



wwPDB EM Validation Summary Report ⓘ

Sep 24, 2026 – 01:04 PM JST

PDB ID : 9WW7 / pdb_00009ww7
EMDB ID : EMD-66301
Title : human 80S ribosome delta eL41 rotated state
Authors : Fujino, M.; Tanaka, Y.; Iwasaki, W.; Ito, T.; Yokoyama, T.
Deposited on : 2025-09-22
Resolution : 2.91 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:

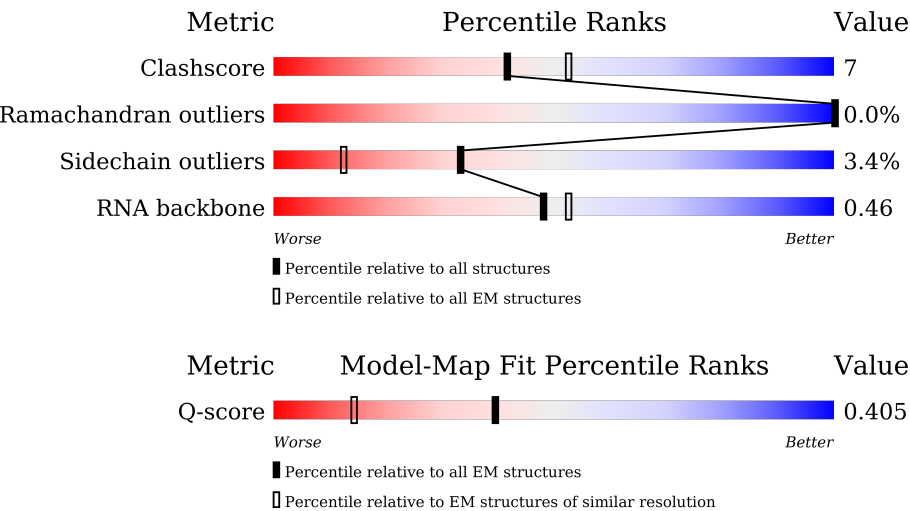
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

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

The reported resolution of this entry is 2.91 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	12972 (2.41 - 3.41)

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	28% 44% 26% • 26%
2	AB	120	33% 72% 27% •
3	AC	157	21% 59% 38% ••

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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	Aq	106	
43	Ar	92	
44	As	137	
45	BA	1869	
46	BB	263	
47	BC	295	
48	BD	264	
49	BE	243	
50	BF	204	
51	BG	194	
52	BH	208	
53	BI	165	

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Mol	Chain	Length	Quality of chain
54	BJ	158	
55	BK	145	
56	BL	146	
57	BM	152	
58	BN	145	
59	BO	119	
60	BP	83	
61	BQ	143	
62	BR	115	
63	BS	69	
64	BT	56	
65	BU	317	
66	BV	293	
67	BW	249	
68	BX	194	
69	BY	132	
70	BZ	151	
71	Ba	151	
72	Bb	130	
73	Bc	133	
74	Bd	125	
75	Be	84	
76	Bf	133	
77	Bg	156	
78	Bh	135	

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 214414 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	134	Total	C	N	O	S	0	0
			1103	707	212	177	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	169	Total	C	N	O	S	0	0
			1408	873	304	222	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	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 42 is a protein called 60S ribosomal protein L36a.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BA	1737	Total	C	N	O	P	0	0
			36892	16481	6588	12086	1737		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BB	262	Total	C	N	O	S	0	0
			2059	1312	384	356	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BE	227	Total	C	N	O	S	0	0
			1762	1122	317	315	8		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BN	143	Total	C	N	O	S	0	0
			1110	696	214	198	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BO	91	Total	C	N	O	S	0	0
			726	457	136	130	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ba	136	Total	C	N	O	S	0	0
			1007	617	196	188	6		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called 40S ribosomal protein S15a.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bg	67	Total	C	N	O	S	0	0
			544	343	101	93	7		

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

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

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

Mol	Chain	Residues	Atoms		AltConf
79	AA	184	Total	Mg	0
			184	184	
79	AB	2	Total	Mg	0
			2	2	
79	AC	4	Total	Mg	0
			4	4	
79	AP	1	Total	Mg	0
			1	1	
79	AR	1	Total	Mg	0
			1	1	
79	AX	1	Total	Mg	0
			1	1	
79	BA	27	Total	Mg	0
			27	27	

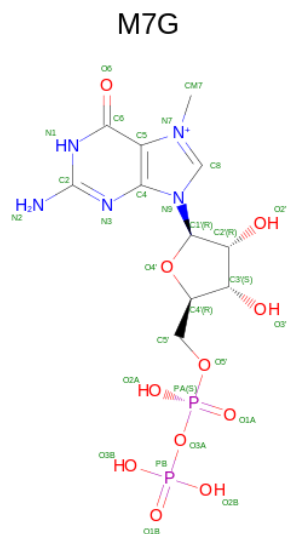
- Molecule 80 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
80	AA	51	Total 51	K 51	0
80	AB	1	Total 1	K 1	0
80	AD	1	Total 1	K 1	0
80	AL	1	Total 1	K 1	0
80	Ag	1	Total 1	K 1	0
80	Ah	1	Total 1	K 1	0
80	Aq	1	Total 1	K 1	0
80	BA	5	Total 5	K 5	0

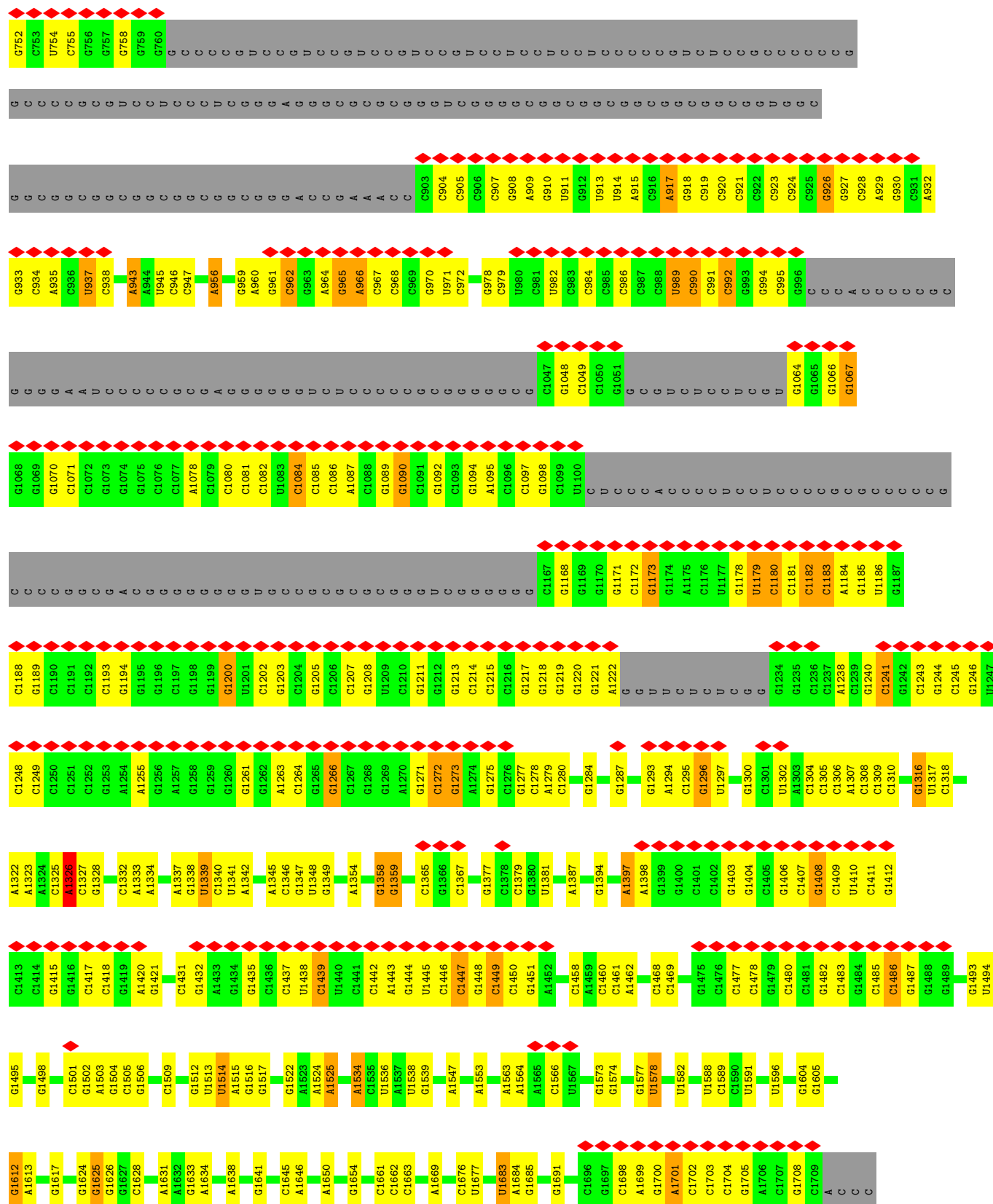
- Molecule 81 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 82 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (CCD ID: M7G) (formula: C₁₁H₁₈N₅O₁₁P₂).

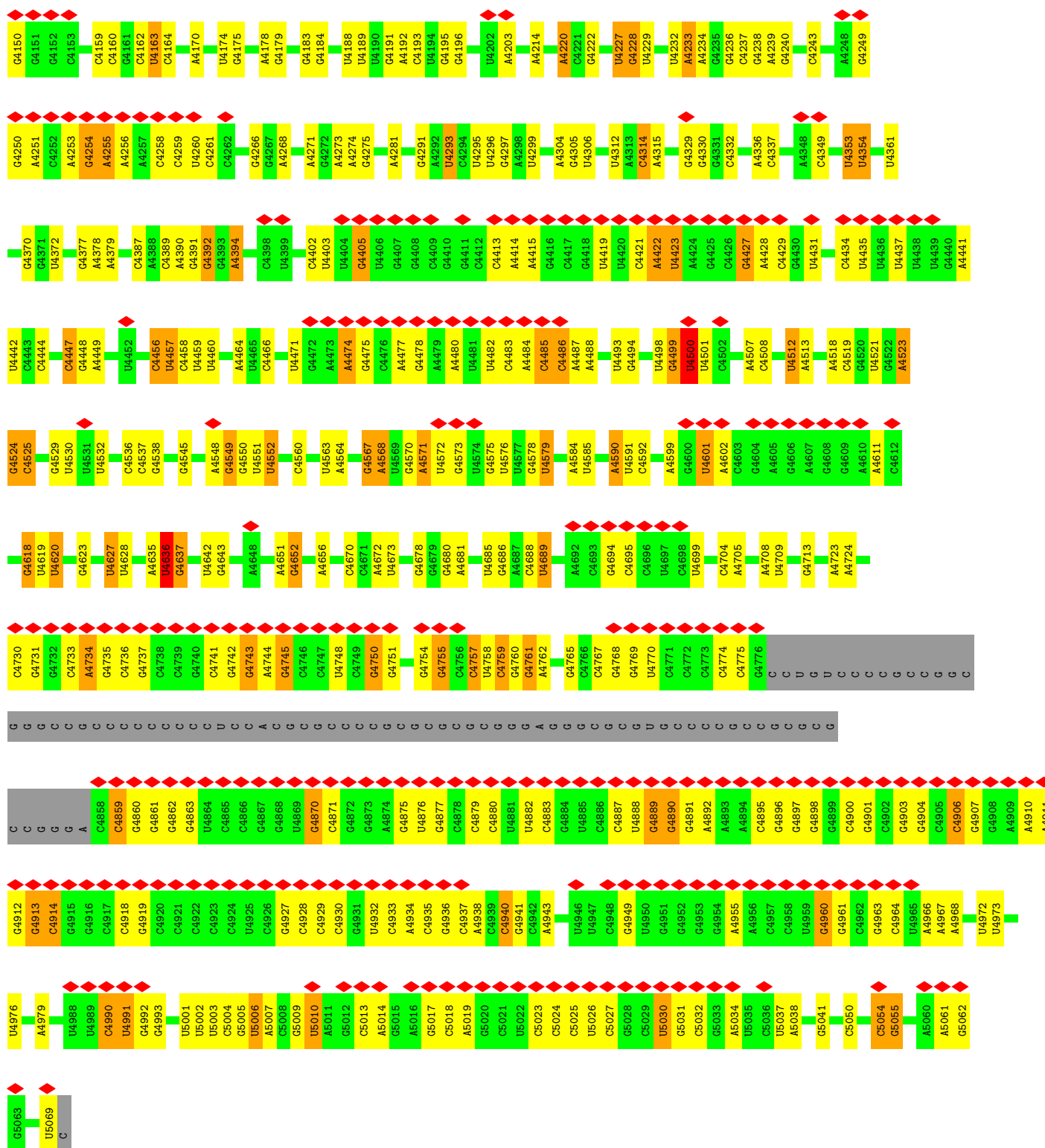


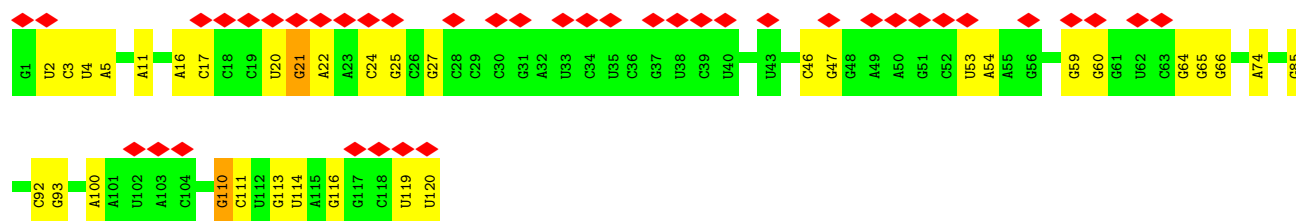
Mol	Chain	Residues	Atoms					AltConf
82	BA	1	Total	C	N	O	P	0
			24	11	5	7	1	



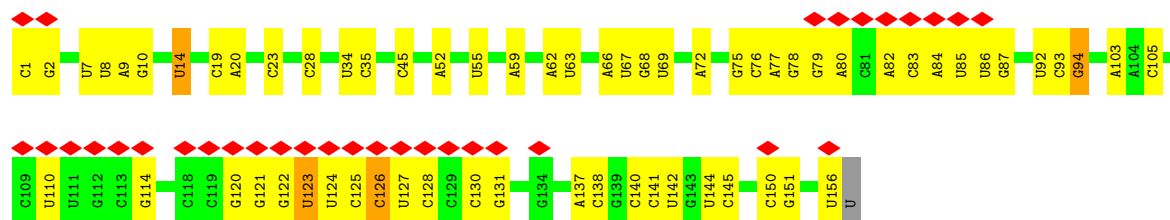
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A2870	C2749	C2672	U2575	G2496	G2391	C	G	A2030	A1970	C1881	C1715
A2871	G2750	G2675	G2576	C2497	C2392	C	G	C2031	C1971	C1785	G1716
G2756	G2756	A2676	C2583	C2498	C	C	G	U2032	G1972	A1786	C1717
A2757	A2757	C2683	G2586	C2499	A2395	C	C	A2041	G1973	A1787	C1718
G2758	G2758	C2684	A2587	G2500	A2396	C	C	G2046	U1974	A1788	A1719
G2759	G2759	C2685	C2588	C2501	A2397	C	C	U2048	G1975	C1893	C1720
G2760	G2760	G2686	C2589	G2502	G2397	C	C	A2048	G1976	U1792	G1721
U2761	U2761	U2687	C2589	G2503	G2400	C	C	U2048	G1977	A1793	C1722
G2762	G2762	C2688	A2601	C2504	A2401	C	C	G2055	C1978	U1794	U1725
U2763	U2763	C2689	A2601	C2505	G2406	C	C	G2056	A1979	U1801	U1726
A2764	A2764	C2690	C2607	C2506	G2406	C	C	G2063	A1980	A1802	C1731
A2765	A2765	G2608	G2608	G2507	C2410	C	C	G2064	U1981	G1803	C1732
A2766	A2766	G2609	G2610	A2507	C2411	C	C	A2069	G1982	A1804	G1733
U2767	U2767	G2610	G2611	U2508	A2412	C	C	A2071	A1983	G1805	C1740
C2768	C2768	G2611	G2612	A2513	U2415	C	C	G2076	U1984	C1806	G1741
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G2770	G2770	G2613	C2616	G2514	A2417	C	C	U2078	U1986	C1807	U1744
G2771	G2771	C2614	C2617	G2522	G2421	C	C	C2078	C1987	C1808	G1745
G2777	G2777	G2615	G2618	G2522	A2423	C	C	U2080	G1988	C1809	A1746
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G2779	G2779	G2620	G2621	A2529	U2425	C	C	C2082	A1990	C1811	U1748
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G2714	G2714	U2630	U2630	A2551	A2477	C	C	G2098	A2002	A1837	G1759
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U2718	U2718	G2634	G2634	G2555	G2481	C	C	G2102	U2006	G1847	C1763
C2719	C2719	U2635	U2635	G2556	G2482	C	C	G2103	G2007	G1848	G1764
G2720	G2720	G2636	G2636	G2557	G2483	C	C	G2104	U2008	G1855	A1765
G2721	G2721	U2637	U2637	C2558	G2484	C	C	A2105	A2009	C1856	A1766
U2722	U2722	G2640	G2640	G2559	A2485	C	C	G2106	G2010	C1857	A1767
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G2724	G2724	G2648	G2648	C2561	G2487	C	C	G2108	A2012	C1859	G1769
A2725	A2725	U2649	U2649	G2562	G2488	C	C	G2109	A2013	U1860	A1770
G2726	G2726	G2652	G2652	G2563	G2489	C	C	G2110	C2014	U1861	U1771
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C2731	C2731	C2669	C2669	C2568	U2494	C	C	G	C2019	C1965	A1776
G2739	G2739	G2670	G2670	G2569		C	C	G	U2020	A1967	C1777
C2742	C2742			U2570		C	C	G	C2021	G1968	C1778
A2743	A2743			C2571		C	C	G	C2022		U1779
A2744	A2744			C2572		C	C	G	C2023		A1780
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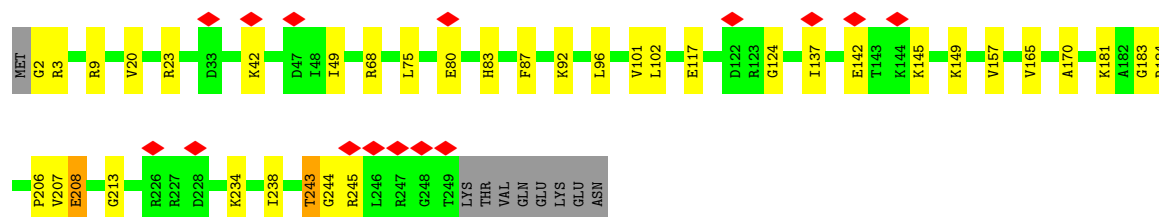
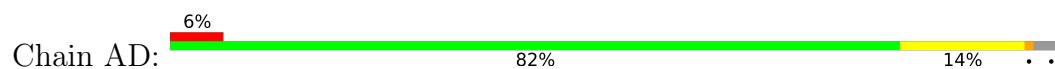




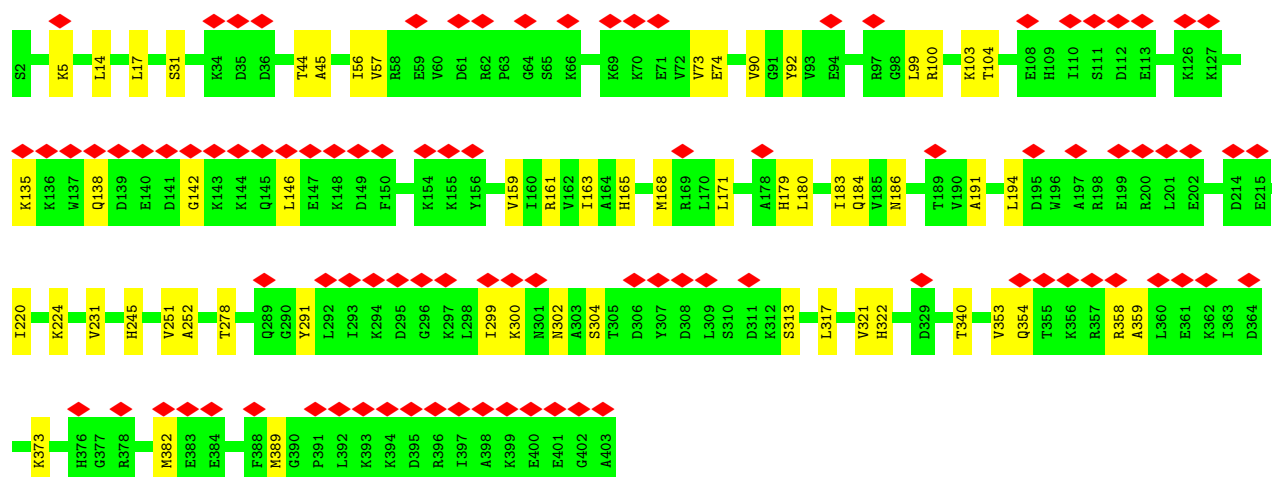
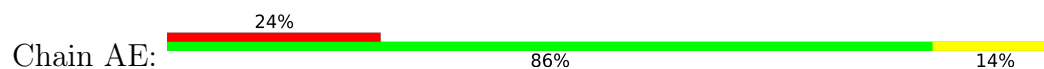
• Molecule 3: 5.8S rRNA (156-MER)



