG	BB	673	4	-	1/5/27/28	0/3/3/3
3	PSU	BA	1258	3	-	2/7/25/26	0/2/2/2
4	A2M	BB	1400	4,86	-	0/5/27/28	0/3/3/3

The worst 5 of 952 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BA	742	1MA	C2-N3	14.16	1.46	1.29
1	AA	1619	PSU	C6-C5	11.69	1.48	1.35
3	BA	452	PSU	C6-C5	11.63	1.48	1.35
4	BB	522	PSU	C6-C5	11.63	1.48	1.35
3	BA	1609	PSU	C6-C5	11.61	1.48	1.35

The worst 5 of 523 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2260	MA6	N1-C6-N6	-12.94	103.43	117.06
1	AA	2261	MA6	N1-C6-N6	-12.05	104.37	117.06
3	BA	746	A2M	C5-C6-N6	10.79	136.75	120.35
3	BA	1620	A2M	C5-C6-N6	10.63	136.51	120.35
1	AA	2096	A2M	C5-C6-N6	10.63	136.50	120.35

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	BC	43	A2M	C1'-C2'-O2'-CM'
5	BC	74	PSU	C3'-C4'-C5'-O5'
5	BC	75	OMG	O4'-C4'-C5'-O5'
5	BC	75	OMG	C3'-C4'-C5'-O5'

Continued on next page...

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Mol	Chain	Res	Type	Atoms
5	BC	163	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 241 ligands modelled in this entry, 241 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	AB	1
1	AA	1
18	Bp	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AB	7:A	O3'	65:G	P	16.40

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1595:C	O3'	1596:B8N	P	3.15
1	Bp	71:SER	C	72:ARG	N	3.01

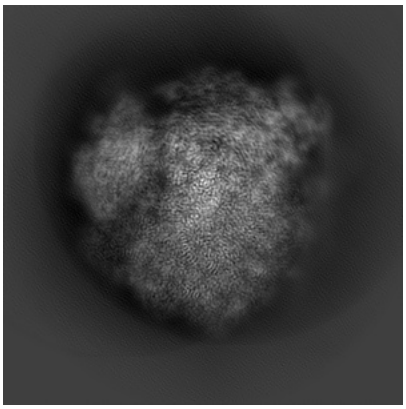
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17212. These allow visual inspection of the internal detail of the map and identification of artifacts.

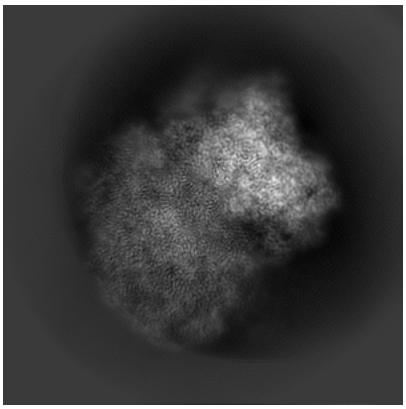
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

