



wwPDB EM Validation Summary Report ⓘ

Sep 8, 2026 – 01:09 PM JST

PDB ID : 9WW4 / pdb_00009ww4
EMDB ID : EMD-66297
Title : human 80S ribosome non-rotated state
Authors : Fujino, M.; Tanaka, Y.; Iwasaki, W.; Ito, T.; Yokoyama, T.
Deposited on : 2025-09-22
Resolution : 2.48 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

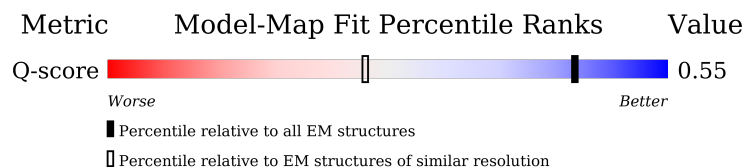
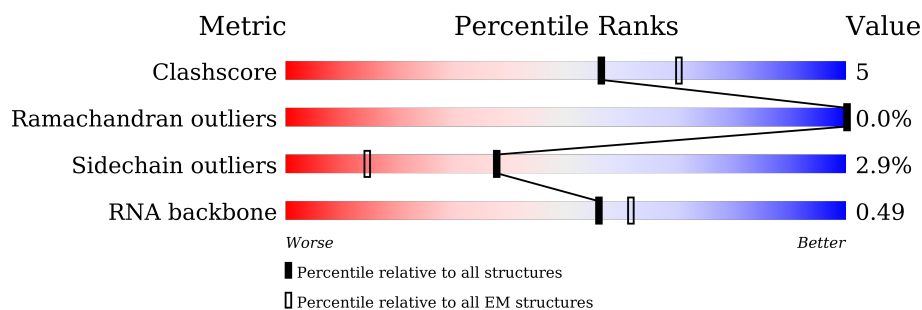
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.48 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.



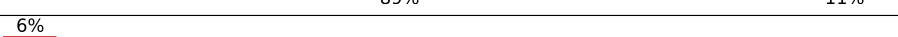
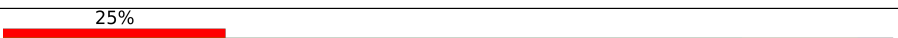
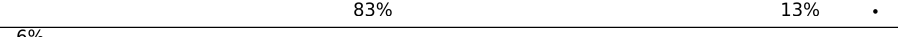
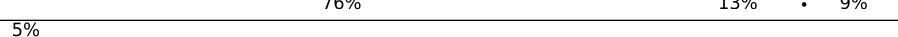
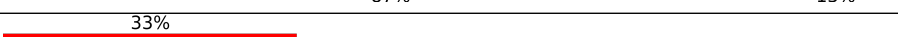
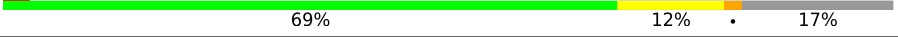
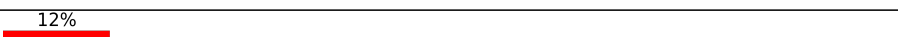
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6178 (1.98 - 2.98)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	5069	
2	AB	120	
3	AC	157	

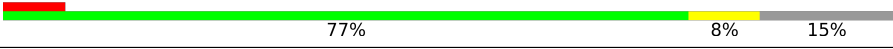
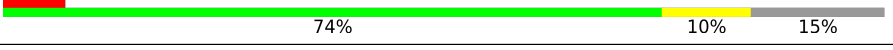
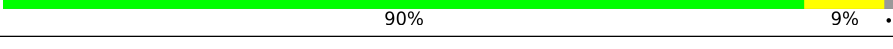
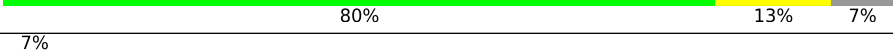
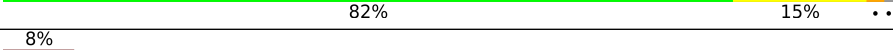
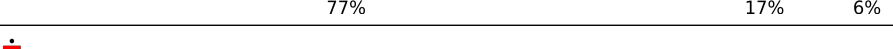
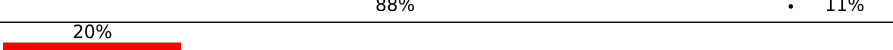
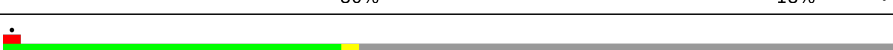
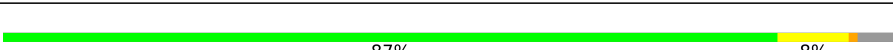
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Mol	Chain	Length	Quality of chain
4	AD	257	
5	AE	402	
6	AF	368	
7	AG	293	
8	AH	247	
9	AI	248	
10	AJ	266	
11	AK	192	
12	AL	214	
13	AM	178	
14	AN	211	
15	AO	215	
16	AP	204	
17	AQ	203	
18	AR	184	
19	AS	188	
20	AT	196	
21	AU	176	
22	AV	160	
23	AW	128	
24	AX	140	
25	AY	157	
26	AZ	156	
27	Aa	145	
28	Ab	136	

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Mol	Chain	Length	Quality of chain
29	Ac	148	
30	Ad	159	
31	Ae	115	
32	Af	125	
33	Ag	135	
34	Ah	110	
35	Ai	117	
36	Aj	123	
37	Ak	105	
38	Al	97	
39	Am	70	
40	An	51	
41	Ao	128	
42	Ap	25	
43	Aq	106	
44	Ar	92	
45	As	137	
46	BA	1869	
47	BB	263	
48	BC	295	
49	BD	264	
50	BE	243	
51	BF	204	
52	BG	194	
53	BH	208	

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Mol	Chain	Length	Quality of chain
54	BI	165	
55	BJ	158	
56	BK	145	
57	BL	146	
58	BM	152	
59	BN	145	
60	BO	119	
61	BP	83	
62	BQ	143	
63	BR	115	
64	BS	69	
65	BT	56	
66	BU	317	
67	BV	293	
68	BW	249	
69	BX	194	
70	BY	132	
71	BZ	151	
72	Ba	151	
73	Bb	130	
74	Bc	133	
75	Bd	125	
76	Be	84	
77	Bf	133	
78	Bg	156	

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Mol	Chain	Length	Quality of chain
79	Bh	135	84% 79% 19% .

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 215529 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 28S rRNA (3773-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	3773	Total	C	N	O	P	0	0
			80205	35722	14588	26123	3772		

- Molecule 2 is a RNA chain called 5S rRNA (120-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S rRNA (156-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

- Molecule 4 is a protein called 60S ribosomal protein L8.

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

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 8 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	213	Total	C	N	O	S	0	0
			1713	1083	329	285	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	49	CYS	GLY	conflict	UNP Q96L21

- Molecule 13 is a protein called 60S ribosomal protein L11.

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

- Molecule 14 is a protein called 60S ribosomal protein L13.

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

- Molecule 15 is a protein called 60S ribosomal protein L14.

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

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

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

- Molecule 18 is a protein called 60S ribosomal protein L17.

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

- Molecule 19 is a protein called 60S ribosomal protein L18.

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

- Molecule 20 is a protein called 60S ribosomal protein L19.

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

- Molecule 21 is a protein called 60S ribosomal protein L18a.

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

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called 60S ribosomal protein L22.

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

- Molecule 24 is a protein called 60S ribosomal protein L23.

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

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	122	Total	C	N	O	S	0	0
			997	622	203	168	4		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

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

- Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Aa	132	Total	C	N	O	S	0	0
			1102	692	223	184	3		

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ac	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ad	99	Total	C	N	O	S	0	0
			808	502	177	125	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Af	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ai	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ak	99	Total	C	N	O	S	0	0
			813	509	173	126	5		

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Am	68	Total	C	N	O	S	0	0
			559	360	101	97	1		

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ao	51	Total	C	N	O	S	0	0
			419	260	88	65	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

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

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Aq	102	Total	C	N	O	S	1	0
			842	527	174	135	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ar	88	Total	C	N	O	S	0	0
			681	430	131	113	7		

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	As	123	Total	C	N	O	S	0	0
			987	612	205	166	4		

- Molecule 46 is a RNA chain called 18S rRNA (1740-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BA	1738	Total	C	N	O	P	0	0
			36916	16492	6593	12093	1738		

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

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

- Molecule 48 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BC	219	Total	C	N	O	S	0	0
			1727	1096	302	320	9		

- Molecule 49 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BD	215	Total	C	N	O	S	0	0
			1747	1109	312	312	14		

- Molecule 50 is a protein called 40S ribosomal protein S3.

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

- Molecule 51 is a protein called 40S ribosomal protein S5.

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

- Molecule 52 is a protein called 40S ribosomal protein S7.

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

- Molecule 53 is a protein called 40S ribosomal protein S8.

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

- Molecule 54 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BI	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 55 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BJ	154	Total	C	N	O	S	0	0
			1258	802	235	215	6		

- Molecule 56 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BK	125	Total	C	N	O	S	0	0
			1027	653	193	174	7		

- Molecule 57 is a protein called 40S ribosomal protein S16.

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

- Molecule 58 is a protein called 40S ribosomal protein S18.

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

- Molecule 59 is a protein called Small ribosomal subunit protein eS19.

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

- Molecule 60 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BO	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 61 is a protein called 40S ribosomal protein S21.

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

- Molecule 62 is a protein called 40S ribosomal protein S23.

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

- Molecule 63 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BR	102	Total	C	N	O	S	1	0
			829	517	174	133	5		

- Molecule 64 is a protein called 40S ribosomal protein S28.

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

- Molecule 65 is a protein called 40S ribosomal protein S29.

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

- Molecule 66 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 67 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BV	221	Total	C	N	O	S	1	0
			1724	1115	298	301	10		

- Molecule 68 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	BW	234	Total	C	N	O	S	0	0
			1903	1188	384	324	7		

- Molecule 69 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	BX	182	Total	C	N	O	S	1	0
			1520	967	306	245	2		

- Molecule 70 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BY	118	Total	C	N	O	S	0	0
			906	568	158	172	8		

- Molecule 71 is a protein called 40S ribosomal protein S13.

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

- Molecule 72 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ba	138	IAS	ASP	conflict	UNP P62263

- Molecule 73 is a protein called 40S ribosomal protein S15a.

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

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bc	128	Total	C	N	O	S	1	0
			1048	661	207	175	5		

- Molecule 75 is a protein called 40S ribosomal protein S25.

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

- Molecule 76 is a protein called 40S ribosomal protein S27.

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

- Molecule 77 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

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

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 79 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bh	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	AA	190	Total	Mg	0
			190	190	
80	AB	1	Total	Mg	0
			1	1	
80	AC	4	Total	Mg	0
			4	4	
80	AL	1	Total	Mg	0
			1	1	
80	AP	1	Total	Mg	0
			1	1	
80	AR	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
80	AX	1	Total 1	Mg 1	0
80	BA	70	Total 70	Mg 70	0

- Molecule 81 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
81	AA	66	Total 66	K 66	0
81	AB	1	Total 1	K 1	0
81	AC	1	Total 1	K 1	0
81	AD	1	Total 1	K 1	0
81	AL	1	Total 1	K 1	0
81	Ag	1	Total 1	K 1	0
81	Ah	1	Total 1	K 1	0
81	Aq	1	Total 1	K 1	0
81	BA	13	Total 13	K 13	0
81	BF	1	Total 1	K 1	0

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	Ai	1	Total 1	Zn 1	0
82	Al	1	Total 1	Zn 1	0
82	Ao	1	Total 1	Zn 1	0
82	Aq	1	Total 1	Zn 1	0
82	Ar	1	Total 1	Zn 1	0

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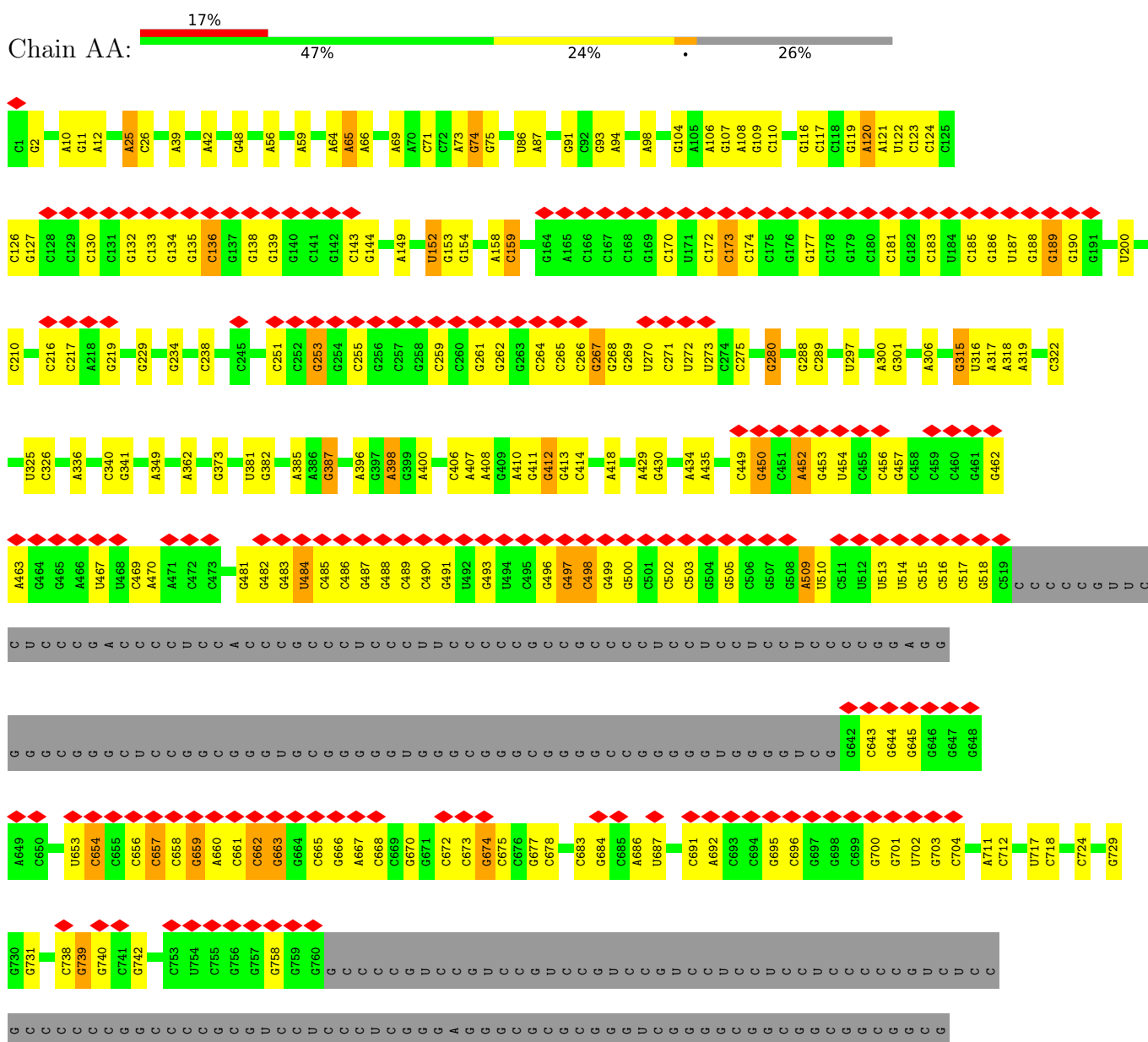
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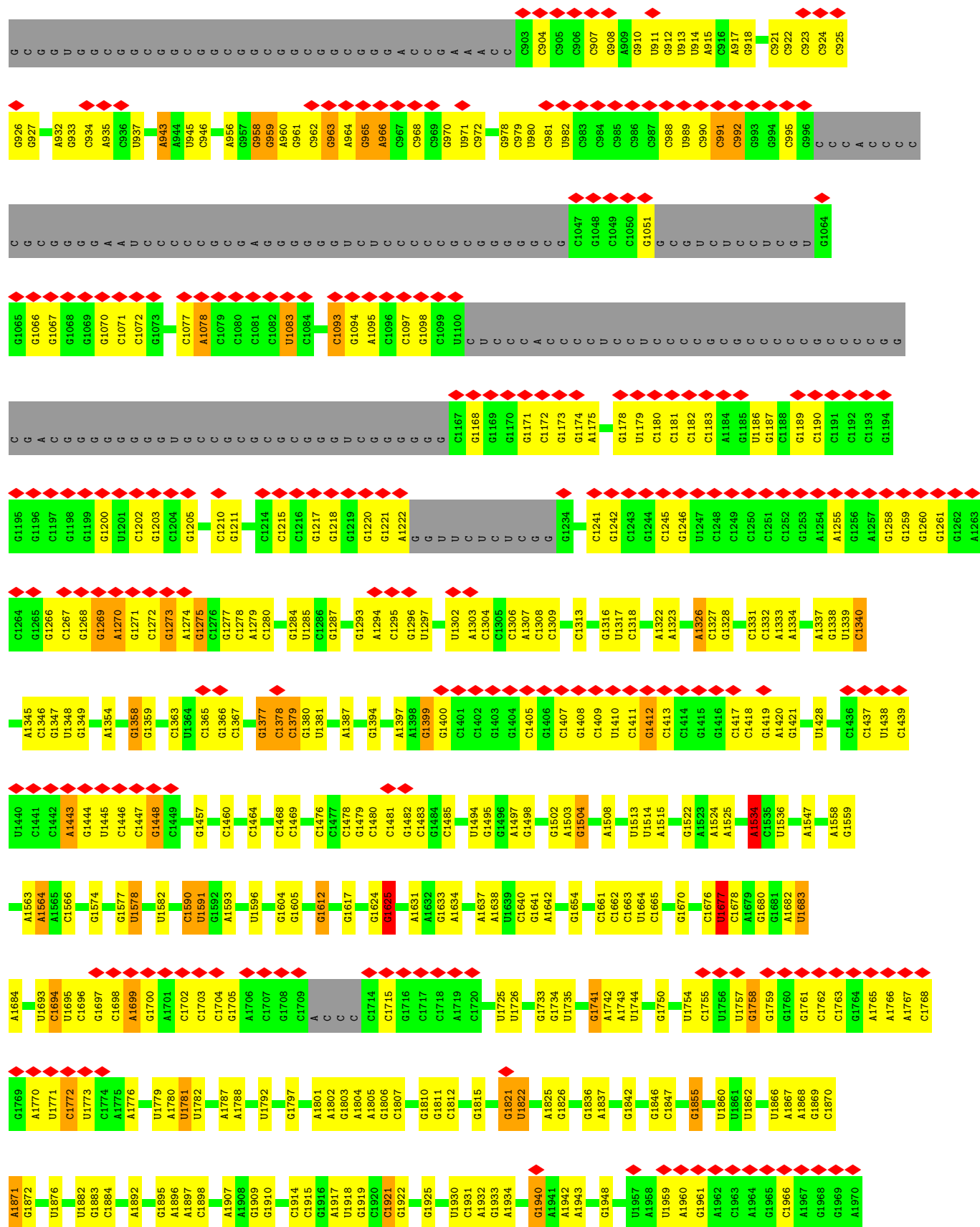
Mol	Chain	Residues	Atoms		AltConf
82	BR	1	Total 1	Zn 1	0
82	BT	1	Total 1	Zn 1	0
82	Bg	1	Total 1	Zn 1	0

3 Residue-property plots

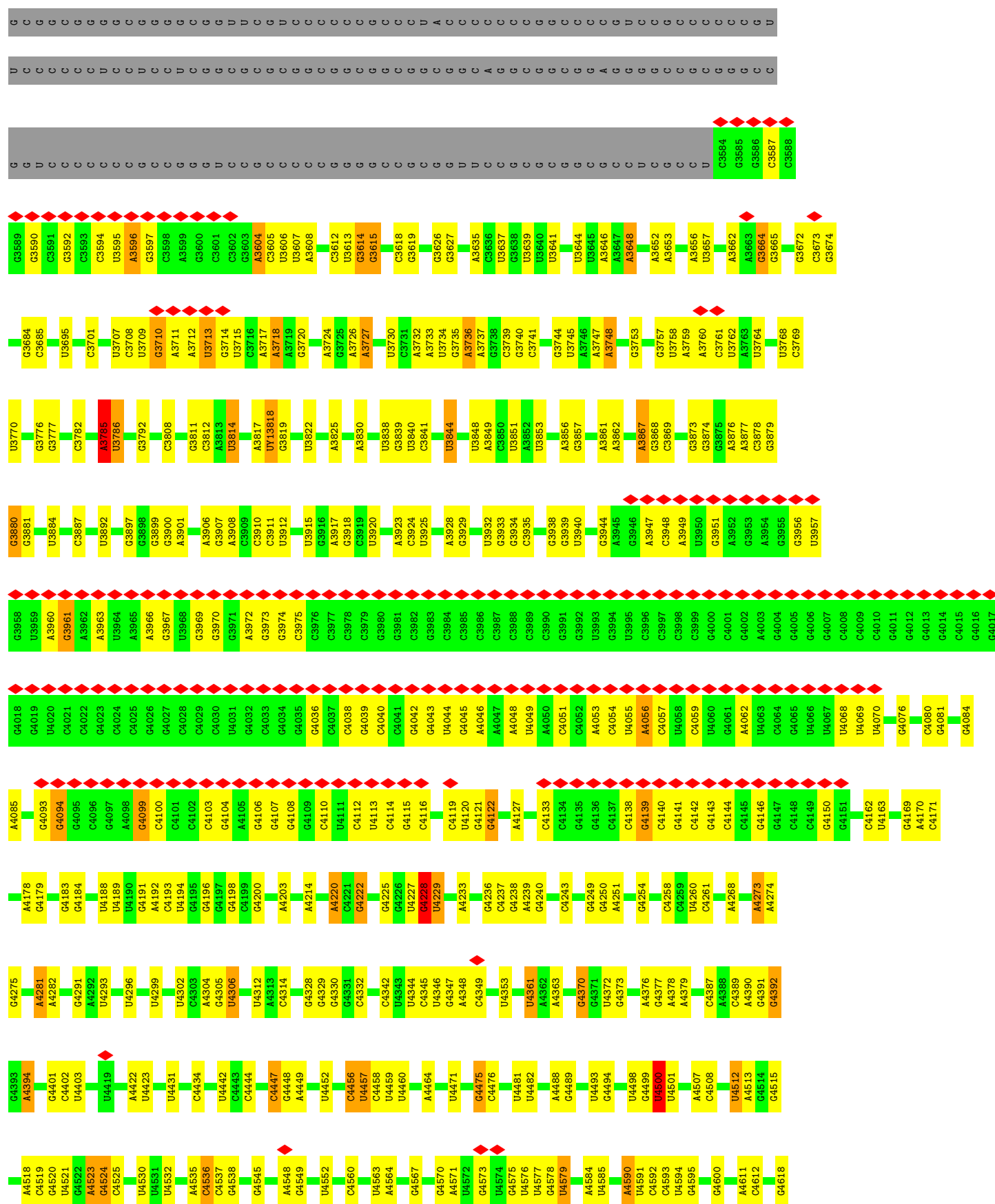
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

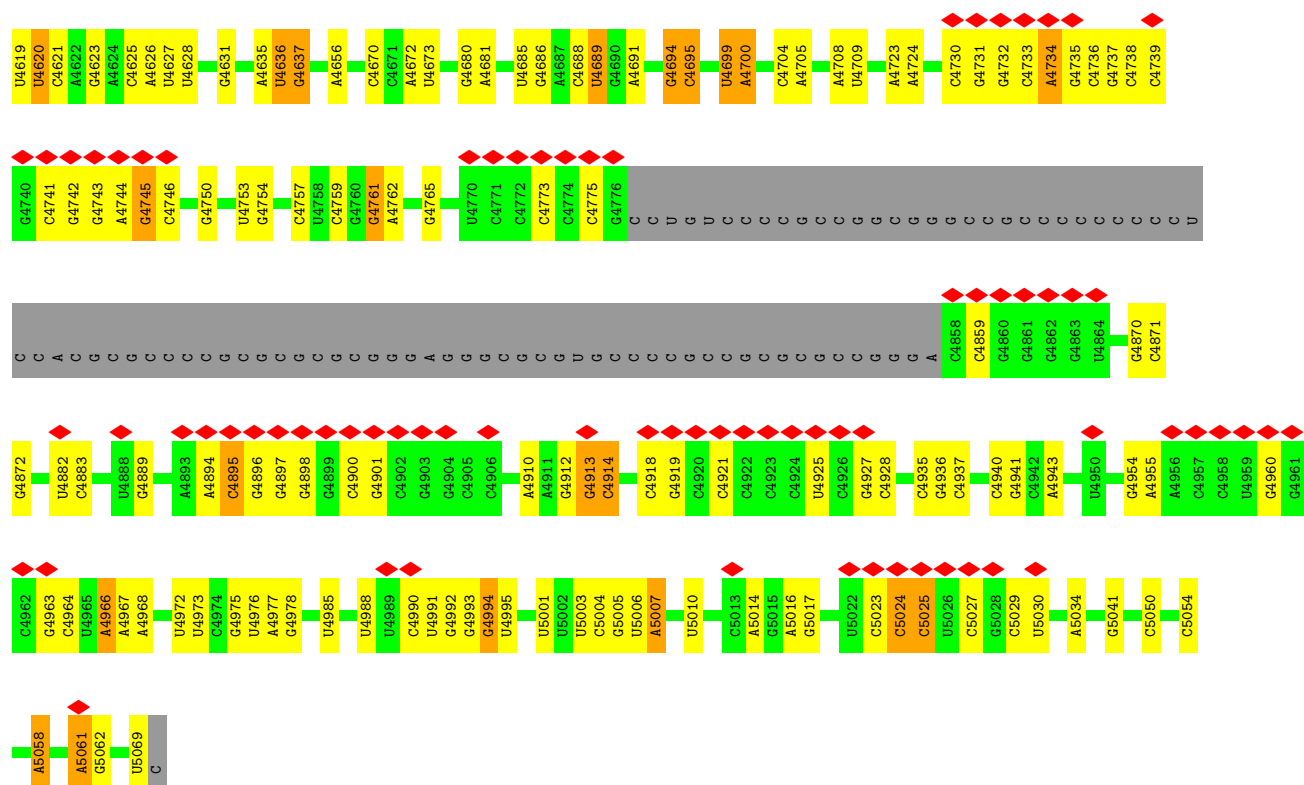
• Molecule 1: 28S rRNA (3773-MER)