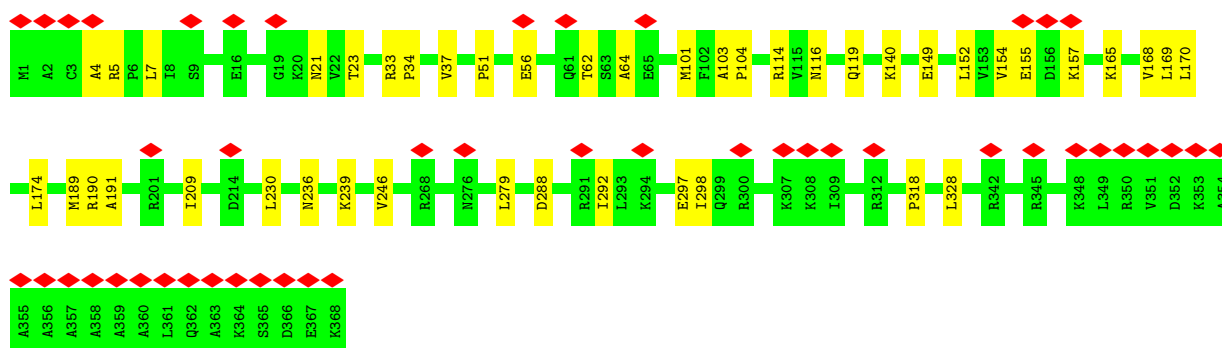
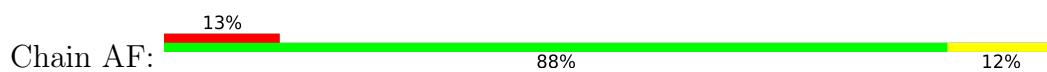
• Molecule 4: 60S ribosomal protein L8



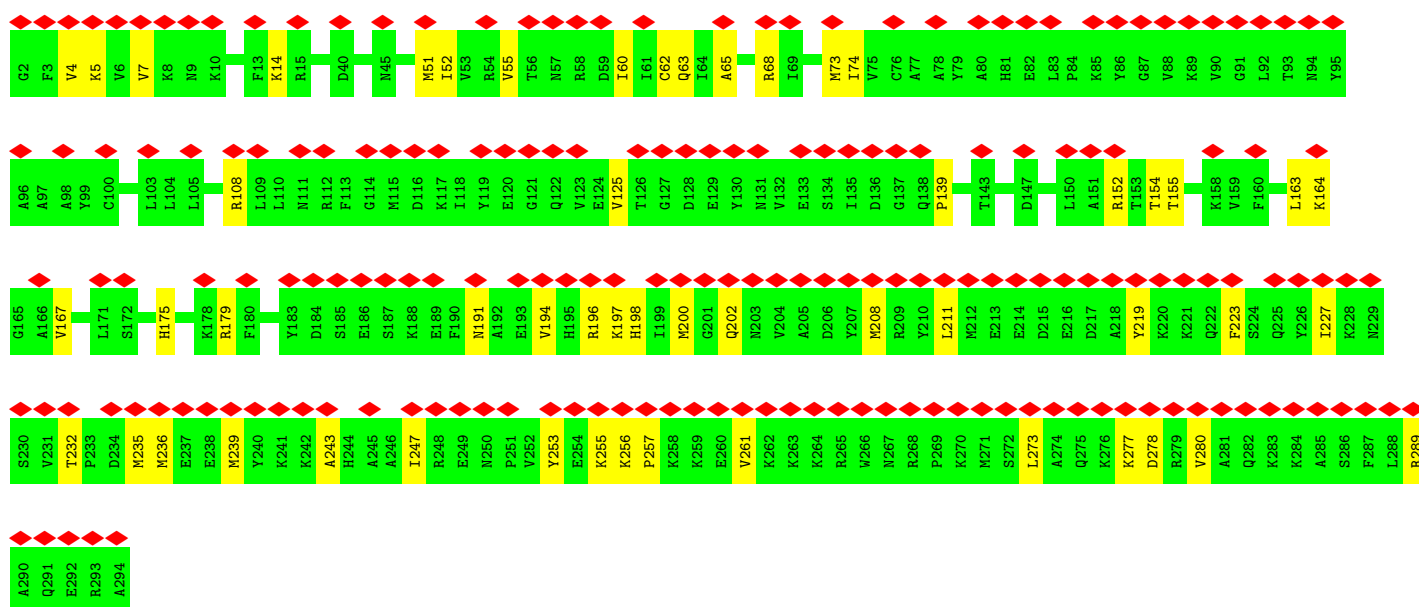
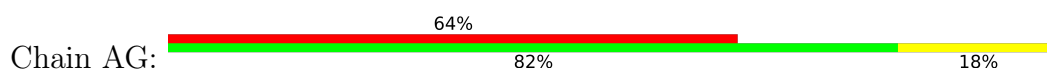
• Molecule 5: Large ribosomal subunit protein uL3



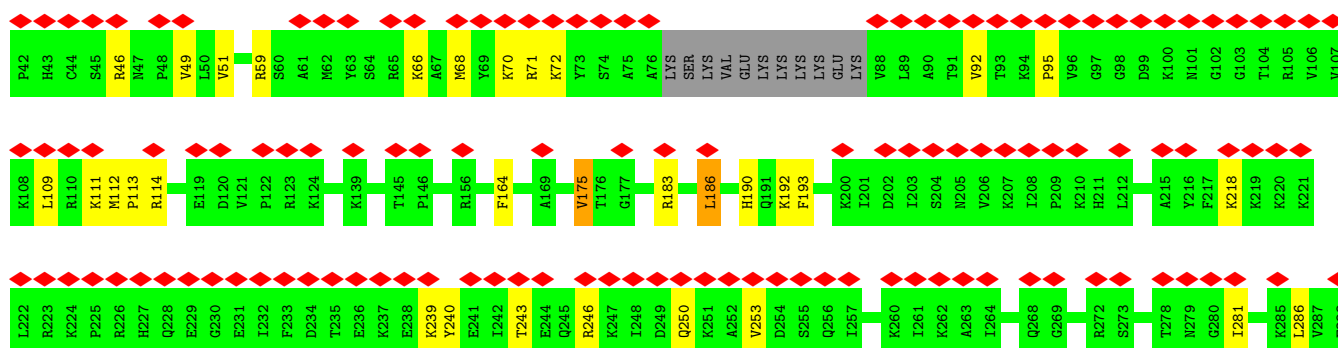
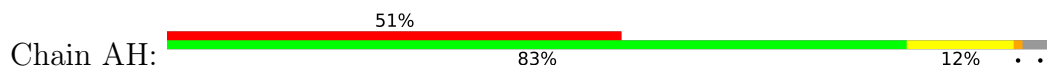
• Molecule 6: Large ribosomal subunit protein uL4



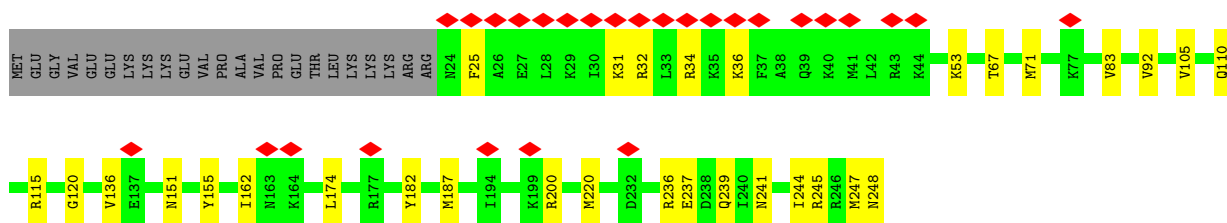
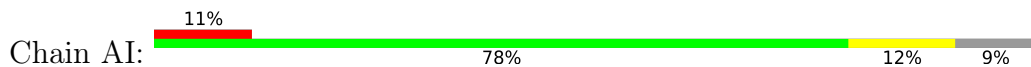
• Molecule 7: Large ribosomal subunit protein uL18



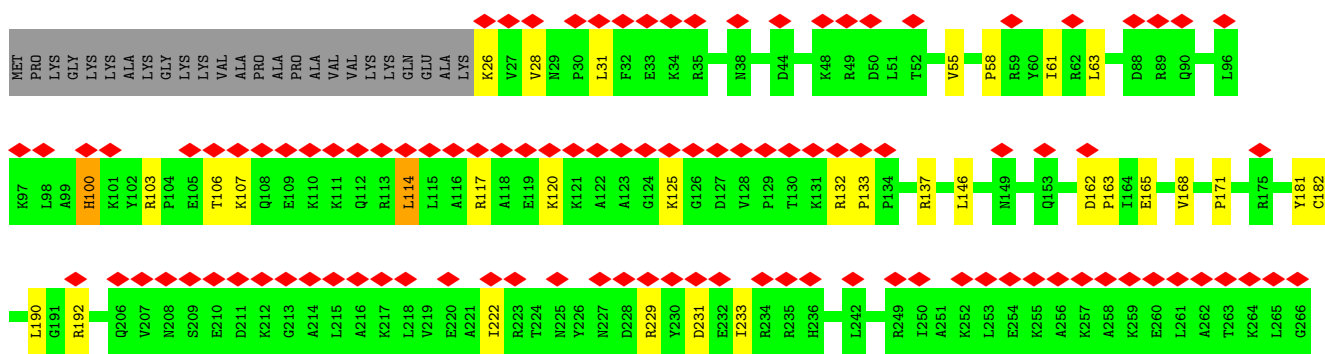
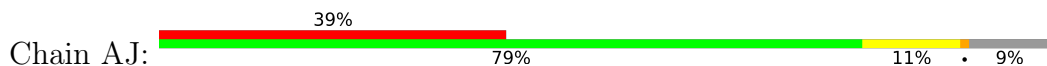
• Molecule 8: Large ribosomal subunit protein eL6



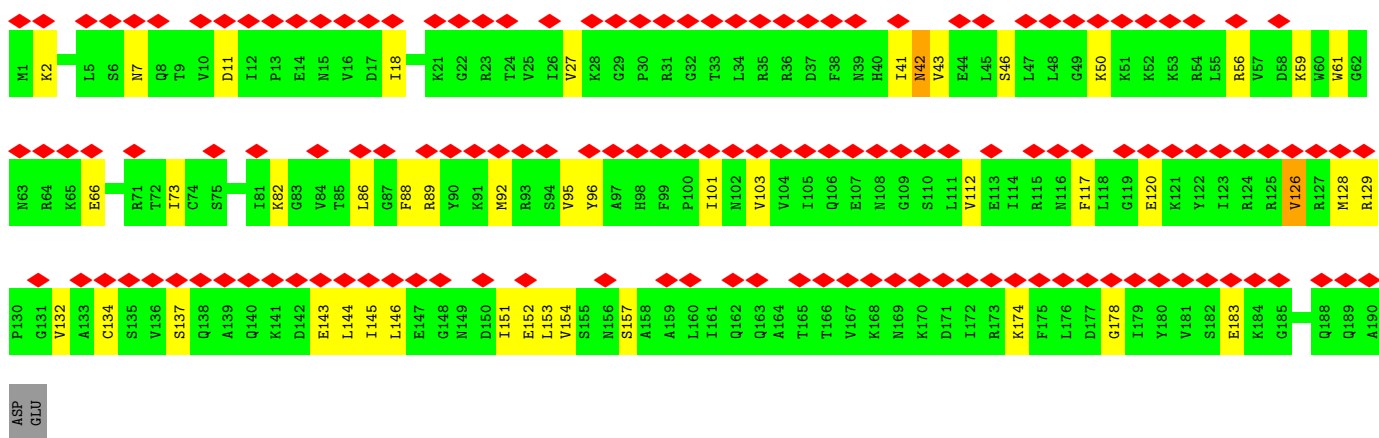
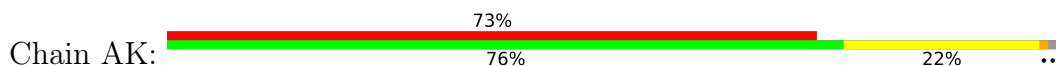
- Molecule 9: 60S ribosomal protein L7



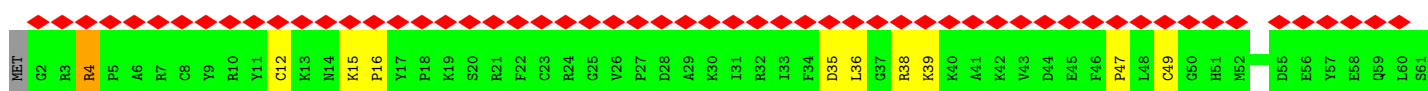
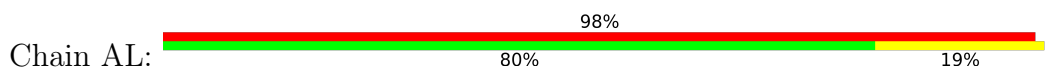
- Molecule 10: 60S ribosomal protein L7a



- Molecule 11: 60S ribosomal protein L9



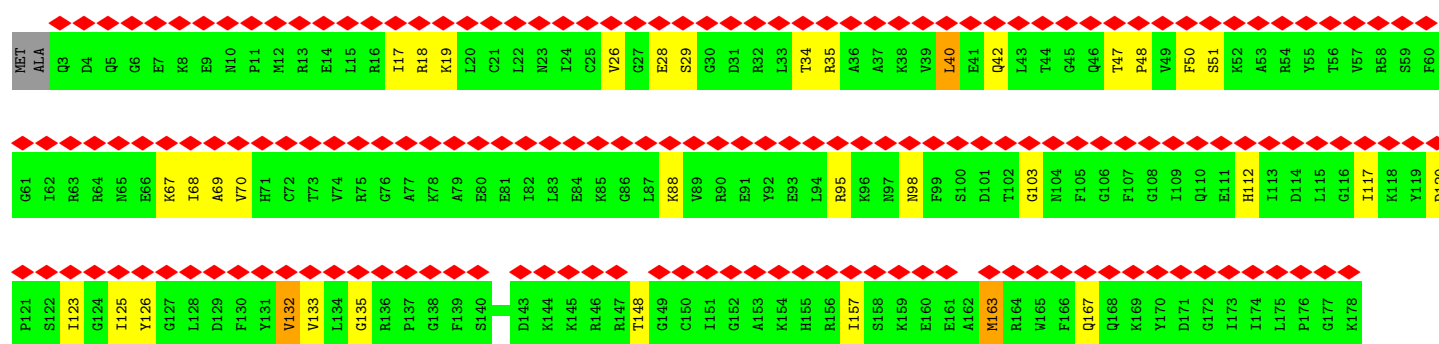
- Molecule 12: Ribosomal protein uL16-like





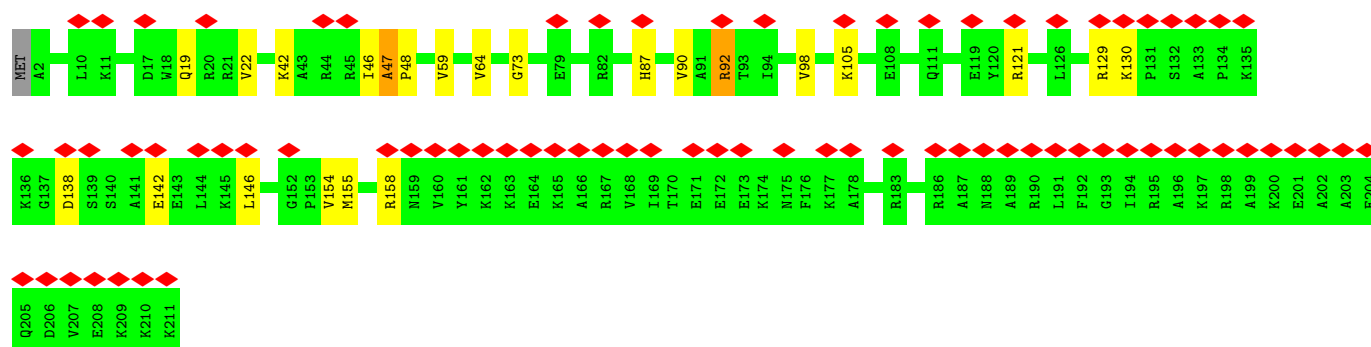
• Molecule 13: 60S ribosomal protein L11

Chain AM: ..



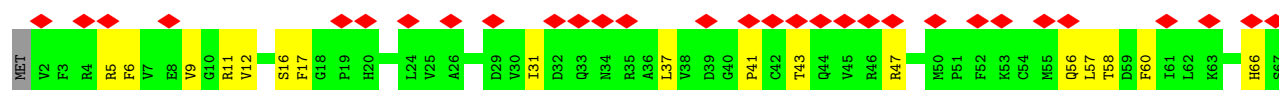
• Molecule 14: 60S ribosomal protein L13

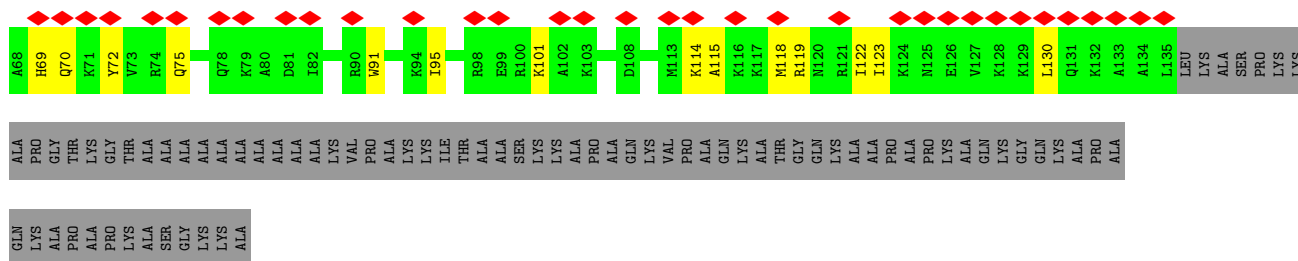
Chain AN: .



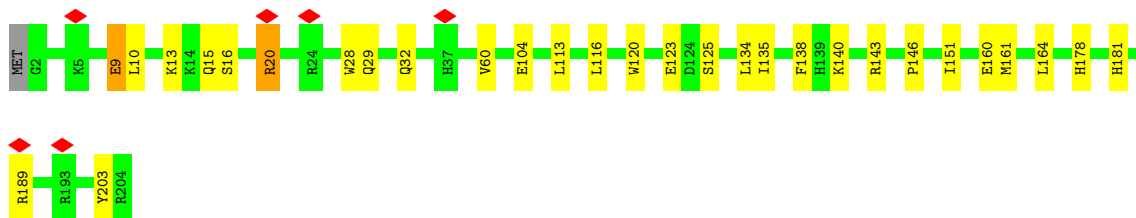
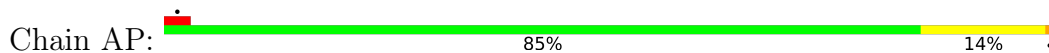
• Molecule 15: 60S ribosomal protein L14

Chain AO: ..