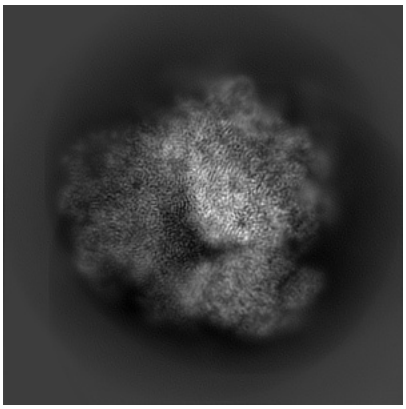
6.1.1 Primary map



X

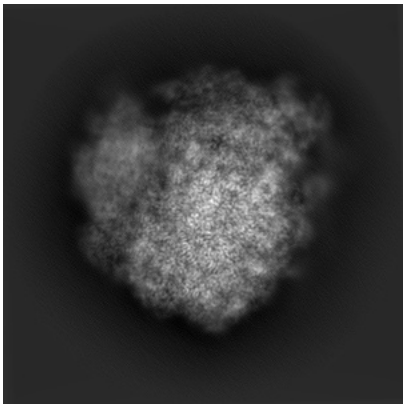


Y

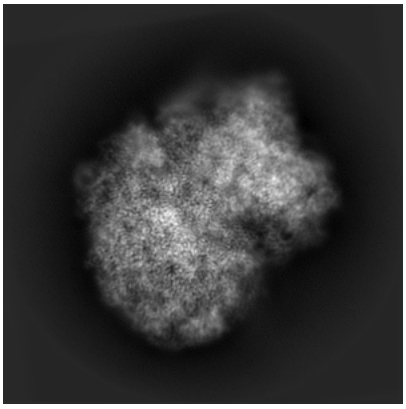


Z

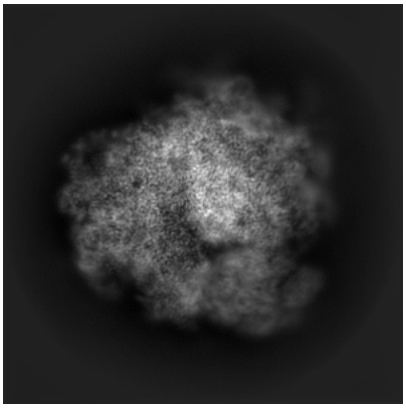
6.1.2 Raw map



X



Y

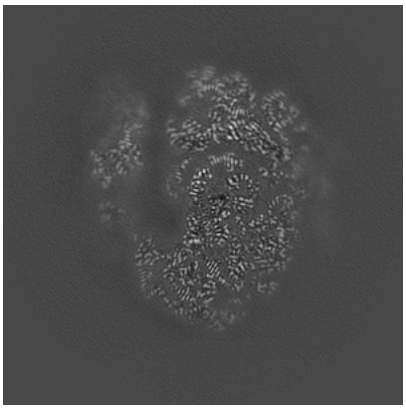


Z

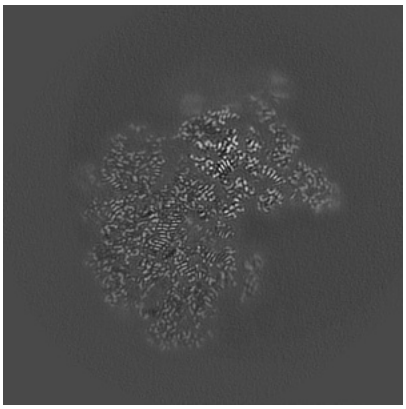
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

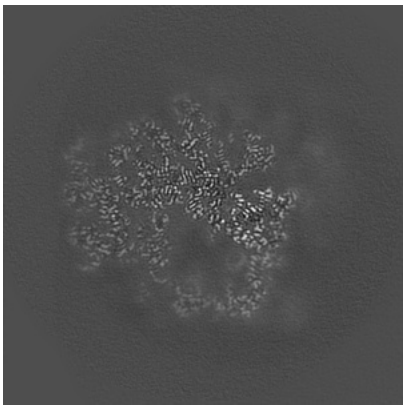
6.2.1 Primary map



X Index: 240

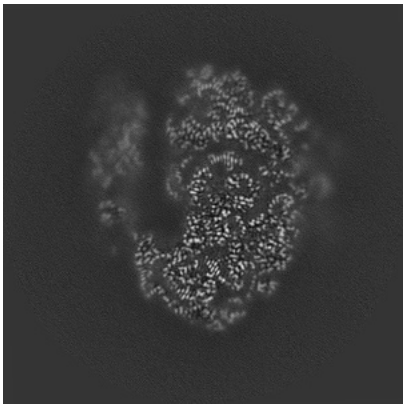


Y Index: 240

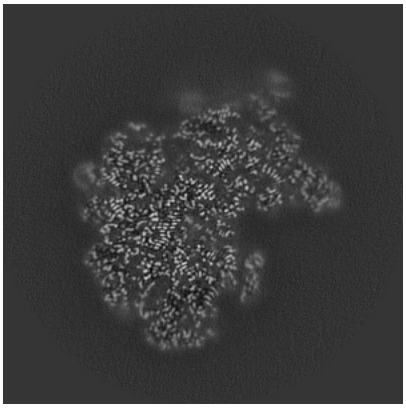


Z Index: 240

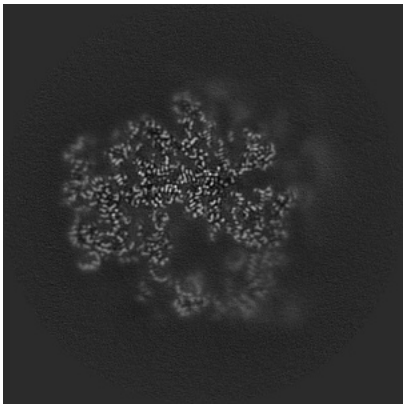
6.2.2 Raw map



X Index: 240



Y Index: 240

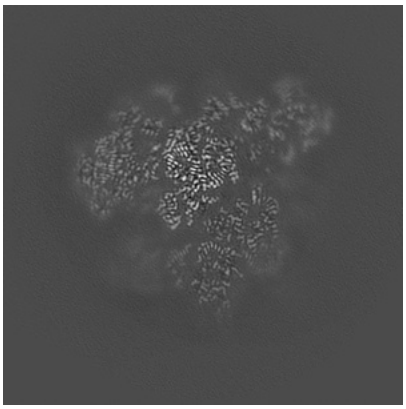


Z Index: 240

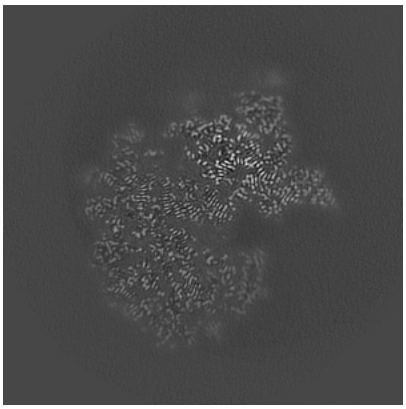
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

