



wwPDB EM Validation Summary Report ⓘ

Sep 8, 2026 – 05:09 PM JST

PDB ID : 9WW5 / pdb_00009ww5
EMDB ID : EMD-66298
Title : human 80S ribosome rotated state
Authors : Fujino, M.; Tanaka, Y.; Iwasaki, W.; Ito, T.; Yokoyama, T.
Deposited on : 2025-09-22
Resolution : 2.69 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

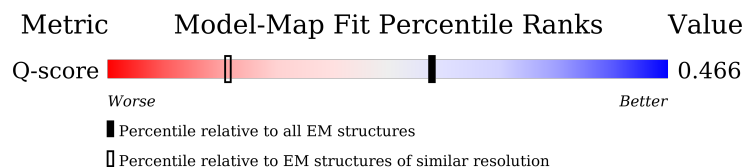
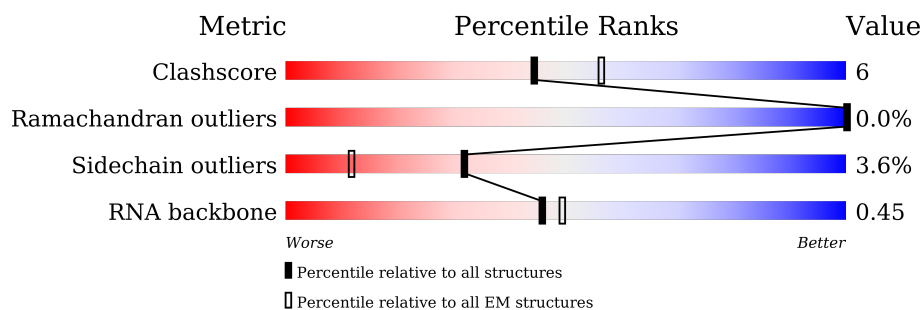
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 Å.

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



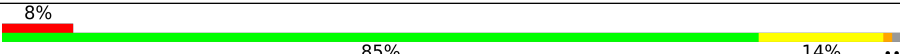
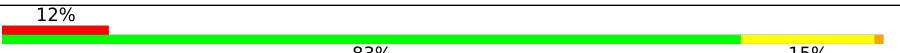
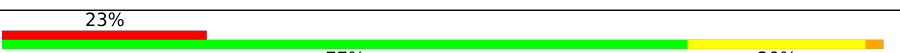
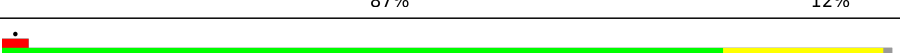
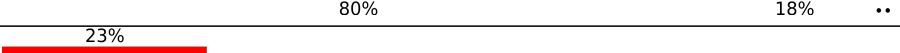
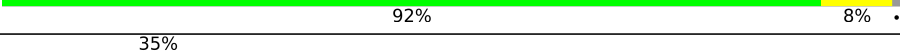
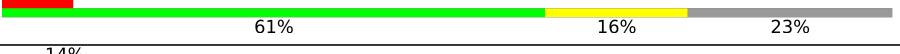
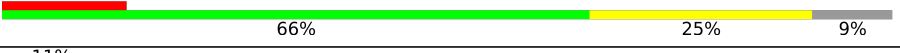
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9309 (2.19 - 3.19)

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

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

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

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

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

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Mol	Chain	Length	Quality of chain
79	Bh	135	97% 67% 29% ..

2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 215368 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S rRNA (3773-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	3773	Total	C	N	O	P	0	0
			80204	35721	14588	26123	3772		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	107	Total	C	N	O	S	0	0
			863	539	174	146	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BB	260	Total	C	N	O	S	0	0
			2060	1315	381	356	8		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BR	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		AltConf
80	AA	197	Total	Mg	0
			197	197	
80	AB	2	Total	Mg	0
			2	2	
80	AC	4	Total	Mg	0
			4	4	
80	AP	1	Total	Mg	0
			1	1	
80	AR	1	Total	Mg	0
			1	1	
80	AX	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
80	BA	62	Total 62	Mg 62	0
80	BL	2	Total 2	Mg 2	0
80	BN	1	Total 1	Mg 1	0

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

Mol	Chain	Residues	Atoms		AltConf
81	AA	65	Total 65	K 65	0
81	AB	1	Total 1	K 1	0
81	AD	1	Total 1	K 1	0
81	AL	1	Total 1	K 1	0
81	Ag	1	Total 1	K 1	0
81	Ah	1	Total 1	K 1	0
81	Aq	1	Total 1	K 1	0
81	BA	12	Total 12	K 12	0

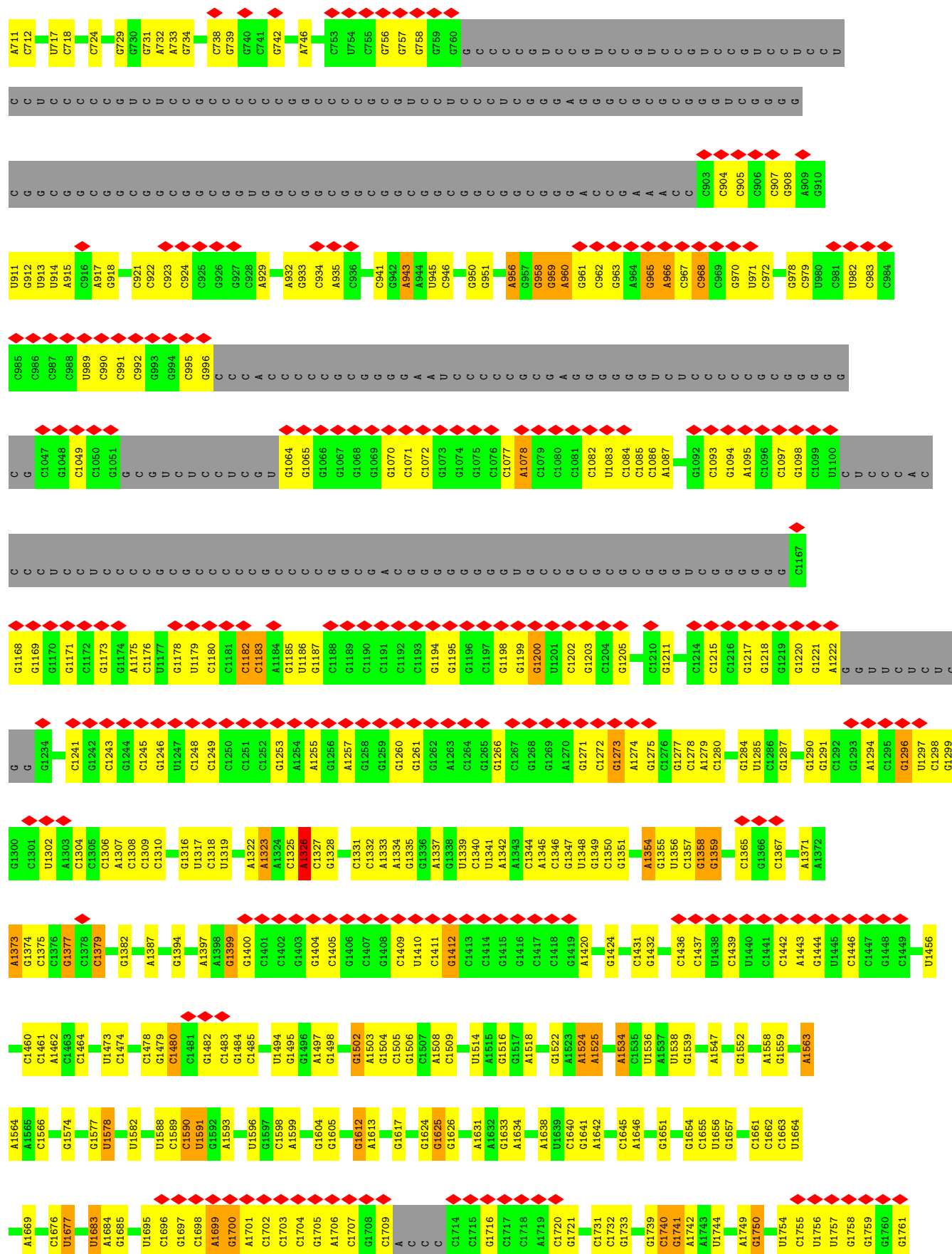
- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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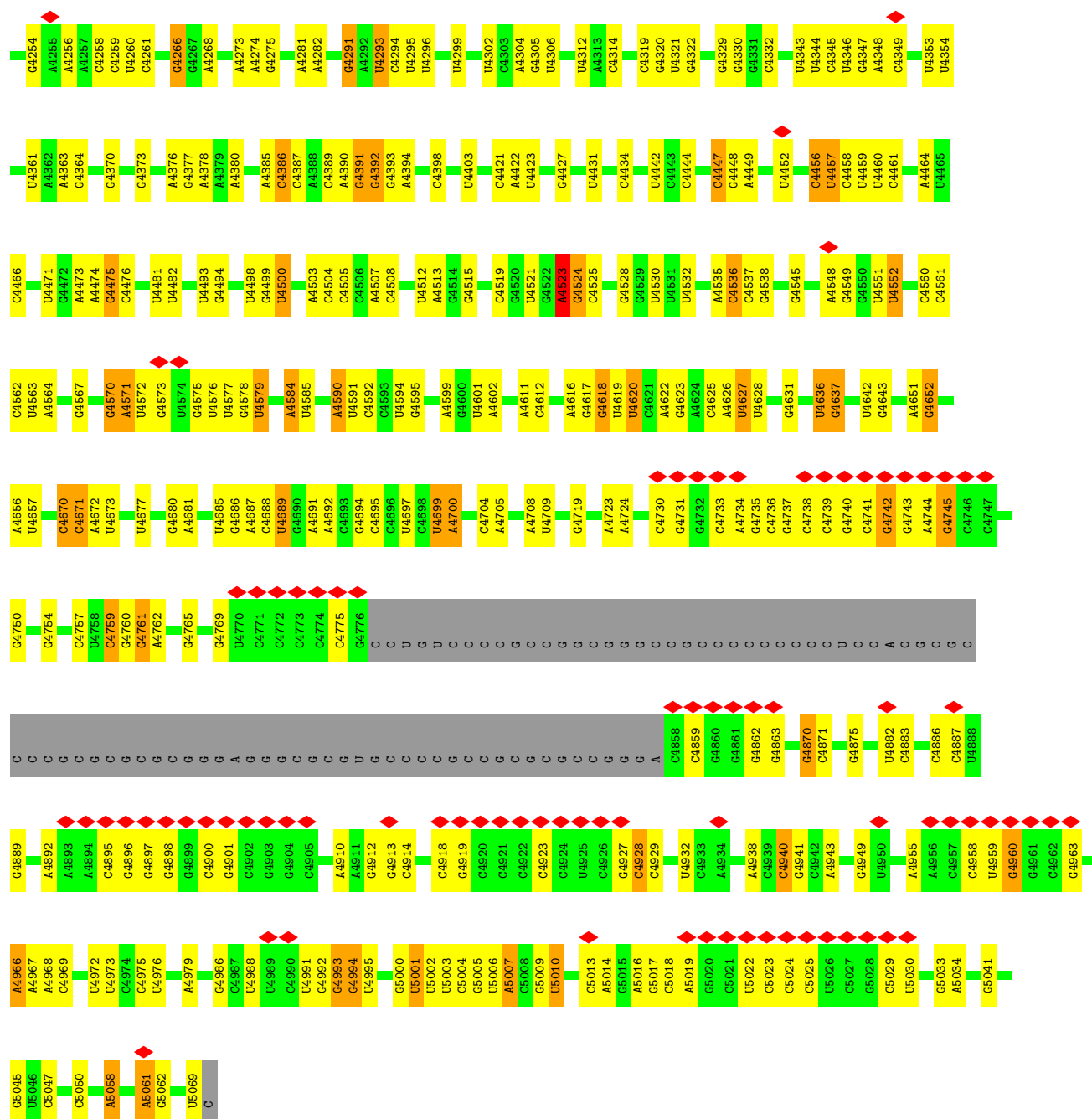
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Mol	Chain	Residues	Atoms		AltConf
82	BT	1	Total 1	Zn 1	0
82	Bg	1	Total 1	Zn 1	0









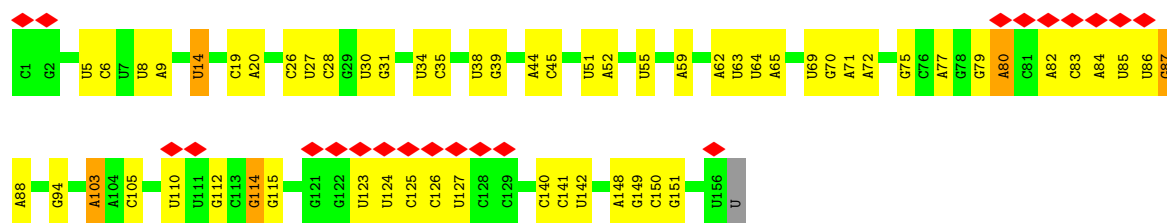
- Molecule 2: 5S rRNA (120-MER)

Chain AB: 84% 15%

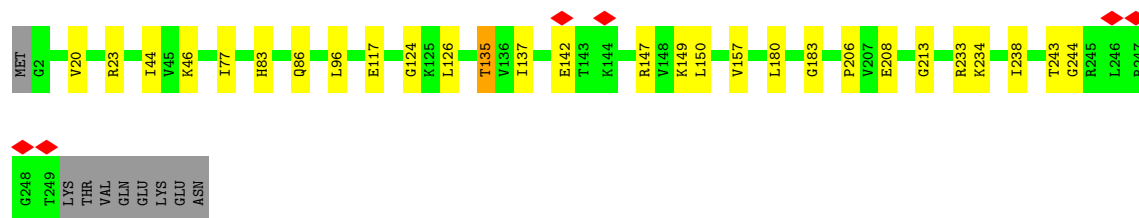
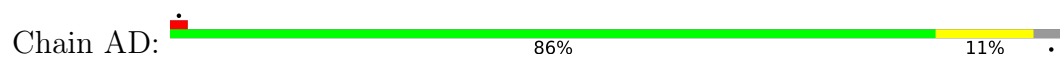


- Molecule 3: 5.8S rRNA (156-MER)

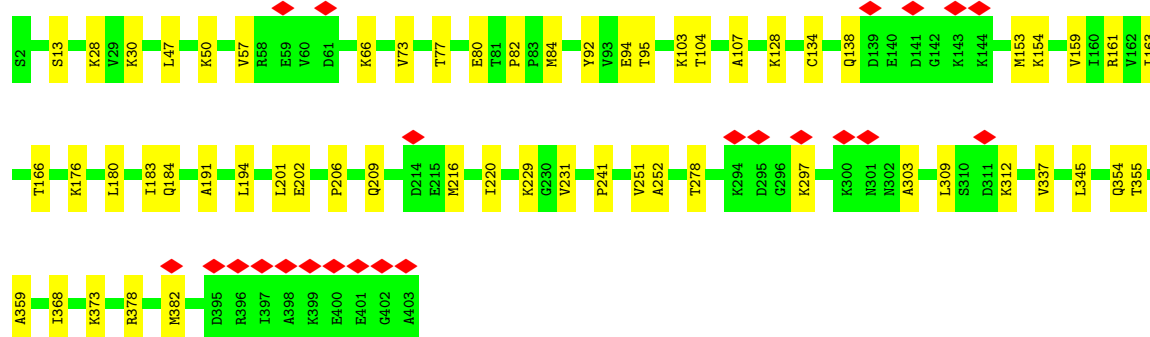
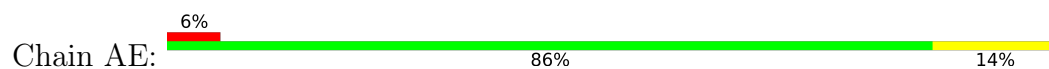
Chain AC: 13% 61% 35%



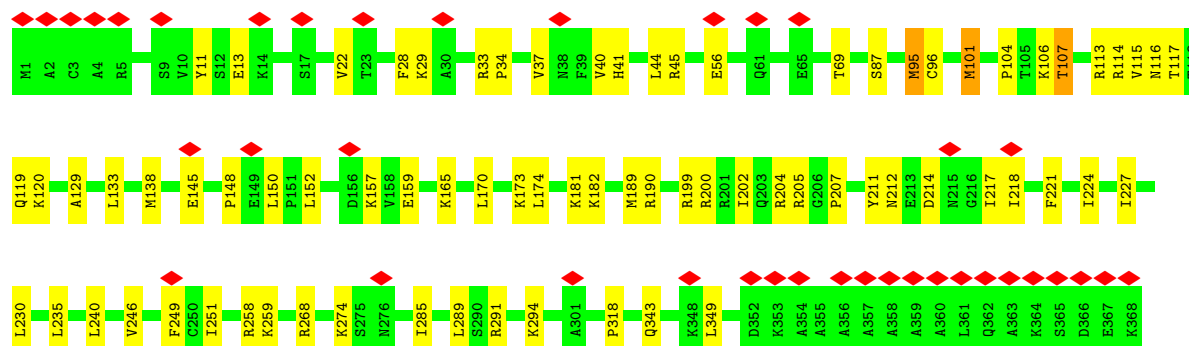
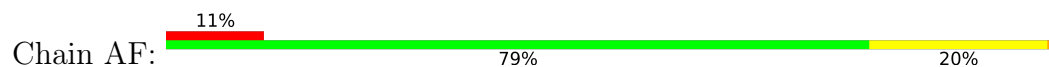
• Molecule 4: 60S ribosomal protein L8



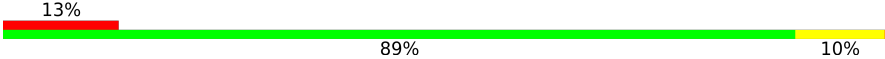
• Molecule 5: Large ribosomal subunit protein uL3

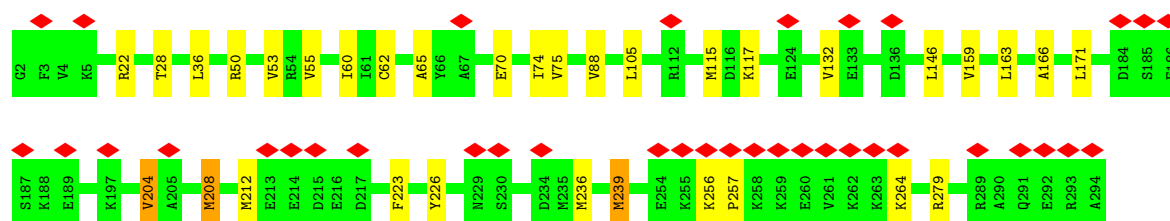


• Molecule 6: Large ribosomal subunit protein uL4



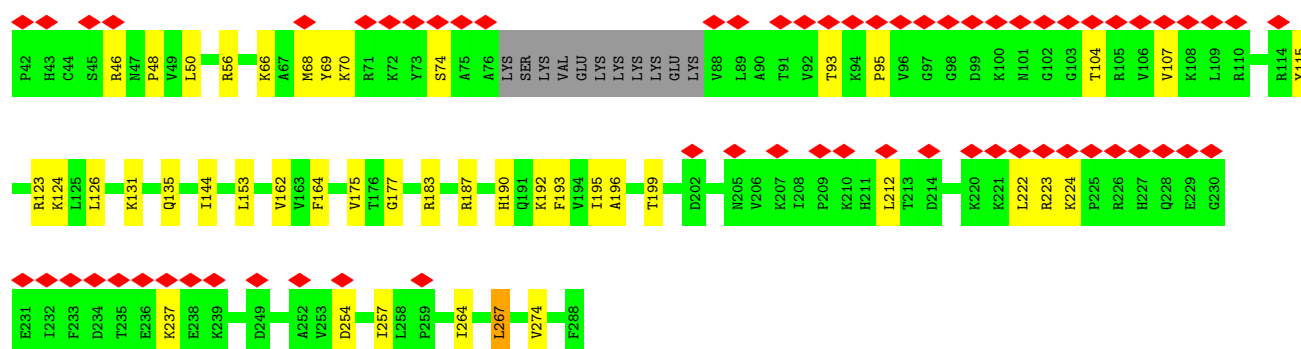
• Molecule 7: Large ribosomal subunit protein uL18

Chain AG: 



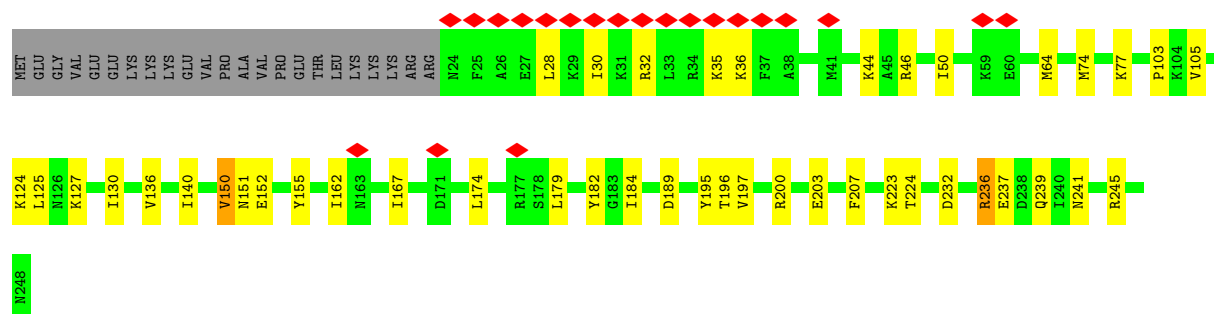
• Molecule 8: Large ribosomal subunit protein eL6

Chain AH: 



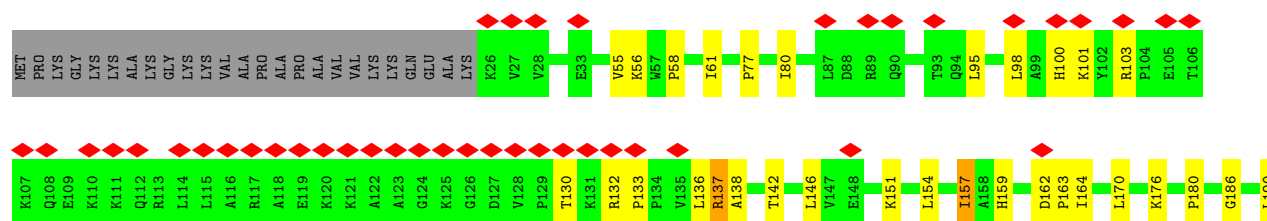
• Molecule 9: 60S ribosomal protein L7

Chain AI: 



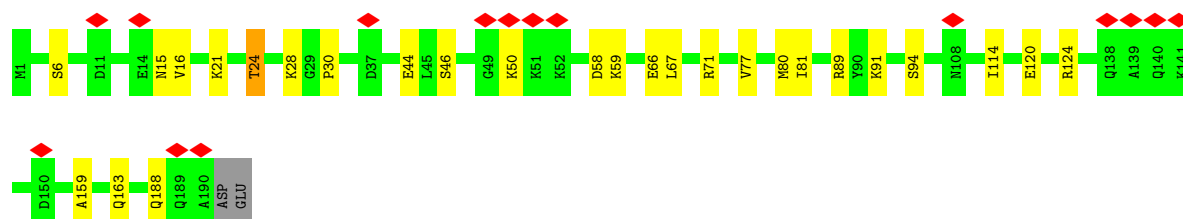
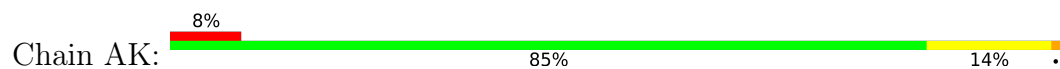
• Molecule 10: 60S ribosomal protein L7a

Chain AJ: 

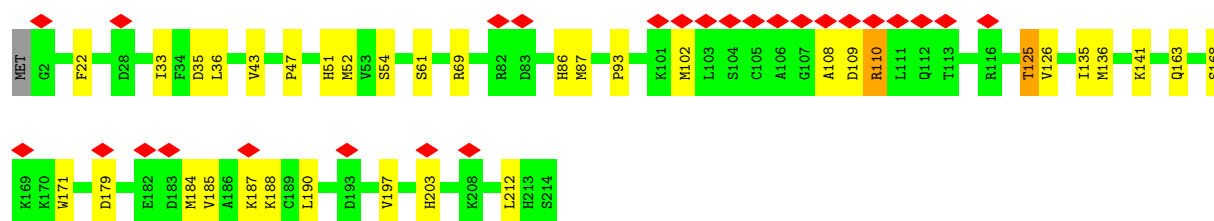
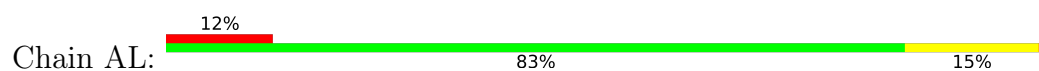




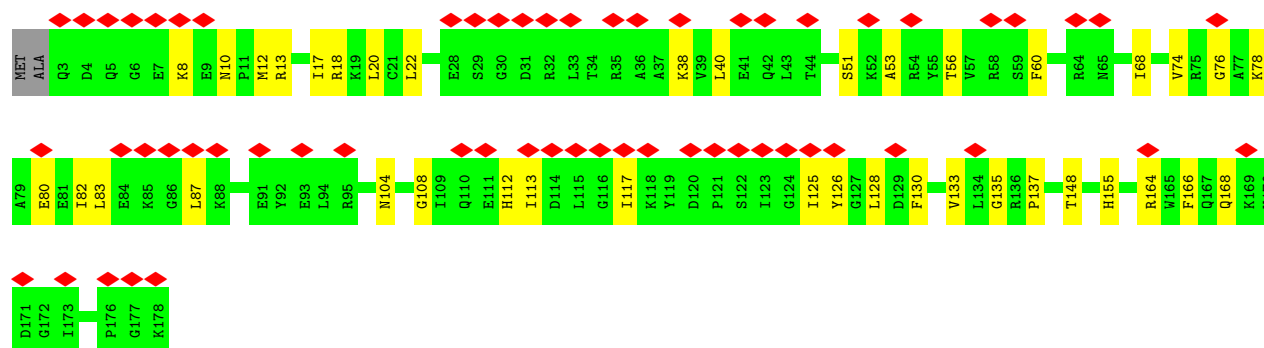
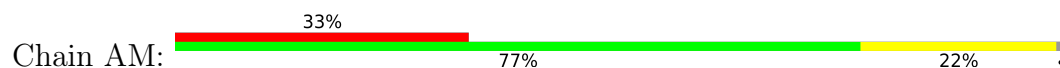
- Molecule 11: 60S ribosomal protein L9



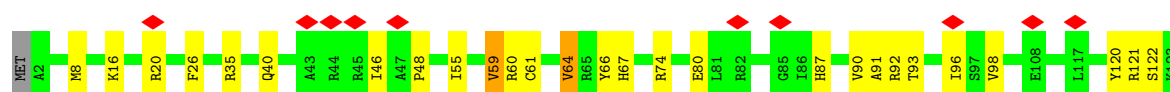
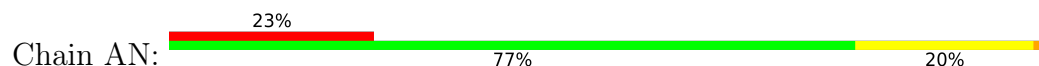
- Molecule 12: Ribosomal protein uL16-like