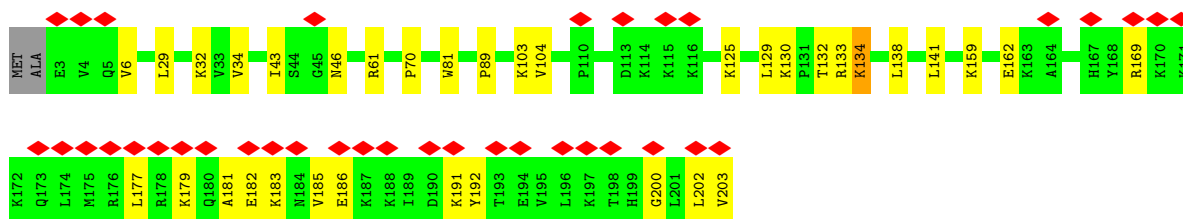
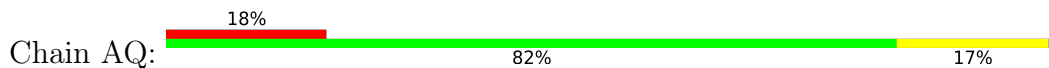




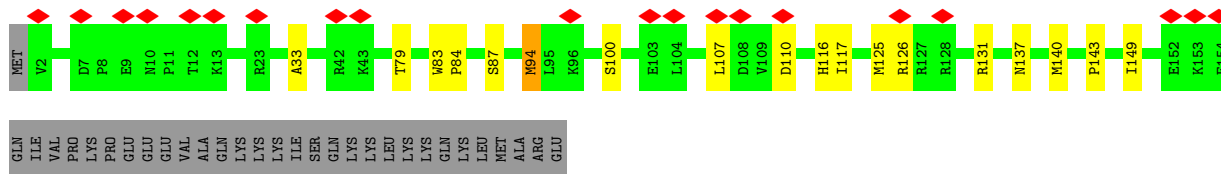
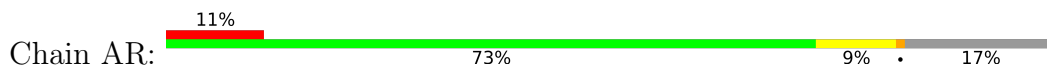
- Molecule 16: 60S ribosomal protein L15



- Molecule 17: 60S ribosomal protein L13a



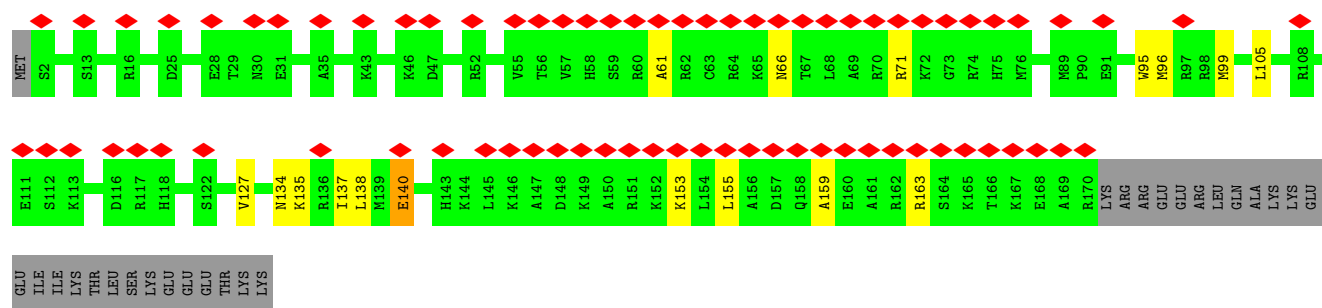
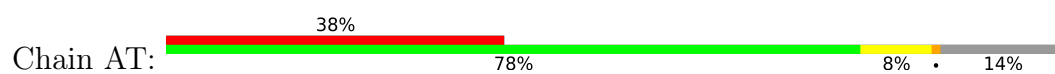
- Molecule 18: 60S ribosomal protein L17



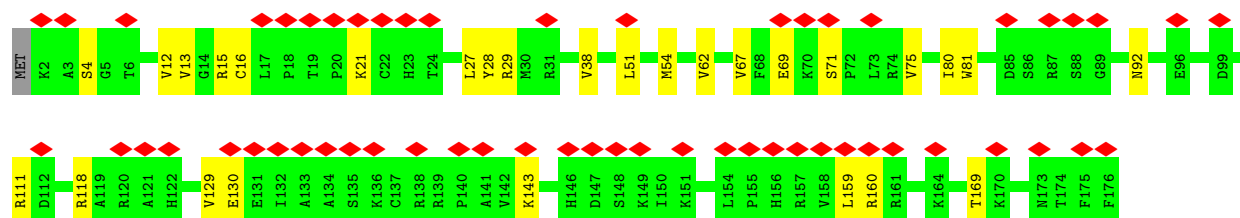
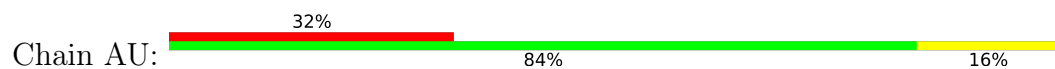
- Molecule 19: 60S ribosomal protein L18



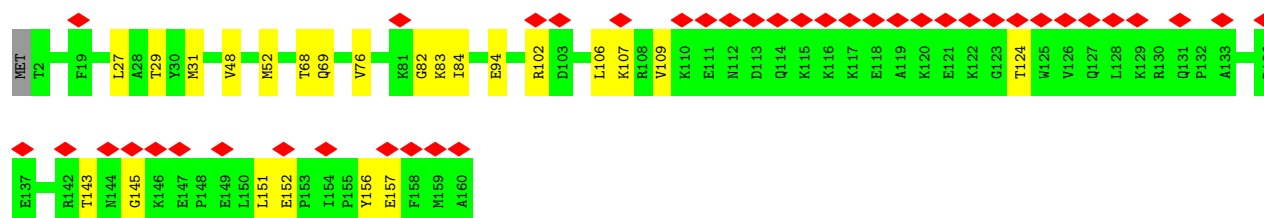
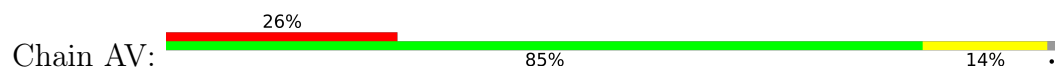
- Molecule 20: 60S ribosomal protein L19



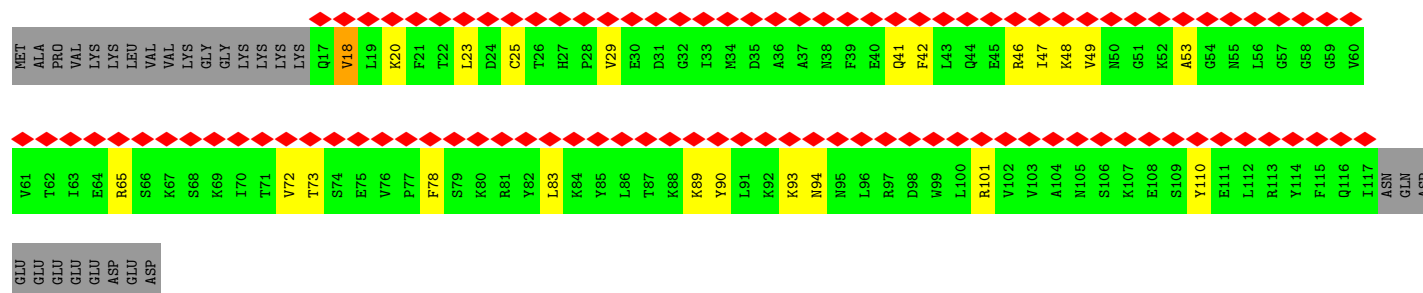
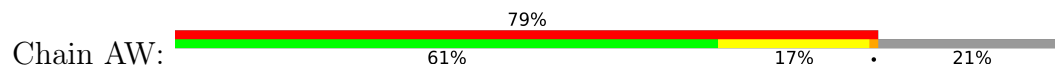
- Molecule 21: 60S ribosomal protein L18a



- Molecule 22: 60S ribosomal protein L21

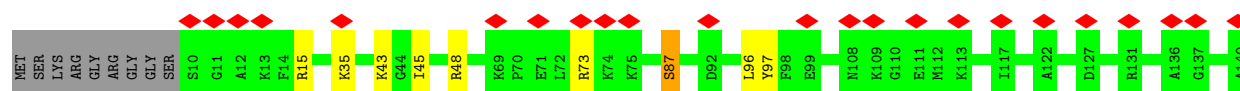


- Molecule 23: 60S ribosomal protein L22



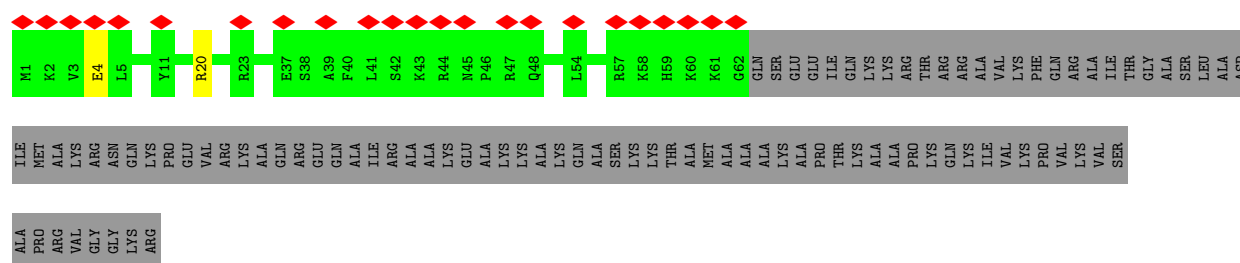
- Molecule 24: 60S ribosomal protein L23

Chain AX: 



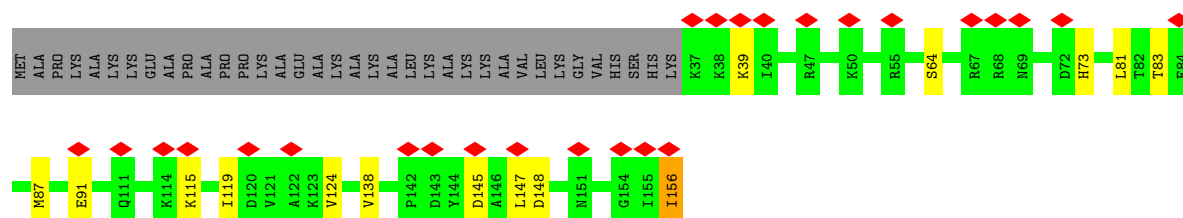
• Molecule 25: 60S ribosomal protein L24

Chain AY: 



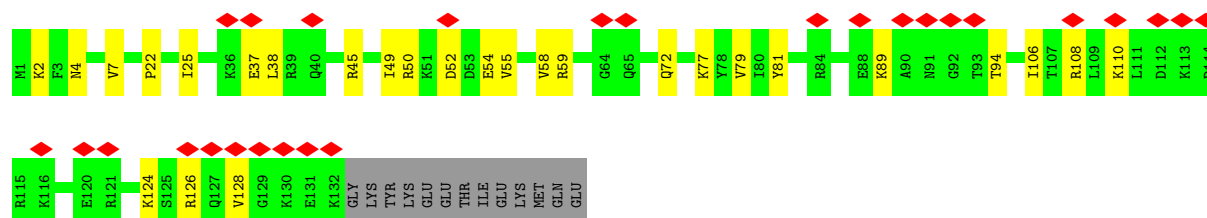
• Molecule 26: 60S ribosomal protein L23a

Chain AZ: 



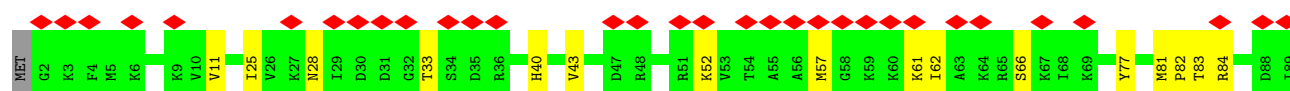
• Molecule 27: 60S ribosomal protein L26

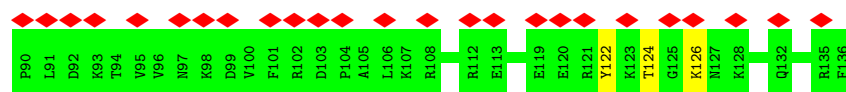
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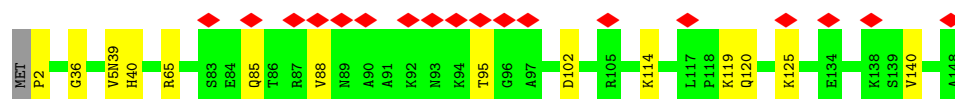
• Molecule 28: 60S ribosomal protein L27

Chain Ab: 

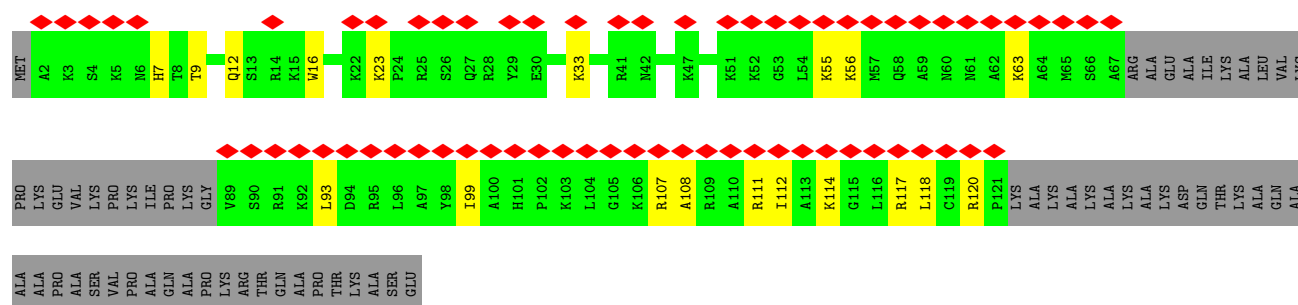
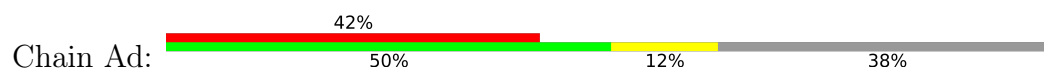




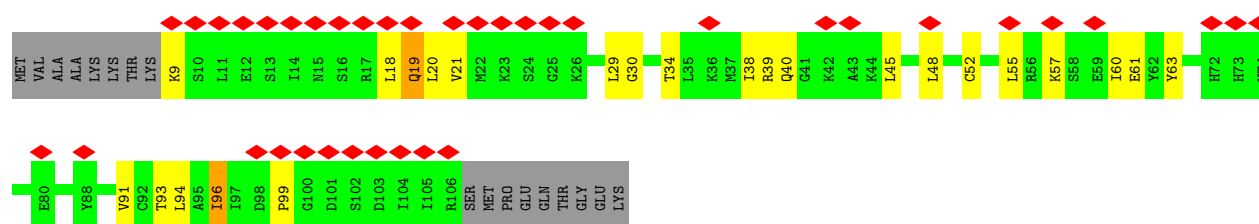
- Molecule 29: Large ribosomal subunit protein uL15



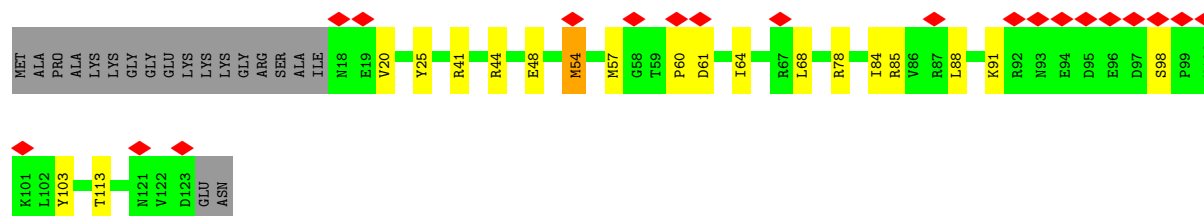
- Molecule 30: 60S ribosomal protein L29



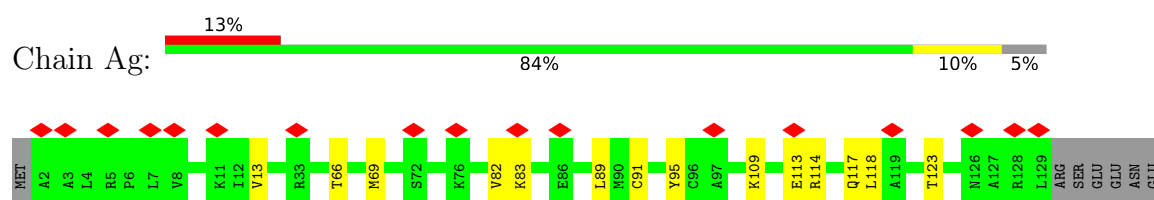
- Molecule 31: 60S ribosomal protein L30



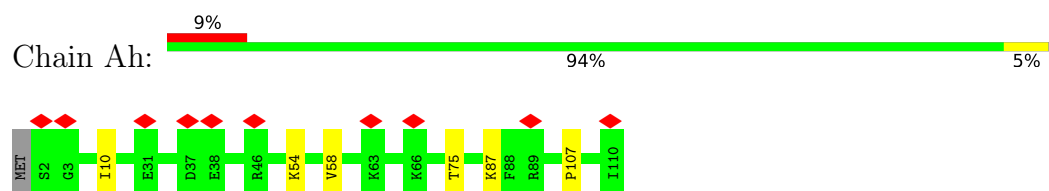
- Molecule 32: 60S ribosomal protein L31



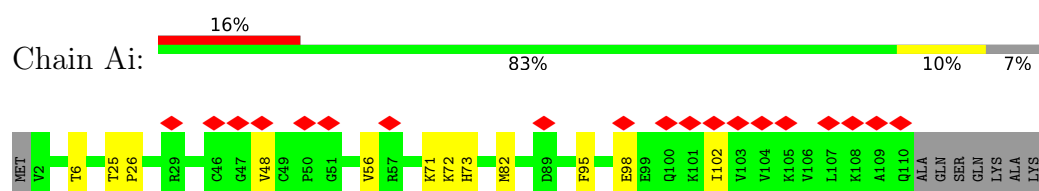
- Molecule 33: 60S ribosomal protein L32



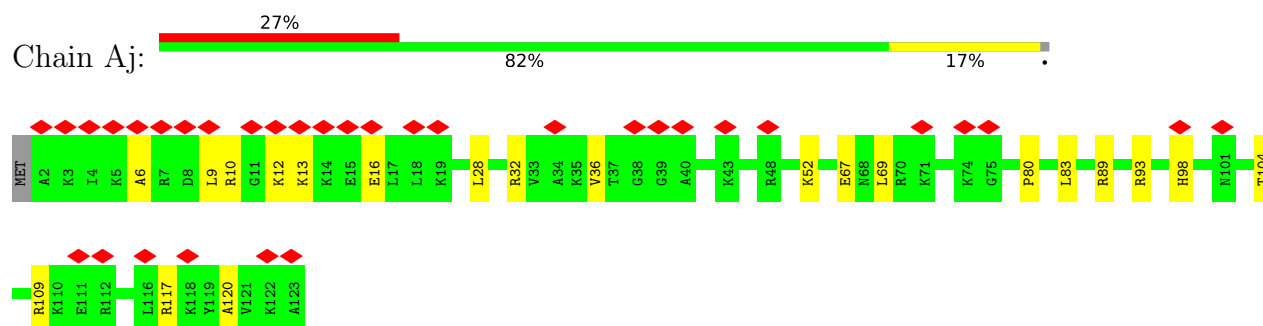
- Molecule 34: 60S ribosomal protein L35a



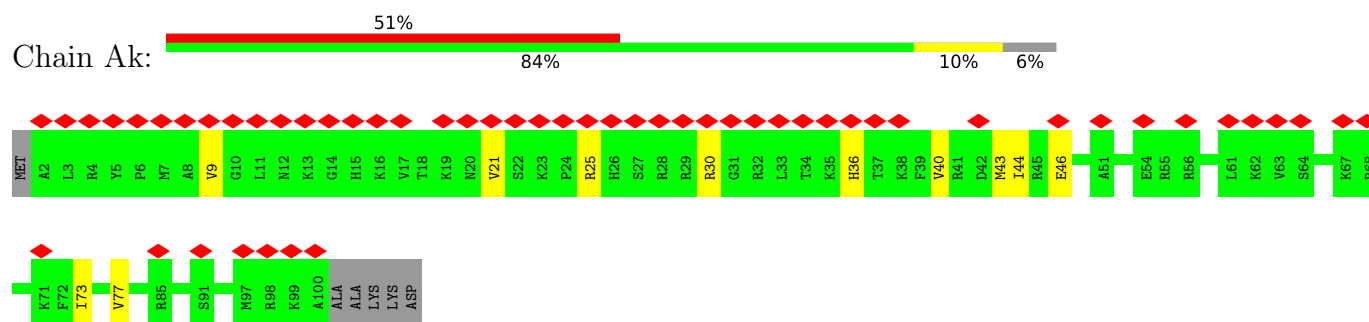
- Molecule 35: 60S ribosomal protein L34