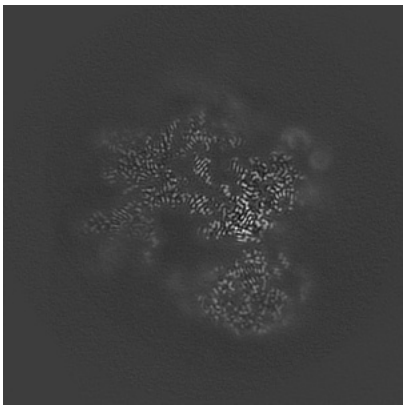
6.3.1 Primary map



X Index: 292

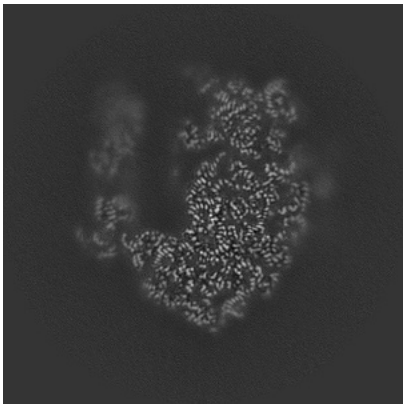


Y Index: 230

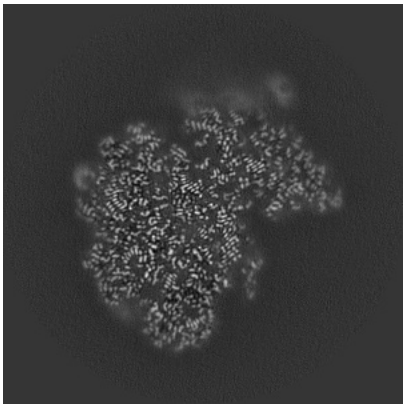


Z Index: 274

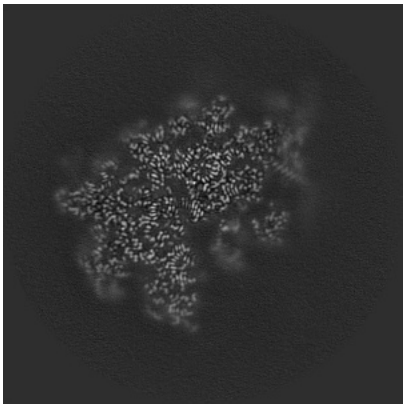
6.3.2 Raw map



X Index: 232



Y Index: 247

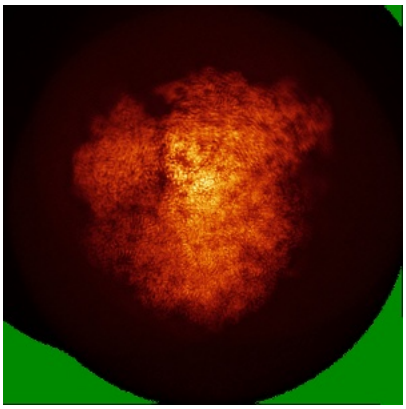


Z Index: 208

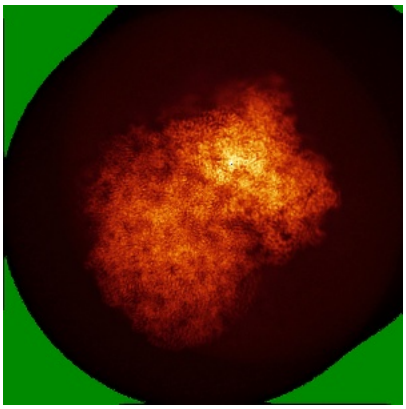
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

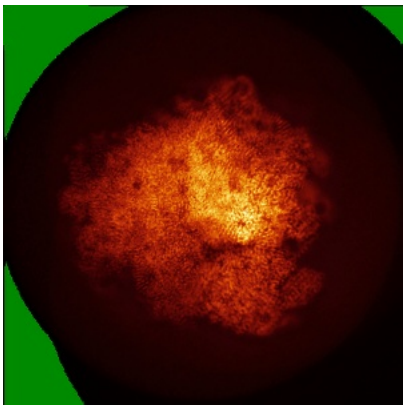
6.4.1 Primary map



X

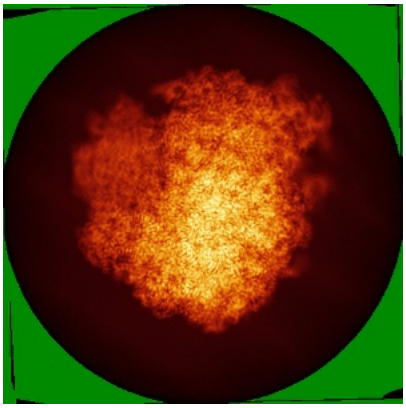


Y

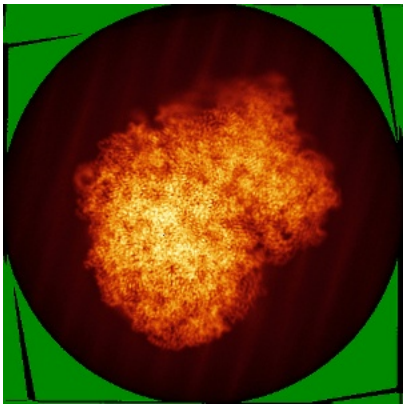


Z

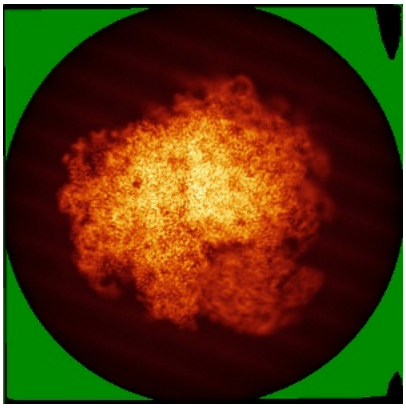
6.4.2 Raw map



X



Y



Z

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

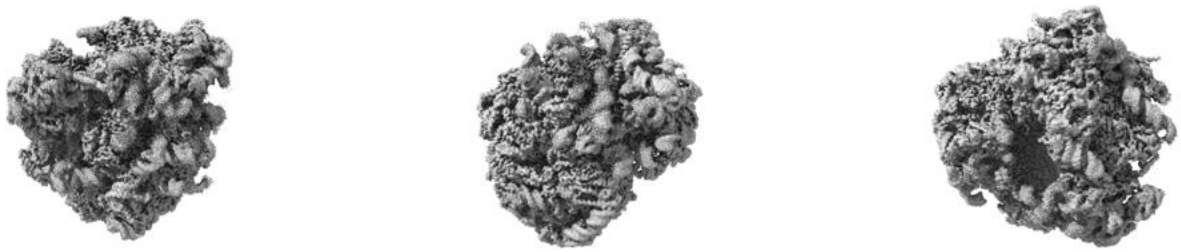
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