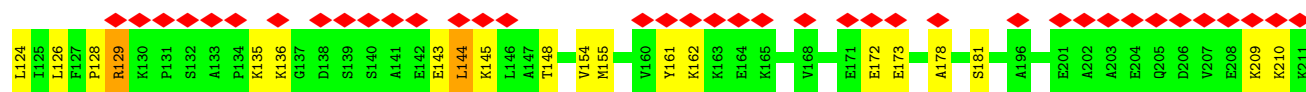


- Molecule 13: 60S ribosomal protein L11

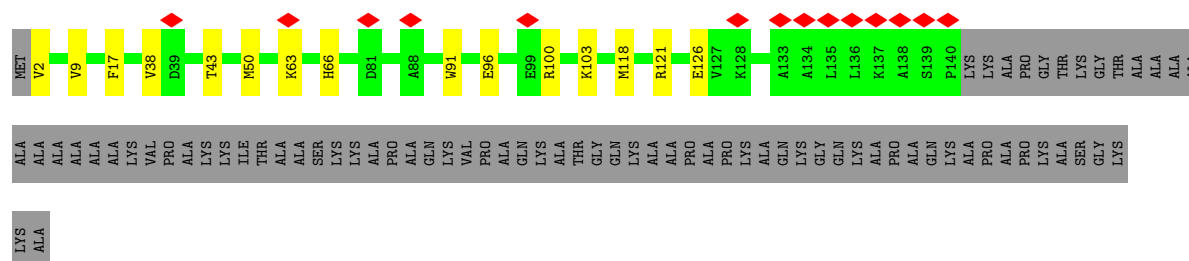


- Molecule 14: 60S ribosomal protein L13

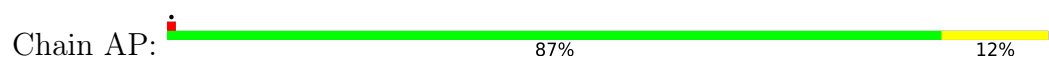




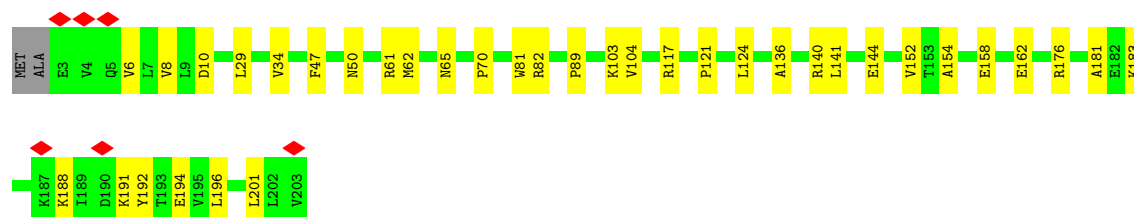
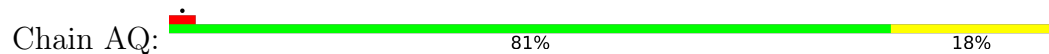
- Molecule 15: 60S ribosomal protein L14



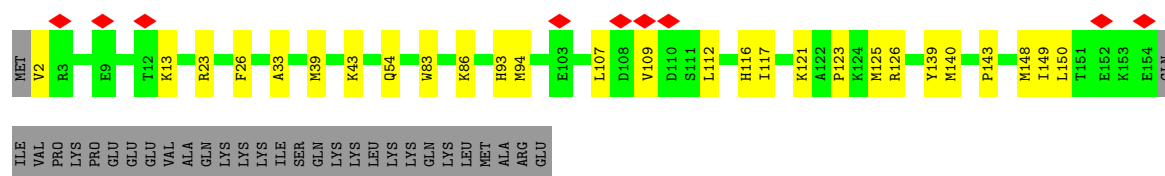
- Molecule 16: 60S ribosomal protein L15



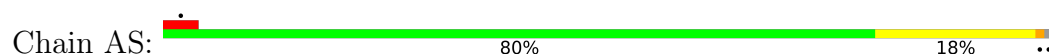
- Molecule 17: 60S ribosomal protein L13a

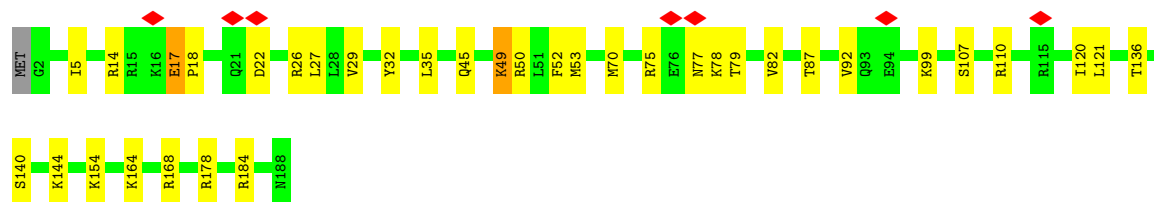


- Molecule 18: 60S ribosomal protein L17

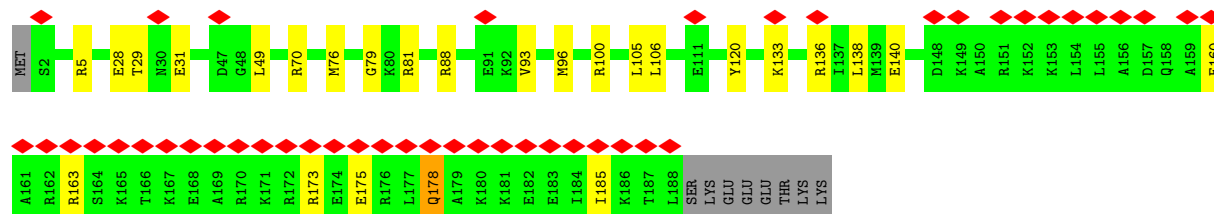
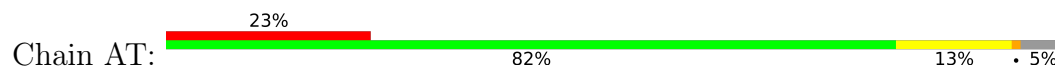


- Molecule 19: 60S ribosomal protein L18

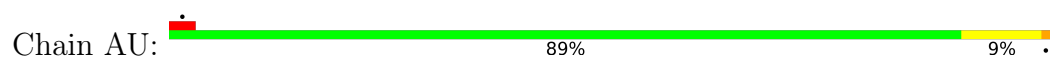




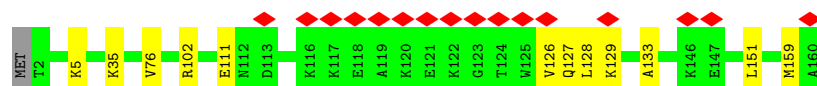
- Molecule 20: 60S ribosomal protein L19



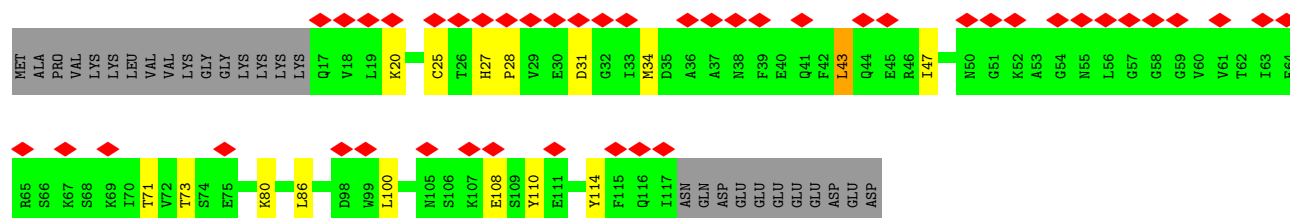
- Molecule 21: 60S ribosomal protein L18a



- Molecule 22: 60S ribosomal protein L21



- Molecule 23: 60S ribosomal protein L22

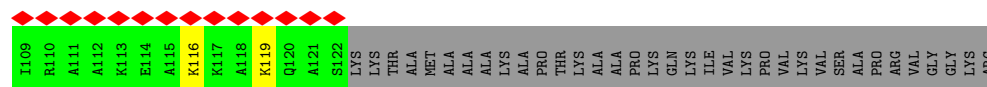
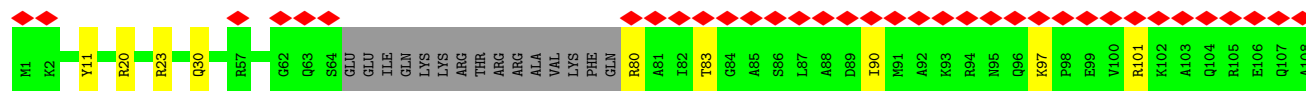


- Molecule 24: 60S ribosomal protein L23

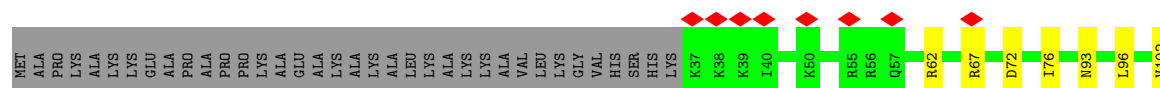




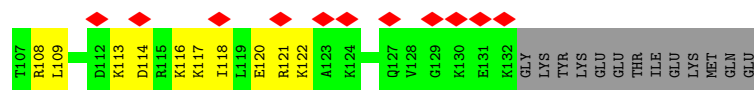
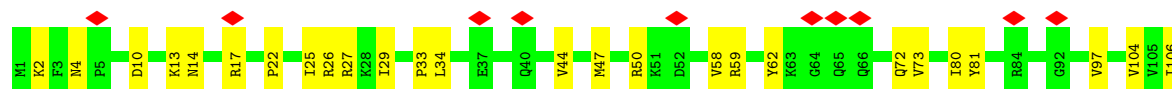
- Molecule 25: 60S ribosomal protein L24



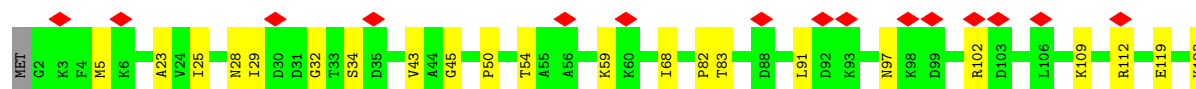
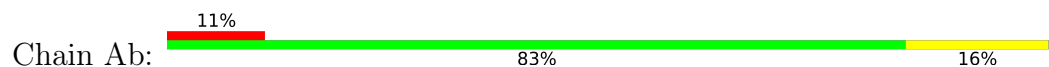
- Molecule 26: 60S ribosomal protein L23a



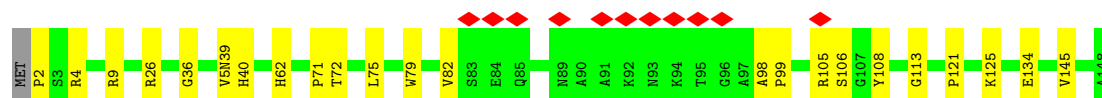
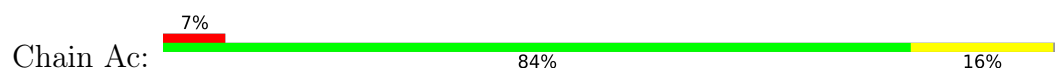
- Molecule 27: 60S ribosomal protein L26



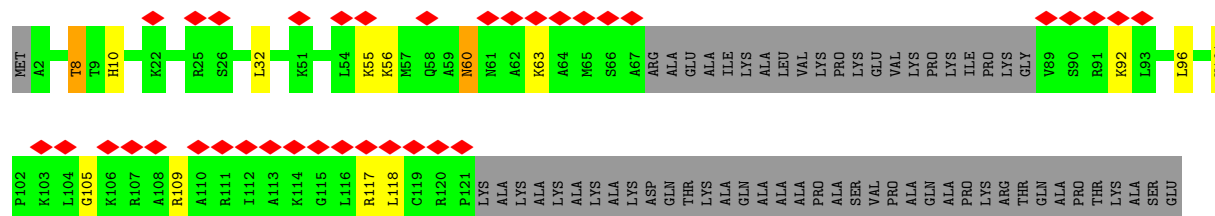
- Molecule 28: 60S ribosomal protein L27



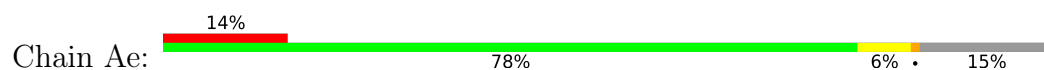
- Molecule 29: Large ribosomal subunit protein uL15



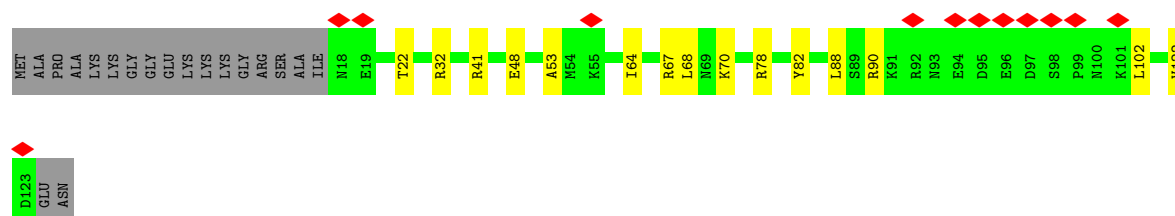
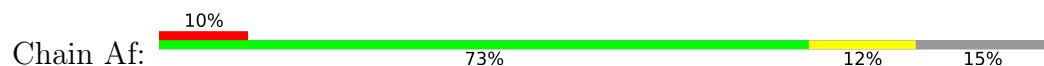
• Molecule 30: 60S ribosomal protein L29



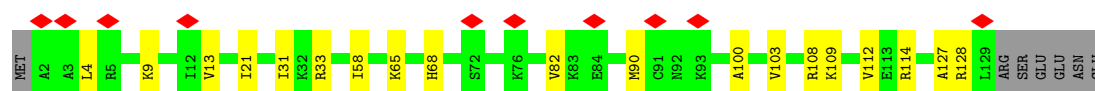
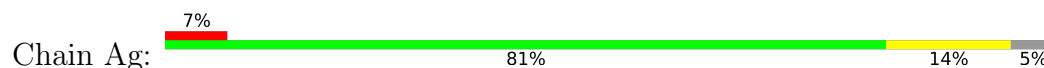
• Molecule 31: 60S ribosomal protein L30



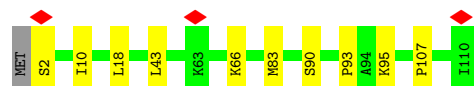
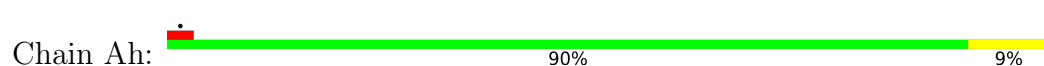
• Molecule 32: 60S ribosomal protein L31



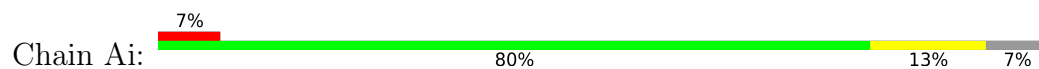
• Molecule 33: 60S ribosomal protein L32



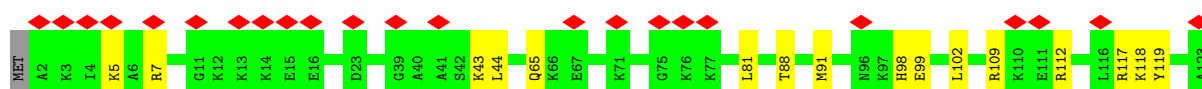
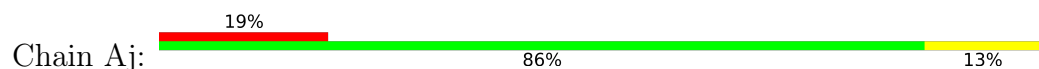
• Molecule 34: 60S ribosomal protein L35a



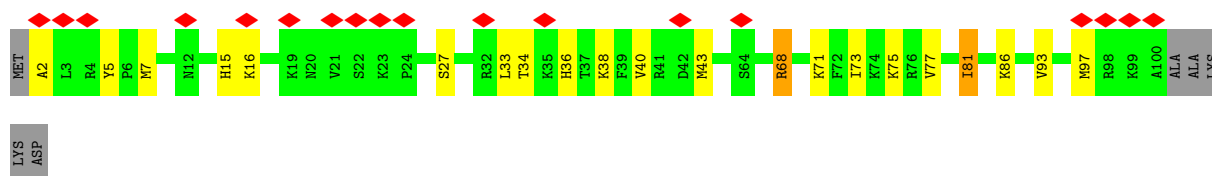
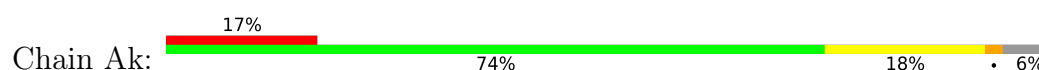
- Molecule 35: 60S ribosomal protein L34



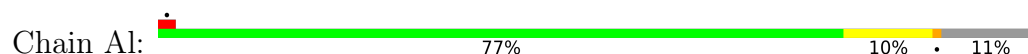
- Molecule 36: 60S ribosomal protein L35



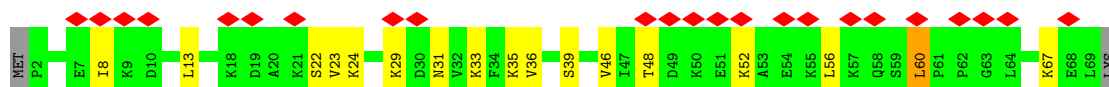
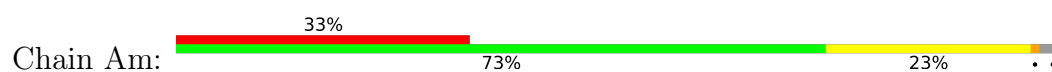
- Molecule 37: 60S ribosomal protein L36



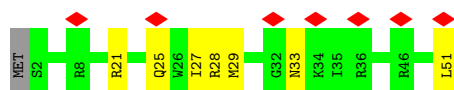
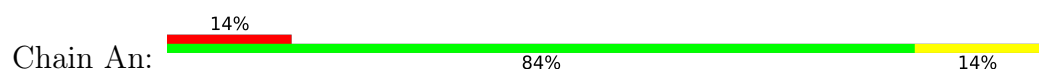
- Molecule 38: 60S ribosomal protein L37



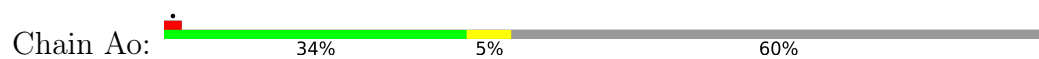
- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39



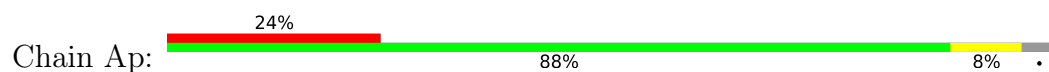
- Molecule 41: Ubiquitin-60S ribosomal protein L40



MET GLN ILE PHE VAL LYS THR LEU THR VAL LEU LYS THR ILE THR LEU VAL VAL GLU VAL PRO SER ASP THR ILE ASN VAL VAL ALA ILE ILE LYS ASP LYS GLU ILE PRO PRO ASP GLN GLN ARG LEU ILE PHE ALA GLY LYS GLN LEU GLU ASP GLY ARG THR LEU SER ASP ASN

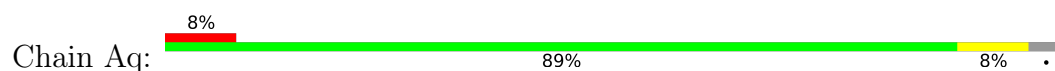
ILE GLN LYS SER THR LEU HIS VAL LEU ARG LEU ARG GLY I77 I78 R83 I95 H104 P105 R106 K125 K126 V127 LYS

- Molecule 42: 60S ribosomal protein L41



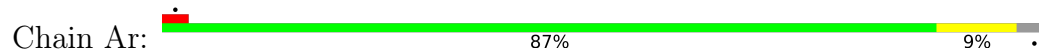
M1 K4 M10 R11 R12 K16 R17 R18 R21 S24 LYS

- Molecule 43: 60S ribosomal protein L36a



MET V2 K14 K30 D31 A35 Q36 R39 R69 E74 P75 N76 C77 C78 R81 D96 R99 K100 G101 Q102 V103 ILE GLN PHE

- Molecule 44: 60S ribosomal protein L37a



MET A2 K3 K6 K7 V8 Y18 L22 T63 N72 R85 L86 K87 E88 L89 LYS ASP GLN

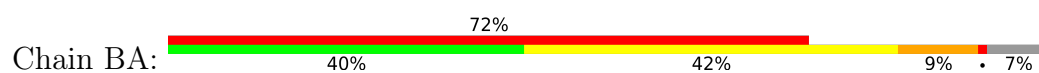
- Molecule 45: 60S ribosomal protein L28



MET S2 A3 H4 L5 Q6 C13 K19 K22 S26 N36 R46 A54 A55 D56 G57 K58 V63 I64 R67 S68 G69 Q70 Q71 R79 T80 N83 K84 N85 A86 L90 S91 S92 I93 M96 I97 R103 P104 D105 L106 R107 M108 A109 A110 I111 R112

R113 I117 P123 V124 MET VAL LYS ARG ARG THR ARG PRO THR LYS SER

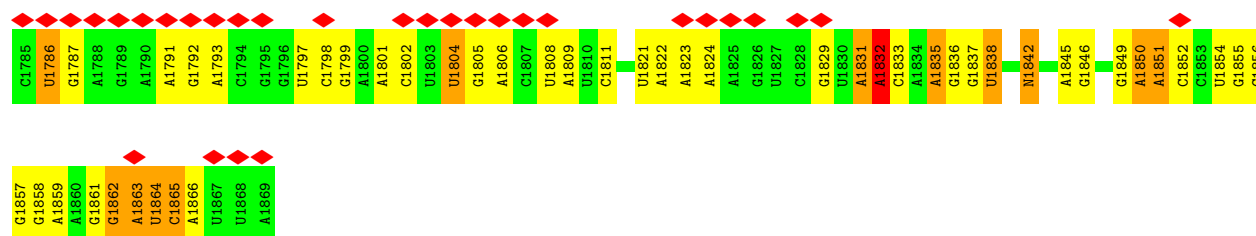
- Molecule 46: 18S rRNA (1740-MER)



