



wwPDB EM Validation Summary Report ⓘ

Sep 16, 2026 – 12:24 AM JST

PDB ID : 9WW6 / pdb_00009ww6
EMDB ID : EMD-66299
Title : human 80S ribosome delta eL41 non-rotated state
Authors : Fujino, M.; Tanaka, Y.; Iwasaki, W.; Ito, T.; Yokoyama, T.
Deposited on : 2025-09-22
Resolution : 2.83 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

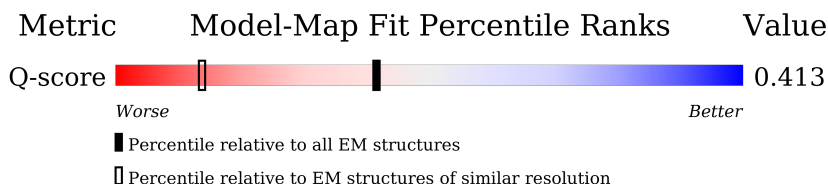
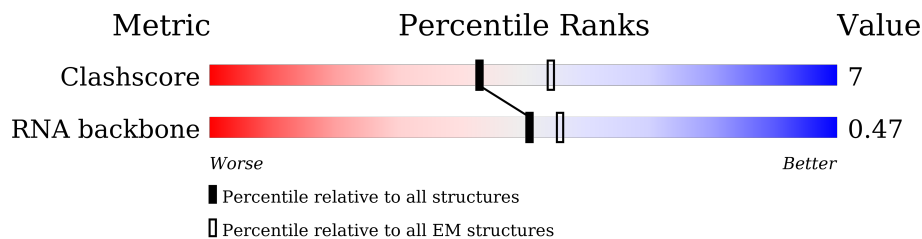
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	
4	AD	257	
5	AE	402	

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Mol	Chain	Length	Quality of chain
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	
29	Ac	148	
30	Ad	159	

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Mol	Chain	Length	Quality of chain
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	Aq	106	
43	Ar	92	
44	As	137	
45	BA	1869	
46	BB	263	
47	BC	295	
48	BD	264	
49	BE	243	
50	BF	204	
51	BG	194	
52	BH	208	
53	BI	165	
54	BJ	158	
55	BK	145	

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Mol	Chain	Length	Quality of chain
56	BL	146	
57	BM	152	
58	BN	145	
59	BO	119	
60	BP	83	
61	BQ	143	
62	BR	115	
63	BS	69	
64	BT	56	
65	BU	317	
66	BV	293	
67	BW	249	
68	BX	194	
69	BY	132	
70	BZ	151	
71	Ba	151	
72	Bb	130	
73	Bc	133	
74	Bd	125	
75	Be	84	
76	Bf	133	
77	Bg	156	
78	Bh	135	

2 Entry composition [i](#)

There are 81 unique types of molecules in this entry. The entry contains 214513 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	3770	Total	C	N	O	P	0	0
			80142	35694	14578	26101	3769		

- 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	364	Total	C	N	O	S	0	0
			2895	1822	578	480	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	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- 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 L36a.

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

- Molecule 43 is a protein called 60S ribosomal protein L37a.

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

- Molecule 44 is a protein called 60S ribosomal protein L28.

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

- Molecule 45 is a RNA chain called 18S rRNA (1740-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BA	1733	Total	C	N	O	P	0	0
			36808	16444	6572	12059	1733		

- Molecule 46 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 47 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 48 is a protein called 40S ribosomal protein S3a.

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

- Molecule 49 is a protein called 40S ribosomal protein S3.

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

- Molecule 50 is a protein called 40S ribosomal protein S5.

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

- Molecule 51 is a protein called 40S ribosomal protein S7.

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

- Molecule 52 is a protein called 40S ribosomal protein S8.

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

- Molecule 53 is a protein called 40S ribosomal protein S10.

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

- Molecule 54 is a protein called 40S ribosomal protein S11.

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

- Molecule 55 is a protein called 40S ribosomal protein S15.

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

- Molecule 56 is a protein called 40S ribosomal protein S16.

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

- Molecule 57 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BM	145	Total	C	N	O	S	0	0
			1194	748	241	203	2		

- Molecule 58 is a protein called Small ribosomal subunit protein eS19.

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

- Molecule 59 is a protein called 40S ribosomal protein S20.

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

- Molecule 60 is a protein called 40S ribosomal protein S21.

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

- Molecule 61 is a protein called 40S ribosomal protein S23.

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

- Molecule 62 is a protein called 40S ribosomal protein S26.

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

- Molecule 63 is a protein called 40S ribosomal protein S28.

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

- Molecule 64 is a protein called 40S ribosomal protein S29.

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

- Molecule 65 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 66 is a protein called 40S ribosomal protein S2.

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

- Molecule 67 is a protein called 40S ribosomal protein S6.

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

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

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

- Molecule 69 is a protein called 40S ribosomal protein S12.

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

- Molecule 70 is a protein called 40S ribosomal protein S13.

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

- Molecule 71 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	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 72 is a protein called 40S ribosomal protein S15a.

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

- Molecule 73 is a protein called 40S ribosomal protein S24.

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

- Molecule 74 is a protein called 40S ribosomal protein S25.

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

- Molecule 75 is a protein called 40S ribosomal protein S27.

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

- Molecule 76 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

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

- Molecule 77 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 78 is a protein called 40S ribosomal protein S17.

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

- Molecule 79 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
79	AA	174	Total	Mg	0
			174	174	
79	AB	2	Total	Mg	0
			2	2	
79	AC	3	Total	Mg	0
			3	3	
79	AE	1	Total	Mg	0
			1	1	
79	AP	1	Total	Mg	0
			1	1	
79	AX	1	Total	Mg	0
			1	1	
79	Al	1	Total	Mg	0
			1	1	
79	BA	6	Total	Mg	0
			6	6	

- Molecule 80 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
80	AA	47	Total K 47 47	0
80	AB	1	Total K 1 1	0
80	AC	1	Total K 1 1	0
80	AD	1	Total K 1 1	0
80	AL	1	Total K 1 1	0
80	Ag	1	Total K 1 1	0
80	Ah	1	Total K 1 1	0
80	Aq	1	Total K 1 1	0
80	BA	2	Total K 2 2	0
80	BT	1	Total K 1 1	0

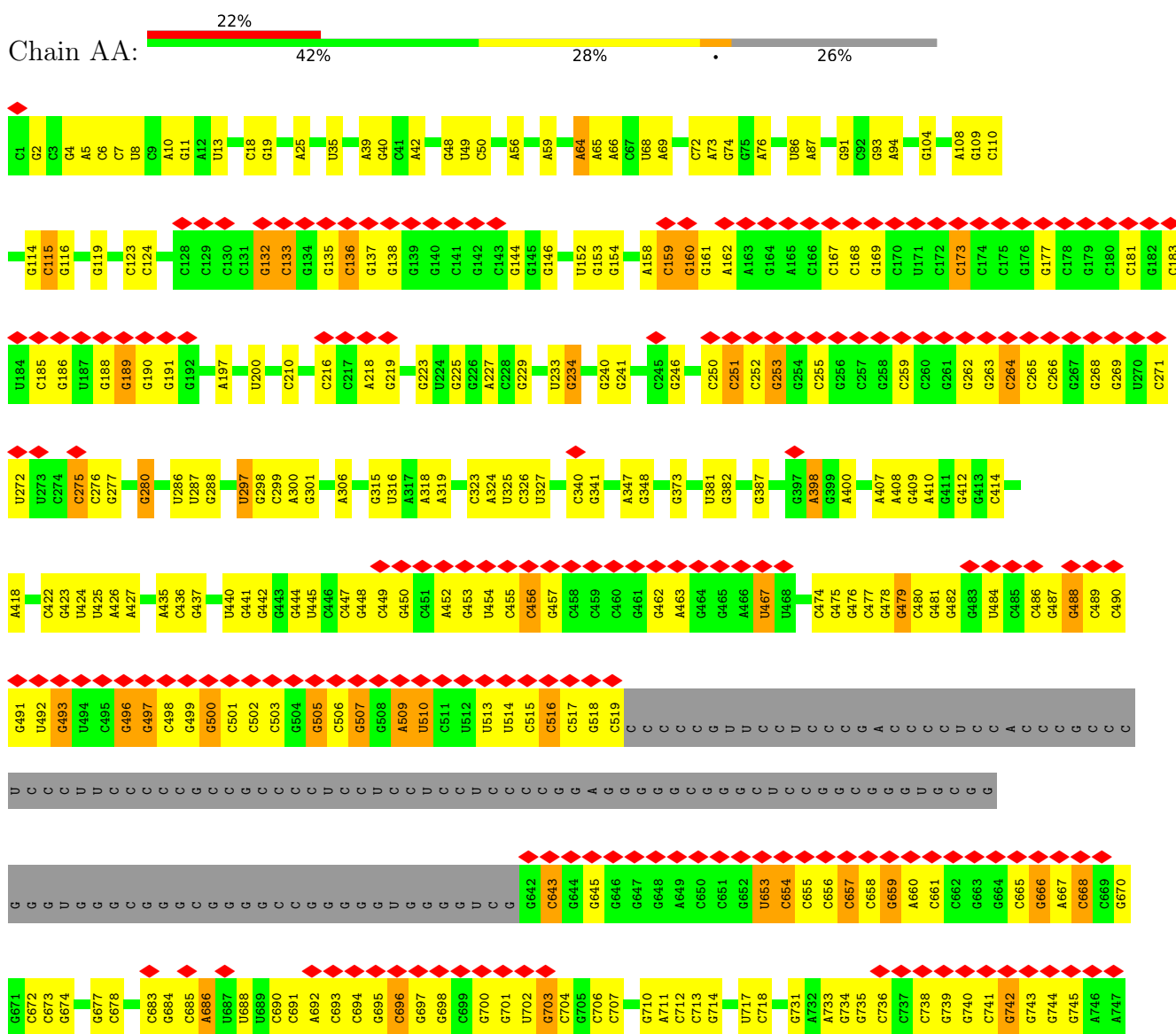
- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

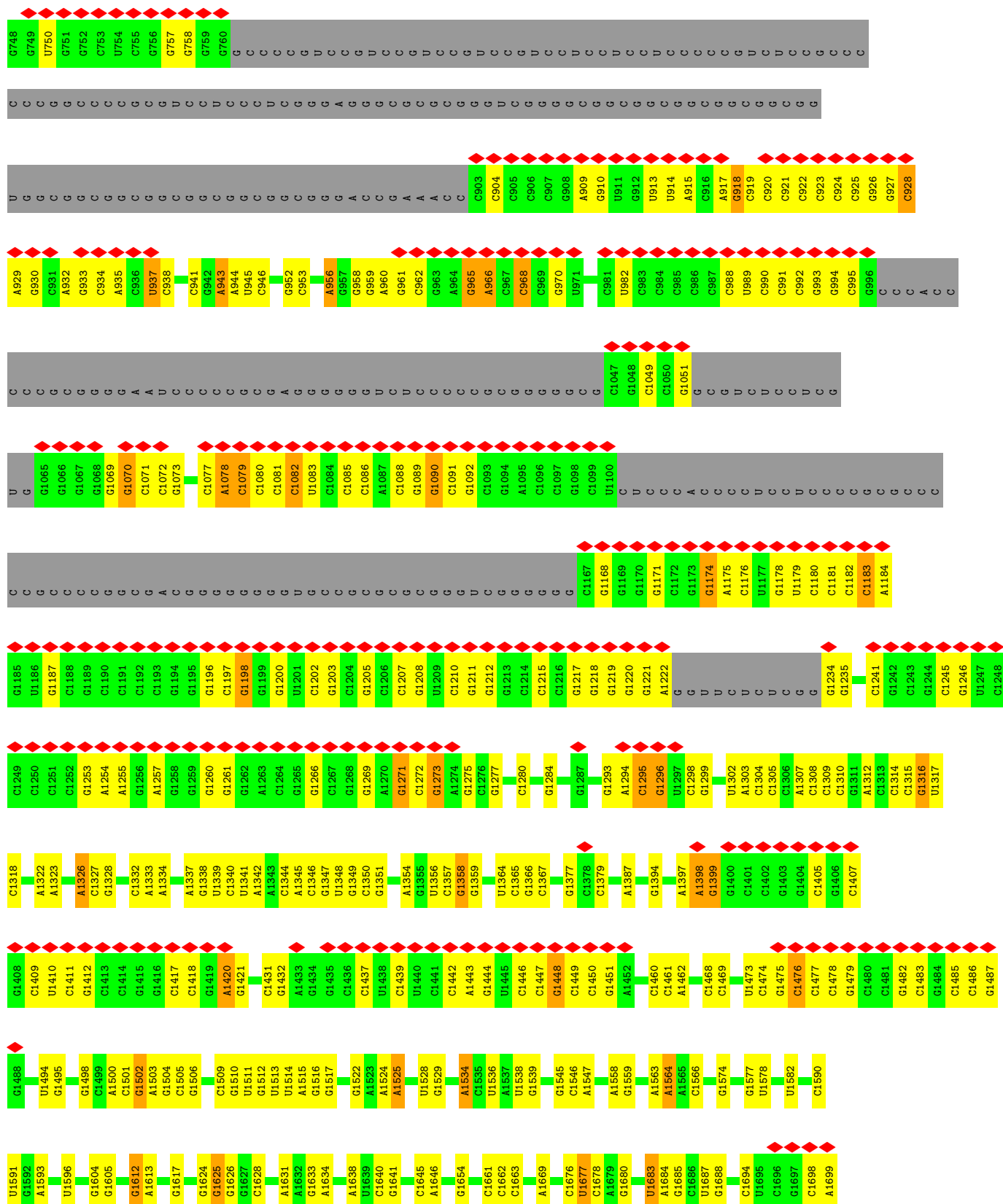
Mol	Chain	Residues	Atoms	AltConf
81	Ai	1	Total Zn 1 1	0
81	Al	1	Total Zn 1 1	0
81	Ao	1	Total Zn 1 1	0
81	Aq	1	Total Zn 1 1	0
81	Ar	1	Total Zn 1 1	0
81	BR	1	Total Zn 1 1	0
81	BT	1	Total Zn 1 1	0
81	Bg	1	Total Zn 1 1	0

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.

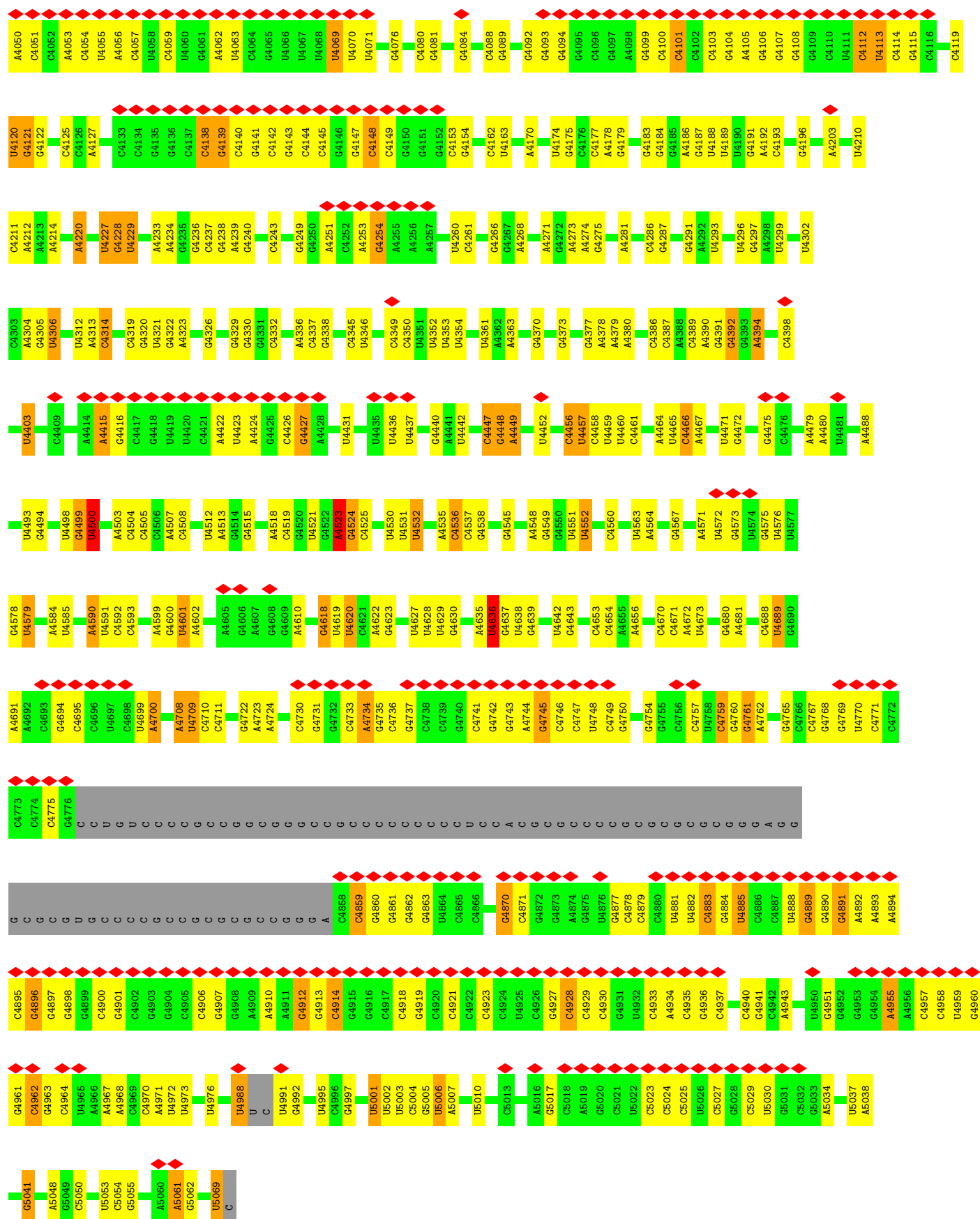
• Molecule 1: 28S rRNA (3773-MER)



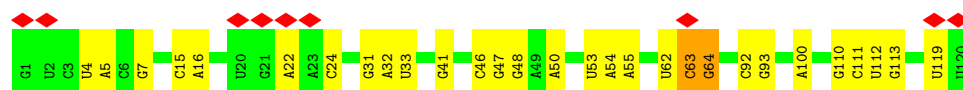
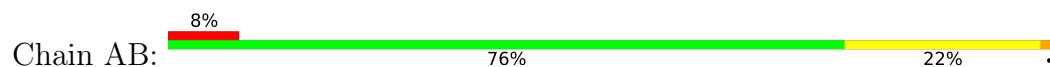




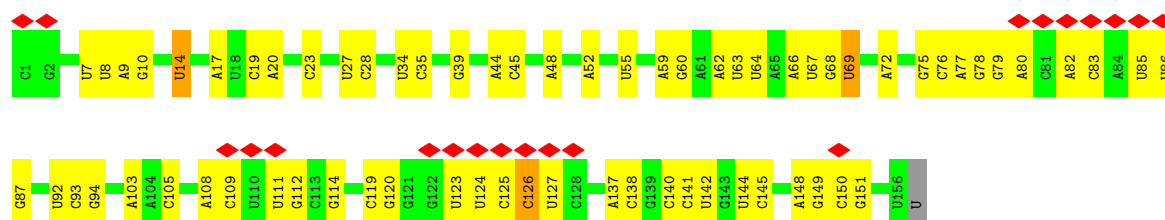




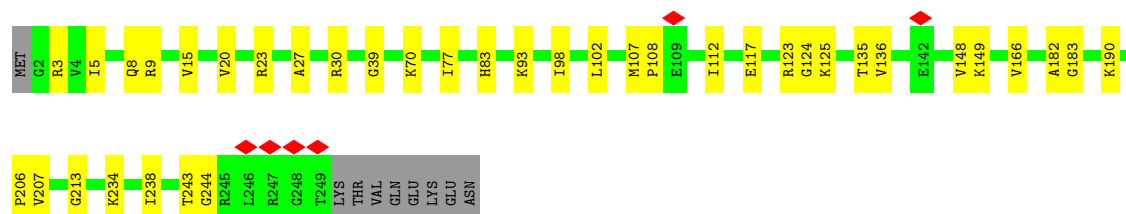
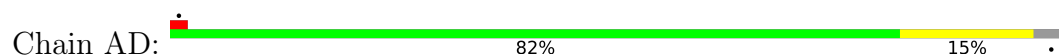
- Molecule 2: 5S rRNA (120-MER)



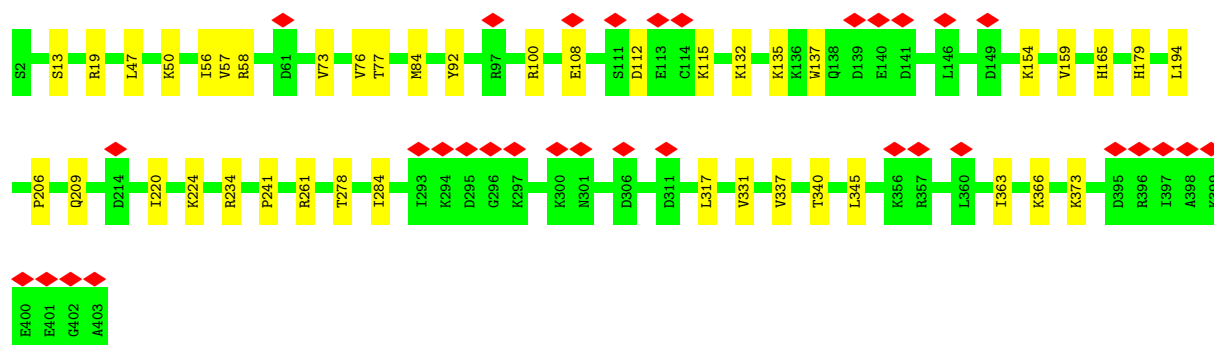
- Molecule 3: 5.8S rRNA (156-MER)



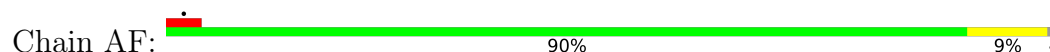
- Molecule 4: 60S ribosomal protein L8

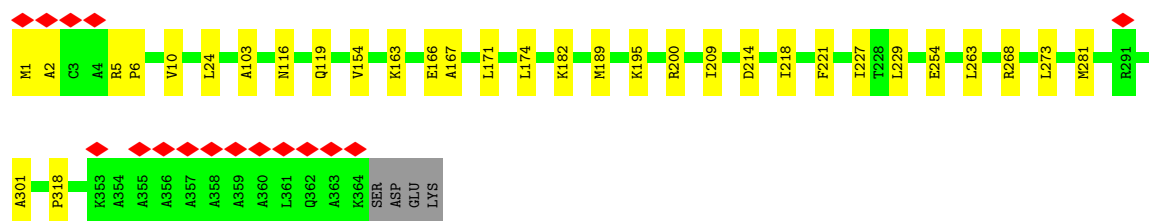


- Molecule 5: Large ribosomal subunit protein uL3

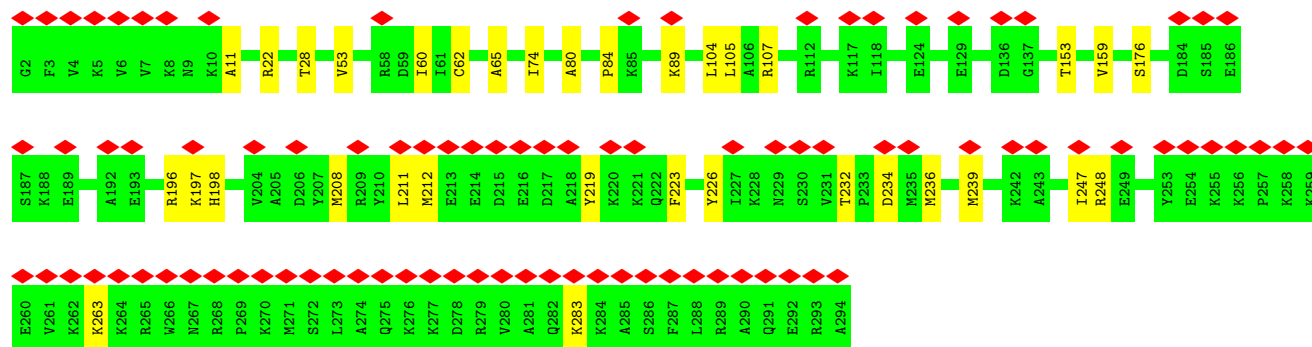
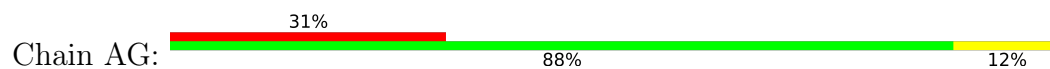