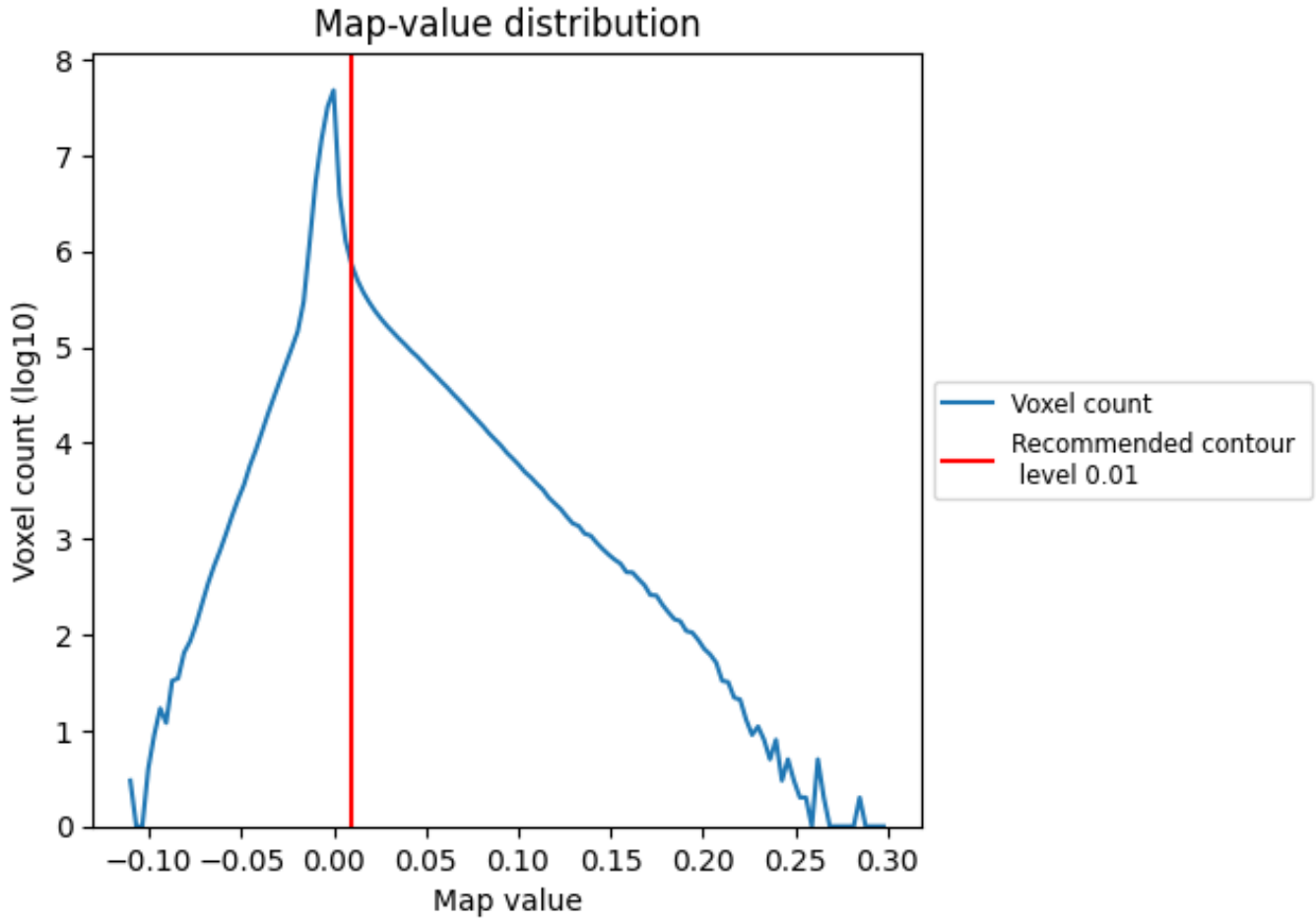
6.6 Mask visualisation (i)