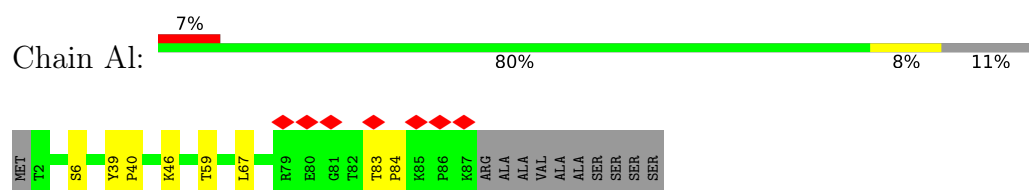
- Molecule 36: 60S ribosomal protein L35



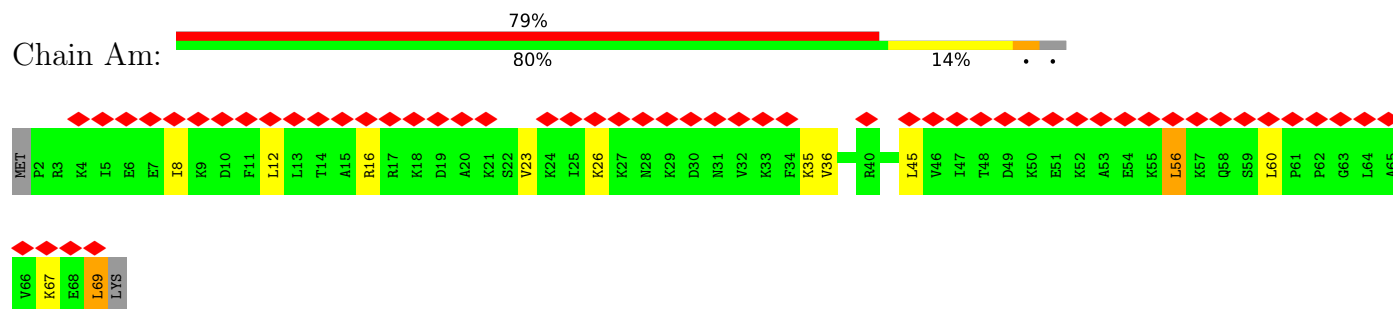
- Molecule 37: 60S ribosomal protein L36



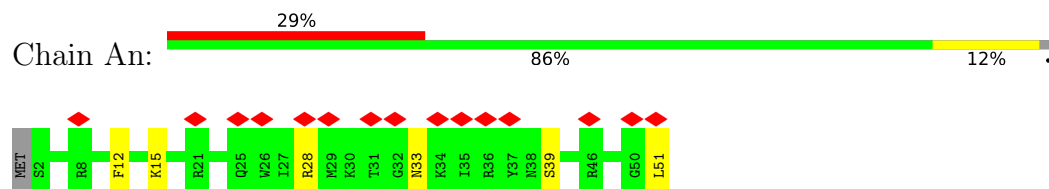
- Molecule 38: 60S ribosomal protein L37



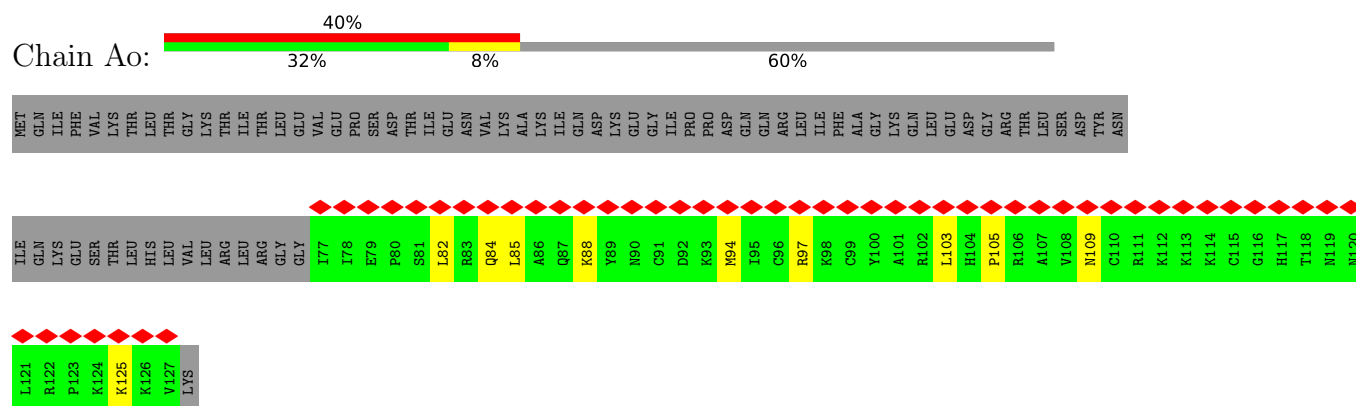
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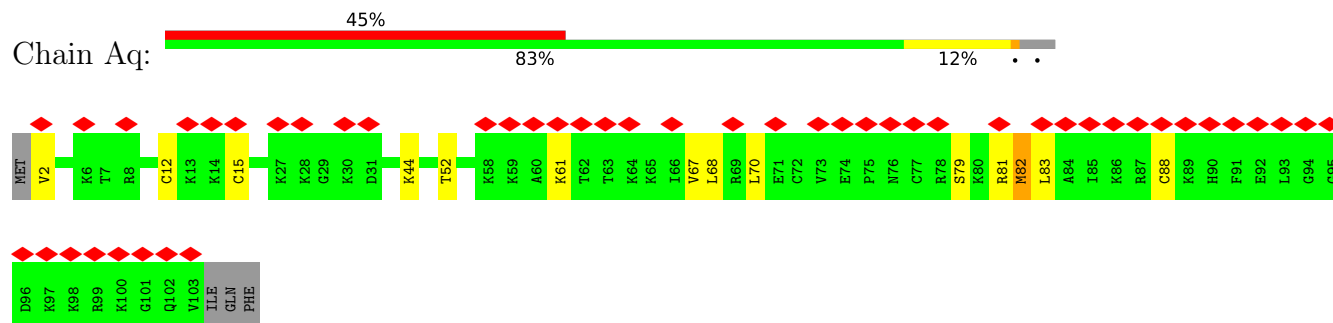
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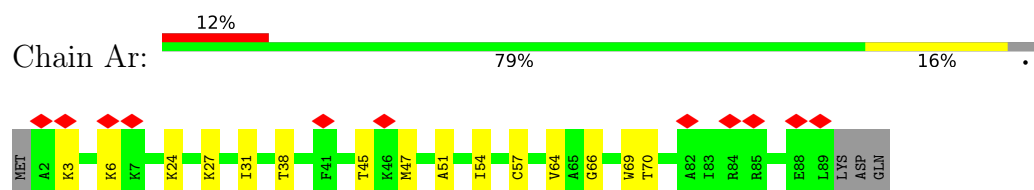
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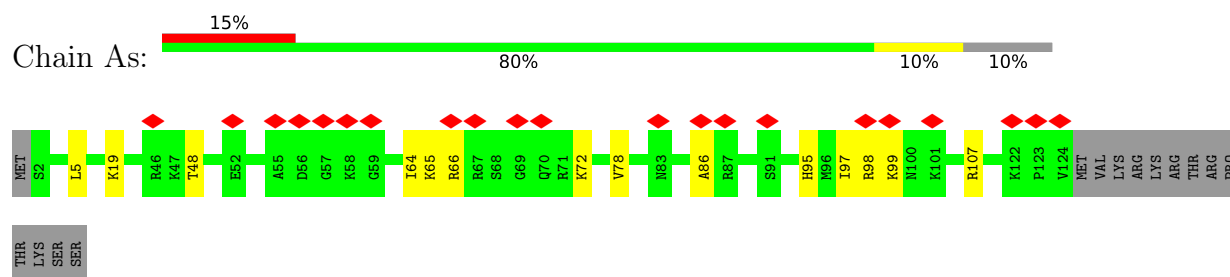
Chain Aq:



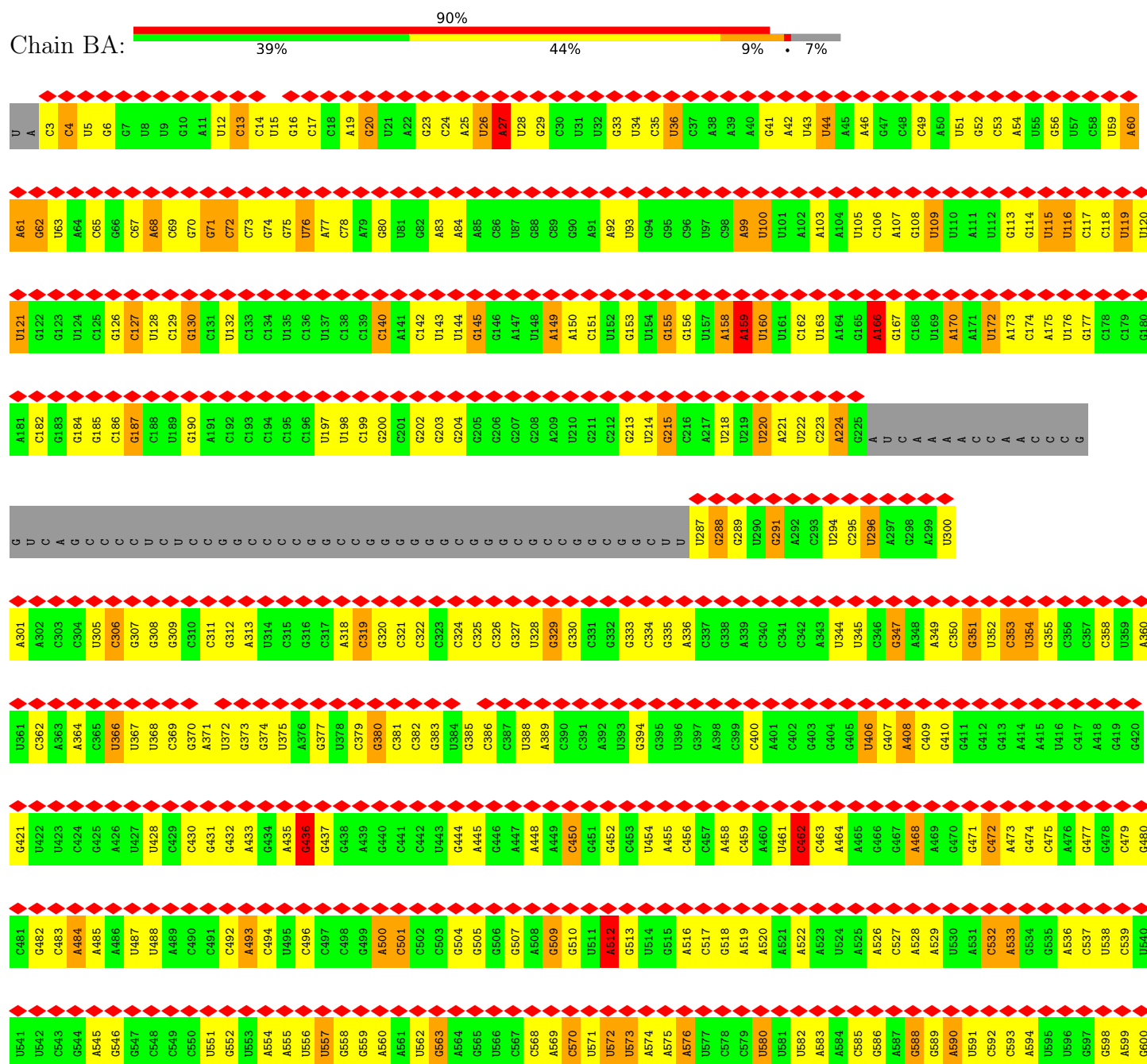
Chain Ar:



- Molecule 44: 60S ribosomal protein L28

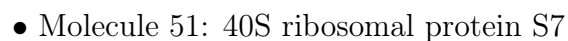
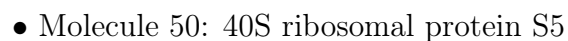


- Molecule 45: 18S rRNA (1740-MER)



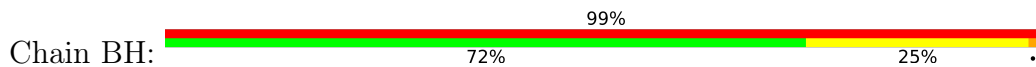
G1327	G1267	G1207	C1147	A1087	A1023	A963	A903	C843	C	G602	G601
G1328	C1268	A1208	A1148	U1088	A1024	A964	A904	U844	A	G603	G602
U1329	G1269	A1209	A1149	G1089		U965	C905	G845	C	A604	C603
G1330	G1270	G1210	A1150	C1090	A1027	U966	U906	G846	C	G605	A604
C1331	C1271	G1211	G1151	C1091	A1028	C967	G907	A847	C	G606	A605
A1332	C1272	G1212	U1152	A1093	G1029	U968	A908	U848		U607	G606
U1333	C1273	C1213	C1153	C1094	A1030	U969	G909	A949		U608	U607
G1334	G1274	A1214	U1154	C1095	A1031	G970	G910	C790		U609	C608
G1335	G1275	C1215	U1155	G1096	C1032	G971	G911	C791		G610	U609
C1336	A1276	C1216	U1156	A972	G1033	A972	C912	C792		G611	U610
U1337	C1277	A1217	G1157	G1097	A1034	C973	A913	G793		A671	G611
G1338	A1278	C1218	C1158	C1098	U1038	C974	U914	A794		A672	U612
U1339	G1279	C1219	C1159	G1099	G1040	G975	G915	A795		G673	G613
U1340	G1280	A1220	U1160	A1100	G1041	G976	A916	G796			G614
C1341	G1281	G1221	U1161	U1101	A1042	C977	U917	G797		G677	C615
U1342	A1282	C1222	C1162	G1102	A1043	G978	U918	A798		U678	A616
U1343	C1283	A1223	G1163	C1103	G1044	C979	A919	G799		G680	G617
A1344	G1284	G1224	G1164	G1104	G1045	A980	A920	U800		U681	C618
G1345	G1285	U1225	G1165	G1105	U1046	A981	G921	U801		U682	A619
U1346	G1286	G1226	G1166	G1106	U1047	G982	A922	A802		G683	G620
U1347	A1287	C1227	G1167	G1107	C1047	A983	G923	A803		G684	C621
G1348	U1288	A1228	G1168	G1108	G1048	C984	G924	U804		G685	C622
U1349	U1289	G1229	G1169	C1109	A1049	G985	G925	U805		U686	G623
U1350	G1290	C1230	A1170	G1110	A1050	G986	A926	U806		G687	C624
G1351	A1291	C1231	G1171	U1111	G1051	A987	G927	G807		U688	G625
G1352	C1292	U1232	U1112	U1112	A1052	C988	G928	A808		U689	G626
A1353	A1293	G1233	A1113	A1113	C1053	C989	G929	A809		G690	U627
G1354	G1294	C1234	U1174	U1114	G1054	A990	C930	A810		G691	A628
A1295	A1295	G1235	G1175	U1115	A1055	G991	C931	A811		G692	A629
G1356	U1296	G1236	G1176	C1116	U1056	A992	G932	A812		A693	U630
U1297	U1297	C1237	U1177	C1117	C1057	G993	G933	G873		G694	U631
G1298	U1298	U1238	U1178	C1118	A1058	C994	G934	G874		C695	C632
U1358	G1299	U1239	G1179	G1119	G1059	G995	G935	A875		G696	C633
U1359	U1300	U1239	A1180	A1119	A1060	A996	G936	C876		G697	A634
U1360	A1301	A1240	U1181	U1120	U1061	A997	C937	C877		G698	G635
G1361	G1302	A1241	G1121	G1121	U1062	A998	A938	G878		C	C636
U1362	C1303	U1242	A1182	A1122	C1063	G999	U939	G879		G	U637
C1363	U1243	U1243	A1183	C1123	C1064	C1000	U940	G880		G	C638
U1364	U1304	U1244	G1184	C1124	C1065	A1001	C941	G881		G	C639
G1365	C1305	G1245	C1185	C1125	U1066	U1002	G942	U822		G	A640
G1366	U1306	U1246	U1186	C1126	G1067	U1003	U943	U823		G	A641
U1367	U1307	C1247	G1187	C1127	U1068	U1004	A944	C824		C	U642
U1368	U1308	B8N1248	A1188	C1128	U1069	G1005	U945	A825		C	A643
A1369	C1309	C1249	A1189	G1129	A1070	C1006	U946	A826		G	G644
U1370	U1310	A1250	A1190	U1130	G1071	C1007	G947	A827		C	C645
U1371	C1311	A1251	C1191	G1131	U1072	A1008	C948	G828		C	G646
U1372	U1372	C1252	U1192	C1132		A1009	G949	C829		C	U647
C1373	A1313	A1253	U1193	C1133	C1075	G1010	C950	A830		C	A648
C1374	U1314	G1254	A1194	A1133	G1076	G1011	C951	G831		C	U649
G1375	U1315	G1255	A1195	G1134	A1077	A1011	G952	G832		A	A650
A1376	C1316	G1256	A1196	C1135	C1078	A1012	G953	G833		C	U651
U1377	G1317	G1257	G1197	U1136	C1079	U1013	C954	C834		C	A652
A1378	C1318	A1258	U1198	U1137	A1080	U1014	U954	C835		A	A653
A1379	U1319	A1259	A1199	C1138	U1081	U1015	A955	G836		C	A654
C1380	G1320	A1260	A1200	U1016	A1082	U1016	G956	U837		C	A655
G1381	G1321	C1261	A1083	U1017	A1083	U1017	A957	G838		C	U657
A1382	C1322	G1262	A1084	U1018	C1084	U1018	G958	C839		C	G656
A1383	U1323	U1263	C1085	C1019	G1086	C1019	G959	C840		C	U658
C1384	G1324	U1264	G1142	A1143		A1020	U960	G841		C	G659
G1385	G1325	A1265	A1144	A1021		U1021	G961	G901		C	C660
A1386	UY11326	C1266	A1145	A1022		U1022	A962	G902			



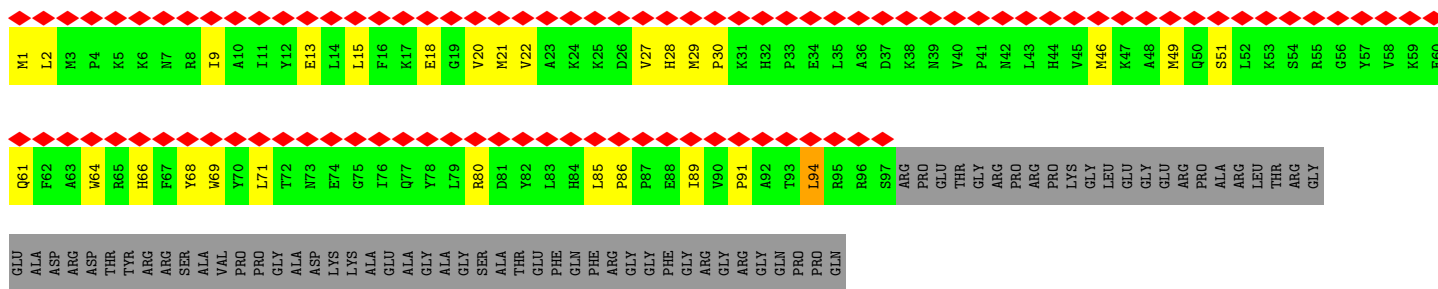
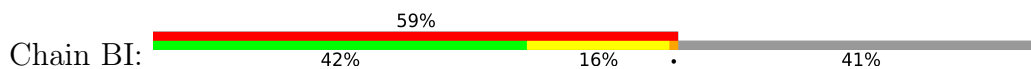




• Molecule 52: 40S ribosomal protein S8

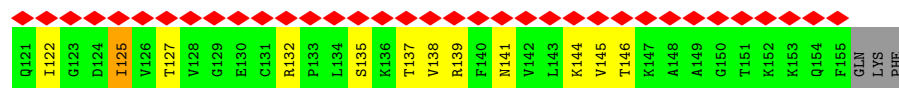


• Molecule 53: 40S ribosomal protein S10

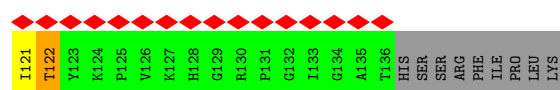
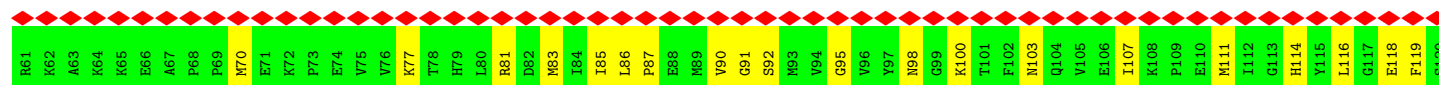
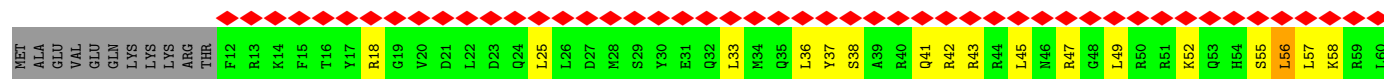
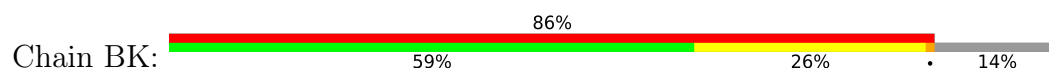