- Molecule 6: Large ribosomal subunit protein uL4

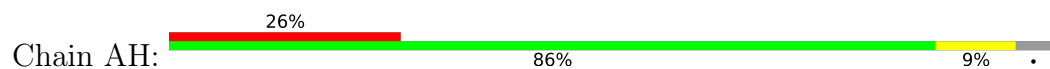




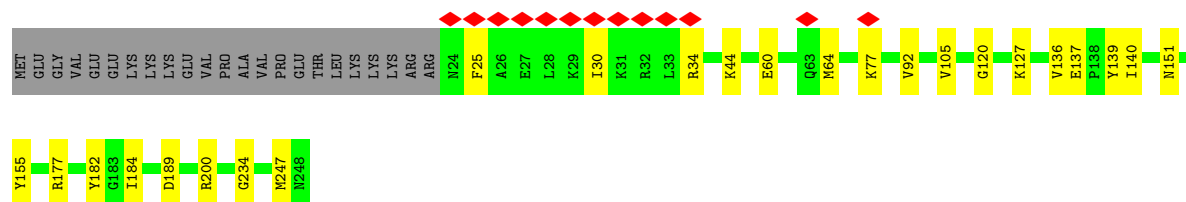
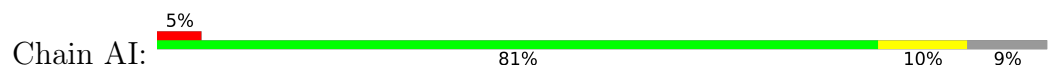
• Molecule 7: Large ribosomal subunit protein uL18



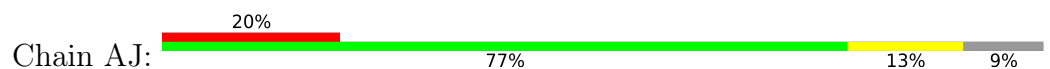
• Molecule 8: Large ribosomal subunit protein eL6

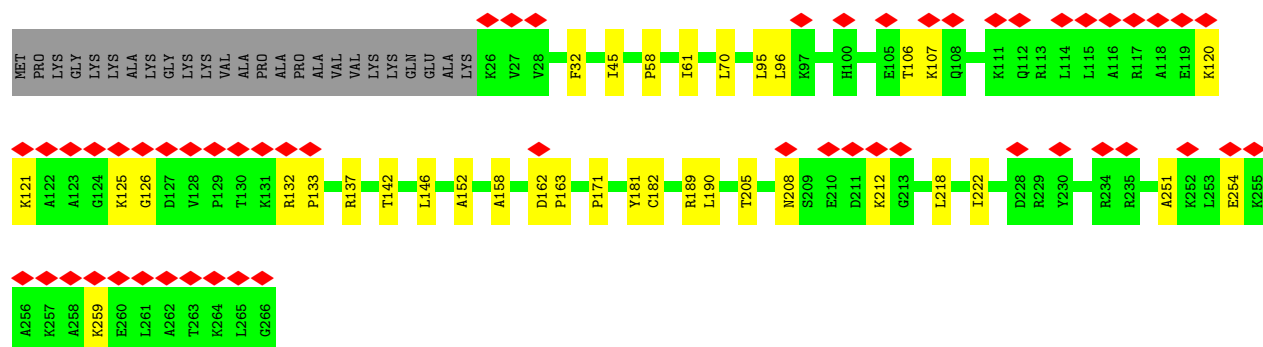


• Molecule 9: 60S ribosomal protein L7

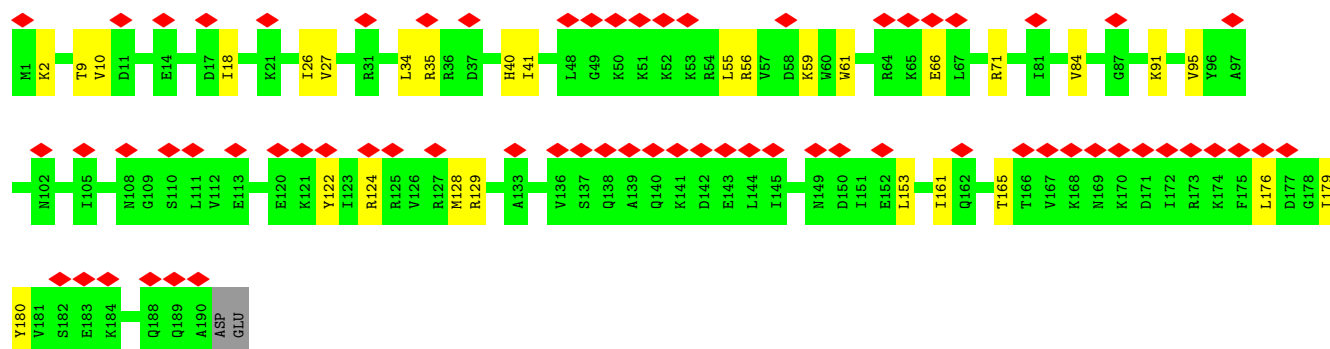
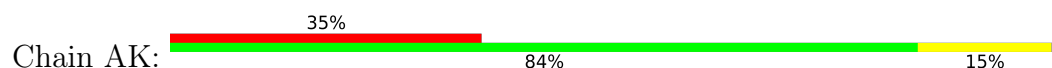


• Molecule 10: 60S ribosomal protein L7a

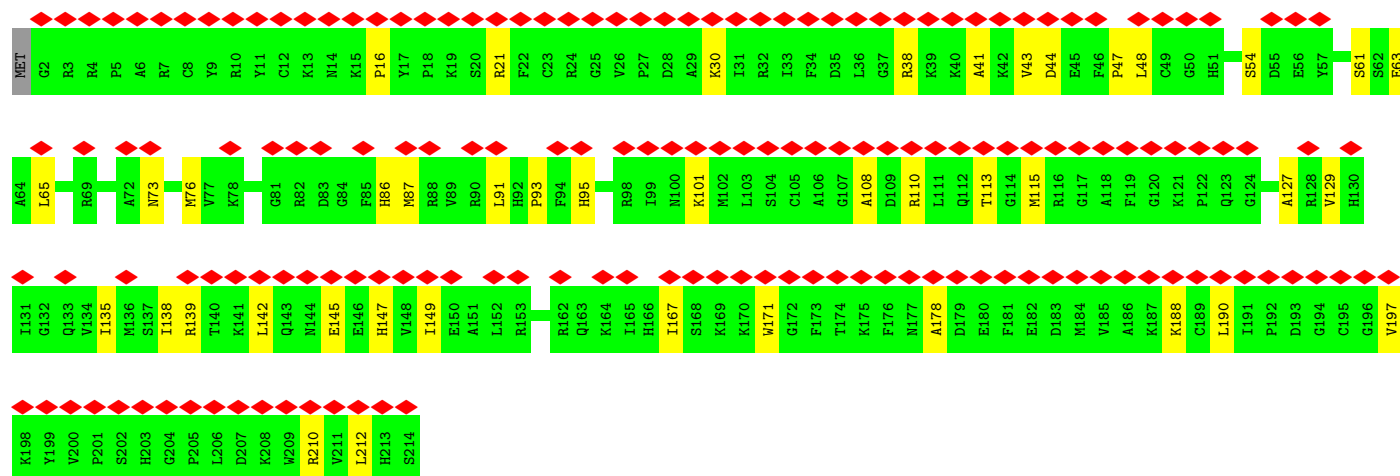
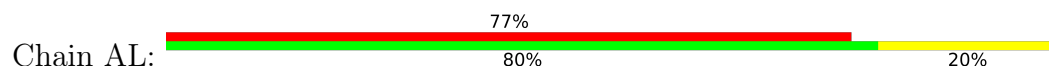




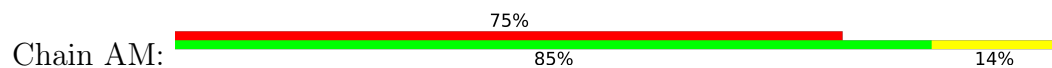
- Molecule 11: 60S ribosomal protein L9

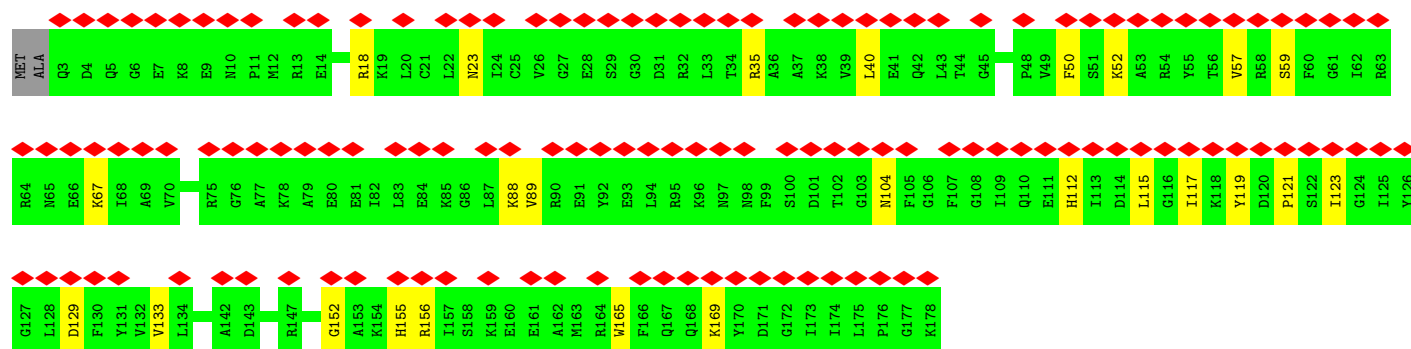


- Molecule 12: Ribosomal protein uL16-like

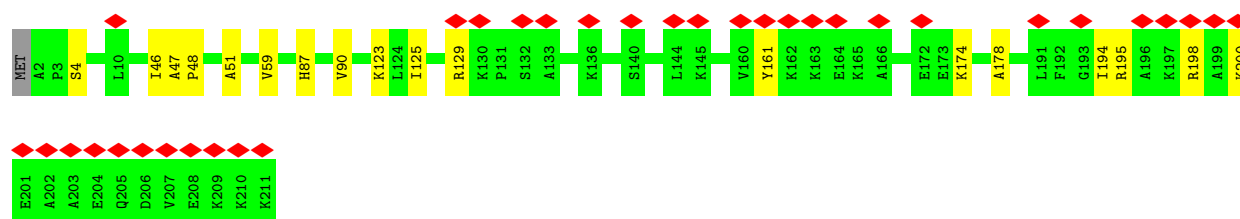


- Molecule 13: 60S ribosomal protein L11

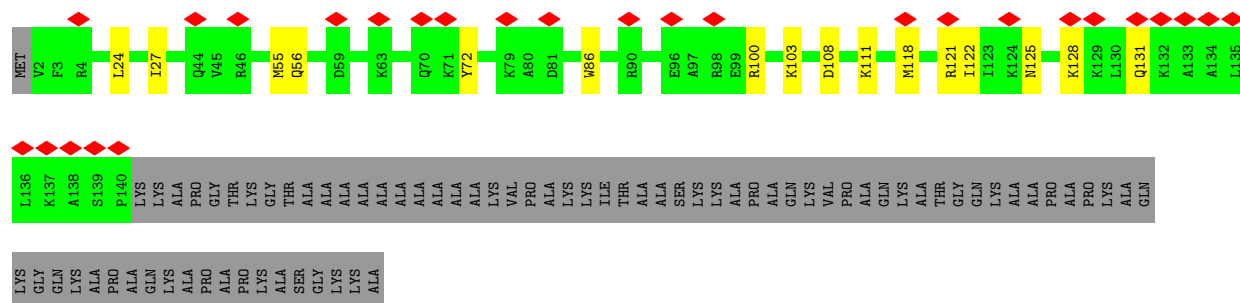




• Molecule 14: 60S ribosomal protein L13



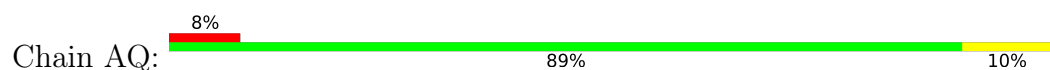
• Molecule 15: 60S ribosomal protein L14



• Molecule 16: 60S ribosomal protein L15

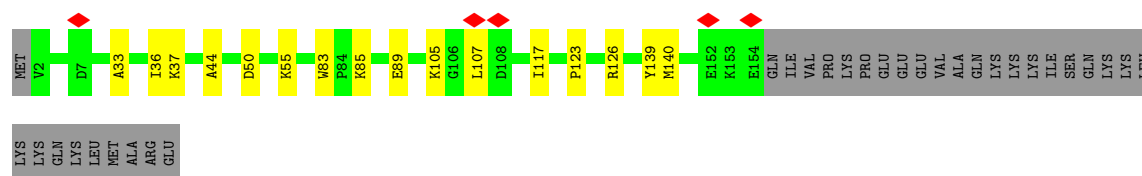


• Molecule 17: 60S ribosomal protein L13a



- Molecule 18: 60S ribosomal protein L17

Chain AR:  74% 9% 17%



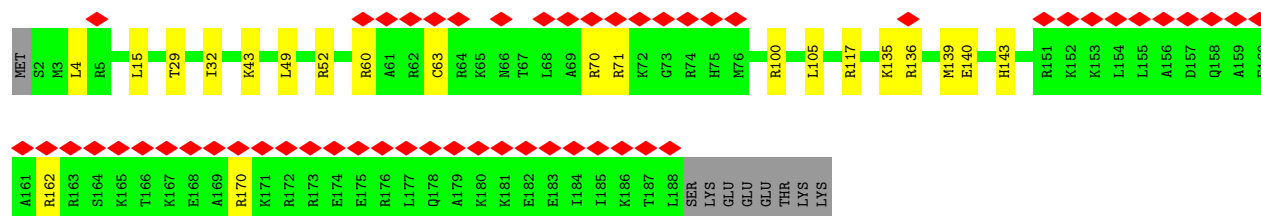
- Molecule 19: 60S ribosomal protein L18

Chain AS:  92% 7%



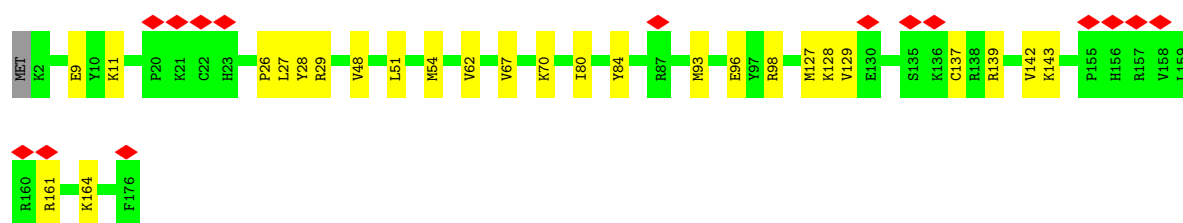
- Molecule 20: 60S ribosomal protein L19

Chain AT:  28% 85% 11% 5%



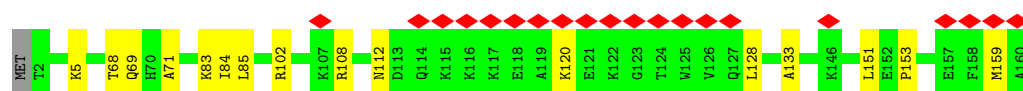
- Molecule 21: 60S ribosomal protein L18a

Chain AU:  9% 85% 15%



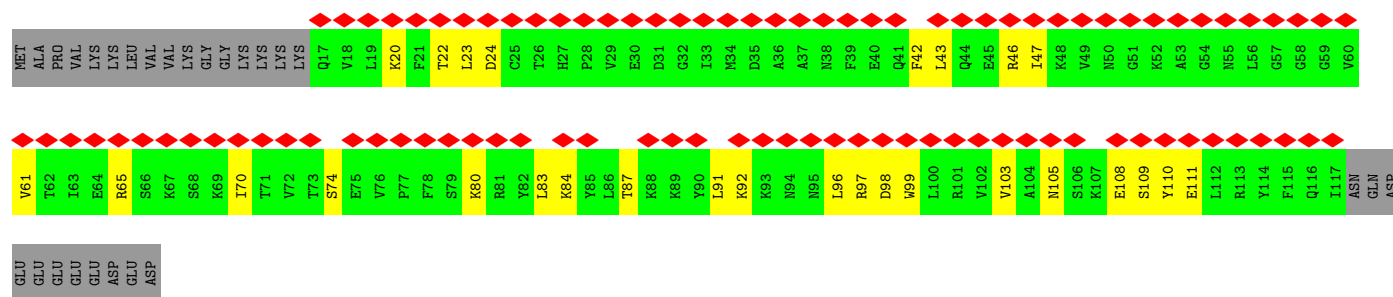
- Molecule 22: 60S ribosomal protein L21

Chain AV:  12% 89% 10%

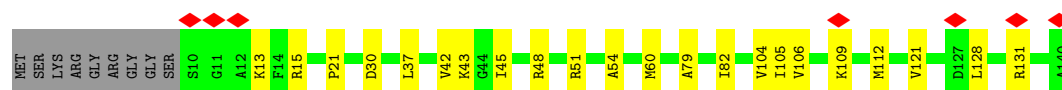
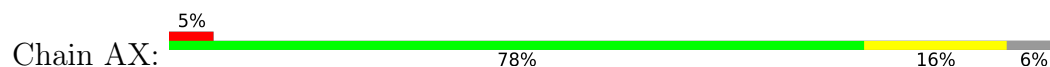


- Molecule 23: 60S ribosomal protein L22

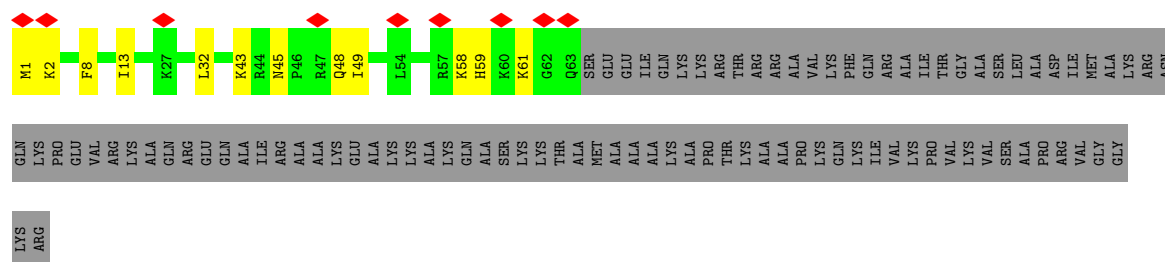
Chain AW:  73% 57% 22% 21%



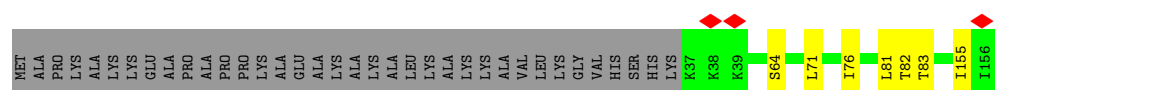
- Molecule 24: 60S ribosomal protein L23



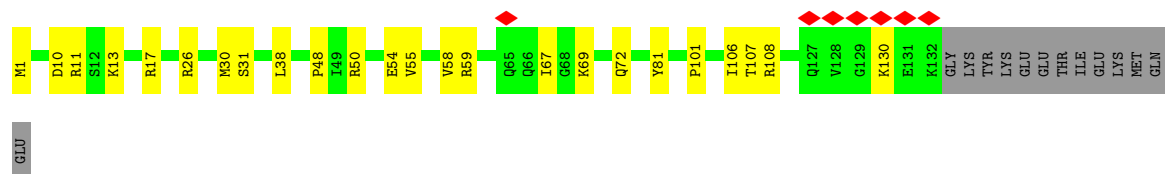
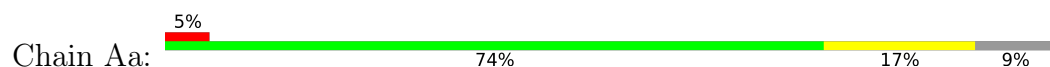
- Molecule 25: 60S ribosomal protein L24



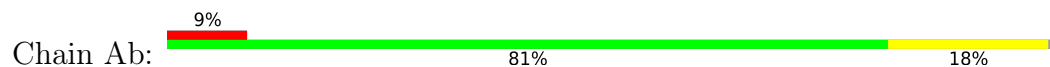
- Molecule 26: 60S ribosomal protein L23a

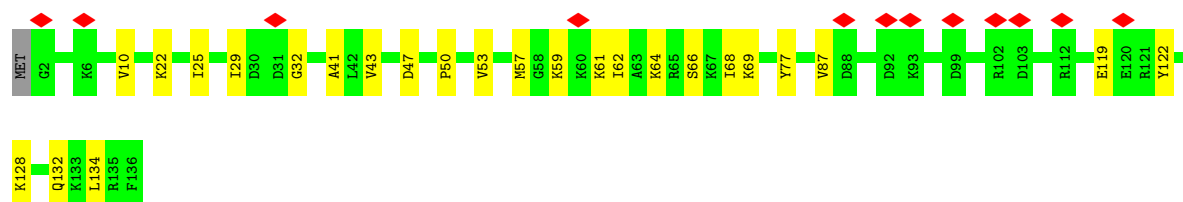


- Molecule 27: 60S ribosomal protein L26

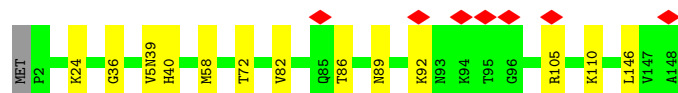


- Molecule 28: 60S ribosomal protein L27

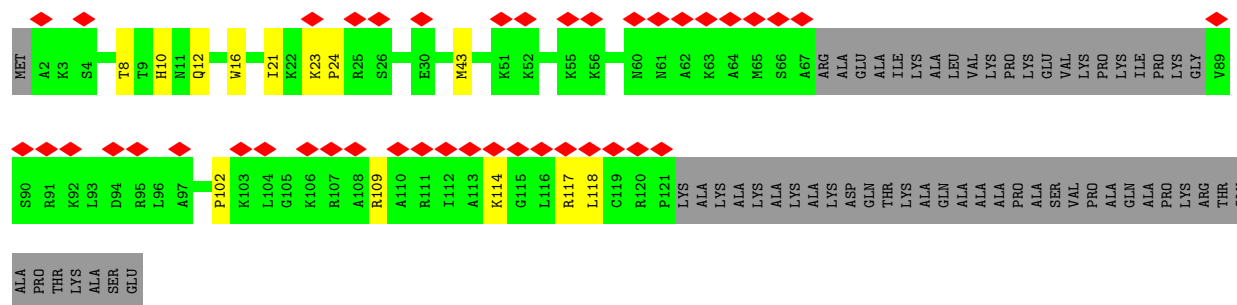




- Molecule 29: Large ribosomal subunit protein uL15



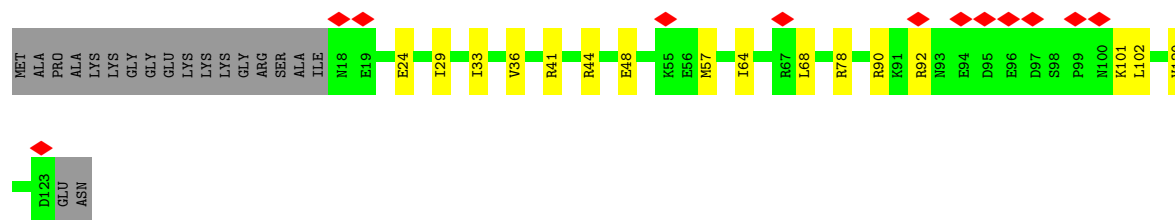
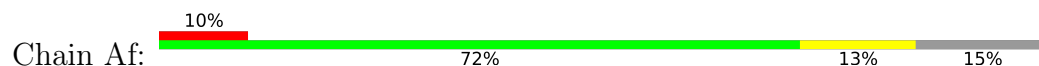
- Molecule 30: 60S ribosomal protein L29