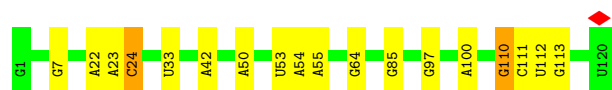






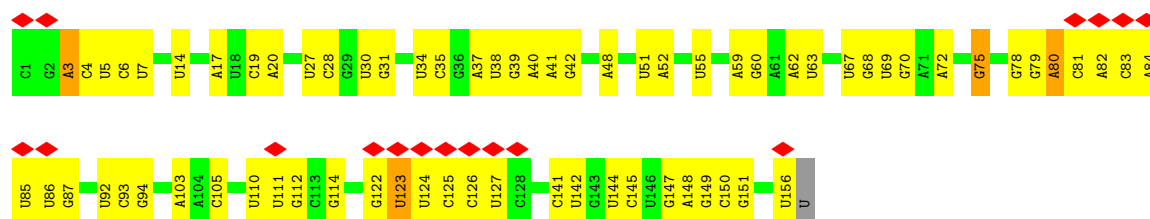
• Molecule 2: 5S rRNA (120-MER)

Chain AB: 85% 13%



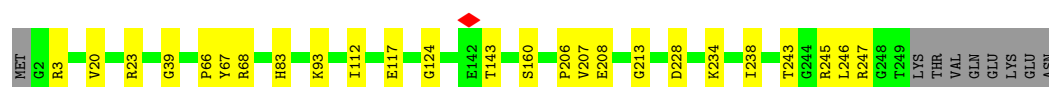
• Molecule 3: 5.8S rRNA (156-MER)

Chain AC: 11% 55% 42%

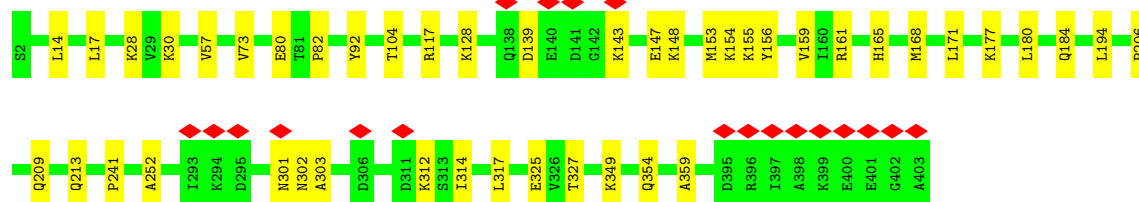
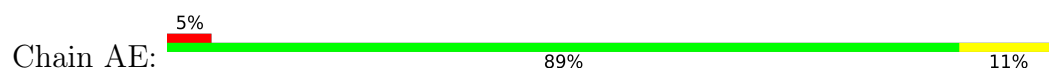


• Molecule 4: 60S ribosomal protein L8

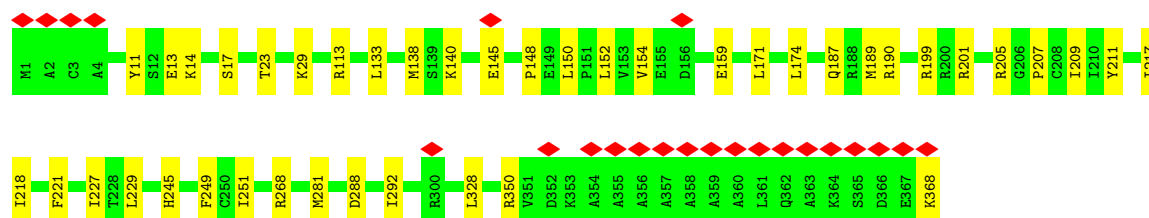
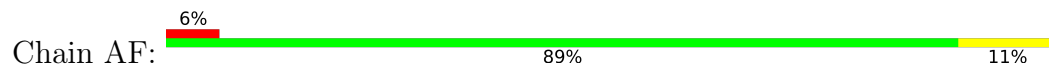
Chain AD: 87% 10%



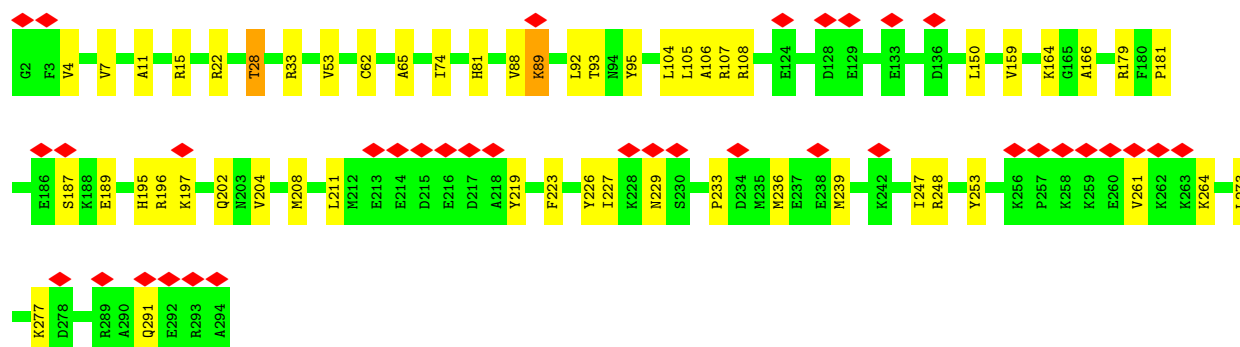
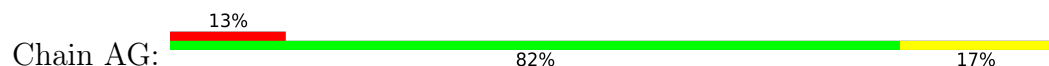
• Molecule 5: Large ribosomal subunit protein uL3



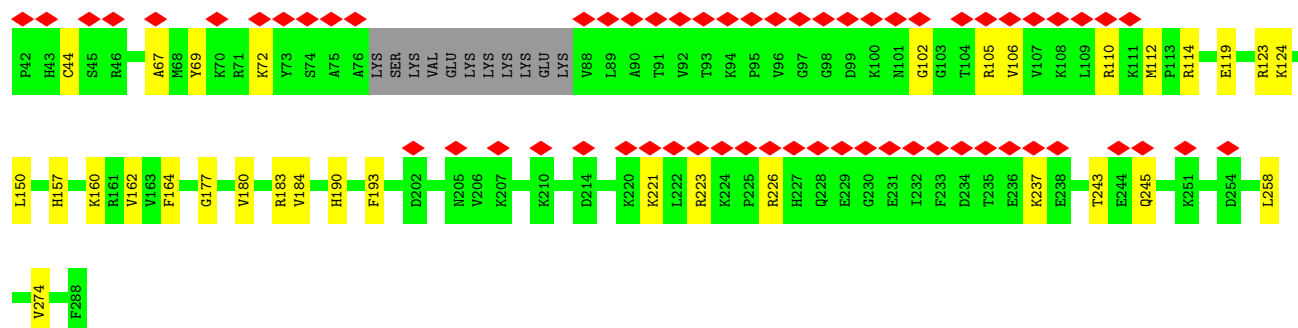
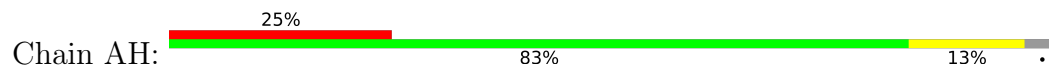
• Molecule 6: Large ribosomal subunit protein uL4



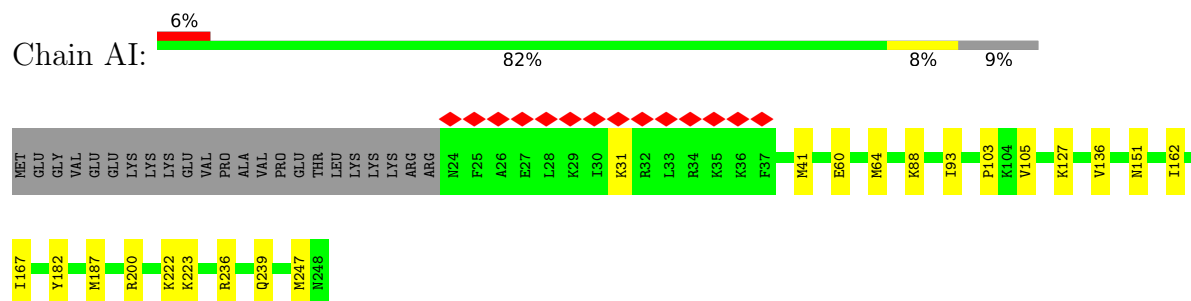
• Molecule 7: Large ribosomal subunit protein uL18



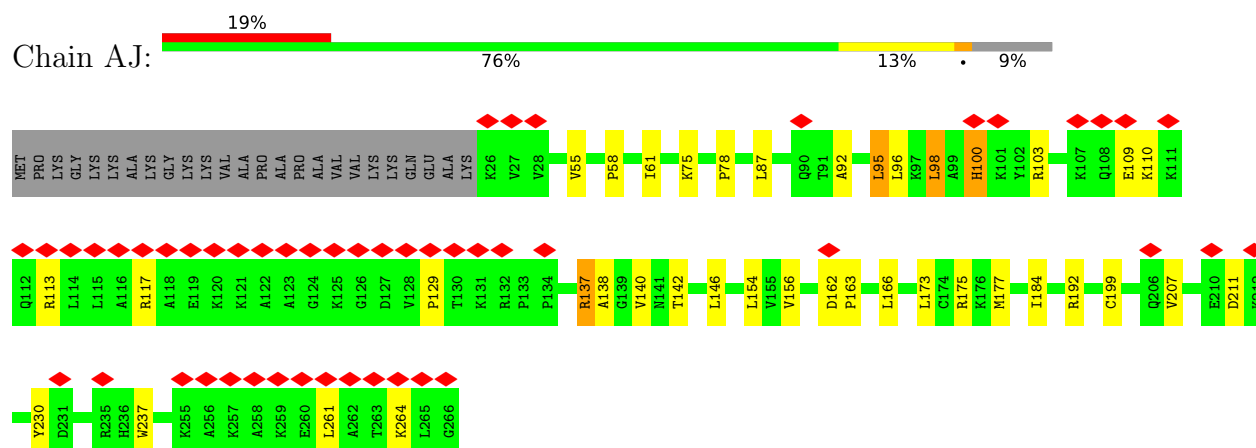
• Molecule 8: Large ribosomal subunit protein eL6



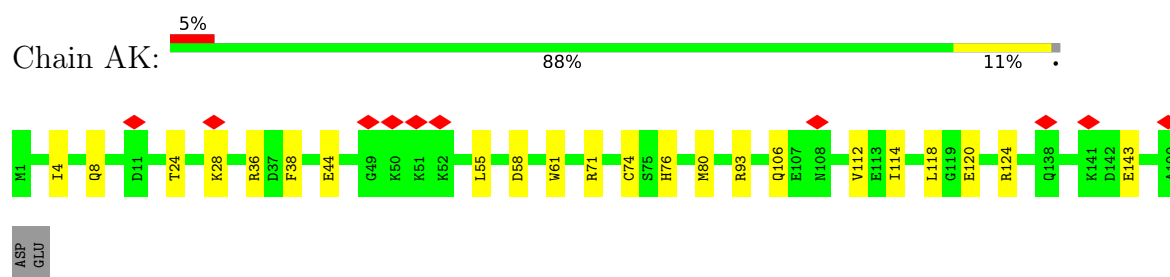
- Molecule 9: 60S ribosomal protein L7



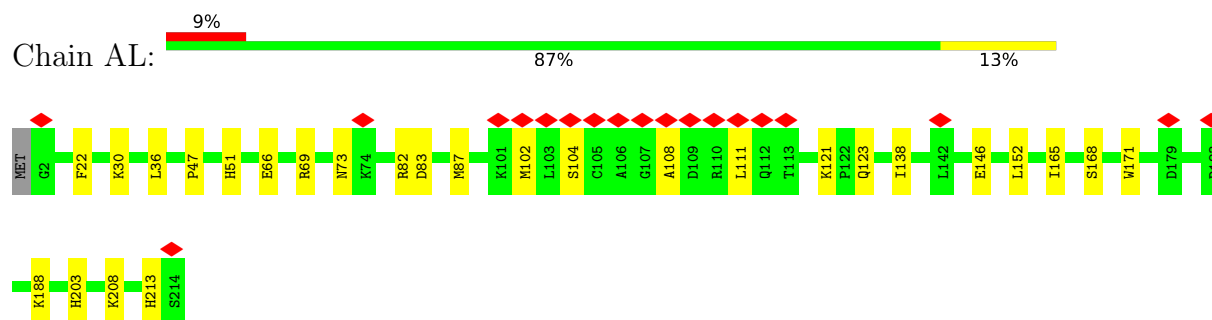
- Molecule 10: 60S ribosomal protein L7a



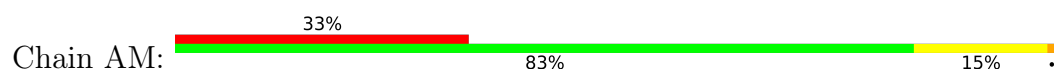
- Molecule 11: 60S ribosomal protein L9

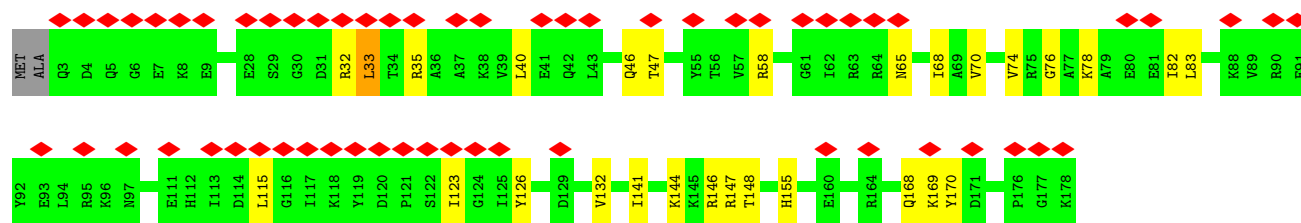


- Molecule 12: Ribosomal protein uL16-like

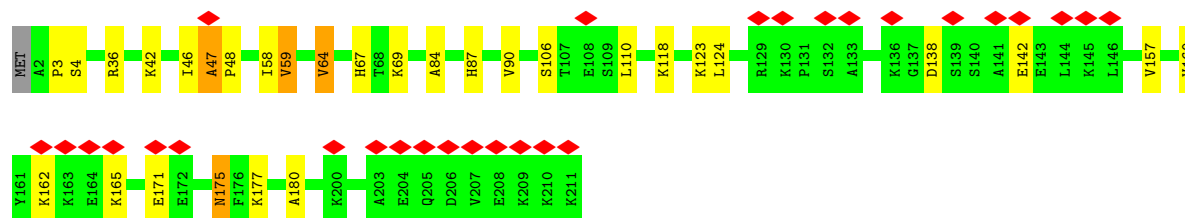
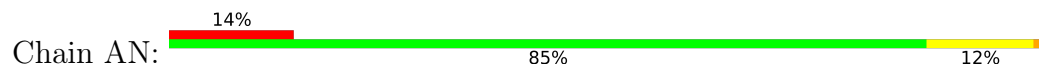


- Molecule 13: 60S ribosomal protein L11

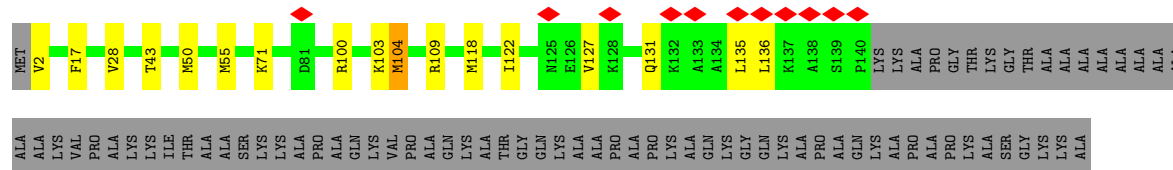




• Molecule 14: 60S ribosomal protein L13



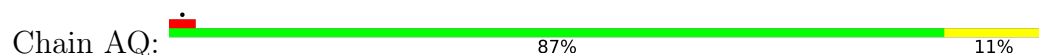
• Molecule 15: 60S ribosomal protein L14



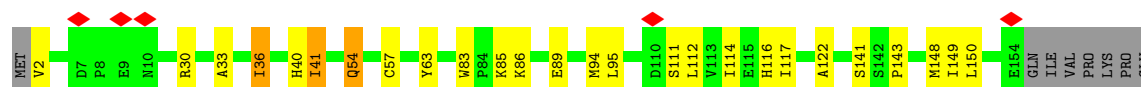
• Molecule 16: 60S ribosomal protein L15



• Molecule 17: 60S ribosomal protein L13a



• Molecule 18: 60S ribosomal protein L17



GLU
GLU
VAL
ALA
GLN
LYS
LYS
ILE
SER
GLN
LYS
LYS
LEU
LYS
GLN
LYS
LEU
MET
ALA
ARG
GLU

- Molecule 19: 60S ribosomal protein L18

Chain AS: 89% 10% ..

MET G2 R14 P18 V29 Y32 L35 T42 K71 E76 N77 V92 K99 R110 S111 R112 I120 L121 K144 E147 P159 K164 R178 R184 N188

- Molecule 20: 60S ribosomal protein L19

Chain AT: 12% 88% 7% 5%

MET S2 M3 M76 G79 R81 R83 M96 H143 L154 Q158 E168 A169 R170 K171 R172 R173 E174 E175 E176 L177 Q178 A179 K180 K181 E182 E183 I184 I185 K186 T187 L188 SER LYS LYS GLU GLU THR LYS

- Molecule 21: 60S ribosomal protein L18a

Chain AU: 89% 11% .

MET K2 A3 S4 E9 Y10 K11 R15 R16 P20 K21 C22 H23 T24 L27 Y28 R29 F33 R43 V48 V67 K76 E96 R111 V142 R161 Q162 H163 K164 F176

- Molecule 22: 60S ribosomal protein L21

Chain AV: 11% 91% 9% .

MET T2 K5 M14 K21 Q44 H58 V76 C82 H95 R102 L106 E111 N112 D113 Q114 K115 K116 K117 E118 A119 K120 E121 K122 G123 T124 W125 V126 A133 E137 K146 A160

- Molecule 23: 60S ribosomal protein L22

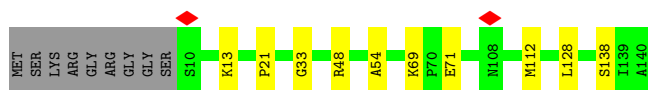
Chain AW: 29% 57% 20% 21%

MET ALA PRO VAL LYS LYS VAL LYS GLY LYS LYS LYS Q17 V18 L19 K20 L23 D24 C25 T26 H27 P28 V29 E30 D31 G32 I33 M34 D35 G36 A37 N38 F39 E40 Q41 F42 L43 Q44 E45 R46 N55 L56 G57 G58 G59 V60 V61 T62 I63 E64 R65 S66 K67 S68

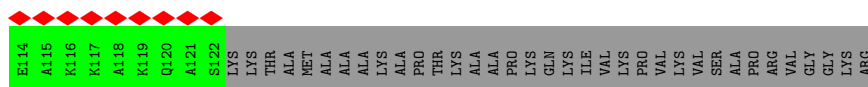
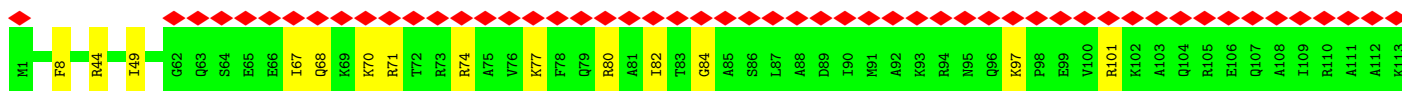
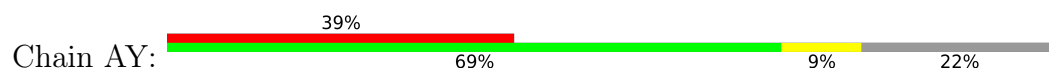
K69 I70 T71 V72 T73 S74 E75 K80 K84 T87 Y90 L91 K92 N95 D98 N105 E108 S109 Y110 E111 L112 Y114 F115 Q116 I117 ASN GLN ASP ASP GLU GLU GLU GLU ASP ASP

- Molecule 24: 60S ribosomal protein L23

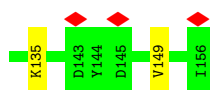
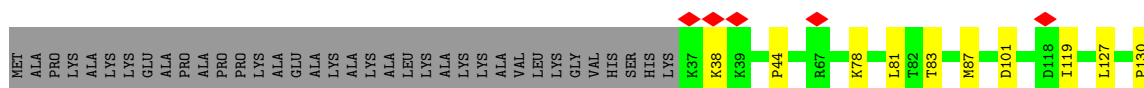
Chain AX: 86% 7% 6%



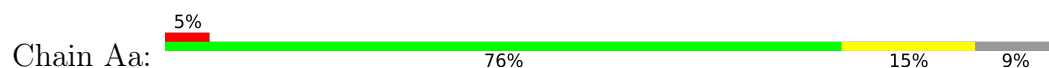
- Molecule 25: 60S ribosomal protein L24



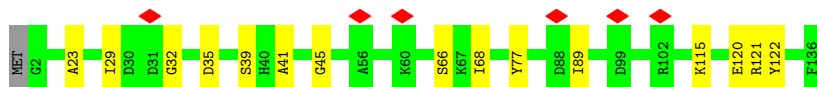
- Molecule 26: 60S ribosomal protein L23a



- Molecule 27: 60S ribosomal protein L26

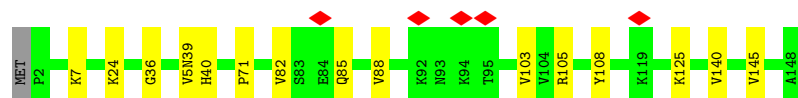


- Molecule 28: 60S ribosomal protein L27

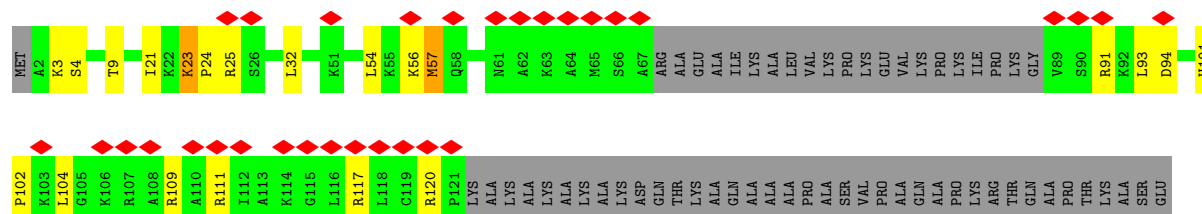


- Molecule 29: Large ribosomal subunit protein uL15

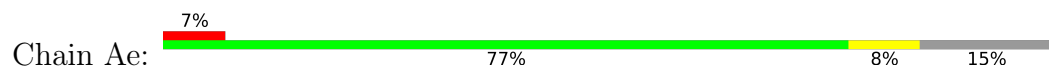




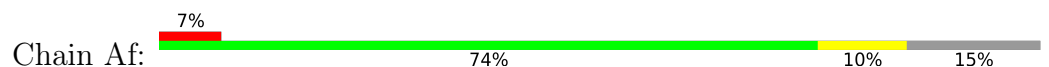
- Molecule 30: 60S ribosomal protein L29



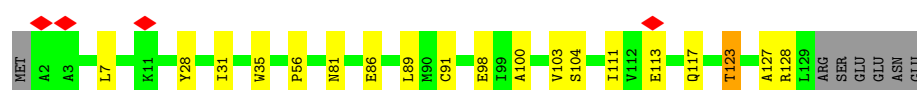
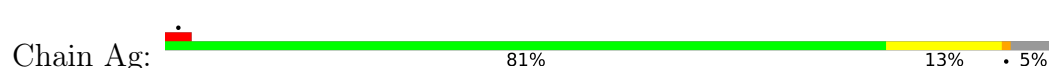
- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31



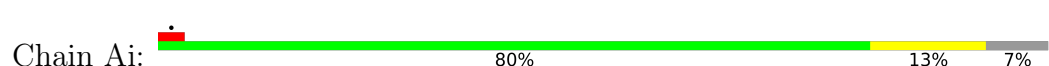
- Molecule 33: 60S ribosomal protein L32

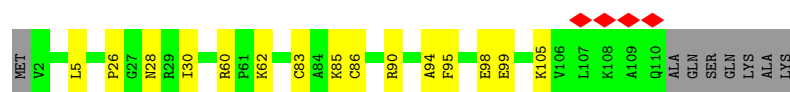


- Molecule 34: 60S ribosomal protein L35a

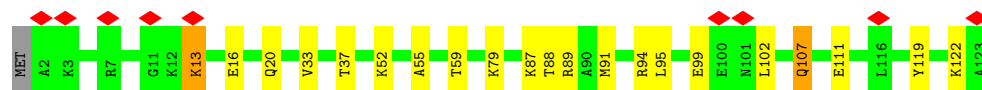
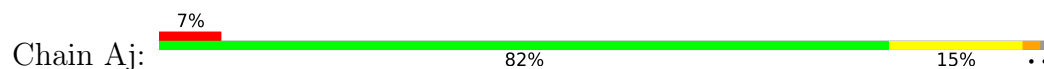


- Molecule 35: 60S ribosomal protein L34

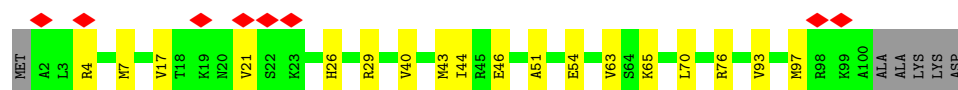
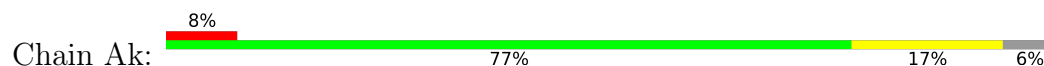




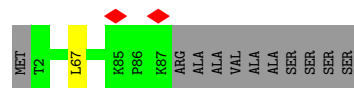
- Molecule 36: 60S ribosomal protein L35



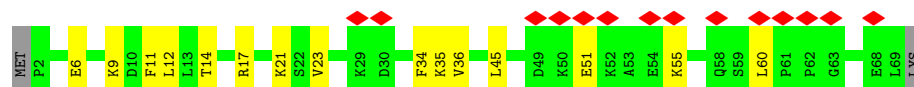
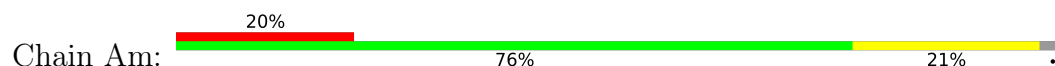
- Molecule 37: 60S ribosomal protein L36



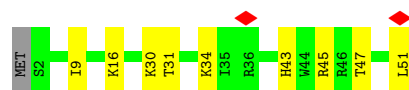
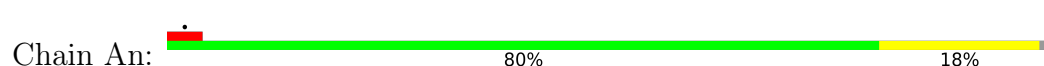
- Molecule 38: 60S ribosomal protein L37



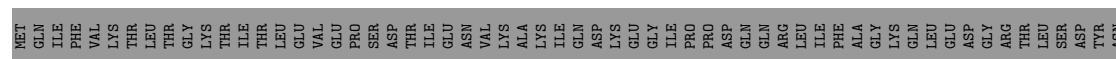
- Molecule 39: 60S ribosomal protein L38

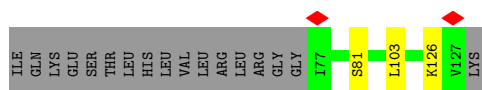


- Molecule 40: 60S ribosomal protein L39



- Molecule 41: Ubiquitin-60S ribosomal protein L40





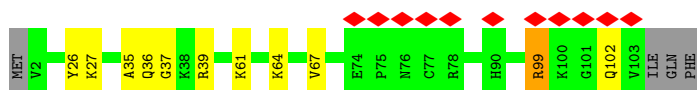
- Molecule 42: 60S ribosomal protein L41

Chain Ap: 88% 8% .