• Molecule 54: 40S ribosomal protein S11

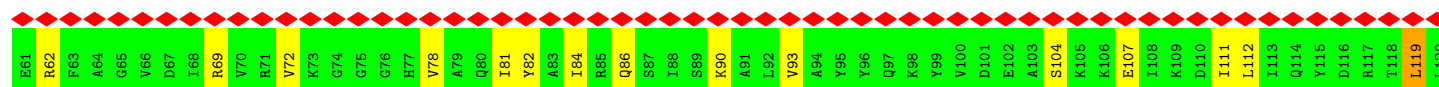
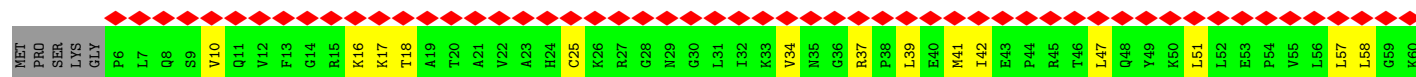
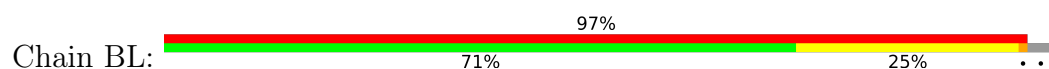




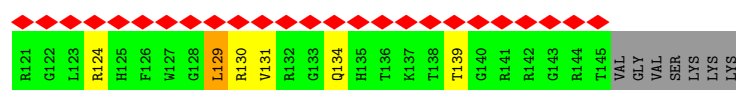
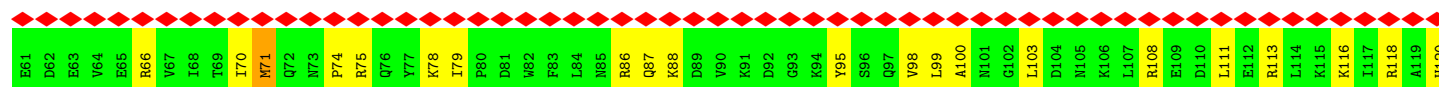
- Molecule 55: 40S ribosomal protein S15



- Molecule 56: 40S ribosomal protein S16

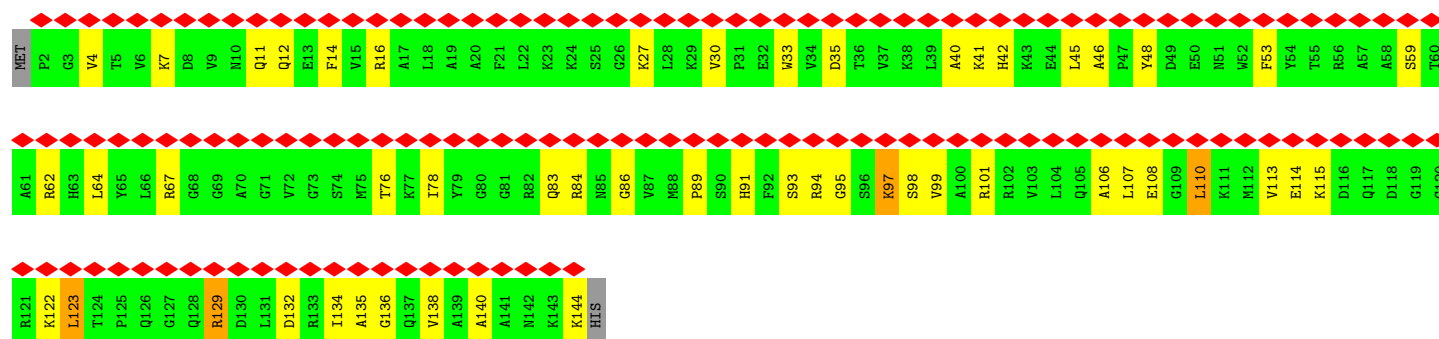


- Molecule 57: 40S ribosomal protein S18

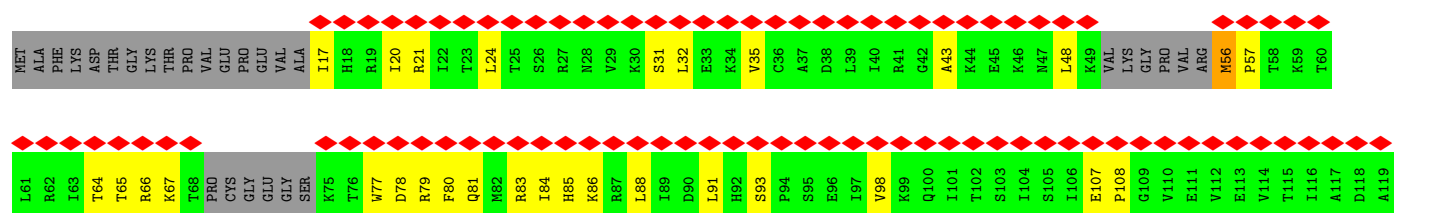
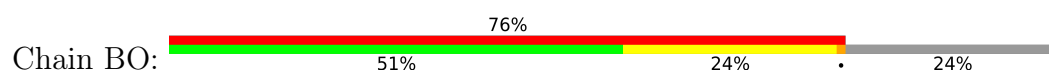


- Molecule 58: Small ribosomal subunit protein eS19

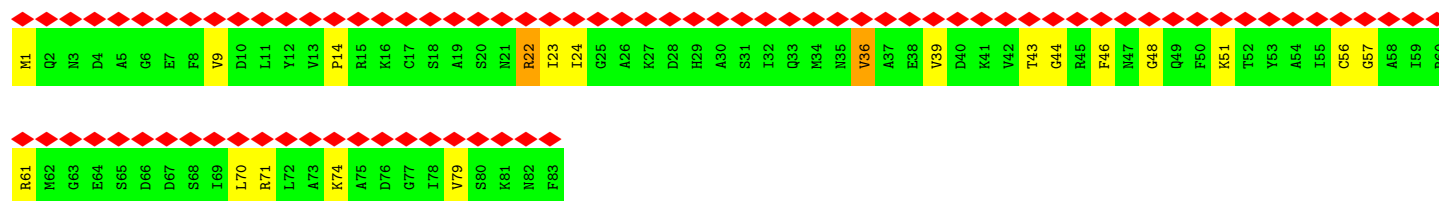
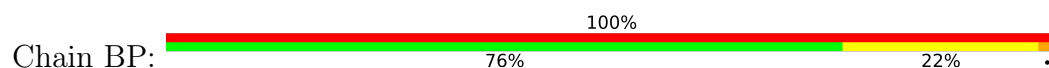




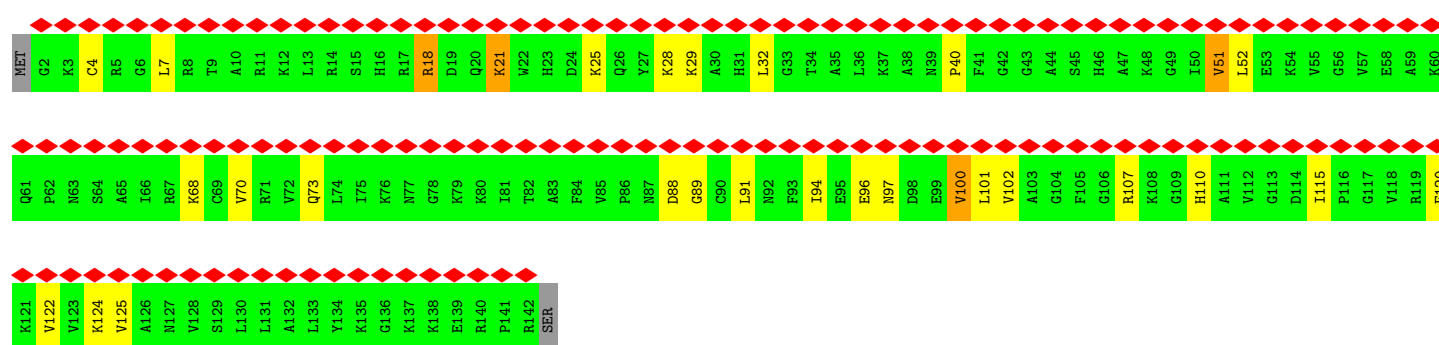
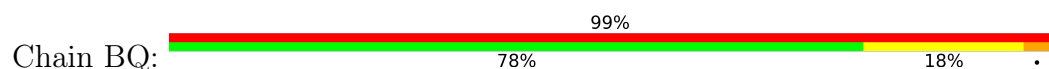
• Molecule 59: 40S ribosomal protein S20



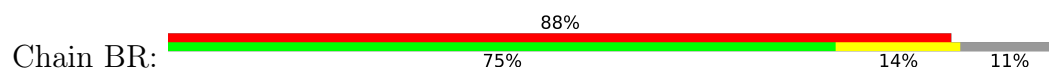
• Molecule 60: 40S ribosomal protein S21



• Molecule 61: 40S ribosomal protein S23

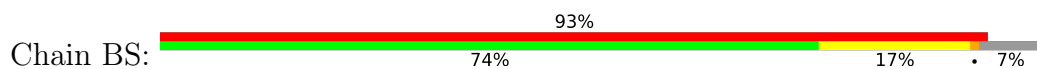


• Molecule 62: 40S ribosomal protein S26

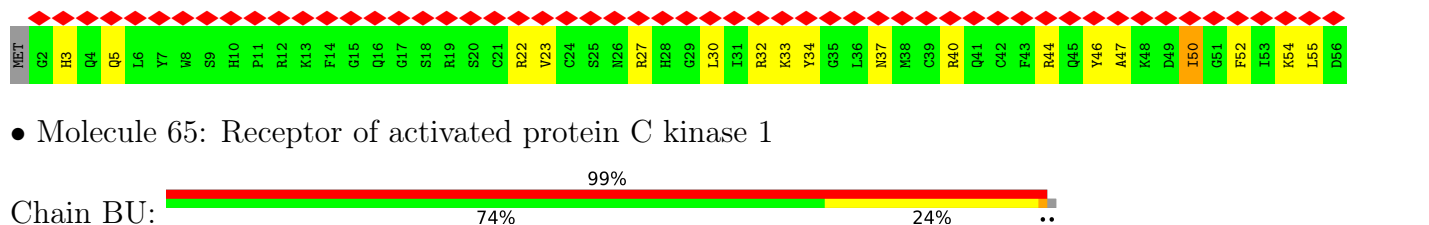




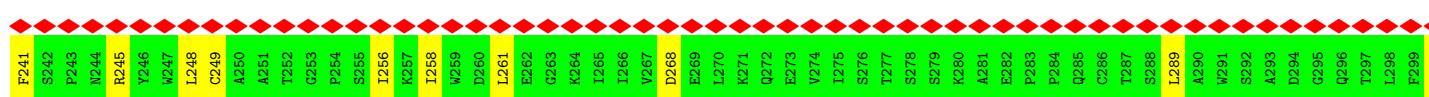
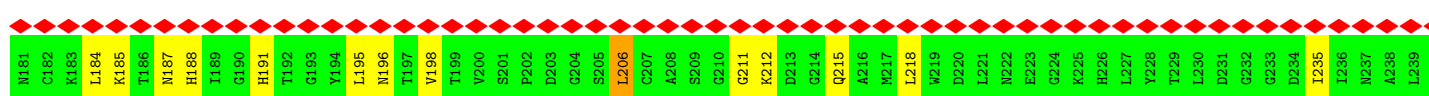
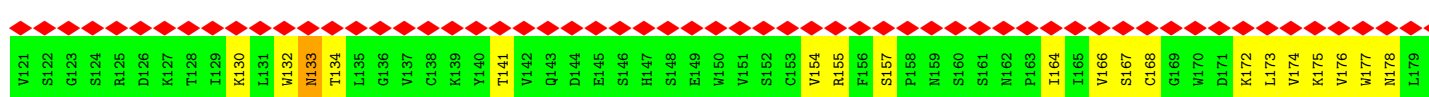
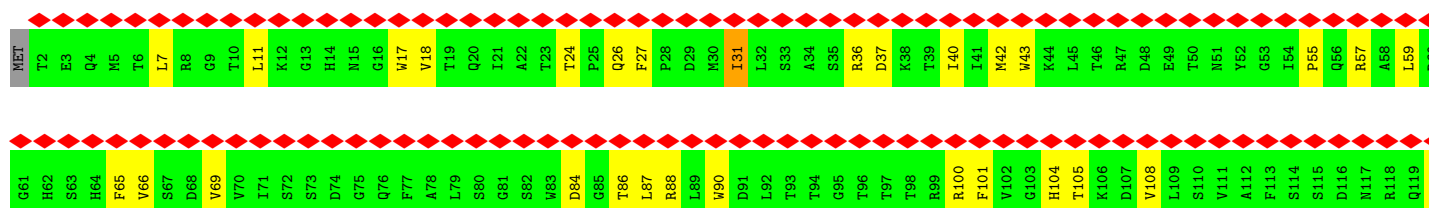
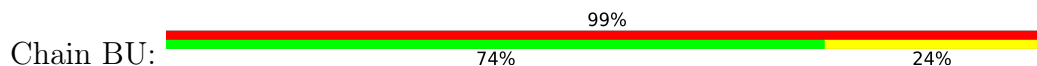
• Molecule 63: 40S ribosomal protein S28



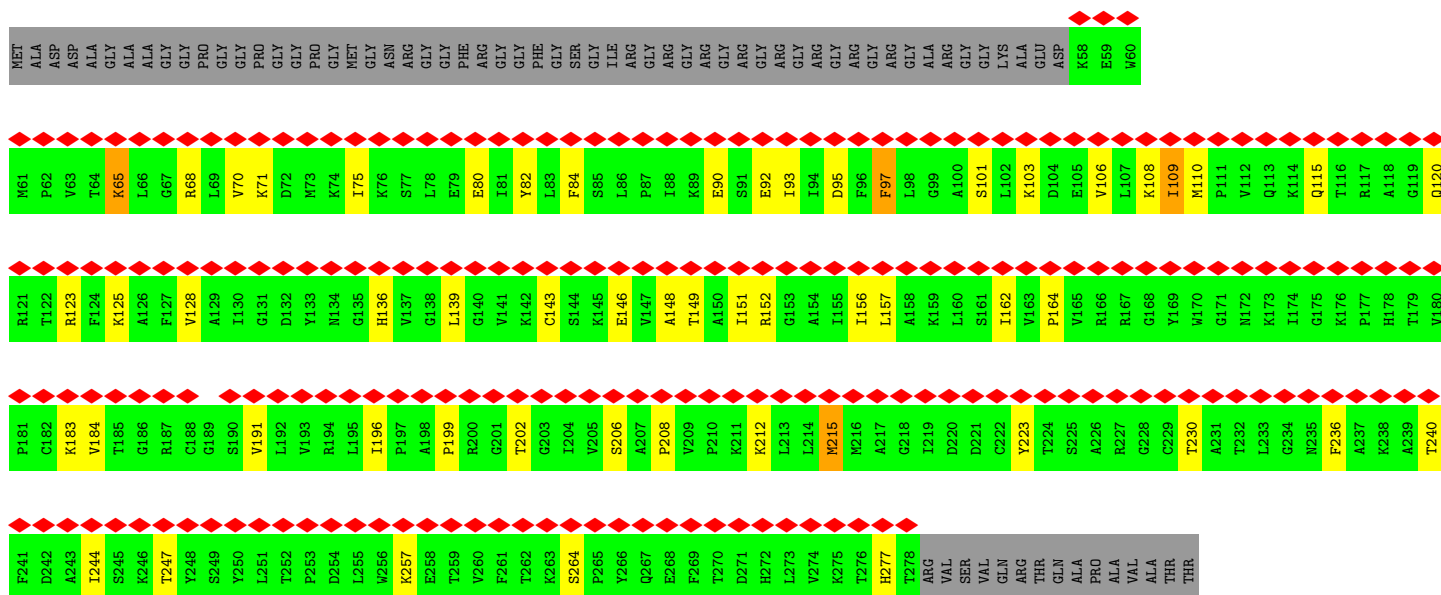
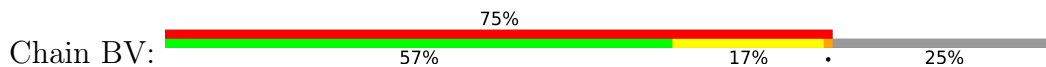
• Molecule 64: 40S ribosomal protein S29



• Molecule 65: Receptor of activated protein C kinase 1



- Molecule 66: 40S ribosomal protein S2



- Molecule 67: 40S ribosomal protein S6

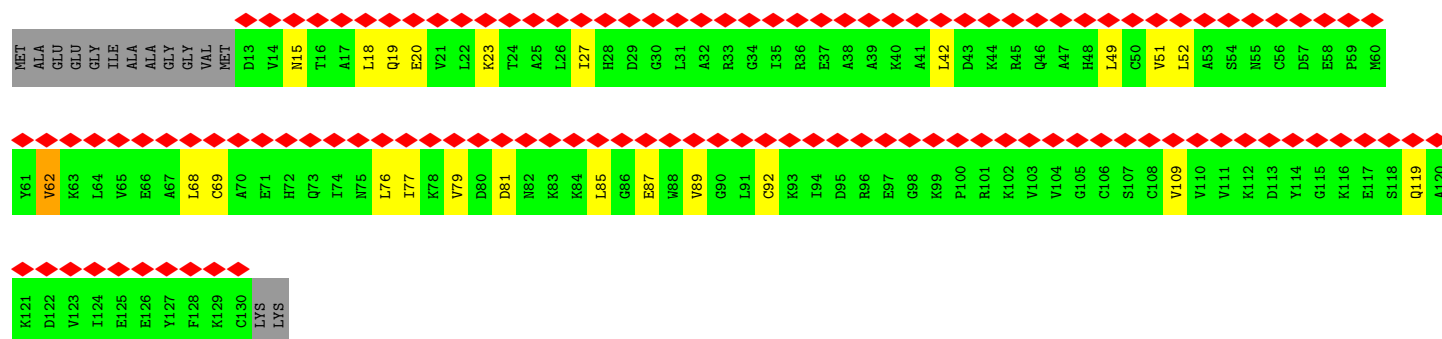
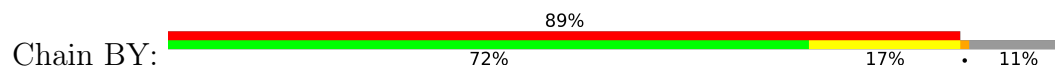


- Molecule 68: 40S ribosomal protein S9





• Molecule 69: 40S ribosomal protein S12

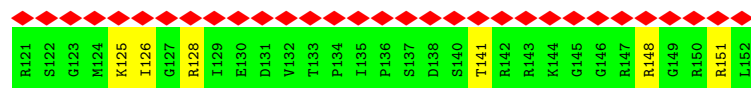


• Molecule 70: 40S ribosomal protein S13



• Molecule 71: Small ribosomal subunit protein uS11





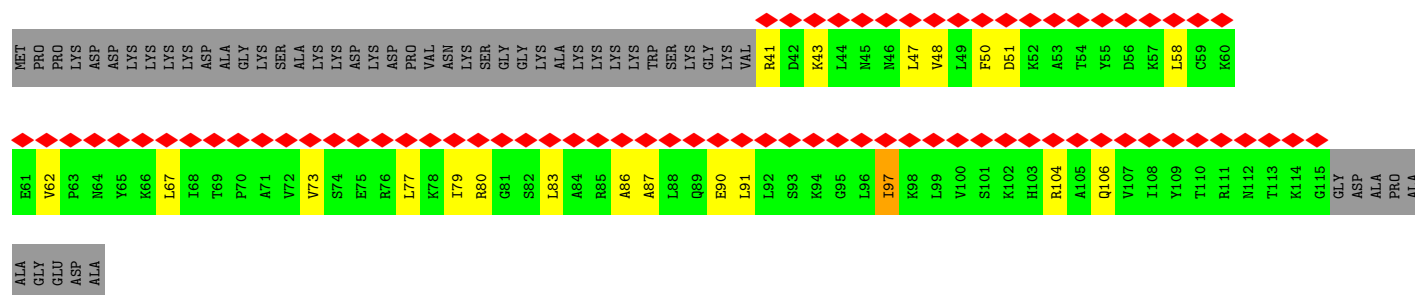
• Molecule 72: 40S ribosomal protein S15a