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

7 Map analysis

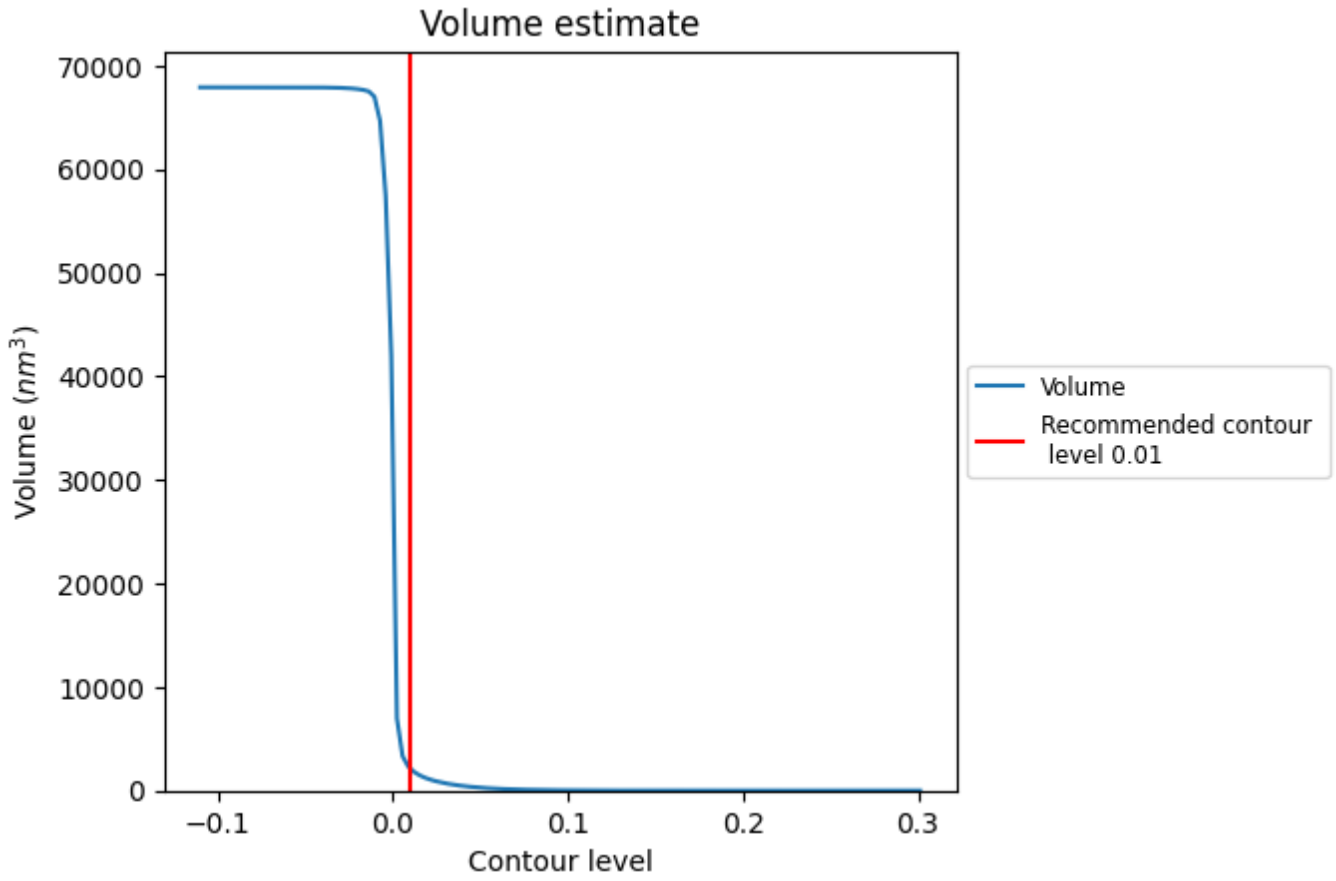
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

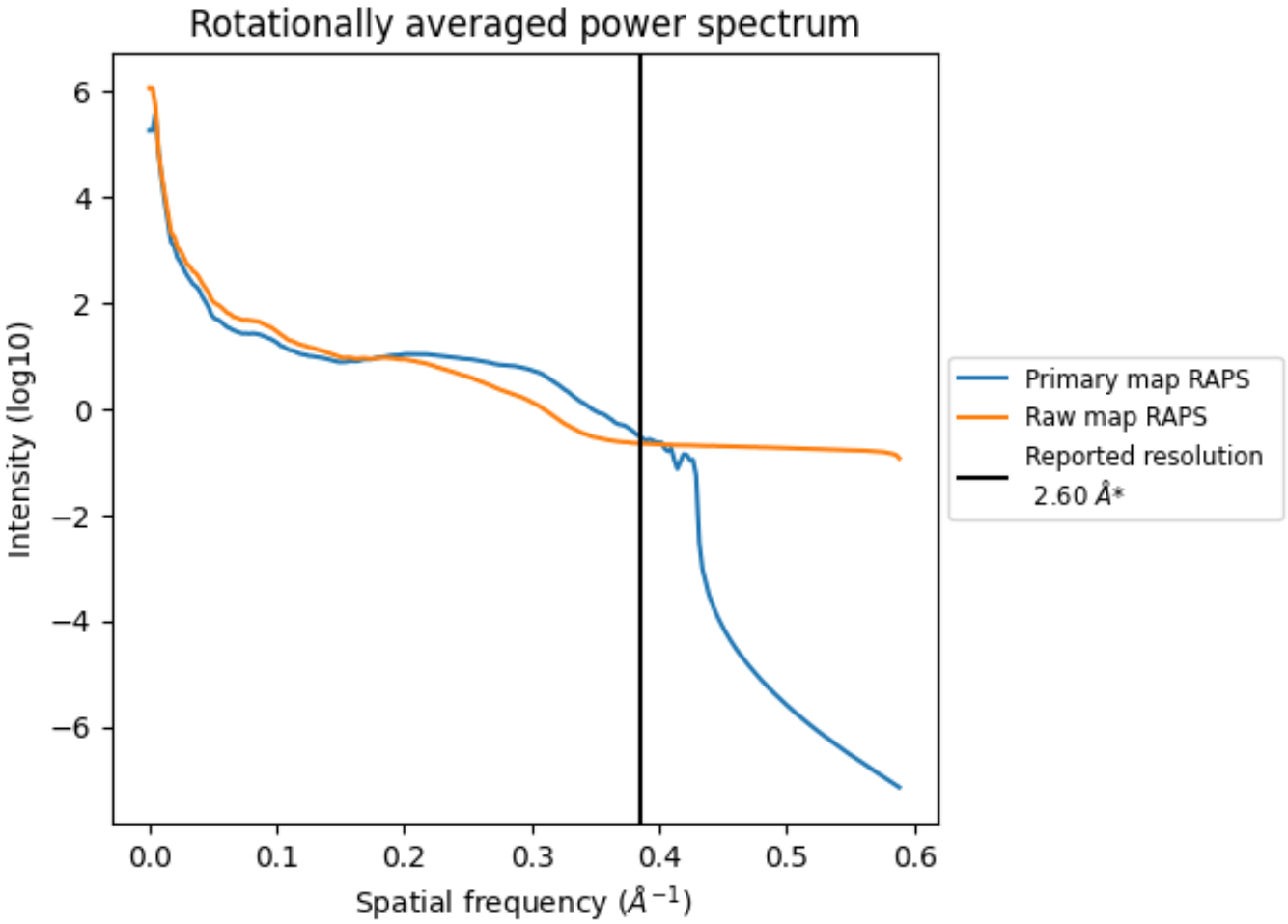
7.2 Volume estimate (i)