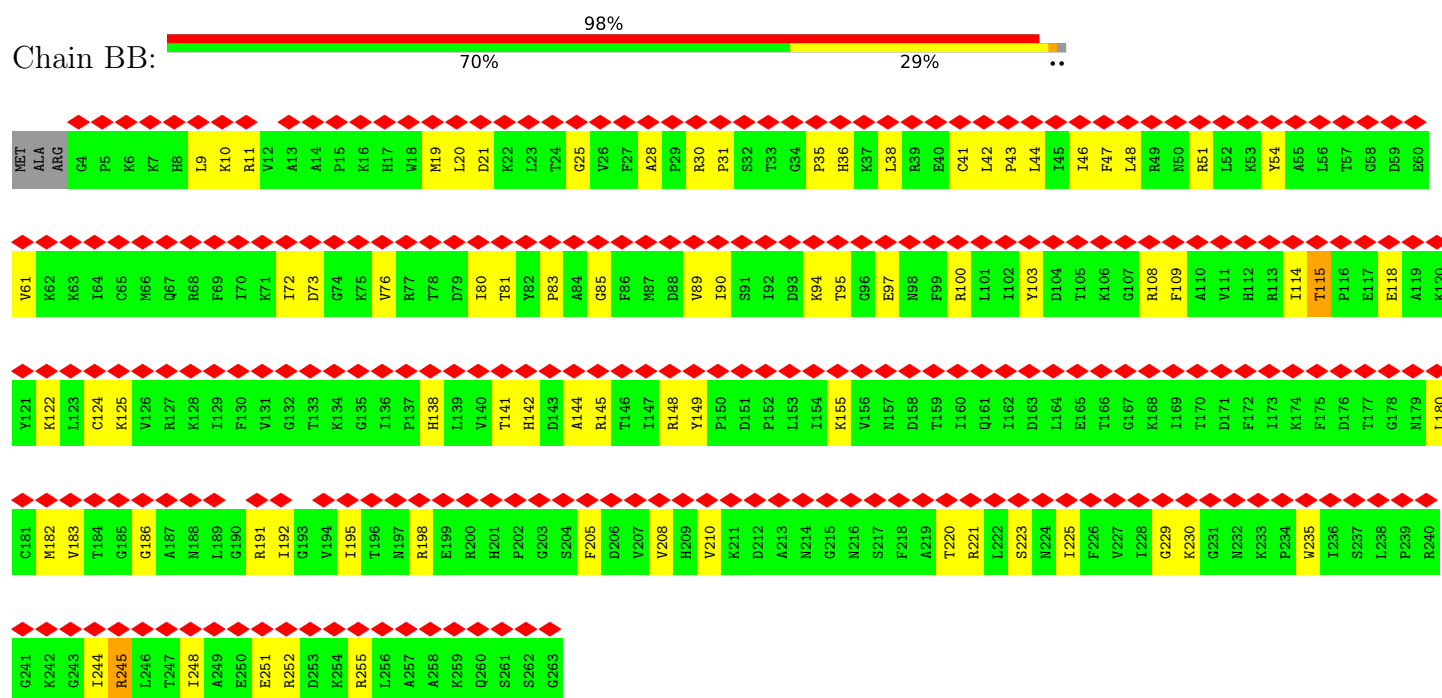
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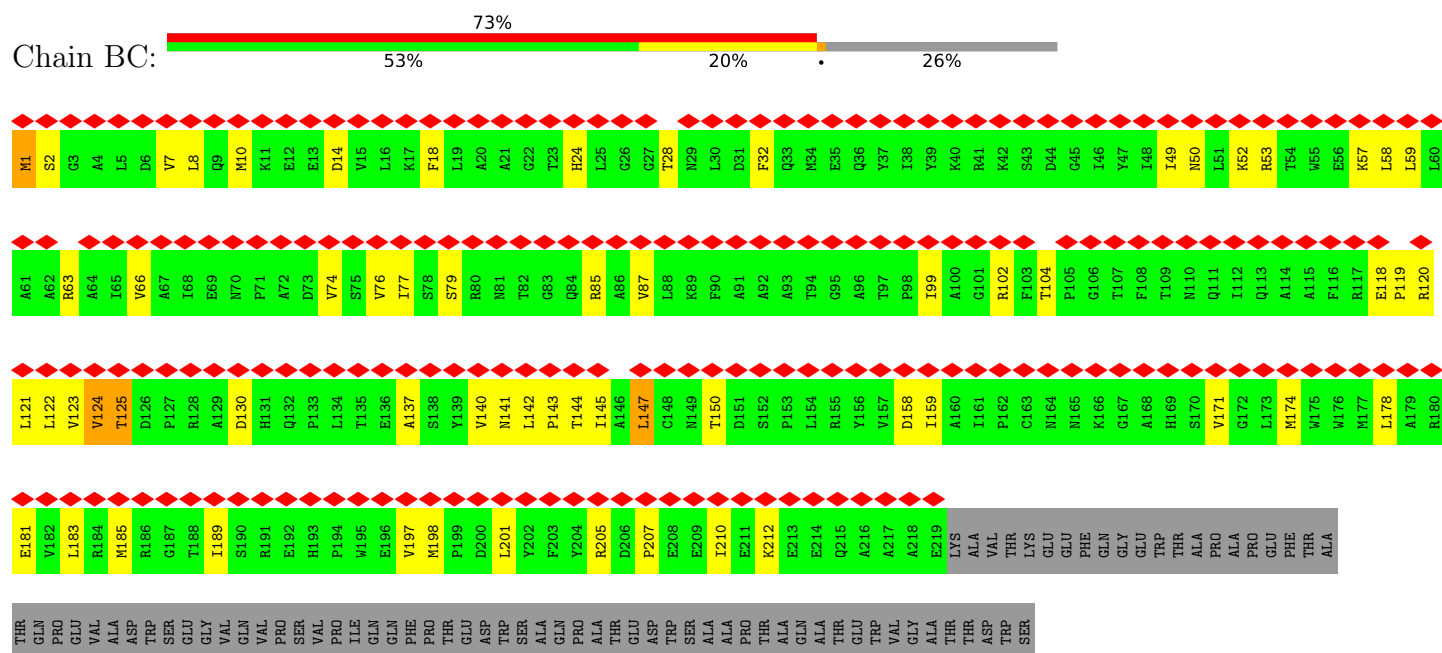
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G1727	G1665	G1605	A1545	U1485	G1425	U1364	G1298	U1238	U1154	G1088	G1005	C941
U1729	C1666	G1606	G1546	A1486	U1426	G1365	A1299	U1239	U1155	C1089	C1006	G942
U1730	U1667	A1607	C1547	C1487	C1427	G1366	U1300	A1240	U1156	G1092	C1007	U943
U1668	U1668	U1608	G1548	C1488	G1428	U1367	A1301	A1241	U1157	A1093	A1008	A944
G1669	G1669	C1609	U1549	A1489	G1429	U1368	G1302	U1242	U1158	C1094	A1009	U945
U1733	C1670	G1610	U1550	C1490	C1430	A1369	C1303	U1243	U1159	G1095	G1010	U946
G1734	G1671	U1611	U1551	G1491	G1431	A1370	U1304	U1244	U1160	G1096	A1011	C947
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G1736	U1673	C1613	C1553	C1493	C1433	U1372	U1306	A1246	U1175	G1098	U1013	G949
G1737	G1674	A1614	C1554	U1494	C1434	C1373	U1307	C1247	U1176	G1099	G1014	C950
U1675	U1675	U1615	U1555	G1495	C1435	C1374	U1308	B8N1248	U1182	A1100	U1015	C951
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C1688	C1688	C1628	C1568	A1508	A1448	A1388	G1321	C1261	C1205	U1113	U1038	A964
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C1696	C1696	C1635	G1575	U1515	A1455	C1395	G1327	C1268	C1213	G1121	C1053	A972
A1697	A1697	G1636	G1576	G1516	G1456	A1396	U1328	G1269	A1214	C1122	G1054	C973
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G1702	G1702	A1641	C1581	C1521	G1461	A1401	G1334	G1274	A1220	C1128	A1058	C978
C1703	C1703	U1642	C1582	A1522	U1462	A1402	G1335	C1275	G1221	G1129	G1059	C979
C1704	C1704	U1643	C1583	C1523	U1463	C1403	C1336	A1276	U1223	G1130	A1060	A980
G1705	G1705	G1644	U1584	G1524	C1464	U1404	N1337	C1277	G1224	G1131	U1061	A981
C1706	C1706	C1645	U1585	C1525	A1465	A1405	G1338	A1278	U1225	C1132	C1063	A983
U1707	U1707	G1646	U1586	G1526	G1466	G1406	U1339	C1279	G1226	G1133	C1064	C984
C1708	C1708	A1647	G1587	C1527	C1467	U1407	U1340	G1280	G1227	C1134	G1065	G985
G1709	G1709	U1648	A1588	G1528	C1468	U1408	U1341	G1281	U1228	U1137	U1066	G986
U1711	U1711	U1649	A1589	C1529	A1469	A1409	U1342	A1282	A1228	C1138	C1074	A987
C1712	C1712	A1650	C1590	U1530	C1470	C1410	U1343	C1283	G1229	C1139	C1075	C988
C1713	C1713	A1651	C1591	A1531	C1471	G1411	A1344	A1284	C1230	G1140	U1081	C989
U1714	U1714	G1652	C1592	C1532	C1472	C1412	G1345	G1285	C1231	C1141	A1082	A996
A1715	A1715	U1653	C1593	A1533	G1473	G1413	U1346	G1286	U1232	A1143	A1083	A997
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C1717	C1717	C1655	U1595	U1535	G1475	C1415	U1348	U1288	C1234	A1145	C1085	G999
U1718	U1718	G1656	U1596	G1536	A1476	C1416	G1349	U1289	G1235	C1146	C1000	A1001
G1719	G1719	C1657	C1597	A1537	U1477	C1417	U1350	A1291			U1002	U1002
C1720	C1720	G1658	U1598	U1538	U1478	C1418	U1351	C1292				
A1781	A1781	U1659	U1599	U1539	U1479	C1419	U1352	C1293				
C1782	C1782	C1660	G1600	A1480	A1480	C1420	U1353	C1294				
G1783	G1783	A1661	U1601	G1541	G1481	A1421	G1361	A1295				
G1784	G1784	U1662	U1602	C1542	G1482	G1422						



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

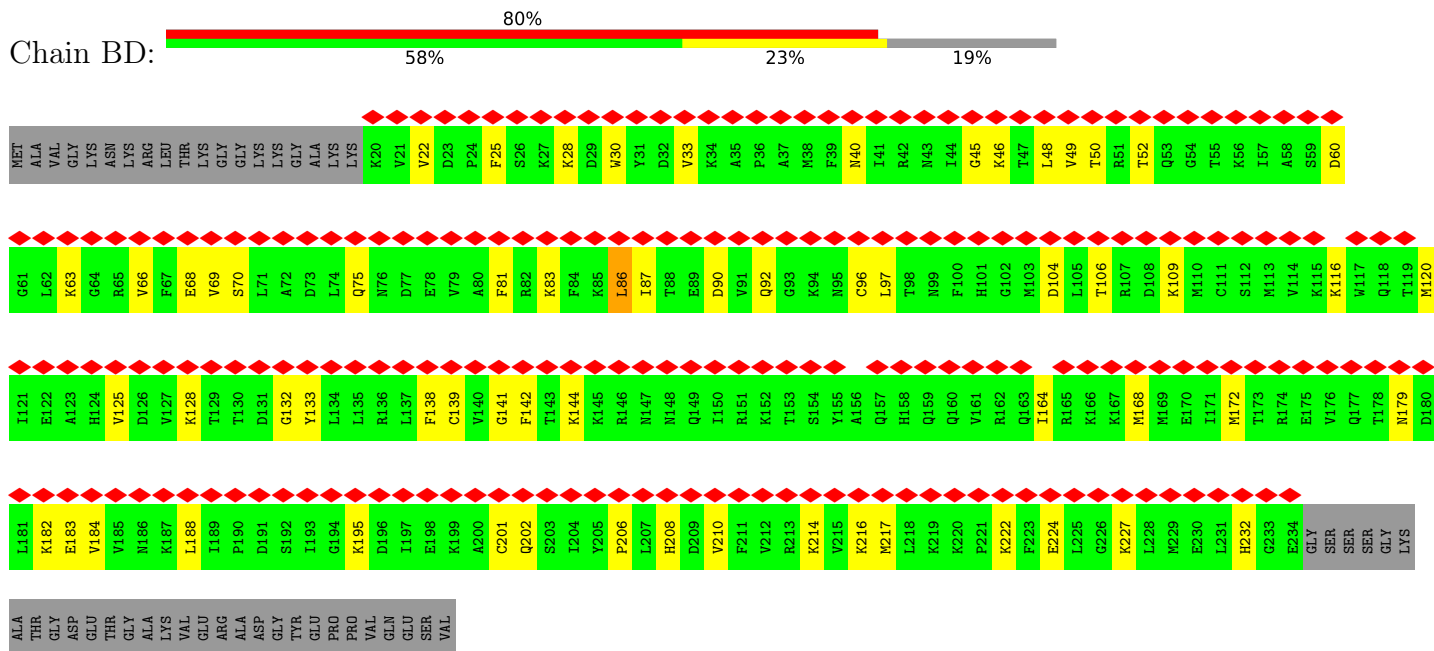


- Molecule 48: Small ribosomal subunit protein uS2



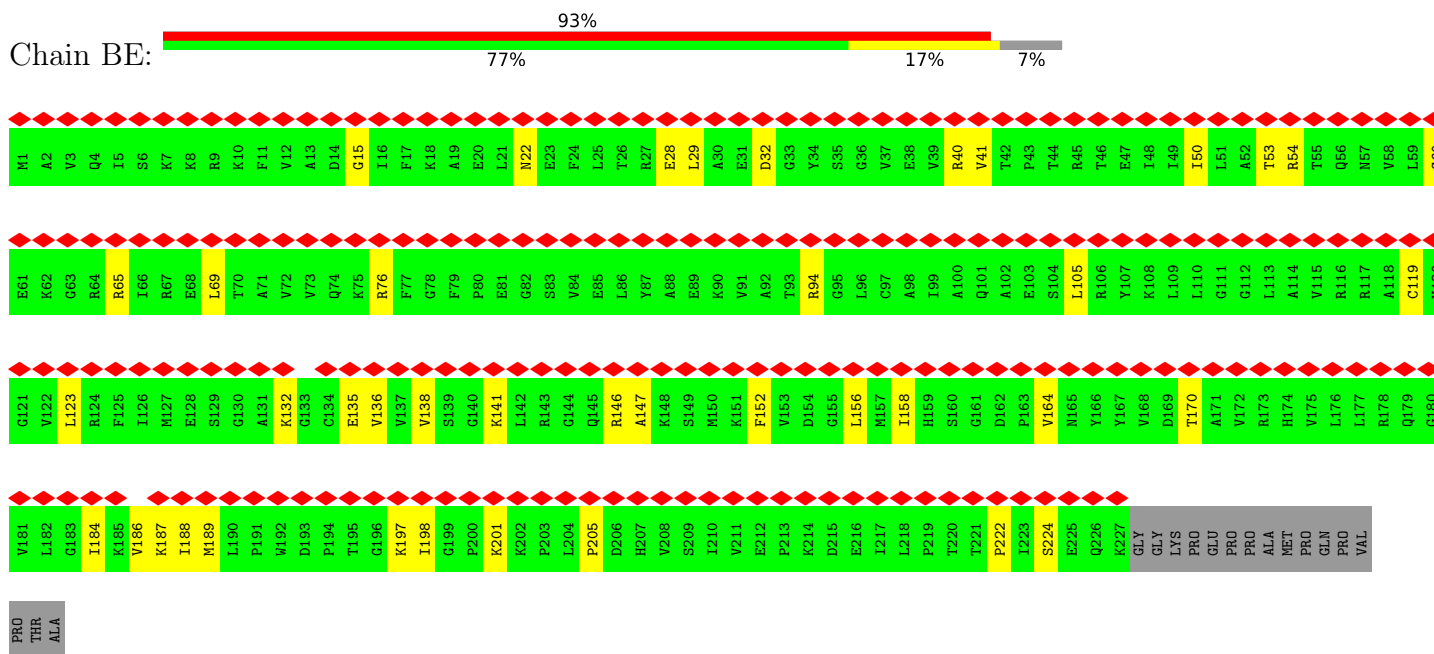
• Molecule 49: 40S ribosomal protein S3a

Chain BD:



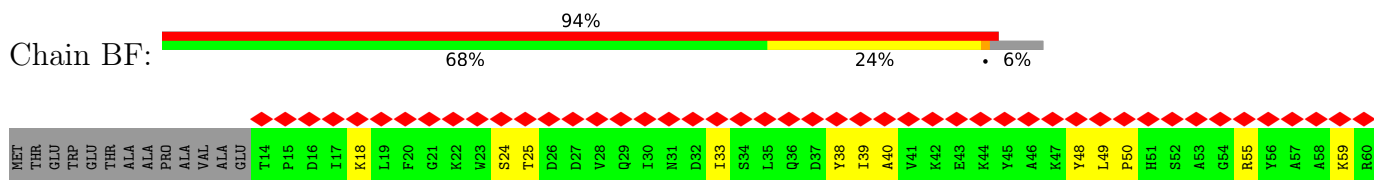
• Molecule 50: 40S ribosomal protein S3

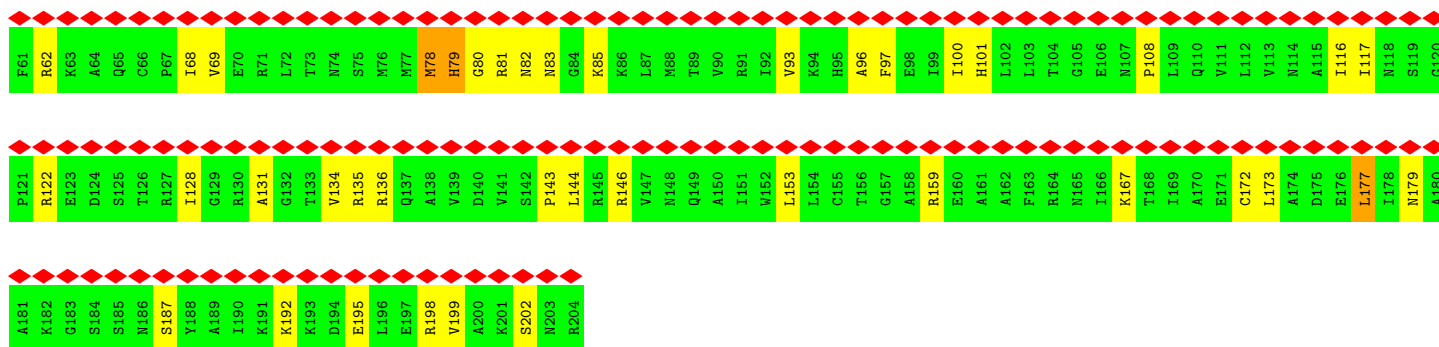
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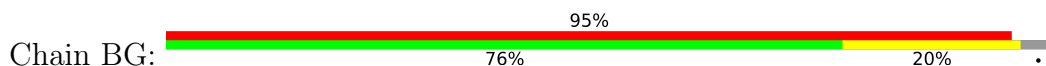
• Molecule 51: 40S ribosomal protein S5

Chain BF:

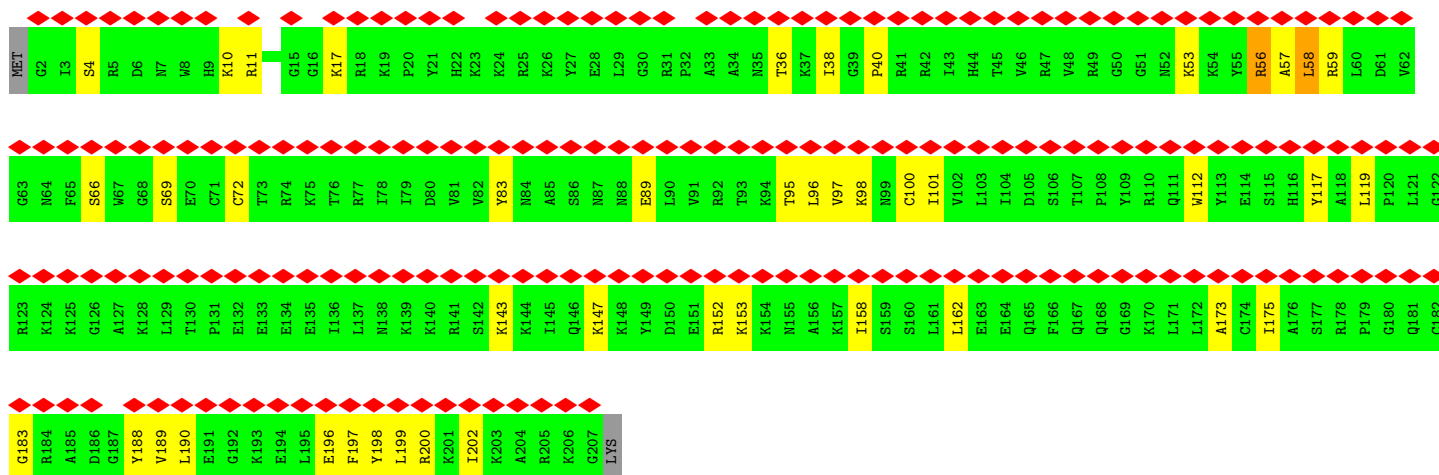
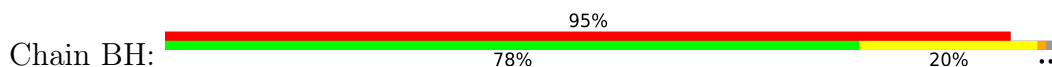




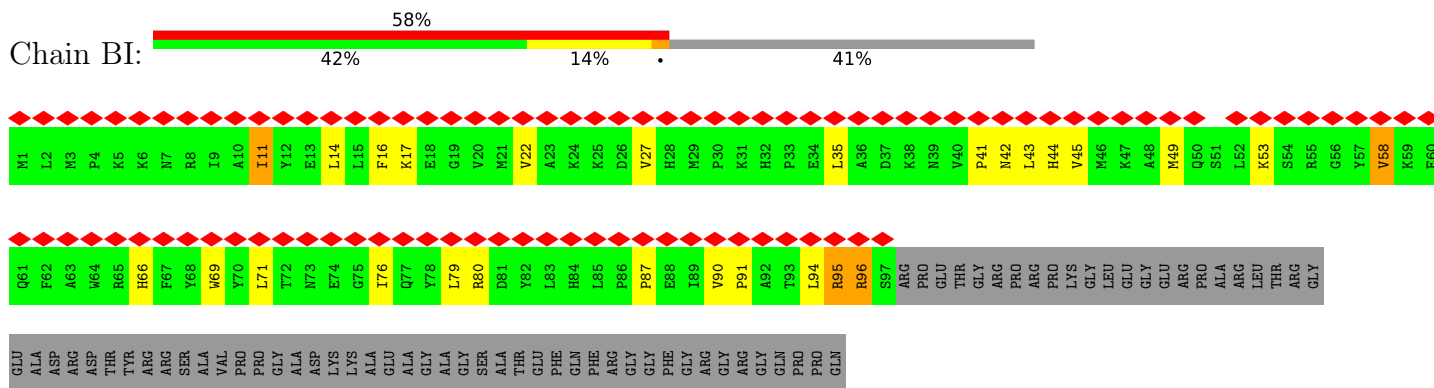
• Molecule 52: 40S ribosomal protein S7



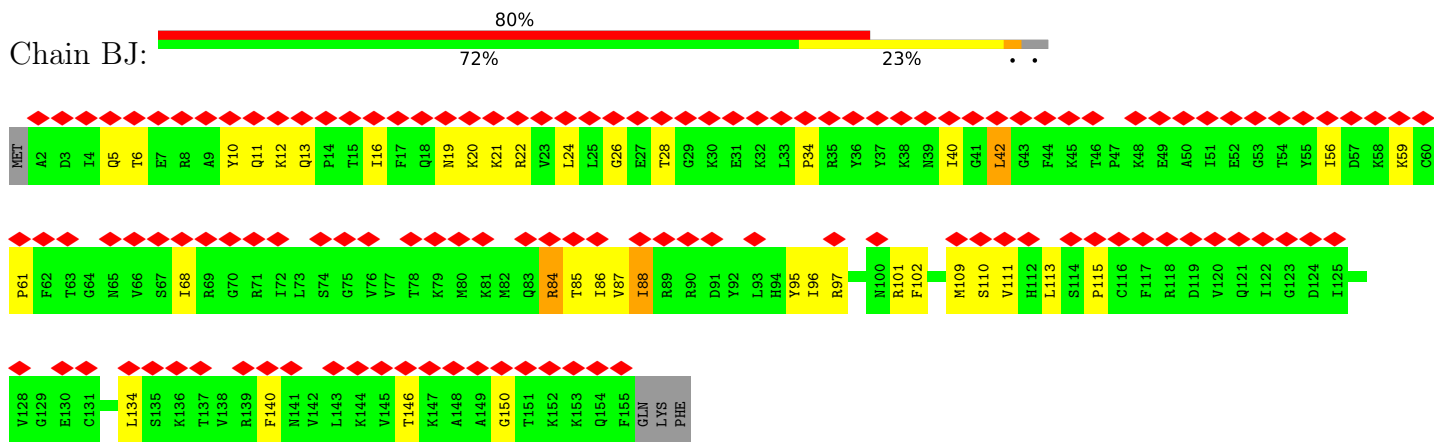
• Molecule 53: 40S ribosomal protein S8



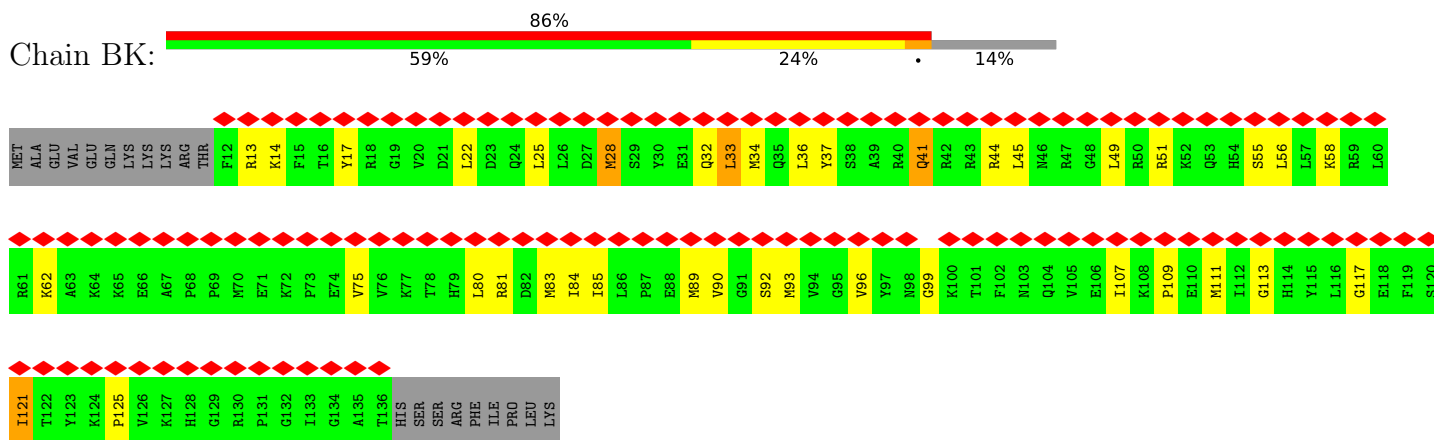
• Molecule 54: 40S ribosomal protein S10



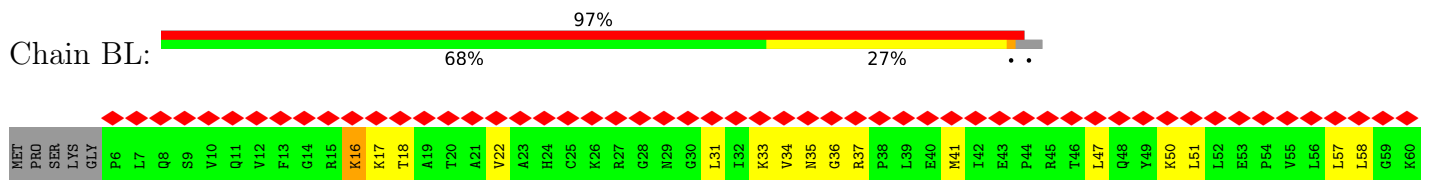
- Molecule 55: 40S ribosomal protein S11

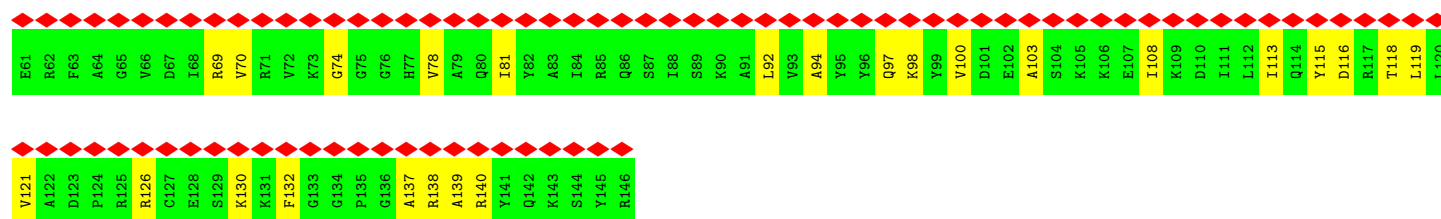


- Molecule 56: 40S ribosomal protein S15



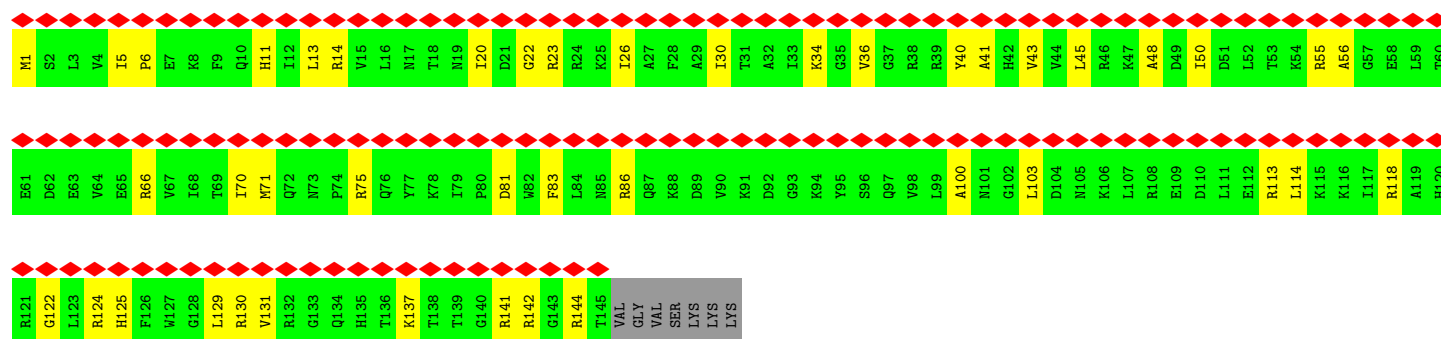
- Molecule 57: 40S ribosomal protein S16