• Molecule 73: 40S ribosomal protein S24



• Molecule 74: 40S ribosomal protein S25

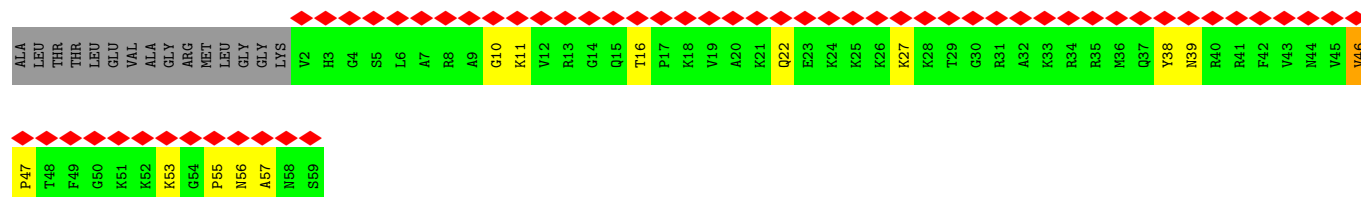
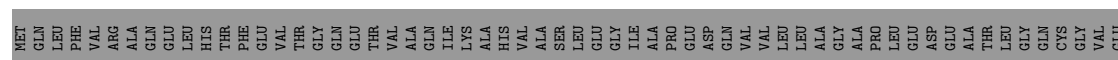
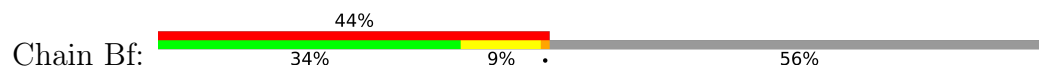


• Molecule 75: 40S ribosomal protein S27

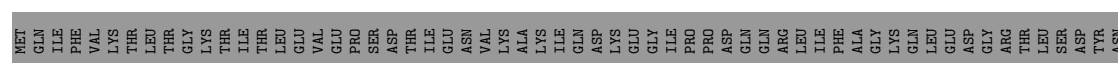
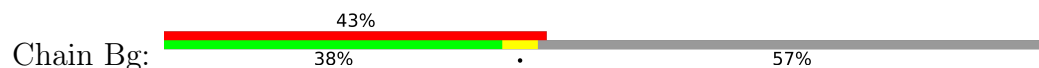




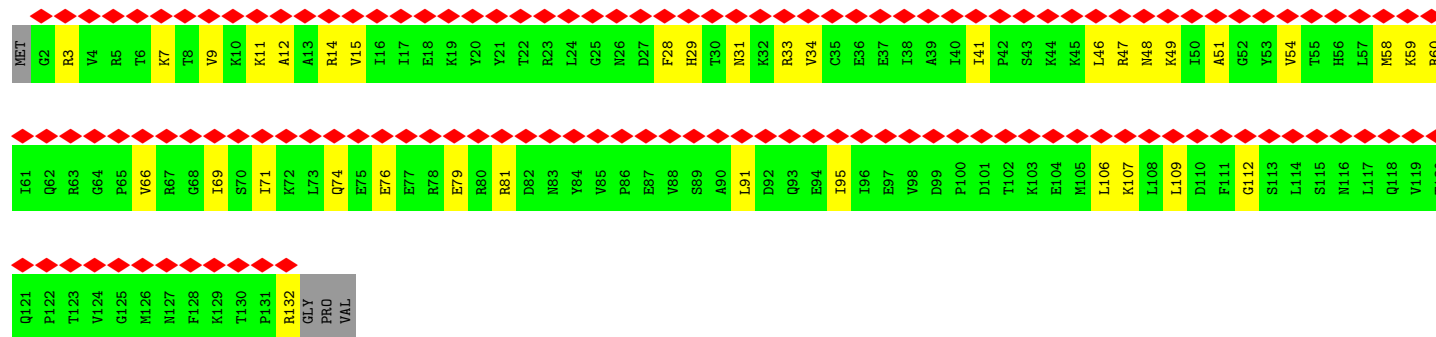
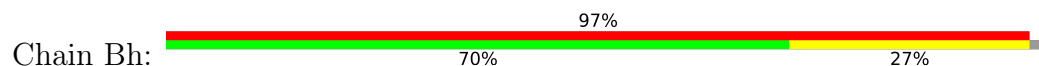
• Molecule 76: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



• Molecule 77: Ubiquitin-40S ribosomal protein S27a



• Molecule 78: 40S ribosomal protein S17



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30153	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	1.354	Depositor
Minimum map value	-0.688	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	528.0, 528.0, 528.0	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NMM, UY1, ZN, OMC, MA6, IAS, 1MA, MG, OMG, M7G, 6MZ, A2M, HIC, V5N, K, UR3, 4AC, B8N, OMU, 5MC, PSU

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	0.17	0/86721	0.28	0/135215
2	AB	0.14	0/2858	0.26	0/4455
3	AC	0.17	0/3609	0.26	0/5623
4	AD	0.18	0/1936	0.37	0/2596
5	AE	0.18	0/3294	0.42	0/4406
6	AF	0.16	0/2981	0.33	0/4002
7	AG	0.16	0/2428	0.42	0/3252
8	AH	0.16	0/1942	0.38	0/2606
9	AI	0.18	0/1916	0.37	0/2553
10	AJ	0.20	0/1971	0.47	0/2651
11	AK	0.18	0/1537	0.45	0/2066
12	AL	0.17	0/1753	0.49	0/2343
13	AM	0.15	0/1433	0.47	0/1915
14	AN	0.17	0/1732	0.42	0/2315
15	AO	0.17	0/1125	0.34	0/1505
16	AP	0.21	0/1746	0.34	0/2338
17	AQ	0.18	0/1682	0.40	0/2250
18	AR	0.19	0/1268	0.44	0/1701
19	AS	0.18	0/1537	0.39	0/2052
20	AT	0.15	0/1424	0.34	0/1884
21	AU	0.18	0/1493	0.45	0/2003
22	AV	0.17	0/1326	0.39	0/1770
23	AW	0.17	0/839	0.49	0/1126
24	AX	0.16	0/993	0.40	0/1332
25	AY	0.17	0/532	0.46	0/708
26	AZ	0.16	0/1002	0.33	0/1345
27	Aa	0.16	0/1119	0.39	0/1488
28	Ab	0.14	0/1130	0.33	0/1507
29	Ac	0.18	0/1179	0.36	0/1573
30	Ad	0.17	0/821	0.45	0/1084
31	Ae	0.17	0/774	0.45	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Af	0.17	0/894	0.44	1/1204 (0.1%)
33	Ag	0.18	0/1071	0.38	0/1429
34	Ah	0.17	0/895	0.30	0/1198
35	Ai	0.16	0/878	0.33	0/1170
36	Aj	0.14	0/1023	0.35	0/1351
37	Ak	0.16	0/824	0.43	0/1090
38	Al	0.16	0/720	0.31	0/952
39	Am	0.19	0/565	0.49	0/750
40	An	0.15	0/454	0.26	0/599
41	Ao	0.25	0/425	0.52	0/564
42	Aq	0.15	0/858	0.34	0/1131
43	Ar	0.15	0/691	0.34	0/919
44	As	0.18	0/1002	0.36	0/1344
45	BA	0.16	0/39081	0.28	0/60888
46	BB	0.13	0/2101	0.39	0/2830
47	BC	0.17	0/1764	0.49	0/2396
48	BD	0.16	0/1774	0.45	0/2373
49	BE	0.16	0/1790	0.43	0/2410
50	BF	0.17	0/1531	0.49	0/2059
51	BG	0.17	0/1519	0.45	0/2033
52	BH	0.14	0/1715	0.41	0/2287
53	BI	0.15	0/840	0.47	0/1133
54	BJ	0.14	0/1280	0.37	0/1712
55	BK	0.19	0/1047	0.55	0/1399
56	BL	0.18	0/1142	0.51	0/1528
57	BM	0.17	0/1212	0.46	0/1624
58	BN	0.17	0/1116	0.45	0/1495
59	BO	0.15	0/732	0.43	0/980
60	BP	0.17	0/643	0.46	0/860
61	BQ	0.14	0/1116	0.43	0/1490
62	BR	0.12	0/836	0.33	0/1121
63	BS	0.16	0/508	0.45	0/680
64	BT	0.14	0/470	0.40	0/623
65	BU	0.15	0/2493	0.45	0/3394
66	BV	0.19	0/1764	0.52	1/2382 (0.0%)
67	BW	0.18	0/1926	0.50	1/2563 (0.0%)
68	BX	0.24	0/1548	0.61	0/2066
69	BY	0.15	0/916	0.42	0/1233
70	BZ	0.19	0/1232	0.48	0/1656
71	Ba	0.16	0/1011	0.49	0/1355
72	Bb	0.18	0/1051	0.48	0/1406
73	Bc	0.14	0/1068	0.36	0/1418
74	Bd	0.14	0/604	0.41	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Be	0.16	0/665	0.45	0/891
76	Bf	0.15	0/465	0.38	0/612
77	Bg	0.13	0/556	0.40	0/741
78	Bh	0.15	0/1078	0.38	0/1447
All	All	0.17	0/224995	0.34	3/330298 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	BW	22	ARG	CA-CB-CG	5.79	125.69	114.10
32	Af	54	MET	CB-CG-SD	5.77	130.01	112.70
66	BV	215	MET	CA-CB-CG	5.41	124.92	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	40485	671	0
2	AB	2558	0	1296	18	0
3	AC	3316	0	1687	29	0
4	AD	1898	0	1993	24	0
5	AE	3239	0	3377	35	0
6	AF	2927	0	3104	28	0
7	AG	2382	0	2410	36	0
8	AH	1904	0	2055	20	0
9	AI	1878	0	2009	24	0
10	AJ	1935	0	2087	18	0
11	AK	1518	0	1601	28	0
12	AL	1713	0	1751	29	0
13	AM	1410	0	1441	19	0
14	AN	1701	0	1818	15	0
15	AO	1103	0	1163	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	AP	1701	0	1749	19	0
17	AQ	1650	0	1794	18	0
18	AR	1242	0	1269	9	0
19	AS	1513	0	1628	8	0
20	AT	1408	0	1550	12	0
21	AU	1453	0	1490	19	0
22	AV	1298	0	1366	13	0
23	AW	825	0	850	13	0
24	AX	979	0	1039	4	0
25	AY	519	0	533	2	0
26	AZ	985	0	1066	7	0
27	Aa	1102	0	1189	15	0
28	Ab	1107	0	1182	13	0
29	Ac	1163	0	1206	6	0
30	Ad	808	0	875	11	0
31	Ae	764	0	804	14	0
32	Af	879	0	924	8	0
33	Ag	1053	0	1147	6	0
34	Ah	876	0	910	5	0
35	Ai	868	0	959	7	0
36	Aj	1015	0	1148	14	0
37	Ak	813	0	894	8	0
38	Al	705	0	737	4	0
39	Am	559	0	624	6	0
40	An	444	0	483	3	0
41	Ao	419	0	452	6	0
42	Aq	842	0	914	8	0
43	Ar	681	0	731	8	0
44	As	987	0	1050	10	0
45	BA	36892	0	18630	564	0
46	BB	2059	0	2137	48	0
47	BC	1727	0	1729	48	0
48	BD	1747	0	1822	44	0
49	BE	1762	0	1856	52	0
50	BF	1509	0	1563	43	0
51	BG	1497	0	1590	41	0
52	BH	1686	0	1772	39	0
53	BI	816	0	841	17	0
54	BJ	1258	0	1332	29	0
55	BK	1027	0	1075	27	0
56	BL	1124	0	1193	27	0
57	BM	1194	0	1250	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	BN	1110	0	1138	41	0
59	BO	726	0	782	21	0
60	BP	636	0	637	16	0
61	BQ	1098	0	1167	19	0
62	BR	821	0	870	12	0
63	BS	506	0	536	10	0
64	BT	459	0	448	16	0
65	BU	2436	0	2393	44	0
66	BV	1724	0	1816	38	0
67	BW	1903	0	2068	43	0
68	BX	1520	0	1642	34	0
69	BY	906	0	921	13	0
70	BZ	1208	0	1294	30	0
71	Ba	1007	0	1025	25	0
72	Bb	1034	0	1080	28	0
73	Bc	1048	0	1119	30	0
74	Bd	598	0	656	18	0
75	Be	651	0	672	17	0
76	Bf	459	0	503	6	0
77	Bg	544	0	539	2	0
78	Bh	1064	0	1118	26	0
79	AA	184	0	0	0	0
79	AB	2	0	0	0	0
79	AC	4	0	0	0	0
79	AP	1	0	0	0	0
79	AR	1	0	0	0	0
79	AX	1	0	0	0	0
79	BA	27	0	0	0	0
80	AA	51	0	0	0	0
80	AB	1	0	0	0	0
80	AD	1	0	0	0	0
80	AL	1	0	0	0	0
80	Ag	1	0	0	0	0
80	Ah	1	0	0	0	0
80	Aq	1	0	0	0	0
80	BA	5	0	0	0	0
81	Ai	1	0	0	0	0
81	Al	1	0	0	0	0
81	Ao	1	0	0	0	0
81	Aq	1	0	0	0	0
81	Ar	1	0	0	0	0
81	BR	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	BT	1	0	0	0	0
81	Bg	1	0	0	0	0
82	BA	24	0	16	0	0
All	All	214414	0	158070	2506	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 2506 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BA:3:C:OP2	66:BV:223:TYR:CE2	1.81	1.31
45:BA:3:C:OP2	66:BV:223:TYR:CZ	1.87	1.26
1:AA:2647:A:H62	1:AA:2686:G:N2	1.44	1.15
1:AA:2647:A:N6	1:AA:2686:G:H21	1.50	1.08
14:AN:142:GLU:O	14:AN:146:LEU:HB2	1.52	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
5	AE	399/402 (99%)	391 (98%)	8 (2%)	0	100	100
6	AF	366/368 (100%)	360 (98%)	6 (2%)	0	100	100
7	AG	291/293 (99%)	275 (94%)	16 (6%)	0	100	100
8	AH	232/247 (94%)	220 (95%)	12 (5%)	0	100	100
9	AI	224/248 (90%)	218 (97%)	6 (3%)	0	100	100
10	AJ	240/266 (90%)	228 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
12	AL	211/214 (99%)	197 (93%)	14 (7%)	0	100	100
13	AM	174/178 (98%)	160 (92%)	14 (8%)	0	100	100
14	AN	208/211 (99%)	196 (94%)	10 (5%)	2 (1%)	12	37
15	AO	132/215 (61%)	129 (98%)	3 (2%)	0	100	100
16	AP	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
17	AQ	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
18	AR	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
19	AS	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
20	AT	167/196 (85%)	164 (98%)	3 (2%)	0	100	100
21	AU	173/176 (98%)	163 (94%)	10 (6%)	0	100	100
22	AV	157/160 (98%)	151 (96%)	5 (3%)	1 (1%)	21	50
23	AW	99/128 (77%)	90 (91%)	9 (9%)	0	100	100
24	AX	129/140 (92%)	125 (97%)	4 (3%)	0	100	100
25	AY	60/157 (38%)	56 (93%)	4 (7%)	0	100	100
26	AZ	118/156 (76%)	117 (99%)	1 (1%)	0	100	100
27	Aa	130/145 (90%)	127 (98%)	3 (2%)	0	100	100
28	Ab	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
29	Ac	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
30	Ad	95/159 (60%)	92 (97%)	3 (3%)	0	100	100
31	Ae	96/115 (84%)	90 (94%)	6 (6%)	0	100	100
32	Af	104/125 (83%)	102 (98%)	2 (2%)	0	100	100
33	Ag	126/135 (93%)	123 (98%)	3 (2%)	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
36	Aj	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
37	Ak	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
38	Al	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
39	Am	66/70 (94%)	64 (97%)	2 (3%)	0	100	100
40	An	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
41	Ao	49/128 (38%)	49 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	Aq	101/106 (95%)	94 (93%)	7 (7%)	0	100	100
43	Ar	86/92 (94%)	84 (98%)	2 (2%)	0	100	100
44	As	121/137 (88%)	116 (96%)	5 (4%)	0	100	100
46	BB	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
47	BC	217/295 (74%)	209 (96%)	8 (4%)	0	100	100
48	BD	213/264 (81%)	203 (95%)	10 (5%)	0	100	100
49	BE	225/243 (93%)	214 (95%)	11 (5%)	0	100	100
50	BF	189/204 (93%)	172 (91%)	17 (9%)	0	100	100
51	BG	182/194 (94%)	169 (93%)	13 (7%)	0	100	100
52	BH	204/208 (98%)	191 (94%)	13 (6%)	0	100	100
53	BI	95/165 (58%)	88 (93%)	7 (7%)	0	100	100
54	BJ	152/158 (96%)	144 (95%)	8 (5%)	0	100	100
55	BK	123/145 (85%)	113 (92%)	10 (8%)	0	100	100
56	BL	139/146 (95%)	132 (95%)	7 (5%)	0	100	100
57	BM	143/152 (94%)	134 (94%)	9 (6%)	0	100	100
58	BN	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
59	BO	85/119 (71%)	77 (91%)	8 (9%)	0	100	100
60	BP	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
61	BQ	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
62	BR	100/115 (87%)	99 (99%)	1 (1%)	0	100	100
63	BS	62/69 (90%)	58 (94%)	4 (6%)	0	100	100
64	BT	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
65	BU	311/317 (98%)	288 (93%)	23 (7%)	0	100	100
66	BV	220/293 (75%)	217 (99%)	3 (1%)	0	100	100
67	BW	232/249 (93%)	226 (97%)	6 (3%)	0	100	100
68	BX	181/194 (93%)	175 (97%)	6 (3%)	0	100	100
69	BY	116/132 (88%)	109 (94%)	7 (6%)	0	100	100
70	BZ	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
71	Ba	132/151 (87%)	125 (95%)	7 (5%)	0	100	100
72	Bb	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
73	Bc	127/133 (96%)	124 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	Bd	73/125 (58%)	64 (88%)	9 (12%)	0	100	100
75	Be	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
76	Bf	56/133 (42%)	49 (88%)	7 (12%)	0	100	100
77	Bg	65/156 (42%)	59 (91%)	6 (9%)	0	100	100
78	Bh	129/135 (96%)	123 (95%)	6 (5%)	0	100	100
All	All	11164/12632 (88%)	10690 (96%)	471 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	AN	47	ALA
14	AN	64	VAL
22	AV	82	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	190/199 (96%)	186 (98%)	4 (2%)	47	76
5	AE	347/347 (100%)	342 (99%)	5 (1%)	59	83
6	AF	306/306 (100%)	300 (98%)	6 (2%)	48	77
7	AG	246/247 (100%)	240 (98%)	6 (2%)	43	73
8	AH	209/220 (95%)	202 (97%)	7 (3%)	33	65
9	AI	195/215 (91%)	194 (100%)	1 (0%)	81	93
10	AJ	204/223 (92%)	198 (97%)	6 (3%)	37	69
11	AK	169/171 (99%)	162 (96%)	7 (4%)	27	60
12	AL	181/182 (100%)	175 (97%)	6 (3%)	33	65
13	AM	148/149 (99%)	140 (95%)	8 (5%)	20	49
14	AN	176/177 (99%)	174 (99%)	2 (1%)	65	86
15	AO	114/161 (71%)	111 (97%)	3 (3%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AP	171/172 (99%)	166 (97%)	5 (3%)	37	69
17	AQ	173/174 (99%)	164 (95%)	9 (5%)	21	50
18	AR	134/163 (82%)	129 (96%)	5 (4%)	30	63
19	AS	164/165 (99%)	162 (99%)	2 (1%)	63	85
20	AT	149/175 (85%)	145 (97%)	4 (3%)	39	71
21	AU	156/157 (99%)	154 (99%)	2 (1%)	61	84
22	AV	139/140 (99%)	132 (95%)	7 (5%)	22	52
23	AW	91/115 (79%)	85 (93%)	6 (7%)	15	41
24	AX	101/107 (94%)	96 (95%)	5 (5%)	22	52
25	AY	54/126 (43%)	53 (98%)	1 (2%)	50	78
26	AZ	108/133 (81%)	104 (96%)	4 (4%)	30	63
27	Aa	123/135 (91%)	121 (98%)	2 (2%)	55	81
28	Ab	117/118 (99%)	116 (99%)	1 (1%)	70	88
29	Ac	119/120 (99%)	116 (98%)	3 (2%)	42	73
30	Ad	83/126 (66%)	80 (96%)	3 (4%)	31	63
31	Ae	83/97 (86%)	77 (93%)	6 (7%)	13	37
32	Af	97/110 (88%)	94 (97%)	3 (3%)	35	67
33	Ag	114/121 (94%)	111 (97%)	3 (3%)	40	72
34	Ah	88/89 (99%)	87 (99%)	1 (1%)	65	86
35	Ai	94/100 (94%)	90 (96%)	4 (4%)	26	58
36	Aj	109/110 (99%)	107 (98%)	2 (2%)	51	79
37	Ak	85/89 (96%)	81 (95%)	4 (5%)	23	55
38	Al	73/80 (91%)	70 (96%)	3 (4%)	27	60
39	Am	63/65 (97%)	58 (92%)	5 (8%)	11	33
40	An	47/48 (98%)	46 (98%)	1 (2%)	47	76
41	Ao	47/116 (40%)	45 (96%)	2 (4%)	26	58
42	Aq	91/94 (97%)	88 (97%)	3 (3%)	33	65
43	Ar	71/75 (95%)	68 (96%)	3 (4%)	26	59
44	As	107/121 (88%)	106 (99%)	1 (1%)	70	88
46	BB	219/225 (97%)	210 (96%)	9 (4%)	27	60
47	BC	182/243 (75%)	171 (94%)	11 (6%)	17	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BD	196/231 (85%)	187 (95%)	9 (5%)	24	56
49	BE	189/202 (94%)	183 (97%)	6 (3%)	34	66
50	BF	161/170 (95%)	157 (98%)	4 (2%)	42	73
51	BG	166/174 (95%)	161 (97%)	5 (3%)	36	68
52	BH	178/180 (99%)	172 (97%)	6 (3%)	32	65
53	BI	88/136 (65%)	85 (97%)	3 (3%)	32	65
54	BJ	138/142 (97%)	134 (97%)	4 (3%)	37	69
55	BK	111/130 (85%)	108 (97%)	3 (3%)	39	71
56	BL	117/121 (97%)	113 (97%)	4 (3%)	32	65
57	BM	125/132 (95%)	117 (94%)	8 (6%)	16	43
58	BN	111/114 (97%)	106 (96%)	5 (4%)	24	56
59	BO	83/107 (78%)	80 (96%)	3 (4%)	31	63
60	BP	67/67 (100%)	64 (96%)	3 (4%)	24	56
61	BQ	113/115 (98%)	104 (92%)	9 (8%)	11	32
62	BR	89/98 (91%)	88 (99%)	1 (1%)	65	86
63	BS	57/62 (92%)	56 (98%)	1 (2%)	51	79
64	BT	48/49 (98%)	44 (92%)	4 (8%)	10	30
65	BU	272/275 (99%)	260 (96%)	12 (4%)	25	57
66	BV	188/225 (84%)	181 (96%)	7 (4%)	30	63
67	BW	204/218 (94%)	198 (97%)	6 (3%)	37	69
68	BX	162/168 (96%)	158 (98%)	4 (2%)	42	73
69	BY	98/108 (91%)	97 (99%)	1 (1%)	68	87
70	BZ	130/131 (99%)	119 (92%)	11 (8%)	10	29
71	Ba	103/118 (87%)	100 (97%)	3 (3%)	37	69
72	Bb	112/113 (99%)	100 (89%)	12 (11%)	6	21
73	Bc	111/115 (96%)	109 (98%)	2 (2%)	51	79
74	Bd	66/103 (64%)	63 (96%)	3 (4%)	24	56
75	Be	75/76 (99%)	73 (97%)	2 (3%)	39	71
76	Bf	47/104 (45%)	41 (87%)	6 (13%)	4	13
77	Bg	59/140 (42%)	56 (95%)	3 (5%)	21	51
78	Bh	119/122 (98%)	115 (97%)	4 (3%)	32	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9720/10752 (90%)	9385 (97%)	335 (3%)	33 65