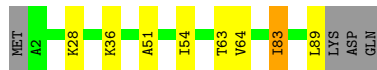
- Molecule 43: 60S ribosomal protein L36a

Chain Aq: 10% 86% 9% . .



- Molecule 44: 60S ribosomal protein L37a

Chain Ar: 87% 8% . .



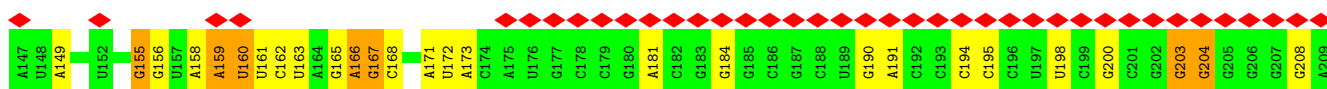
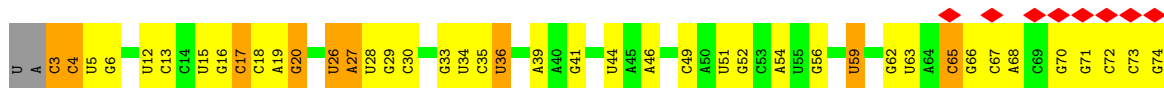
- Molecule 45: 60S ribosomal protein L28

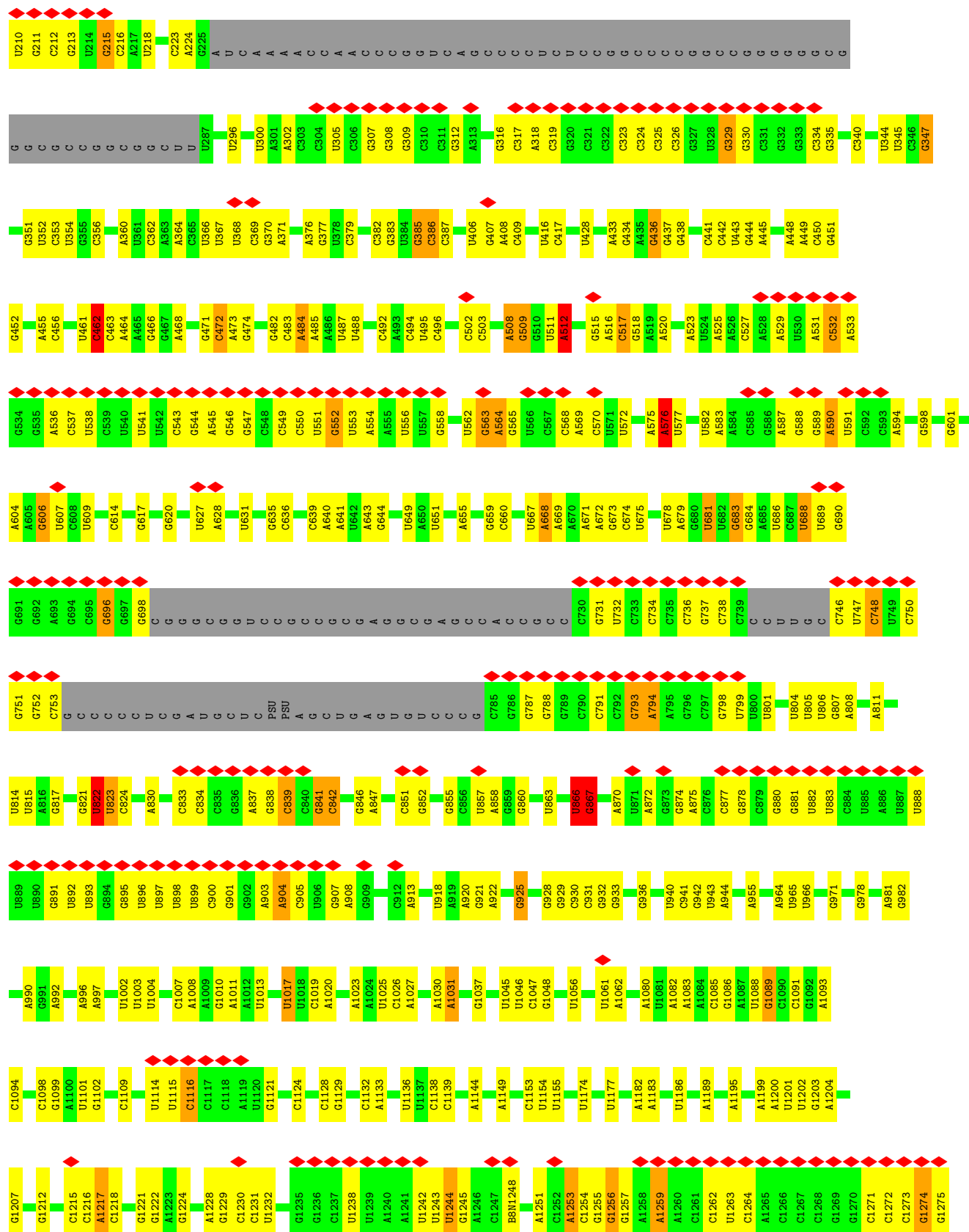
Chain As: 80% 9% 10%

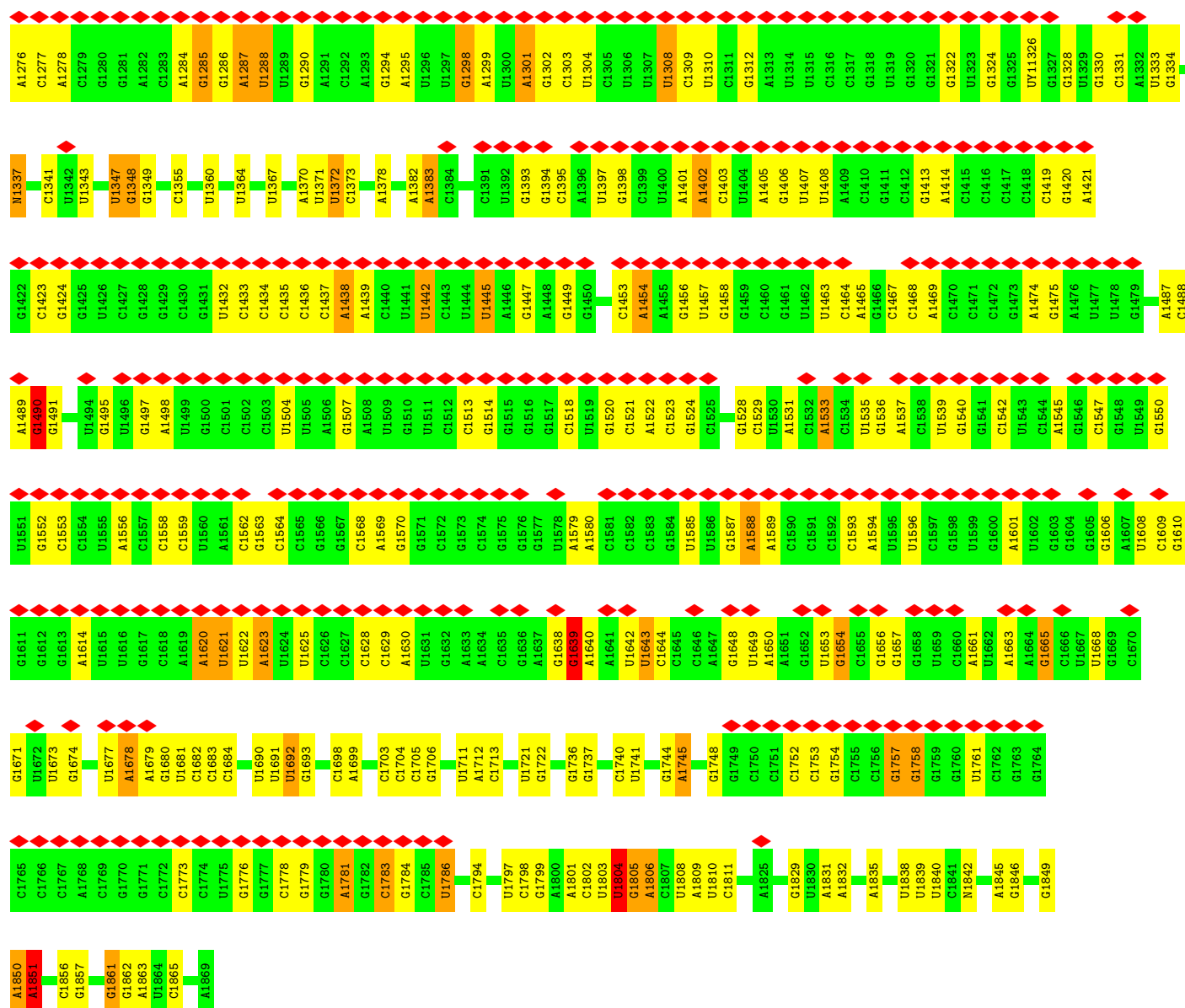


- Molecule 46: 18S rRNA (1740-MER)

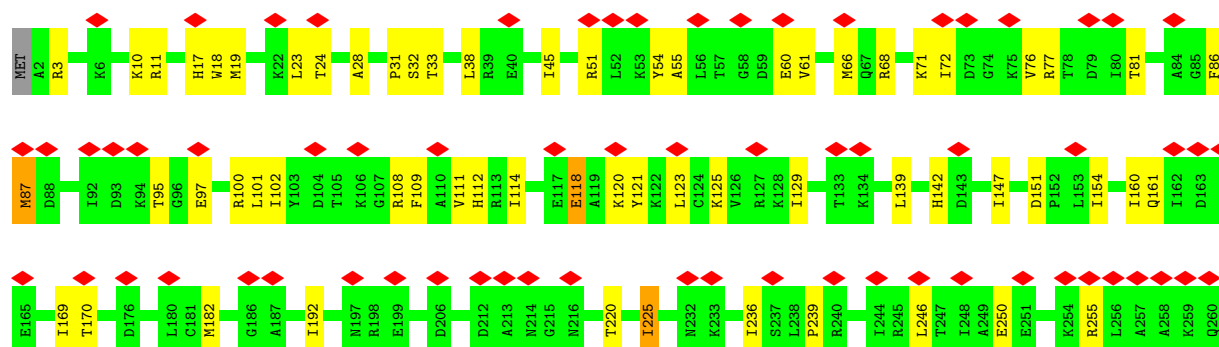
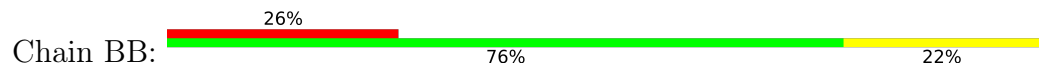
Chain BA: 33% 52% 35% 5% . 7%



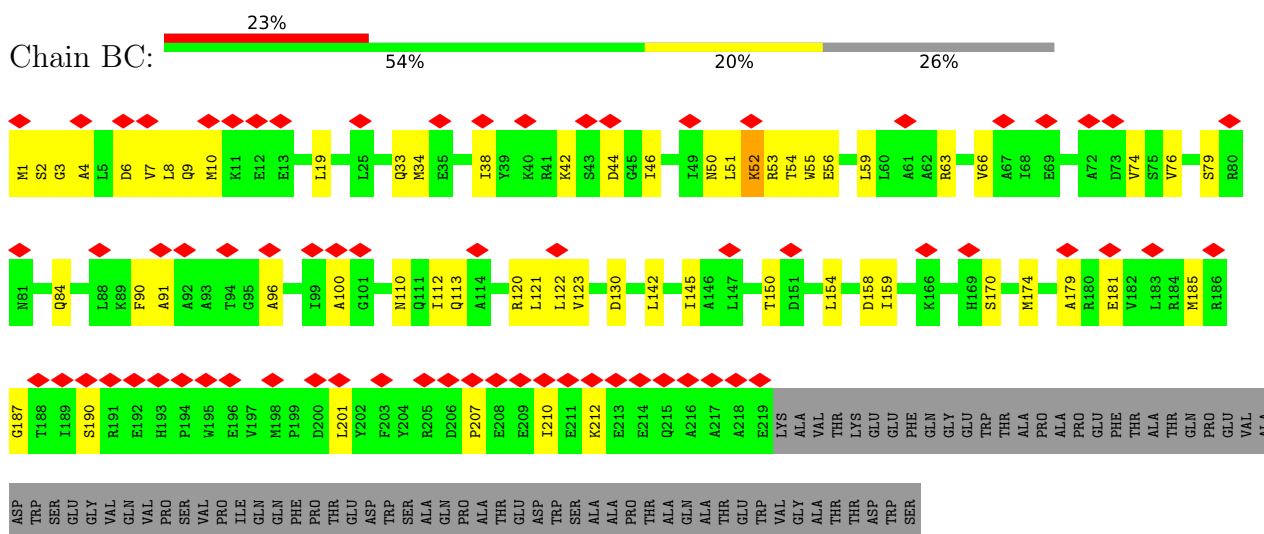




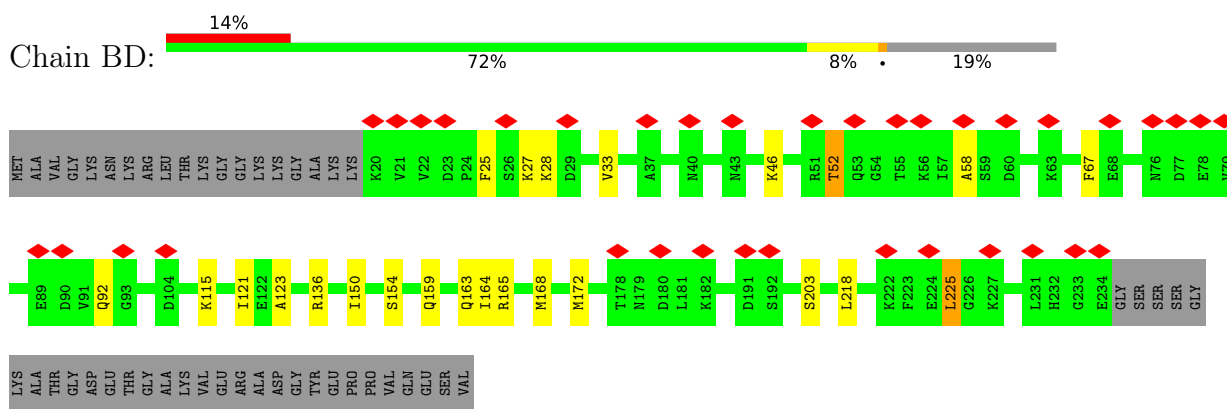
- Molecule 47: 40S ribosomal protein S4, X isoform



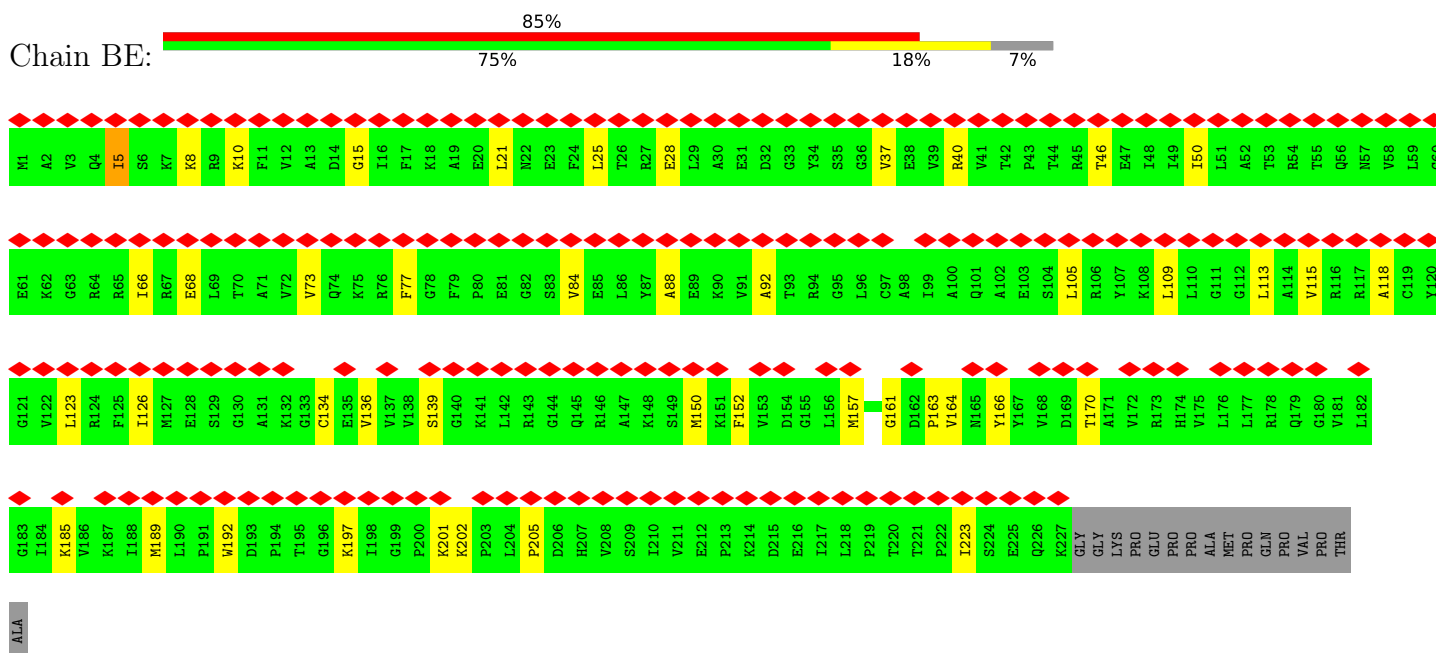
- Molecule 48: Small ribosomal subunit protein uS2



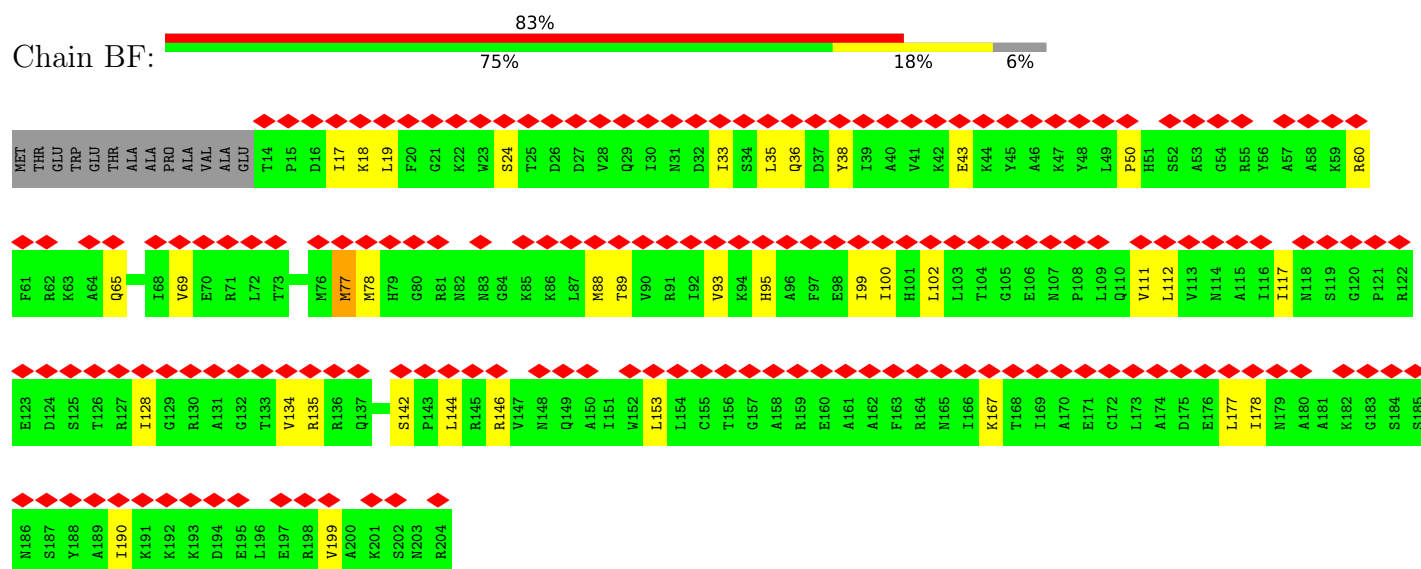
- Molecule 49: 40S ribosomal protein S3a



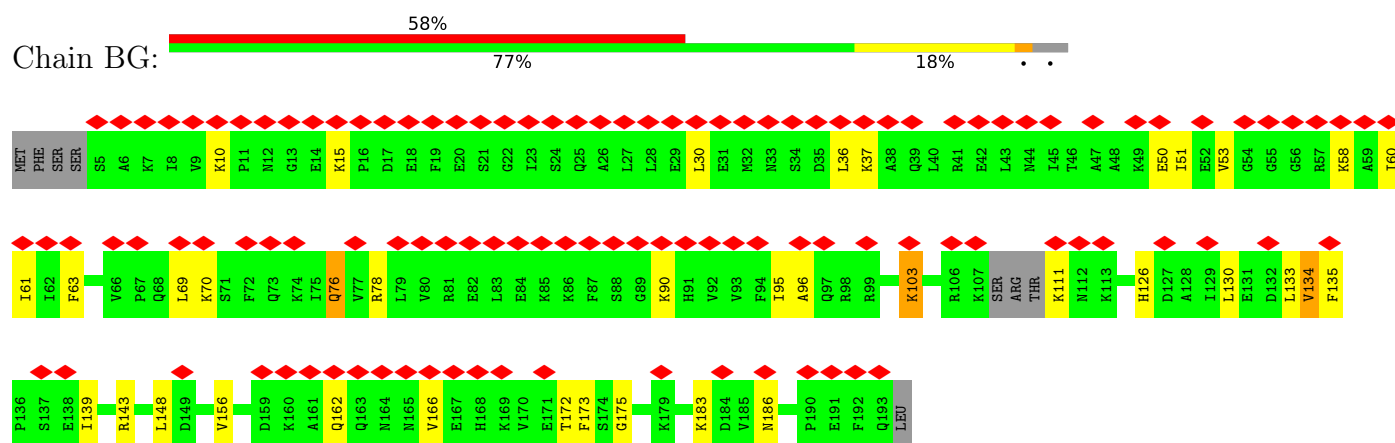
- Molecule 50: 40S ribosomal protein S3



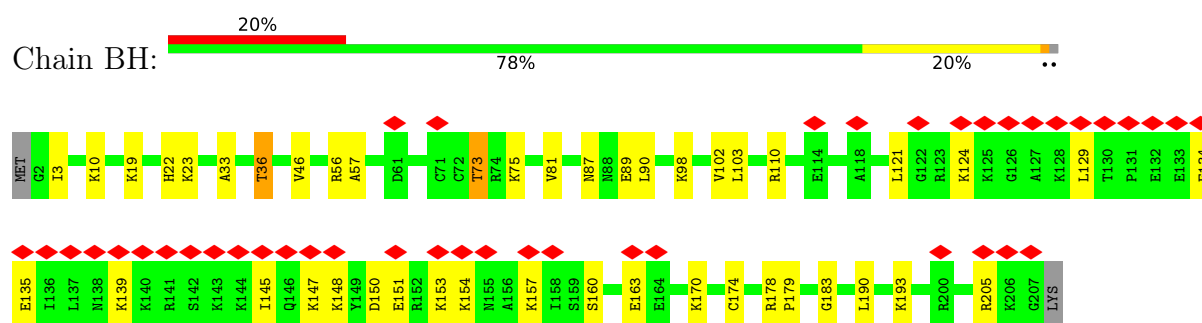
- Molecule 51: 40S ribosomal protein S5



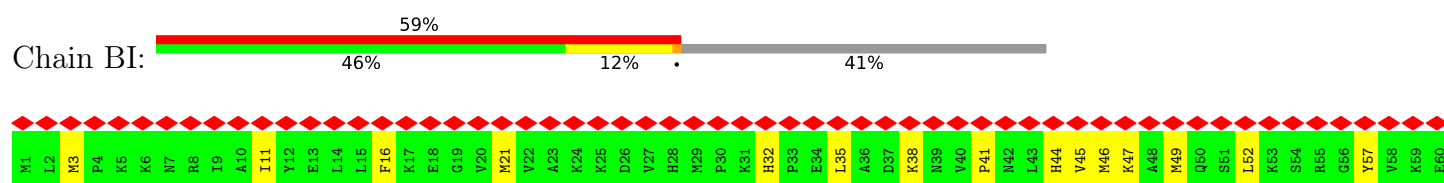
- Molecule 52: 40S ribosomal protein S7

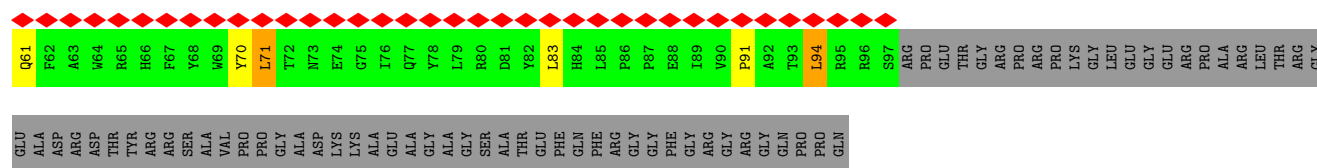


- Molecule 53: 40S ribosomal protein S8

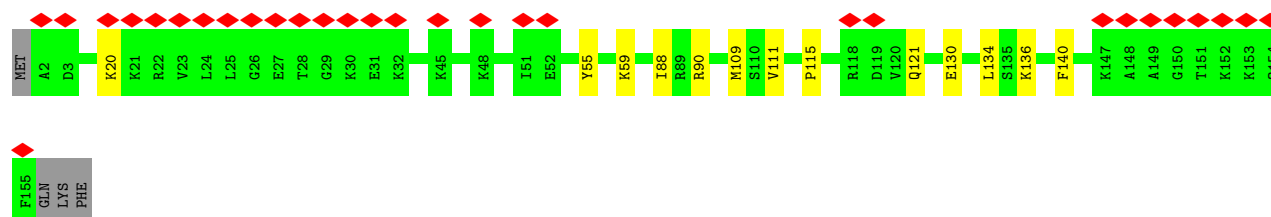
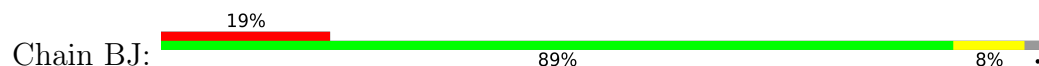