The volume at the recommended contour level is 2123 nm^3; this corresponds to an approximate mass of 1918 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 (i)

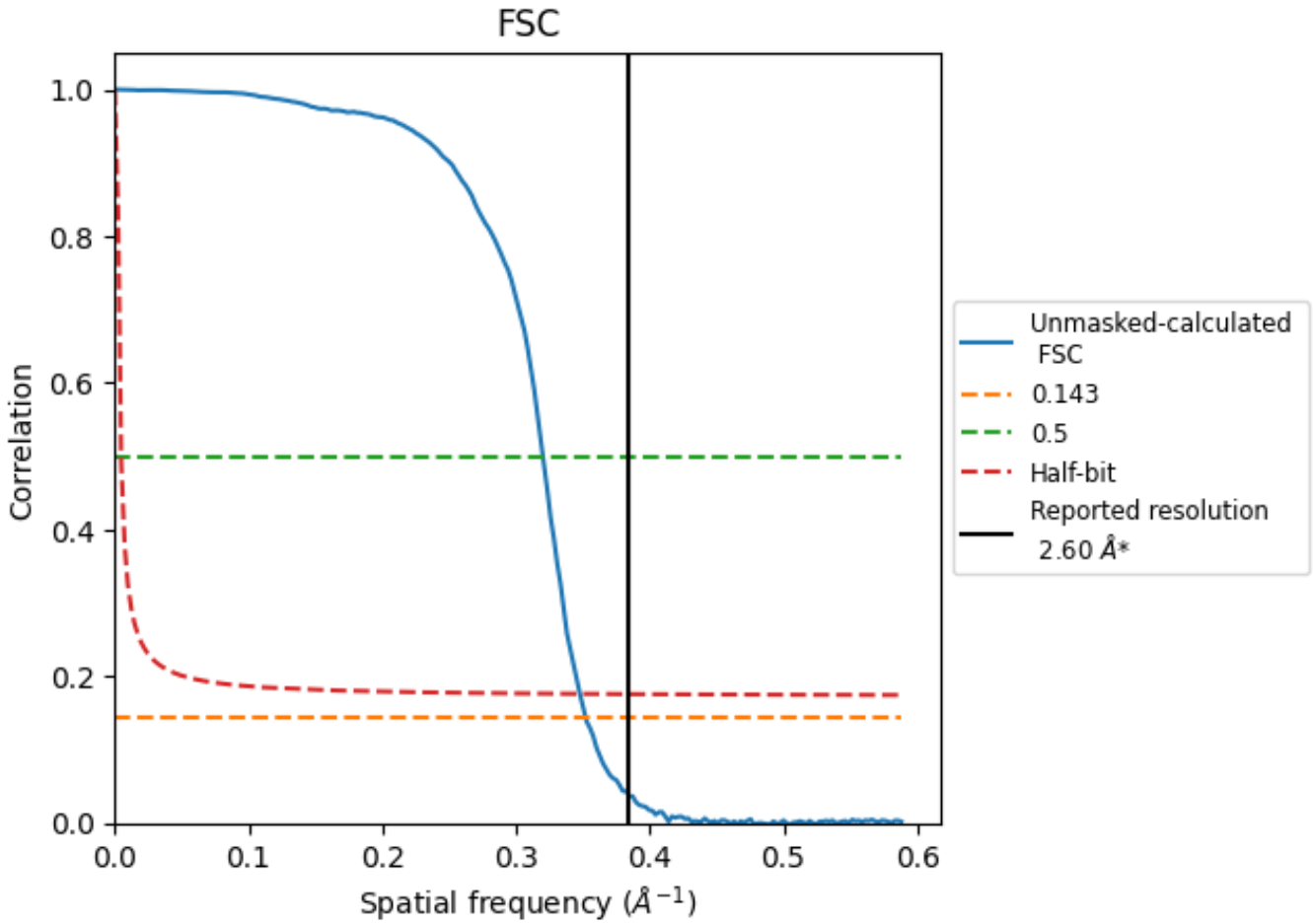


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

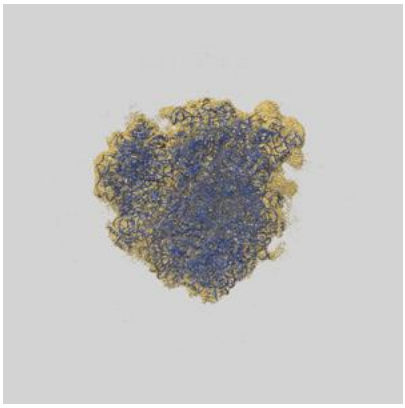
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.84	3.12	2.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

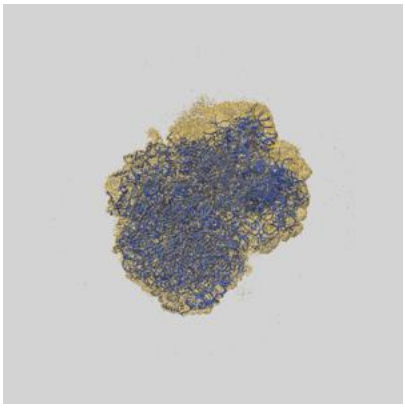
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17212 and PDB model 8OVE. Per-residue inclusion information can be found in section 3 on page 23.