5 of 335 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	BM	78	LYS
68	BX	125	HIS
59	BO	56	MET
65	BU	31	ILE
71	Ba	95	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
53	BI	84	HIS
70	BZ	69	ASN
55	BK	54	HIS
61	BQ	31	HIS
78	Bh	116	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	3705/5069 (73%)	846 (22%)	10 (0%)
2	AB	119/120 (99%)	12 (10%)	0
3	AC	155/157 (98%)	27 (17%)	1 (0%)
45	BA	1711/1869 (91%)	467 (27%)	4 (0%)
All	All	5690/7215 (78%)	1352 (23%)	15 (0%)

5 of 1352 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	21	G
1	AA	25	A
1	AA	39	A
1	AA	42	A
1	AA	48	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	3673	C
45	BA	866	PSU
1	AA	4120	U
45	BA	1520	G
45	BA	369	C

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

223 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	A2M	AA	400	1	22,25,26	1.46	4 (18%)	31,36,39	2.04	7 (22%)
1	OMC	AA	3887	1	19,22,23	0.84	0	26,31,34	0.90	1 (3%)
45	PSU	BA	1596	45	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	AA	4571	1	22,25,26	1.47	4 (18%)	31,36,39	2.10	7 (22%)
29	V5N	Ac	39	29	9,11,12	0.82	0	9,14,16	1.50	2 (22%)
1	OMG	AA	3792	1	23,26,27	1.22	3 (13%)	33,38,41	1.96	6 (18%)
1	PSU	AA	4673	80,1	18,21,22	1.40	3 (16%)	22,30,33	1.85	3 (13%)
1	PSU	AA	4521	79,1	18,21,22	1.40	3 (16%)	22,30,33	1.90	3 (13%)
1	A2M	AA	3718	1	22,25,26	1.48	4 (18%)	31,36,39	1.98	7 (22%)
1	PSU	AA	3764	1	18,21,22	1.36	2 (11%)	22,30,33	1.80	3 (13%)
45	PSU	BA	815	45	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	AA	1782	1	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	AA	1326	1	22,25,26	1.45	4 (18%)	31,36,39	2.09	8 (25%)
45	PSU	BA	1174	45	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
45	6MZ	BA	1832	79,45	22,25,26	1.42	4 (18%)	30,36,39	2.18	9 (30%)
1	PSU	AA	3822	1	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)
45	A2M	BA	668	79,45	22,25,26	1.46	4 (18%)	31,36,39	2.13	10 (32%)
58	NMM	BN	67	58	9,11,12	1.68	1 (11%)	6,12,14	1.25	1 (16%)
1	OMG	AA	2364	79,1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	AA	4576	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	4 (18%)
1	A2M	AA	2363	79,1	22,25,26	1.44	4 (18%)	31,36,39	2.07	9 (29%)
1	OMC	AA	1340	1	19,22,23	0.85	0	26,31,34	0.87	0
1	PSU	AA	5001	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
1	OMG	AA	2424	1	23,26,27	1.20	3 (13%)	33,38,41	1.91	6 (18%)
1	PSU	AA	4532	1	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	AA	3844	1	18,21,22	1.38	3 (16%)	22,30,33	1.87	3 (13%)
45	PSU	BA	866	45	18,21,22	1.32	2 (11%)	22,30,33	2.04	5 (22%)
45	OMC	BA	1391	45	19,22,23	0.84	0	26,31,34	0.94	1 (3%)
1	OMU	AA	2415	1	19,22,23	1.22	3 (15%)	26,31,34	1.70	5 (19%)
1	PSU	AA	4552	1	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
45	A2M	BA	484	45	22,25,26	1.48	4 (18%)	31,36,39	2.28	8 (25%)
45	PSU	BA	1136	45	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
1	PSU	AA	4689	1	18,21,22	1.36	2 (11%)	22,30,33	1.75	3 (13%)
1	OMU	AA	2837	1	19,22,23	1.25	3 (15%)	26,31,34	1.74	4 (15%)
1	OMC	AA	4456	1	19,22,23	0.84	0	26,31,34	0.99	1 (3%)
1	PSU	AA	3695	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
45	PSU	BA	36	45	18,21,22	1.33	2 (11%)	22,30,33	1.87	4 (18%)
1	PSU	AA	1744	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	AA	2422	79,1	19,22,23	0.80	0	26,31,34	0.80	0
1	PSU	AA	4296	1	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
45	PSU	BA	1046	45	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
1	OMC	AA	2365	1	19,22,23	0.80	0	26,31,34	0.76	0
1	OMG	AA	1522	1	23,26,27	1.20	3 (13%)	33,38,41	1.93	5 (15%)
1	OMG	AA	3899	79,1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	PSU	AA	4442	1	18,21,22	1.38	3 (16%)	22,30,33	1.96	4 (18%)
1	OMG	AA	4499	1	23,26,27	1.24	3 (13%)	33,38,41	1.97	6 (18%)
45	MA6	BA	1851	45	23,26,27	1.48	4 (17%)	34,38,41	2.41	13 (38%)
1	OMU	AA	4620	1	19,22,23	1.25	3 (15%)	26,31,34	1.66	4 (15%)
1	OMC	AA	2351	79,1	19,22,23	0.83	0	26,31,34	0.98	2 (7%)
45	OMU	BA	1288	45	19,22,23	1.17	3 (15%)	26,31,34	1.73	4 (15%)
1	PSU	AA	4471	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	4579	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	A2M	AA	1524	1	22,25,26	1.44	4 (18%)	31,36,39	2.15	11 (35%)
1	OMG	AA	4637	80,1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	AA	3701	80,1	19,22,23	0.80	0	26,31,34	0.76	0
3	PSU	AC	69	3	18,21,22	1.39	2 (11%)	22,30,33	1.91	4 (18%)
45	OMU	BA	428	45	19,22,23	1.19	2 (10%)	26,31,34	1.69	5 (19%)
1	A2M	AA	4523	79,1	22,25,26	1.41	4 (18%)	31,36,39	2.15	10 (32%)
3	PSU	AC	55	3	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	4361	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	AA	4628	1	18,21,22	1.37	2 (11%)	22,30,33	1.95	3 (13%)
45	OMU	BA	172	45	19,22,23	1.19	3 (15%)	26,31,34	1.71	4 (15%)
45	OMC	BA	174	45	19,22,23	0.81	0	26,31,34	0.84	0
45	PSU	BA	609	45	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	1186	45	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	AA	3715	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
45	A2M	BA	27	45	22,25,26	1.49	4 (18%)	31,36,39	2.12	9 (29%)
45	PSU	BA	300	45	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
45	OMC	BA	1272	45	19,22,23	0.81	0	26,31,34	0.85	1 (3%)
45	OMG	BA	1447	45	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
45	PSU	BA	63	45	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
1	OMC	AA	2824	1	19,22,23	0.82	0	26,31,34	0.89	1 (3%)
1	PSU	AA	3920	79,1	18,21,22	1.39	3 (16%)	22,30,33	1.89	4 (18%)
1	PSU	AA	3768	1	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
45	PSU	BA	1625	45	18,21,22	1.39	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	AA	1781	1	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	34	45	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
45	OMG	BA	509	79,45	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
45	A2M	BA	1678	45	22,25,26	1.48	4 (18%)	31,36,39	2.14	10 (32%)
45	A2M	BA	99	45	22,25,26	1.45	4 (18%)	31,36,39	2.15	8 (25%)
45	PSU	BA	651	45	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	AA	4493	80,1	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
45	PSU	BA	1003	45	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
45	A2M	BA	1031	45	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
45	PSU	BA	801	45	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
1	A2M	AA	2401	1	22,25,26	1.45	4 (18%)	31,36,39	2.14	10 (32%)
1	OMC	AA	3869	1	19,22,23	0.83	0	26,31,34	0.73	0
1	OMG	AA	4228	1	23,26,27	1.18	4 (17%)	33,38,41	1.95	6 (18%)
1	A2M	AA	1534	79,1	22,25,26	1.44	4 (18%)	31,36,39	2.09	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMG	BA	683	45	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
1	A2M	AA	3724	1	22,25,26	1.47	4 (18%)	31,36,39	2.10	9 (29%)
45	OMU	BA	354	45	19,22,23	1.18	3 (15%)	26,31,34	1.71	5 (19%)
45	A2M	BA	159	45	22,25,26	1.46	4 (18%)	31,36,39	2.17	9 (29%)
1	1MA	AA	1322	79,1	21,25,26	1.38	4 (19%)	31,37,40	1.66	6 (19%)
45	4AC	BA	1337	45	21,24,25	1.09	1 (4%)	29,34,37	1.60	5 (17%)
1	OMC	AA	3808	1	19,22,23	0.84	0	26,31,34	1.00	1 (3%)
45	PSU	BA	1045	45	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	AA	3825	1	22,25,26	1.46	4 (18%)	31,36,39	2.05	8 (25%)
1	OMU	AA	4498	1	19,22,23	1.22	3 (15%)	26,31,34	1.71	5 (19%)
1	A2M	AA	2787	79,1	22,25,26	1.43	4 (18%)	31,36,39	2.13	8 (25%)
45	PSU	BA	822	45	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
45	PSU	BA	1445	45	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
45	OMU	BA	1804	45	19,22,23	1.24	4 (21%)	26,31,34	1.68	5 (19%)
1	PSU	AA	1862	1	18,21,22	1.35	3 (16%)	22,30,33	1.86	3 (13%)
45	A2M	BA	590	45	22,25,26	1.47	4 (18%)	31,36,39	2.26	6 (19%)
1	PSU	AA	4431	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
45	PSU	BA	1347	45	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
1	OMG	AA	4623	1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	5MC	AA	4447	80,1	18,22,23	0.99	2 (11%)	26,32,35	1.22	2 (7%)
1	PSU	AA	2632	1	18,21,22	1.39	2 (11%)	22,30,33	1.78	3 (13%)
1	PSU	AA	3639	1	18,21,22	1.38	2 (11%)	22,30,33	1.86	3 (13%)
45	PSU	BA	406	45	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	AA	1677	79,1	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
1	UR3	AA	4530	1	19,22,23	0.98	0	26,32,35	1.40	1 (3%)
1	PSU	AA	2508	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	AA	4618	1	23,26,27	1.18	3 (13%)	33,38,41	1.98	6 (18%)
45	PSU	BA	105	45	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
45	PSU	BA	1367	45	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	A2M	AA	4590	1	22,25,26	1.45	4 (18%)	31,36,39	2.07	9 (29%)
45	PSU	BA	1056	45	18,21,22	1.36	2 (11%)	22,30,33	1.88	4 (18%)
1	PSU	AA	3770	1	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
1	PSU	AA	5010	1	18,21,22	1.35	2 (11%)	22,30,33	1.80	3 (13%)
1	OMG	AA	3627	1	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
45	A2M	BA	576	45	22,25,26	1.49	4 (18%)	31,36,39	2.05	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	OMU	BA	121	45	19,22,23	1.20	2 (10%)	26,31,34	1.68	5 (19%)
1	PSU	AA	3730	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	AA	2843	1	18,21,22	1.38	3 (16%)	22,30,33	1.87	3 (13%)
45	OMC	BA	462	45	19,22,23	0.81	0	26,31,34	0.85	1 (3%)
45	PSU	BA	366	45	18,21,22	1.37	2 (11%)	22,30,33	1.82	3 (13%)
1	PSU	AA	1683	1	18,21,22	1.42	3 (16%)	22,30,33	1.89	3 (13%)
1	OMG	AA	1625	80,1	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
1	A2M	AA	1323	1	22,25,26	1.46	4 (18%)	31,36,39	2.08	8 (25%)
45	PSU	BA	109	45	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	AA	1860	1	18,21,22	1.38	3 (16%)	22,30,33	1.82	3 (13%)
1	PSU	AA	4500	1	18,21,22	1.36	2 (11%)	22,30,33	1.96	4 (18%)
45	PSU	BA	966	45	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
1	PSU	AA	3853	79,1	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
45	PSU	BA	218	45	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
1	A2M	AA	3867	1	22,25,26	1.46	4 (18%)	31,36,39	2.09	7 (22%)
1	OMG	AA	4196	79,1	23,26,27	1.23	3 (13%)	33,38,41	1.95	6 (18%)
45	OMG	BA	601	45	23,26,27	1.23	3 (13%)	33,38,41	2.01	6 (18%)
45	OMG	BA	867	45	23,26,27	1.24	3 (13%)	33,38,41	1.94	6 (18%)
45	PSU	BA	1244	45	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
5	HIC	AE	245	5	10,11,12	0.52	0	8,14,16	0.49	0
1	OMC	AA	2861	1	19,22,23	0.84	0	26,31,34	0.99	2 (7%)
1	OMG	AA	4494	1	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
45	PSU	BA	1238	45	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
45	PSU	BA	649	45	18,21,22	1.34	2 (11%)	22,30,33	1.93	3 (13%)
1	PSU	AA	1582	1	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
45	PSU	BA	572	45	18,21,22	1.37	3 (16%)	22,30,33	1.93	4 (18%)
1	A2M	AA	1871	79,1	22,25,26	1.47	4 (18%)	31,36,39	2.07	8 (25%)
45	PSU	BA	119	45	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
45	OMU	BA	116	45	19,22,23	1.22	3 (15%)	26,31,34	1.65	5 (19%)
1	PSU	AA	4353	1	18,21,22	1.38	2 (11%)	22,30,33	1.90	3 (13%)
45	PSU	BA	100	45	18,21,22	1.37	2 (11%)	22,30,33	1.86	3 (13%)
1	6MZ	AA	4220	1	22,25,26	1.42	4 (18%)	30,36,39	2.15	9 (30%)
1	PSU	AA	3884	1	18,21,22	1.38	3 (16%)	22,30,33	1.88	3 (13%)
1	PSU	AA	4973	1	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)
1	OMC	AA	1881	79,1	19,22,23	0.82	0	26,31,34	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	PSU	BA	686	45	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
1	OMG	AA	3744	1	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	AA	1316	1	23,26,27	1.22	3 (13%)	33,38,41	1.93	6 (18%)
45	A2M	BA	1383	45	22,25,26	1.47	4 (18%)	31,36,39	2.25	10 (32%)
1	OMG	AA	4370	1	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
71	IAS	Ba	138	71	6,7,8	1.07	0	6,8,10	1.47	0
1	PSU	AA	1792	1	18,21,22	1.39	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	AA	3851	1	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
3	OMG	AC	75	3	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
1	OMU	AA	4306	1	19,22,23	1.26	3 (15%)	26,31,34	1.63	4 (15%)
1	A2M	AA	398	1	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
45	OMC	BA	1703	45	19,22,23	0.80	0	26,31,34	0.77	0
1	PSU	AA	1536	1	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	AA	2804	1	19,22,23	0.82	0	26,31,34	0.76	0
1	A2M	AA	2815	1	22,25,26	1.47	4 (18%)	31,36,39	2.18	7 (22%)
1	PSU	AA	4293	1	18,21,22	1.36	3 (16%)	22,30,33	1.89	4 (18%)
45	OMG	BA	436	45	23,26,27	1.18	3 (13%)	33,38,41	1.98	6 (18%)
1	A2M	AA	3830	1	22,25,26	1.45	4 (18%)	31,36,39	2.14	8 (25%)
1	PSU	AA	4403	1	18,21,22	1.36	2 (11%)	22,30,33	1.92	5 (22%)
45	4AC	BA	1842	45	21,24,25	1.06	1 (4%)	29,34,37	1.49	5 (17%)
45	PSU	BA	1692	45	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
3	OMU	AC	14	3,1	19,22,23	1.27	3 (15%)	26,31,34	1.83	5 (19%)
45	PSU	BA	681	45	18,21,22	1.37	2 (11%)	22,30,33	1.80	3 (13%)
45	OMG	BA	1328	45	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
45	OMG	BA	644	45	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
45	PSU	BA	1232	45	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	OMU	AA	3925	1	19,22,23	1.23	3 (15%)	26,31,34	1.73	5 (19%)
1	UY1	AA	3818	80,1	19,22,23	4.31	7 (36%)	22,31,34	1.78	5 (22%)
1	OMG	AA	4392	1	23,26,27	1.21	3 (13%)	33,38,41	1.93	5 (15%)
1	5MC	AA	3782	79,1	18,22,23	0.95	2 (11%)	26,32,35	1.18	3 (11%)
45	PSU	BA	814	45	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
45	PSU	BA	1004	45	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	AA	4972	1	18,21,22	1.32	2 (11%)	22,30,33	1.90	3 (13%)
45	OMU	BA	1442	45	19,22,23	1.30	4 (21%)	26,31,34	1.78	6 (23%)
45	PSU	BA	1360	45	18,21,22	1.42	5 (27%)	22,30,33	1.90	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	AA	4536	1	19,22,23	0.83	0	26,31,34	0.88	1 (3%)
1	PSU	AA	1779	1	18,21,22	1.31	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	AA	3637	80,1	18,21,22	1.43	3 (16%)	22,30,33	1.95	5 (22%)
45	PSU	BA	863	45	18,21,22	1.34	2 (11%)	22,30,33	1.74	3 (13%)
45	OMG	BA	1490	45	23,26,27	1.21	3 (13%)	33,38,41	1.92	6 (18%)
45	PSU	BA	918	45	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
45	OMC	BA	517	45	19,22,23	0.83	0	26,31,34	0.99	1 (3%)
45	B8N	BA	1248	45	24,29,30	0.91	1 (4%)	29,42,45	1.32	2 (6%)
1	PSU	AA	4312	1	18,21,22	1.39	2 (11%)	22,30,33	1.90	3 (13%)
45	PSU	BA	1177	45	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	AA	2839	1	18,21,22	1.38	3 (16%)	22,30,33	1.85	3 (13%)
1	A2M	AA	3785	1	22,25,26	1.41	4 (18%)	31,36,39	2.29	11 (35%)
45	A2M	BA	468	45	22,25,26	1.47	4 (18%)	31,36,39	2.13	10 (32%)
45	A2M	BA	166	45	22,25,26	1.44	4 (18%)	31,36,39	2.25	9 (29%)
1	PSU	AA	3762	1	18,21,22	1.35	2 (11%)	22,30,33	1.81	3 (13%)
1	PSU	AA	4423	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	OMG	AA	2876	1	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
1	PSU	AA	4299	1	18,21,22	1.38	3 (16%)	22,30,33	1.82	3 (13%)
45	MA6	BA	1850	45	23,26,27	1.47	4 (17%)	34,38,41	2.40	13 (38%)
45	UY1	BA	1326	45	19,22,23	4.40	7 (36%)	22,31,34	1.75	5 (22%)
45	PSU	BA	93	45	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
45	A2M	BA	512	45	22,25,26	1.47	4 (18%)	31,36,39	2.20	8 (25%)
1	PSU	AA	4457	1	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
1	OMC	AA	3841	1	19,22,23	0.81	0	26,31,34	0.74	0
1	OMU	AA	4227	1	19,22,23	1.25	3 (15%)	26,31,34	1.73	4 (15%)
45	PSU	BA	296	45	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
45	PSU	BA	667	45	18,21,22	1.39	3 (16%)	22,30,33	1.85	4 (18%)
45	PSU	BA	1643	45	18,21,22	1.41	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	AA	4636	1	18,21,22	1.38	2 (11%)	22,30,33	1.94	5 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	AA	400	1	-	0/9/27/28	0/3/3/3
1	OMC	AA	3887	1	-	1/9/27/28	0/2/2/2
45	PSU	BA	1596	45	-	1/7/25/26	0/2/2/2
1	A2M	AA	4571	1	-	0/9/27/28	0/3/3/3
29	V5N	Ac	39	29	-	0/9/10/12	0/1/1/1
1	OMG	AA	3792	1	-	1/9/27/28	0/3/3/3
1	PSU	AA	4673	80,1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4521	79,1	-	1/7/25/26	0/2/2/2
1	A2M	AA	3718	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	3764	1	-	2/7/25/26	0/2/2/2
45	PSU	BA	815	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1782	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	1326	1	-	3/9/27/28	0/3/3/3
45	PSU	BA	1174	45	-	0/7/25/26	0/2/2/2
45	6MZ	BA	1832	79,45	-	2/9/27/28	0/3/3/3
1	PSU	AA	3822	1	-	0/7/25/26	0/2/2/2
45	A2M	BA	668	79,45	-	4/9/27/28	0/3/3/3
58	NMM	BN	67	58	-	1/9/11/13	-
1	OMG	AA	2364	79,1	-	2/9/27/28	0/3/3/3
1	PSU	AA	4576	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	2363	79,1	-	0/9/27/28	0/3/3/3
1	OMC	AA	1340	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	5001	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	2424	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4532	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3844	1	-	3/7/25/26	0/2/2/2
45	PSU	BA	866	45	-	0/7/25/26	0/2/2/2
45	OMC	BA	1391	45	-	0/9/27/28	0/2/2/2
1	OMU	AA	2415	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	4552	1	-	0/7/25/26	0/2/2/2
45	A2M	BA	484	45	-	1/9/27/28	0/3/3/3
45	PSU	BA	1136	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	4689	1	-	0/7/25/26	0/2/2/2
1	OMU	AA	2837	1	-	1/9/27/28	0/2/2/2
1	OMC	AA	4456	1	-	1/9/27/28	0/2/2/2
1	PSU	AA	3695	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	36	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1744	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	2422	79,1	-	1/9/27/28	0/2/2/2
1	PSU	AA	4296	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1046	45	-	0/7/25/26	0/2/2/2
1	OMC	AA	2365	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	AA	1522	1	-	1/9/27/28	0/3/3/3
1	OMG	AA	3899	79,1	-	2/9/27/28	0/3/3/3
1	PSU	AA	4442	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	4499	1	-	0/9/27/28	0/3/3/3
45	MA6	BA	1851	45	-	4/11/29/30	0/3/3/3
1	OMU	AA	4620	1	-	0/9/27/28	0/2/2/2
1	OMC	AA	2351	79,1	-	1/9/27/28	0/2/2/2
45	OMU	BA	1288	45	-	2/9/27/28	0/2/2/2
1	PSU	AA	4471	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4579	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	1524	1	-	1/9/27/28	0/3/3/3
1	OMG	AA	4637	80,1	-	0/9/27/28	0/3/3/3
1	OMC	AA	3701	80,1	-	4/9/27/28	0/2/2/2
3	PSU	AC	69	3	-	0/7/25/26	0/2/2/2
45	OMU	BA	428	45	-	4/9/27/28	0/2/2/2
1	A2M	AA	4523	79,1	-	1/9/27/28	0/3/3/3
3	PSU	AC	55	3	-	0/7/25/26	0/2/2/2
1	PSU	AA	4361	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4628	1	-	0/7/25/26	0/2/2/2
45	OMU	BA	172	45	-	0/9/27/28	0/2/2/2
45	OMC	BA	174	45	-	2/9/27/28	0/2/2/2
45	PSU	BA	609	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	1186	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	3715	1	-	0/7/25/26	0/2/2/2
45	A2M	BA	27	45	-	2/9/27/28	0/3/3/3
45	PSU	BA	300	45	-	0/7/25/26	0/2/2/2
45	OMC	BA	1272	45	-	0/9/27/28	0/2/2/2
45	OMG	BA	1447	45	-	0/9/27/28	0/3/3/3
45	PSU	BA	63	45	-	0/7/25/26	0/2/2/2
1	OMC	AA	2824	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	3920	79,1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3768	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1625	45	-	1/7/25/26	0/2/2/2
1	PSU	AA	1781	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	34	45	-	0/7/25/26	0/2/2/2
45	OMG	BA	509	79,45	-	1/9/27/28	0/3/3/3
45	A2M	BA	1678	45	-	1/9/27/28	0/3/3/3
45	A2M	BA	99	45	-	2/9/27/28	0/3/3/3
45	PSU	BA	651	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	4493	80,1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PSU	BA	1003	45	-	0/7/25/26	0/2/2/2
45	A2M	BA	1031	45	-	0/9/27/28	0/3/3/3
45	PSU	BA	801	45	-	1/7/25/26	0/2/2/2
1	A2M	AA	2401	1	-	0/9/27/28	0/3/3/3
1	OMC	AA	3869	1	-	0/9/27/28	0/2/2/2
1	OMG	AA	4228	1	-	0/9/27/28	0/3/3/3
1	A2M	AA	1534	79,1	-	1/9/27/28	0/3/3/3
45	OMG	BA	683	45	-	2/9/27/28	0/3/3/3
1	A2M	AA	3724	1	-	0/9/27/28	0/3/3/3
45	OMU	BA	354	45	-	0/9/27/28	0/2/2/2
45	A2M	BA	159	45	-	0/9/27/28	0/3/3/3
1	1MA	AA	1322	79,1	-	1/7/25/26	0/3/3/3
45	4AC	BA	1337	45	-	2/11/29/30	0/2/2/2
1	OMC	AA	3808	1	-	0/9/27/28	0/2/2/2
45	PSU	BA	1045	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	3825	1	-	0/9/27/28	0/3/3/3
1	OMU	AA	4498	1	-	0/9/27/28	0/2/2/2
1	A2M	AA	2787	79,1	-	5/9/27/28	0/3/3/3
45	PSU	BA	822	45	-	1/7/25/26	0/2/2/2
45	PSU	BA	1445	45	-	0/7/25/26	0/2/2/2
45	OMU	BA	1804	45	-	0/9/27/28	0/2/2/2
1	PSU	AA	1862	1	-	0/7/25/26	0/2/2/2
45	A2M	BA	590	45	-	5/9/27/28	0/3/3/3
1	PSU	AA	4431	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	1347	45	-	0/7/25/26	0/2/2/2
1	OMG	AA	4623	1	-	2/9/27/28	0/3/3/3
1	5MC	AA	4447	80,1	-	4/7/25/26	0/2/2/2
1	PSU	AA	2632	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3639	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	406	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1677	79,1	-	4/7/25/26	0/2/2/2
1	UR3	AA	4530	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	2508	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	4618	1	-	0/9/27/28	0/3/3/3
45	PSU	BA	105	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	1367	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	4590	1	-	3/9/27/28	0/3/3/3
45	PSU	BA	1056	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	3770	1	-	2/7/25/26	0/2/2/2
1	PSU	AA	5010	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	AA	3627	1	-	0/9/27/28	0/3/3/3
45	A2M	BA	576	45	-	0/9/27/28	0/3/3/3
45	OMU	BA	121	45	-	0/9/27/28	0/2/2/2
1	PSU	AA	3730	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	2843	1	-	0/7/25/26	0/2/2/2
45	OMC	BA	462	45	-	0/9/27/28	0/2/2/2
45	PSU	BA	366	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1683	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	1625	80,1	-	2/9/27/28	0/3/3/3
1	A2M	AA	1323	1	-	2/9/27/28	0/3/3/3
45	PSU	BA	109	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1860	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4500	1	-	3/7/25/26	0/2/2/2
45	PSU	BA	966	45	-	1/7/25/26	0/2/2/2
1	PSU	AA	3853	79,1	-	0/7/25/26	0/2/2/2
45	PSU	BA	218	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	3867	1	-	1/9/27/28	0/3/3/3
1	OMG	AA	4196	79,1	-	0/9/27/28	0/3/3/3
45	OMG	BA	601	45	-	2/9/27/28	0/3/3/3
45	OMG	BA	867	45	-	1/9/27/28	0/3/3/3
45	PSU	BA	1244	45	-	0/7/25/26	0/2/2/2
5	HIC	AE	245	5	-	0/5/6/8	0/1/1/1
1	OMC	AA	2861	1	-	0/9/27/28	0/2/2/2
1	OMG	AA	4494	1	-	0/9/27/28	0/3/3/3
45	PSU	BA	1238	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	649	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	1582	1	-	2/7/25/26	0/2/2/2
45	PSU	BA	572	45	-	0/7/25/26	0/2/2/2
1	A2M	AA	1871	79,1	-	0/9/27/28	0/3/3/3
45	PSU	BA	119	45	-	0/7/25/26	0/2/2/2
45	OMU	BA	116	45	-	0/9/27/28	0/2/2/2
1	PSU	AA	4353	1	-	0/7/25/26	0/2/2/2
45	PSU	BA	100	45	-	2/7/25/26	0/2/2/2
1	6MZ	AA	4220	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	3884	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4973	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	1881	79,1	-	2/9/27/28	0/2/2/2
45	PSU	BA	686	45	-	0/7/25/26	0/2/2/2
1	OMG	AA	3744	1	-	0/9/27/28	0/3/3/3
1	OMG	AA	1316	1	-	0/9/27/28	0/3/3/3
45	A2M	BA	1383	45	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	AA	4370	1	-	0/9/27/28	0/3/3/3
71	IAS	Ba	138	71	-	1/7/7/8	-
1	PSU	AA	1792	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3851	1	-	2/7/25/26	0/2/2/2
3	OMG	AC	75	3	-	1/9/27/28	0/3/3/3
1	OMU	AA	4306	1	-	0/9/27/28	0/2/2/2
1	A2M	AA	398	1	-	2/9/27/28	0/3/3/3
45	OMC	BA	1703	45	-	0/9/27/28	0/2/2/2
1	PSU	AA	1536	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	2804	1	-	1/9/27/28	0/2/2/2
1	A2M	AA	2815	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4293	1	-	0/7/25/26	0/2/2/2
45	OMG	BA	436	45	-	4/9/27/28	0/3/3/3
1	A2M	AA	3830	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4403	1	-	0/7/25/26	0/2/2/2
45	4AC	BA	1842	45	-	0/11/29/30	0/2/2/2
45	PSU	BA	1692	45	-	0/7/25/26	0/2/2/2
3	OMU	AC	14	3,1	-	0/9/27/28	0/2/2/2
45	PSU	BA	681	45	-	0/7/25/26	0/2/2/2
45	OMG	BA	1328	45	-	0/9/27/28	0/3/3/3
45	OMG	BA	644	45	-	2/9/27/28	0/3/3/3
45	PSU	BA	1232	45	-	0/7/25/26	0/2/2/2
1	OMU	AA	3925	1	-	0/9/27/28	0/2/2/2
1	UY1	AA	3818	80,1	-	2/9/27/28	0/2/2/2
1	OMG	AA	4392	1	-	0/9/27/28	0/3/3/3
1	5MC	AA	3782	79,1	-	0/7/25/26	0/2/2/2
45	PSU	BA	814	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	1004	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	4972	1	-	0/7/25/26	0/2/2/2
45	OMU	BA	1442	45	-	2/9/27/28	0/2/2/2
45	PSU	BA	1360	45	-	4/7/25/26	0/2/2/2
1	OMC	AA	4536	1	-	0/9/27/28	0/2/2/2
1	PSU	AA	1779	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	3637	80,1	-	0/7/25/26	0/2/2/2
45	PSU	BA	863	45	-	0/7/25/26	0/2/2/2
45	OMG	BA	1490	45	-	2/9/27/28	0/3/3/3
45	PSU	BA	918	45	-	0/7/25/26	0/2/2/2
45	OMC	BA	517	45	-	0/9/27/28	0/2/2/2
45	B8N	BA	1248	45	-	8/16/34/35	0/2/2/2
1	PSU	AA	4312	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PSU	BA	1177	45	-	0/7/25/26	0/2/2/2
1	PSU	AA	2839	1	-	0/7/25/26	0/2/2/2
1	A2M	AA	3785	1	-	2/9/27/28	0/3/3/3
45	A2M	BA	468	45	-	2/9/27/28	0/3/3/3
45	A2M	BA	166	45	-	2/9/27/28	0/3/3/3
1	PSU	AA	3762	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	4423	1	-	0/7/25/26	0/2/2/2
1	OMG	AA	2876	1	-	0/9/27/28	0/3/3/3
1	PSU	AA	4299	1	-	0/7/25/26	0/2/2/2
45	MA6	BA	1850	45	-	5/11/29/30	0/3/3/3
45	UY1	BA	1326	45	-	5/9/27/28	0/2/2/2
45	PSU	BA	93	45	-	0/7/25/26	0/2/2/2
45	A2M	BA	512	45	-	2/9/27/28	0/3/3/3
1	PSU	AA	4457	1	-	0/7/25/26	0/2/2/2
1	OMC	AA	3841	1	-	0/9/27/28	0/2/2/2
1	OMU	AA	4227	1	-	0/9/27/28	0/2/2/2
45	PSU	BA	296	45	-	0/7/25/26	0/2/2/2
45	PSU	BA	667	45	-	4/7/25/26	0/2/2/2
45	PSU	BA	1643	45	-	2/7/25/26	0/2/2/2
1	PSU	AA	4636	1	-	4/7/25/26	0/2/2/2