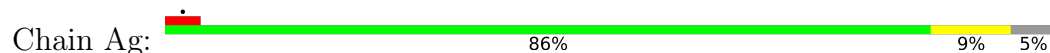
- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31



- Molecule 33: 60S ribosomal protein L32

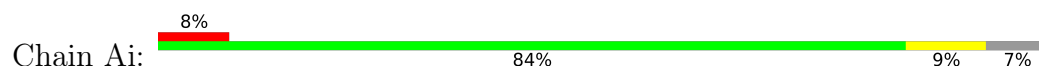




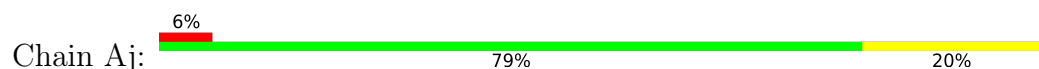
- Molecule 34: 60S ribosomal protein L35a



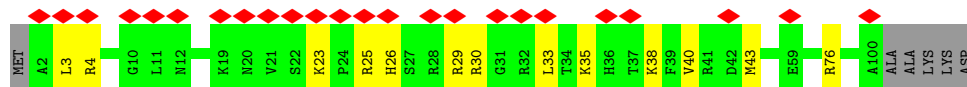
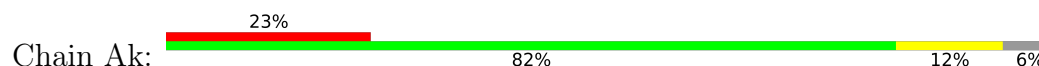
- Molecule 35: 60S ribosomal protein L34



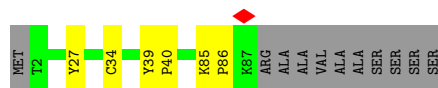
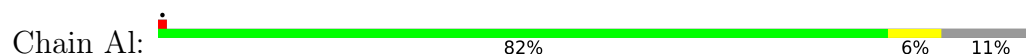
- Molecule 36: 60S ribosomal protein L35



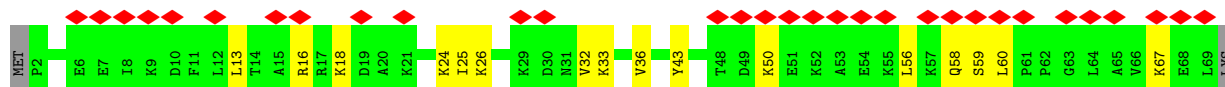
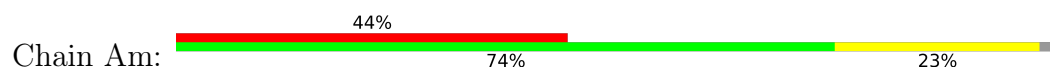
- Molecule 37: 60S ribosomal protein L36



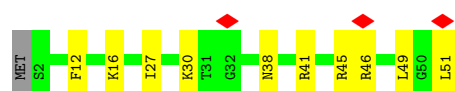
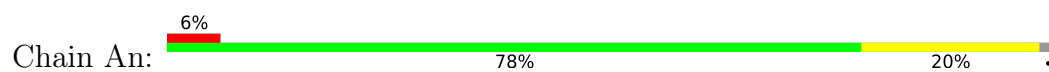
- Molecule 38: 60S ribosomal protein L37



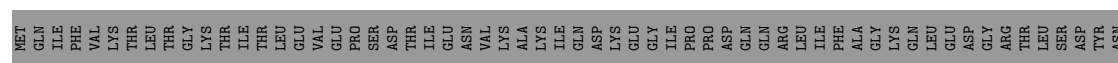
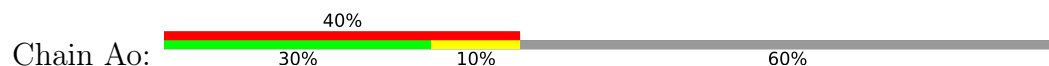
- Molecule 39: 60S ribosomal protein L38



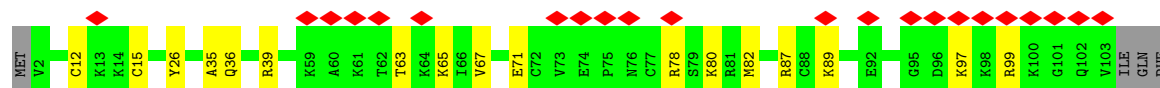
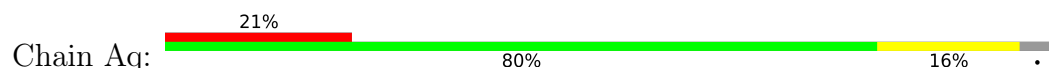
- Molecule 40: 60S ribosomal protein L39



- Molecule 41: Ubiquitin-60S ribosomal protein L40



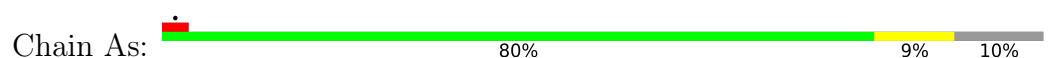
- Molecule 42: 60S ribosomal protein L36a



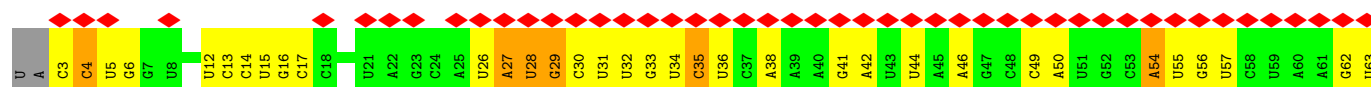
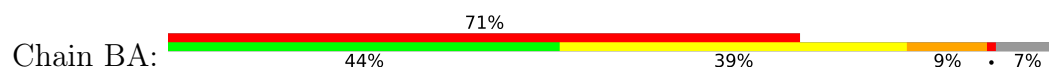
- Molecule 43: 60S ribosomal protein L37a



- Molecule 44: 60S ribosomal protein L28

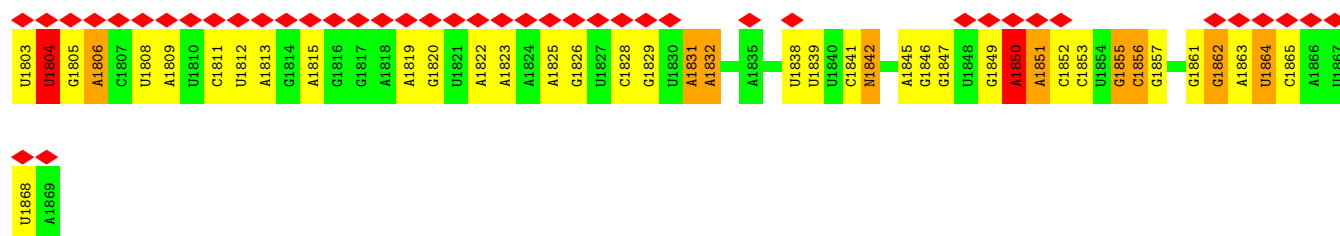


- Molecule 45: 18S rRNA (1740-MER)

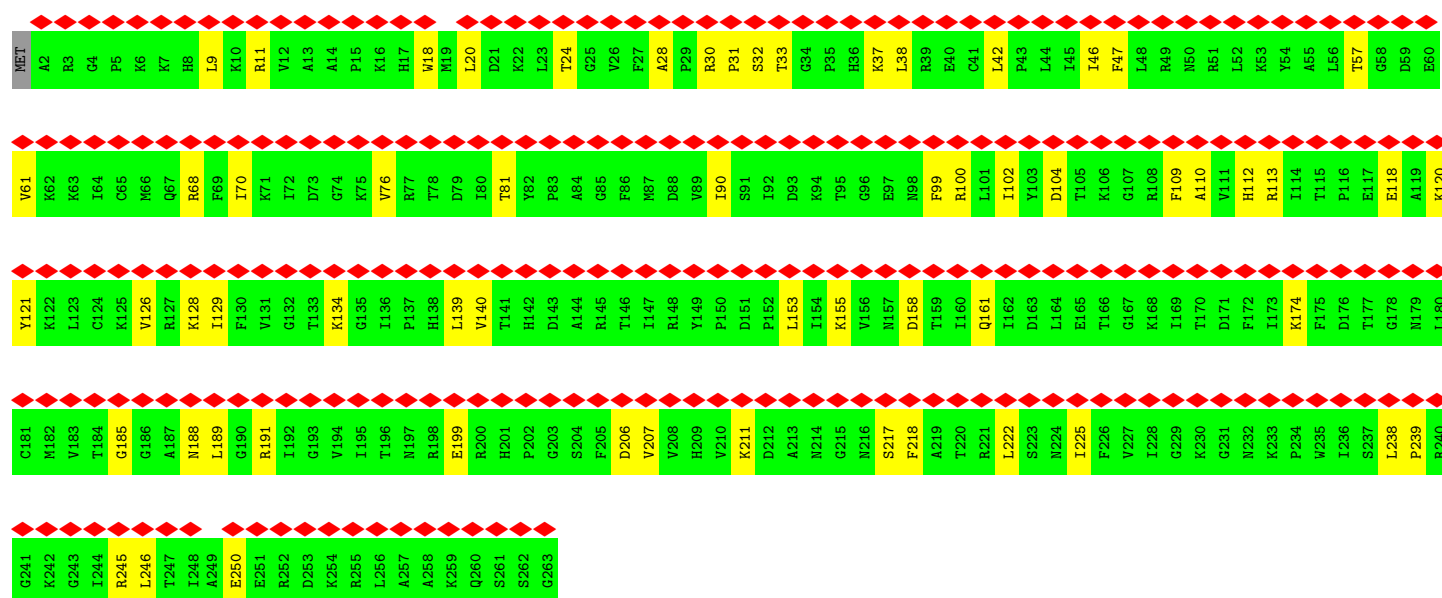
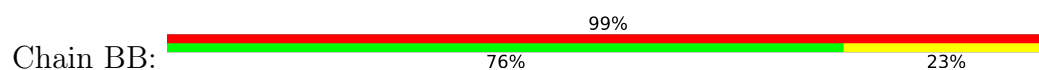




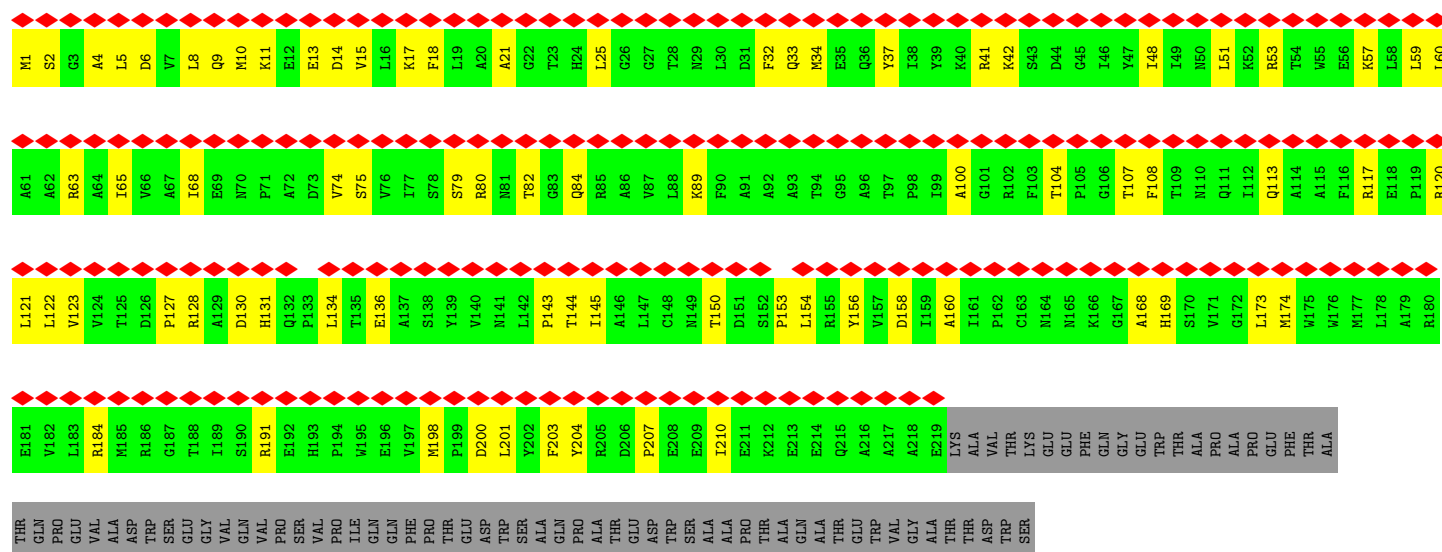
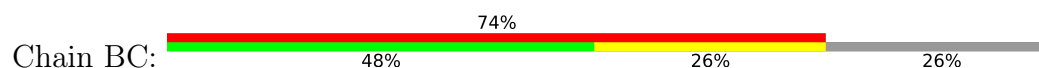
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C1683	C1684	U1685	G1686	C1687	C1688	C1689	U1690	U1691	U1692	U1693	U1694	A1695	C1696	A1697	C1698	A1699	C1700	G1701	C1702	C1703	C1704	G1705	G1706	C1765	C1766	C1767	A1768	C1769	G1770	A1771	C1772	C1773	C1774	U1775	C1776	C1777	G1778	C1779	U1780	A1781	G1782	C1783	G1784	U1785	U1786	G1787	A1788	G1789	A1790	A1791	G1792	G1793	C1794	G1795	G1796	U1797	C1798	U1799	U1741	A1800	A1801	C1802																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
A1623	U1624	U1625	C1626	C1627	C1628	C1629	A1630	G1631	G1632	A1633	A1634	C1635	G1636	A1637	G1638	C1639	A1640	A1641	U1642	U1643	C1644	C1645	C1646	A1647	G1648	U1649	A1650	A1651	G1652	U1653	G1654	C1655	G1656	C1657	G1658	U1659	C1660	A1661	U1662	A1663	A1664	C1665	C1666	U1667	U1668	G1669	C1670	G1671	U1672	U1673	G1674	A1675	U1676	U1677	A1678	U1679	A1680	U1681	C1682																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
C1563	C1564	C1565	G1566	C1567	C1568	A1569	G1570	G1571	C1572	G1573	C1574	G1575	G1576	G1577	U1578	A1579	G1580	C1581	C1582	C1583	G1584	U1585	U1586	G1587	A1588	C1589	U1590	G1591	C1592	G1593	A1594	U1595	U1596	C1597	G1598	U1599	G1600	A1601	U1602	G1603	G1604	G1605	G1606	A1607	U1608	C1609	G1610	G1611	G1612	G1613	A1614	U1615	U1616	G1617	C1618	A1619	U1620	U1621	U1622																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
A1623	U1624	U1625	C1626	C1627	C1628	C1629	A1630	G1631	G1632	A1633	A1634	C1635	G1636	A1637	G1638	C1639	A1640	A1641	U1642	U1643	C1644	C1645	C1646	A1647	G1648	U1649	A1650	A1651	G1652	U1653	G1654	C1655	G1656	C1657	G1658	U1659	C1660	A1661	U1662	A1663	A1664	C1665	C1666	U1667	U1668	G1669	C1670	G1671	U1672	U1673	G1674	A1675	U1676	U1677	A1678	U1679	A1680	U1681	C1682																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
C1683	C1684	U1685	G1686	C1687	C1688	C1689	U1690	U1691	U1692	U1693	U1694	A1695	C1696	A1697	C1698	A1699	C1700	G1701	C1702	C1703	C1704	G1705	G1706	C1765	C1766	C1767	A1768	C1769	G1770	A1771	C1772	C1773	C1774	U1775	C1776	C1777	G1778	C1779	U1780	A1781	G1782	C1783	G1784	U1785	U1786	G1787	A1788	G1789	A1790	A1791	G1792	G1793	C1794	G1795	G1796	U1797	C1798	U1799	U1741	A1800	A1801	C1802																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
A1030	A1031	G1125	G1126	G1127	C1128	G1129	U1045	U1046	C1132	A1133	G1134	C1135	U1136	U1137	C1138	C1139	G1140	A1144	A1145	A1148	A1149	A1150	C1153	U1154	U1155	U1156	C1163	G1164	G1165	G1166	A1170	G1171	U1172	A1173	U1174	G1175	G1176	U1177	U1178	G1179	C1180	A1181	U1111	U1112	A1113	G1184	C1185	U1186	C1116	C1117	U1192	U1193	A1194	A1195	G1198	A1199																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								



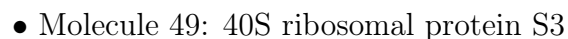
- Molecule 46: 40S ribosomal protein S4, X isoform



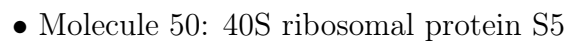
- Molecule 47: Small ribosomal subunit protein uS2



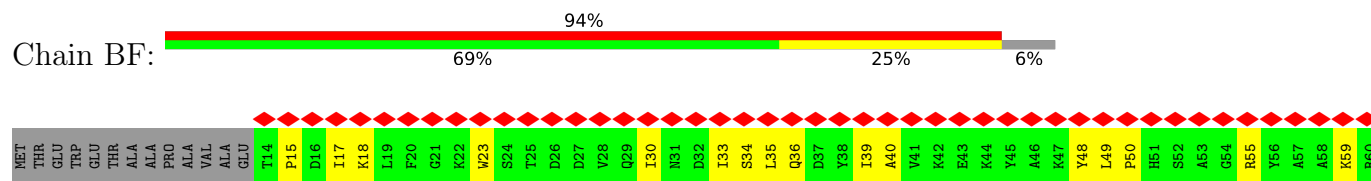
Chain BD:

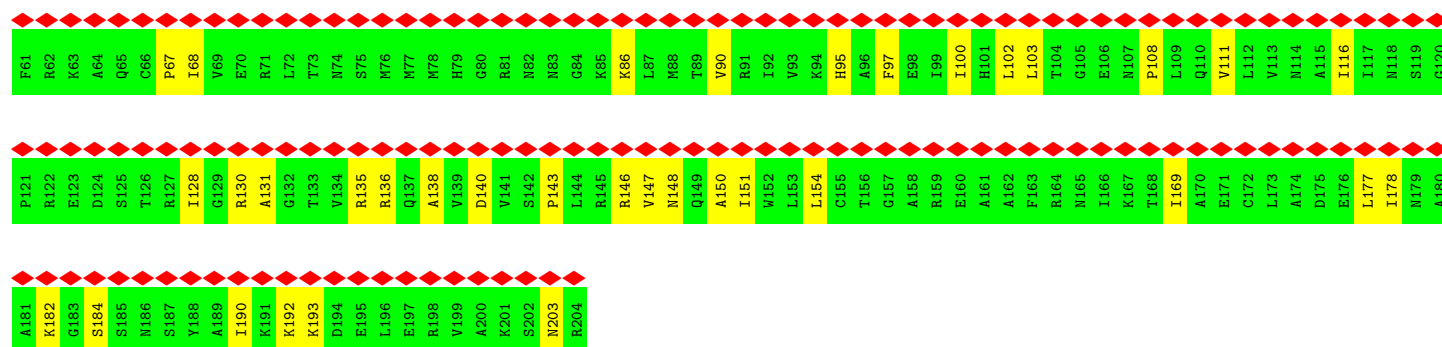


Chain BE:

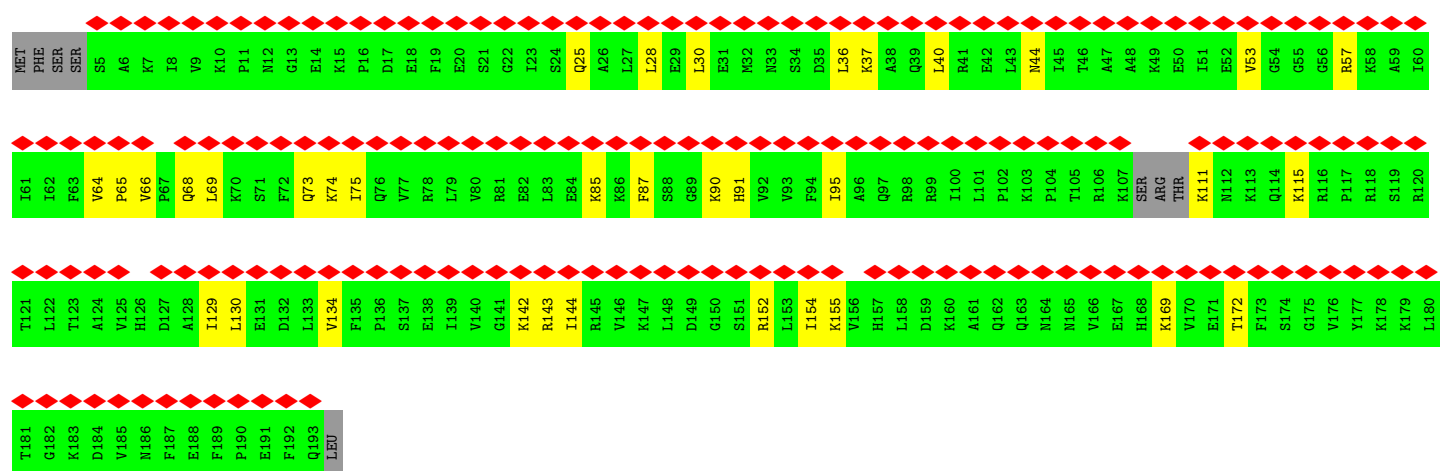
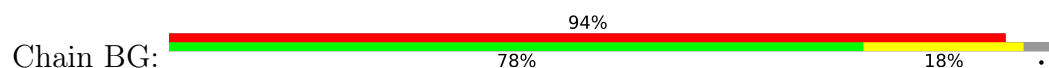


Chain BF:

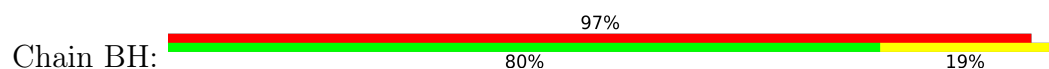




• Molecule 51: 40S ribosomal protein S7

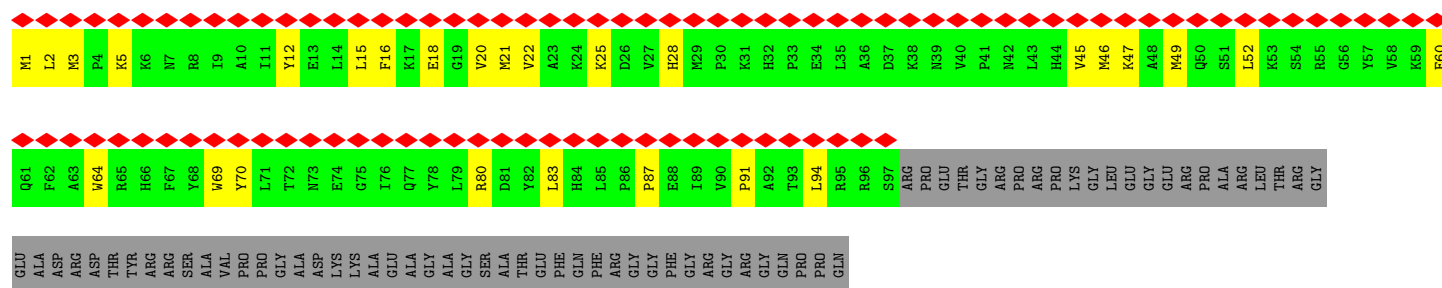


• Molecule 52: 40S ribosomal protein S8

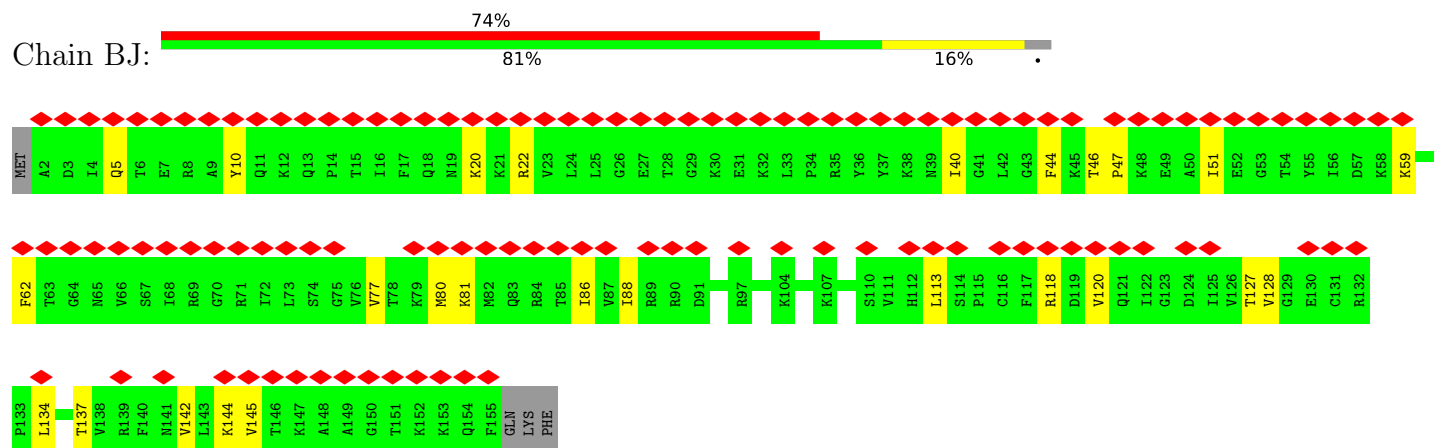


• Molecule 53: 40S ribosomal protein S10

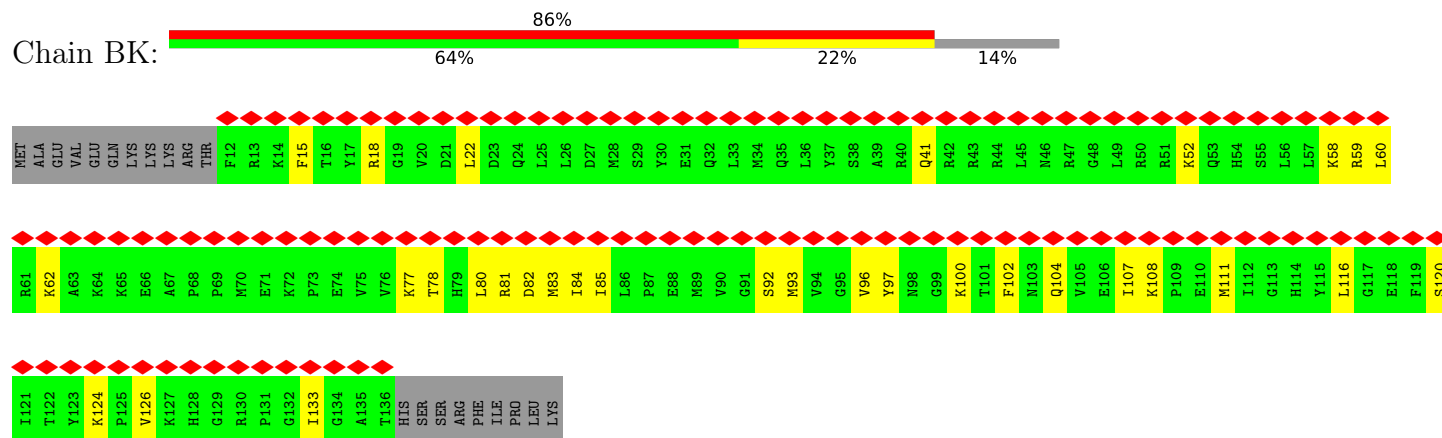




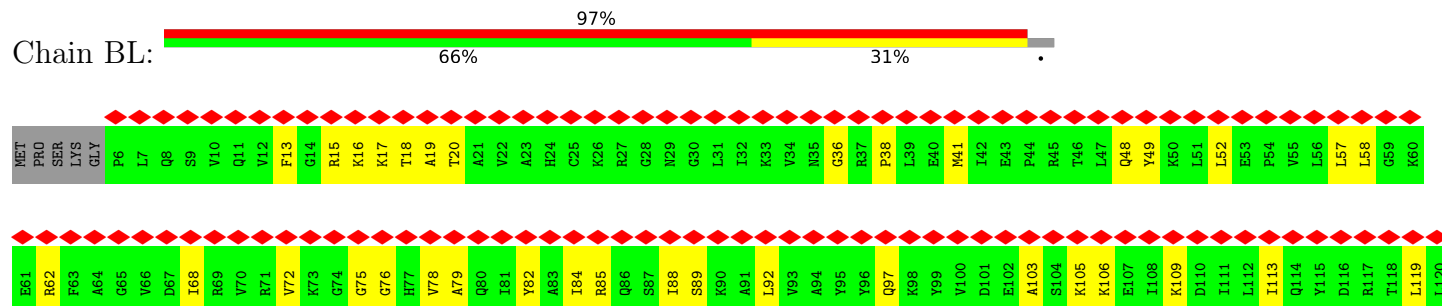
• Molecule 54: 40S ribosomal protein S11



• Molecule 55: 40S ribosomal protein S15

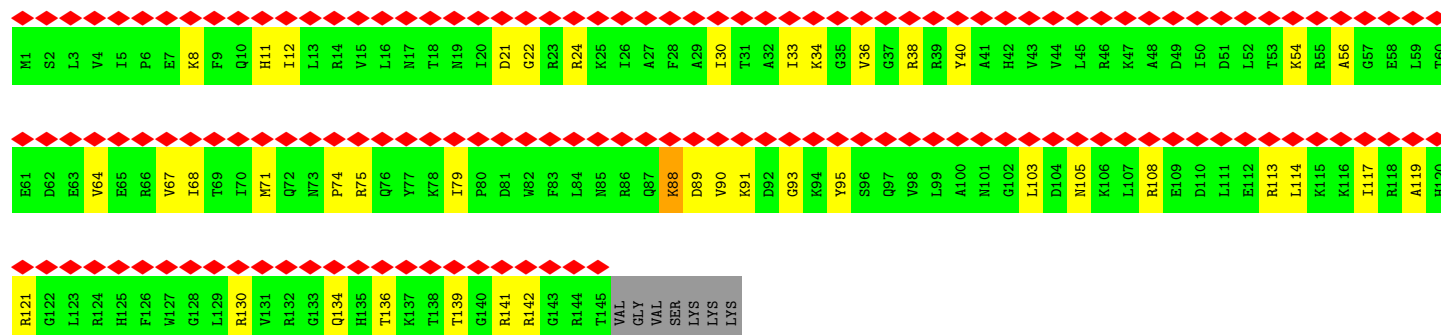


• Molecule 56: 40S ribosomal protein S16

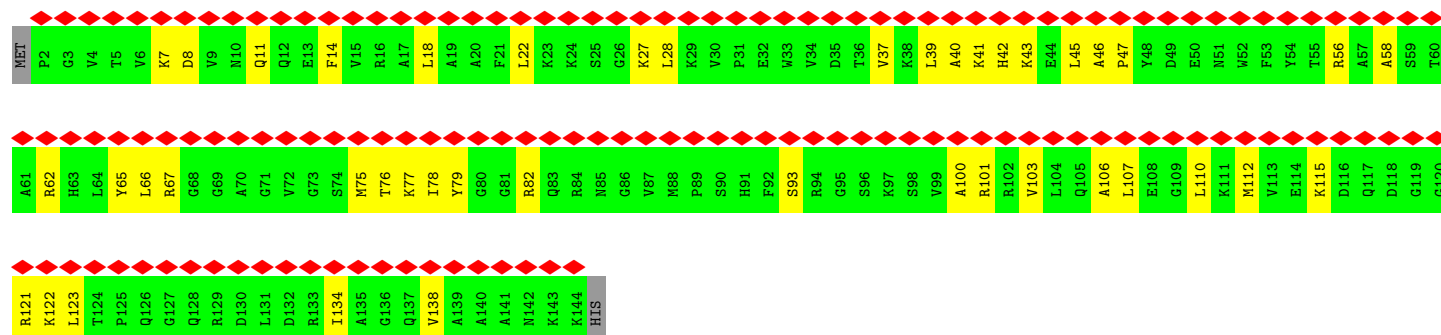




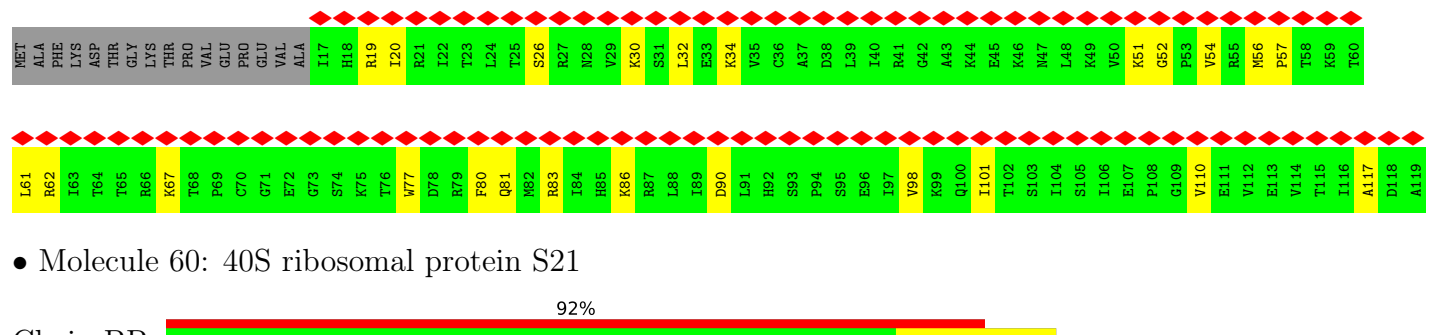
• Molecule 57: 40S ribosomal protein S18



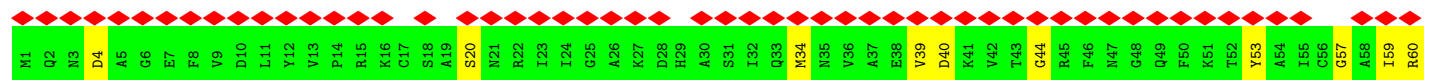
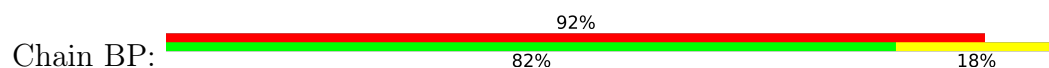
• Molecule 58: Small ribosomal subunit protein eS19



• Molecule 59: 40S ribosomal protein S20

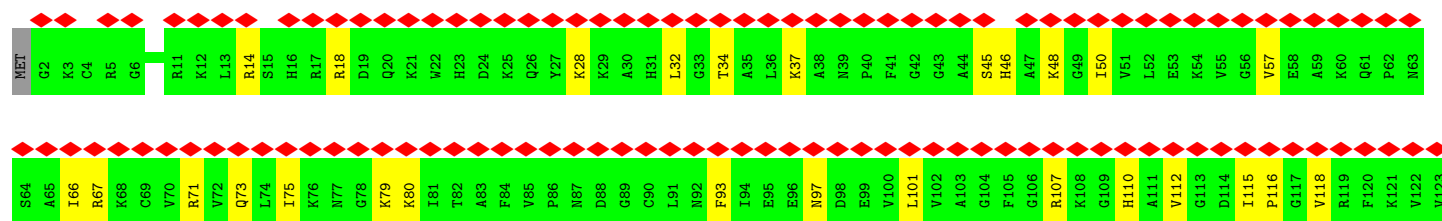
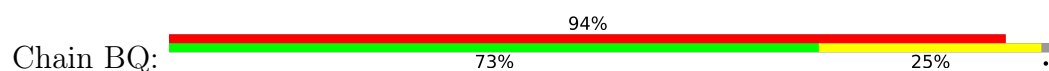


• Molecule 60: 40S ribosomal protein S21

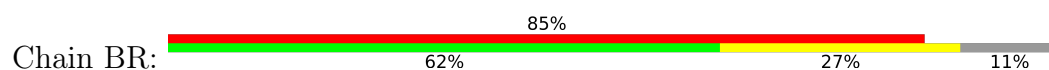




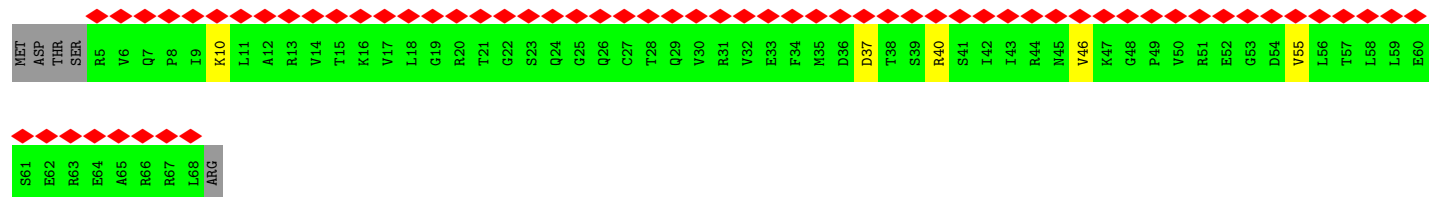
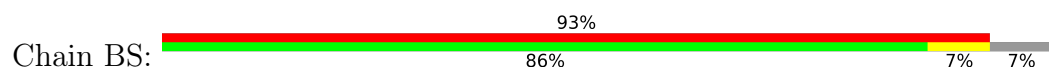
- Molecule 61: 40S ribosomal protein S23



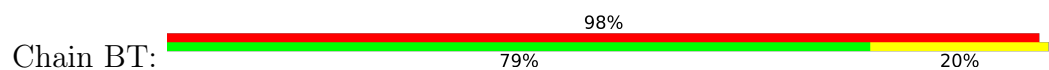
- Molecule 62: 40S ribosomal protein S26



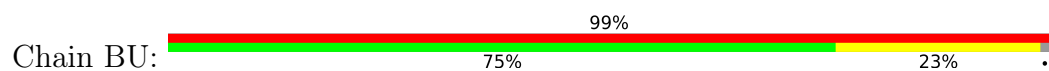
- Molecule 63: 40S ribosomal protein S28

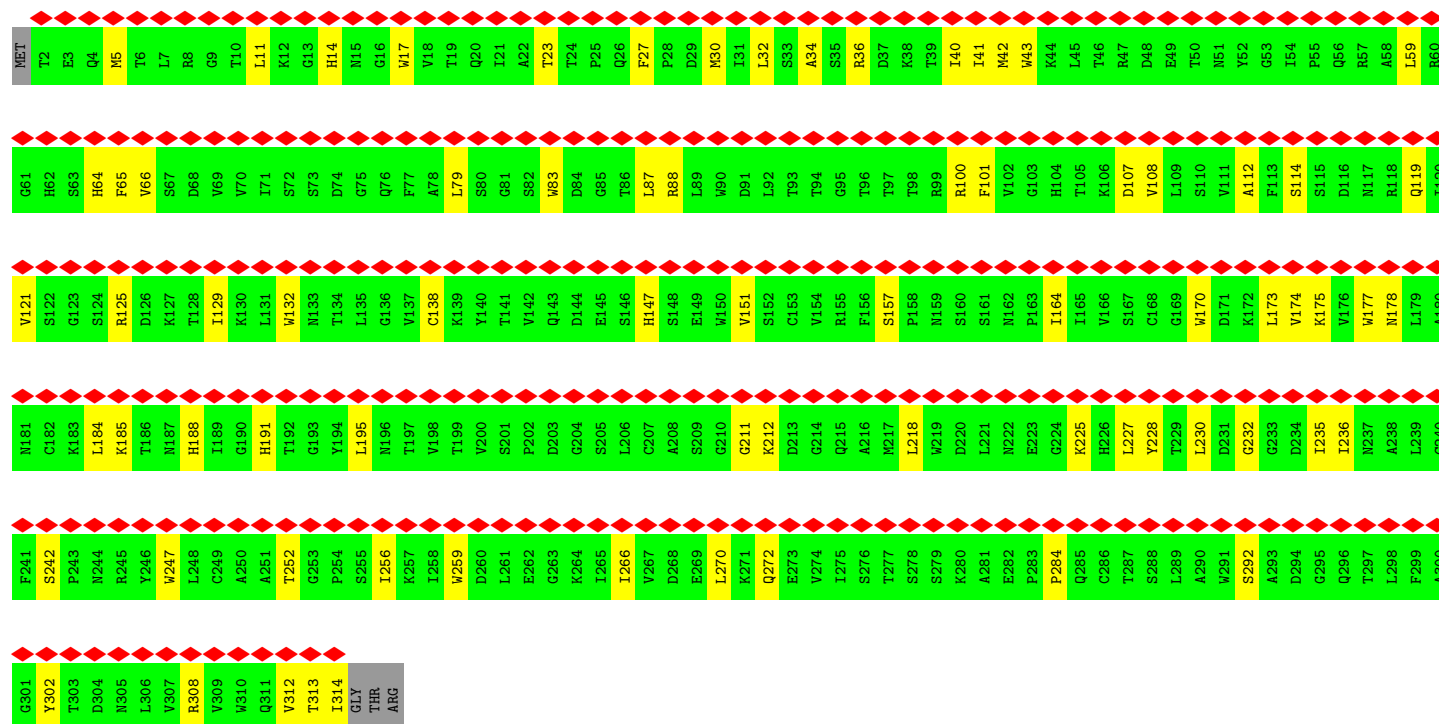


- Molecule 64: 40S ribosomal protein S29

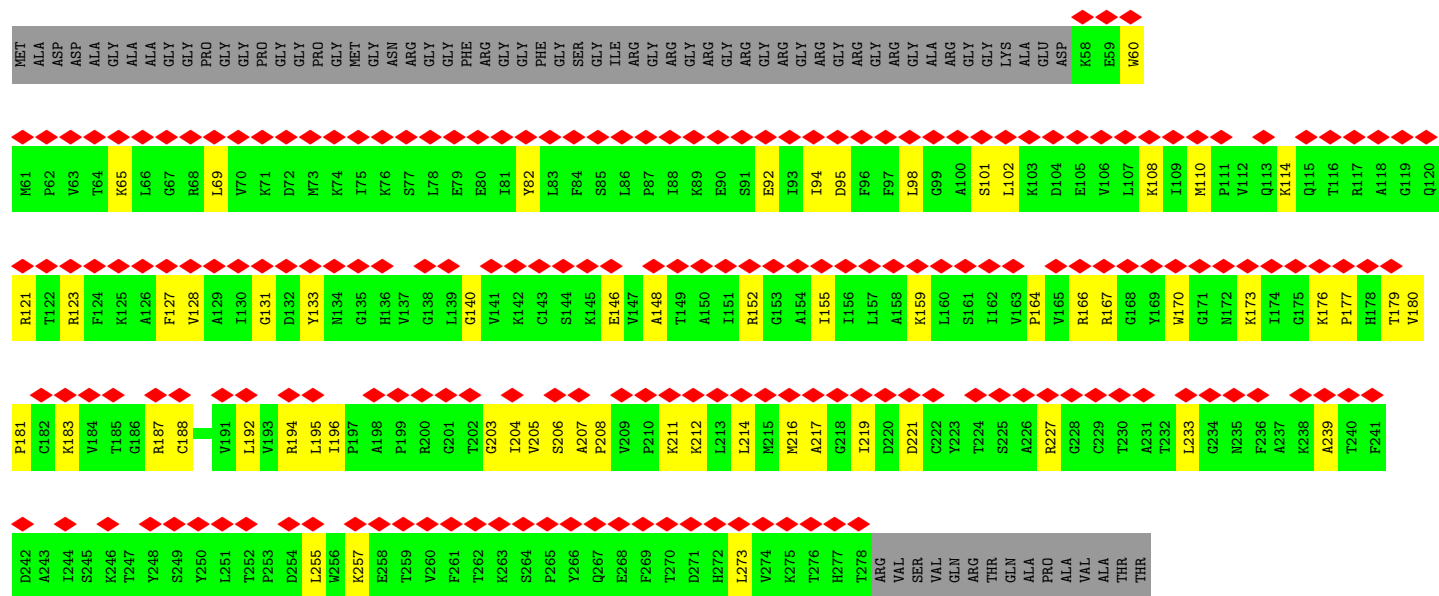


- Molecule 65: Receptor of activated protein C kinase 1

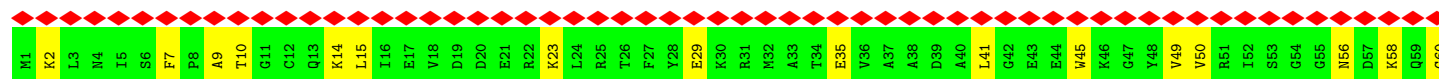
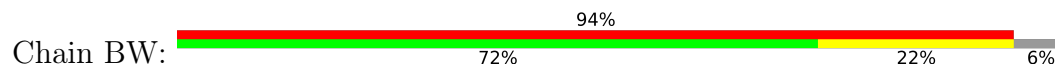




• Molecule 66: 40S ribosomal protein S2



• Molecule 67: 40S ribosomal protein S6

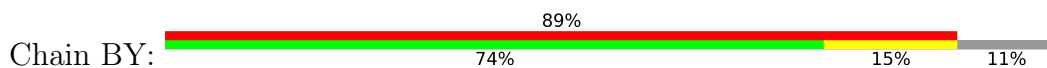




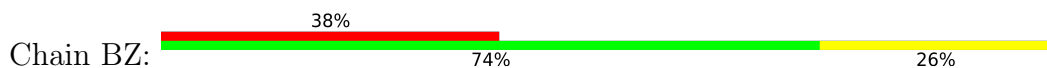
• Molecule 68: 40S ribosomal protein S9

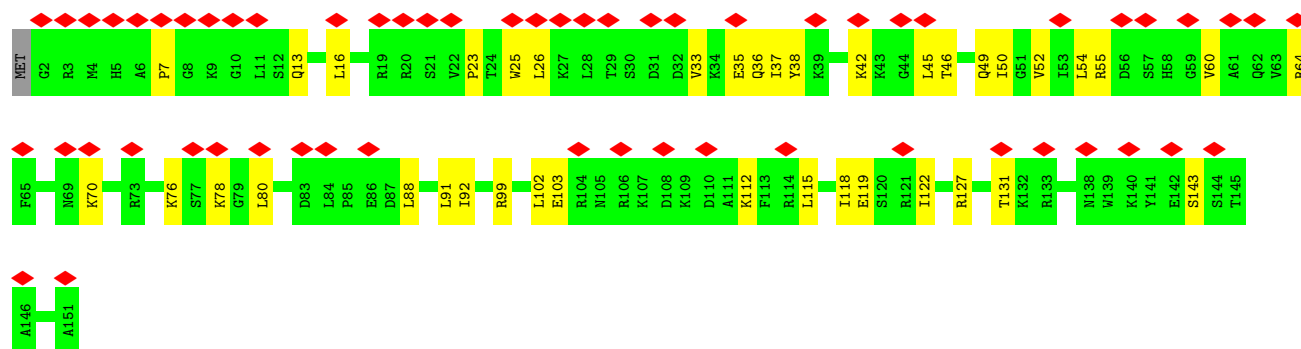


• Molecule 69: 40S ribosomal protein S12

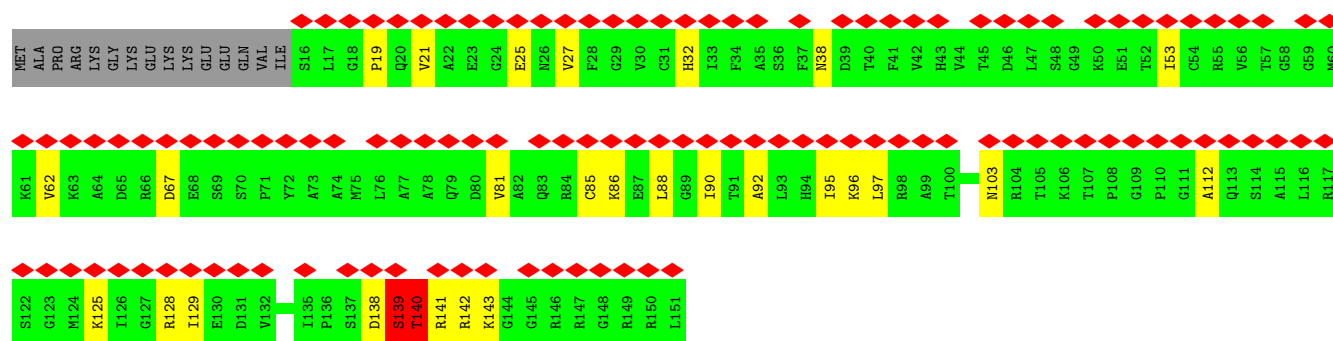
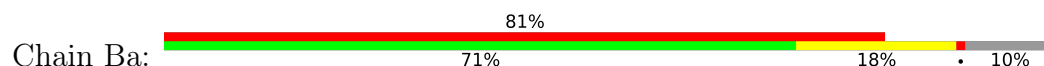