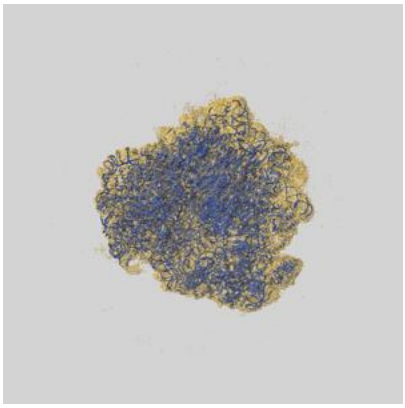
9.1 Map-model overlay



X



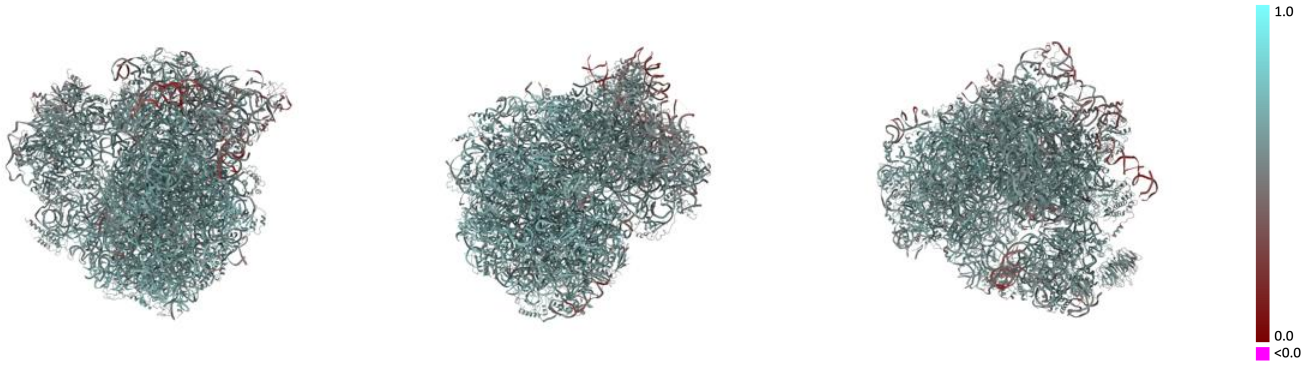
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

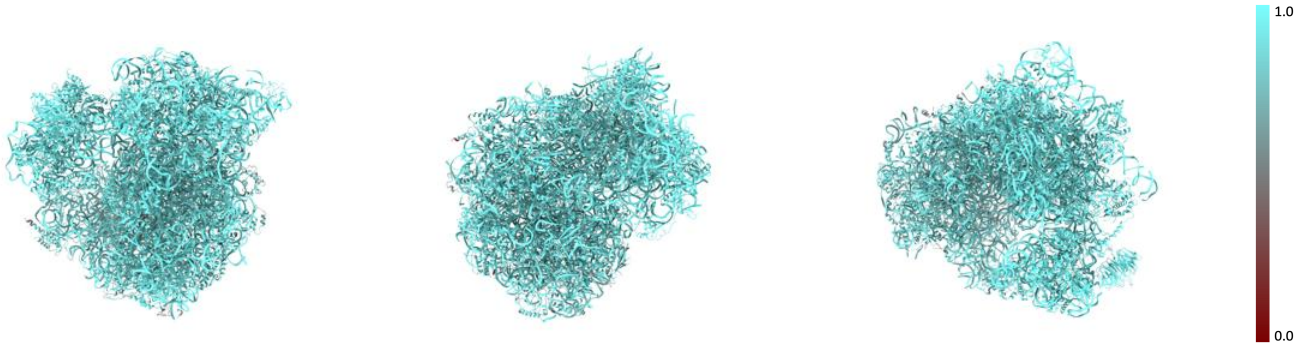
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