- Molecule 54: 40S ribosomal protein S10

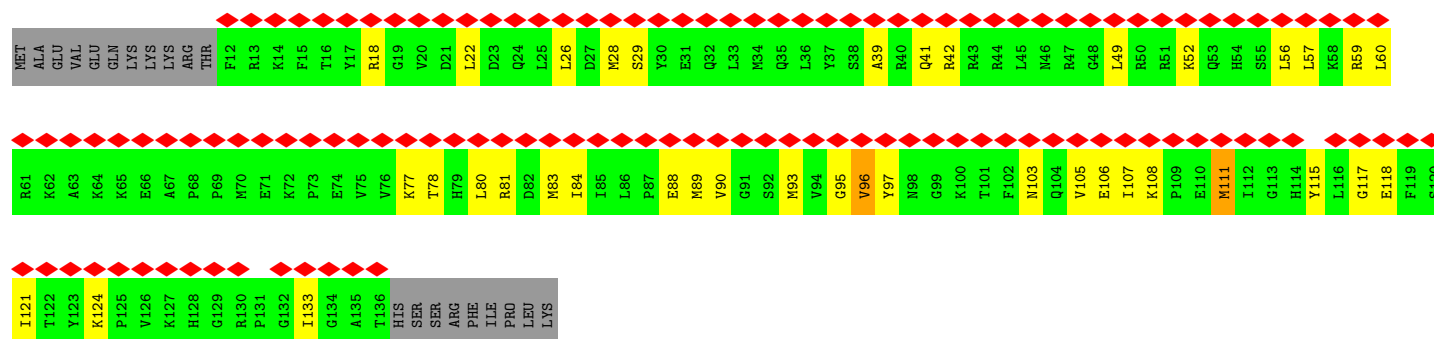
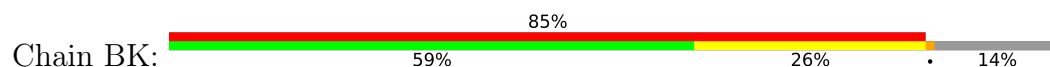




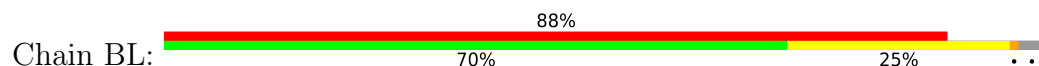
• Molecule 55: 40S ribosomal protein S11



• Molecule 56: 40S ribosomal protein S15

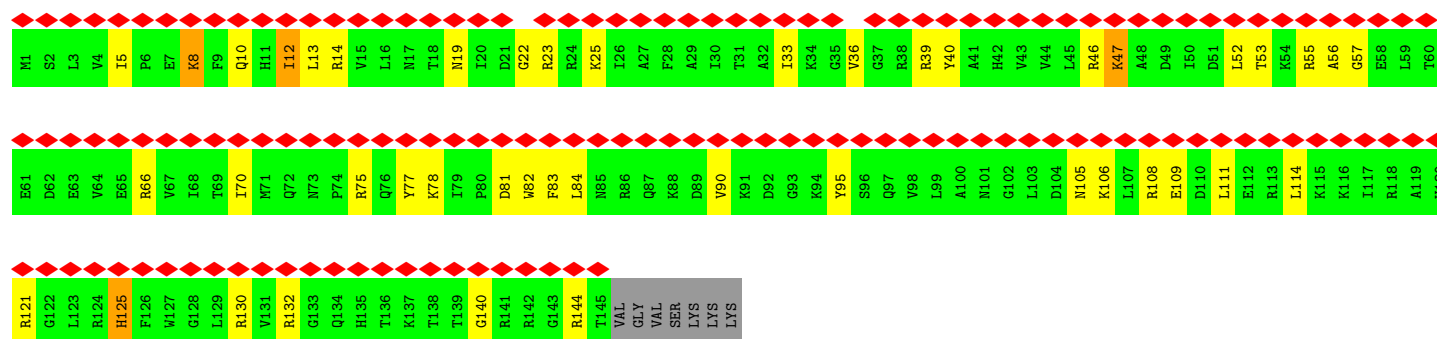


• Molecule 57: 40S ribosomal protein S16

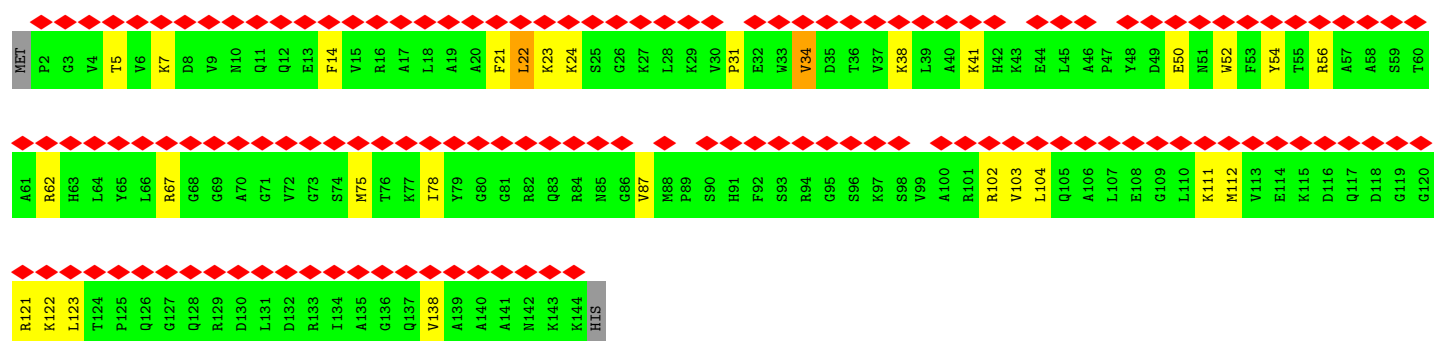
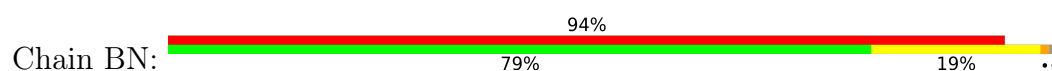


• Molecule 58: 40S ribosomal protein S18

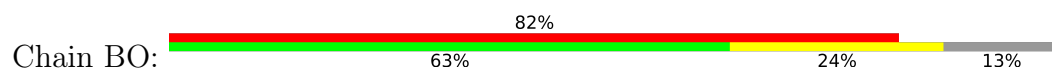




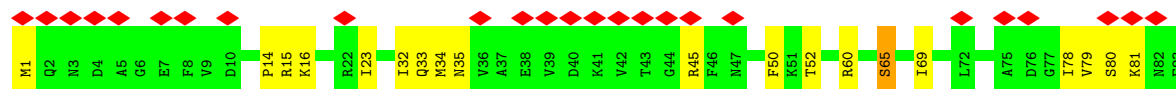
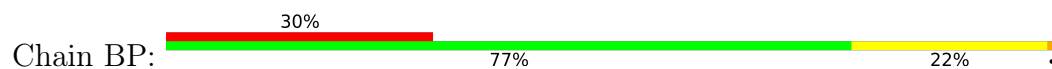
• Molecule 59: Small ribosomal subunit protein eS19



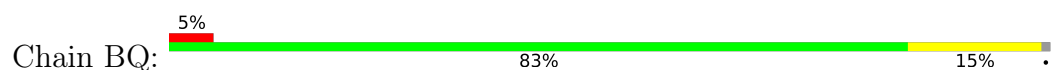
• Molecule 60: 40S ribosomal protein S20

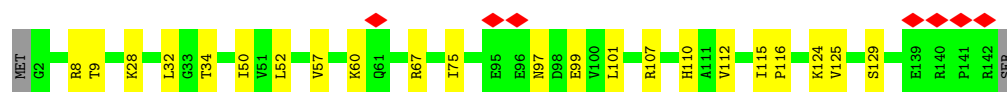


• Molecule 61: 40S ribosomal protein S21

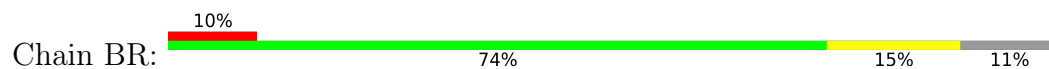


• Molecule 62: 40S ribosomal protein S23

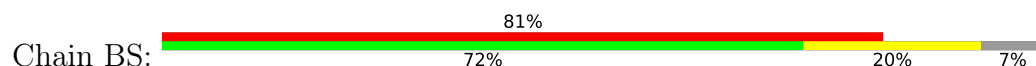




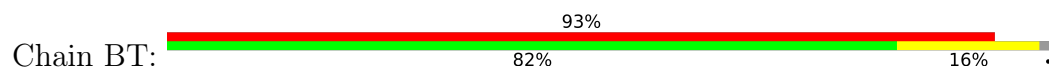
- Molecule 63: 40S ribosomal protein S26



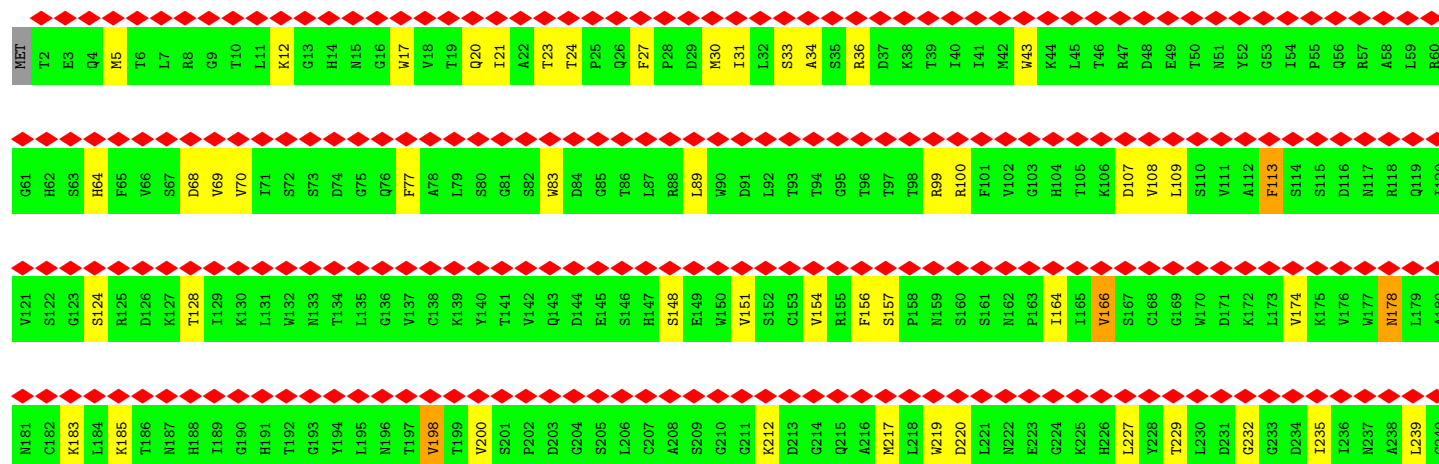
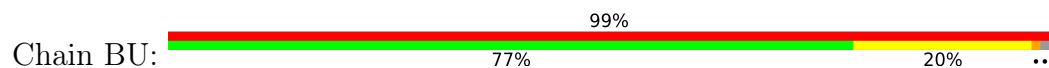
- Molecule 64: 40S ribosomal protein S28

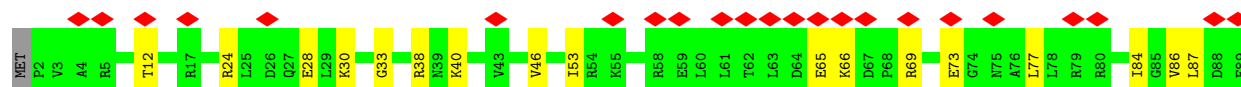


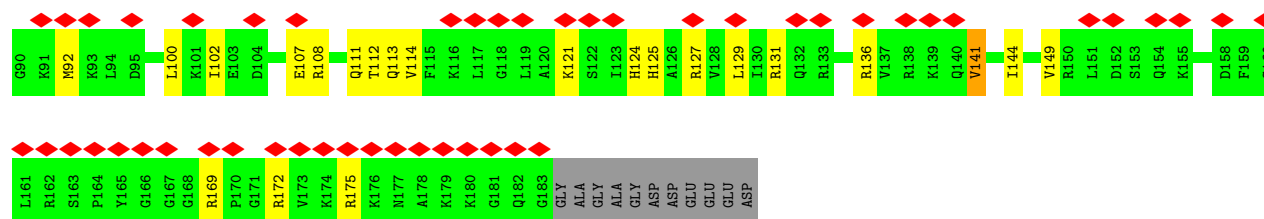
- Molecule 65: 40S ribosomal protein S29



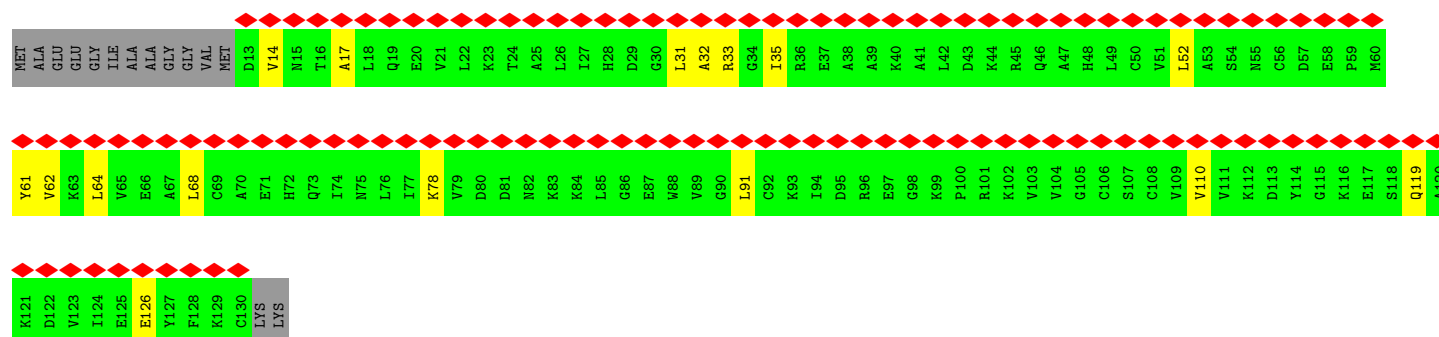
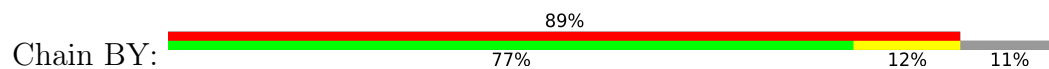
- Molecule 66: Receptor of activated protein C kinase 1



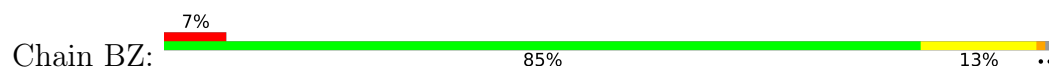




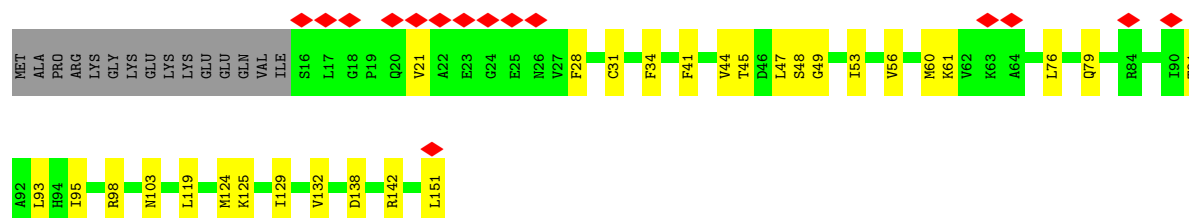
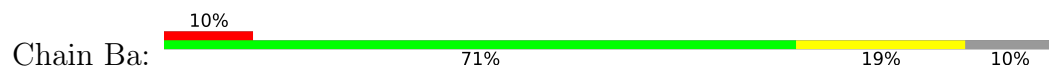
- Molecule 70: 40S ribosomal protein S12



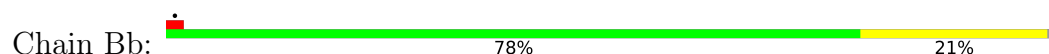
- Molecule 71: 40S ribosomal protein S13



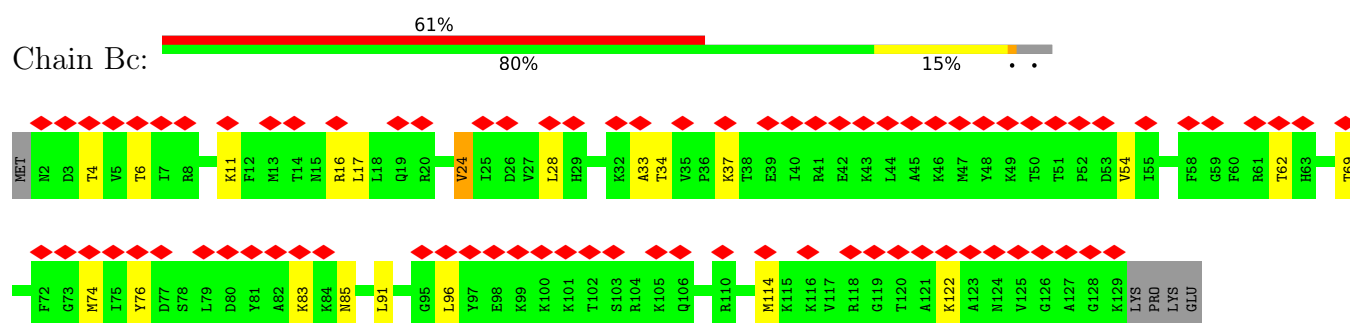
- Molecule 72: Small ribosomal subunit protein uS11



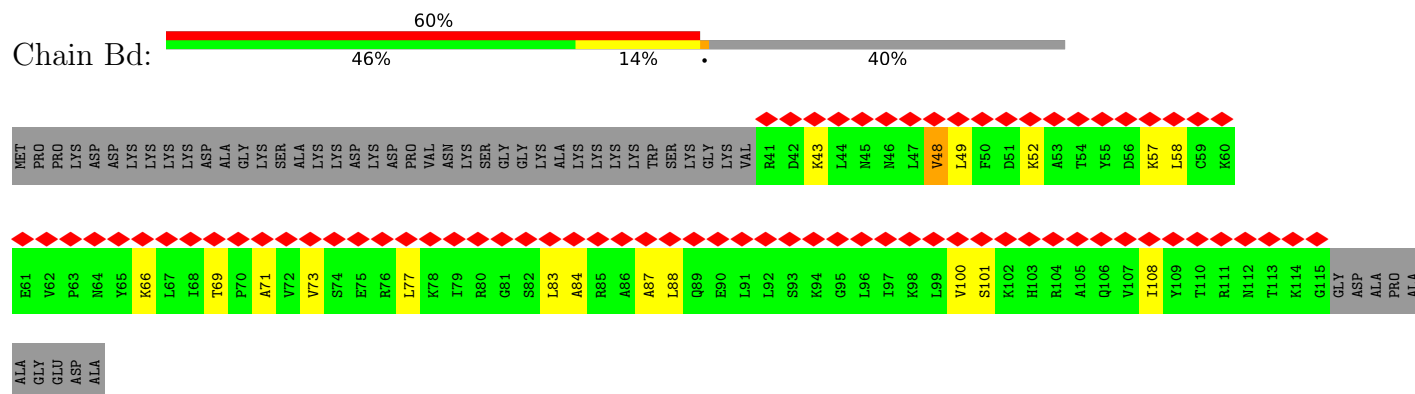
- Molecule 73: 40S ribosomal protein S15a



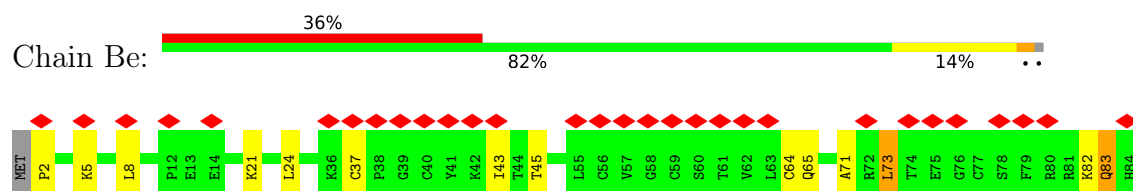
- Molecule 74: 40S ribosomal protein S24



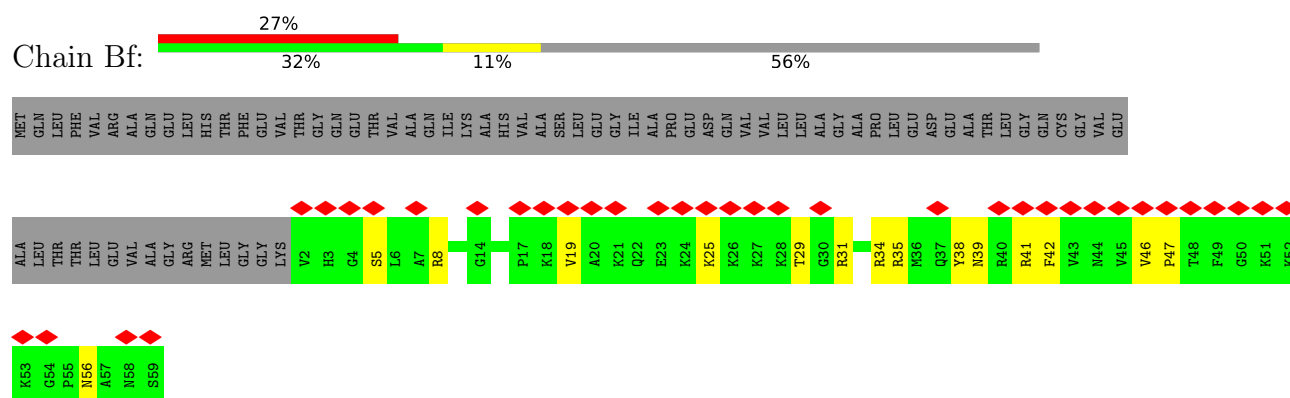
- Molecule 75: 40S ribosomal protein S25



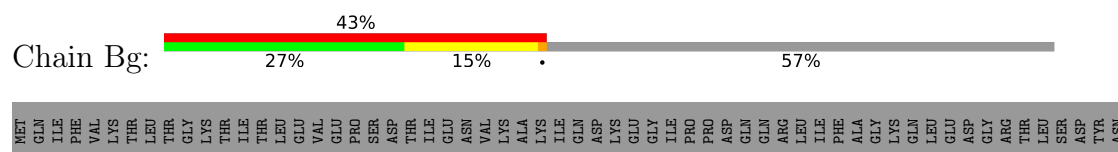
- Molecule 76: 40S ribosomal protein S27



- Molecule 77: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



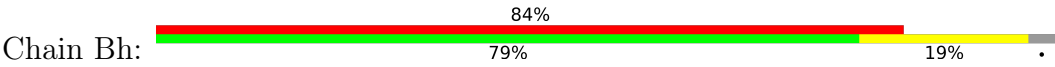
- Molecule 78: Ubiquitin-40S ribosomal protein S27a



ILE	GLN	LYS	GLU	SER	THR	LEU	HIS	LEU	VAL	LEU	ARG	LEU	ARG	ARG	GLY	GLY	ALA	LYS	LYS	ARG	ARG	LYS	LYS	LYS	SER	Y65	T86	T87	P88	K69	K90	N91	K92	H93	K94	R95	K96	K97	V98	K99	L100	A101	V102	L103	K104	Y105	Y106	K107	V108	D109	E110	N111	G112	K113	I114	S115	R116	L117	R118	R119	E120
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C121	P122	S123	D124	E125	C126	G127	A128	G129	V130	F131	M132	A133	S134	H135	F136	D137	R138	H139	Y140	C141	G142	K143	C144	C145	L146	T147	Y148	C149	F150	N151	LYS	PRO	GLU	ASP	LYS
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• Molecule 79: 40S ribosomal protein S17



MET	G2	R3	V4	R5	T6	K7	T8	V9	K10	K11	A12	A13	R14	V15	I16	I17	E18	K19	Y20	Y21	T22	R23	L24	G25	N26	D27	H29	T30	N31	K32	R33	V34	C35	E36	E37	I38	A39	I40	I41	P42	S43	K44	K45	L46	R47	N48	K49	I50	A51	G52	Y53	V54	T55	H56	L57	M58	K59	R60
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I61	Q62	R63	G64	P65	V66	R67	G68	S69	I70	I71	K72	L73	Q74	E75	E76	E77	R78	E79	R80	R81	D82	R83	Y84	V85	P86	E87	V88	S89	A90	L91	D92	Q93	E94	I95	I96	E97	V98	D99	P100	D101	T102	K103	E104	M105	L106	K107	L108	L109	D110	F111	G112	S113	L114	S115	N116	L117	Q118	V119	T120
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Q121	P122	T123	V124	N127	T130	P131	R132	GLY	PRO	VAL
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128805	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.963	Depositor
Minimum map value	-1.545	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	515.83997, 515.83997, 515.83997	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.80599993, 0.80599993, 0.80599993	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NMM, MG, B8N, 5MC, UR3, IAS, OMG, MA6, OMU, V5N, UY1, HIC, PSU, G7M, OMC, 6MZ, 4AC, K, ZN, 1MA, A2M