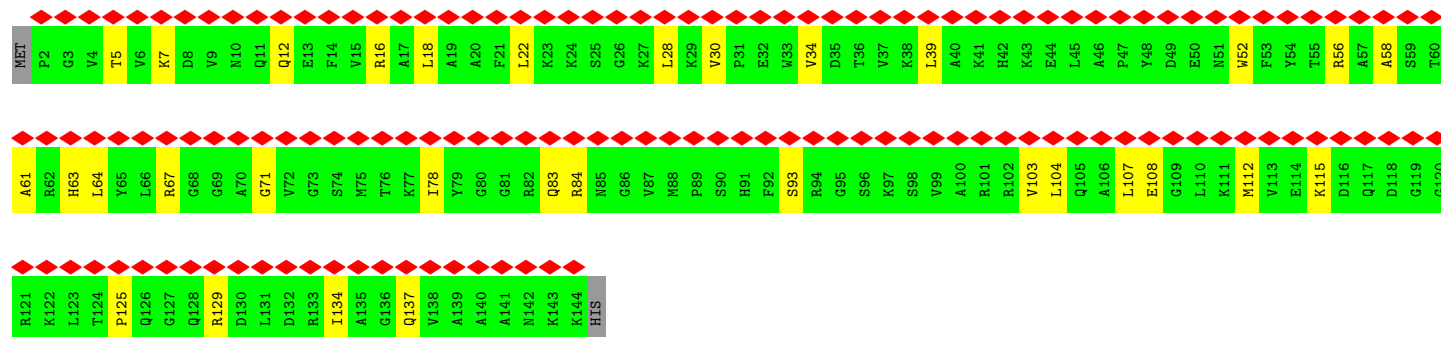
• Molecule 58: 40S ribosomal protein S18

Chain BM:



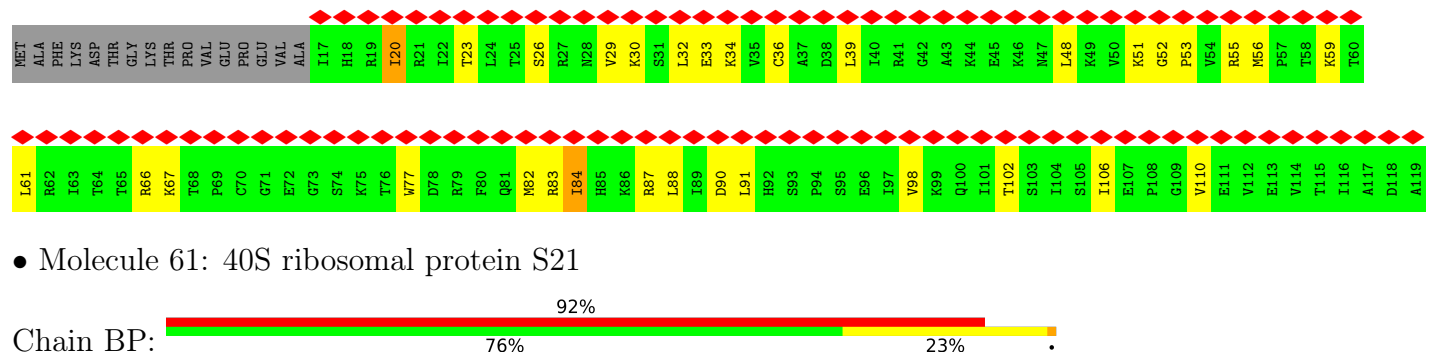
• Molecule 59: Small ribosomal subunit protein eS19

Chain BN:



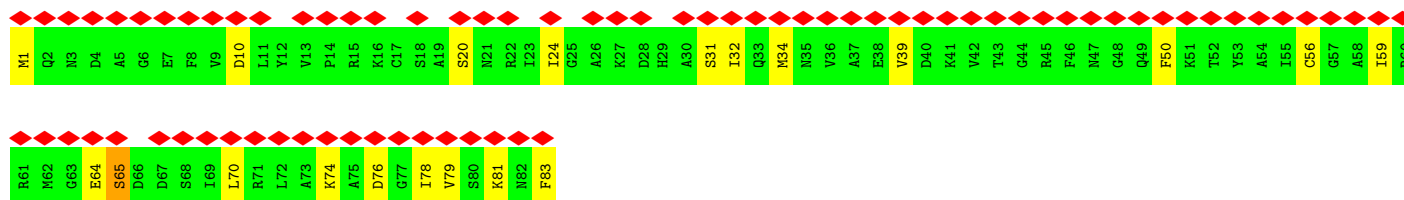
• Molecule 60: 40S ribosomal protein S20

Chain BO:

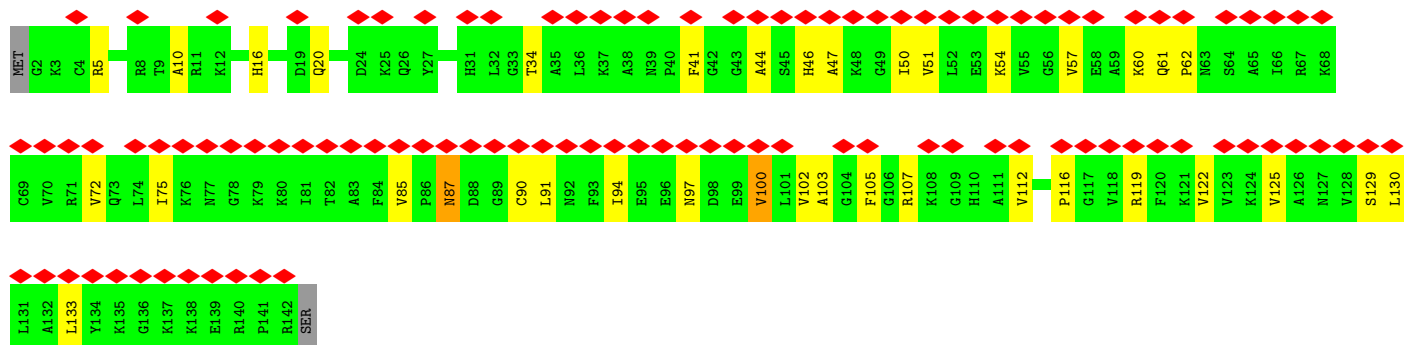
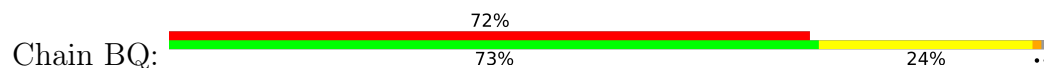


• Molecule 61: 40S ribosomal protein S21

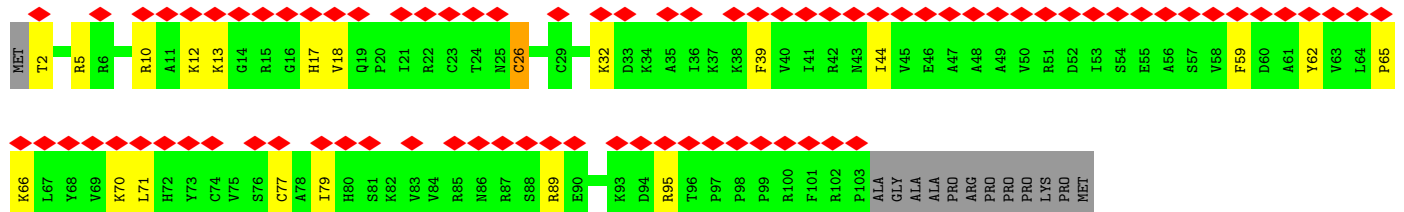
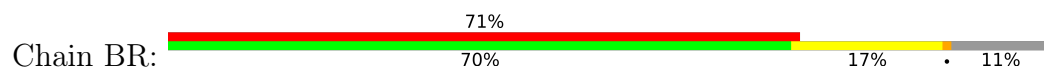
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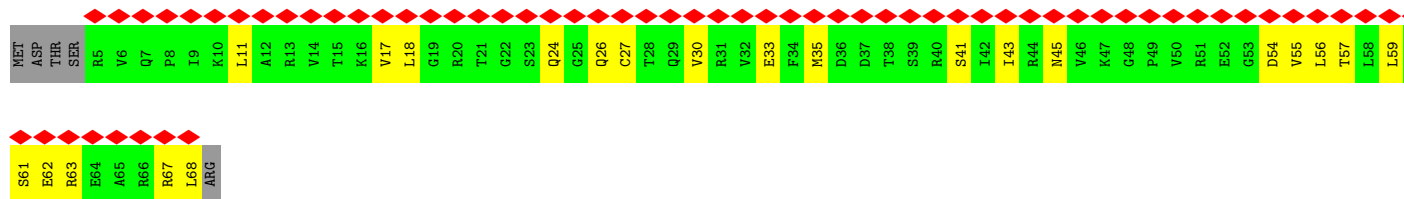
• Molecule 62: 40S ribosomal protein S23



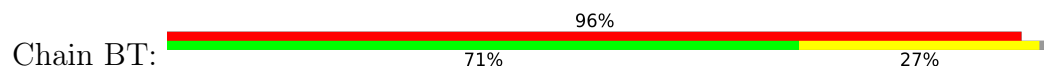
• Molecule 63: 40S ribosomal protein S26



• Molecule 64: 40S ribosomal protein S28

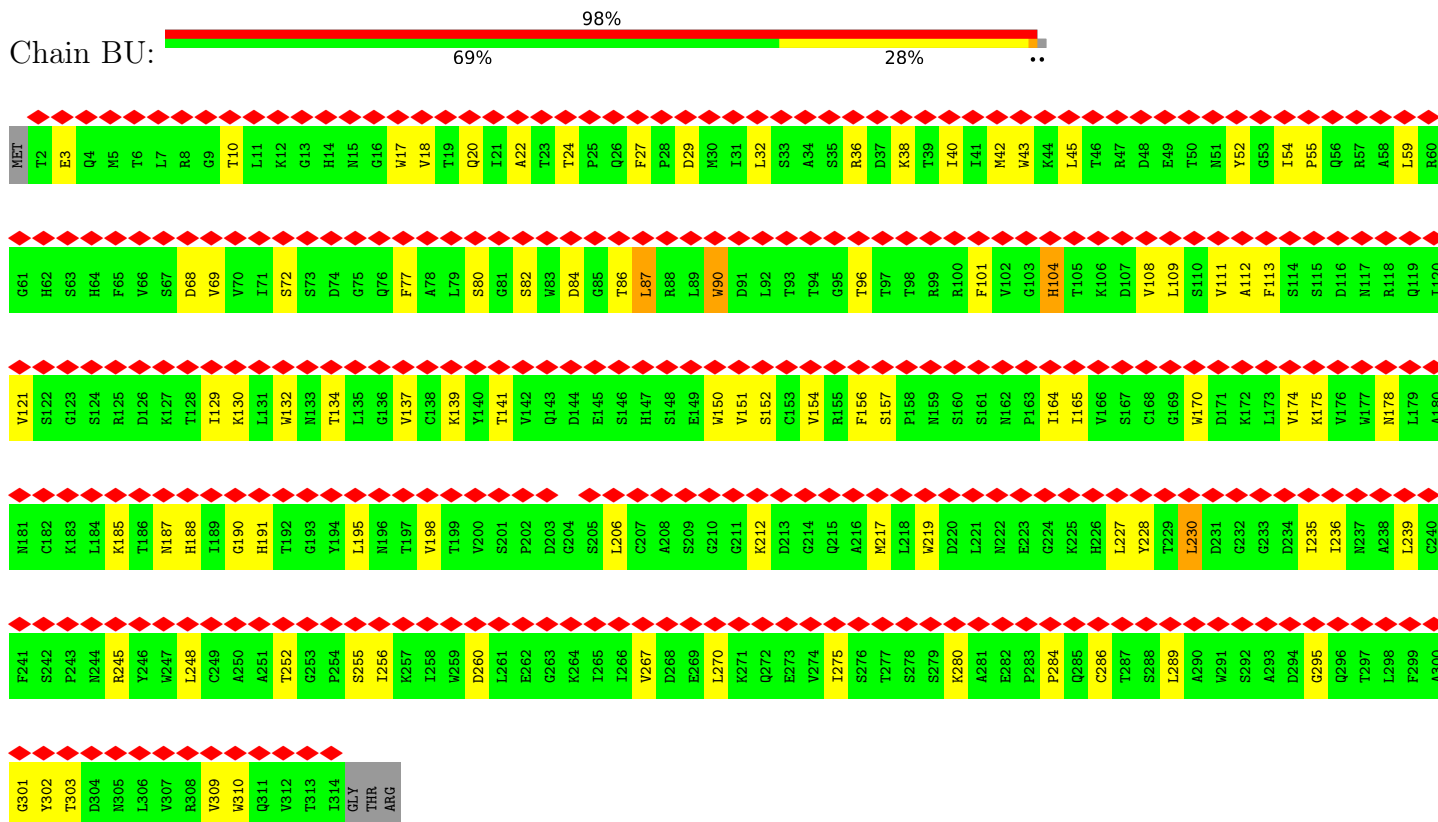


• Molecule 65: 40S ribosomal protein S29



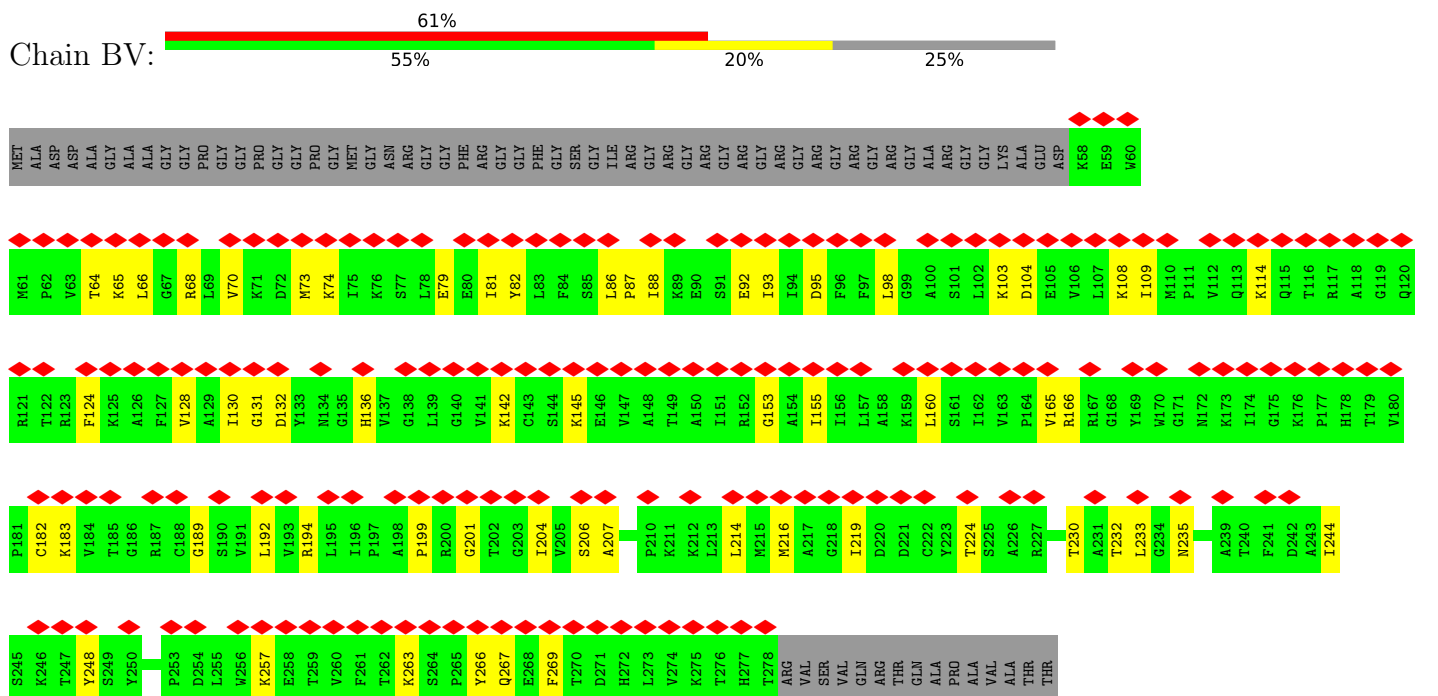
- Molecule 66: Receptor of activated protein C kinase 1

Chain BU:



- Molecule 67: 40S ribosomal protein S2

Chain BV:



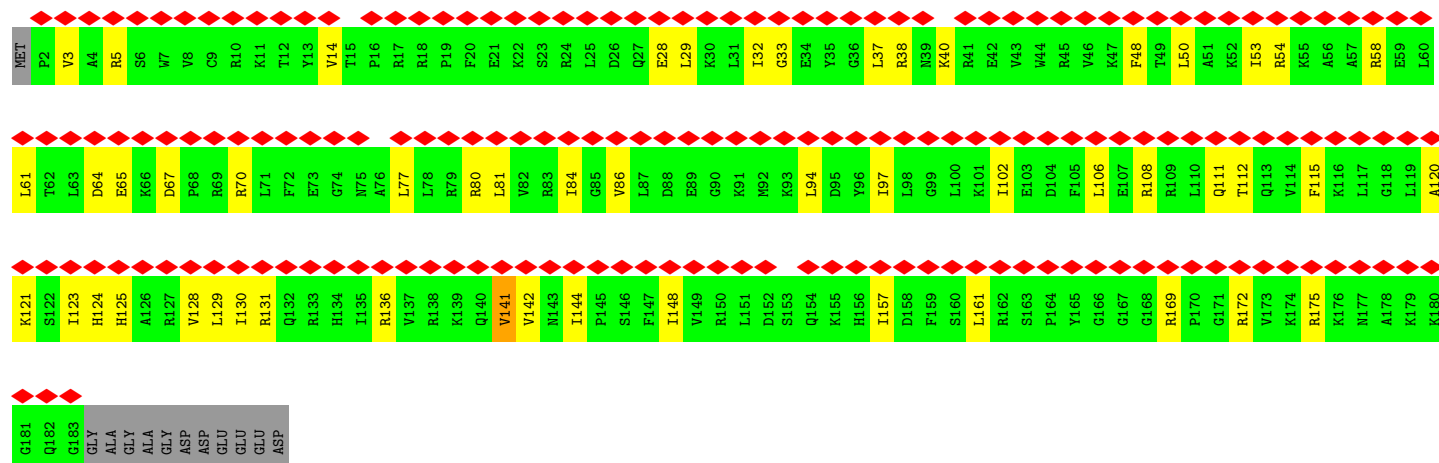
- Molecule 68: 40S ribosomal protein S6

Chain BW:

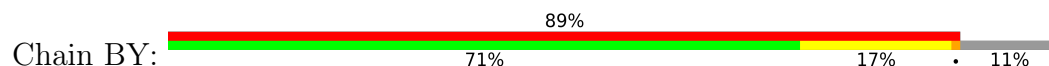




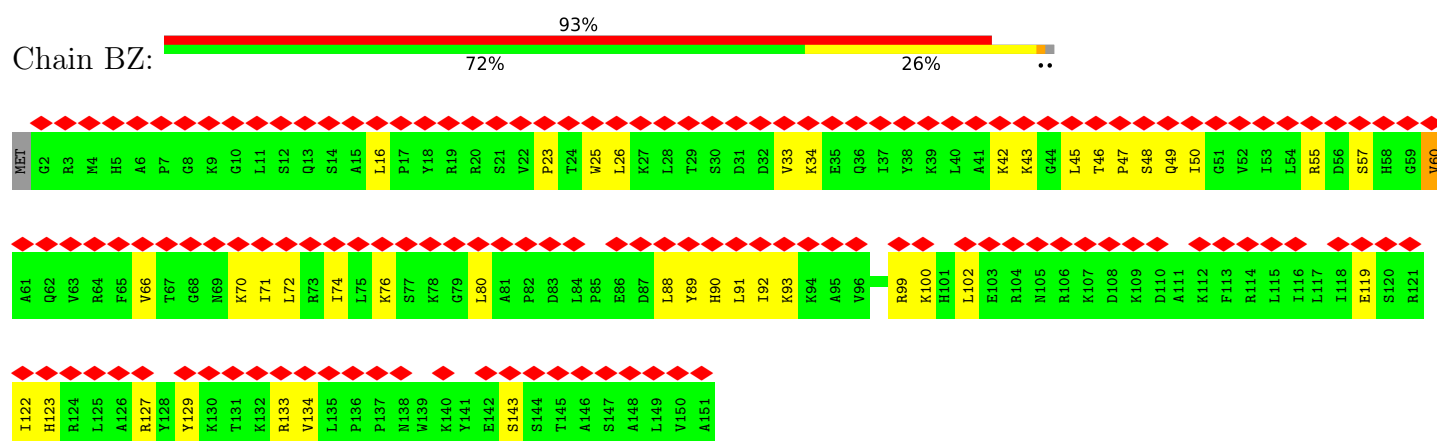
• Molecule 69: 40S ribosomal protein S9



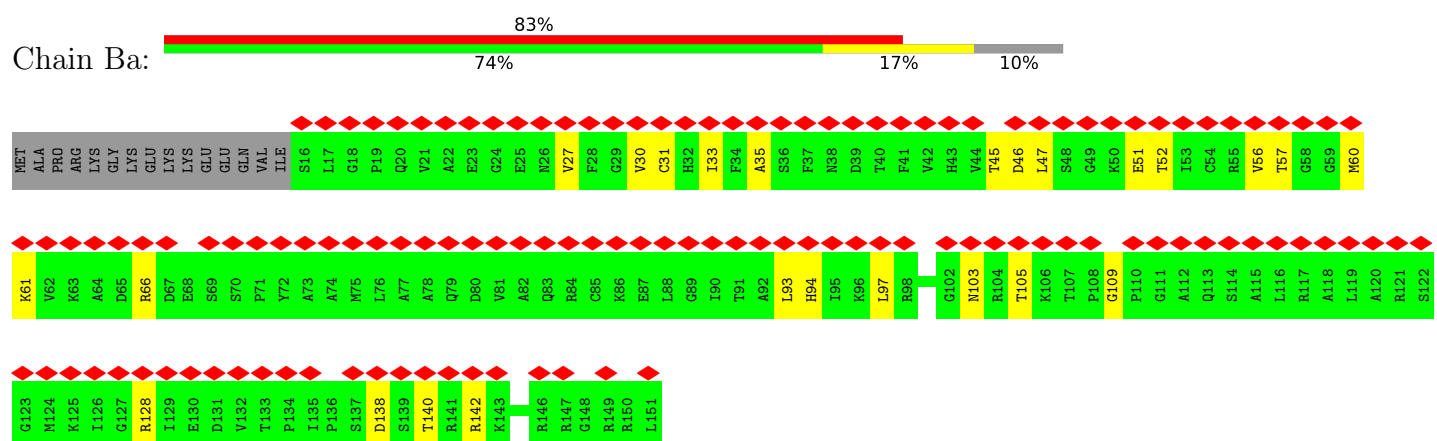
• Molecule 70: 40S ribosomal protein S12



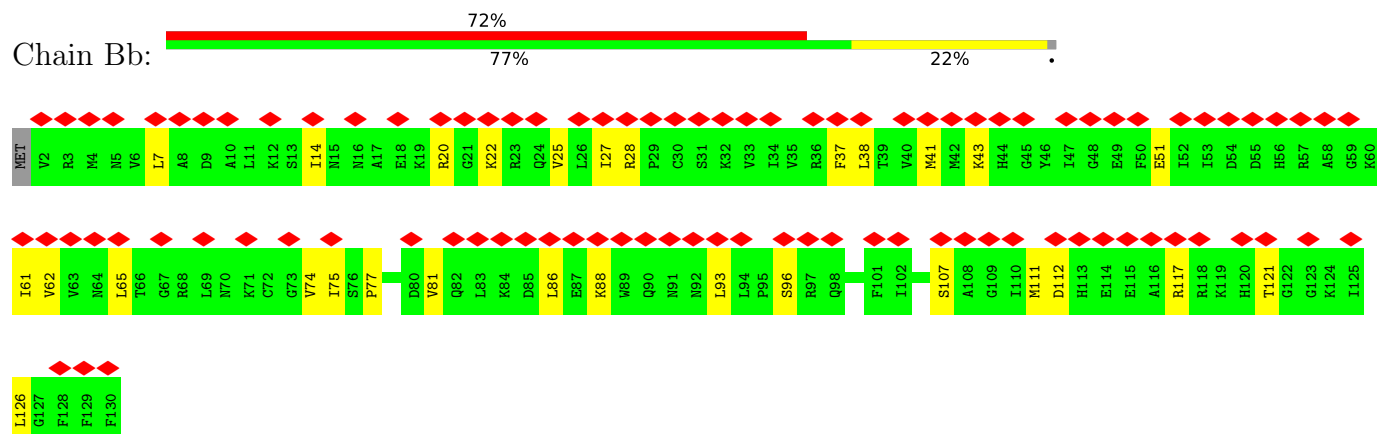
• Molecule 71: 40S ribosomal protein S13



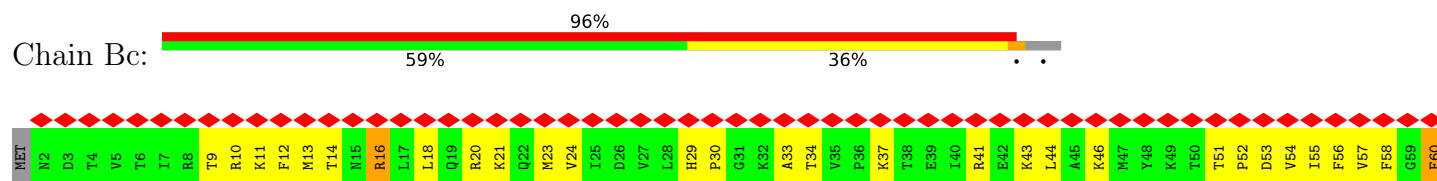
• Molecule 72: Small ribosomal subunit protein uS11



• Molecule 73: 40S ribosomal protein S15a

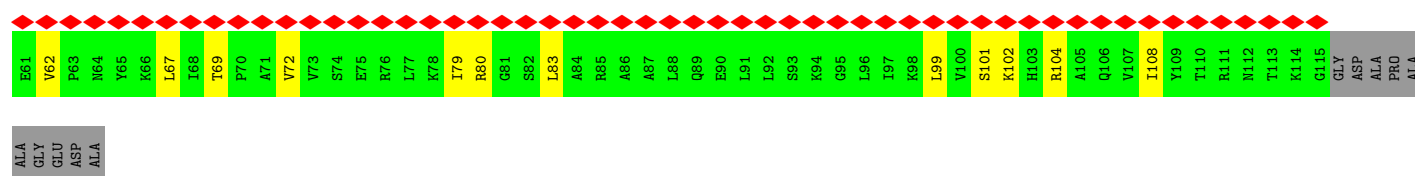
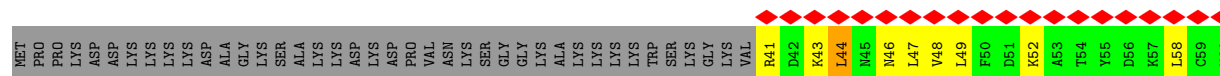
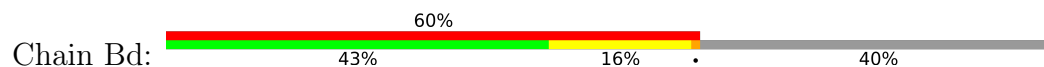