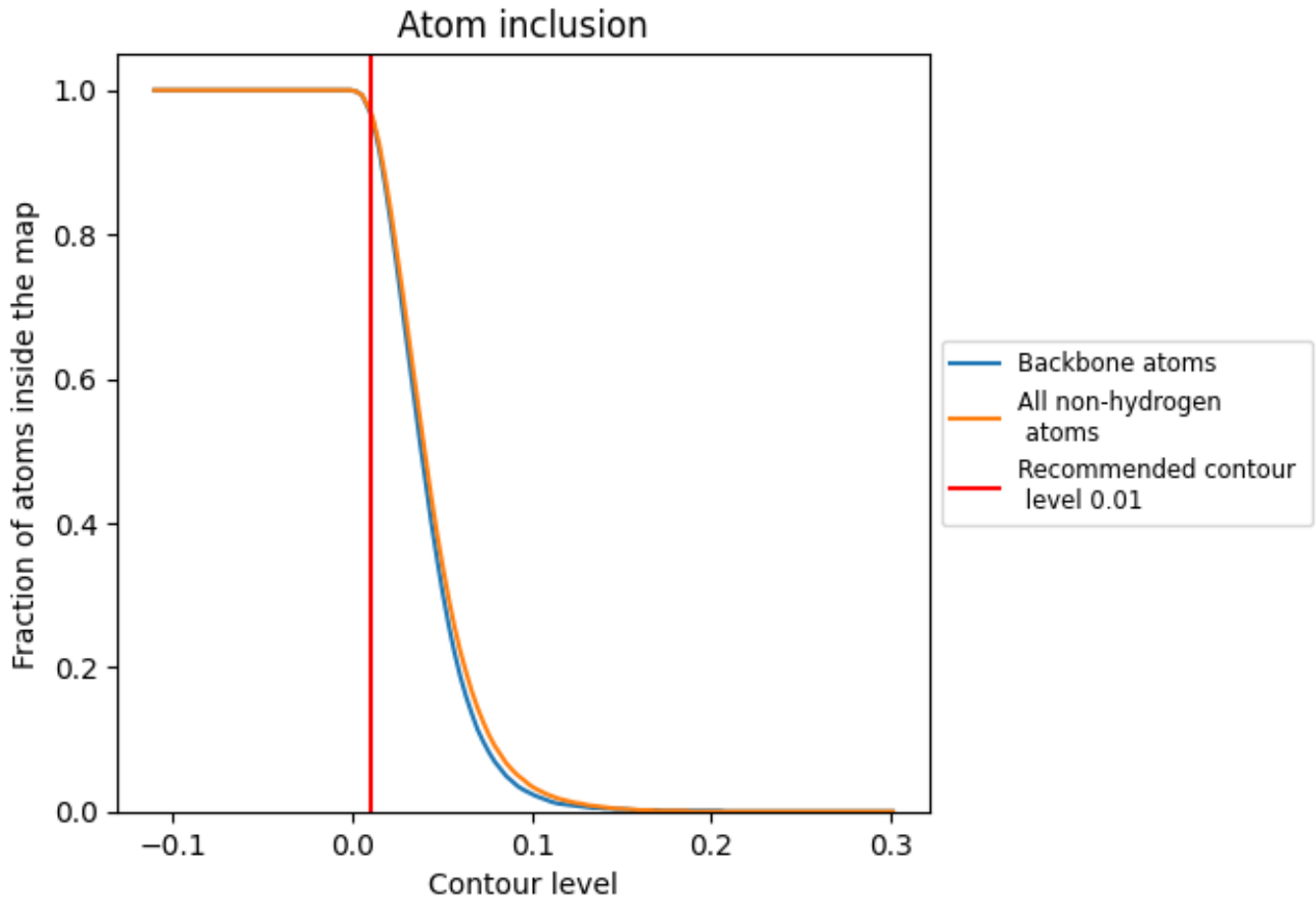
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9720	0.6050
A	1.0000	0.5020
A0	0.9920	0.6190
A1	0.9820	0.5640
A2	0.9910	0.5810
A3	0.9860	0.5420
A4	0.9920	0.5480
A5	0.9860	0.5690
A6	0.9900	0.5690
A7	0.9820	0.5330
A8	0.9840	0.5950
AA	0.9930	0.5580
AB	0.8490	0.4950
AC	0.9940	0.5680
AD	0.9860	0.5360
AE	0.9780	0.5780
AG	0.9940	0.6070
AH	0.9920	0.6180
AI	0.9860	0.5650
AJ	0.9890	0.6010
AK	0.9930	0.5810
AL	0.9950	0.5400
AM	0.9900	0.5610
AO	0.9940	0.5780
AP	0.9900	0.5850
AQ	0.9830	0.5380
AR	0.9940	0.5720
AS	0.9890	0.6090
AT	0.9930	0.5620
AU	0.9930	0.5590
AV	0.9920	0.6290
AW	0.9840	0.5770
AX	0.9780	0.5610
AY	0.9670	0.5390
AZ	0.9910	0.5690

Continued on next page...

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Chain	Atom inclusion	Q-score
Az	0.9910	0.4630
BA	0.9790	0.6380
BB	0.9790	0.6300
BC	0.9830	0.6360
BD	0.9760	0.5910
BE	0.9830	0.6170
BF	0.9210	0.5810
BG	0.9760	0.6230
BH	0.9650	0.6020
BI	0.9690	0.6540
BK	0.9380	0.6150
BL	0.8750	0.5320
BN	0.9110	0.6300
BO	0.9490	0.6410
BP	0.8710	0.6040
BQ	0.9930	0.6710
BR	0.9860	0.6710
BS	0.9440	0.6320
BT	0.9520	0.6030
BU	0.8920	0.6150
BV	0.8260	0.5330
BW	0.9800	0.6550
BX	0.9680	0.6470
BY	0.9840	0.6460
BZ	0.9520	0.6330
Ba	0.9390	0.6160
Bb	0.9540	0.6570
Bc	0.9270	0.6280
Bd	0.9760	0.6480
Be	0.9950	0.6760
Bf	0.9620	0.6510
Bg	0.9780	0.6290
Bh	0.9160	0.6150
Bi	0.9430	0.6570
Bj	0.9510	0.6440
Bk	0.9050	0.6050
Bl	0.9620	0.6510
Bm	0.9340	0.6130
Bn	0.9920	0.6760
Bo	0.9870	0.6640
Bp	0.8570	0.5860
Bq	0.9840	0.6540

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Chain	Atom inclusion	Q-score
Br	0.9490	0.6430
Bs	0.7090	0.5470
Bt	0.9540	0.6300
Bu	0.8950	0.5960
Bv	0.9150	0.5940
Bw	0.9590	0.6450
Bx	0.9300	0.6220
By	0.9010	0.5830
Bz	0.9740	0.6400