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	0.32	0/86723	0.32	0/135219
2	AB	0.30	0/2858	0.28	0/4455
3	AC	0.32	0/3609	0.30	0/5623
4	AD	0.31	0/1936	0.38	0/2596
5	AE	0.29	0/3294	0.35	0/4406
6	AF	0.28	0/2981	0.36	0/4002
7	AG	0.23	0/2428	0.41	1/3252 (0.0%)
8	AH	0.22	0/1942	0.35	0/2606
9	AI	0.29	0/1916	0.35	0/2553
10	AJ	0.24	0/1971	0.38	0/2651
11	AK	0.25	0/1537	0.29	0/2066
12	AL	0.26	0/1753	0.39	0/2343
13	AM	0.19	0/1433	0.34	0/1915
14	AN	0.25	0/1732	0.37	0/2315
15	AO	0.23	0/1161	0.32	0/1554
16	AP	0.32	0/1746	0.32	0/2338
17	AQ	0.29	0/1682	0.37	0/2250
18	AR	0.29	0/1268	0.35	0/1701
19	AS	0.29	0/1537	0.37	0/2052
20	AT	0.25	0/1582	0.30	0/2091
21	AU	0.29	0/1493	0.35	0/2003
22	AV	0.29	0/1326	0.38	0/1770
23	AW	0.21	0/839	0.44	0/1126
24	AX	0.29	0/993	0.35	0/1332
25	AY	0.23	0/1012	0.34	0/1342
26	AZ	0.25	0/1002	0.32	0/1345
27	Aa	0.24	0/1119	0.33	0/1488
28	Ab	0.25	0/1130	0.32	0/1507
29	Ac	0.30	0/1179	0.34	0/1573
30	Ad	0.23	0/821	0.37	0/1084
31	Ae	0.27	0/774	0.38	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Af	0.27	0/894	0.31	0/1204
33	Ag	0.31	0/1071	0.37	0/1429
34	Ah	0.31	0/895	0.32	0/1198
35	Ai	0.27	0/878	0.34	0/1170
36	Aj	0.24	0/1023	0.33	1/1351 (0.1%)
37	Ak	0.21	0/824	0.32	0/1090
38	Al	0.31	0/720	0.34	0/952
39	Am	0.25	0/565	0.39	0/750
40	An	0.27	0/454	0.32	0/599
41	Ao	0.26	0/425	0.39	0/564
42	Ap	0.27	0/231	0.28	0/294
43	Aq	0.26	0/858	0.32	0/1131
44	Ar	0.29	0/691	0.36	0/919
45	As	0.28	0/1002	0.42	0/1344
46	BA	0.25	0/39082	0.32	5/60892 (0.0%)
47	BB	0.20	0/2118	0.35	0/2849
48	BC	0.22	0/1764	0.42	0/2396
49	BD	0.21	0/1774	0.32	0/2373
50	BE	0.14	0/1793	0.34	0/2414
51	BF	0.15	0/1531	0.38	0/2059
52	BG	0.19	0/1519	0.39	0/2033
53	BH	0.23	0/1715	0.36	0/2287
54	BI	0.13	0/840	0.37	0/1133
55	BJ	0.24	0/1280	0.37	0/1712
56	BK	0.17	0/1047	0.42	0/1399
57	BL	0.16	0/1142	0.41	0/1528
58	BM	0.14	0/1216	0.36	0/1628
59	BN	0.13	0/1119	0.32	0/1498
60	BO	0.14	0/827	0.35	0/1110
61	BP	0.24	0/643	0.47	0/860
62	BQ	0.23	0/1116	0.37	0/1490
63	BR	0.24	0/847	0.39	0/1135
64	BS	0.15	0/508	0.35	0/680
65	BT	0.16	0/470	0.32	0/623
66	BU	0.14	0/2493	0.38	0/3394
67	BV	0.22	0/1764	0.39	0/2382
68	BW	0.17	0/1926	0.40	0/2563
69	BX	0.20	0/1548	0.42	0/2066
70	BY	0.12	0/916	0.35	0/1233
71	BZ	0.23	0/1232	0.29	0/1656
72	Ba	0.22	0/1020	0.39	0/1366
73	Bb	0.24	0/1051	0.36	0/1406
74	Bc	0.19	0/1068	0.40	0/1418

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Bd	0.13	0/604	0.36	0/810
76	Be	0.20	0/665	0.33	0/891
77	Bf	0.15	0/465	0.31	0/612
78	Bg	0.12	0/560	0.35	0/745
79	Bh	0.20	0/1078	0.53	0/1447
All	All	0.28	0/226049	0.34	7/331679 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BA	3	C	O3'-P-O5'	-22.84	69.74	104.00
46	BA	1639	G7M	O3'-P-O5'	-13.32	78.69	104.00
46	BA	3	C	P-O3'-C3'	-11.48	102.98	120.20
46	BA	3	C	OP1-P-O3'	6.03	126.08	108.00
7	AG	93	THR	N-CA-C	-5.81	98.43	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	80205	0	40481	510	0
2	AB	2558	0	1295	7	0
3	AC	3316	0	1687	30	0
4	AD	1898	0	1993	13	0
5	AE	3239	0	3377	29	0
6	AF	2927	0	3104	26	0
7	AG	2382	0	2410	27	0
8	AH	1904	0	2055	21	0
9	AI	1878	0	2009	15	0
10	AJ	1935	0	2087	21	0
11	AK	1518	0	1601	11	0
12	AL	1713	0	1751	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AM	1410	0	1441	15	0
14	AN	1701	0	1818	20	0
15	AO	1138	0	1204	11	0
16	AP	1701	0	1749	15	0
17	AQ	1650	0	1794	13	0
18	AR	1242	0	1269	15	0
19	AS	1513	0	1628	12	0
20	AT	1566	0	1729	12	0
21	AU	1453	0	1490	10	0
22	AV	1298	0	1366	8	0
23	AW	825	0	850	14	0
24	AX	979	0	1039	7	0
25	AY	997	0	1053	13	0
26	AZ	985	0	1066	8	0
27	Aa	1102	0	1189	14	0
28	Ab	1107	0	1182	8	0
29	Ac	1163	0	1206	8	0
30	Ad	808	0	875	14	0
31	Ae	764	0	804	5	0
32	Af	879	0	924	6	0
33	Ag	1053	0	1147	11	0
34	Ah	876	0	911	6	0
35	Ai	868	0	959	9	0
36	Aj	1015	0	1148	13	0
37	Ak	813	0	894	11	0
38	Al	705	0	737	1	0
39	Am	559	0	624	7	0
40	An	444	0	483	8	0
41	Ao	419	0	452	0	0
42	Ap	230	0	276	1	0
43	Aq	842	0	914	7	0
44	Ar	681	0	731	4	0
45	As	987	0	1050	10	0
46	BA	36916	0	18646	359	0
47	BB	2076	0	2177	39	0
48	BC	1727	0	1729	44	0
49	BD	1747	0	1822	12	0
50	BE	1765	0	1865	29	0
51	BF	1509	0	1563	28	0
52	BG	1497	0	1590	21	0
53	BH	1686	0	1772	26	0
54	BI	816	0	841	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BJ	1258	0	1332	7	0
56	BK	1027	0	1075	24	0
57	BL	1124	0	1193	23	0
58	BM	1198	0	1261	34	0
59	BN	1113	0	1145	20	0
60	BO	817	0	882	18	0
61	BP	636	0	637	20	0
62	BQ	1098	0	1167	14	0
63	BR	829	0	883	10	0
64	BS	506	0	536	10	0
65	BT	459	0	448	9	0
66	BU	2436	0	2393	35	0
67	BV	1724	0	1817	30	0
68	BW	1903	0	2068	33	0
69	BX	1520	0	1642	35	0
70	BY	906	0	921	11	0
71	BZ	1208	0	1293	11	0
72	Ba	1016	0	1038	19	0
73	Bb	1034	0	1080	15	0
74	Bc	1048	0	1122	14	0
75	Bd	598	0	656	13	0
76	Be	651	0	672	8	0
77	Bf	459	0	503	15	0
78	Bg	548	0	552	20	0
79	Bh	1064	0	1118	19	0
80	AA	190	0	0	0	0
80	AB	1	0	0	0	0
80	AC	4	0	0	0	0
80	AL	1	0	0	0	0
80	AP	1	0	0	0	0
80	AR	1	0	0	0	0
80	AX	1	0	0	0	0
80	BA	70	0	0	0	0
81	AA	66	0	0	0	0
81	AB	1	0	0	0	0
81	AC	1	0	0	0	0
81	AD	1	0	0	0	0
81	AL	1	0	0	0	0
81	Ag	1	0	0	0	0
81	Ah	1	0	0	0	0
81	Aq	1	0	0	0	0
81	BA	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	BF	1	0	0	0	0
82	Ai	1	0	0	0	0
82	Al	1	0	0	0	0
82	Ao	1	0	0	0	0
82	Aq	1	0	0	0	0
82	Ar	1	0	0	0	0
82	BR	1	0	0	0	0
82	BT	1	0	0	0	0
82	Bg	1	0	0	0	0
All	All	215529	0	159291	1820	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1820 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:70:G:N2	46:BA:79:A:H62	1.56	1.04
46:BA:39:A:H62	46:BA:515:G:H21	1.03	1.00
46:BA:1748:G:H1	46:BA:1786:U:H3	1.14	0.94
46:BA:70:G:H21	46:BA:79:A:N6	1.65	0.92
46:BA:39:A:H62	46:BA:515:G:N2	1.68	0.91

There are no symmetry-related clashes.

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	
4	AD	246/257 (96%)	237 (96%)	9 (4%)	0	100	100
5	AE	399/402 (99%)	384 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AF	366/368 (100%)	355 (97%)	11 (3%)	0	100	100
7	AG	291/293 (99%)	277 (95%)	13 (4%)	1 (0%)	36	53
8	AH	232/247 (94%)	218 (94%)	14 (6%)	0	100	100
9	AI	224/248 (90%)	219 (98%)	5 (2%)	0	100	100
10	AJ	240/266 (90%)	230 (96%)	10 (4%)	0	100	100
11	AK	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
12	AL	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
13	AM	174/178 (98%)	162 (93%)	12 (7%)	0	100	100
14	AN	208/211 (99%)	196 (94%)	10 (5%)	2 (1%)	12	22
15	AO	137/215 (64%)	133 (97%)	4 (3%)	0	100	100
16	AP	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
17	AQ	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
18	AR	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
19	AS	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
20	AT	185/196 (94%)	182 (98%)	3 (2%)	0	100	100
21	AU	173/176 (98%)	166 (96%)	7 (4%)	0	100	100
22	AV	157/160 (98%)	150 (96%)	6 (4%)	1 (1%)	21	35
23	AW	99/128 (77%)	91 (92%)	8 (8%)	0	100	100
24	AX	129/140 (92%)	128 (99%)	1 (1%)	0	100	100
25	AY	120/157 (76%)	112 (93%)	8 (7%)	0	100	100
26	AZ	118/156 (76%)	118 (100%)	0	0	100	100
27	Aa	130/145 (90%)	128 (98%)	2 (2%)	0	100	100
28	Ab	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
29	Ac	144/148 (97%)	138 (96%)	6 (4%)	0	100	100
30	Ad	95/159 (60%)	93 (98%)	2 (2%)	0	100	100
31	Ae	96/115 (84%)	90 (94%)	6 (6%)	0	100	100
32	Af	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
33	Ag	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
34	Ah	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
35	Ai	107/117 (92%)	106 (99%)	1 (1%)	0	100	100
36	Aj	120/123 (98%)	119 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Ak	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
38	Al	84/97 (87%)	84 (100%)	0	0	100	100
39	Am	66/70 (94%)	64 (97%)	2 (3%)	0	100	100
40	An	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
41	Ao	49/128 (38%)	49 (100%)	0	0	100	100
42	Ap	22/25 (88%)	22 (100%)	0	0	100	100
43	Aq	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
44	Ar	86/92 (94%)	82 (95%)	4 (5%)	0	100	100
45	As	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
47	BB	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
48	BC	217/295 (74%)	209 (96%)	8 (4%)	0	100	100
49	BD	213/264 (81%)	208 (98%)	5 (2%)	0	100	100
50	BE	225/243 (93%)	216 (96%)	9 (4%)	0	100	100
51	BF	189/204 (93%)	174 (92%)	15 (8%)	0	100	100
52	BG	182/194 (94%)	169 (93%)	12 (7%)	1 (0%)	24	40
53	BH	204/208 (98%)	196 (96%)	8 (4%)	0	100	100
54	BI	95/165 (58%)	88 (93%)	7 (7%)	0	100	100
55	BJ	152/158 (96%)	144 (95%)	8 (5%)	0	100	100
56	BK	123/145 (85%)	118 (96%)	5 (4%)	0	100	100
57	BL	139/146 (95%)	127 (91%)	12 (9%)	0	100	100
58	BM	143/152 (94%)	136 (95%)	7 (5%)	0	100	100
59	BN	140/145 (97%)	135 (96%)	5 (4%)	0	100	100
60	BO	101/119 (85%)	94 (93%)	7 (7%)	0	100	100
61	BP	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
62	BQ	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
63	BR	101/115 (88%)	100 (99%)	1 (1%)	0	100	100
64	BS	62/69 (90%)	54 (87%)	8 (13%)	0	100	100
65	BT	53/56 (95%)	53 (100%)	0	0	100	100
66	BU	311/317 (98%)	293 (94%)	18 (6%)	0	100	100
67	BV	220/293 (75%)	213 (97%)	7 (3%)	0	100	100
68	BW	232/249 (93%)	223 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	BX	181/194 (93%)	177 (98%)	4 (2%)	0	100	100
70	BY	116/132 (88%)	110 (95%)	6 (5%)	0	100	100
71	BZ	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
72	Ba	132/151 (87%)	124 (94%)	8 (6%)	0	100	100
73	Bb	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
74	Bc	127/133 (96%)	123 (97%)	4 (3%)	0	100	100
75	Bd	73/125 (58%)	68 (93%)	5 (7%)	0	100	100
76	Be	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
77	Bf	56/133 (42%)	52 (93%)	4 (7%)	0	100	100
78	Bg	65/156 (42%)	61 (94%)	4 (6%)	0	100	100
79	Bh	129/135 (96%)	127 (98%)	2 (2%)	0	100	100
All	All	11286/12657 (89%)	10871 (96%)	410 (4%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	BG	15	LYS
7	AG	95	TYR
14	AN	47	ALA
14	AN	64	VAL
22	AV	82	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	190/199 (96%)	185 (97%)	5 (3%)	40	65
5	AE	347/347 (100%)	344 (99%)	3 (1%)	70	86
6	AF	306/306 (100%)	302 (99%)	4 (1%)	61	80
7	AG	246/247 (100%)	237 (96%)	9 (4%)	30	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AH	209/220 (95%)	206 (99%)	3 (1%)	59	79
9	AI	195/215 (91%)	195 (100%)	0	100	100
10	AJ	204/223 (92%)	196 (96%)	8 (4%)	28	52
11	AK	169/171 (99%)	163 (96%)	6 (4%)	31	55
12	AL	181/182 (100%)	178 (98%)	3 (2%)	53	75
13	AM	148/149 (99%)	141 (95%)	7 (5%)	23	44
14	AN	176/177 (99%)	170 (97%)	6 (3%)	32	57
15	AO	118/161 (73%)	114 (97%)	4 (3%)	32	57
16	AP	171/172 (99%)	168 (98%)	3 (2%)	51	74
17	AQ	173/174 (99%)	169 (98%)	4 (2%)	44	69
18	AR	134/163 (82%)	128 (96%)	6 (4%)	24	46
19	AS	164/165 (99%)	162 (99%)	2 (1%)	63	81
20	AT	166/175 (95%)	164 (99%)	2 (1%)	63	81
21	AU	156/157 (99%)	153 (98%)	3 (2%)	50	73
22	AV	139/140 (99%)	137 (99%)	2 (1%)	59	79
23	AW	91/115 (79%)	84 (92%)	7 (8%)	12	23
24	AX	101/107 (94%)	100 (99%)	1 (1%)	68	84
25	AY	101/126 (80%)	100 (99%)	1 (1%)	68	84
26	AZ	108/133 (81%)	108 (100%)	0	100	100
27	Aa	123/135 (91%)	119 (97%)	4 (3%)	33	58
28	Ab	117/118 (99%)	115 (98%)	2 (2%)	53	75
29	Ac	119/120 (99%)	117 (98%)	2 (2%)	53	75
30	Ad	83/126 (66%)	79 (95%)	4 (5%)	23	43
31	Ae	83/97 (86%)	82 (99%)	1 (1%)	63	81
32	Af	97/110 (88%)	95 (98%)	2 (2%)	47	71
33	Ag	114/121 (94%)	110 (96%)	4 (4%)	32	55
34	Ah	88/89 (99%)	87 (99%)	1 (1%)	65	83
35	Ai	94/100 (94%)	92 (98%)	2 (2%)	47	71
36	Aj	109/110 (99%)	105 (96%)	4 (4%)	30	54
37	Ak	85/89 (96%)	82 (96%)	3 (4%)	32	55
38	Al	73/80 (91%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Am	63/65 (97%)	58 (92%)	5 (8%)	11	22
40	An	47/48 (98%)	46 (98%)	1 (2%)	47	71
41	Ao	47/116 (40%)	44 (94%)	3 (6%)	16	31
42	Ap	23/24 (96%)	23 (100%)	0	100	100
43	Aq	91/94 (97%)	89 (98%)	2 (2%)	45	70
44	Ar	71/75 (95%)	67 (94%)	4 (6%)	19	37
45	As	107/121 (88%)	106 (99%)	1 (1%)	70	86
47	BB	224/225 (100%)	215 (96%)	9 (4%)	28	51
48	BC	182/243 (75%)	179 (98%)	3 (2%)	55	77
49	BD	196/231 (85%)	190 (97%)	6 (3%)	35	60
50	BE	190/202 (94%)	186 (98%)	4 (2%)	47	71
51	BF	161/170 (95%)	155 (96%)	6 (4%)	30	54
52	BG	166/174 (95%)	160 (96%)	6 (4%)	31	55
53	BH	178/180 (99%)	169 (95%)	9 (5%)	21	40
54	BI	88/136 (65%)	84 (96%)	4 (4%)	24	46
55	BJ	138/142 (97%)	136 (99%)	2 (1%)	59	79
56	BK	111/130 (85%)	105 (95%)	6 (5%)	20	38
57	BL	117/121 (97%)	108 (92%)	9 (8%)	12	23
58	BM	126/132 (96%)	117 (93%)	9 (7%)	13	26
59	BN	112/114 (98%)	110 (98%)	2 (2%)	51	74
60	BO	94/107 (88%)	91 (97%)	3 (3%)	34	58
61	BP	67/67 (100%)	64 (96%)	3 (4%)	24	46
62	BQ	113/115 (98%)	110 (97%)	3 (3%)	39	64
63	BR	90/98 (92%)	88 (98%)	2 (2%)	45	70
64	BS	57/62 (92%)	54 (95%)	3 (5%)	20	39
65	BT	48/49 (98%)	48 (100%)	0	100	100
66	BU	272/275 (99%)	256 (94%)	16 (6%)	18	34
67	BV	188/225 (84%)	187 (100%)	1 (0%)	81	91
68	BW	204/218 (94%)	193 (95%)	11 (5%)	20	38
69	BX	162/168 (96%)	161 (99%)	1 (1%)	78	90
70	BY	98/108 (91%)	97 (99%)	1 (1%)	68	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	BZ	130/131 (99%)	125 (96%)	5 (4%)	29	53
72	Ba	105/118 (89%)	104 (99%)	1 (1%)	68	84
73	Bb	112/113 (99%)	106 (95%)	6 (5%)	20	38
74	Bc	111/115 (96%)	108 (97%)	3 (3%)	39	64
75	Bd	66/103 (64%)	64 (97%)	2 (3%)	36	61
76	Be	75/76 (99%)	69 (92%)	6 (8%)	11	21
77	Bf	47/104 (45%)	45 (96%)	2 (4%)	26	48
78	Bg	60/140 (43%)	58 (97%)	2 (3%)	33	58
79	Bh	119/122 (98%)	116 (98%)	3 (2%)	42	66
All	All	9834/10776 (91%)	9551 (97%)	283 (3%)	38	62

5 of 283 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
66	BU	166	VAL
66	BU	313	THR
73	Bb	26	LEU
30	Ad	9	THR
28	Ab	120	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
57	BL	8	GLN
67	BV	136	HIS
58	BM	73	ASN
62	BQ	16	HIS
72	Ba	103	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	3705/5069 (73%)	786 (21%)	13 (0%)
2	AB	119/120 (99%)	11 (9%)	0
3	AC	155/157 (98%)	33 (21%)	0
46	BA	1714/1869 (91%)	340 (19%)	6 (0%)
All	All	5693/7215 (78%)	1170 (20%)	19 (0%)

5 of 1170 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	G
1	AA	25	A
1	AA	39	A
1	AA	42	A
1	AA	48	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	BA	563	G
46	BA	1520	G
46	BA	1805	G
46	BA	866	PSU
1	AA	2760	G