• Molecule 74: 40S ribosomal protein S24

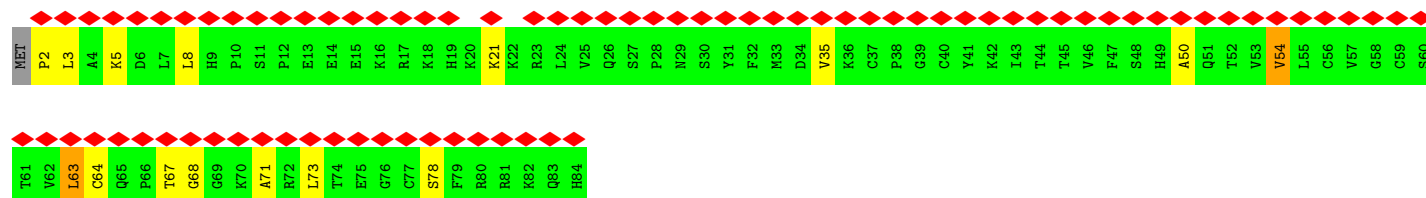
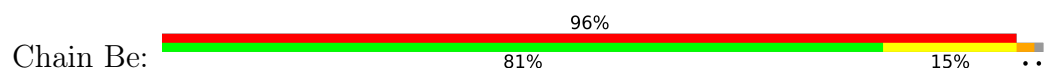




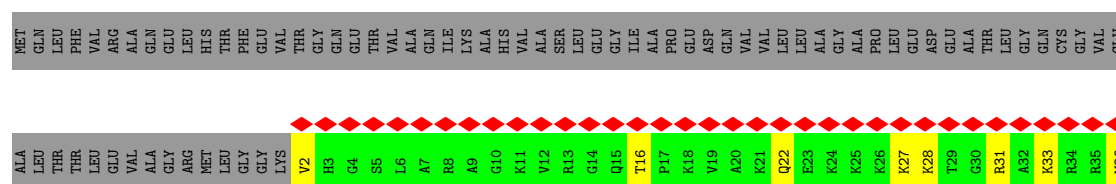
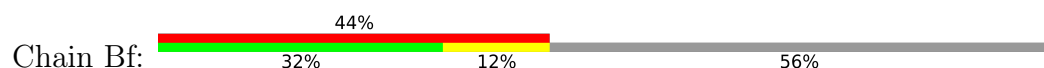
- Molecule 75: 40S ribosomal protein S25



- Molecule 76: 40S ribosomal protein S27



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



ILE	GLN	LYS	GLU	SER	THR	LEU	HIS	LEU	VAL	LEU	ARG	LEU	ARG	ARG	GLY	GLY	ALA	LYS	LYS	ARG	LYS	LYS	LYS	SER	Y85	T86	T87	P88	K89	K90	N91	K92	H93	H94	R95	K96	K97	V98	K99	L100	A101	V102	L103	K104	Y105	Y106	K107	V108	D109	E110	N111	G112	K113	I114	S115	R116	L117	R118	R119	E120
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C121	P122	S123	D124	E125	C126	G127	A128	G129	V130	F131	M132	A133	S134	H135	F136	D137	R138	H139	Y140	C141	G142	K143	C144	C145	L146	T147	Y148	C149	F150	N151	LYS	PRO	GLU	ASP	LYS
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● Molecule 79: 40S ribosomal protein S17



MET	G2	R3	V4	R5	T6	K7	T8	V9	K10	K11	A12	A13	R14	V15	I16	I17	E18	K19	Y20	Y21	T22	R23	L24	G25	N26	D27	F28	H29	T30	N31	K32	R33	V34	C35	E36	E37	I38	A39	I40	I41	P42	S43	K44	K45	L46	R47	M48	K49	I50	A51	G52	V53	V54	T55	H56	L57	M58	K59	R60
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I61	Q62	R63	G64	P65	V66	R67	G68	I69	S70	I71	K72	L73	Q74	E75	E76	E77	R78	E79	R80	R81	D82	N83	Y84	V85	P86	E87	V88	S89	A90	L91	D92	Q93	E94	I95	I96	E97	V98	D99	P100	D101	T102	K103	E104	M105	L106	K107	L108	L109	D110	F111	G112	S113	L114	S115	N116	L117	Q118	V119	T120
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Q121	P122	T123	V124	G125	M126	N127	F128	K129	T130	P131	R132	GLY	PRO	VAL
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64802	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	1.939	Depositor
Minimum map value	-1.142	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.29	Depositor
Map size (Å)	515.83997, 515.83997, 515.83997	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.80599993, 0.80599993, 0.80599993	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.21	0/86721	0.30	0/135215
2	AB	0.19	0/2858	0.26	0/4455
3	AC	0.20	0/3609	0.28	0/5623
4	AD	0.20	0/1936	0.33	0/2596
5	AE	0.19	0/3294	0.32	0/4406
6	AF	0.18	0/2981	0.36	0/4002
7	AG	0.16	0/2428	0.32	0/3252
8	AH	0.16	0/1942	0.34	0/2606
9	AI	0.20	0/1916	0.35	0/2553
10	AJ	0.19	0/1971	0.42	0/2651
11	AK	0.17	0/1537	0.29	0/2066
12	AL	0.18	0/1753	0.34	0/2343
13	AM	0.16	0/1433	0.41	0/1915
14	AN	0.18	0/1732	0.40	0/2315
15	AO	0.16	0/1161	0.30	0/1554
16	AP	0.20	0/1746	0.36	0/2338
17	AQ	0.19	0/1682	0.31	0/2250
18	AR	0.19	0/1268	0.33	0/1701
19	AS	0.18	0/1537	0.34	0/2052
20	AT	0.15	0/1582	0.28	0/2091
21	AU	0.20	0/1493	0.32	0/2003
22	AV	0.19	0/1326	0.34	0/1770
23	AW	0.20	0/839	0.52	0/1126
24	AX	0.19	0/993	0.32	0/1332
25	AY	0.15	0/876	0.32	0/1162
26	AZ	0.18	0/1002	0.37	0/1345
27	Aa	0.19	0/1119	0.42	0/1488
28	Ab	0.17	0/1130	0.34	0/1507
29	Ac	0.19	0/1179	0.32	0/1573
30	Ad	0.16	0/821	0.36	0/1084
31	Ae	0.17	0/774	0.36	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Af	0.18	0/894	0.32	0/1204
33	Ag	0.20	0/1071	0.44	0/1429
34	Ah	0.20	0/895	0.30	0/1198
35	Ai	0.23	0/878	0.36	0/1170
36	Aj	0.14	0/1023	0.33	0/1351
37	Ak	0.16	0/824	0.35	0/1090
38	Al	0.19	0/720	0.33	0/952
39	Am	0.21	0/565	0.45	0/750
40	An	0.20	0/454	0.39	0/599
41	Ao	0.16	0/425	0.31	0/564
42	Ap	0.16	0/231	0.41	0/294
43	Aq	0.17	0/858	0.28	0/1131
44	Ar	0.19	0/691	0.36	0/919
45	As	0.20	0/1002	0.39	0/1344
46	BA	0.17	2/39082 (0.0%)	0.32	5/60892 (0.0%)
47	BB	0.13	0/2102	0.38	0/2828
48	BC	0.16	0/1764	0.38	0/2396
49	BD	0.13	0/1774	0.38	0/2373
50	BE	0.14	0/1793	0.36	0/2414
51	BF	0.15	0/1531	0.42	0/2059
52	BG	0.14	0/1519	0.38	0/2033
53	BH	0.13	0/1715	0.34	0/2287
54	BI	0.15	0/840	0.44	0/1133
55	BJ	0.15	0/1280	0.41	0/1712
56	BK	0.18	0/1047	0.52	0/1399
57	BL	0.14	0/1142	0.42	0/1528
58	BM	0.13	0/1216	0.44	0/1628
59	BN	0.12	0/1119	0.34	0/1498
60	BO	0.17	0/827	0.42	0/1110
61	BP	0.14	0/643	0.38	0/860
62	BQ	0.16	0/1116	0.40	0/1490
63	BR	0.12	0/836	0.29	0/1121
64	BS	0.14	0/508	0.42	0/680
65	BT	0.13	0/470	0.34	0/623
66	BU	0.15	0/2493	0.43	0/3394
67	BV	0.15	0/1764	0.41	0/2382
68	BW	0.15	0/1926	0.43	0/2563
69	BX	0.17	0/1548	0.44	0/2066
70	BY	0.11	0/916	0.35	0/1233
71	BZ	0.17	0/1232	0.42	0/1656
72	Ba	0.13	0/1020	0.36	0/1366
73	Bb	0.15	0/1051	0.41	0/1406
74	Bc	0.16	0/1068	0.42	0/1418

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Bd	0.13	0/604	0.37	0/810
76	Be	0.15	0/665	0.41	0/891
77	Bf	0.13	0/465	0.35	0/612
78	Bg	0.11	0/560	0.35	0/745
79	Bh	0.13	0/1078	0.39	0/1447
All	All	0.19	2/225884 (0.0%)	0.33	5/331460 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	BA	668	A2M	O3'-P	5.18	1.61	1.56
46	BA	590	A2M	O3'-P	5.02	1.61	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BA	1639	G7M	O3'-P-O5'	-23.84	58.71	104.00
46	BA	1639	G7M	P-O3'-C3'	18.30	141.66	119.70
46	BA	3	C	C4'-C3'-O3'	8.73	126.10	113.00
46	BA	1639	G7M	OP1-P-O3'	8.42	123.73	105.20
46	BA	3	C	C2'-C3'-O3'	-6.95	103.28	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	80204	0	40480	668	0
2	AB	2558	0	1295	8	0
3	AC	3316	0	1687	25	0
4	AD	1898	0	1993	18	0
5	AE	3239	0	3374	35	0
6	AF	2927	0	3104	52	0
7	AG	2382	0	2410	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AH	1904	0	2055	27	0
9	AI	1878	0	2009	26	0
10	AJ	1935	0	2087	24	0
11	AK	1518	0	1601	15	0
12	AL	1713	0	1751	18	0
13	AM	1410	0	1441	21	0
14	AN	1701	0	1818	34	0
15	AO	1138	0	1204	8	0
16	AP	1701	0	1749	15	0
17	AQ	1650	0	1794	22	0
18	AR	1242	0	1269	17	0
19	AS	1513	0	1628	20	0
20	AT	1566	0	1729	16	0
21	AU	1453	0	1490	13	0
22	AV	1298	0	1366	7	0
23	AW	825	0	850	7	0
24	AX	979	0	1039	4	0
25	AY	863	0	905	4	0
26	AZ	985	0	1066	12	0
27	Aa	1102	0	1189	23	0
28	Ab	1107	0	1182	11	0
29	Ac	1163	0	1206	17	0
30	Ad	808	0	875	12	0
31	Ae	764	0	804	3	0
32	Af	879	0	924	11	0
33	Ag	1053	0	1147	12	0
34	Ah	876	0	910	6	0
35	Ai	868	0	959	10	0
36	Aj	1015	0	1148	10	0
37	Ak	813	0	894	15	0
38	Al	705	0	737	6	0
39	Am	559	0	624	11	0
40	An	444	0	483	3	0
41	Ao	419	0	452	5	0
42	Ap	230	0	276	2	0
43	Aq	842	0	914	6	0
44	Ar	681	0	731	4	0
45	As	987	0	1050	19	0
46	BA	36916	0	18641	506	0
47	BB	2060	0	2157	57	0
48	BC	1727	0	1729	45	0
49	BD	1747	0	1822	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	BE	1765	0	1865	26	0
51	BF	1509	0	1563	37	0
52	BG	1497	0	1590	21	0
53	BH	1686	0	1772	36	0
54	BI	816	0	841	17	0
55	BJ	1258	0	1332	23	0
56	BK	1027	0	1073	28	0
57	BL	1124	0	1192	31	0
58	BM	1198	0	1261	33	0
59	BN	1113	0	1145	22	0
60	BO	817	0	880	28	0
61	BP	636	0	637	13	0
62	BQ	1098	0	1167	25	0
63	BR	821	0	870	12	0
64	BS	506	0	536	14	0
65	BT	459	0	448	11	0
66	BU	2436	0	2393	61	0
67	BV	1724	0	1817	42	0
68	BW	1903	0	2068	43	0
69	BX	1520	0	1642	41	0
70	BY	906	0	921	13	0
71	BZ	1208	0	1294	29	0
72	Ba	1016	0	1037	17	0
73	Bb	1034	0	1080	19	0
74	Bc	1048	0	1122	41	0
75	Bd	598	0	656	20	0
76	Be	651	0	672	11	0
77	Bf	459	0	503	14	0
78	Bg	548	0	552	8	0
79	Bh	1064	0	1118	26	0
80	AA	197	0	0	0	0
80	AB	2	0	0	0	0
80	AC	4	0	0	0	0
80	AP	1	0	0	0	0
80	AR	1	0	0	0	0
80	AX	1	0	0	0	0
80	BA	62	0	0	0	0
80	BL	2	0	0	0	0
80	BN	1	0	0	0	0
81	AA	65	0	0	0	0
81	AB	1	0	0	0	0
81	AD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	AL	1	0	0	0	0
81	Ag	1	0	0	0	0
81	Ah	1	0	0	0	0
81	Aq	1	0	0	0	0
81	BA	12	0	0	0	0
82	Ai	1	0	0	0	0
82	Al	1	0	0	0	0
82	Ao	1	0	0	0	0
82	Aq	1	0	0	0	0
82	Ar	1	0	0	0	0
82	BR	1	0	0	0	0
82	BT	1	0	0	0	0
82	Bg	1	0	0	0	0
All	All	215368	0	159095	2401	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 6.

The worst 5 of 2401 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BA:1451:G:H21	46:BA:1474:A:N6	1.56	1.03
46:BA:1451:G:N2	46:BA:1474:A:H61	1.57	1.01
46:BA:1560:U:H3	46:BA:1575:G:H1	1.06	1.01
46:BA:1656:G:H1	46:BA:1668:U:H3	1.10	0.98
46:BA:1260:A:C2	46:BA:1617:G:N2	2.33	0.97

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	246/257 (96%)	236 (96%)	10 (4%)	0	100	100
5	AE	399/402 (99%)	388 (97%)	11 (3%)	0	100	100
6	AF	366/368 (100%)	352 (96%)	14 (4%)	0	100	100
7	AG	291/293 (99%)	276 (95%)	15 (5%)	0	100	100
8	AH	232/247 (94%)	221 (95%)	11 (5%)	0	100	100
9	AI	224/248 (90%)	219 (98%)	5 (2%)	0	100	100
10	AJ	240/266 (90%)	233 (97%)	7 (3%)	0	100	100
11	AK	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
12	AL	211/214 (99%)	200 (95%)	11 (5%)	0	100	100
13	AM	174/178 (98%)	160 (92%)	14 (8%)	0	100	100
14	AN	208/211 (99%)	196 (94%)	11 (5%)	1 (0%)	24	48
15	AO	137/215 (64%)	132 (96%)	5 (4%)	0	100	100
16	AP	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
17	AQ	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
18	AR	151/184 (82%)	149 (99%)	2 (1%)	0	100	100
19	AS	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
20	AT	185/196 (94%)	185 (100%)	0	0	100	100
21	AU	173/176 (98%)	167 (96%)	6 (4%)	0	100	100
22	AV	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
23	AW	99/128 (77%)	94 (95%)	5 (5%)	0	100	100
24	AX	129/140 (92%)	127 (98%)	2 (2%)	0	100	100
25	AY	103/157 (66%)	98 (95%)	5 (5%)	0	100	100
26	AZ	118/156 (76%)	114 (97%)	4 (3%)	0	100	100
27	Aa	130/145 (90%)	125 (96%)	5 (4%)	0	100	100
28	Ab	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
29	Ac	144/148 (97%)	138 (96%)	6 (4%)	0	100	100
30	Ad	95/159 (60%)	93 (98%)	2 (2%)	0	100	100
31	Ae	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
32	Af	104/125 (83%)	102 (98%)	2 (2%)	0	100	100
33	Ag	126/135 (93%)	126 (100%)	0	0	100	100
34	Ah	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
35	Ai	107/117 (92%)	107 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Aj	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
37	Ak	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
38	Al	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
39	Am	66/70 (94%)	66 (100%)	0	0	100	100
40	An	48/51 (94%)	48 (100%)	0	0	100	100
41	Ao	49/128 (38%)	49 (100%)	0	0	100	100
42	Ap	22/25 (88%)	22 (100%)	0	0	100	100
43	Aq	101/106 (95%)	98 (97%)	3 (3%)	0	100	100
44	Ar	86/92 (94%)	83 (96%)	3 (4%)	0	100	100
45	As	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
47	BB	258/263 (98%)	250 (97%)	8 (3%)	0	100	100
48	BC	217/295 (74%)	210 (97%)	7 (3%)	0	100	100
49	BD	213/264 (81%)	206 (97%)	7 (3%)	0	100	100
50	BE	225/243 (93%)	214 (95%)	11 (5%)	0	100	100
51	BF	189/204 (93%)	176 (93%)	13 (7%)	0	100	100
52	BG	182/194 (94%)	169 (93%)	12 (7%)	1 (0%)	24	48
53	BH	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
54	BI	95/165 (58%)	88 (93%)	7 (7%)	0	100	100
55	BJ	152/158 (96%)	140 (92%)	12 (8%)	0	100	100
56	BK	123/145 (85%)	116 (94%)	7 (6%)	0	100	100
57	BL	139/146 (95%)	127 (91%)	12 (9%)	0	100	100
58	BM	143/152 (94%)	135 (94%)	8 (6%)	0	100	100
59	BN	140/145 (97%)	135 (96%)	5 (4%)	0	100	100
60	BO	101/119 (85%)	92 (91%)	9 (9%)	0	100	100
61	BP	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
62	BQ	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
63	BR	100/115 (87%)	97 (97%)	3 (3%)	0	100	100
64	BS	62/69 (90%)	57 (92%)	5 (8%)	0	100	100
65	BT	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
66	BU	311/317 (98%)	285 (92%)	26 (8%)	0	100	100
67	BV	220/293 (75%)	214 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	BW	232/249 (93%)	220 (95%)	12 (5%)	0	100	100
69	BX	181/194 (93%)	175 (97%)	6 (3%)	0	100	100
70	BY	116/132 (88%)	113 (97%)	3 (3%)	0	100	100
71	BZ	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
72	Ba	132/151 (87%)	121 (92%)	11 (8%)	0	100	100
73	Bb	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
74	Bc	127/133 (96%)	118 (93%)	9 (7%)	0	100	100
75	Bd	73/125 (58%)	63 (86%)	10 (14%)	0	100	100
76	Be	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
77	Bf	56/133 (42%)	48 (86%)	8 (14%)	0	100	100
78	Bg	65/156 (42%)	59 (91%)	6 (9%)	0	100	100
79	Bh	129/135 (96%)	127 (98%)	2 (2%)	0	100	100
All	All	11266/12657 (89%)	10806 (96%)	458 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	BG	15	LYS
14	AN	64	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	190/199 (96%)	185 (97%)	5 (3%)	40	70
5	AE	347/347 (100%)	339 (98%)	8 (2%)	44	73
6	AF	306/306 (100%)	298 (97%)	8 (3%)	40	70
7	AG	246/247 (100%)	239 (97%)	7 (3%)	38	68
8	AH	209/220 (95%)	203 (97%)	6 (3%)	37	67
9	AI	195/215 (91%)	189 (97%)	6 (3%)	35	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AJ	204/223 (92%)	195 (96%)	9 (4%)	25	53
11	AK	169/171 (99%)	164 (97%)	5 (3%)	36	66
12	AL	181/182 (100%)	175 (97%)	6 (3%)	33	63
13	AM	148/149 (99%)	141 (95%)	7 (5%)	23	51
14	AN	176/177 (99%)	165 (94%)	11 (6%)	16	39
15	AO	118/161 (73%)	115 (98%)	3 (2%)	42	71
16	AP	171/172 (99%)	163 (95%)	8 (5%)	23	51
17	AQ	173/174 (99%)	170 (98%)	3 (2%)	53	79
18	AR	134/163 (82%)	131 (98%)	3 (2%)	45	74
19	AS	164/165 (99%)	154 (94%)	10 (6%)	17	40
20	AT	166/175 (95%)	161 (97%)	5 (3%)	36	66
21	AU	156/157 (99%)	154 (99%)	2 (1%)	61	83
22	AV	139/140 (99%)	134 (96%)	5 (4%)	31	60
23	AW	91/115 (79%)	86 (94%)	5 (6%)	19	45
24	AX	101/107 (94%)	97 (96%)	4 (4%)	28	56
25	AY	87/126 (69%)	83 (95%)	4 (5%)	24	51
26	AZ	108/133 (81%)	104 (96%)	4 (4%)	30	59
27	Aa	123/135 (91%)	121 (98%)	2 (2%)	55	80
28	Ab	117/118 (99%)	112 (96%)	5 (4%)	26	54
29	Ac	119/120 (99%)	117 (98%)	2 (2%)	53	79
30	Ad	83/126 (66%)	81 (98%)	2 (2%)	43	72
31	Ae	83/97 (86%)	80 (96%)	3 (4%)	31	60
32	Af	97/110 (88%)	97 (100%)	0	100	100
33	Ag	114/121 (94%)	110 (96%)	4 (4%)	32	61
34	Ah	88/89 (99%)	85 (97%)	3 (3%)	32	62
35	Ai	94/100 (94%)	93 (99%)	1 (1%)	65	85
36	Aj	109/110 (99%)	105 (96%)	4 (4%)	30	59
37	Ak	85/89 (96%)	80 (94%)	5 (6%)	18	42
38	Al	73/80 (91%)	71 (97%)	2 (3%)	39	69
39	Am	63/65 (97%)	61 (97%)	2 (3%)	34	64
40	An	47/48 (98%)	43 (92%)	4 (8%)	10	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	Ao	47/116 (40%)	46 (98%)	1 (2%)	47	75
42	Ap	23/24 (96%)	23 (100%)	0	100	100
43	Aq	91/94 (97%)	89 (98%)	2 (2%)	45	74
44	Ar	71/75 (95%)	68 (96%)	3 (4%)	26	55
45	As	107/121 (88%)	100 (94%)	7 (6%)	15	37
47	BB	223/225 (99%)	218 (98%)	5 (2%)	45	74
48	BC	182/243 (75%)	170 (93%)	12 (7%)	15	36
49	BD	196/231 (85%)	188 (96%)	8 (4%)	27	56
50	BE	190/202 (94%)	182 (96%)	8 (4%)	26	55
51	BF	161/170 (95%)	157 (98%)	4 (2%)	42	71
52	BG	166/174 (95%)	159 (96%)	7 (4%)	26	55
53	BH	178/180 (99%)	173 (97%)	5 (3%)	38	68
54	BI	88/136 (65%)	84 (96%)	4 (4%)	24	52
55	BJ	138/142 (97%)	127 (92%)	11 (8%)	11	28
56	BK	111/130 (85%)	106 (96%)	5 (4%)	24	52
57	BL	117/121 (97%)	111 (95%)	6 (5%)	21	48
58	BM	126/132 (96%)	122 (97%)	4 (3%)	34	64
59	BN	112/114 (98%)	109 (97%)	3 (3%)	39	69
60	BO	94/107 (88%)	92 (98%)	2 (2%)	47	75
61	BP	67/67 (100%)	65 (97%)	2 (3%)	36	66
62	BQ	113/115 (98%)	107 (95%)	6 (5%)	20	46
63	BR	89/98 (91%)	84 (94%)	5 (6%)	19	44
64	BS	57/62 (92%)	53 (93%)	4 (7%)	14	34
65	BT	48/49 (98%)	46 (96%)	2 (4%)	26	55
66	BU	272/275 (99%)	257 (94%)	15 (6%)	19	45
67	BV	188/225 (84%)	182 (97%)	6 (3%)	34	64
68	BW	204/218 (94%)	191 (94%)	13 (6%)	16	38
69	BX	162/168 (96%)	156 (96%)	6 (4%)	30	59
70	BY	98/108 (91%)	96 (98%)	2 (2%)	48	76
71	BZ	130/131 (99%)	127 (98%)	3 (2%)	44	73
72	Ba	105/118 (89%)	104 (99%)	1 (1%)	68	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	Bb	112/113 (99%)	106 (95%)	6 (5%)	20	45
74	Bc	111/115 (96%)	108 (97%)	3 (3%)	39	69
75	Bd	66/103 (64%)	64 (97%)	2 (3%)	36	66
76	Be	75/76 (99%)	73 (97%)	2 (3%)	39	69
77	Bf	47/104 (45%)	44 (94%)	3 (6%)	16	38
78	Bg	60/140 (43%)	59 (98%)	1 (2%)	53	79
79	Bh	119/122 (98%)	112 (94%)	7 (6%)	18	42
All	All	9818/10776 (91%)	9459 (96%)	359 (4%)	32	59

5 of 359 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	BH	56	ARG
64	BS	57	THR
54	BI	96	ARG
57	BL	121	VAL
66	BU	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
53	BH	64	ASN
60	BO	47	ASN
54	BI	50	GLN
58	BM	101	ASN
65	BT	26	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	3705/5069 (73%)	831 (22%)	12 (0%)
2	AB	119/120 (99%)	8 (6%)	0
3	AC	155/157 (98%)	30 (19%)	0
46	BA	1713/1869 (91%)	479 (27%)	4 (0%)
All	All	5692/7215 (78%)	1348 (23%)	16 (0%)

5 of 1348 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	3	C
1	AA	12	A
1	AA	13	U
1	AA	15	A
1	AA	21	G

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	BA	866	PSU
46	BA	688	U
1	AA	3614	G
46	BA	369	C
1	AA	2675	G