• Molecule 70: 40S ribosomal protein S13

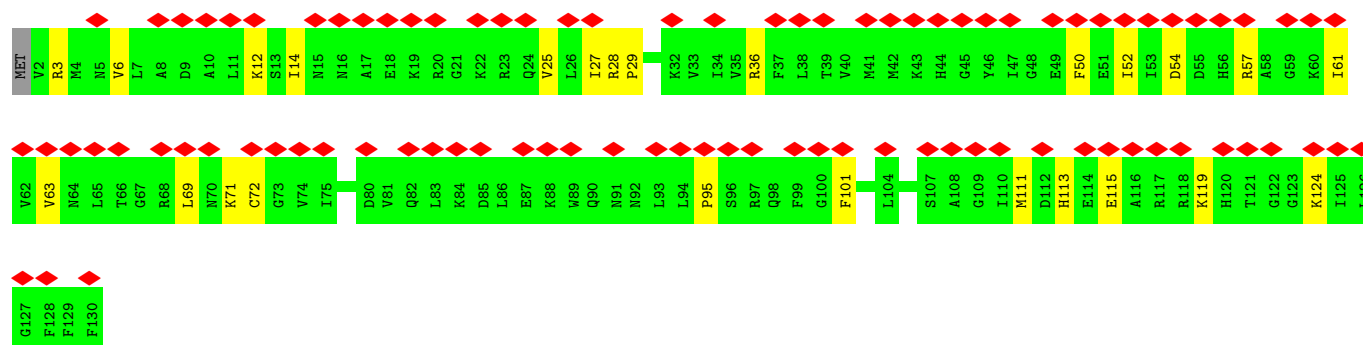
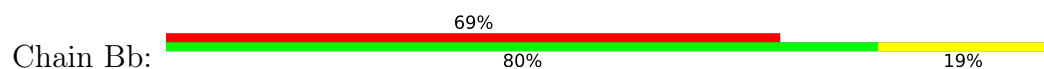




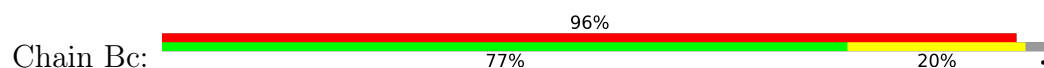
- Molecule 71: Small ribosomal subunit protein uS11

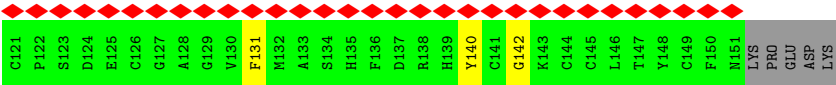


- Molecule 72: 40S ribosomal protein S15a

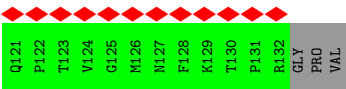
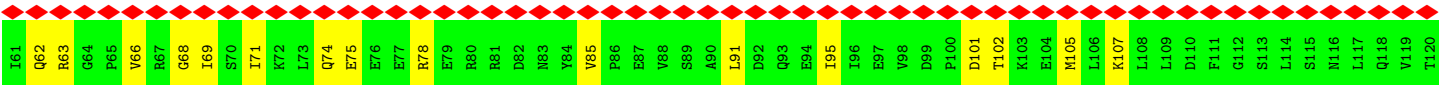
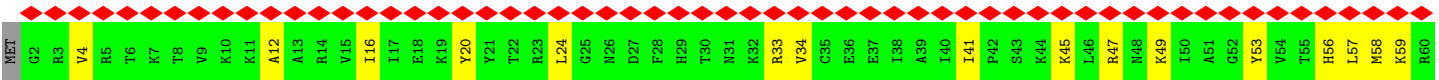
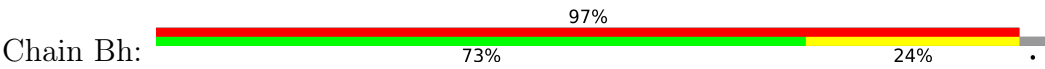


- Molecule 73: 40S ribosomal protein S24





• Molecule 78: 40S ribosomal protein S17



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30970	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	1.684	Depositor
Minimum map value	-0.777	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.14	3/86652 (0.0%)	0.27	0/135106
2	AB	0.10	0/2858	0.25	0/4455
3	AC	0.13	0/3609	0.26	0/5623
4	AD	0.12	0/1936	0.33	0/2596
5	AE	0.12	0/3294	0.34	0/4406
6	AF	0.12	0/2949	0.31	0/3960
7	AG	0.13	0/2428	0.39	0/3252
8	AH	0.14	0/1942	0.37	0/2606
9	AI	0.13	0/1916	0.30	0/2553
10	AJ	0.16	0/1971	0.44	0/2651
11	AK	0.15	0/1537	0.40	0/2066
12	AL	0.15	0/1753	0.39	0/2343
13	AM	0.15	0/1433	0.45	0/1915
14	AN	0.14	0/1732	0.35	0/2315
15	AO	0.15	0/1161	0.39	0/1554
16	AP	0.11	0/1746	0.29	0/2338
17	AQ	0.15	0/1682	0.38	0/2250
18	AR	0.15	0/1268	0.39	0/1701
19	AS	0.11	0/1537	0.29	0/2052
20	AT	0.12	0/1582	0.33	0/2091
21	AU	0.15	0/1493	0.38	0/2003
22	AV	0.16	0/1326	0.43	0/1770
23	AW	0.20	0/839	0.60	0/1126
24	AX	0.13	0/993	0.37	0/1332
25	AY	0.13	0/541	0.38	0/720
26	AZ	0.13	0/1002	0.35	0/1345
27	Aa	0.14	0/1119	0.40	0/1488
28	Ab	0.14	0/1130	0.36	0/1507
29	Ac	0.10	0/1179	0.27	0/1573
30	Ad	0.13	0/821	0.35	0/1084
31	Ae	0.18	0/774	0.50	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Af	0.12	0/894	0.34	0/1204
33	Ag	0.11	0/1071	0.29	0/1429
34	Ah	0.12	0/895	0.30	0/1198
35	Ai	0.12	0/878	0.30	0/1170
36	Aj	0.11	0/1023	0.32	0/1351
37	Ak	0.14	0/824	0.42	0/1090
38	Al	0.10	0/720	0.28	0/952
39	Am	0.13	0/565	0.36	0/750
40	An	0.14	0/454	0.28	0/599
41	Ao	0.10	0/425	0.28	0/564
42	Aq	0.14	0/858	0.38	0/1131
43	Ar	0.12	0/691	0.37	0/919
44	As	0.13	0/1002	0.35	0/1344
45	BA	0.15	2/38960 (0.0%)	0.27	2/60699 (0.0%)
46	BB	0.14	0/2118	0.36	0/2849
47	BC	0.23	0/1764	0.51	0/2396
48	BD	0.15	0/1774	0.46	0/2373
49	BE	0.15	0/1793	0.42	0/2414
50	BF	0.17	0/1531	0.49	0/2059
51	BG	0.15	0/1519	0.41	0/2033
52	BH	0.13	0/1715	0.37	0/2287
53	BI	0.15	0/840	0.41	0/1133
54	BJ	0.14	0/1280	0.39	0/1712
55	BK	0.15	0/1047	0.40	0/1399
56	BL	0.14	0/1142	0.45	0/1528
57	BM	0.16	0/1212	0.52	1/1624 (0.1%)
58	BN	0.16	0/1119	0.44	0/1498
59	BO	0.12	0/827	0.35	0/1110
60	BP	0.16	0/643	0.46	0/860
61	BQ	0.14	0/1116	0.43	0/1490
62	BR	0.14	0/847	0.37	0/1135
63	BS	0.13	0/508	0.38	0/680
64	BT	0.13	0/470	0.34	0/623
65	BU	0.16	0/2493	0.41	0/3394
66	BV	0.16	0/1764	0.44	0/2382
67	BW	0.13	0/1926	0.35	0/2563
68	BX	0.18	0/1548	0.48	0/2066
69	BY	0.14	0/916	0.38	0/1233
70	BZ	0.16	0/1232	0.41	0/1656
71	Ba	0.29	0/1020	0.61	2/1366 (0.1%)
72	Bb	0.15	0/1051	0.43	0/1406
73	Bc	0.14	0/1068	0.43	0/1418
74	Bd	0.12	0/604	0.36	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Be	0.17	0/665	0.46	0/891
76	Bf	0.15	0/465	0.39	0/612
77	Bg	0.13	0/560	0.36	0/745
78	Bh	0.18	0/1078	0.51	0/1447
All	All	0.14	5/225118 (0.0%)	0.32	5/330411 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
71	Ba	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	484	A2M	O3'-P	5.18	1.61	1.56
1	AA	2415	OMU	O3'-P	5.10	1.61	1.56
1	AA	4523	A2M	O3'-P	5.04	1.61	1.56
1	AA	3785	A2M	O3'-P	5.03	1.61	1.56
45	BA	1288	OMU	O3'-P	5.01	1.61	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	1639	G7M	OP1-P-O3'	10.17	127.57	105.20
71	Ba	140	THR	O-C-N	-8.60	112.99	122.88
45	BA	1639	G7M	O3'-P-O5'	-8.59	87.69	104.00
71	Ba	139	SER	O-C-N	-6.29	112.93	123.00
57	BM	88	LYS	CA-CB-CG	5.44	124.98	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
71	Ba	139	SER	Mainchain
71	Ba	140	THR	Mainchain
71	Ba	141	ARG	Mainchain

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	80142	0	40458	688	0
2	AB	2558	0	1296	14	0
3	AC	3316	0	1687	34	0
4	AD	1898	0	1993	25	0
5	AE	3239	0	3377	24	0
6	AF	2895	0	3076	20	0
7	AG	2382	0	2410	27	0
8	AH	1904	0	2055	13	0
9	AI	1878	0	2009	18	0
10	AJ	1935	0	2087	21	0
11	AK	1518	0	1601	20	0
12	AL	1713	0	1751	27	0
13	AM	1410	0	1441	17	0
14	AN	1701	0	1818	15	0
15	AO	1138	0	1204	12	0
16	AP	1701	0	1749	12	0
17	AQ	1650	0	1794	15	0
18	AR	1242	0	1269	11	0
19	AS	1513	0	1628	9	0
20	AT	1566	0	1729	16	0
21	AU	1453	0	1490	17	0
22	AV	1298	0	1366	14	0
23	AW	825	0	850	20	0
24	AX	979	0	1039	14	0
25	AY	528	0	541	8	0
26	AZ	985	0	1066	6	0
27	Aa	1102	0	1189	16	0
28	Ab	1107	0	1182	16	0
29	Ac	1163	0	1206	10	0
30	Ad	808	0	875	10	0
31	Ae	764	0	804	12	0
32	Af	879	0	924	9	0
33	Ag	1053	0	1147	8	0
34	Ah	876	0	911	4	0
35	Ai	868	0	959	7	0
36	Aj	1015	0	1148	21	0
37	Ak	813	0	894	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Al	705	0	737	3	0
39	Am	559	0	624	12	0
40	An	444	0	483	7	0
41	Ao	419	0	452	11	0
42	Aq	842	0	914	10	0
43	Ar	681	0	731	6	0
44	As	987	0	1050	7	0
45	BA	36808	0	18593	493	0
46	BB	2076	0	2177	40	0
47	BC	1727	0	1729	58	0
48	BD	1747	0	1822	39	0
49	BE	1765	0	1865	35	0
50	BF	1509	0	1563	38	0
51	BG	1497	0	1590	26	0
52	BH	1686	0	1772	36	0
53	BI	816	0	841	29	0
54	BJ	1258	0	1332	17	0
55	BK	1027	0	1075	30	0
56	BL	1124	0	1193	36	0
57	BM	1194	0	1250	29	0
58	BN	1113	0	1145	35	0
59	BO	817	0	882	20	0
60	BP	636	0	637	13	0
61	BQ	1098	0	1167	27	0
62	BR	829	0	883	24	0
63	BS	506	0	536	5	0
64	BT	459	0	448	11	0
65	BU	2436	0	2393	51	0
66	BV	1724	0	1817	61	0
67	BW	1903	0	2068	46	0
68	BX	1520	0	1642	51	0
69	BY	906	0	921	13	0
70	BZ	1208	0	1292	29	0
71	Ba	1016	0	1038	26	0
72	Bb	1034	0	1080	20	0
73	Bc	1048	0	1122	17	0
74	Bd	598	0	656	11	0
75	Be	651	0	672	15	0
76	Bf	459	0	503	7	0
77	Bg	548	0	549	8	0
78	Bh	1064	0	1118	26	0
79	AA	174	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	AB	2	0	0	0	0
79	AC	3	0	0	0	0
79	AE	1	0	0	0	0
79	AP	1	0	0	0	0
79	AX	1	0	0	0	0
79	Al	1	0	0	0	0
79	BA	6	0	0	0	0
80	AA	47	0	0	0	0
80	AB	1	0	0	0	0
80	AC	1	0	0	0	0
80	AD	1	0	0	0	0
80	AL	1	0	0	0	0
80	Ag	1	0	0	0	0
80	Ah	1	0	0	0	0
80	Aq	1	0	0	0	0
80	BA	2	0	0	0	0
80	BT	1	0	0	0	0
81	Ai	1	0	0	0	0
81	Al	1	0	0	0	0
81	Ao	1	0	0	0	0
81	Aq	1	0	0	0	0
81	Ar	1	0	0	0	0
81	BR	1	0	0	0	0
81	BT	1	0	0	0	0
81	Bg	1	0	0	0	0
All	All	214513	0	158385	2440	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 7.

The worst 5 of 2440 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)
45:BA:3:C:C5'	66:BV:205:VAL:HG22	1.59	1.32
45:BA:3:C:H5'	66:BV:205:VAL:CG2	1.82	1.07
45:BA:3:C:H5'	66:BV:205:VAL:HG22	1.08	1.05
45:BA:3:C:C5	68:BX:17:ARG:NH1	2.27	1.03
1:AA:4745:G:H1	1:AA:4955:A:N6	1.60	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	3701/5069 (73%)	822 (22%)	0
2	AB	119/120 (99%)	11 (9%)	0
3	AC	155/157 (98%)	27 (17%)	0
45	BA	1707/1869 (91%)	442 (25%)	0
All	All	5682/7215 (78%)	1302 (22%)	0

5 of 1302 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	G
1	AA	13	U
1	AA	25	A
1	AA	39	A
1	AA	42	A

There are no RNA pucker outliers to report.

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

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
45	PSU	BA	918	45	18,21,22	1.43	3 (16%)	22,30,33	1.88	3 (13%)
45	PSU	BA	36	45	18,21,22	1.37	2 (11%)	22,30,33	1.80	4 (18%)
1	PSU	AA	1792	1	18,21,22	1.40	2 (11%)	22,30,33	1.81	3 (13%)
1	OMU	AA	4306	1	19,22,23	1.23	4 (21%)	26,31,34	1.63	4 (15%)
1	PSU	AA	3822	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
1	OMG	AA	1625	80,1	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
45	A2M	BA	166	45	22,25,26	1.47	4 (18%)	31,36,39	2.20	8 (25%)
45	PSU	BA	649	45	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	4576	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	4 (18%)
45	OMG	BA	867	45	23,26,27	1.23	3 (13%)	33,38,41	2.06	6 (18%)
45	PSU	BA	1186	45	18,21,22	1.33	2 (11%)	22,30,33	1.83	3 (13%)
45	OMU	BA	354	45	19,22,23	1.21	3 (15%)	26,31,34	1.68	4 (15%)
1	A2M	AA	1534	79,1	22,25,26	1.47	4 (18%)	31,36,39	2.10	8 (25%)
1	A2M	AA	3718	1	22,25,26	1.48	4 (18%)	31,36,39	2.04	7 (22%)
1	PSU	AA	4579	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	AA	1582	1	18,21,22	1.39	2 (11%)	22,30,33	1.80	3 (13%)
1	PSU	AA	1536	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	296	45	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
1	OMC	AA	2804	1	19,22,23	0.82	0	26,31,34	0.79	0
1	A2M	AA	1326	1	22,25,26	1.46	4 (18%)	31,36,39	2.12	7 (22%)
1	OMC	AA	2861	1	19,22,23	0.83	0	26,31,34	1.02	2 (7%)
1	PSU	AA	3764	1	18,21,22	1.37	2 (11%)	22,30,33	1.82	3 (13%)
45	G7M	BA	1639	45	23,26,27	5.05	20 (86%)	35,39,42	1.72	7 (20%)
45	OMC	BA	462	45	19,22,23	0.81	0	26,31,34	0.76	0
1	PSU	AA	4500	1	18,21,22	1.39	2 (11%)	22,30,33	1.82	3 (13%)
45	OMG	BA	1447	45	23,26,27	1.18	3 (13%)	33,38,41	1.94	6 (18%)
1	PSU	AA	4689	1	18,21,22	1.35	2 (11%)	22,30,33	1.79	3 (13%)
1	OMC	AA	3808	1	19,22,23	0.83	0	26,31,34	0.96	1 (3%)
45	PSU	BA	1596	45	18,21,22	1.38	2 (11%)	22,30,33	1.85	4 (18%)
45	A2M	BA	99	45	22,25,26	1.46	4 (18%)	31,36,39	2.13	8 (25%)
45	PSU	BA	651	45	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	1781	1	18,21,22	1.32	2 (11%)	22,30,33	1.87	3 (13%)
45	PSU	BA	801	45	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
45	OMG	BA	1490	45	23,26,27	1.21	3 (13%)	33,38,41	1.89	6 (18%)
45	MA6	BA	1850	45	23,26,27	1.49	4 (17%)	34,38,41	2.41	12 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	A2M	BA	590	45	22,25,26	1.50	4 (18%)	31,36,39	2.25	6 (19%)
1	5MC	AA	4447	80,1	18,22,23	1.01	2 (11%)	26,32,35	1.21	2 (7%)
45	OMU	BA	121	45	19,22,23	1.18	2 (10%)	26,31,34	1.68	5 (19%)
3	PSU	AC	55	3	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
45	A2M	BA	468	45	22,25,26	1.48	4 (18%)	31,36,39	2.09	10 (32%)
1	UR3	AA	4530	1	19,22,23	1.01	1 (5%)	26,32,35	1.40	1 (3%)
45	PSU	BA	667	45	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
1	OMG	AA	4228	1	23,26,27	1.18	3 (13%)	33,38,41	1.94	6 (18%)
1	OMC	AA	1340	1	19,22,23	0.82	0	26,31,34	0.88	0
1	OMC	AA	2365	1	19,22,23	0.80	0	26,31,34	0.76	0
1	A2M	AA	3867	1	22,25,26	1.49	4 (18%)	31,36,39	2.11	7 (22%)
1	OMG	AA	4637	1	23,26,27	1.22	3 (13%)	33,38,41	1.98	6 (18%)
1	PSU	AA	1677	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	AA	2787	79,1	22,25,26	1.45	4 (18%)	31,36,39	2.20	8 (25%)
45	PSU	BA	686	45	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
45	OMC	BA	1272	45	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
45	OMU	BA	428	45	19,22,23	1.17	2 (10%)	26,31,34	1.68	5 (19%)
1	PSU	AA	1744	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	1174	45	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	AA	2815	1	22,25,26	1.47	4 (18%)	31,36,39	2.18	7 (22%)
1	UY1	AA	3818	80,1	19,22,23	4.37	7 (36%)	22,31,34	1.89	6 (27%)
45	A2M	BA	576	45	22,25,26	1.48	4 (18%)	31,36,39	2.05	9 (29%)
45	PSU	BA	1056	45	18,21,22	1.38	2 (11%)	22,30,33	1.83	4 (18%)
1	PSU	AA	5001	1	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
45	OMC	BA	517	45	19,22,23	0.85	0	26,31,34	1.17	2 (7%)
45	PSU	BA	1347	45	18,21,22	1.39	2 (11%)	22,30,33	1.81	3 (13%)
1	PSU	AA	4628	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
45	PSU	BA	93	45	18,21,22	1.32	2 (11%)	22,30,33	1.84	3 (13%)
45	A2M	BA	1383	45	22,25,26	1.48	4 (18%)	31,36,39	2.12	9 (29%)
45	PSU	BA	63	45	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
45	MA6	BA	1851	45	23,26,27	1.48	4 (17%)	34,38,41	2.39	13 (38%)
45	PSU	BA	218	45	18,21,22	1.35	2 (11%)	22,30,33	1.81	3 (13%)
45	PSU	BA	300	45	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	AA	3825	1	22,25,26	1.49	4 (18%)	31,36,39	2.07	8 (25%)
45	UY1	BA	1326	45	19,22,23	4.40	7 (36%)	22,31,34	1.85	5 (22%)