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

224 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	$\# Z > 2$
1	PSU	AA	4532	1	18,21,22	1.47	4 (22%)	22,30,33	1.98	3 (13%)
1	A2M	AA	3724	1	22,25,26	1.43	4 (18%)	31,36,39	2.06	9 (29%)
46	PSU	BA	918	46	18,21,22	1.40	3 (16%)	22,30,33	1.99	4 (18%)
1	OMG	AA	4370	1	23,26,27	1.20	4 (17%)	33,38,41	1.94	6 (18%)
1	PSU	AA	1683	81,1	18,21,22	1.49	4 (22%)	22,30,33	1.96	3 (13%)
1	OMU	AA	2415	1	19,22,23	1.29	3 (15%)	26,31,34	1.79	5 (19%)
29	V5N	Ac	39	29	9,11,12	0.99	0	9,14,16	1.65	2 (22%)
1	PSU	AA	3762	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
46	A2M	BA	159	46	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
46	OMG	BA	436	46	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	AA	1781	1	18,21,22	1.40	3 (16%)	22,30,33	1.93	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	AA	4628	1	18,21,22	1.45	4 (22%)	22,30,33	2.04	3 (13%)
46	OMU	BA	428	46	19,22,23	1.20	3 (15%)	26,31,34	1.77	5 (19%)
1	OMC	AA	2351	80,1	19,22,23	0.85	1 (5%)	26,31,34	1.07	2 (7%)
1	PSU	AA	2508	1	18,21,22	1.44	4 (22%)	22,30,33	1.88	3 (13%)
1	PSU	AA	3695	1	18,21,22	1.43	4 (22%)	22,30,33	1.95	3 (13%)
1	OMC	AA	2861	1	19,22,23	0.84	0	26,31,34	0.89	1 (3%)
1	PSU	AA	1744	1	18,21,22	1.41	4 (22%)	22,30,33	1.96	3 (13%)
1	PSU	AA	3851	1	18,21,22	1.47	4 (22%)	22,30,33	1.91	3 (13%)
46	PSU	BA	681	46	18,21,22	1.48	4 (22%)	22,30,33	1.90	3 (13%)
46	OMG	BA	683	46	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	AA	1625	81,1	23,26,27	1.26	3 (13%)	33,38,41	1.89	6 (18%)
46	PSU	BA	100	80,46	18,21,22	1.39	3 (16%)	22,30,33	1.92	3 (13%)
1	PSU	AA	1582	1	18,21,22	1.48	4 (22%)	22,30,33	1.90	4 (18%)
1	OMG	AA	4196	80,1	23,26,27	1.25	3 (13%)	33,38,41	1.90	6 (18%)
46	OMG	BA	867	46	23,26,27	1.20	3 (13%)	33,38,41	1.90	6 (18%)
46	PSU	BA	1445	80,46	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
46	OMG	BA	1447	46	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
46	PSU	BA	651	46	18,21,22	1.40	3 (16%)	22,30,33	1.93	3 (13%)
46	MA6	BA	1851	46	23,26,27	1.42	5 (21%)	34,38,41	2.38	14 (41%)
1	OMG	AA	3792	1	23,26,27	1.23	3 (13%)	33,38,41	1.91	6 (18%)
1	PSU	AA	3768	1	18,21,22	1.39	3 (16%)	22,30,33	1.89	3 (13%)
46	PSU	BA	1177	46	18,21,22	1.41	4 (22%)	22,30,33	1.97	3 (13%)
46	MA6	BA	1850	46	23,26,27	1.41	3 (13%)	34,38,41	2.41	13 (38%)
1	A2M	AA	1323	1	22,25,26	1.44	3 (13%)	31,36,39	2.09	8 (25%)
1	PSU	AA	5001	1	18,21,22	1.43	3 (16%)	22,30,33	1.95	3 (13%)
1	OMG	AA	4499	1	23,26,27	1.23	3 (13%)	33,38,41	1.90	6 (18%)
46	PSU	BA	814	46	18,21,22	1.38	3 (16%)	22,30,33	1.83	4 (18%)
46	A2M	BA	99	80,46	22,25,26	1.41	3 (13%)	31,36,39	2.12	8 (25%)
46	OMU	BA	116	46	19,22,23	1.21	3 (15%)	26,31,34	1.72	6 (23%)
1	PSU	AA	3853	80,1	18,21,22	1.48	4 (22%)	22,30,33	1.92	3 (13%)
46	PSU	BA	863	46	18,21,22	1.41	3 (16%)	22,30,33	2.02	3 (13%)
46	UY1	BA	1326	46	19,22,23	4.35	8 (42%)	22,31,34	1.79	5 (22%)
46	PSU	BA	1643	80,46	18,21,22	1.38	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	3764	1	18,21,22	1.40	4 (22%)	22,30,33	1.86	3 (13%)
46	PSU	BA	572	46	18,21,22	1.37	3 (16%)	22,30,33	1.88	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	AA	3718	1	22,25,26	1.50	4 (18%)	31,36,39	1.86	6 (19%)
46	PSU	BA	1136	46	18,21,22	1.39	3 (16%)	22,30,33	1.97	4 (18%)
1	A2M	AA	2815	81,1	22,25,26	1.45	3 (13%)	31,36,39	2.14	8 (25%)
46	OMC	BA	517	46	19,22,23	0.81	0	26,31,34	0.88	1 (3%)
46	PSU	BA	1244	46	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
1	OMC	AA	2804	1	19,22,23	0.85	1 (5%)	26,31,34	0.70	0
1	PSU	AA	4636	1	18,21,22	1.43	4 (22%)	22,30,33	2.07	5 (22%)
1	OMG	AA	4228	1	23,26,27	1.20	4 (17%)	33,38,41	1.97	6 (18%)
46	PSU	BA	1625	46	18,21,22	1.37	2 (11%)	22,30,33	1.82	3 (13%)
1	A2M	AA	2401	1	22,25,26	1.40	4 (18%)	31,36,39	2.09	10 (32%)
1	PSU	AA	3884	1	18,21,22	1.52	4 (22%)	22,30,33	1.95	3 (13%)
1	PSU	AA	2632	1	18,21,22	1.42	4 (22%)	22,30,33	1.84	3 (13%)
1	PSU	AA	3822	1	18,21,22	1.40	3 (16%)	22,30,33	1.99	4 (18%)
1	OMC	AA	4456	1	19,22,23	0.86	1 (5%)	26,31,34	0.91	1 (3%)
1	OMU	AA	4498	1	19,22,23	1.28	3 (15%)	26,31,34	1.75	5 (19%)
46	A2M	BA	1031	46	22,25,26	1.41	5 (22%)	31,36,39	2.04	11 (35%)
46	A2M	BA	590	46	22,25,26	1.46	4 (18%)	31,36,39	2.17	8 (25%)
46	A2M	BA	668	80,46	22,25,26	1.47	5 (22%)	31,36,39	2.03	10 (32%)
46	PSU	BA	1692	46	18,21,22	1.42	4 (22%)	22,30,33	1.96	3 (13%)
1	A2M	AA	4590	1	22,25,26	1.43	5 (22%)	31,36,39	2.11	11 (35%)
1	OMU	AA	4620	1	19,22,23	1.33	3 (15%)	26,31,34	1.76	4 (15%)
46	PSU	BA	119	46	18,21,22	1.39	4 (22%)	22,30,33	1.88	3 (13%)
1	OMU	AA	2837	1	19,22,23	1.31	3 (15%)	26,31,34	1.85	5 (19%)
46	OMG	BA	1328	46	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
46	OMC	BA	1703	46	19,22,23	0.80	0	26,31,34	0.71	0
3	PSU	AC	55	3	18,21,22	1.44	4 (22%)	22,30,33	1.93	3 (13%)
46	OMC	BA	174	46	19,22,23	0.81	0	26,31,34	0.75	0
46	PSU	BA	649	46	18,21,22	1.42	3 (16%)	22,30,33	1.82	3 (13%)
1	OMC	AA	4536	1	19,22,23	0.86	0	26,31,34	0.86	1 (3%)
3	PSU	AC	69	3	18,21,22	1.40	3 (16%)	22,30,33	1.93	4 (18%)
1	5MC	AA	4447	81,1	18,22,23	1.01	2 (11%)	26,32,35	1.35	4 (15%)
1	PSU	AA	1677	1	18,21,22	1.45	5 (27%)	22,30,33	1.87	3 (13%)
1	A2M	AA	4523	80,1	22,25,26	1.41	4 (18%)	31,36,39	2.20	10 (32%)
46	OMU	BA	1804	46	19,22,23	1.27	3 (15%)	26,31,34	1.73	4 (15%)
46	PSU	BA	1056	46	18,21,22	1.39	4 (22%)	22,30,33	1.90	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	BA	406	46	18,21,22	1.44	4 (22%)	22,30,33	1.94	3 (13%)
46	A2M	BA	1383	46	22,25,26	1.46	4 (18%)	31,36,39	2.10	9 (29%)
46	PSU	BA	1003	46	18,21,22	1.42	4 (22%)	22,30,33	1.96	3 (13%)
72	IAS	Ba	138	72	6,7,8	1.08	0	6,8,10	1.51	1 (16%)
5	HIC	AE	245	5	10,11,12	0.60	0	8,14,16	0.66	0
1	UR3	AA	4530	1	19,22,23	0.95	0	26,32,35	1.41	2 (7%)
1	PSU	AA	4973	1	18,21,22	1.40	3 (16%)	22,30,33	1.97	4 (18%)
46	PSU	BA	36	46	18,21,22	1.40	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	AA	1326	1	22,25,26	1.44	4 (18%)	31,36,39	2.10	9 (29%)
1	PSU	AA	1779	1	18,21,22	1.42	4 (22%)	22,30,33	1.95	3 (13%)
1	5MC	AA	3782	80,1	18,22,23	0.94	2 (11%)	26,32,35	1.20	4 (15%)
1	PSU	AA	4579	1	18,21,22	1.42	4 (22%)	22,30,33	1.98	3 (13%)
46	PSU	BA	966	46	18,21,22	1.40	4 (22%)	22,30,33	1.92	3 (13%)
46	PSU	BA	1347	46	18,21,22	1.36	3 (16%)	22,30,33	1.86	3 (13%)
46	OMG	BA	1490	80,46	23,26,27	1.23	3 (13%)	33,38,41	1.88	6 (18%)
46	4AC	BA	1842	46	21,24,25	1.07	1 (4%)	29,34,37	1.37	3 (10%)
1	PSU	AA	1862	1	18,21,22	1.43	4 (22%)	22,30,33	1.98	3 (13%)
46	PSU	BA	105	46	18,21,22	1.41	3 (16%)	22,30,33	1.93	3 (13%)
1	OMC	AA	3869	1	19,22,23	0.84	1 (5%)	26,31,34	0.71	0
1	PSU	AA	4299	1	18,21,22	1.47	4 (22%)	22,30,33	1.83	3 (13%)
1	PSU	AA	5010	1	18,21,22	1.42	3 (16%)	22,30,33	1.90	3 (13%)
1	OMU	AA	4227	1	19,22,23	1.30	3 (15%)	26,31,34	1.78	4 (15%)
1	OMG	AA	4618	1	23,26,27	1.23	4 (17%)	33,38,41	1.96	6 (18%)
46	6MZ	BA	1832	80,46,81	22,25,26	1.49	5 (22%)	30,36,39	2.19	9 (30%)
1	A2M	AA	3867	1	22,25,26	1.46	4 (18%)	31,36,39	2.04	8 (25%)
1	PSU	AA	3920	80,1	18,21,22	1.51	4 (22%)	22,30,33	1.91	4 (18%)
1	OMG	AA	4623	1	23,26,27	1.26	4 (17%)	33,38,41	1.92	6 (18%)
1	PSU	AA	3770	1	18,21,22	1.45	4 (22%)	22,30,33	1.84	3 (13%)
1	OMU	AA	3925	1	19,22,23	1.32	3 (15%)	26,31,34	1.77	5 (19%)
46	OMG	BA	601	46	23,26,27	1.22	3 (13%)	33,38,41	1.92	6 (18%)
46	A2M	BA	484	46	22,25,26	1.47	3 (13%)	31,36,39	2.14	8 (25%)
1	PSU	AA	4442	1	18,21,22	1.44	4 (22%)	22,30,33	2.02	5 (22%)
1	A2M	AA	398	1	22,25,26	1.42	4 (18%)	31,36,39	2.14	10 (32%)
1	OMC	AA	3887	1	19,22,23	0.85	0	26,31,34	0.92	1 (3%)
46	PSU	BA	218	46	18,21,22	1.39	3 (16%)	22,30,33	1.91	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	AA	3701	81,1	19,22,23	0.82	0	26,31,34	0.89	0
1	PSU	AA	1860	1	18,21,22	1.46	4 (22%)	22,30,33	1.89	3 (13%)
3	OMG	AC	75	3	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
3	OMU	AC	14	1,3	19,22,23	1.29	3 (15%)	26,31,34	1.75	5 (19%)
1	OMG	AA	4392	1	23,26,27	1.25	4 (17%)	33,38,41	1.94	7 (21%)
1	OMG	AA	4637	81,1	23,26,27	1.25	4 (17%)	33,38,41	1.93	7 (21%)
46	PSU	BA	1174	46	18,21,22	1.43	4 (22%)	22,30,33	1.95	3 (13%)
1	PSU	AA	3730	1	18,21,22	1.39	3 (16%)	22,30,33	1.93	4 (18%)
1	OMG	AA	3899	80,1	23,26,27	1.25	4 (17%)	33,38,41	1.95	6 (18%)
1	OMC	AA	1881	80,1	19,22,23	0.88	0	26,31,34	0.88	0
1	PSU	AA	4423	1	18,21,22	1.40	4 (22%)	22,30,33	1.91	3 (13%)
1	PSU	AA	4500	1	18,21,22	1.42	3 (16%)	22,30,33	2.01	3 (13%)
1	A2M	AA	4571	1	22,25,26	1.46	5 (22%)	31,36,39	2.06	10 (32%)
46	PSU	BA	801	46	18,21,22	1.44	4 (22%)	22,30,33	1.89	3 (13%)
1	OMG	AA	3627	1	23,26,27	1.24	4 (17%)	33,38,41	1.97	6 (18%)
46	PSU	BA	1232	46	18,21,22	1.36	2 (11%)	22,30,33	1.96	3 (13%)
1	PSU	AA	3715	1	18,21,22	1.39	3 (16%)	22,30,33	1.89	4 (18%)
1	PSU	AA	2843	1	18,21,22	1.44	4 (22%)	22,30,33	1.92	3 (13%)
1	PSU	AA	1782	1	18,21,22	1.40	4 (22%)	22,30,33	1.93	3 (13%)
1	PSU	AA	4296	1	18,21,22	1.41	3 (16%)	22,30,33	1.97	3 (13%)
46	OMU	BA	172	46	19,22,23	1.21	3 (15%)	26,31,34	1.74	5 (19%)
46	PSU	BA	667	46	18,21,22	1.45	5 (27%)	22,30,33	1.91	4 (18%)
46	PSU	BA	866	46	18,21,22	1.36	3 (16%)	22,30,33	2.06	4 (18%)
1	1MA	AA	1322	80,1	21,25,26	1.36	4 (19%)	31,37,40	1.70	6 (19%)
46	PSU	BA	366	46	18,21,22	1.44	4 (22%)	22,30,33	1.89	4 (18%)
1	PSU	AA	4293	1	18,21,22	1.43	4 (22%)	22,30,33	1.92	4 (18%)
46	PSU	BA	296	46	18,21,22	1.38	3 (16%)	22,30,33	1.86	3 (13%)
1	OMG	AA	3744	1	23,26,27	1.23	4 (17%)	33,38,41	1.89	6 (18%)
1	PSU	AA	4521	80,81,1	18,21,22	1.46	4 (22%)	22,30,33	1.91	3 (13%)
1	A2M	AA	1534	80,1	22,25,26	1.43	4 (18%)	31,36,39	2.09	10 (32%)
1	PSU	AA	1536	1	18,21,22	1.47	4 (22%)	22,30,33	1.88	3 (13%)
46	PSU	BA	686	46	18,21,22	1.41	2 (11%)	22,30,33	1.93	3 (13%)
1	PSU	AA	4972	1	18,21,22	1.39	3 (16%)	22,30,33	2.00	4 (18%)
1	PSU	AA	3639	1	18,21,22	1.50	4 (22%)	22,30,33	1.86	3 (13%)
1	OMG	AA	2424	1	23,26,27	1.23	3 (13%)	33,38,41	1.89	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	BA	93	46	18,21,22	1.33	3 (16%)	22,30,33	1.89	3 (13%)
46	A2M	BA	512	46	22,25,26	1.46	4 (18%)	31,36,39	2.17	9 (29%)
1	OMC	AA	2365	80,1	19,22,23	0.83	0	26,31,34	0.78	0
1	OMC	AA	2422	80,1	19,22,23	0.84	0	26,31,34	0.79	0
1	PSU	AA	4493	81,1	18,21,22	1.44	4 (22%)	22,30,33	1.93	3 (13%)
46	PSU	BA	1004	46	18,21,22	1.42	3 (16%)	22,30,33	1.87	3 (13%)
46	PSU	BA	1238	46	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	AA	3637	81,1	18,21,22	1.51	4 (22%)	22,30,33	2.04	5 (22%)
1	PSU	AA	4457	1	18,21,22	1.44	4 (22%)	22,30,33	1.96	3 (13%)
1	PSU	AA	3844	1	18,21,22	1.44	3 (16%)	22,30,33	1.92	4 (18%)
46	PSU	BA	815	46	18,21,22	1.38	3 (16%)	22,30,33	1.87	3 (13%)
46	PSU	BA	109	46	18,21,22	1.40	3 (16%)	22,30,33	1.97	3 (13%)
1	UY1	AA	3818	81,1	19,22,23	4.11	9 (47%)	22,31,34	2.02	6 (27%)
46	A2M	BA	1678	46	22,25,26	1.45	4 (18%)	31,36,39	2.09	9 (29%)
46	PSU	BA	300	46	18,21,22	1.38	3 (16%)	22,30,33	1.89	3 (13%)
46	PSU	BA	1186	46	18,21,22	1.41	3 (16%)	22,30,33	1.93	4 (18%)
46	PSU	BA	1046	46	18,21,22	1.41	4 (22%)	22,30,33	1.97	3 (13%)
46	G7M	BA	1639	46	23,26,27	4.99	20 (86%)	35,39,42	1.73	8 (22%)
46	OMU	BA	121	46	19,22,23	1.29	3 (15%)	26,31,34	1.61	4 (15%)
46	B8N	BA	1248	46	24,29,30	0.98	2 (8%)	29,42,45	1.40	3 (10%)
46	PSU	BA	1596	46	18,21,22	1.37	2 (11%)	22,30,33	1.83	3 (13%)
46	OMU	BA	1288	46	19,22,23	1.29	4 (21%)	26,31,34	1.75	6 (23%)
46	OMC	BA	462	46	19,22,23	0.84	0	26,31,34	0.99	1 (3%)
1	OMU	AA	4306	1	19,22,23	1.33	3 (15%)	26,31,34	1.66	4 (15%)
46	A2M	BA	166	46	22,25,26	1.48	4 (18%)	31,36,39	2.20	8 (25%)
46	OMG	BA	644	46	23,26,27	1.23	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	AA	4576	1	18,21,22	1.42	4 (22%)	22,30,33	1.89	4 (18%)
1	OMG	AA	1316	81,1	23,26,27	1.29	4 (17%)	33,38,41	1.92	6 (18%)
46	OMU	BA	354	46	19,22,23	1.28	3 (15%)	26,31,34	1.74	4 (15%)
46	A2M	BA	576	46	22,25,26	1.44	5 (22%)	31,36,39	2.09	10 (32%)
1	OMG	AA	2364	1	23,26,27	1.20	4 (17%)	33,38,41	1.95	6 (18%)
46	OMG	BA	509	80,46	23,26,27	1.23	3 (13%)	33,38,41	1.89	6 (18%)
46	OMU	BA	1442	46	19,22,23	1.26	4 (21%)	26,31,34	1.74	5 (19%)
1	PSU	AA	4353	1	18,21,22	1.41	4 (22%)	22,30,33	1.96	3 (13%)
1	A2M	AA	3825	1	22,25,26	1.44	4 (18%)	31,36,39	2.03	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	6MZ	AA	4220	1	22,25,26	1.39	4 (18%)	30,36,39	2.13	10 (33%)
1	PSU	AA	4689	1	18,21,22	1.49	4 (22%)	22,30,33	1.87	3 (13%)
1	A2M	AA	3830	1	22,25,26	1.42	5 (22%)	31,36,39	2.05	10 (32%)
1	PSU	AA	1792	1	18,21,22	1.46	4 (22%)	22,30,33	1.86	4 (18%)
1	A2M	AA	2363	80,1	22,25,26	1.44	5 (22%)	31,36,39	2.00	8 (25%)
1	PSU	AA	4312	1	18,21,22	1.47	4 (22%)	22,30,33	1.87	3 (13%)
1	PSU	AA	4361	1	18,21,22	1.49	4 (22%)	22,30,33	1.96	3 (13%)
1	PSU	AA	4471	1	18,21,22	1.49	4 (22%)	22,30,33	1.90	3 (13%)
1	PSU	AA	4673	81,1	18,21,22	1.46	4 (22%)	22,30,33	1.87	3 (13%)
46	4AC	BA	1337	46	21,24,25	1.10	1 (4%)	29,34,37	1.66	7 (24%)
1	PSU	AA	4431	1	18,21,22	1.43	4 (22%)	22,30,33	1.91	3 (13%)
1	A2M	AA	3785	80,1	22,25,26	1.37	4 (18%)	31,36,39	2.42	11 (35%)
1	A2M	AA	400	1	22,25,26	1.44	5 (22%)	31,36,39	2.02	8 (25%)
1	OMG	AA	2876	1	23,26,27	1.25	3 (13%)	33,38,41	1.98	6 (18%)
59	NMM	BN	67	59	9,11,12	1.70	1 (11%)	6,12,14	1.22	1 (16%)
1	OMG	AA	4494	1	23,26,27	1.24	4 (17%)	33,38,41	1.89	6 (18%)
1	OMC	AA	2824	1	19,22,23	0.83	0	26,31,34	0.76	0
1	PSU	AA	4403	1	18,21,22	1.51	5 (27%)	22,30,33	1.96	5 (22%)
46	PSU	BA	1045	46	18,21,22	1.39	3 (16%)	22,30,33	1.93	4 (18%)
1	OMG	AA	1522	1	23,26,27	1.24	4 (17%)	33,38,41	1.94	7 (21%)
1	OMC	AA	3841	1	19,22,23	0.84	0	26,31,34	0.84	1 (3%)
1	PSU	AA	2839	1	18,21,22	1.45	4 (22%)	22,30,33	1.87	3 (13%)
1	OMC	AA	3808	1	19,22,23	0.86	1 (5%)	26,31,34	0.84	1 (3%)
46	OMC	BA	1391	46	19,22,23	0.80	0	26,31,34	0.71	0
46	PSU	BA	822	46	18,21,22	1.40	3 (16%)	22,30,33	1.96	3 (13%)
46	A2M	BA	27	80,46	22,25,26	1.46	4 (18%)	31,36,39	1.98	8 (25%)
46	A2M	BA	468	46	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
1	A2M	AA	1871	80,1	22,25,26	1.44	4 (18%)	31,36,39	2.16	11 (35%)
1	A2M	AA	1524	1	22,25,26	1.42	4 (18%)	31,36,39	2.19	11 (35%)
1	PSU	AA	4552	1	18,21,22	1.45	4 (22%)	22,30,33	2.02	3 (13%)
1	A2M	AA	2787	80,1	22,25,26	1.39	4 (18%)	31,36,39	2.13	8 (25%)
46	PSU	BA	1367	46	18,21,22	1.39	3 (16%)	22,30,33	1.89	4 (18%)
46	PSU	BA	1360	80,46,81	18,21,22	1.40	3 (16%)	22,30,33	1.96	5 (22%)
46	PSU	BA	63	46	18,21,22	1.39	2 (11%)	22,30,33	1.92	4 (18%)
46	PSU	BA	609	46	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	BA	34	46	18,21,22	1.40	3 (16%)	22,30,33	1.88	3 (13%)
46	OMC	BA	1272	46	19,22,23	0.80	0	26,31,34	0.76	0
1	OMC	AA	1340	1	19,22,23	0.89	2 (10%)	26,31,34	0.90	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	4532	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	3724	1	-	0/9/27/28	0/3/3/3
46	PSU	BA	918	46	-	0/7/25/26	0/2/2/2
1	OMG	AA	4370	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	1683	81,1	-	0/7/25/26	0/2/2/2
1	OMU	AA	2415	1	-	0/9/27/28	0/2/2/2
29	V5N	Ac	39	29	-	1/9/10/12	0/1/1/1
1	PSU	AA	3762	1	-	0/7/25/26	0/2/2/2
46	A2M	BA	159	46	-	0/9/27/28	0/3/3/3
46	OMG	BA	436	46	-	2/9/27/28	0/3/3/3
1	PSU	AA	1781	1	-	1/7/25/26	0/2/2/2
1	PSU	AA	4628	1	-	0/7/25/26	0/2/2/2
46	OMU	BA	428	46	-	6/9/27/28	0/2/2/2
1	OMC	AA	2351	80,1	-	3/9/27/28	0/2/2/2
1	PSU	AA	2508	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3695	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	2861	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	1744	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3851	1	-	1/7/25/26	0/2/2/2
46	PSU	BA	681	46	-	0/7/25/26	0/2/2/2
46	OMG	BA	683	46	-	2/9/27/28	0/3/3/3
1	OMG	AA	1625	81,1	-	2/9/27/28	0/3/3/3
46	PSU	BA	100	80,46	-	2/7/25/26	0/2/2/2
1	PSU	AA	1582	1	-	2/7/25/26	0/2/2/2
1	OMG	AA	4196	80,1	-	0/9/27/28	0/3/3/3
46	OMG	BA	867	46	-	2/9/27/28	0/3/3/3
46	PSU	BA	1445	80,46	-	0/7/25/26	0/2/2/2
46	OMG	BA	1447	46	-	2/9/27/28	0/3/3/3
46	PSU	BA	651	46	-	0/7/25/26	0/2/2/2
46	MA6	BA	1851	46	-	4/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	AA	3792	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	3768	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	1177	46	-	0/7/25/26	0/2/2/2
46	MA6	BA	1850	46	-	2/11/29/30	0/3/3/3
1	A2M	AA	1323	1	-	2/9/27/28	0/3/3/3
1	PSU	AA	5001	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	4499	1	-	1/9/27/28	0/3/3/3
46	PSU	BA	814	46	-	0/7/25/26	0/2/2/2
46	A2M	BA	99	80,46	-	1/9/27/28	0/3/3/3
46	OMU	BA	116	46	-	0/9/27/28	0/2/2/2
1	PSU	AA	3853	80,1	-	0/7/25/26	0/2/2/2
46	PSU	BA	863	46	-	0/7/25/26	0/2/2/2
46	UY1	BA	1326	46	-	1/9/27/28	0/2/2/2
46	PSU	BA	1643	80,46	-	0/7/25/26	0/2/2/2
1	PSU	AA	3764	1	-	1/7/25/26	0/2/2/2
46	PSU	BA	572	46	-	0/7/25/26	0/2/2/2
1	A2M	AA	3718	1	-	0/9/27/28	0/3/3/3
46	PSU	BA	1136	46	-	0/7/25/26	0/2/2/2
1	A2M	AA	2815	81,1	-	3/9/27/28	0/3/3/3
46	OMC	BA	517	46	-	0/9/27/28	0/2/2/2
46	PSU	BA	1244	46	-	0/7/25/26	0/2/2/2
1	OMC	AA	2804	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	4636	1	-	4/7/25/26	0/2/2/2
1	OMG	AA	4228	1	-	1/9/27/28	0/3/3/3
46	PSU	BA	1625	46	-	0/7/25/26	0/2/2/2
1	A2M	AA	2401	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	3884	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	2632	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3822	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	4456	1	-	0/9/27/28	0/2/2/2
1	OMU	AA	4498	1	-	0/9/27/28	0/2/2/2
46	A2M	BA	1031	46	-	0/9/27/28	0/3/3/3
46	A2M	BA	590	46	-	3/9/27/28	0/3/3/3
46	A2M	BA	668	80,46	-	3/9/27/28	0/3/3/3
46	PSU	BA	1692	46	-	0/7/25/26	0/2/2/2
1	A2M	AA	4590	1	-	1/9/27/28	0/3/3/3
1	OMU	AA	4620	1	-	0/9/27/28	0/2/2/2
46	PSU	BA	119	46	-	0/7/25/26	0/2/2/2
1	OMU	AA	2837	1	-	0/9/27/28	0/2/2/2
46	OMG	BA	1328	46	-	0/9/27/28	0/3/3/3
46	OMC	BA	1703	46	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	AC	55	3	-	0/7/25/26	0/2/2/2
46	OMC	BA	174	46	-	0/9/27/28	0/2/2/2
46	PSU	BA	649	46	-	0/7/25/26	0/2/2/2
1	OMC	AA	4536	1	-	0/9/27/28	0/2/2/2
3	PSU	AC	69	3	-	0/7/25/26	0/2/2/2
1	5MC	AA	4447	81,1	-	4/7/25/26	0/2/2/2
1	PSU	AA	1677	1	-	3/7/25/26	0/2/2/2
1	A2M	AA	4523	80,1	-	1/9/27/28	0/3/3/3
46	OMU	BA	1804	46	-	2/9/27/28	0/2/2/2
46	PSU	BA	1056	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	406	46	-	0/7/25/26	0/2/2/2
46	A2M	BA	1383	46	-	0/9/27/28	0/3/3/3
46	PSU	BA	1003	46	-	0/7/25/26	0/2/2/2
72	IAS	Ba	138	72	-	0/7/7/8	-
5	HIC	AE	245	5	-	0/5/6/8	0/1/1/1
1	UR3	AA	4530	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4973	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	36	46	-	0/7/25/26	0/2/2/2
1	A2M	AA	1326	1	-	1/9/27/28	0/3/3/3
1	PSU	AA	1779	1	-	0/7/25/26	0/2/2/2
1	5MC	AA	3782	80,1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4579	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	966	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	1347	46	-	0/7/25/26	0/2/2/2
46	OMG	BA	1490	80,46	-	2/9/27/28	0/3/3/3
46	4AC	BA	1842	46	-	0/11/29/30	0/2/2/2
1	PSU	AA	1862	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	105	46	-	0/7/25/26	0/2/2/2
1	OMC	AA	3869	1	-	1/9/27/28	0/2/2/2
1	PSU	AA	4299	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	5010	1	-	0/7/25/26	0/2/2/2
1	OMU	AA	4227	1	-	0/9/27/28	0/2/2/2
1	OMG	AA	4618	1	-	0/9/27/28	0/3/3/3
46	6MZ	BA	1832	80,46,81	-	1/9/27/28	0/3/3/3
1	A2M	AA	3867	1	-	2/9/27/28	0/3/3/3
1	PSU	AA	3920	80,1	-	0/7/25/26	0/2/2/2
1	OMG	AA	4623	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	3770	1	-	0/7/25/26	0/2/2/2
1	OMU	AA	3925	1	-	0/9/27/28	0/2/2/2
46	OMG	BA	601	46	-	0/9/27/28	0/3/3/3
46	A2M	BA	484	46	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	4442	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	398	1	-	2/9/27/28	0/3/3/3
1	OMC	AA	3887	1	-	1/9/27/28	0/2/2/2
46	PSU	BA	218	46	-	0/7/25/26	0/2/2/2
1	OMC	AA	3701	81,1	-	4/9/27/28	0/2/2/2
1	PSU	AA	1860	1	-	0/7/25/26	0/2/2/2
3	OMG	AC	75	3	-	1/9/27/28	0/3/3/3
3	OMU	AC	14	1,3	-	1/9/27/28	0/2/2/2
1	OMG	AA	4392	1	-	0/9/27/28	0/3/3/3
1	OMG	AA	4637	81,1	-	0/9/27/28	0/3/3/3
46	PSU	BA	1174	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	3730	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	3899	80,1	-	0/9/27/28	0/3/3/3
1	OMC	AA	1881	80,1	-	0/9/27/28	0/2/2/2
1	PSU	AA	4423	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4500	1	-	3/7/25/26	0/2/2/2
1	A2M	AA	4571	1	-	1/9/27/28	0/3/3/3
46	PSU	BA	801	46	-	0/7/25/26	0/2/2/2
1	OMG	AA	3627	1	-	0/9/27/28	0/3/3/3
46	PSU	BA	1232	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	3715	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	2843	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	1782	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4296	1	-	0/7/25/26	0/2/2/2
46	OMU	BA	172	46	-	0/9/27/28	0/2/2/2
46	PSU	BA	667	46	-	2/7/25/26	0/2/2/2
46	PSU	BA	866	46	-	0/7/25/26	0/2/2/2
1	1MA	AA	1322	80,1	-	2/7/25/26	0/3/3/3
46	PSU	BA	366	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	4293	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	296	46	-	0/7/25/26	0/2/2/2
1	OMG	AA	3744	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4521	80,81,1	-	1/7/25/26	0/2/2/2
1	A2M	AA	1534	80,1	-	2/9/27/28	0/3/3/3
1	PSU	AA	1536	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	686	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	4972	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3639	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	2424	1	-	0/9/27/28	0/3/3/3
46	PSU	BA	93	46	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	A2M	BA	512	46	-	2/9/27/28	0/3/3/3
1	OMC	AA	2365	80,1	-	0/9/27/28	0/2/2/2
1	OMC	AA	2422	80,1	-	1/9/27/28	0/2/2/2
1	PSU	AA	4493	81,1	-	0/7/25/26	0/2/2/2
46	PSU	BA	1004	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	1238	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	3637	81,1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4457	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3844	1	-	3/7/25/26	0/2/2/2
46	PSU	BA	815	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	109	46	-	0/7/25/26	0/2/2/2
1	UY1	AA	3818	81,1	-	4/9/27/28	0/2/2/2
46	A2M	BA	1678	46	-	0/9/27/28	0/3/3/3
46	PSU	BA	300	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	1186	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	1046	46	-	0/7/25/26	0/2/2/2
46	G7M	BA	1639	46	-	2/7/25/26	0/3/3/3
46	OMU	BA	121	46	-	0/9/27/28	0/2/2/2
46	B8N	BA	1248	46	-	2/16/34/35	0/2/2/2
46	PSU	BA	1596	46	-	0/7/25/26	0/2/2/2
46	OMU	BA	1288	46	-	3/9/27/28	0/2/2/2
46	OMC	BA	462	46	-	0/9/27/28	0/2/2/2
1	OMU	AA	4306	1	-	0/9/27/28	0/2/2/2
46	A2M	BA	166	46	-	2/9/27/28	0/3/3/3
46	OMG	BA	644	46	-	1/9/27/28	0/3/3/3
1	PSU	AA	4576	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	1316	81,1	-	0/9/27/28	0/3/3/3
46	OMU	BA	354	46	-	0/9/27/28	0/2/2/2
46	A2M	BA	576	46	-	2/9/27/28	0/3/3/3
1	OMG	AA	2364	1	-	2/9/27/28	0/3/3/3
46	OMG	BA	509	80,46	-	0/9/27/28	0/3/3/3
46	OMU	BA	1442	46	-	0/9/27/28	0/2/2/2
1	PSU	AA	4353	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	3825	1	-	0/9/27/28	0/3/3/3
1	6MZ	AA	4220	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4689	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	3830	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	1792	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	2363	80,1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4312	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	4361	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4471	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4673	81,1	-	0/7/25/26	0/2/2/2
46	4AC	BA	1337	46	-	4/11/29/30	0/2/2/2
1	PSU	AA	4431	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	3785	80,1	-	1/9/27/28	0/3/3/3
1	A2M	AA	400	1	-	0/9/27/28	0/3/3/3
1	OMG	AA	2876	1	-	1/9/27/28	0/3/3/3
59	NMM	BN	67	59	-	3/9/11/13	-
1	OMG	AA	4494	1	-	0/9/27/28	0/3/3/3
1	OMC	AA	2824	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	4403	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	1045	46	-	2/7/25/26	0/2/2/2
1	OMG	AA	1522	1	-	2/9/27/28	0/3/3/3
1	OMC	AA	3841	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	2839	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	3808	1	-	0/9/27/28	0/2/2/2
46	OMC	BA	1391	46	-	0/9/27/28	0/2/2/2
46	PSU	BA	822	46	-	0/7/25/26	0/2/2/2
46	A2M	BA	27	80,46	-	0/9/27/28	0/3/3/3
46	A2M	BA	468	46	-	0/9/27/28	0/3/3/3
1	A2M	AA	1871	80,1	-	0/9/27/28	0/3/3/3
1	A2M	AA	1524	1	-	1/9/27/28	0/3/3/3
1	PSU	AA	4552	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	2787	80,1	-	4/9/27/28	0/3/3/3
46	PSU	BA	1367	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	1360	80,46,81	-	0/7/25/26	0/2/2/2
46	PSU	BA	63	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	609	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	34	46	-	0/7/25/26	0/2/2/2
46	OMC	BA	1272	46	-	2/9/27/28	0/2/2/2
1	OMC	AA	1340	1	-	0/9/27/28	0/2/2/2