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	$\# Z > 2$
1	OMU	AA	2837	1	19,22,23	1.26	3 (15%)	26,31,34	1.78	4 (15%)
1	A2M	AA	2787	1	22,25,26	1.42	4 (18%)	31,36,39	2.27	8 (25%)
3	OMG	AC	75	3	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
46	OMU	BA	116	46	19,22,23	1.22	4 (21%)	26,31,34	1.68	5 (19%)
46	A2M	BA	1383	46	22,25,26	1.47	4 (18%)	31,36,39	2.14	9 (29%)
1	PSU	AA	3851	1	18,21,22	1.41	3 (16%)	22,30,33	1.89	3 (13%)
1	PSU	AA	1683	81,1	18,21,22	1.42	3 (16%)	22,30,33	1.90	3 (13%)
1	OMG	AA	2424	1	23,26,27	1.20	3 (13%)	33,38,41	1.90	6 (18%)
46	A2M	BA	166	46	22,25,26	1.45	4 (18%)	31,36,39	2.26	10 (32%)
3	PSU	AC	55	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	3 (13%)
46	PSU	BA	801	46	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	AA	2422	80,1	19,22,23	0.81	0	26,31,34	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	AA	3718	1	22,25,26	1.48	4 (18%)	31,36,39	1.91	6 (19%)
1	PSU	AA	3764	1	18,21,22	1.39	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	AA	4471	1	18,21,22	1.42	3 (16%)	22,30,33	1.83	3 (13%)
46	OMU	BA	172	46	19,22,23	1.22	3 (15%)	26,31,34	1.75	5 (19%)
46	G7M	BA	1639	46	23,26,27	5.05	20 (86%)	35,39,42	1.71	7 (20%)
46	A2M	BA	468	46	22,25,26	1.48	4 (18%)	31,36,39	2.01	9 (29%)
46	PSU	BA	1643	46	18,21,22	1.34	2 (11%)	22,30,33	1.96	5 (22%)
1	A2M	AA	3830	1	22,25,26	1.46	4 (18%)	31,36,39	2.07	10 (32%)
1	PSU	AA	4457	1	18,21,22	1.39	3 (16%)	22,30,33	1.95	5 (22%)
46	OMC	BA	1391	46	19,22,23	0.85	0	26,31,34	1.11	2 (7%)
1	PSU	AA	4689	1	18,21,22	1.42	4 (22%)	22,30,33	1.81	3 (13%)
1	A2M	AA	3825	1	22,25,26	1.45	4 (18%)	31,36,39	2.04	8 (25%)
1	PSU	AA	4973	1	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
46	OMC	BA	1703	46	19,22,23	0.81	0	26,31,34	0.79	0
1	PSU	AA	3844	1	18,21,22	1.39	3 (16%)	22,30,33	1.88	3 (13%)
46	OMG	BA	1447	46	23,26,27	1.18	3 (13%)	33,38,41	1.92	6 (18%)
1	PSU	AA	4299	1	18,21,22	1.39	3 (16%)	22,30,33	1.81	3 (13%)
1	OMG	AA	1625	81,1	23,26,27	1.22	3 (13%)	33,38,41	1.91	6 (18%)
46	OMG	BA	1490	46,80	23,26,27	1.23	3 (13%)	33,38,41	1.94	6 (18%)
46	PSU	BA	1445	46	18,21,22	1.39	2 (11%)	22,30,33	1.81	3 (13%)
46	PSU	BA	1232	46	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	AA	3724	1	22,25,26	1.44	4 (18%)	31,36,39	2.09	10 (32%)
1	OMU	AA	4227	1	19,22,23	1.28	4 (21%)	26,31,34	1.73	4 (15%)
1	OMC	AA	3841	1	19,22,23	0.80	0	26,31,34	0.72	0
1	PSU	AA	3762	1	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
1	OMU	AA	4620	1	19,22,23	1.29	3 (15%)	26,31,34	1.69	4 (15%)
1	PSU	AA	1744	1	18,21,22	1.39	3 (16%)	22,30,33	1.92	3 (13%)
46	PSU	BA	1177	46	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	AA	1323	1	22,25,26	1.46	4 (18%)	31,36,39	2.10	8 (25%)
46	A2M	BA	484	46	22,25,26	1.47	4 (18%)	31,36,39	2.27	9 (29%)
1	PSU	AA	4673	81,1	18,21,22	1.41	3 (16%)	22,30,33	1.81	3 (13%)
46	OMG	BA	867	46	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
1	PSU	AA	1862	1	18,21,22	1.37	3 (16%)	22,30,33	1.92	3 (13%)
1	OMU	AA	2415	1	19,22,23	1.24	4 (21%)	26,31,34	1.75	5 (19%)
1	5MC	AA	3782	80,1	18,22,23	0.94	2 (11%)	26,32,35	1.23	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	AA	4494	1	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
1	PSU	AA	3768	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
46	PSU	BA	1692	46	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	AA	4590	1	22,25,26	1.43	4 (18%)	31,36,39	2.07	9 (29%)
46	PSU	BA	1056	46	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
46	OMC	BA	1272	46	19,22,23	0.83	0	26,31,34	0.87	1 (3%)
3	OMU	AC	14	1,3	19,22,23	1.25	3 (15%)	26,31,34	1.81	6 (23%)
72	IAS	Ba	138	72	6,7,8	1.08	0	6,8,10	1.45	0
46	OMG	BA	436	46	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	AA	3770	1	18,21,22	1.39	2 (11%)	22,30,33	1.82	3 (13%)
1	OMC	AA	3869	1	19,22,23	0.82	0	26,31,34	0.78	0
1	OMC	AA	3701	81,1	19,22,23	0.79	0	26,31,34	0.77	0
1	PSU	AA	1582	1	18,21,22	1.41	3 (16%)	22,30,33	1.84	3 (13%)
1	OMG	AA	2876	1	23,26,27	1.21	3 (13%)	33,38,41	1.98	6 (18%)
1	OMC	AA	3808	1	19,22,23	0.85	0	26,31,34	0.91	1 (3%)
1	PSU	AA	3730	1	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
1	6MZ	AA	4220	1	22,25,26	1.40	4 (18%)	30,36,39	2.17	9 (30%)
46	OMU	BA	354	46	19,22,23	1.23	3 (15%)	26,31,34	1.72	4 (15%)
1	UY1	AA	3818	81,1	19,22,23	4.26	8 (42%)	22,31,34	1.98	6 (27%)
46	PSU	BA	822	46	18,21,22	1.41	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	AA	4636	1	18,21,22	1.39	3 (16%)	22,30,33	2.00	5 (22%)
1	PSU	AA	4353	1	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
46	PSU	BA	649	46	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
3	PSU	AC	69	3	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	AA	4361	1	18,21,22	1.41	3 (16%)	22,30,33	1.90	3 (13%)
46	OMC	BA	462	46	19,22,23	0.83	0	26,31,34	0.92	1 (3%)
1	OMC	AA	3887	1	19,22,23	0.83	0	26,31,34	0.91	1 (3%)
46	OMC	BA	174	46	19,22,23	0.84	0	26,31,34	0.93	1 (3%)
1	A2M	AA	2401	1	22,25,26	1.44	5 (22%)	31,36,39	2.08	9 (29%)
1	OMU	AA	4498	80,1	19,22,23	1.22	3 (15%)	26,31,34	1.70	5 (19%)
46	PSU	BA	1046	46	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	AA	2815	81,1	22,25,26	1.45	4 (18%)	31,36,39	2.19	7 (22%)
46	PSU	BA	119	46,80	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
46	PSU	BA	63	46	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
46	OMU	BA	1442	46	19,22,23	1.19	2 (10%)	26,31,34	1.69	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	BA	1625	46	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	AA	4576	1	18,21,22	1.38	2 (11%)	22,30,33	1.85	4 (18%)
1	PSU	AA	3884	1	18,21,22	1.41	3 (16%)	22,30,33	1.86	3 (13%)
46	PSU	BA	1244	46	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
46	PSU	BA	1347	46	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
46	PSU	BA	109	46	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
46	PSU	BA	1003	46	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
46	PSU	BA	651	46	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	AA	1860	1	18,21,22	1.43	4 (22%)	22,30,33	1.87	3 (13%)
1	PSU	AA	2508	1	18,21,22	1.37	3 (16%)	22,30,33	1.86	3 (13%)
1	PSU	AA	4493	81,1	18,21,22	1.41	3 (16%)	22,30,33	1.91	3 (13%)
1	OMG	AA	1522	1	23,26,27	1.20	4 (17%)	33,38,41	1.93	5 (15%)
1	A2M	AA	1534	80,1	22,25,26	1.45	4 (18%)	31,36,39	2.07	8 (25%)
1	OMG	AA	1316	1	23,26,27	1.22	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	AA	1792	1	18,21,22	1.39	3 (16%)	22,30,33	1.82	4 (18%)
1	OMC	AA	1881	80,1	19,22,23	0.84	0	26,31,34	0.90	0
1	PSU	AA	4972	1	18,21,22	1.36	3 (16%)	22,30,33	1.89	3 (13%)
46	PSU	BA	918	46	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
1	OMG	AA	2364	1	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
1	OMU	AA	3925	1	19,22,23	1.26	3 (15%)	26,31,34	1.76	5 (19%)
46	UY1	BA	1326	46	19,22,23	4.41	7 (36%)	22,31,34	1.81	5 (22%)
46	OMU	BA	121	46	19,22,23	1.23	3 (15%)	26,31,34	1.68	4 (15%)
1	PSU	AA	2632	1	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
46	PSU	BA	572	46	18,21,22	1.39	3 (16%)	22,30,33	1.94	4 (18%)
46	PSU	BA	866	46	18,21,22	1.34	2 (11%)	22,30,33	1.99	5 (22%)
1	OMG	AA	4499	1	23,26,27	1.21	3 (13%)	33,38,41	1.94	6 (18%)
1	1MA	AA	1322	80,1	21,25,26	1.36	4 (19%)	31,37,40	1.63	6 (19%)
46	PSU	BA	1174	46	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	OMC	AA	2351	80,1	19,22,23	0.82	0	26,31,34	0.90	1 (3%)
1	PSU	AA	5010	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
46	PSU	BA	406	46	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	AA	5001	1	18,21,22	1.39	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	AA	3920	80,1	18,21,22	1.41	3 (16%)	22,30,33	1.91	4 (18%)
1	A2M	AA	400	1	22,25,26	1.43	4 (18%)	31,36,39	2.07	9 (29%)
1	PSU	AA	4442	1	18,21,22	1.39	3 (16%)	22,30,33	1.92	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	AA	4456	1	19,22,23	0.84	0	26,31,34	0.91	1 (3%)
1	PSU	AA	3637	81,1	18,21,22	1.44	3 (16%)	22,30,33	1.97	5 (22%)
1	PSU	AA	4312	1	18,21,22	1.39	3 (16%)	22,30,33	1.88	3 (13%)
46	PSU	BA	34	46	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	AA	2839	1	18,21,22	1.42	4 (22%)	22,30,33	1.82	3 (13%)
1	OMG	AA	4370	1	23,26,27	1.19	3 (13%)	33,38,41	1.91	6 (18%)
46	A2M	BA	512	46	22,25,26	1.50	4 (18%)	31,36,39	2.02	6 (19%)
1	OMC	AA	2365	80,1	19,22,23	0.81	0	26,31,34	0.75	0
46	OMG	BA	601	46	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
46	4AC	BA	1337	46	21,24,25	1.09	1 (4%)	29,34,37	1.59	6 (20%)
1	PSU	AA	1779	1	18,21,22	1.39	3 (16%)	22,30,33	1.86	3 (13%)
46	PSU	BA	1360	46,80,81	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	AA	3853	80,1	18,21,22	1.40	3 (16%)	22,30,33	1.90	3 (13%)
46	A2M	BA	668	46,80	22,25,26	1.46	4 (18%)	31,36,39	2.08	10 (32%)
1	PSU	AA	4552	1	18,21,22	1.37	3 (16%)	22,30,33	1.97	3 (13%)
46	PSU	BA	1136	46	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	AA	4628	1	18,21,22	1.40	3 (16%)	22,30,33	2.01	3 (13%)
1	PSU	AA	4532	1	18,21,22	1.40	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	AA	4623	1	23,26,27	1.21	4 (17%)	33,38,41	1.96	6 (18%)
1	PSU	AA	4423	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
46	PSU	BA	1596	46	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
46	PSU	BA	863	46	18,21,22	1.36	2 (11%)	22,30,33	1.82	3 (13%)
1	PSU	AA	4403	1	18,21,22	1.39	3 (16%)	22,30,33	1.91	4 (18%)
1	OMG	AA	3627	1	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
46	PSU	BA	1045	46	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	3695	1	18,21,22	1.37	3 (16%)	22,30,33	1.94	4 (18%)
46	MA6	BA	1851	46	23,26,27	1.45	4 (17%)	34,38,41	2.41	13 (38%)
46	PSU	BA	1367	46	18,21,22	1.65	4 (22%)	22,30,33	2.35	7 (31%)
1	A2M	AA	3867	1	22,25,26	1.46	4 (18%)	31,36,39	2.09	7 (22%)
1	OMG	AA	4196	80,1	23,26,27	1.23	3 (13%)	33,38,41	1.94	6 (18%)
46	OMG	BA	644	46	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
46	OMU	BA	428	46	19,22,23	1.21	3 (15%)	26,31,34	1.72	4 (15%)
46	A2M	BA	576	46	22,25,26	1.47	4 (18%)	31,36,39	2.17	9 (29%)
59	NMM	BN	67	59	9,11,12	1.71	1 (11%)	6,12,14	1.06	0
46	OMC	BA	517	46	19,22,23	0.82	0	26,31,34	0.85	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	BA	1004	46	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	AA	2843	1	18,21,22	1.39	3 (16%)	22,30,33	1.91	4 (18%)
1	PSU	AA	3715	1	18,21,22	1.39	2 (11%)	22,30,33	1.82	3 (13%)
1	OMU	AA	4306	1	19,22,23	1.25	3 (15%)	26,31,34	1.60	4 (15%)
46	PSU	BA	93	46	18,21,22	1.38	2 (11%)	22,30,33	1.82	3 (13%)
46	A2M	BA	99	46,80	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
46	PSU	BA	300	46	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
1	OMG	AA	4392	1	23,26,27	1.22	3 (13%)	33,38,41	1.91	5 (15%)
1	PSU	AA	1781	1	18,21,22	1.37	3 (16%)	22,30,33	1.87	3 (13%)
1	OMC	AA	2824	1	19,22,23	0.80	0	26,31,34	0.80	0
1	A2M	AA	398	1	22,25,26	1.43	4 (18%)	31,36,39	2.14	10 (32%)
1	PSU	AA	4579	1	18,21,22	1.38	4 (22%)	22,30,33	1.91	3 (13%)
1	OMG	AA	4618	1	23,26,27	1.20	4 (17%)	33,38,41	1.94	6 (18%)
46	PSU	BA	100	46,80	18,21,22	1.37	2 (11%)	22,30,33	1.84	3 (13%)
46	PSU	BA	966	46	18,21,22	1.36	2 (11%)	22,30,33	1.80	3 (13%)
46	6MZ	BA	1832	46,81	22,25,26	1.49	4 (18%)	30,36,39	2.13	8 (26%)
46	PSU	BA	686	46	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
46	PSU	BA	667	46	18,21,22	1.43	4 (22%)	22,30,33	1.88	4 (18%)
1	OMG	AA	3744	1	23,26,27	1.22	3 (13%)	33,38,41	1.91	6 (18%)
1	OMG	AA	4637	81,1	23,26,27	1.22	3 (13%)	33,38,41	1.96	6 (18%)
1	OMG	AA	3899	80,1	23,26,27	1.21	4 (17%)	33,38,41	1.89	6 (18%)
1	OMC	AA	4536	1	19,22,23	0.84	0	26,31,34	0.91	1 (3%)
1	OMG	AA	4228	1	23,26,27	1.20	4 (17%)	33,38,41	1.94	6 (18%)
1	PSU	AA	3639	1	18,21,22	1.42	3 (16%)	22,30,33	1.87	3 (13%)
1	A2M	AA	4571	1	22,25,26	1.46	4 (18%)	31,36,39	2.05	7 (22%)
46	PSU	BA	609	46	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
46	A2M	BA	27	46,80	22,25,26	1.47	4 (18%)	31,36,39	2.08	9 (29%)
46	PSU	BA	105	46	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	1536	1	18,21,22	1.40	2 (11%)	22,30,33	1.91	3 (13%)
1	A2M	AA	1871	80,1	22,25,26	1.43	5 (22%)	31,36,39	2.20	10 (32%)
46	OMG	BA	509	46,80	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
1	PSU	AA	4296	1	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
46	PSU	BA	366	46	18,21,22	1.33	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	AA	3822	1	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
1	A2M	AA	4523	80,1	22,25,26	1.41	4 (18%)	31,36,39	2.18	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	AA	2363	80,1	22,25,26	1.46	4 (18%)	31,36,39	2.04	8 (25%)
1	UR3	AA	4530	1	19,22,23	0.97	0	26,32,35	1.41	1 (3%)
46	A2M	BA	1678	46	22,25,26	1.45	4 (18%)	31,36,39	2.28	10 (32%)
46	PSU	BA	815	46	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
46	PSU	BA	814	46	18,21,22	1.36	2 (11%)	22,30,33	1.82	3 (13%)
46	PSU	BA	681	46	18,21,22	1.36	2 (11%)	22,30,33	1.81	3 (13%)
1	OMC	AA	2804	1	19,22,23	0.82	0	26,31,34	0.76	0
46	OMU	BA	1288	46	19,22,23	1.23	3 (15%)	26,31,34	1.66	4 (15%)
46	A2M	BA	590	46	22,25,26	1.50	4 (18%)	31,36,39	2.12	6 (19%)
46	PSU	BA	1186	46	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	AA	3792	1	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	AA	1782	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
46	OMG	BA	683	46	23,26,27	1.18	3 (13%)	33,38,41	1.97	6 (18%)
46	4AC	BA	1842	46	21,24,25	1.09	1 (4%)	29,34,37	1.34	3 (10%)
46	PSU	BA	296	46	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
46	PSU	BA	218	46	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
1	A2M	AA	1326	1	22,25,26	1.46	4 (18%)	31,36,39	2.05	7 (22%)
1	A2M	AA	3785	80,1	22,25,26	1.40	4 (18%)	31,36,39	2.38	11 (35%)
46	OMU	BA	1804	46	19,22,23	1.23	4 (21%)	26,31,34	1.72	5 (19%)
1	OMC	AA	1340	1	19,22,23	0.81	0	26,31,34	0.79	0
46	B8N	BA	1248	46	24,29,30	0.84	1 (4%)	29,42,45	1.31	2 (6%)
1	PSU	AA	4500	1	18,21,22	1.37	2 (11%)	22,30,33	1.95	3 (13%)
1	PSU	AA	4521	80,81,1	18,21,22	1.39	3 (16%)	22,30,33	1.93	4 (18%)
1	5MC	AA	4447	81,1	18,22,23	1.00	2 (11%)	26,32,35	1.35	3 (11%)
5	HIC	AE	245	5	10,11,12	0.54	0	8,14,16	0.58	0
46	MA6	BA	1850	46	23,26,27	1.44	4 (17%)	34,38,41	2.43	14 (41%)
1	PSU	AA	1677	1	18,21,22	1.41	2 (11%)	22,30,33	1.92	4 (18%)
29	V5N	Ac	39	29	9,11,12	0.82	0	9,14,16	1.75	2 (22%)
46	OMG	BA	1328	46	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	AA	4293	1	18,21,22	1.39	4 (22%)	22,30,33	1.90	3 (13%)
46	PSU	BA	1238	46	18,21,22	1.32	2 (11%)	22,30,33	1.86	4 (18%)
46	PSU	BA	36	46	18,21,22	1.33	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	AA	4431	1	18,21,22	1.40	2 (11%)	22,30,33	1.86	3 (13%)
1	OMC	AA	2861	1	19,22,23	0.83	0	26,31,34	0.93	2 (7%)
1	A2M	AA	1524	1	22,25,26	1.44	4 (18%)	31,36,39	2.19	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	A2M	BA	1031	46	22,25,26	1.46	4 (18%)	31,36,39	2.05	8 (25%)
46	A2M	BA	159	46	22,25,26	1.47	4 (18%)	31,36,39	2.22	10 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	AA	2837	1	-	1/9/27/28	0/2/2/2
1	A2M	AA	2787	1	-	3/9/27/28	0/3/3/3
3	OMG	AC	75	3	-	1/9/27/28	0/3/3/3
46	OMU	BA	116	46	-	1/9/27/28	0/2/2/2
46	A2M	BA	1383	46	-	0/9/27/28	0/3/3/3
1	PSU	AA	3851	1	-	1/7/25/26	0/2/2/2
1	PSU	AA	1683	81,1	-	0/7/25/26	0/2/2/2
1	OMG	AA	2424	1	-	0/9/27/28	0/3/3/3
46	A2M	BA	166	46	-	2/9/27/28	0/3/3/3
3	PSU	AC	55	3	-	0/7/25/26	0/2/2/2
46	PSU	BA	801	46	-	1/7/25/26	0/2/2/2
1	OMC	AA	2422	80,1	-	1/9/27/28	0/2/2/2
1	A2M	AA	3718	1	-	2/9/27/28	0/3/3/3
1	PSU	AA	3764	1	-	2/7/25/26	0/2/2/2
1	PSU	AA	4471	1	-	0/7/25/26	0/2/2/2
46	OMU	BA	172	46	-	0/9/27/28	0/2/2/2
46	G7M	BA	1639	46	-	2/7/25/26	0/3/3/3
46	A2M	BA	468	46	-	3/9/27/28	0/3/3/3
46	PSU	BA	1643	46	-	0/7/25/26	0/2/2/2
1	A2M	AA	3830	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4457	1	-	0/7/25/26	0/2/2/2
46	OMC	BA	1391	46	-	1/9/27/28	0/2/2/2
1	PSU	AA	4689	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	3825	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4973	1	-	0/7/25/26	0/2/2/2
46	OMC	BA	1703	46	-	1/9/27/28	0/2/2/2
1	PSU	AA	3844	1	-	3/7/25/26	0/2/2/2
46	OMG	BA	1447	46	-	0/9/27/28	0/3/3/3
1	PSU	AA	4299	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	1625	81,1	-	2/9/27/28	0/3/3/3
46	OMG	BA	1490	46,80	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PSU	BA	1445	46	-	1/7/25/26	0/2/2/2
46	PSU	BA	1232	46	-	4/7/25/26	0/2/2/2
1	A2M	AA	3724	1	-	0/9/27/28	0/3/3/3
1	OMU	AA	4227	1	-	0/9/27/28	0/2/2/2
1	OMC	AA	3841	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	3762	1	-	2/7/25/26	0/2/2/2
1	OMU	AA	4620	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	1744	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	1177	46	-	0/7/25/26	0/2/2/2
1	A2M	AA	1323	1	-	4/9/27/28	0/3/3/3
46	A2M	BA	484	46	-	1/9/27/28	0/3/3/3
1	PSU	AA	4673	81,1	-	0/7/25/26	0/2/2/2
46	OMG	BA	867	46	-	0/9/27/28	0/3/3/3
1	PSU	AA	1862	1	-	0/7/25/26	0/2/2/2
1	OMU	AA	2415	1	-	0/9/27/28	0/2/2/2
1	5MC	AA	3782	80,1	-	0/7/25/26	0/2/2/2
1	OMG	AA	4494	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	3768	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	1692	46	-	0/7/25/26	0/2/2/2
1	A2M	AA	4590	1	-	1/9/27/28	0/3/3/3
46	PSU	BA	1056	46	-	0/7/25/26	0/2/2/2
46	OMC	BA	1272	46	-	0/9/27/28	0/2/2/2
3	OMU	AC	14	1,3	-	0/9/27/28	0/2/2/2
72	IAS	Ba	138	72	-	1/7/7/8	-
46	OMG	BA	436	46	-	0/9/27/28	0/3/3/3
1	PSU	AA	3770	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	3869	1	-	0/9/27/28	0/2/2/2
1	OMC	AA	3701	81,1	-	4/9/27/28	0/2/2/2
1	PSU	AA	1582	1	-	3/7/25/26	0/2/2/2
1	OMG	AA	2876	1	-	0/9/27/28	0/3/3/3
1	OMC	AA	3808	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	3730	1	-	0/7/25/26	0/2/2/2
1	6MZ	AA	4220	1	-	0/9/27/28	0/3/3/3
46	OMU	BA	354	46	-	0/9/27/28	0/2/2/2
1	UY1	AA	3818	81,1	-	4/9/27/28	0/2/2/2
46	PSU	BA	822	46	-	1/7/25/26	0/2/2/2
1	PSU	AA	4636	1	-	3/7/25/26	0/2/2/2
1	PSU	AA	4353	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	649	46	-	0/7/25/26	0/2/2/2
3	PSU	AC	69	3	-	0/7/25/26	0/2/2/2
1	PSU	AA	4361	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	OMC	BA	462	46	-	0/9/27/28	0/2/2/2
1	OMC	AA	3887	1	-	1/9/27/28	0/2/2/2
46	OMC	BA	174	46	-	0/9/27/28	0/2/2/2
1	A2M	AA	2401	1	-	0/9/27/28	0/3/3/3
1	OMU	AA	4498	80,1	-	0/9/27/28	0/2/2/2
46	PSU	BA	1046	46	-	0/7/25/26	0/2/2/2
1	A2M	AA	2815	81,1	-	0/9/27/28	0/3/3/3
46	PSU	BA	119	46,80	-	0/7/25/26	0/2/2/2
46	PSU	BA	63	46	-	0/7/25/26	0/2/2/2
46	OMU	BA	1442	46	-	0/9/27/28	0/2/2/2
46	PSU	BA	1625	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	4576	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3884	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	1244	46	-	2/7/25/26	0/2/2/2
46	PSU	BA	1347	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	109	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	1003	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	651	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	1860	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	2508	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4493	81,1	-	0/7/25/26	0/2/2/2
1	OMG	AA	1522	1	-	0/9/27/28	0/3/3/3
1	A2M	AA	1534	80,1	-	2/9/27/28	0/3/3/3
1	OMG	AA	1316	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	1792	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	1881	80,1	-	0/9/27/28	0/2/2/2
1	PSU	AA	4972	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	918	46	-	2/7/25/26	0/2/2/2
1	OMG	AA	2364	1	-	2/9/27/28	0/3/3/3
1	OMU	AA	3925	1	-	0/9/27/28	0/2/2/2
46	UY1	BA	1326	46	-	4/9/27/28	0/2/2/2
46	OMU	BA	121	46	-	0/9/27/28	0/2/2/2
1	PSU	AA	2632	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	572	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	866	46	-	0/7/25/26	0/2/2/2
1	OMG	AA	4499	1	-	0/9/27/28	0/3/3/3
1	1MA	AA	1322	80,1	-	1/7/25/26	0/3/3/3
46	PSU	BA	1174	46	-	0/7/25/26	0/2/2/2
1	OMC	AA	2351	80,1	-	1/9/27/28	0/2/2/2
1	PSU	AA	5010	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	406	46	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	5001	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3920	80,1	-	0/7/25/26	0/2/2/2
1	A2M	AA	400	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4442	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	4456	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	3637	81,1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4312	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	34	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	2839	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	4370	1	-	0/9/27/28	0/3/3/3
46	A2M	BA	512	46	-	2/9/27/28	0/3/3/3
1	OMC	AA	2365	80,1	-	0/9/27/28	0/2/2/2
46	OMG	BA	601	46	-	0/9/27/28	0/3/3/3
46	4AC	BA	1337	46	-	1/11/29/30	0/2/2/2
1	PSU	AA	1779	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	1360	46,80,81	-	0/7/25/26	0/2/2/2
1	PSU	AA	3853	80,1	-	0/7/25/26	0/2/2/2
46	A2M	BA	668	46,80	-	2/9/27/28	0/3/3/3
1	PSU	AA	4552	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	1136	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	4628	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4532	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	4623	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4423	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	1596	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	863	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	4403	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	3627	1	-	0/9/27/28	0/3/3/3
46	PSU	BA	1045	46	-	2/7/25/26	0/2/2/2
1	PSU	AA	3695	1	-	0/7/25/26	0/2/2/2
46	MA6	BA	1851	46	-	5/11/29/30	0/3/3/3
46	PSU	BA	1367	46	-	1/7/25/26	0/2/2/2
1	A2M	AA	3867	1	-	1/9/27/28	0/3/3/3
1	OMG	AA	4196	80,1	-	0/9/27/28	0/3/3/3
46	OMG	BA	644	46	-	0/9/27/28	0/3/3/3
46	OMU	BA	428	46	-	6/9/27/28	0/2/2/2
46	A2M	BA	576	46	-	1/9/27/28	0/3/3/3
59	NMM	BN	67	59	-	2/9/11/13	-
46	OMC	BA	517	46	-	0/9/27/28	0/2/2/2
46	PSU	BA	1004	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	2843	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	AA	3715	1	-	0/7/25/26	0/2/2/2
1	OMU	AA	4306	1	-	0/9/27/28	0/2/2/2
46	PSU	BA	93	46	-	0/7/25/26	0/2/2/2
46	A2M	BA	99	46,80	-	2/9/27/28	0/3/3/3
46	PSU	BA	300	46	-	0/7/25/26	0/2/2/2
1	OMG	AA	4392	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	1781	1	-	1/7/25/26	0/2/2/2
1	OMC	AA	2824	1	-	0/9/27/28	0/2/2/2
1	A2M	AA	398	1	-	2/9/27/28	0/3/3/3
1	PSU	AA	4579	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	4618	1	-	0/9/27/28	0/3/3/3
46	PSU	BA	100	46,80	-	2/7/25/26	0/2/2/2
46	PSU	BA	966	46	-	1/7/25/26	0/2/2/2
46	6MZ	BA	1832	46,81	-	4/9/27/28	0/3/3/3
46	PSU	BA	686	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	667	46	-	4/7/25/26	0/2/2/2
1	OMG	AA	3744	1	-	0/9/27/28	0/3/3/3
1	OMG	AA	4637	81,1	-	2/9/27/28	0/3/3/3
1	OMG	AA	3899	80,1	-	0/9/27/28	0/3/3/3
1	OMC	AA	4536	1	-	0/9/27/28	0/2/2/2
1	OMG	AA	4228	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	3639	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	4571	1	-	0/9/27/28	0/3/3/3
46	PSU	BA	609	46	-	0/7/25/26	0/2/2/2
46	A2M	BA	27	46,80	-	0/9/27/28	0/3/3/3
46	PSU	BA	105	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	1536	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	1871	80,1	-	0/9/27/28	0/3/3/3
46	OMG	BA	509	46,80	-	1/9/27/28	0/3/3/3
1	PSU	AA	4296	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	366	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	3822	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	4523	80,1	-	0/9/27/28	0/3/3/3
1	A2M	AA	2363	80,1	-	0/9/27/28	0/3/3/3
1	UR3	AA	4530	1	-	0/7/25/26	0/2/2/2
46	A2M	BA	1678	46	-	0/9/27/28	0/3/3/3
46	PSU	BA	815	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	814	46	-	0/7/25/26	0/2/2/2
46	PSU	BA	681	46	-	0/7/25/26	0/2/2/2
1	OMC	AA	2804	1	-	0/9/27/28	0/2/2/2
46	OMU	BA	1288	46	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	A2M	BA	590	46	-	5/9/27/28	0/3/3/3
46	PSU	BA	1186	46	-	0/7/25/26	0/2/2/2
1	OMG	AA	3792	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	1782	1	-	0/7/25/26	0/2/2/2
46	OMG	BA	683	46	-	0/9/27/28	0/3/3/3
46	4AC	BA	1842	46	-	0/11/29/30	0/2/2/2
46	PSU	BA	296	46	-	2/7/25/26	0/2/2/2
46	PSU	BA	218	46	-	0/7/25/26	0/2/2/2
1	A2M	AA	1326	1	-	2/9/27/28	0/3/3/3
1	A2M	AA	3785	80,1	-	2/9/27/28	0/3/3/3
46	OMU	BA	1804	46	-	3/9/27/28	0/2/2/2
1	OMC	AA	1340	1	-	0/9/27/28	0/2/2/2
46	B8N	BA	1248	46	-	3/16/34/35	0/2/2/2
1	PSU	AA	4500	1	-	3/7/25/26	0/2/2/2
1	PSU	AA	4521	80,81,1	-	0/7/25/26	0/2/2/2
1	5MC	AA	4447	81,1	-	4/7/25/26	0/2/2/2
5	HIC	AE	245	5	-	0/5/6/8	0/1/1/1
46	MA6	BA	1850	46	-	2/11/29/30	0/3/3/3
1	PSU	AA	1677	1	-	1/7/25/26	0/2/2/2
29	V5N	Ac	39	29	-	0/9/10/12	0/1/1/1
46	OMG	BA	1328	46	-	0/9/27/28	0/3/3/3
1	PSU	AA	4293	1	-	0/7/25/26	0/2/2/2
46	PSU	BA	1238	46	-	1/7/25/26	0/2/2/2
46	PSU	BA	36	46	-	0/7/25/26	0/2/2/2
1	PSU	AA	4431	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	2861	1	-	0/9/27/28	0/2/2/2
1	A2M	AA	1524	1	-	2/9/27/28	0/3/3/3
46	A2M	BA	1031	46	-	0/9/27/28	0/3/3/3
46	A2M	BA	159	46	-	1/9/27/28	0/3/3/3