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	1.45	4 (18%)	30,36,39	2.18	9 (30%)
1	PSU	AA	4299	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	AA	4552	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	4973	1	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	34	45	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
45	PSU	BA	866	45	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
45	PSU	BA	100	45	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	AA	1862	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	AA	3695	1	18,21,22	1.33	2 (11%)	22,30,33	1.91	4 (18%)
3	OMG	AC	75	3	23,26,27	1.22	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	AA	4293	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	4 (18%)
45	PSU	BA	105	45	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
45	OMG	BA	683	45	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
45	PSU	BA	1046	45	18,21,22	1.33	2 (11%)	22,30,33	1.83	3 (13%)
1	OMG	AA	1316	1	23,26,27	1.22	3 (13%)	33,38,41	1.97	6 (18%)
1	OMC	AA	1881	79,1	19,22,23	0.81	0	26,31,34	0.93	0
1	PSU	AA	3768	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	AA	2363	79,1	22,25,26	1.46	4 (18%)	31,36,39	2.07	8 (25%)
1	OMG	AA	3744	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	5 (15%)
45	OMU	BA	1442	45	19,22,23	1.23	3 (15%)	26,31,34	1.66	5 (19%)
1	OMG	AA	1522	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	5 (15%)
1	PSU	AA	1782	1	18,21,22	1.33	2 (11%)	22,30,33	1.84	3 (13%)
45	PSU	BA	1625	45	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	AA	1871	79,1	22,25,26	1.45	4 (18%)	31,36,39	2.17	9 (29%)
1	PSU	AA	3762	1	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
45	PSU	BA	1136	45	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	AA	3730	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	4532	1	18,21,22	1.38	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	609	45	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
45	PSU	BA	1445	45	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	AA	3884	1	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	AA	4423	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	AA	2824	1	19,22,23	0.82	0	26,31,34	0.88	1 (3%)
45	PSU	BA	1177	45	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
45	PSU	BA	1232	45	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	B8N	BA	1248	45	24,29,30	0.92	1 (4%)	29,42,45	1.36	4 (13%)
1	PSU	AA	2632	1	18,21,22	1.37	2 (11%)	22,30,33	1.81	3 (13%)
1	OMC	AA	3701	80,1	19,22,23	0.79	0	26,31,34	0.75	0
1	PSU	AA	3770	1	18,21,22	1.38	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	AA	4521	79,1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
45	OMG	BA	436	45	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
1	1MA	AA	1322	79,1	21,25,26	1.37	4 (19%)	31,37,40	1.69	6 (19%)
45	A2M	BA	159	45	22,25,26	1.47	4 (18%)	31,36,39	2.10	7 (22%)
1	A2M	AA	1524	1	22,25,26	1.47	4 (18%)	31,36,39	2.13	9 (29%)
1	OMC	AA	3841	1	19,22,23	0.80	0	26,31,34	0.74	0
1	PSU	AA	1779	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	3637	80,1	18,21,22	1.41	3 (16%)	22,30,33	1.95	4 (18%)
45	OMU	BA	116	45	19,22,23	1.20	3 (15%)	26,31,34	1.63	4 (15%)
1	OMC	AA	2422	79,1	19,22,23	0.81	0	26,31,34	0.78	0
45	OMU	BA	1288	45	19,22,23	1.20	2 (10%)	26,31,34	1.62	5 (19%)
45	PSU	BA	109	45	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
58	NMM	BN	67	58	9,11,12	1.71	1 (11%)	6,12,14	1.08	1 (16%)
1	PSU	AA	4431	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	3844	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	AA	4536	1	19,22,23	0.83	0	26,31,34	0.90	1 (3%)
1	OMG	AA	4623	1	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
45	6MZ	BA	1832	45	22,25,26	1.46	4 (18%)	30,36,39	2.15	9 (30%)
45	PSU	BA	1004	45	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	366	45	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	AA	4590	1	22,25,26	1.47	4 (18%)	31,36,39	2.09	8 (25%)
1	OMG	AA	3792	1	23,26,27	1.22	3 (13%)	33,38,41	1.97	6 (18%)
1	OMG	AA	4196	1	23,26,27	1.22	3 (13%)	33,38,41	1.99	6 (18%)
1	OMC	AA	2351	79,1	19,22,23	0.86	0	26,31,34	1.33	4 (15%)
45	OMG	BA	601	45	23,26,27	1.24	3 (13%)	33,38,41	1.97	6 (18%)
1	OMU	AA	2837	1	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
1	OMG	AA	4392	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	5 (15%)
45	A2M	BA	484	45	22,25,26	1.48	4 (18%)	31,36,39	2.11	8 (25%)
1	OMG	AA	3899	79,1	23,26,27	1.20	3 (13%)	33,38,41	1.93	5 (15%)
1	PSU	AA	4353	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	AA	3724	1	22,25,26	1.47	4 (18%)	31,36,39	2.08	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	AA	2508	1	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	AA	1860	1	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	AA	4493	80,1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
45	PSU	BA	1045	45	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
45	OMG	BA	644	45	23,26,27	1.20	3 (13%)	33,38,41	1.89	6 (18%)
1	PSU	AA	4457	1	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)
45	OMG	BA	1328	45	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	AA	1683	1	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
45	PSU	BA	1367	45	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
45	PSU	BA	1643	45	18,21,22	1.32	2 (11%)	22,30,33	1.90	4 (18%)
45	A2M	BA	1678	45	22,25,26	1.47	4 (18%)	31,36,39	2.16	9 (29%)
45	OMG	BA	509	45	23,26,27	1.17	3 (13%)	33,38,41	1.97	6 (18%)
45	PSU	BA	966	45	18,21,22	1.33	2 (11%)	22,30,33	1.84	3 (13%)
45	PSU	BA	1003	45	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
45	PSU	BA	681	45	18,21,22	1.36	2 (11%)	22,30,33	1.81	3 (13%)
45	OMC	BA	1703	45	19,22,23	0.80	0	26,31,34	0.74	0
1	OMC	AA	3887	1	19,22,23	0.83	0	26,31,34	0.92	1 (3%)
1	A2M	AA	4523	79,1	22,25,26	1.45	4 (18%)	31,36,39	2.19	10 (32%)
45	A2M	BA	1031	45	22,25,26	1.47	4 (18%)	31,36,39	2.07	8 (25%)
1	PSU	AA	4636	1	18,21,22	1.35	2 (11%)	22,30,33	1.95	5 (22%)
1	A2M	AA	3830	1	22,25,26	1.46	4 (18%)	31,36,39	2.16	8 (25%)
1	PSU	AA	5010	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	AA	3853	79,1	18,21,22	1.38	2 (11%)	22,30,33	1.81	3 (13%)
45	PSU	BA	119	45	18,21,22	1.32	2 (11%)	22,30,33	1.81	3 (13%)
1	OMG	AA	4370	1	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
45	A2M	BA	668	45	22,25,26	1.47	4 (18%)	31,36,39	2.19	9 (29%)
1	PSU	AA	4673	80,1	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
3	PSU	AC	69	3	18,21,22	1.36	2 (11%)	22,30,33	1.86	4 (18%)
1	PSU	AA	3920	79,1	18,21,22	1.35	2 (11%)	22,30,33	1.89	4 (18%)
1	A2M	AA	4571	1	22,25,26	1.46	4 (18%)	31,36,39	2.15	9 (29%)
1	OMG	AA	4499	1	23,26,27	1.21	3 (13%)	33,38,41	1.97	6 (18%)
1	OMG	AA	2424	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
45	OMU	BA	172	45	19,22,23	1.19	2 (10%)	26,31,34	1.72	4 (15%)
1	A2M	AA	400	1	22,25,26	1.46	4 (18%)	31,36,39	2.10	10 (32%)
1	PSU	AA	3715	79,1	18,21,22	1.36	2 (11%)	22,30,33	1.82	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	AA	3639	1	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
45	A2M	BA	512	45	22,25,26	1.47	4 (18%)	31,36,39	2.19	9 (29%)
45	PSU	BA	572	45	18,21,22	1.34	2 (11%)	22,30,33	1.83	4 (18%)
1	PSU	AA	4442	1	18,21,22	1.37	2 (11%)	22,30,33	1.91	4 (18%)
45	PSU	BA	1360	45	18,21,22	1.35	2 (11%)	22,30,33	1.84	4 (18%)
1	A2M	AA	1323	1	22,25,26	1.48	4 (18%)	31,36,39	2.08	8 (25%)
1	PSU	AA	3851	1	18,21,22	1.38	2 (11%)	22,30,33	1.84	3 (13%)
71	IAS	Ba	138	71	6,7,8	1.10	0	6,8,10	1.45	0
1	A2M	AA	398	1	22,25,26	1.47	4 (18%)	31,36,39	2.22	10 (32%)
1	OMU	AA	4620	1	19,22,23	1.24	4 (21%)	26,31,34	1.67	4 (15%)
1	OMG	AA	2364	1	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
1	OMC	AA	4456	1	19,22,23	0.83	0	26,31,34	1.04	2 (7%)
45	OMC	BA	1391	45	19,22,23	0.82	0	26,31,34	0.85	1 (3%)
45	PSU	BA	863	45	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
45	PSU	BA	814	45	18,21,22	1.38	3 (16%)	22,30,33	1.92	4 (18%)
1	OMU	AA	3925	1	19,22,23	1.22	2 (10%)	26,31,34	1.69	4 (15%)
1	PSU	AA	2839	1	18,21,22	1.35	2 (11%)	22,30,33	1.81	3 (13%)
1	OMC	AA	3869	1	19,22,23	0.81	0	26,31,34	0.76	0
45	4AC	BA	1337	45	21,24,25	1.08	1 (4%)	29,34,37	1.53	5 (17%)
45	PSU	BA	1238	45	18,21,22	1.32	2 (11%)	22,30,33	1.78	3 (13%)
1	PSU	AA	4312	1	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
5	HIC	AE	245	5	10,11,12	0.50	0	8,14,16	0.55	0
1	5MC	AA	3782	79,1	18,22,23	0.97	2 (11%)	26,32,35	1.20	3 (11%)
1	PSU	AA	2843	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
45	4AC	BA	1842	45	21,24,25	1.09	1 (4%)	29,34,37	1.52	5 (17%)
1	OMG	AA	3627	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
45	A2M	BA	27	45	22,25,26	1.50	4 (18%)	31,36,39	2.04	7 (22%)
45	OMU	BA	1804	45	19,22,23	1.25	4 (21%)	26,31,34	1.68	5 (19%)
1	PSU	AA	4471	1	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	406	45	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	1692	45	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	AA	2401	1	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
1	A2M	AA	3785	1	22,25,26	1.42	4 (18%)	31,36,39	2.25	11 (35%)
1	OMG	AA	4618	1	23,26,27	1.18	3 (13%)	33,38,41	1.99	6 (18%)
45	OMC	BA	174	45	19,22,23	0.81	0	26,31,34	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	AA	2415	1	19,22,23	1.23	3 (15%)	26,31,34	1.67	5 (19%)
1	OMU	AA	4227	1	19,22,23	1.25	3 (15%)	26,31,34	1.72	4 (15%)
1	PSU	AA	4403	1	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
1	OMG	AA	2876	1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	AA	4296	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
1	PSU	AA	4361	1	18,21,22	1.34	2 (11%)	22,30,33	1.83	3 (13%)
29	V5N	Ac	39	29	9,11,12	0.81	0	9,14,16	1.42	2 (22%)
45	PSU	BA	822	45	18,21,22	1.34	2 (11%)	22,30,33	1.87	4 (18%)
1	OMU	AA	4498	1	19,22,23	1.21	2 (10%)	26,31,34	1.69	5 (19%)
45	PSU	BA	815	45	18,21,22	1.38	2 (11%)	22,30,33	1.87	4 (18%)
3	OMU	AC	14	1,3	19,22,23	1.25	4 (21%)	26,31,34	1.80	5 (19%)
1	PSU	AA	4972	1	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
1	OMG	AA	4494	1	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
45	PSU	BA	1244	45	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)

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
45	PSU	BA	918	45	-	2/7/25/26	0/2/2/2
45	PSU	BA	36	45	-	1/7/25/26	0/2/2/2
1	PSU	AA	1792	1	-	2/7/25/26	0/2/2/2
1	OMU	AA	4306	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	3822	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	1625	80,1	-	2/9/27/28	0/3/3/3
45	A2M	BA	166	45	-	2/9/27/28	0/3/3/3
45	PSU	BA	649	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	4576	1	-	0/7/25/26	0/2/2/2
45	OMG	BA	867	45	-	3/9/27/28	0/3/3/3
45	PSU	BA	1186	45	-	0/7/25/26	0/2/2/2
45	OMU	BA	354	45	-	1/9/27/28	0/2/2/2
1	A2M	AA	1534	79,1	-	1/9/27/28	0/3/3/3
1	A2M	AA	3718	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4579	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	1582	1	-	3/7/25/26	0/2/2/2
1	PSU	AA	1536	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PSU	BA	296	45	-	0/7/25/26	0/2/2/2
1	OMC	AA	2804	1	-	0/9/27/28	0/2/2/2
1	A2M	AA	1326	1	-	3/9/27/28	0/3/3/3
1	OMC	AA	2861	1	-	1/9/27/28	0/2/2/2
1	PSU	AA	3764	1	-	2/7/25/26	0/2/2/2
45	G7M	BA	1639	45	-	0/7/25/26	0/3/3/3
45	OMC	BA	462	45	-	2/9/27/28	0/2/2/2
1	PSU	AA	4500	1	-	3/7/25/26	0/2/2/2
45	OMG	BA	1447	45	-	1/9/27/28	0/3/3/3
1	PSU	AA	4689	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	3808	1	-	0/9/27/28	0/2/2/2
45	PSU	BA	1596	45	-	2/7/25/26	0/2/2/2
45	A2M	BA	99	45	-	2/9/27/28	0/3/3/3
45	PSU	BA	651	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1781	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	801	45	-	0/7/25/26	0/2/2/2
45	OMG	BA	1490	45	-	3/9/27/28	0/3/3/3
45	MA6	BA	1850	45	-	7/11/29/30	0/3/3/3
45	A2M	BA	590	45	-	3/9/27/28	0/3/3/3
1	5MC	AA	4447	80,1	-	4/7/25/26	0/2/2/2
45	OMU	BA	121	45	-	0/9/27/28	0/2/2/2
3	PSU	AC	55	3	-	0/7/25/26	0/2/2/2
45	A2M	BA	468	45	-	2/9/27/28	0/3/3/3
1	UR3	AA	4530	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	667	45	-	1/7/25/26	0/2/2/2
1	OMG	AA	4228	1	-	0/9/27/28	0/3/3/3
1	OMC	AA	1340	1	-	0/9/27/28	0/2/2/2
1	OMC	AA	2365	1	-	0/9/27/28	0/2/2/2
1	A2M	AA	3867	1	-	1/9/27/28	0/3/3/3
1	OMG	AA	4637	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	1677	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	2787	79,1	-	3/9/27/28	0/3/3/3
45	PSU	BA	686	45	-	0/7/25/26	0/2/2/2
45	OMC	BA	1272	45	-	0/9/27/28	0/2/2/2
45	OMU	BA	428	45	-	7/9/27/28	0/2/2/2
1	PSU	AA	1744	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1174	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	2815	1	-	0/9/27/28	0/3/3/3
1	UY1	AA	3818	80,1	-	3/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	A2M	BA	576	45	-	2/9/27/28	0/3/3/3
45	PSU	BA	1056	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	5001	1	-	0/7/25/26	0/2/2/2
45	OMC	BA	517	45	-	7/9/27/28	0/2/2/2
45	PSU	BA	1347	45	-	2/7/25/26	0/2/2/2
1	PSU	AA	4628	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	93	45	-	3/7/25/26	0/2/2/2
45	A2M	BA	1383	45	-	0/9/27/28	0/3/3/3
45	PSU	BA	63	45	-	0/7/25/26	0/2/2/2
45	MA6	BA	1851	45	-	4/11/29/30	0/3/3/3
45	PSU	BA	218	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	300	45	-	2/7/25/26	0/2/2/2
1	A2M	AA	3825	1	-	0/9/27/28	0/3/3/3
45	UY1	BA	1326	45	-	1/9/27/28	0/2/2/2
1	6MZ	AA	4220	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4299	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4552	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4973	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	34	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	866	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	100	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1862	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3695	1	-	0/7/25/26	0/2/2/2
3	OMG	AC	75	3	-	0/9/27/28	0/3/3/3
1	PSU	AA	4293	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	105	45	-	0/7/25/26	0/2/2/2
45	OMG	BA	683	45	-	0/9/27/28	0/3/3/3
45	PSU	BA	1046	45	-	0/7/25/26	0/2/2/2
1	OMG	AA	1316	1	-	0/9/27/28	0/3/3/3
1	OMC	AA	1881	79,1	-	2/9/27/28	0/2/2/2
1	PSU	AA	3768	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	2363	79,1	-	0/9/27/28	0/3/3/3
1	OMG	AA	3744	1	-	0/9/27/28	0/3/3/3
45	OMU	BA	1442	45	-	1/9/27/28	0/2/2/2
1	OMG	AA	1522	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	1782	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1625	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	1871	79,1	-	0/9/27/28	0/3/3/3
1	PSU	AA	3762	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1136	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	3730	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	4532	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	609	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	1445	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	3884	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4423	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	2824	1	-	0/9/27/28	0/2/2/2
45	PSU	BA	1177	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	1232	45	-	4/7/25/26	0/2/2/2
45	B8N	BA	1248	45	-	6/16/34/35	0/2/2/2
1	PSU	AA	2632	1	-	1/7/25/26	0/2/2/2
1	OMC	AA	3701	80,1	-	4/9/27/28	0/2/2/2
1	PSU	AA	3770	1	-	2/7/25/26	0/2/2/2
1	PSU	AA	4521	79,1	-	0/7/25/26	0/2/2/2
45	OMG	BA	436	45	-	2/9/27/28	0/3/3/3
1	1MA	AA	1322	79,1	-	0/7/25/26	0/3/3/3
45	A2M	BA	159	45	-	0/9/27/28	0/3/3/3
1	A2M	AA	1524	1	-	1/9/27/28	0/3/3/3
1	OMC	AA	3841	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	1779	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3637	80,1	-	0/7/25/26	0/2/2/2
45	OMU	BA	116	45	-	0/9/27/28	0/2/2/2
1	OMC	AA	2422	79,1	-	1/9/27/28	0/2/2/2
45	OMU	BA	1288	45	-	0/9/27/28	0/2/2/2
45	PSU	BA	109	45	-	0/7/25/26	0/2/2/2
58	NMM	BN	67	58	-	4/9/11/13	-
1	PSU	AA	4431	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3844	1	-	3/7/25/26	0/2/2/2
1	OMC	AA	4536	1	-	0/9/27/28	0/2/2/2
1	OMG	AA	4623	1	-	2/9/27/28	0/3/3/3
45	6MZ	BA	1832	45	-	0/9/27/28	0/3/3/3
45	PSU	BA	1004	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	366	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	4590	1	-	2/9/27/28	0/3/3/3
1	OMG	AA	3792	1	-	0/9/27/28	0/3/3/3
1	OMG	AA	4196	1	-	0/9/27/28	0/3/3/3
1	OMC	AA	2351	79,1	-	3/9/27/28	0/2/2/2
45	OMG	BA	601	45	-	2/9/27/28	0/3/3/3
1	OMU	AA	2837	1	-	1/9/27/28	0/2/2/2
1	OMG	AA	4392	1	-	0/9/27/28	0/3/3/3
45	A2M	BA	484	45	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	AA	3899	79,1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4353	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	3724	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	2508	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	1860	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4493	80,1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1045	45	-	2/7/25/26	0/2/2/2
45	OMG	BA	644	45	-	1/9/27/28	0/3/3/3
1	PSU	AA	4457	1	-	0/7/25/26	0/2/2/2
45	OMG	BA	1328	45	-	0/9/27/28	0/3/3/3
1	PSU	AA	1683	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1367	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	1643	45	-	0/7/25/26	0/2/2/2
45	A2M	BA	1678	45	-	0/9/27/28	0/3/3/3
45	OMG	BA	509	45	-	0/9/27/28	0/3/3/3
45	PSU	BA	966	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	1003	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	681	45	-	0/7/25/26	0/2/2/2
45	OMC	BA	1703	45	-	1/9/27/28	0/2/2/2
1	OMC	AA	3887	1	-	1/9/27/28	0/2/2/2
1	A2M	AA	4523	79,1	-	2/9/27/28	0/3/3/3
45	A2M	BA	1031	45	-	0/9/27/28	0/3/3/3
1	PSU	AA	4636	1	-	5/7/25/26	0/2/2/2
1	A2M	AA	3830	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	5010	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3853	79,1	-	0/7/25/26	0/2/2/2
45	PSU	BA	119	45	-	0/7/25/26	0/2/2/2
1	OMG	AA	4370	1	-	0/9/27/28	0/3/3/3
45	A2M	BA	668	45	-	6/9/27/28	0/3/3/3
1	PSU	AA	4673	80,1	-	0/7/25/26	0/2/2/2
3	PSU	AC	69	3	-	0/7/25/26	0/2/2/2
1	PSU	AA	3920	79,1	-	0/7/25/26	0/2/2/2
1	A2M	AA	4571	1	-	0/9/27/28	0/3/3/3
1	OMG	AA	4499	1	-	0/9/27/28	0/3/3/3
1	OMG	AA	2424	1	-	0/9/27/28	0/3/3/3
45	OMU	BA	172	45	-	0/9/27/28	0/2/2/2
1	A2M	AA	400	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	3715	79,1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3639	1	-	0/7/25/26	0/2/2/2
45	A2M	BA	512	45	-	1/9/27/28	0/3/3/3
45	PSU	BA	572	45	-	1/7/25/26	0/2/2/2

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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
45	PSU	BA	1360	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	1323	1	-	2/9/27/28	0/3/3/3
1	PSU	AA	3851	1	-	0/7/25/26	0/2/2/2
71	IAS	Ba	138	71	-	3/7/7/8	-
1	A2M	AA	398	1	-	2/9/27/28	0/3/3/3
1	OMU	AA	4620	1	-	0/9/27/28	0/2/2/2
1	OMG	AA	2364	1	-	2/9/27/28	0/3/3/3
1	OMC	AA	4456	1	-	1/9/27/28	0/2/2/2
45	OMC	BA	1391	45	-	2/9/27/28	0/2/2/2
45	PSU	BA	863	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	814	45	-	4/7/25/26	0/2/2/2
1	OMU	AA	3925	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	3869	1	-	0/9/27/28	0/2/2/2
45	4AC	BA	1337	45	-	3/11/29/30	0/2/2/2
45	PSU	BA	1238	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	4312	1	-	0/7/25/26	0/2/2/2
5	HIC	AE	245	5	-	0/5/6/8	0/1/1/1
1	5MC	AA	3782	79,1	-	0/7/25/26	0/2/2/2
1	PSU	AA	2843	1	-	0/7/25/26	0/2/2/2
45	4AC	BA	1842	45	-	0/11/29/30	0/2/2/2
1	OMG	AA	3627	1	-	0/9/27/28	0/3/3/3
45	A2M	BA	27	45	-	0/9/27/28	0/3/3/3
45	OMU	BA	1804	45	-	2/9/27/28	0/2/2/2
1	PSU	AA	4471	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	406	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	1692	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	2401	1	-	0/9/27/28	0/3/3/3
1	A2M	AA	3785	1	-	2/9/27/28	0/3/3/3
1	OMG	AA	4618	1	-	1/9/27/28	0/3/3/3
45	OMC	BA	174	45	-	0/9/27/28	0/2/2/2
1	OMU	AA	2415	1	-	0/9/27/28	0/2/2/2
1	OMU	AA	4227	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	4403	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	2876	1	-	1/9/27/28	0/3/3/3
1	PSU	AA	4296	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4361	1	-	0/7/25/26	0/2/2/2
29	V5N	Ac	39	29	-	0/9/10/12	0/1/1/1
45	PSU	BA	822	45	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	AA	4498	1	-	0/9/27/28	0/2/2/2
45	PSU	BA	815	45	-	3/7/25/26	0/2/2/2
3	OMU	AC	14	1,3	-	0/9/27/28	0/2/2/2
1	PSU	AA	4972	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	4494	1	-	0/9/27/28	0/3/3/3
45	PSU	BA	1244	45	-	0/7/25/26	0/2/2/2

The worst 5 of 545 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	1326	UY1	C6-C5	11.84	1.49	1.35
1	AA	3818	UY1	C6-C5	11.74	1.49	1.35
45	BA	1639	G7M	C8-N7	10.61	1.52	1.33
45	BA	1639	G7M	C2'-C3'	-10.54	1.24	1.53
45	BA	1326	UY1	C2-N1	9.59	1.49	1.36

The worst 5 of 968 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	590	A2M	C5-C4-N3	-7.25	117.29	126.75
45	BA	867	OMG	C5-C4-N3	-6.93	117.22	128.46
1	AA	2815	A2M	C5-C4-N3	-6.91	117.73	126.75
1	AA	3867	A2M	C5-C4-N3	-6.69	118.03	126.75
45	BA	484	A2M	C5-C4-N3	-6.54	118.21	126.75

There are no chirality outliers.

5 of 182 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BN	67	NMM	C-CA-CB-CG
58	BN	67	NMM	N-CA-CB-CG
58	BN	67	NMM	O-C-CA-CB
1	AA	1582	PSU	C2'-C1'-C5-C4
1	AA	1582	PSU	O4'-C1'-C5-C4

There are no ring outliers.