The worst 5 of 730 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	BA	1326	UY1	C6-C5	11.68	1.48	1.35
1	AA	3818	UY1	C6-C5	10.89	1.48	1.35
46	BA	1639	G7M	C8-N7	10.52	1.52	1.33
46	BA	1639	G7M	C2'-C3'	-10.50	1.24	1.53
46	BA	1326	UY1	C2-N1	9.49	1.49	1.36

The worst 5 of 1018 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BA	166	A2M	C5-C4-N3	-6.77	117.92	126.75
46	BA	590	A2M	C5-C4-N3	-6.66	118.06	126.75
1	AA	3637	PSU	N1-C2-N3	6.64	122.65	115.13
1	AA	4628	PSU	N1-C2-N3	6.50	122.50	115.13
46	BA	484	A2M	C5-C4-N3	-6.50	118.27	126.75

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AC	14	OMU	C1'-C2'-O2'-CM2
59	BN	67	NMM	C-CA-CB-CG
59	BN	67	NMM	N-CA-CB-CG
1	AA	1582	PSU	O4'-C1'-C5-C4
1	AA	1582	PSU	O4'-C1'-C5-C6

There are no ring outliers.

70 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	4370	OMG	1	0
1	AA	1683	PSU	1	0
1	AA	2415	OMU	1	0
46	BA	159	A2M	2	0
46	BA	436	OMG	1	0
1	AA	1781	PSU	1	0
1	AA	2351	OMC	1	0
46	BA	681	PSU	2	0
46	BA	683	OMG	1	0
1	AA	1625	OMG	1	0
46	BA	867	OMG	2	0
46	BA	1445	PSU	1	0
46	BA	1851	MA6	1	0
46	BA	1850	MA6	1	0
46	BA	99	A2M	1	0
46	BA	116	OMU	3	0
46	BA	1643	PSU	2	0
1	AA	3718	A2M	4	0
46	BA	517	OMC	1	0
46	BA	1244	PSU	2	0
1	AA	4228	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	4456	OMC	1	0
46	BA	1031	A2M	1	0
46	BA	590	A2M	1	0
46	BA	1692	PSU	1	0
1	AA	4620	OMU	1	0
46	BA	1703	OMC	1	0
1	AA	4536	OMC	2	0
1	AA	4447	5MC	1	0
1	AA	1677	PSU	1	0
1	AA	4523	A2M	1	0
46	BA	1804	OMU	1	0
46	BA	1383	A2M	1	0
46	BA	36	PSU	1	0
1	AA	4579	PSU	2	0
46	BA	1347	PSU	1	0
46	BA	1490	OMG	1	0
46	BA	484	A2M	2	0
1	AA	398	A2M	1	0
1	AA	3701	OMC	1	0
3	AC	75	OMG	1	0
1	AA	4392	OMG	2	0
1	AA	4500	PSU	1	0
46	BA	866	PSU	1	0
1	AA	1534	A2M	1	0
1	AA	2424	OMG	2	0
46	BA	512	A2M	1	0
1	AA	4457	PSU	1	0
46	BA	1678	A2M	2	0
46	BA	1639	G7M	1	0
46	BA	121	OMU	1	0
46	BA	1288	OMU	2	0
46	BA	462	OMC	2	0
1	AA	4306	OMU	1	0
46	BA	166	A2M	2	0
46	BA	576	A2M	2	0
46	BA	509	OMG	2	0
46	BA	1442	OMU	1	0
1	AA	4220	6MZ	1	0
1	AA	4689	PSU	1	0
1	AA	2363	A2M	1	0
1	AA	4361	PSU	1	0
1	AA	3785	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	2876	OMG	1	0
1	AA	2839	PSU	1	0
46	BA	822	PSU	1	0
46	BA	27	A2M	1	0
1	AA	1871	A2M	2	0
46	BA	1272	OMC	1	0
1	AA	1340	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 364 ligands modelled in this entry, 364 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](#)

There are no chain breaks in this entry.

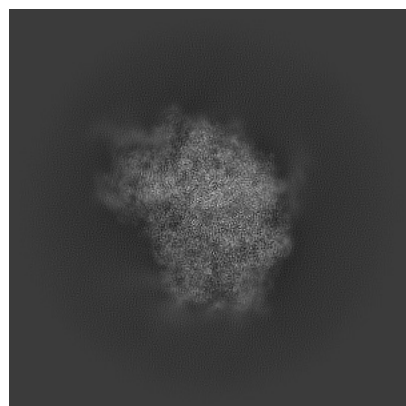
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66297. These allow visual inspection of the internal detail of the map and identification of artifacts.

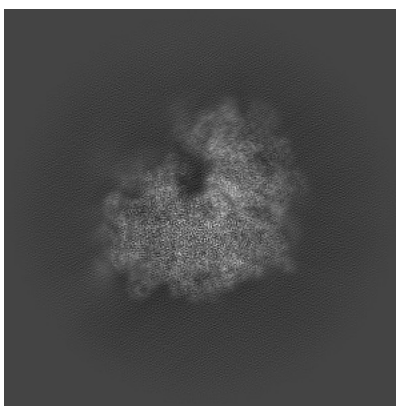
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

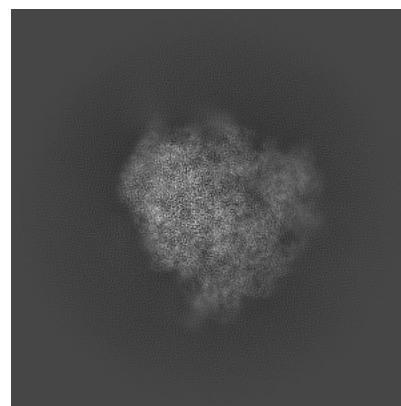
6.1.1 Primary map



X

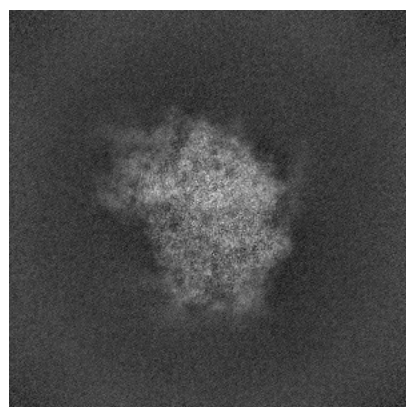


Y

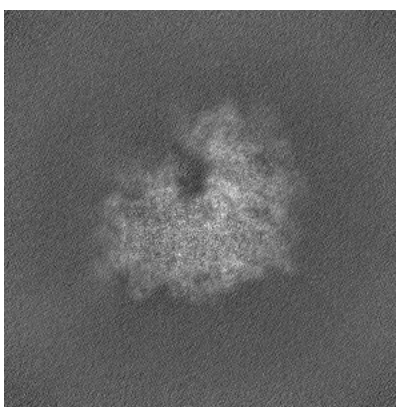


Z

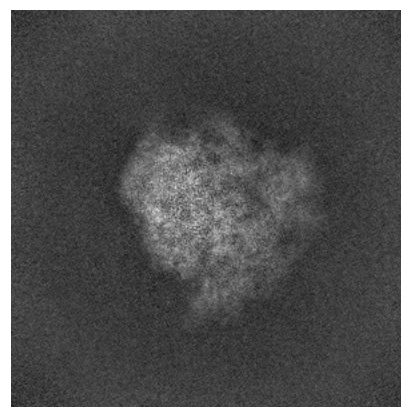
6.1.2 Raw map



X



Y

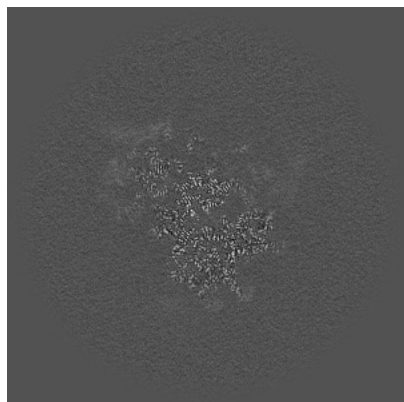


Z

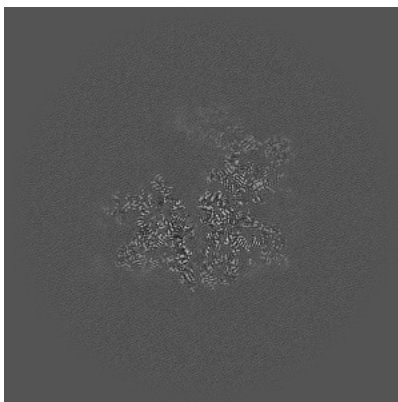
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

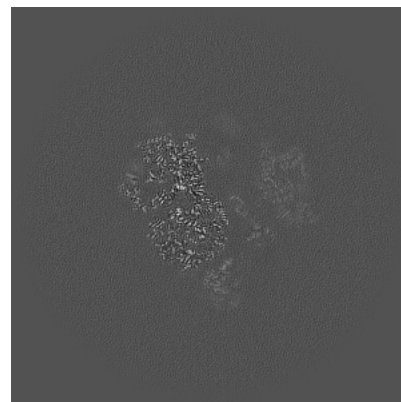
6.2.1 Primary map



X Index: 320

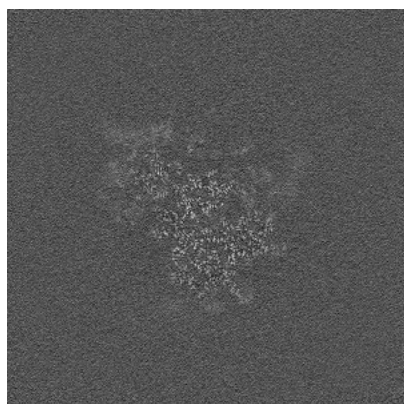


Y Index: 320

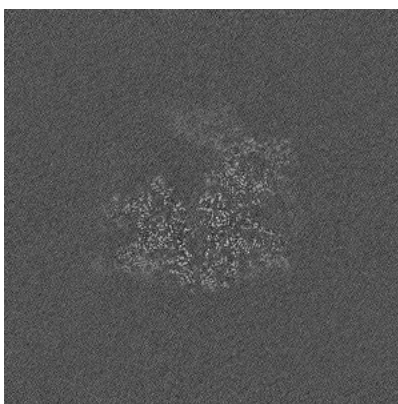


Z Index: 320

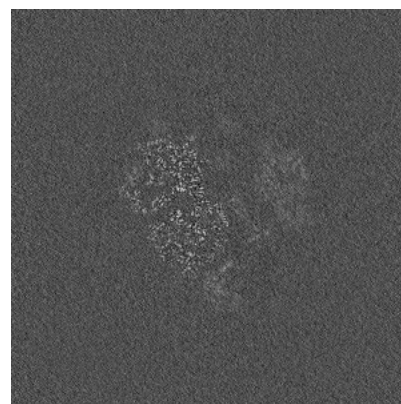
6.2.2 Raw map



X Index: 320



Y Index: 320

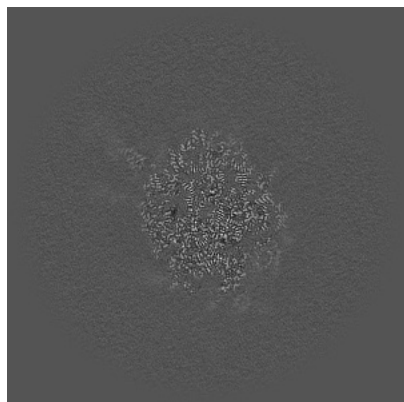


Z Index: 320

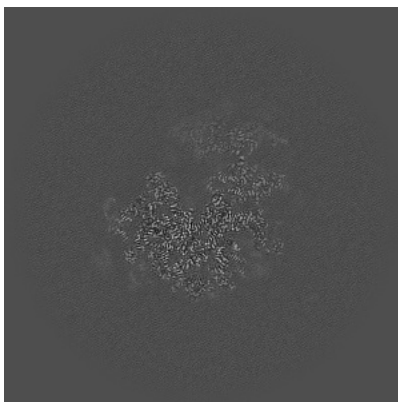
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

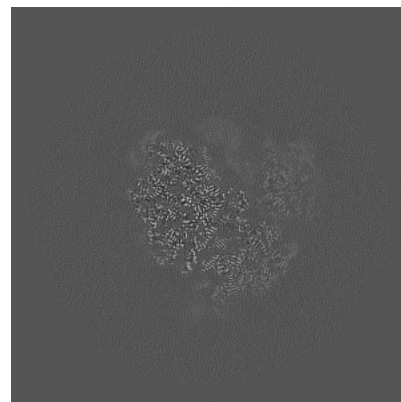
6.3.1 Primary map



X Index: 289

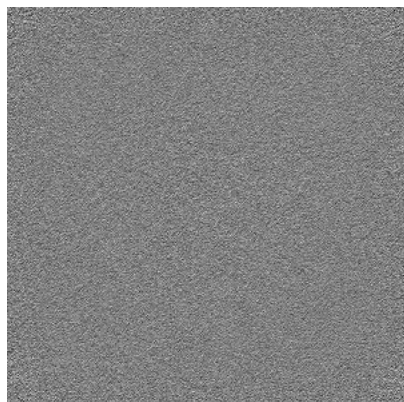


Y Index: 338

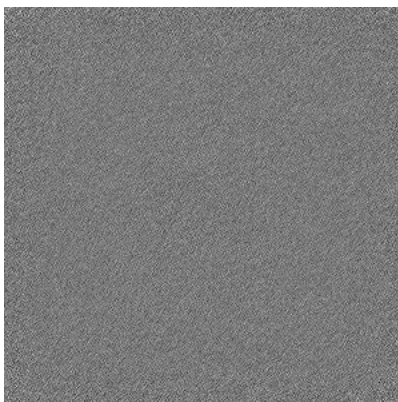


Z Index: 349

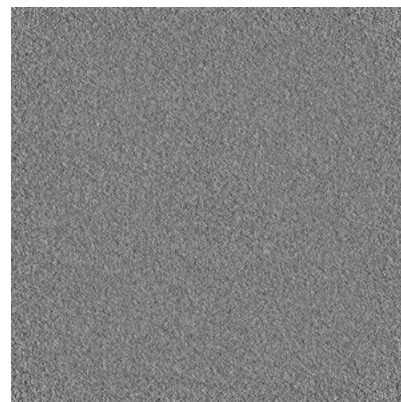
6.3.2 Raw map



X Index: 0



Y Index: 0

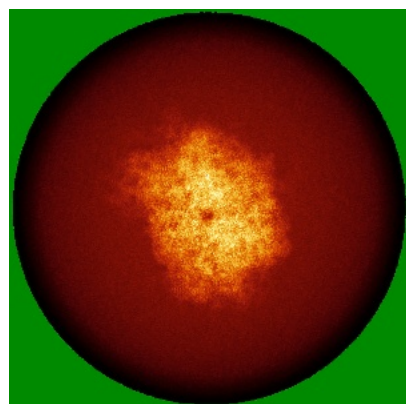


Z Index: 0

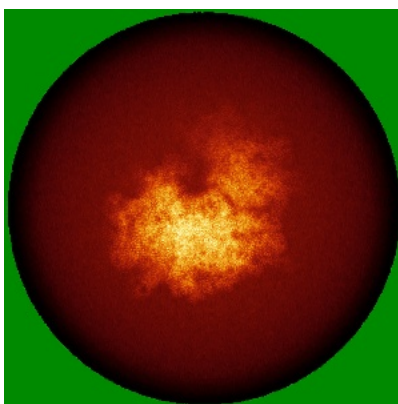
The images above show the largest variance slices of the map in three orthogonal directions.

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

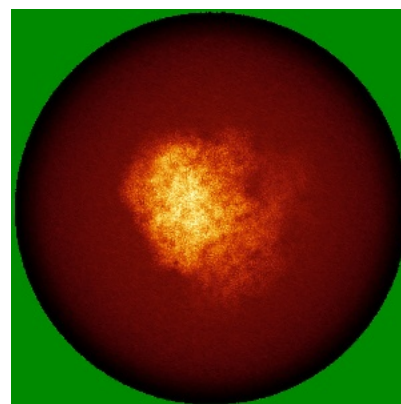
6.4.1 Primary map



X

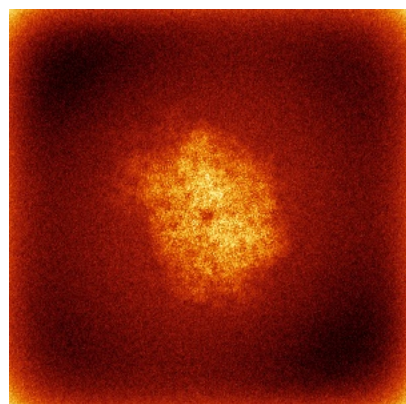


Y

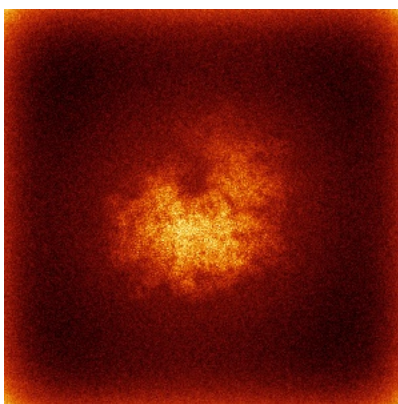


Z

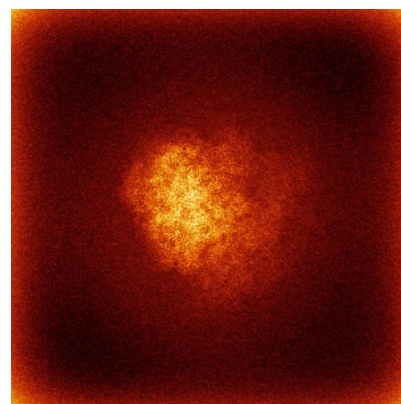
6.4.2 Raw map



X



Y

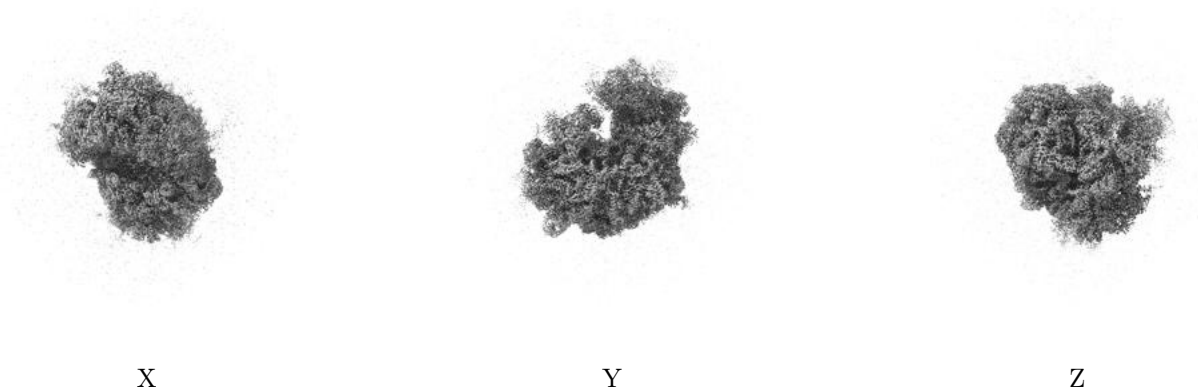


Z

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

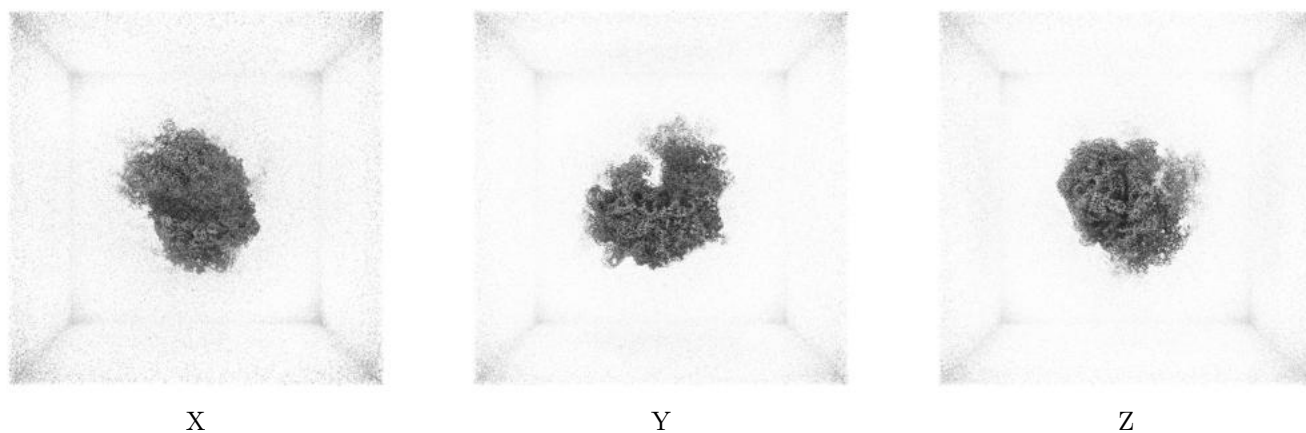
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