The worst 5 of 601 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	BA	1326	UY1	C6-C5	11.93	1.49	1.35
1	AA	3818	UY1	C6-C5	11.36	1.48	1.35
46	BA	1639	G7M	C8-N7	10.68	1.52	1.33
46	BA	1639	G7M	C2'-C3'	-10.42	1.24	1.53
46	BA	1326	UY1	C2-N1	9.67	1.49	1.36

The worst 5 of 982 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2815	A2M	C5-C4-N3	-6.86	117.80	126.75
46	BA	590	A2M	C5-C4-N3	-6.80	117.88	126.75
46	BA	576	A2M	C5-C4-N3	-6.59	118.15	126.75
1	AA	3637	PSU	N1-C2-N3	6.51	122.50	115.13
1	AA	3867	A2M	C5-C4-N3	-6.50	118.27	126.75

There are no chirality outliers.

5 of 150 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	BN	67	NMM	O-C-CA-CB
1	AA	1323	A2M	O4'-C4'-C5'-O5'
1	AA	1582	PSU	C2'-C1'-C5-C4
1	AA	1582	PSU	O4'-C1'-C5-C4
1	AA	1582	PSU	O4'-C1'-C5-C6

There are no ring outliers.

81 monomers are involved in 104 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	2787	A2M	1	0
46	BA	116	OMU	3	0
46	BA	1383	A2M	2	0
1	AA	1683	PSU	1	0
1	AA	2424	OMG	1	0
46	BA	166	A2M	1	0
1	AA	3718	A2M	4	0
46	BA	1639	G7M	1	0
46	BA	468	A2M	3	0
46	BA	1643	PSU	1	0
1	AA	4457	PSU	2	0
46	BA	1391	OMC	2	0
1	AA	4689	PSU	1	0
46	BA	1703	OMC	1	0
46	BA	1490	OMG	1	0
46	BA	1445	PSU	1	0
46	BA	1232	PSU	1	0
1	AA	4620	OMU	1	0
46	BA	484	A2M	2	0
46	BA	867	OMG	1	0
1	AA	2415	OMU	1	0
46	BA	1692	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	BA	1272	OMC	2	0
3	AC	14	OMU	2	0
72	Ba	138	IAS	1	0
1	AA	4220	6MZ	1	0
46	BA	822	PSU	2	0
46	BA	462	OMC	2	0
1	AA	3887	OMC	1	0
46	BA	1046	PSU	2	0
46	BA	63	PSU	1	0
46	BA	1442	OMU	1	0
46	BA	1625	PSU	1	0
46	BA	121	OMU	1	0
46	BA	866	PSU	1	0
1	AA	2351	OMC	2	0
1	AA	5010	PSU	1	0
1	AA	5001	PSU	1	0
1	AA	3920	PSU	1	0
1	AA	400	A2M	1	0
1	AA	4456	OMC	2	0
1	AA	2839	PSU	1	0
46	BA	512	A2M	3	0
46	BA	1337	4AC	1	0
1	AA	4552	PSU	1	0
46	BA	1045	PSU	1	0
46	BA	1367	PSU	3	0
46	BA	576	A2M	1	0
46	BA	517	OMC	1	0
46	BA	99	A2M	1	0
46	BA	300	PSU	1	0
1	AA	4392	OMG	1	0
1	AA	1781	PSU	1	0
1	AA	398	A2M	1	0
1	AA	4579	PSU	2	0
1	AA	4618	OMG	1	0
46	BA	1832	6MZ	2	0
1	AA	4536	OMC	1	0
1	AA	4228	OMG	1	0
1	AA	4571	A2M	2	0
46	BA	27	A2M	1	0
1	AA	1871	A2M	1	0
46	BA	509	OMG	1	0
46	BA	366	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	4523	A2M	1	0
1	AA	2363	A2M	1	0
46	BA	1678	A2M	1	0
46	BA	815	PSU	1	0
46	BA	1288	OMU	1	0
46	BA	590	A2M	1	0
46	BA	1842	4AC	1	0
46	BA	296	PSU	1	0
1	AA	1326	A2M	1	0
1	AA	3785	A2M	1	0
1	AA	1340	OMC	2	0
1	AA	4447	5MC	2	0
46	BA	1850	MA6	1	0
1	AA	4293	PSU	1	0
1	AA	1524	A2M	1	0
46	BA	1031	A2M	2	0
46	BA	159	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 362 ligands modelled in this entry, 362 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 ⓘ

There are no chain breaks in this entry.

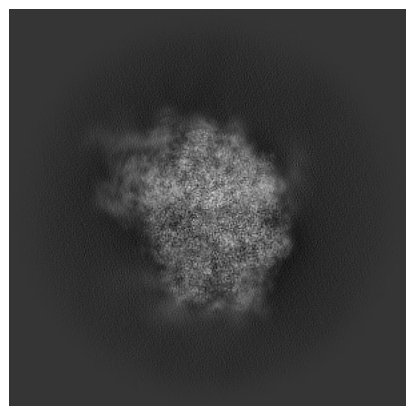
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66298. These allow visual inspection of the internal detail of the map and identification of artifacts.

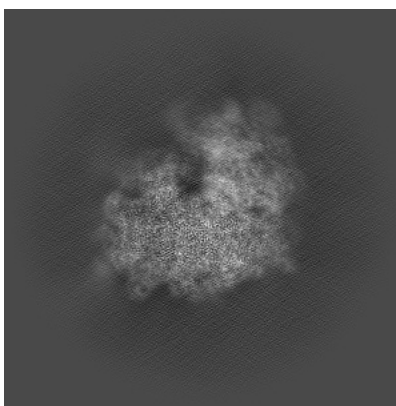
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

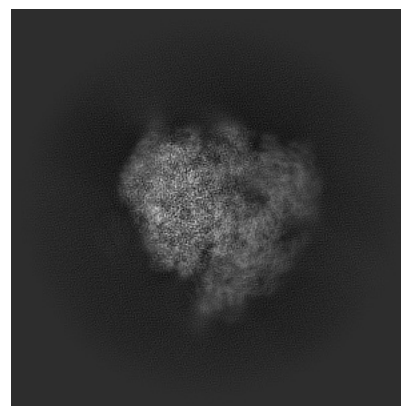
6.1.1 Primary map



X

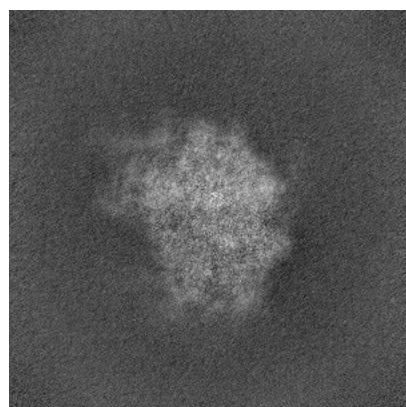


Y

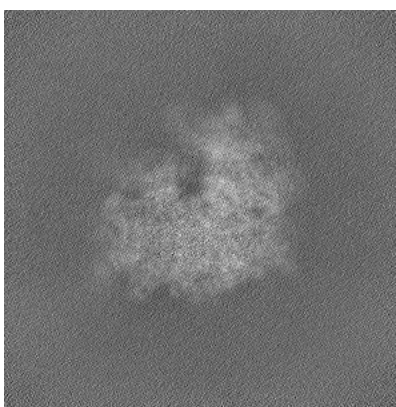


Z

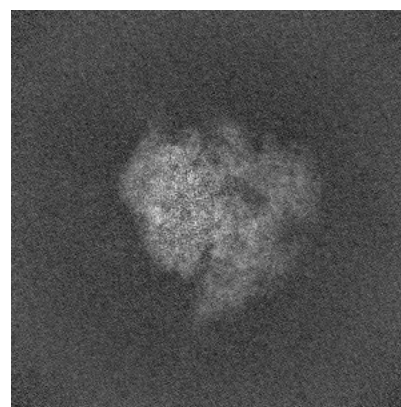
6.1.2 Raw map



X



Y

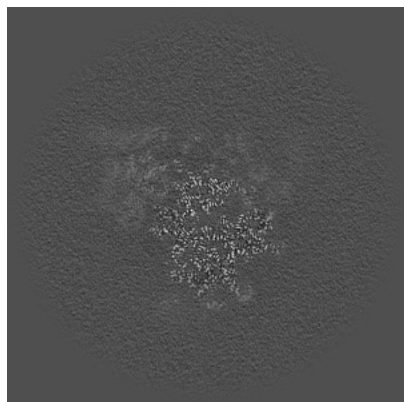


Z

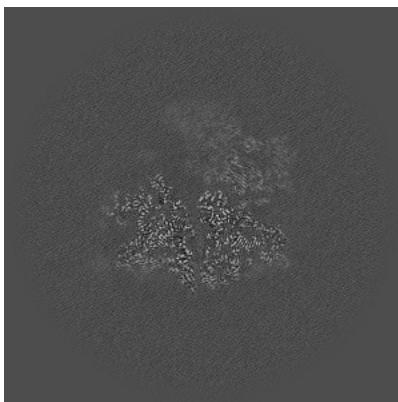
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

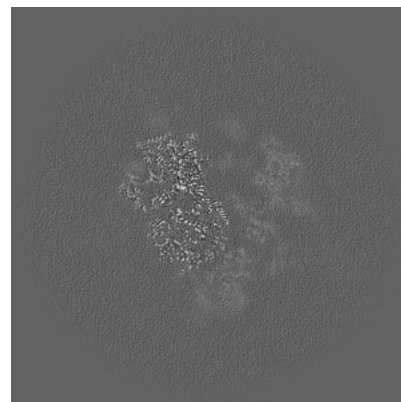
6.2.1 Primary map



X Index: 320

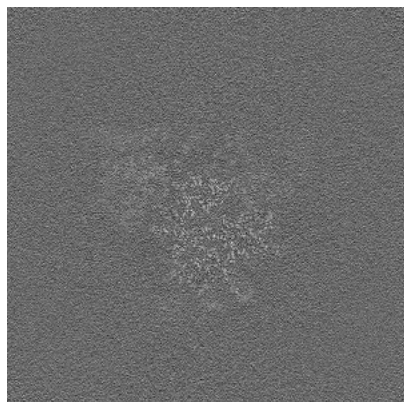


Y Index: 320

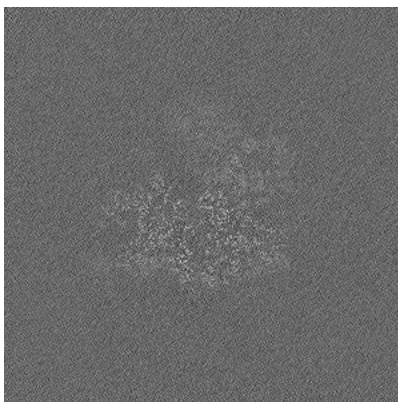


Z Index: 320

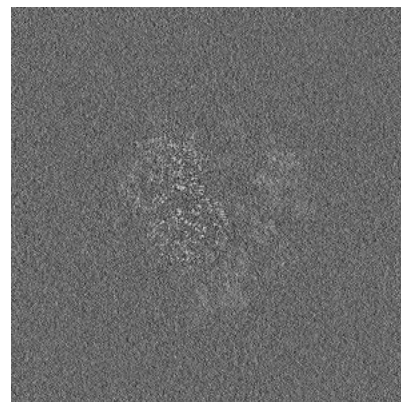
6.2.2 Raw map



X Index: 320



Y Index: 320

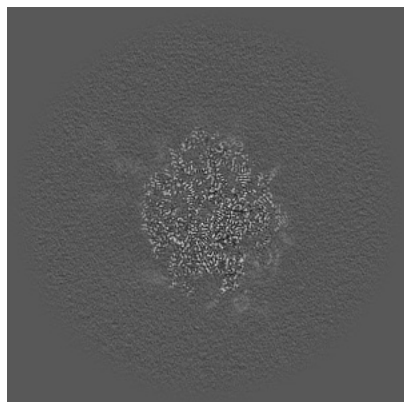


Z Index: 320

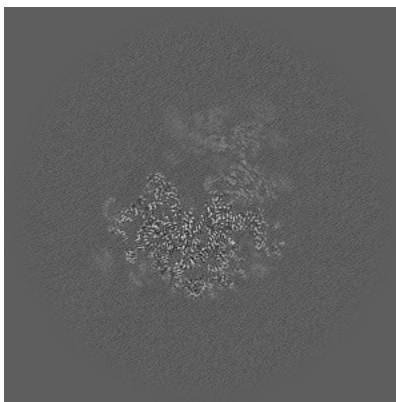
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

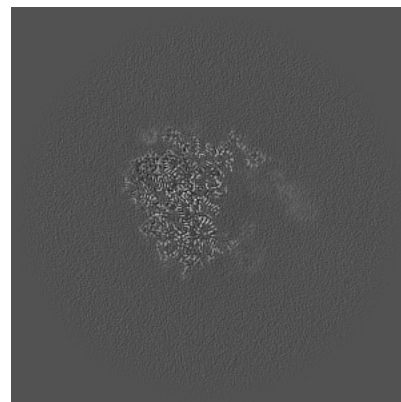
6.3.1 Primary map



X Index: 288

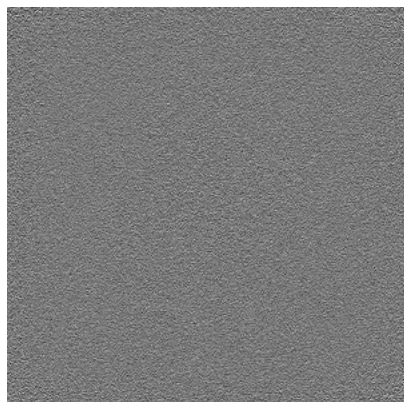


Y Index: 337

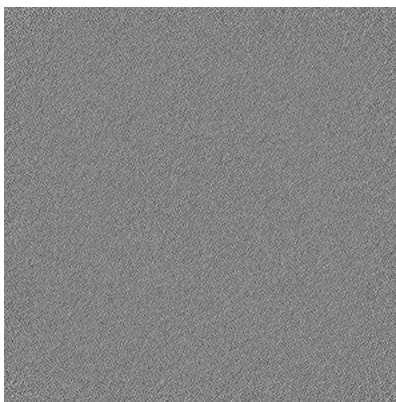


Z Index: 279

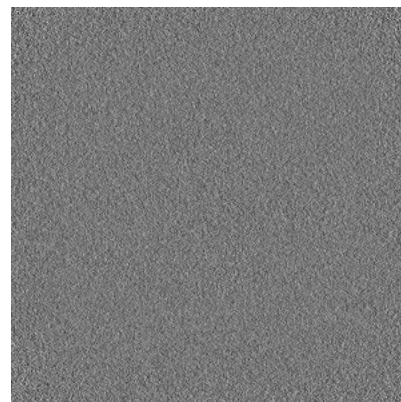
6.3.2 Raw map



X Index: 0



Y Index: 0

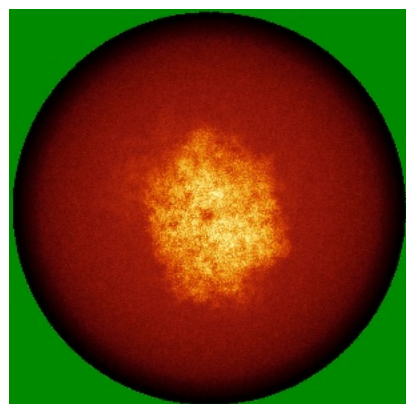


Z Index: 0

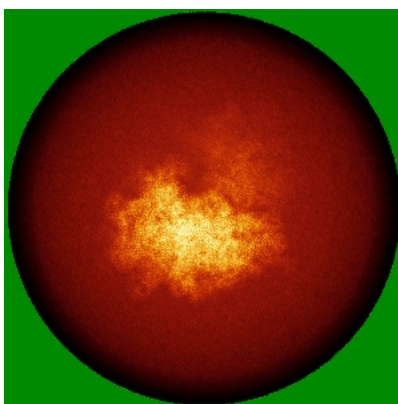
The images above show the largest variance slices of the map in three orthogonal directions.

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

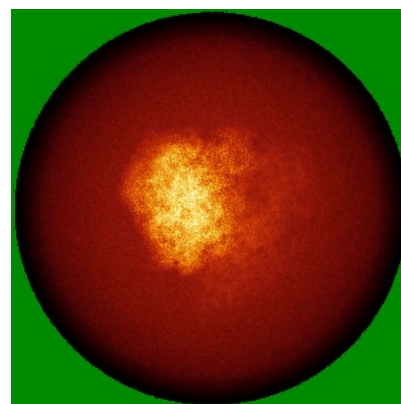
6.4.1 Primary map



X

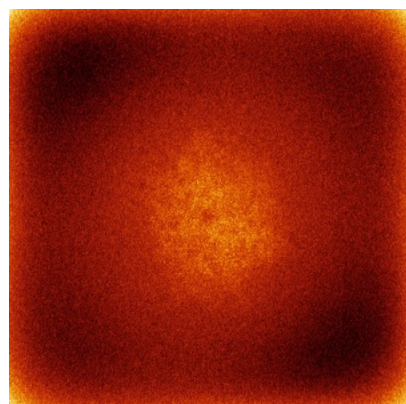


Y

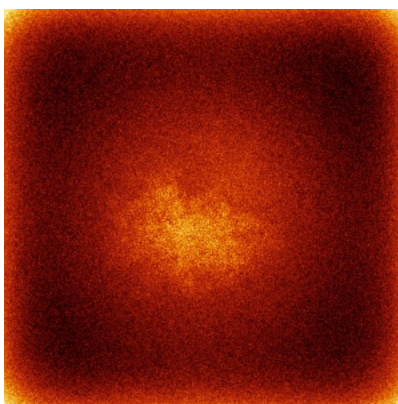


Z

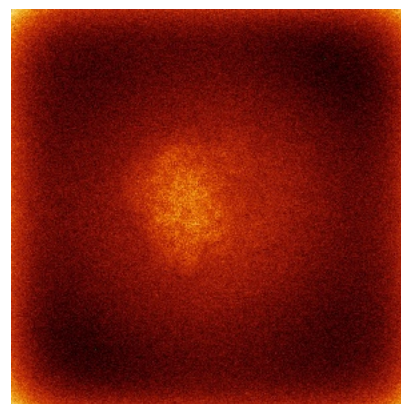
6.4.2 Raw map



X



Y

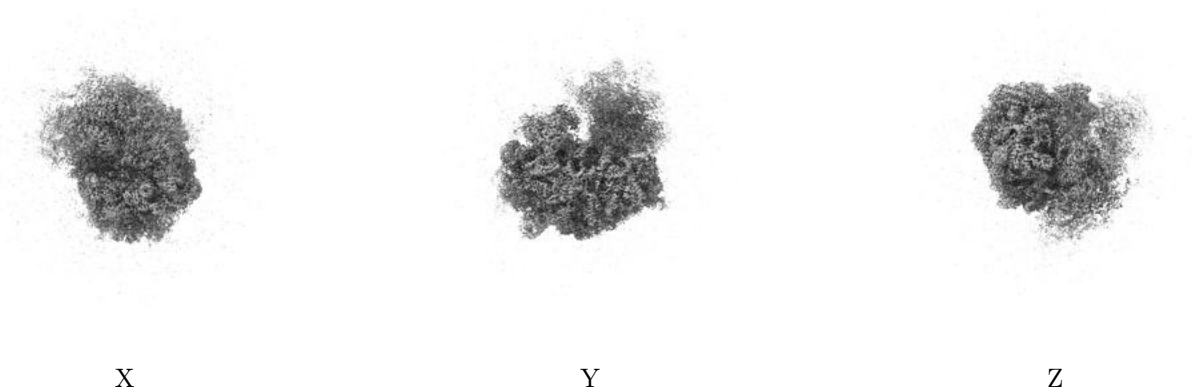


Z

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.

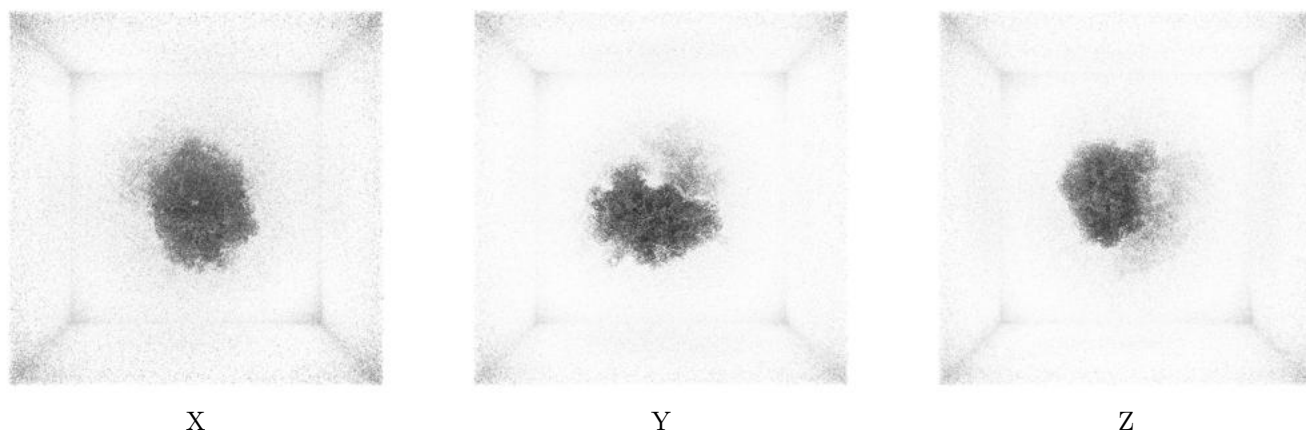
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.29. 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.