94 monomers are involved in 128 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	BA	649	PSU	3	0
45	BA	867	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	BA	354	OMU	1	0
1	AA	3718	A2M	3	0
1	AA	4579	PSU	2	0
1	AA	2804	OMC	1	0
1	AA	2861	OMC	1	0
45	BA	462	OMC	1	0
1	AA	4500	PSU	1	0
45	BA	1447	OMG	1	0
1	AA	4689	PSU	1	0
45	BA	99	A2M	1	0
45	BA	801	PSU	1	0
45	BA	1850	MA6	3	0
1	AA	4447	5MC	1	0
45	BA	121	OMU	2	0
45	BA	468	A2M	1	0
1	AA	4228	OMG	1	0
1	AA	1340	OMC	1	0
1	AA	3867	A2M	1	0
45	BA	1272	OMC	2	0
45	BA	1174	PSU	2	0
1	AA	2815	A2M	1	0
45	BA	576	A2M	2	0
45	BA	1056	PSU	1	0
1	AA	5001	PSU	1	0
45	BA	517	OMC	1	0
45	BA	93	PSU	1	0
45	BA	1383	A2M	1	0
1	AA	3825	A2M	1	0
1	AA	4220	6MZ	1	0
1	AA	4552	PSU	2	0
45	BA	100	PSU	1	0
1	AA	1316	OMG	2	0
1	AA	3768	PSU	1	0
1	AA	2363	A2M	1	0
45	BA	1442	OMU	1	0
45	BA	1625	PSU	1	0
1	AA	1871	A2M	2	0
1	AA	4532	PSU	1	0
45	BA	609	PSU	1	0
1	AA	2824	OMC	1	0
45	BA	436	OMG	1	0
45	BA	159	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	BA	116	OMU	3	0
45	BA	1288	OMU	1	0
45	BA	109	PSU	1	0
1	AA	3844	PSU	1	0
1	AA	4536	OMC	1	0
45	BA	1832	6MZ	1	0
45	BA	1004	PSU	2	0
1	AA	3792	OMG	1	0
1	AA	2351	OMC	1	0
45	BA	601	OMG	4	0
1	AA	4392	OMG	2	0
45	BA	484	A2M	1	0
45	BA	644	OMG	2	0
1	AA	4457	PSU	1	0
45	BA	1328	OMG	2	0
1	AA	1683	PSU	2	0
45	BA	1643	PSU	1	0
45	BA	1678	A2M	2	0
45	BA	509	OMG	3	0
45	BA	1703	OMC	1	0
1	AA	3887	OMC	1	0
1	AA	4523	A2M	1	0
45	BA	1031	A2M	1	0
1	AA	4636	PSU	1	0
1	AA	3830	A2M	1	0
45	BA	119	PSU	1	0
45	BA	668	A2M	4	0
3	AC	69	PSU	1	0
1	AA	4499	OMG	1	0
1	AA	2424	OMG	1	0
45	BA	512	A2M	3	0
45	BA	1360	PSU	1	0
71	Ba	138	IAS	2	0
1	AA	398	A2M	1	0
1	AA	4620	OMU	1	0
1	AA	4456	OMC	2	0
1	AA	3925	OMU	1	0
1	AA	2839	PSU	1	0
45	BA	1238	PSU	3	0
45	BA	1842	4AC	1	0
45	BA	27	A2M	2	0
45	BA	1804	OMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	BA	1692	PSU	1	0
1	AA	3785	A2M	1	0
1	AA	4618	OMG	1	0
1	AA	2415	OMU	1	0
1	AA	4227	OMU	1	0
1	AA	4403	PSU	1	0
3	AC	14	OMU	1	0
45	BA	1244	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 254 ligands modelled in this entry, 254 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.

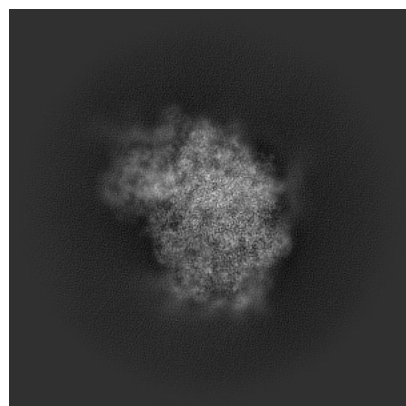
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66299. These allow visual inspection of the internal detail of the map and identification of artifacts.

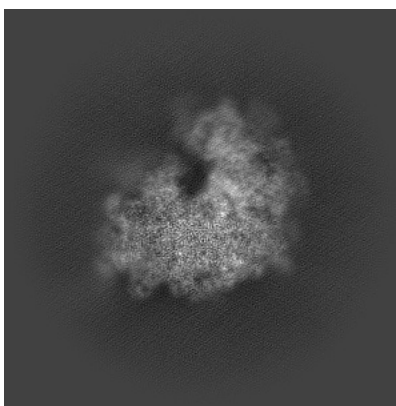
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

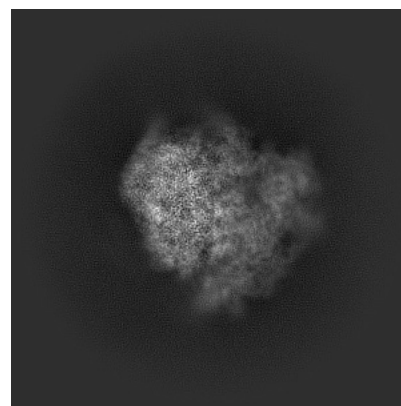
6.1.1 Primary map



X

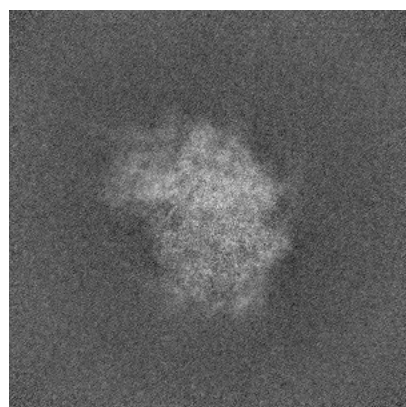


Y

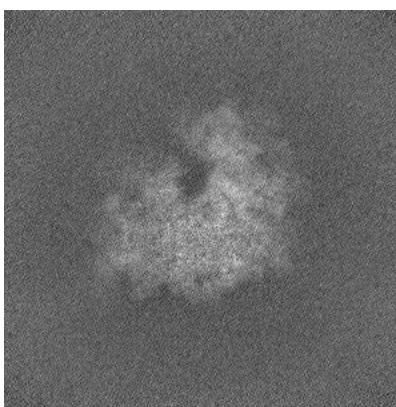


Z

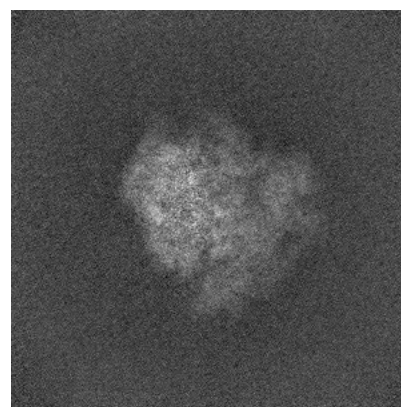
6.1.2 Raw map



X



Y

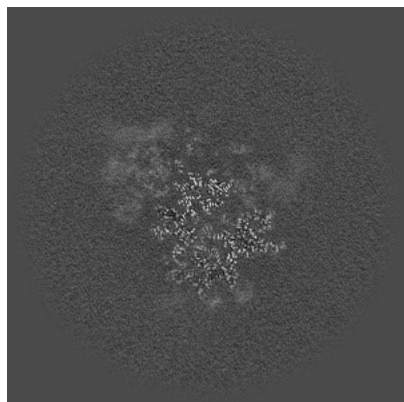


Z

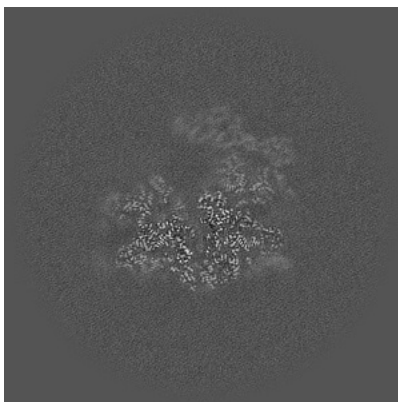
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

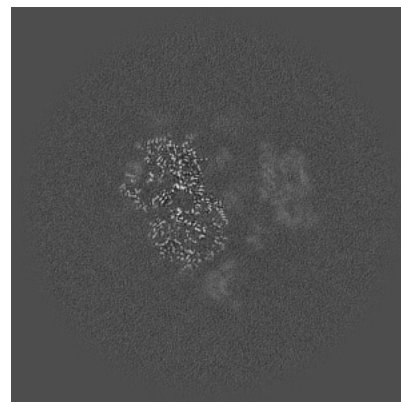
6.2.1 Primary map



X Index: 320

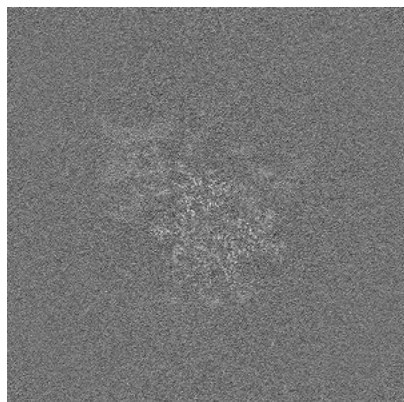


Y Index: 320

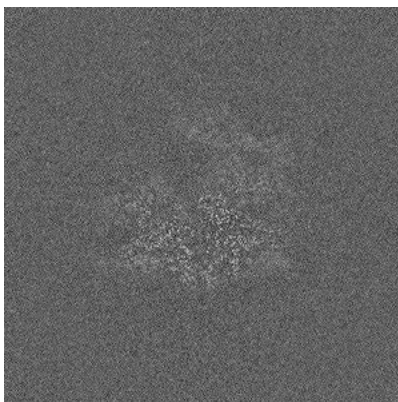


Z Index: 320

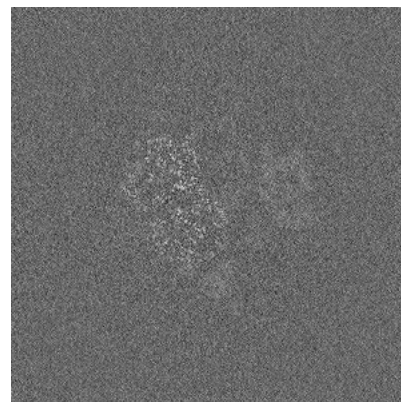
6.2.2 Raw map



X Index: 320



Y Index: 320

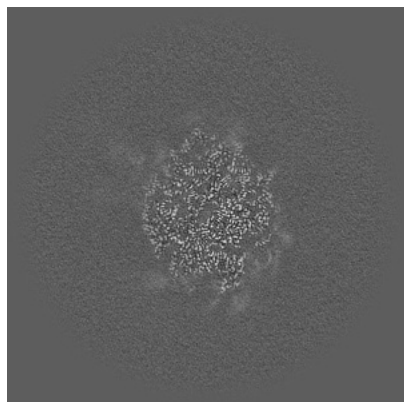


Z Index: 320

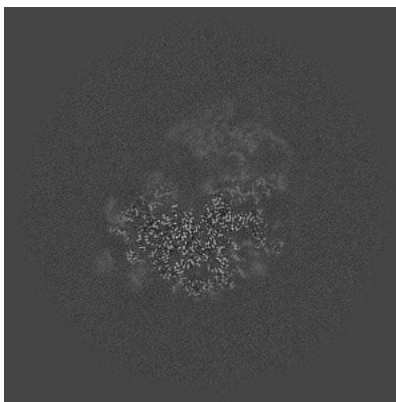
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

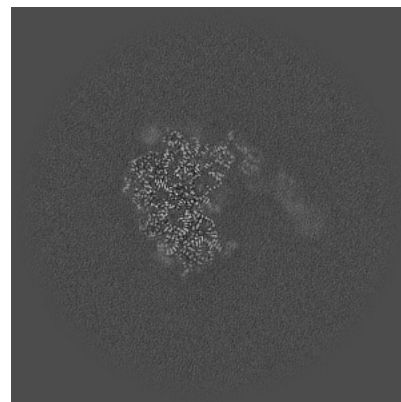
6.3.1 Primary map



X Index: 287

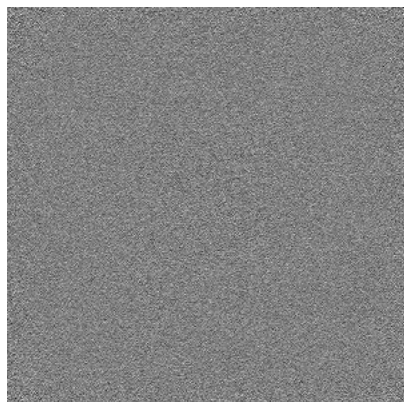


Y Index: 338

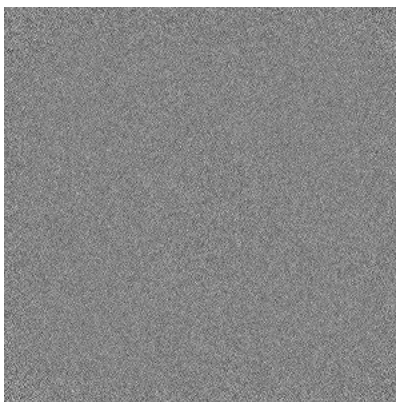


Z Index: 282

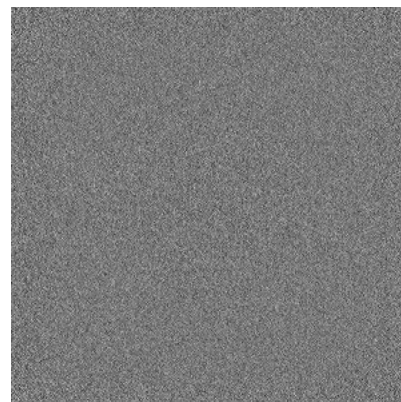
6.3.2 Raw map



X Index: 0



Y Index: 0

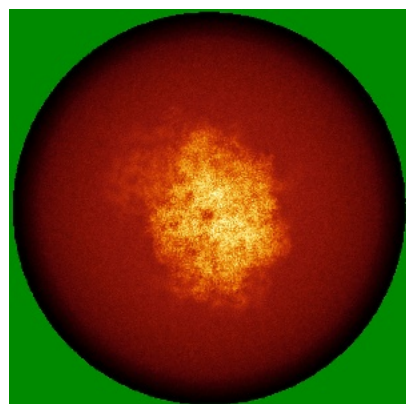


Z Index: 0

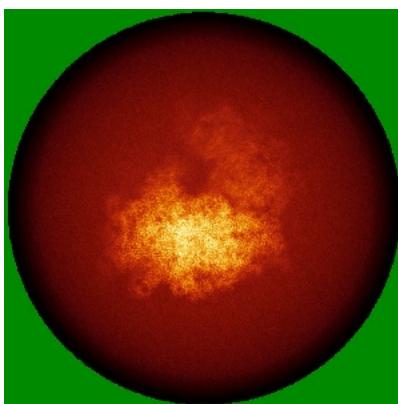
The images above show the largest variance slices of the map in three orthogonal directions.

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

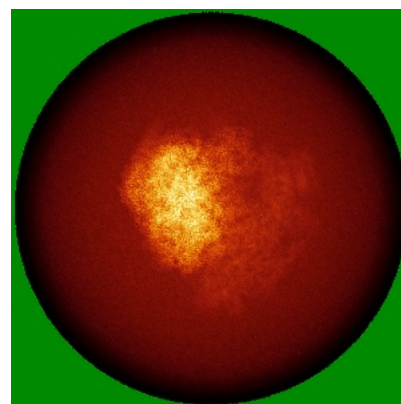
6.4.1 Primary map



X

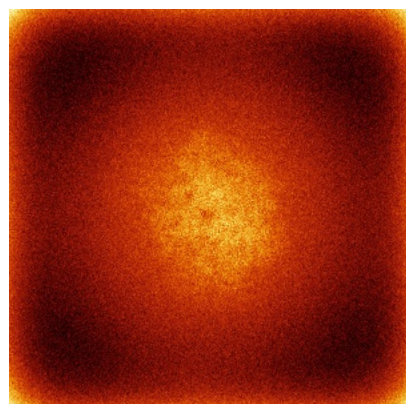


Y

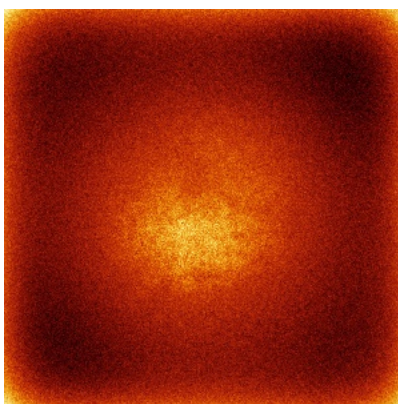


Z

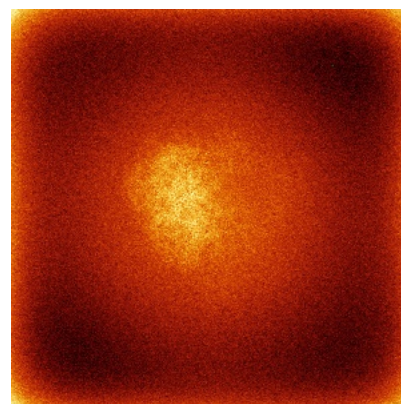
6.4.2 Raw map



X



Y

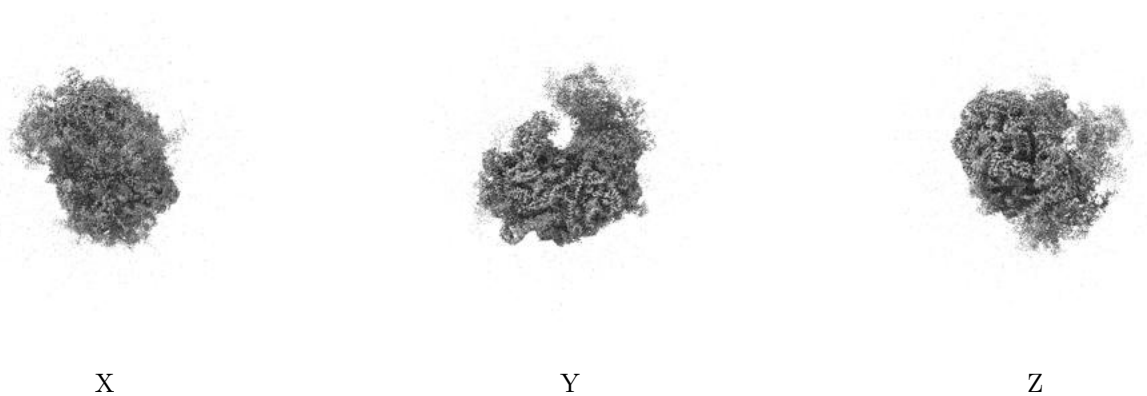


Z

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.

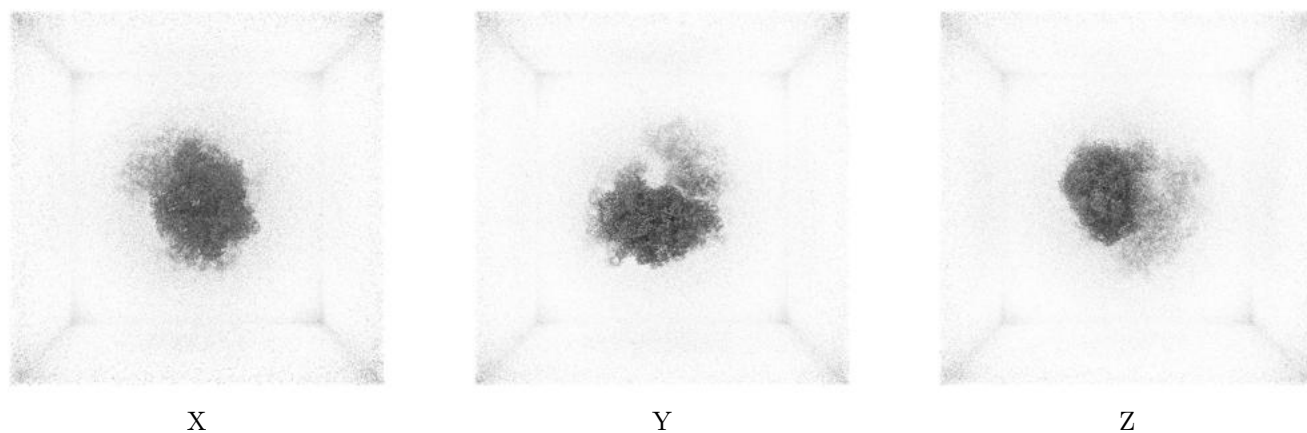
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. 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.