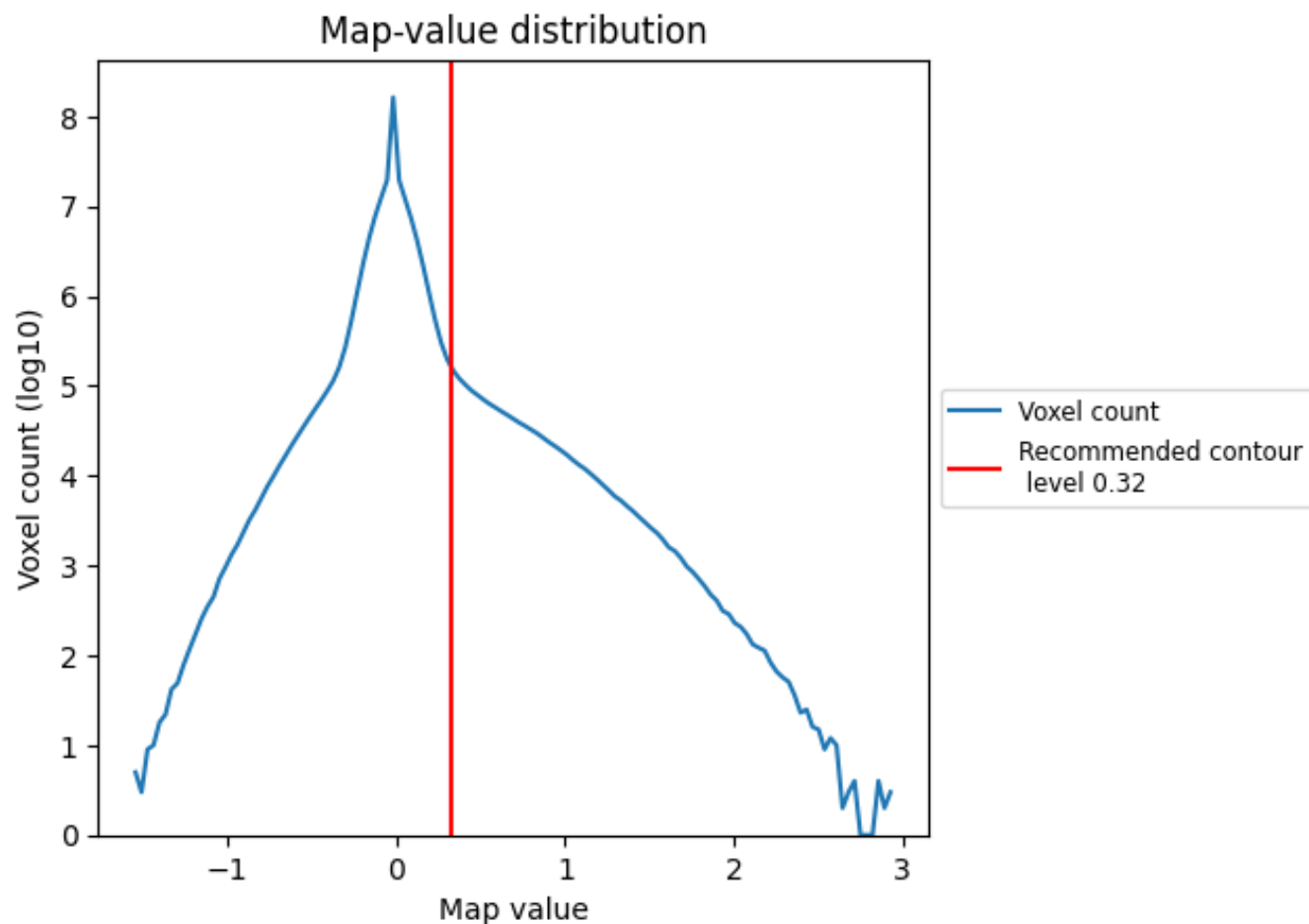
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

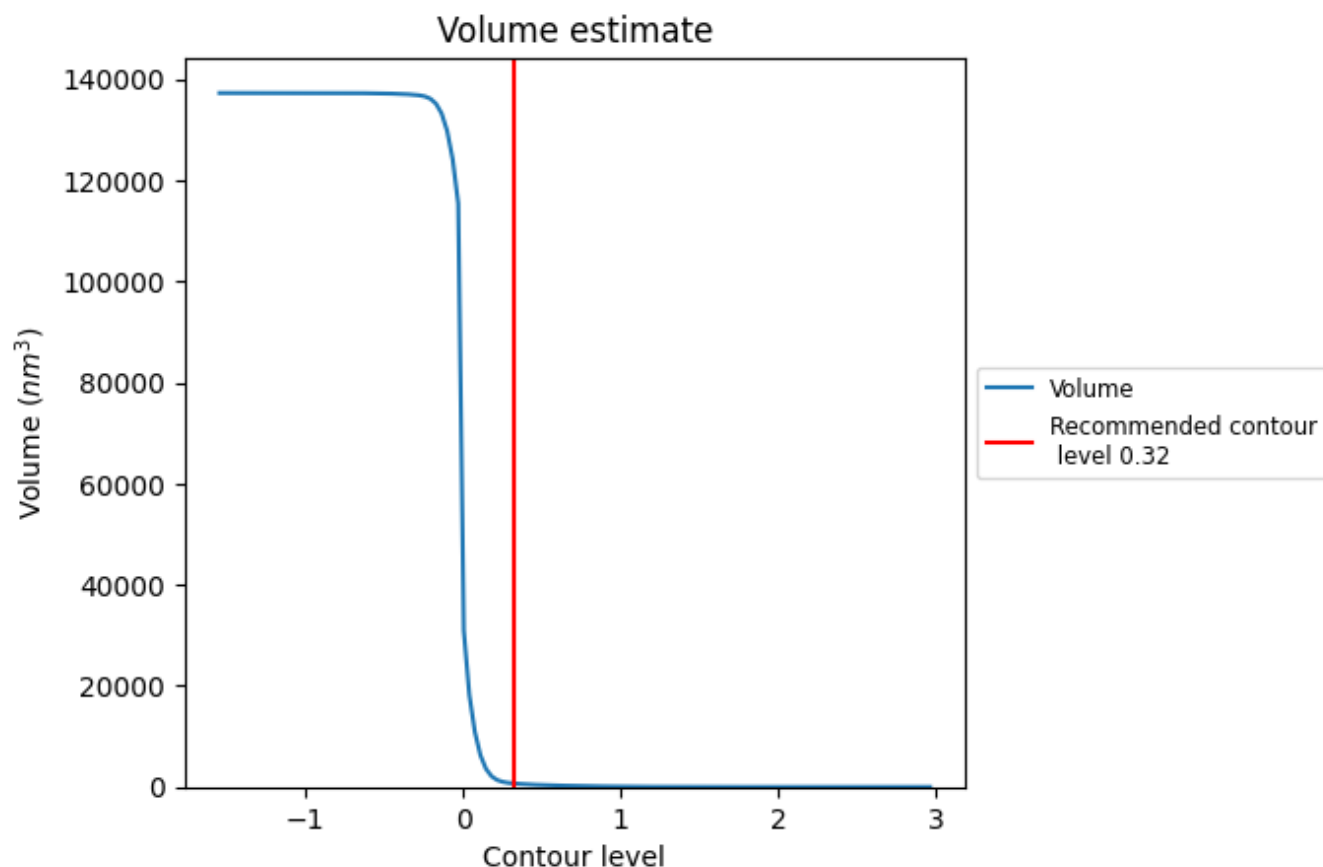
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

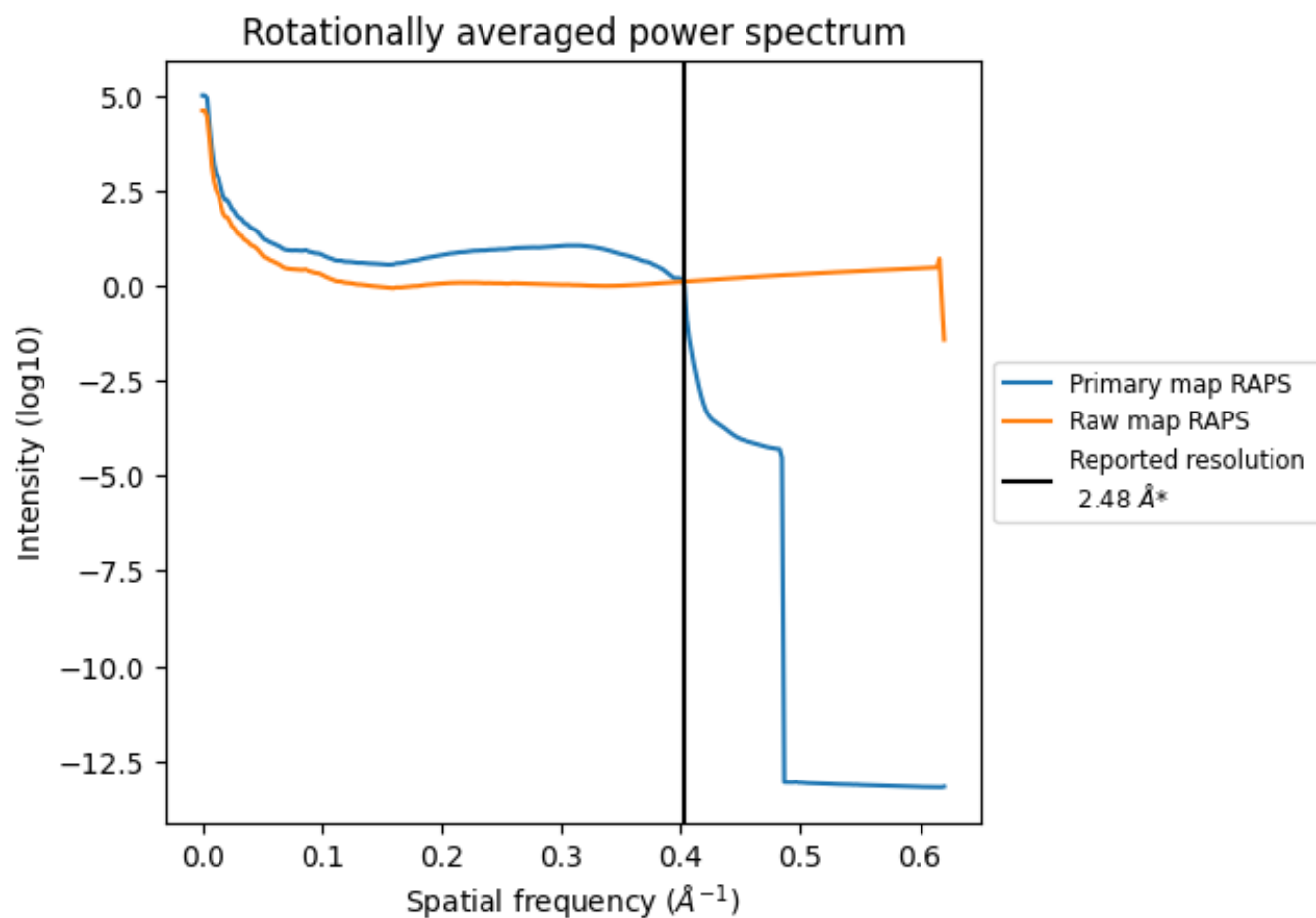
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 697 nm³; this corresponds to an approximate mass of 630 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

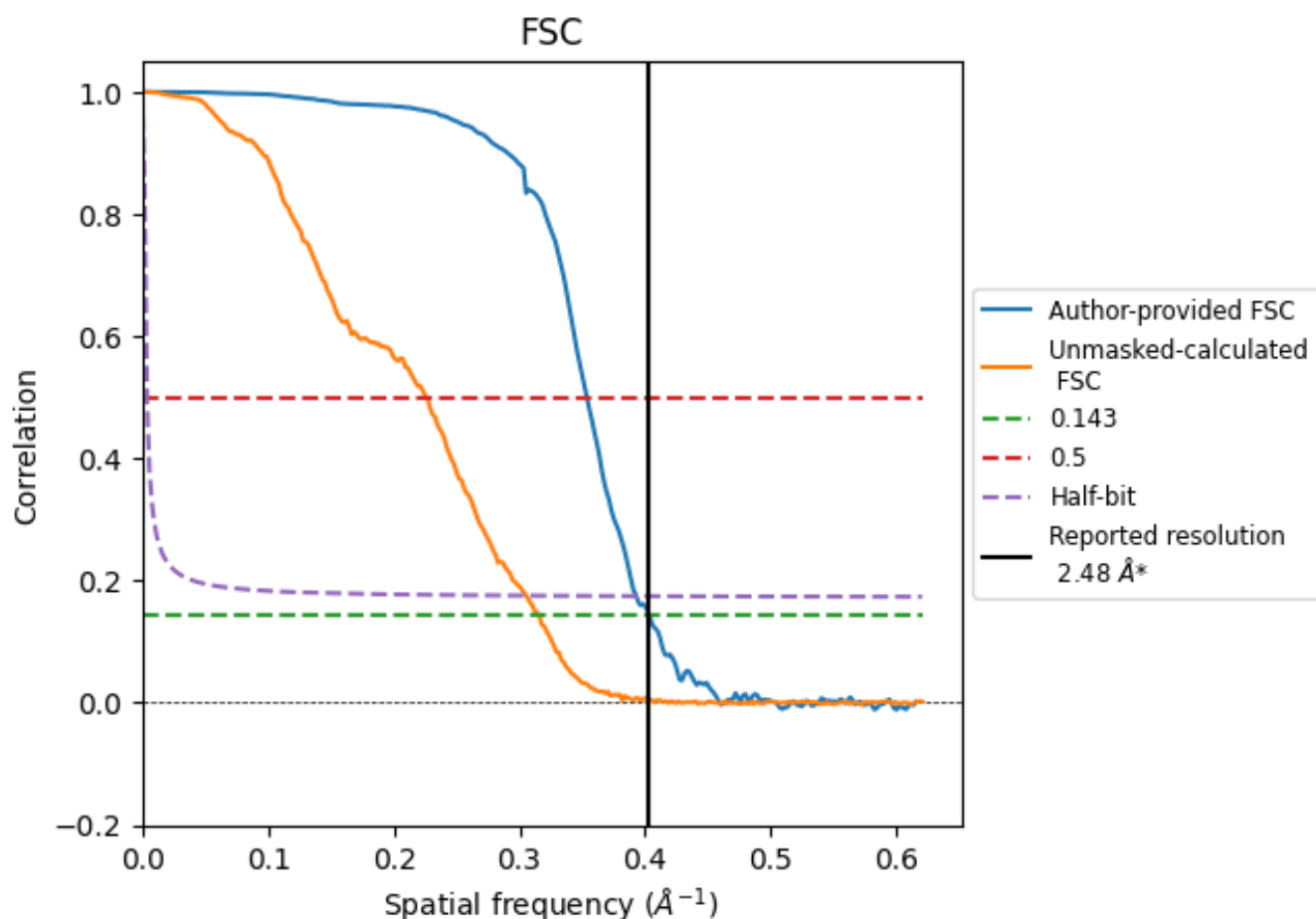


*Reported resolution corresponds to spatial frequency of 0.403 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.403 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

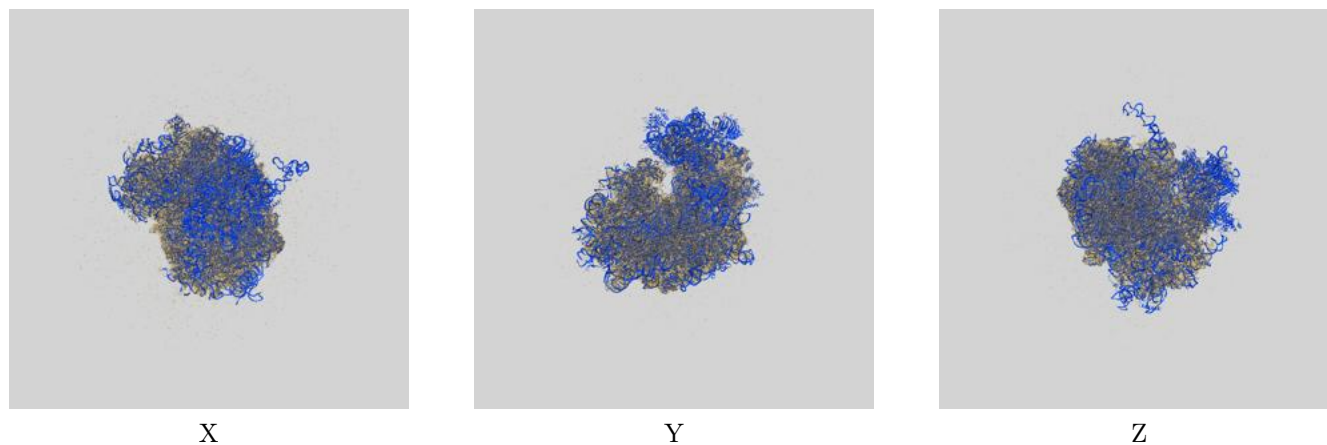
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.48	2.83	2.55
Unmasked-calculated*	3.17	4.42	3.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.17 differs from the reported value 2.48 by more than 10 %

9 Map-model fit [i](#)

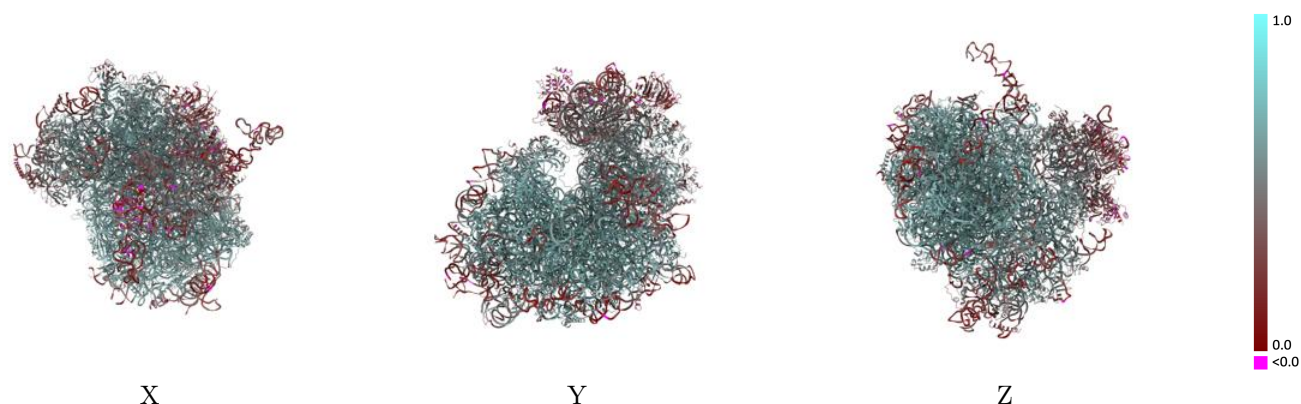
This section contains information regarding the fit between EMDB map EMD-66297 and PDB model 9WW4. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



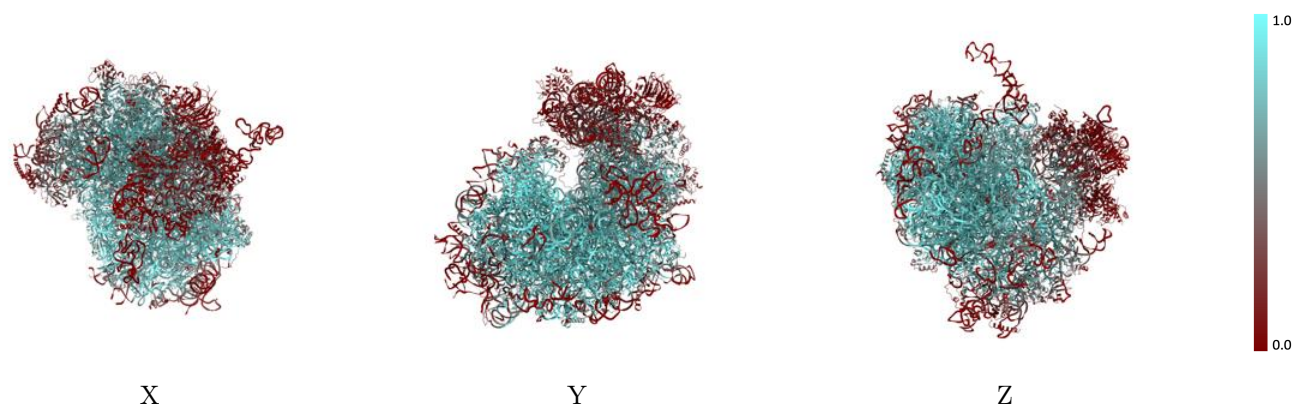
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



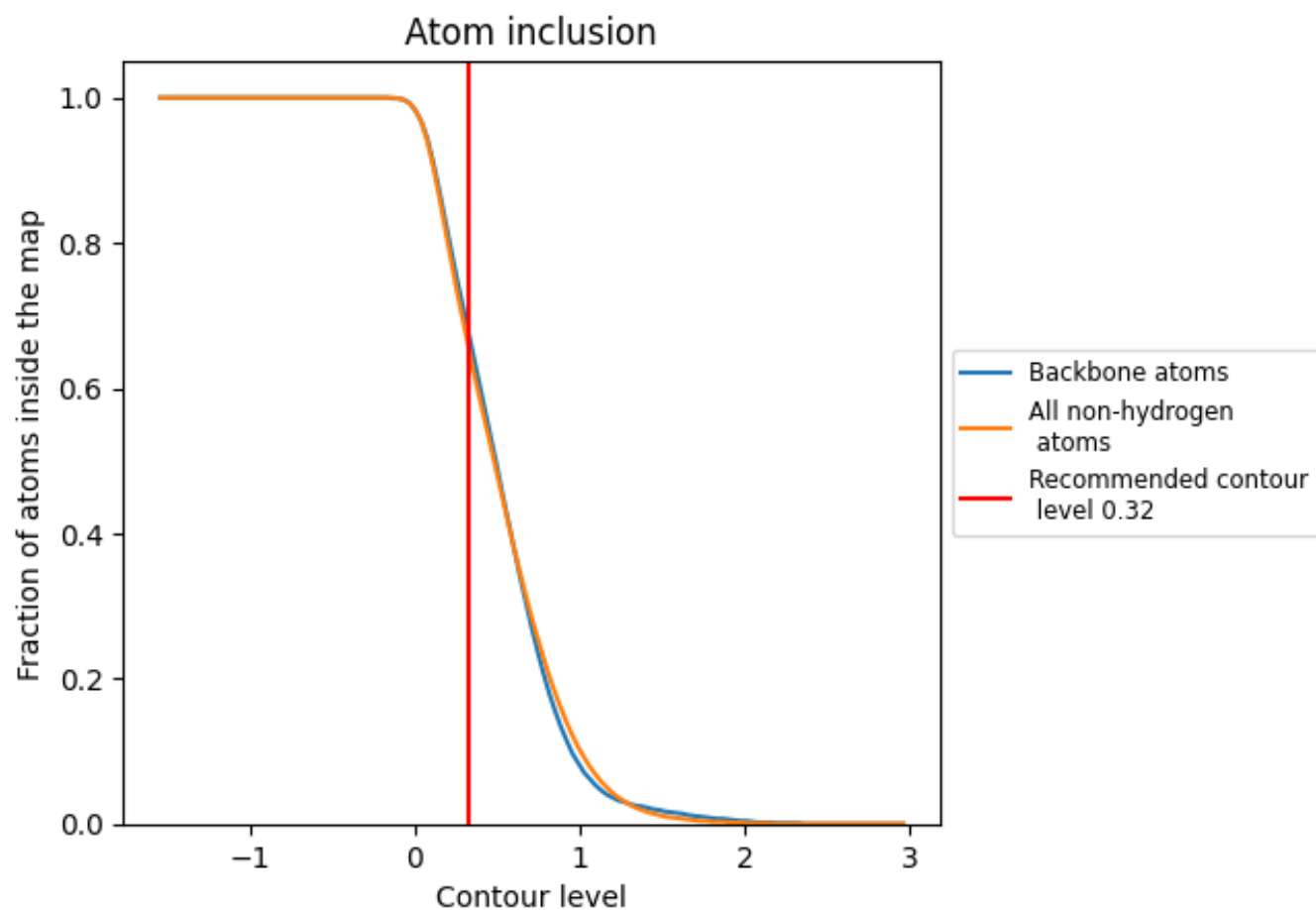
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 66% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6620	 0.5500
AA	 0.7360	 0.5560
AB	 0.9100	 0.6400
AC	 0.8250	 0.5960
AD	 0.9410	 0.6810
AE	 0.8660	 0.6550
AF	 0.8370	 0.6240
AG	 0.7440	 0.6110
AH	 0.6220	 0.5620
AI	 0.8640	 0.6450
AJ	 0.6740	 0.5750
AK	 0.8030	 0.6370
AL	 0.8040	 0.6260
AM	 0.5220	 0.5590
AN	 0.7470	 0.6030
AO	 0.7960	 0.6230
AP	 0.9510	 0.6730
AQ	 0.8780	 0.6560
AR	 0.8910	 0.6610
AS	 0.9120	 0.6570
AT	 0.7720	 0.6190
AU	 0.9000	 0.6620
AV	 0.8230	 0.6400
AW	 0.5240	 0.5400
AX	 0.8930	 0.6640
AY	 0.4580	 0.4430
AZ	 0.8140	 0.6350
Aa	 0.7910	 0.6180
Ab	 0.8040	 0.6370
Ac	 0.8880	 0.6510
Ad	 0.6390	 0.5720
Ae	 0.8060	 0.6230
Af	 0.8150	 0.6380
Ag	 0.8800	 0.6540
Ah	 0.9200	 0.6740



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Chain	Atom inclusion	Q-score
Ai	 0.8790	 0.6570
Aj	 0.7700	 0.6220
Ak	 0.7510	 0.6180
Al	 0.9240	 0.6660
Am	 0.6490	 0.5960
An	 0.8460	 0.6420
Ao	 0.8700	 0.6500
Ap	 0.8280	 0.6550
Aq	 0.8370	 0.6490
Ar	 0.9200	 0.6730
As	 0.8340	 0.6270
BA	 0.5730	 0.5020
BB	 0.5490	 0.5590
BC	 0.5210	 0.5310
BD	 0.6530	 0.5990
BE	 0.1210	 0.3900
BF	 0.1770	 0.4230
BG	 0.3440	 0.4670
BH	 0.6440	 0.5790
BI	 0.0300	 0.2760
BJ	 0.7010	 0.5930
BK	 0.0580	 0.3440
BL	 0.1380	 0.3870
BM	 0.0820	 0.3820
BN	 0.0970	 0.3600
BO	 0.1030	 0.3470
BP	 0.5290	 0.5430
BQ	 0.7150	 0.6020
BR	 0.7120	 0.5980
BS	 0.1910	 0.4520
BT	 0.1290	 0.3920
BU	 0.0210	 0.2630
BV	 0.6070	 0.5640
BW	 0.2720	 0.4540
BX	 0.4710	 0.5270
BY	 0.0010	 0.1480
BZ	 0.7550	 0.6270
Ba	 0.6990	 0.5910
Bb	 0.7570	 0.6070
Bc	 0.3350	 0.4740
Bd	 0.0620	 0.3590
Be	 0.5290	 0.5360

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Chain	Atom inclusion	Q-score
Bf	 0.3380	 0.4660
Bg	 0.0000	 0.1530
Bh	 0.2070	 0.4320