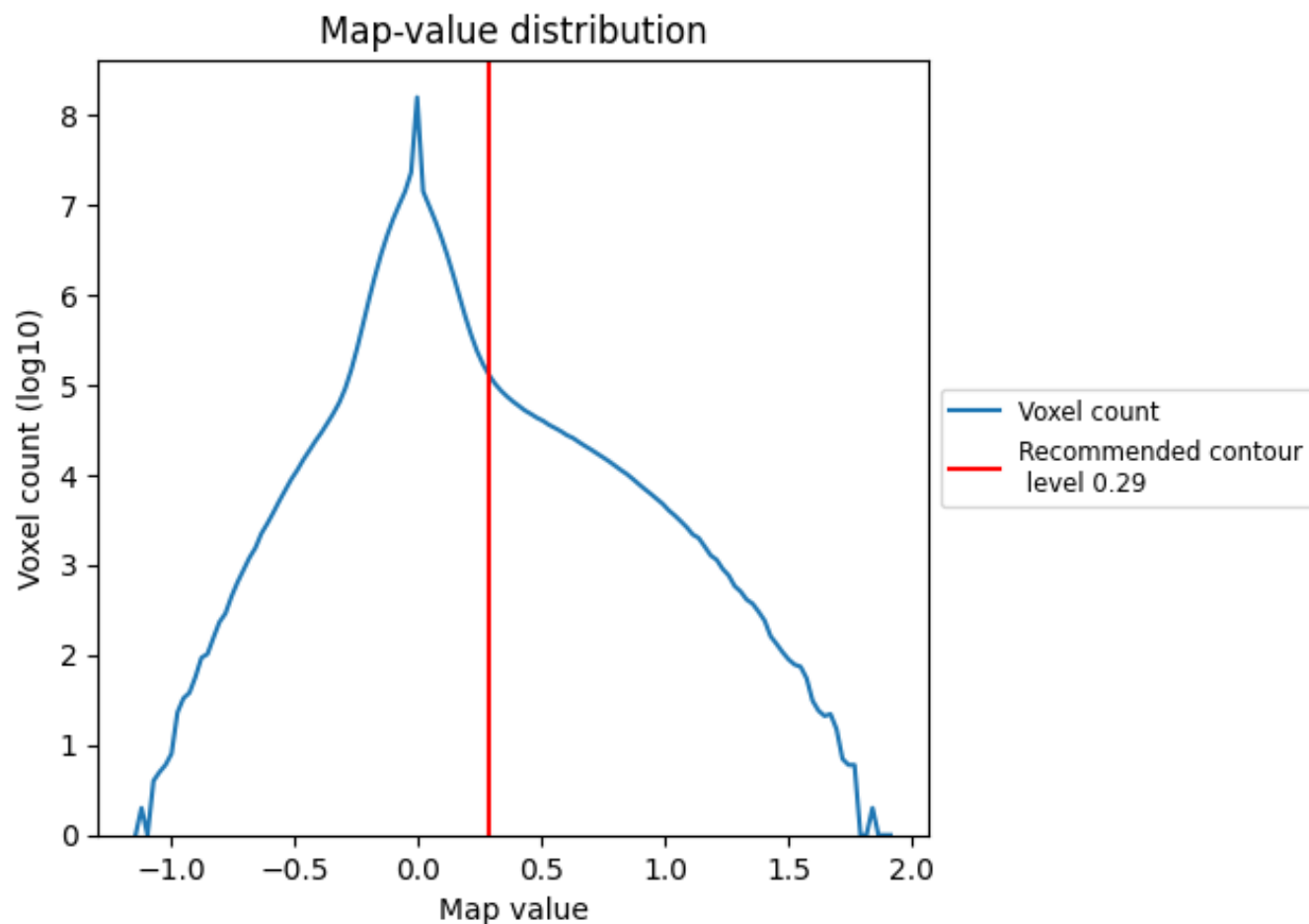
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

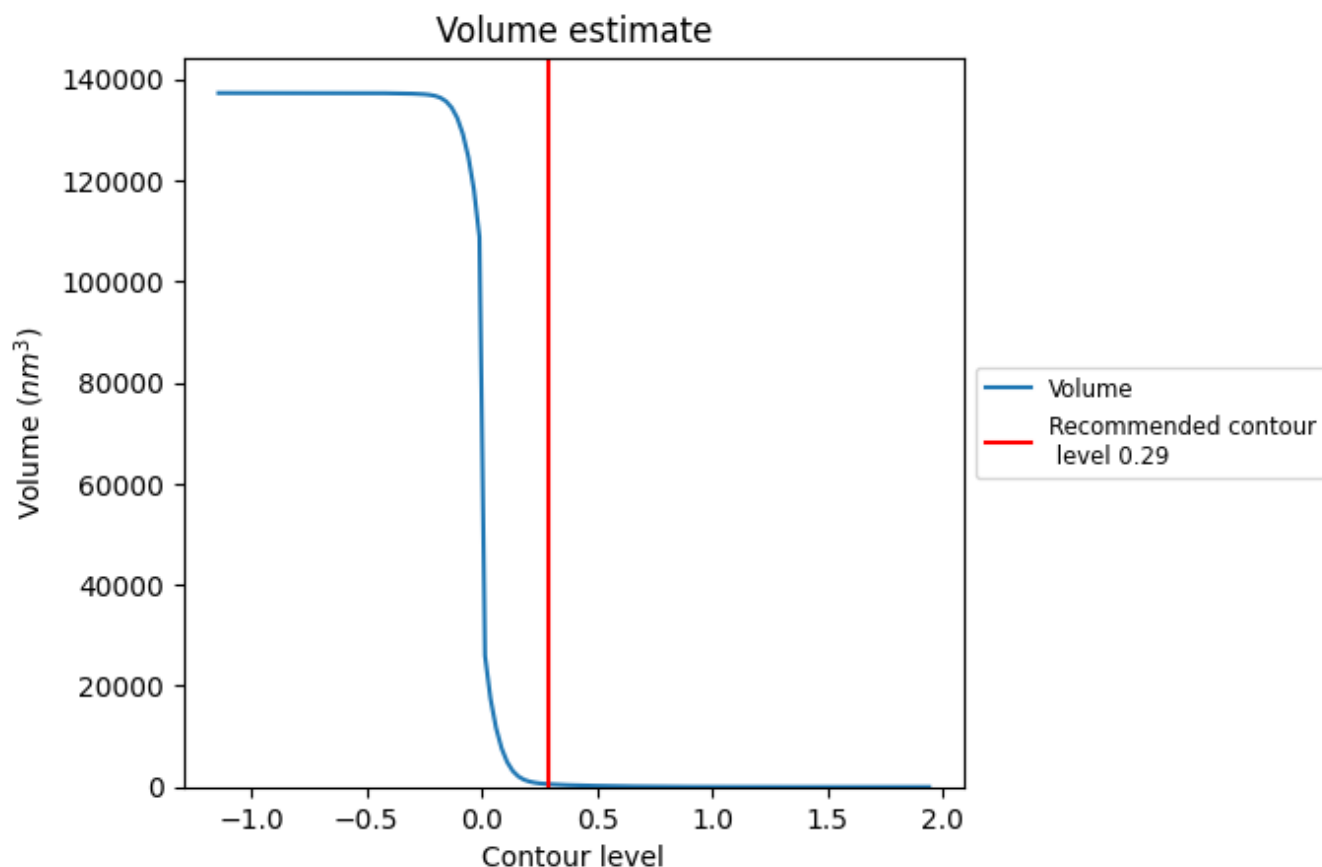
This section contains the results of statistical analysis of the map.

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.

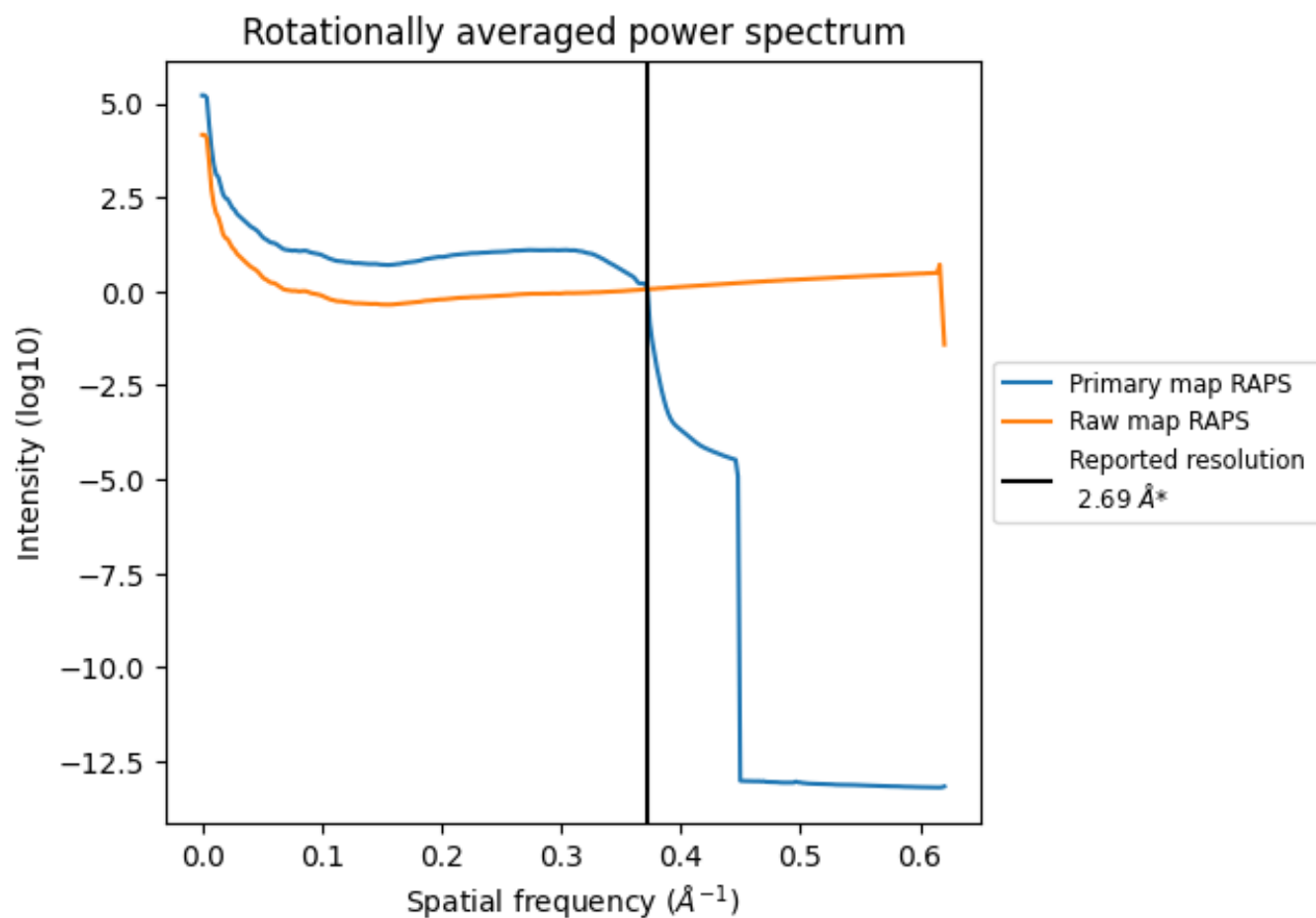
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 555 nm³; this corresponds to an approximate mass of 501 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 ⓘ

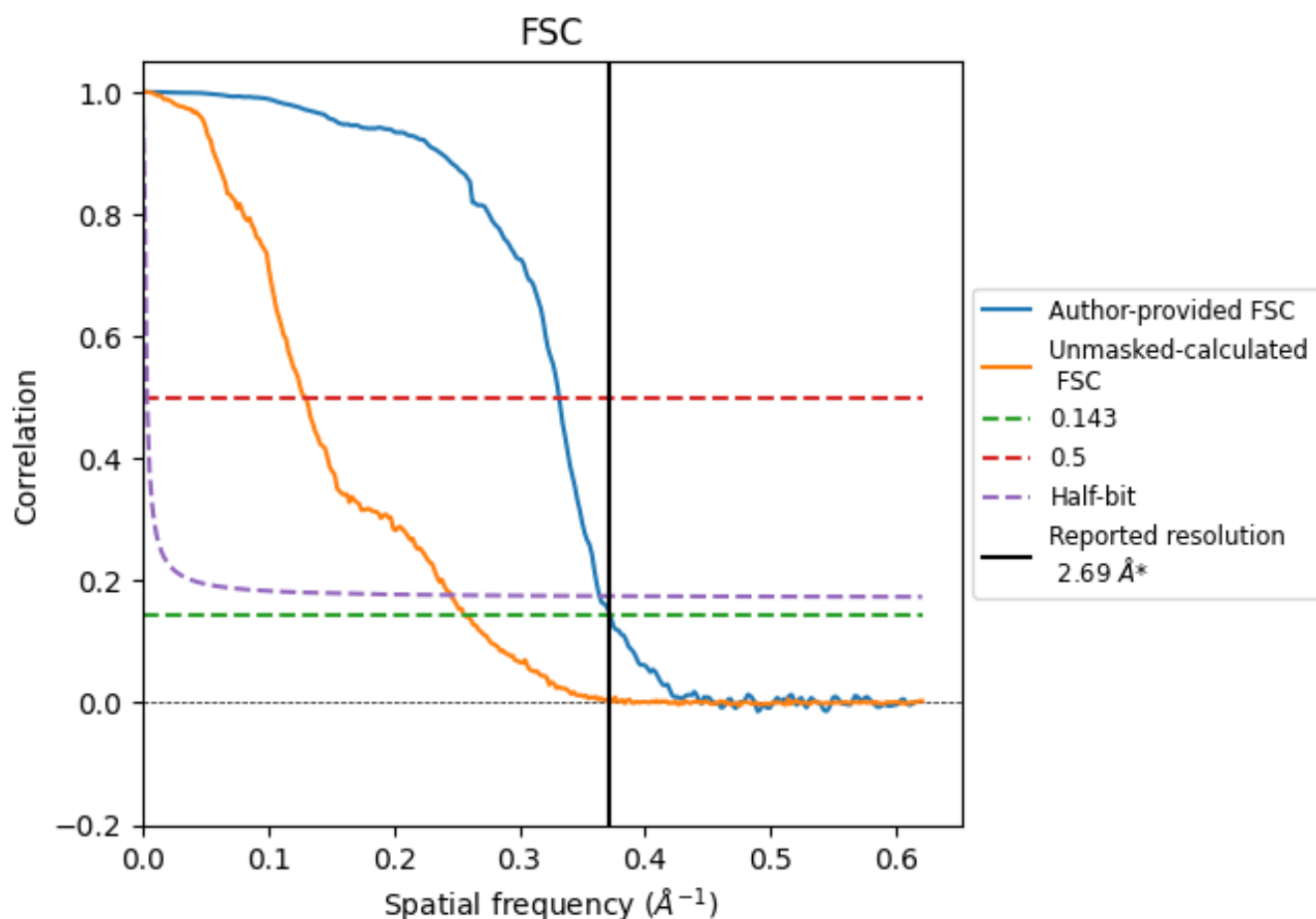


*Reported resolution corresponds to spatial frequency of 0.372 Å⁻¹

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 $0.372 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

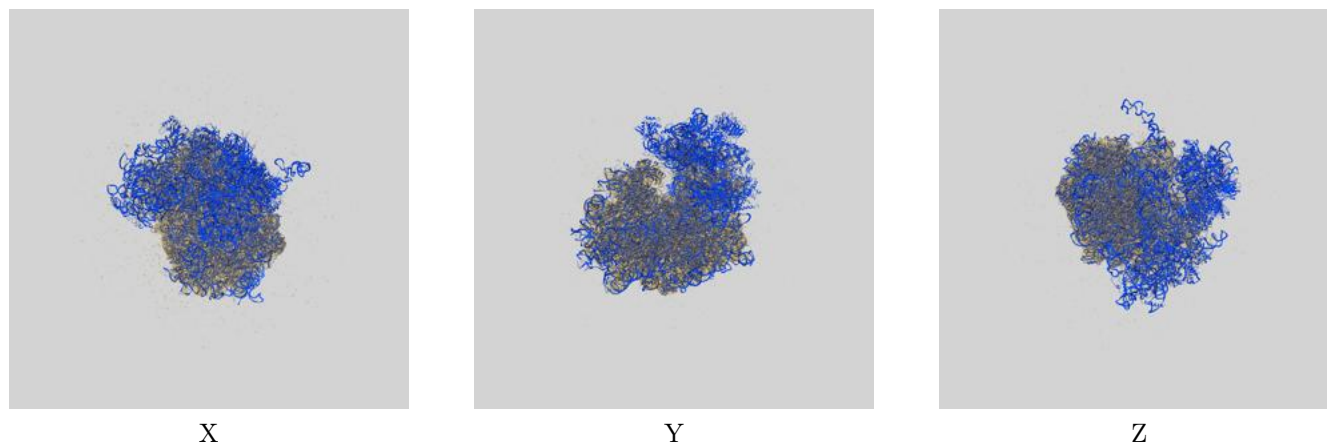
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	3.02	2.75
Unmasked-calculated*	3.90	7.69	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 2.69 by more than 10 %

9 Map-model fit [i](#)

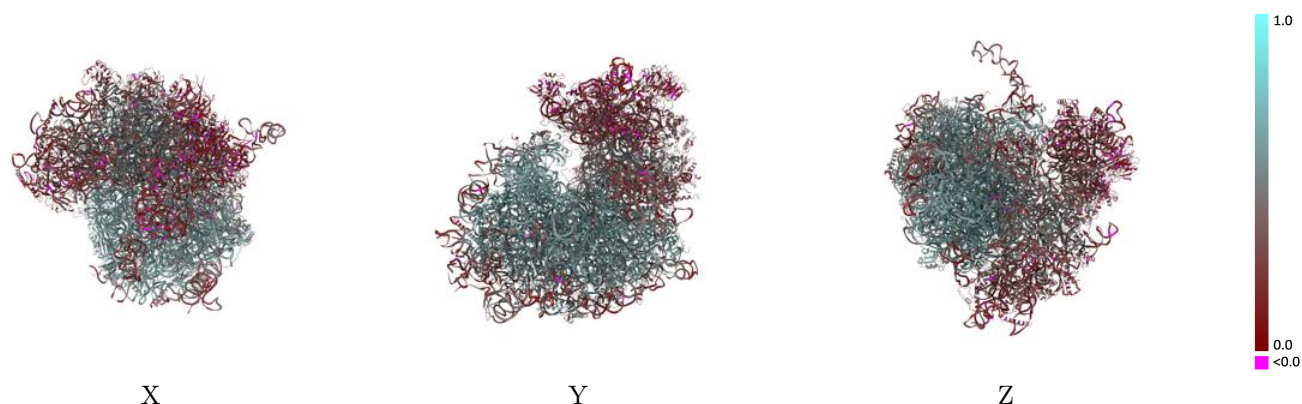
This section contains information regarding the fit between EMDB map EMD-66298 and PDB model 9WW5. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

9.1 Map-model overlay [i](#)



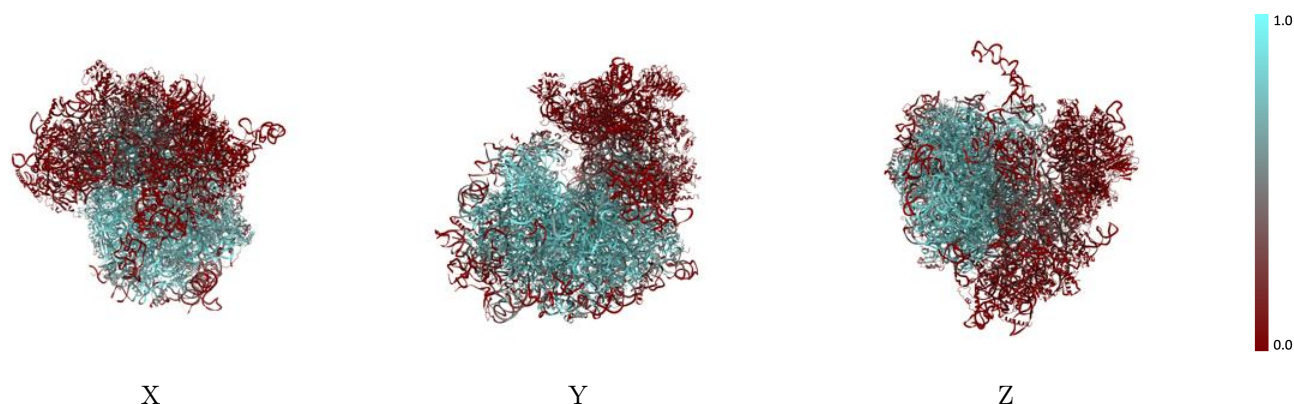
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



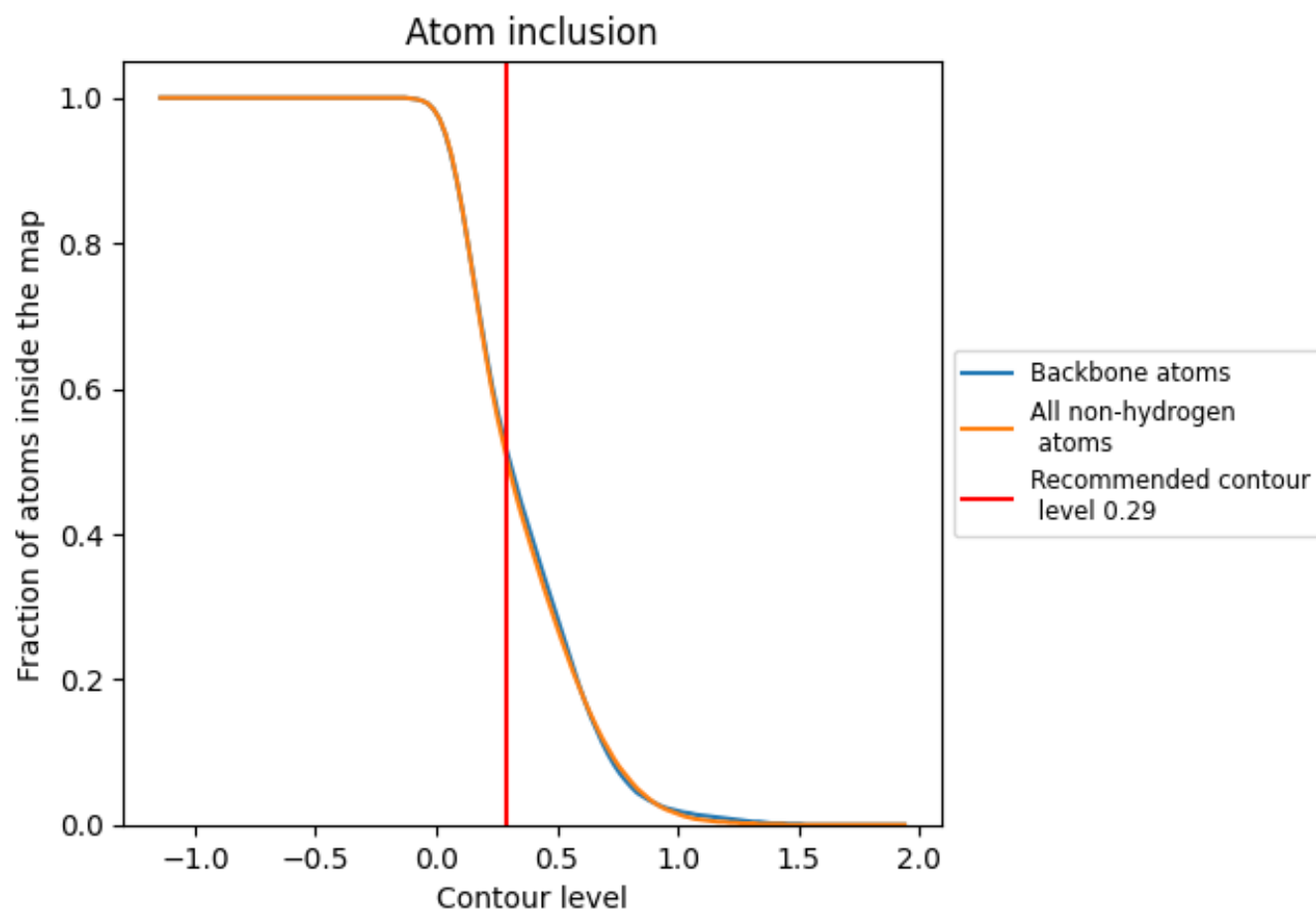
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.29).

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 51% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5060	0.4660
AA	0.6880	0.5240
AB	0.8640	0.6100
AC	0.7420	0.5350
AD	0.8500	0.6450
AE	0.7840	0.6230
AF	0.7020	0.5470
AG	0.6770	0.5790
AH	0.5380	0.5190
AI	0.7720	0.6030
AJ	0.5720	0.5280
AK	0.7120	0.6040
AL	0.7330	0.6010
AM	0.5070	0.5360
AN	0.6210	0.5270
AO	0.7280	0.6000
AP	0.8430	0.6110
AQ	0.8150	0.6250
AR	0.7970	0.6130
AS	0.7860	0.5880
AT	0.6180	0.5460
AU	0.8390	0.6320
AV	0.7380	0.6090
AW	0.4610	0.5210
AX	0.7900	0.6250
AY	0.4640	0.4400
AZ	0.6810	0.5680
Aa	0.6300	0.5270
Ab	0.6880	0.5890
Ac	0.7590	0.5880
Ad	0.5480	0.5370
Ae	0.6470	0.5570
Af	0.7450	0.6030
Ag	0.7400	0.5830
Ah	0.8430	0.6270



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Chain	Atom inclusion	Q-score
Ai	 0.7780	 0.6140
Aj	 0.6270	 0.5440
Ak	 0.6390	 0.5650
Al	 0.8080	 0.6000
Am	 0.5720	 0.5580
An	 0.7350	 0.5900
Ao	 0.7930	 0.6120
Ap	 0.5020	 0.5720
Aq	 0.7690	 0.6250
Ar	 0.7780	 0.6380
As	 0.6610	 0.5440
BA	 0.2300	 0.3310
BB	 0.0590	 0.3460
BC	 0.0890	 0.3580
BD	 0.0720	 0.3430
BE	 0.0310	 0.2750
BF	 0.0110	 0.1920
BG	 0.0530	 0.3090
BH	 0.0810	 0.3520
BI	 0.0090	 0.1740
BJ	 0.1980	 0.4160
BK	 0.0190	 0.2720
BL	 0.0120	 0.2490
BM	 0.0110	 0.2470
BN	 0.0170	 0.2170
BO	 0.0110	 0.2150
BP	 0.1560	 0.3900
BQ	 0.2750	 0.4430
BR	 0.2080	 0.4230
BS	 0.0040	 0.1820
BT	 0.0430	 0.2730
BU	 0.0040	 0.1900
BV	 0.2050	 0.4100
BW	 0.0280	 0.2710
BX	 0.0870	 0.3380
BY	 0.0000	 0.1580
BZ	 0.1380	 0.4370
Ba	 0.1080	 0.3410
Bb	 0.2960	 0.4720
Bc	 0.0170	 0.2550
Bd	 0.0100	 0.1940
Be	 0.0770	 0.2910

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Chain	Atom inclusion	Q-score
Bf	 0.0450	 0.2590
Bg	 0.0000	 0.1530
Bh	 0.0210	 0.3000