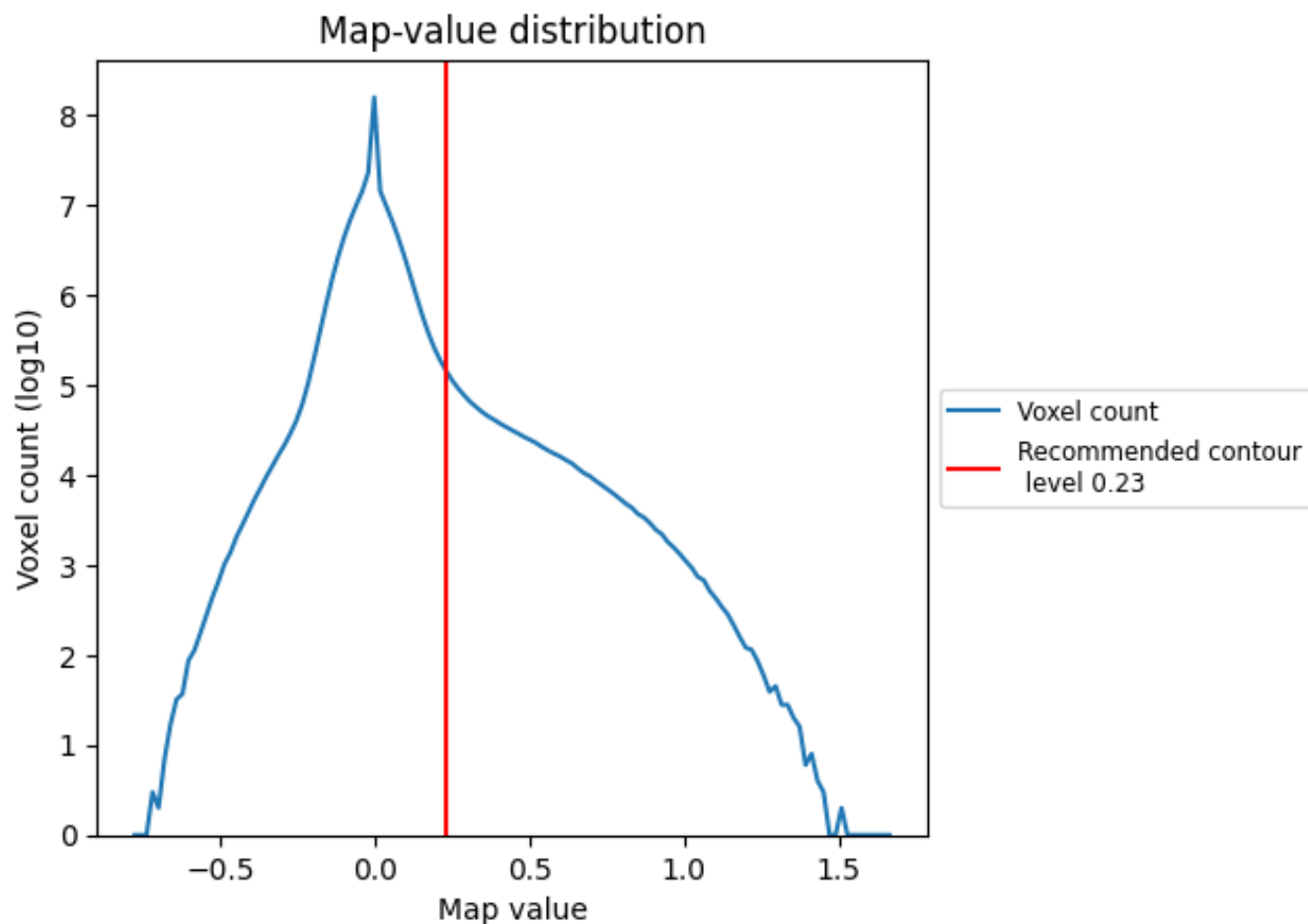
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

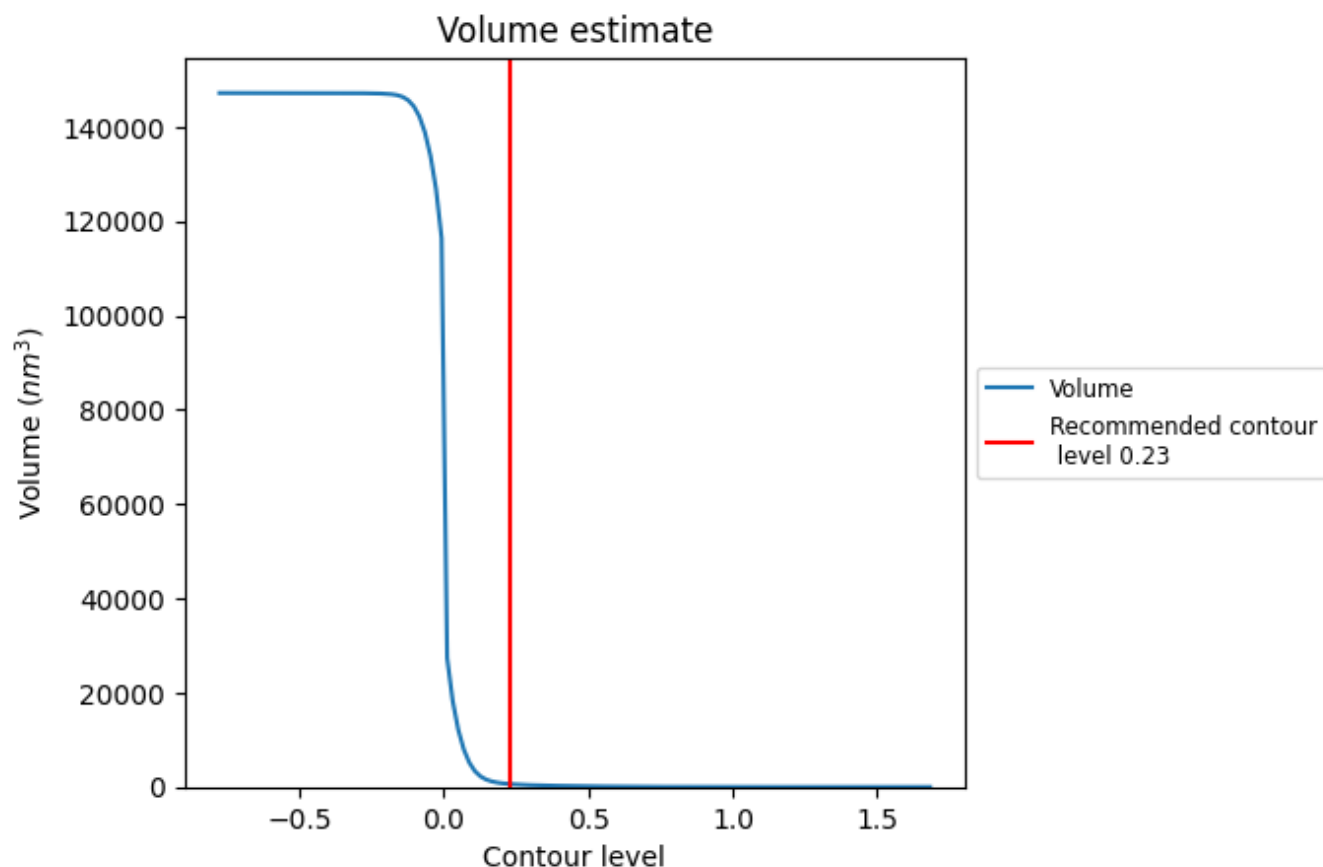
This section contains the results of statistical analysis of the map.

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.

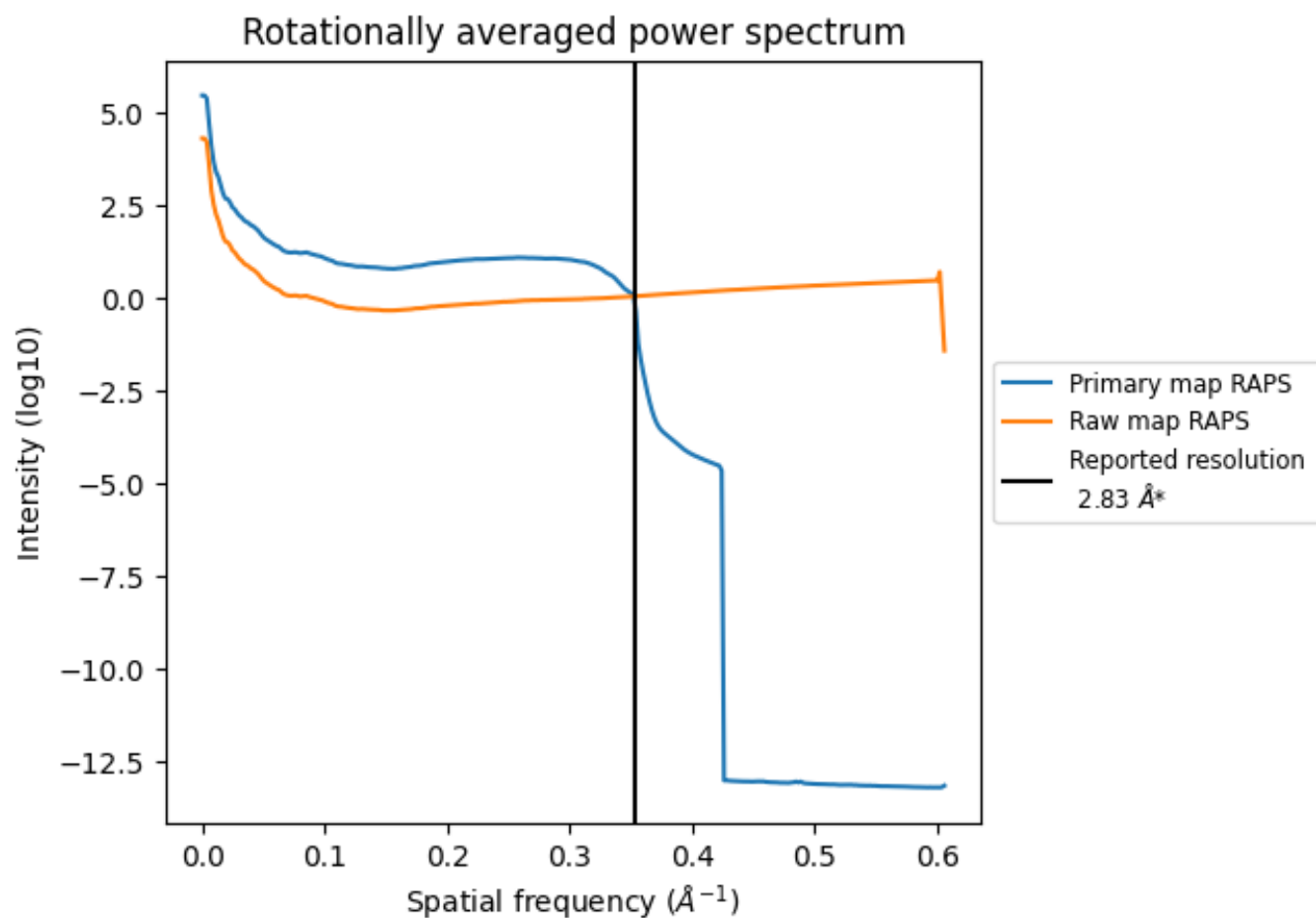
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 617 nm³; this corresponds to an approximate mass of 557 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 ⓘ

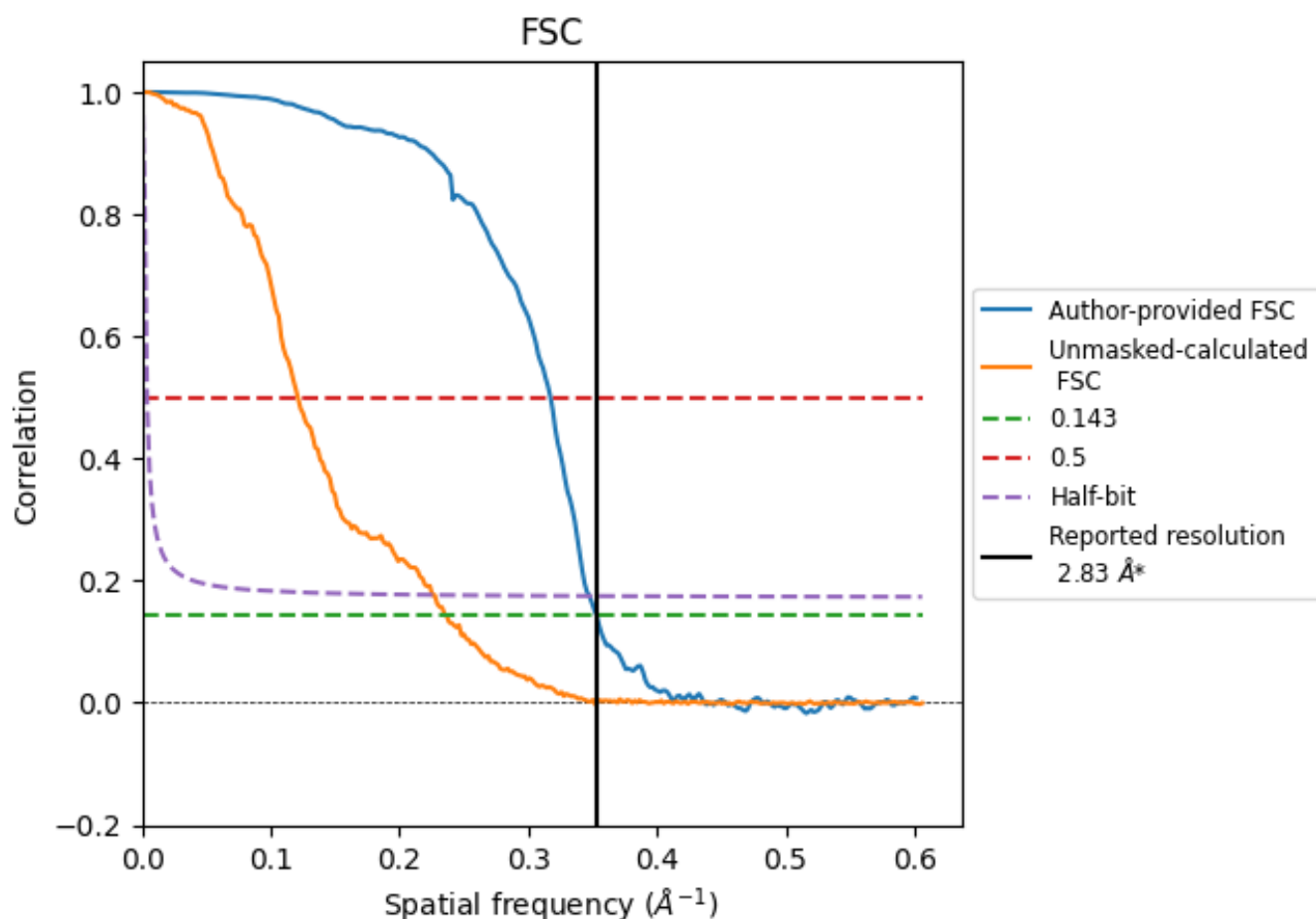


*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

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 0.353 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

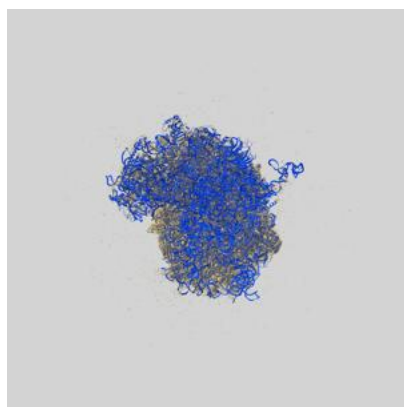
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.15	2.88
Unmasked-calculated*	4.24	8.27	4.43

*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 4.24 differs from the reported value 2.83 by more than 10 %

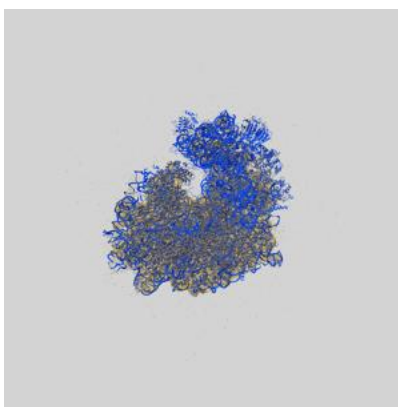
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66299 and PDB model 9WW6. Per-residue inclusion information can be found in section [3](#) on page [19](#).

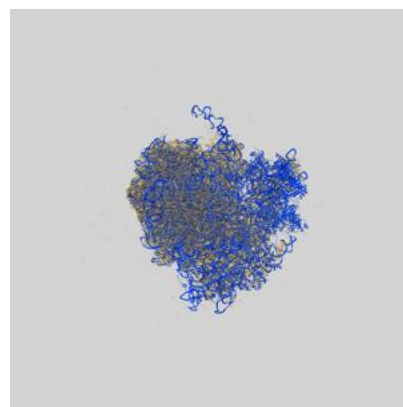
9.1 Map-model overlay [i](#)



X



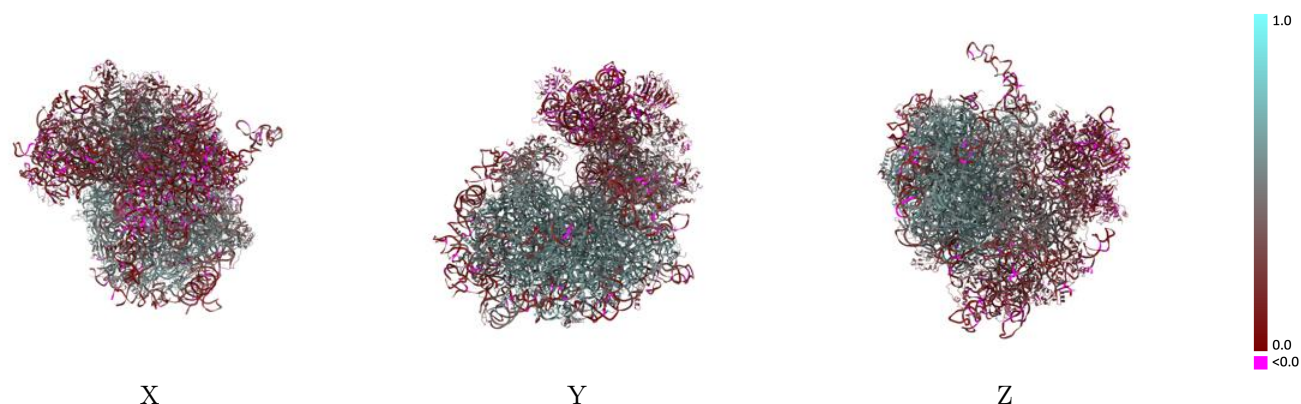
Y



Z

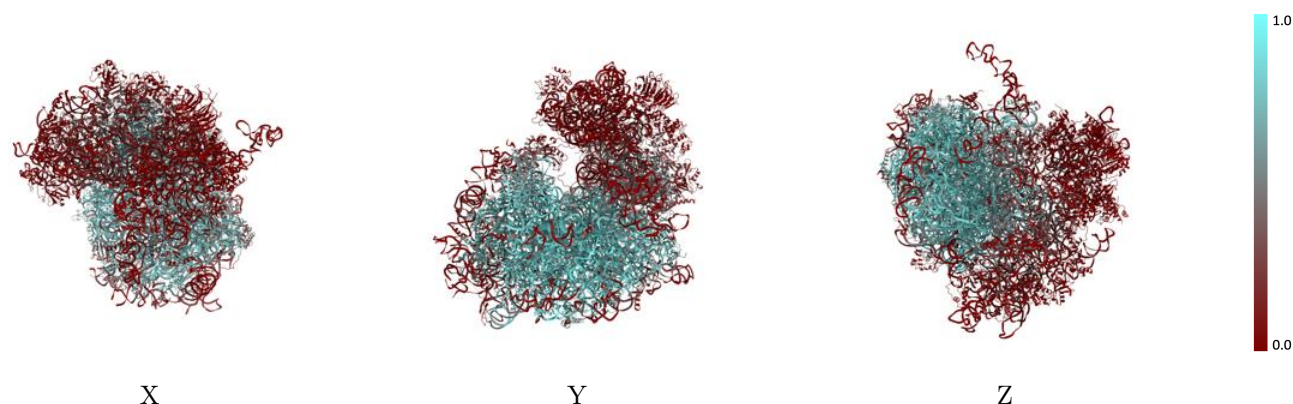
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



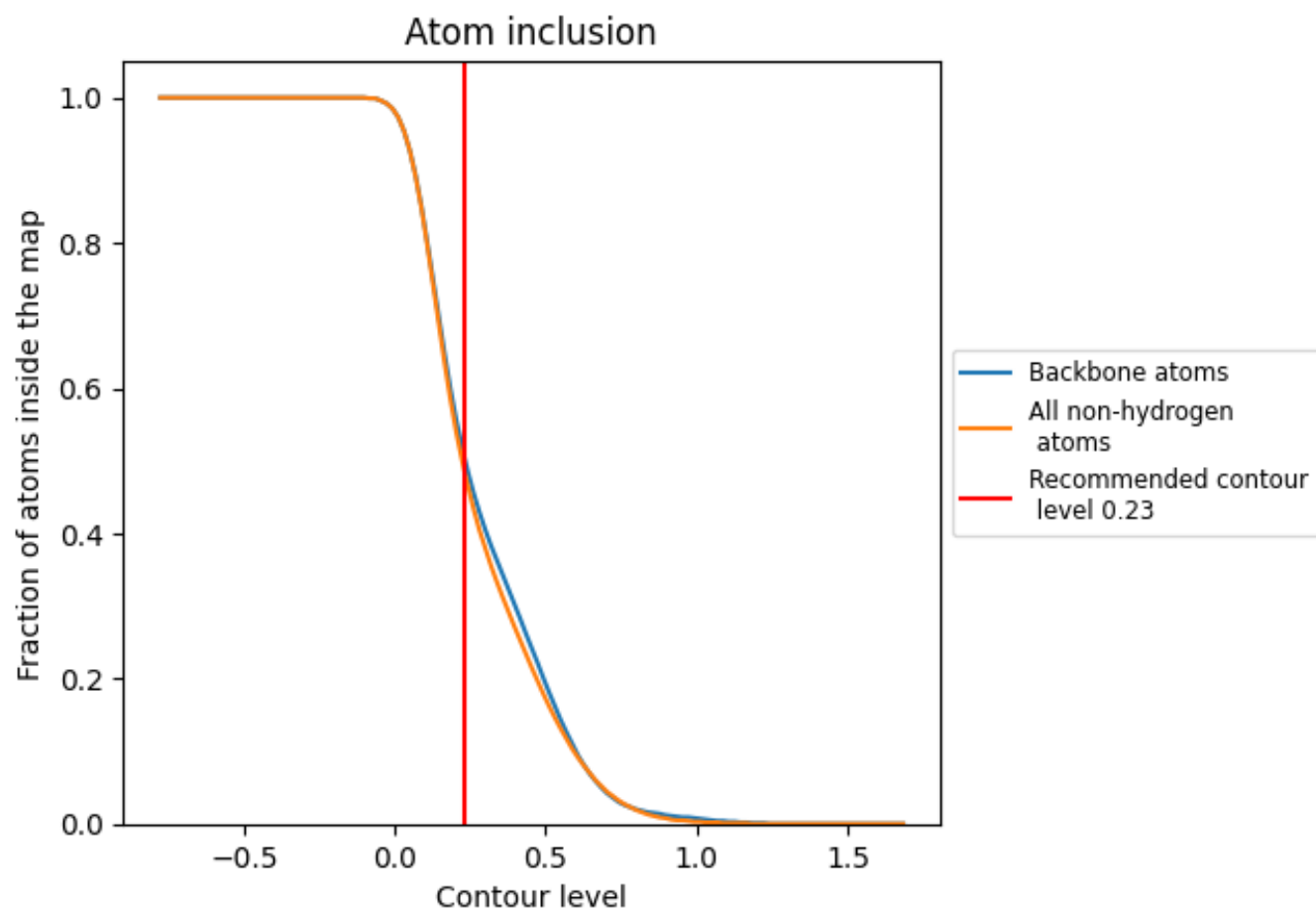
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 49% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4860	0.4130
AA	0.6520	0.4610
AB	0.7310	0.4880
AC	0.7950	0.5390
AD	0.8460	0.6220
AE	0.7430	0.5820
AF	0.8120	0.5990
AG	0.5170	0.4700
AH	0.5590	0.4990
AI	0.7800	0.5870
AJ	0.6010	0.5150
AK	0.4730	0.4880
AL	0.2110	0.4060
AM	0.2590	0.3950
AN	0.6710	0.5460
AO	0.5830	0.5110
AP	0.8880	0.6280
AQ	0.7410	0.5850
AR	0.7980	0.6030
AS	0.8570	0.6180
AT	0.5630	0.5040
AU	0.7180	0.5640
AV	0.7130	0.5690
AW	0.1520	0.3460
AX	0.7700	0.5960
AY	0.6860	0.5710
AZ	0.7650	0.5950
Aa	0.7540	0.5750
Ab	0.6820	0.5540
Ac	0.8340	0.6090
Ad	0.5060	0.4860
Ae	0.6870	0.5490
Af	0.7110	0.5770
Ag	0.8240	0.6180
Ah	0.8430	0.6160



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Chain	Atom inclusion	Q-score
Ai	 0.7680	 0.5940
Aj	 0.7110	 0.5800
Ak	 0.5820	 0.5340
Al	 0.8640	 0.6210
Am	 0.4410	 0.4870
An	 0.7640	 0.5960
Ao	 0.0000	 0.1390
Aq	 0.6170	 0.5420
Ar	 0.7730	 0.6020
As	 0.8110	 0.5990
BA	 0.2390	 0.2530
BB	 0.0610	 0.2910
BC	 0.0850	 0.2830
BD	 0.2570	 0.4040
BE	 0.0260	 0.2130
BF	 0.0310	 0.2050
BG	 0.0690	 0.2800
BH	 0.0890	 0.3280
BI	 0.0060	 0.1410
BJ	 0.2310	 0.4130
BK	 0.0080	 0.1640
BL	 0.0230	 0.2040
BM	 0.0200	 0.2010
BN	 0.0160	 0.1950
BO	 0.0230	 0.1800
BP	 0.1210	 0.3280
BQ	 0.1080	 0.3460
BR	 0.0730	 0.2970
BS	 0.0210	 0.2380
BT	 0.0200	 0.1790
BU	 0.0050	 0.1400
BV	 0.1490	 0.3340
BW	 0.0220	 0.2230
BX	 0.0730	 0.2450
BY	 0.0040	 0.1260
BZ	 0.4550	 0.4970
Ba	 0.2110	 0.3810
Bb	 0.3250	 0.4490
Bc	 0.0340	 0.1990
Bd	 0.0050	 0.1460
Be	 0.2130	 0.3800
Bf	 0.0470	 0.2650

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Chain	Atom inclusion	Q-score
Bg	 0.0070	 0.0600
Bh	 0.0250	 0.2120