The worst 5 of 544 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	1326	UY1	C6-C5	11.87	1.49	1.35
1	AA	3818	UY1	C6-C5	11.51	1.48	1.35
45	BA	1326	UY1	C2-N1	9.54	1.49	1.36
1	AA	3818	UY1	C2-N1	9.37	1.49	1.36
45	BA	1326	UY1	C2-N3	7.79	1.50	1.37

The worst 5 of 976 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	590	A2M	C5-C4-N3	-7.19	117.37	126.75
1	AA	2815	A2M	C5-C4-N3	-6.91	117.73	126.75
45	BA	867	OMG	C5-C4-N3	-6.62	117.71	128.46
45	BA	512	A2M	C5-C4-N3	-6.61	118.12	126.75
45	BA	601	OMG	C5-C4-N3	-6.58	117.79	128.46

There are no chirality outliers.

5 of 164 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1582	PSU	O4'-C1'-C5-C4
1	AA	1582	PSU	O4'-C1'-C5-C6
1	AA	1625	OMG	O4'-C4'-C5'-O5'
1	AA	1625	OMG	C3'-C4'-C5'-O5'
1	AA	1677	PSU	C2'-C1'-C5-C4

There are no ring outliers.

94 monomers are involved in 126 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	400	A2M	1	0
1	AA	4571	A2M	2	0
1	AA	3792	OMG	1	0
1	AA	3718	A2M	4	0
1	AA	1326	A2M	1	0
45	BA	1174	PSU	1	0
45	BA	1832	6MZ	1	0
1	AA	2363	A2M	1	0
1	AA	1340	OMC	1	0
45	BA	1391	OMC	1	0
1	AA	4552	PSU	1	0
45	BA	484	A2M	2	0
45	BA	1136	PSU	2	0
1	AA	4689	PSU	1	0
1	AA	4456	OMC	1	0
45	BA	36	PSU	1	0
1	AA	3899	OMG	1	0
1	AA	4499	OMG	1	0
45	BA	1851	MA6	2	0
1	AA	4620	OMU	1	0
1	AA	2351	OMC	1	0
1	AA	4579	PSU	2	0
1	AA	4523	A2M	1	0
45	BA	172	OMU	1	0
45	BA	174	OMC	1	0
45	BA	609	PSU	2	0
45	BA	27	A2M	1	0
45	BA	1447	OMG	1	0
45	BA	1625	PSU	1	0
45	BA	509	OMG	2	0
45	BA	1678	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	BA	99	A2M	1	0
45	BA	651	PSU	2	0
45	BA	1003	PSU	1	0
45	BA	1031	A2M	2	0
45	BA	354	OMU	3	0
45	BA	159	A2M	3	0
45	BA	1337	4AC	1	0
45	BA	822	PSU	2	0
45	BA	1445	PSU	2	0
45	BA	1804	OMU	2	0
1	AA	4447	5MC	1	0
1	AA	2632	PSU	1	0
45	BA	406	PSU	1	0
1	AA	4618	OMG	1	0
1	AA	3770	PSU	1	0
1	AA	5010	PSU	1	0
45	BA	576	A2M	2	0
45	BA	121	OMU	2	0
45	BA	462	OMC	2	0
45	BA	366	PSU	1	0
1	AA	1683	PSU	1	0
45	BA	109	PSU	1	0
1	AA	4500	PSU	1	0
45	BA	601	OMG	1	0
45	BA	867	OMG	2	0
45	BA	1244	PSU	3	0
5	AE	245	HIC	1	0
45	BA	649	PSU	2	0
45	BA	572	PSU	1	0
1	AA	1871	A2M	1	0
45	BA	119	PSU	1	0
45	BA	116	OMU	3	0
1	AA	4353	PSU	1	0
45	BA	100	PSU	1	0
1	AA	4220	6MZ	1	0
1	AA	1316	OMG	1	0
45	BA	1383	A2M	1	0
1	AA	398	A2M	1	0
45	BA	1703	OMC	1	0
1	AA	2804	OMC	1	0
1	AA	2815	A2M	1	0
1	AA	4293	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	BA	436	OMG	1	0
1	AA	3830	A2M	1	0
45	BA	1842	4AC	1	0
45	BA	1692	PSU	2	0
3	AC	14	OMU	1	0
45	BA	681	PSU	2	0
45	BA	1232	PSU	1	0
1	AA	4392	OMG	2	0
45	BA	1004	PSU	1	0
45	BA	1360	PSU	2	0
1	AA	1779	PSU	1	0
45	BA	468	A2M	1	0
45	BA	166	A2M	1	0
1	AA	4423	PSU	2	0
45	BA	1850	MA6	3	0
45	BA	512	A2M	1	0
1	AA	4457	PSU	2	0
1	AA	4227	OMU	1	0
45	BA	296	PSU	1	0
45	BA	1643	PSU	3	0
1	AA	4636	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 291 ligands modelled in this entry, 290 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
82	M7G	BA	1933	-	24,26,31	4.92	20 (83%)	34,39,49	1.79	9 (26%)

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
82	M7G	BA	1933	-	-	1/7/25/32	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	BA	1933	M7G	C8-N7	10.42	1.51	1.33
82	BA	1933	M7G	C2'-C3'	-10.37	1.24	1.53
82	BA	1933	M7G	C2-N3	6.55	1.49	1.33
82	BA	1933	M7G	O4'-C4'	-6.34	1.30	1.45
82	BA	1933	M7G	C4-N3	6.12	1.48	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	BA	1933	M7G	C2-N3-C4	4.39	120.11	112.30
82	BA	1933	M7G	C5-C4-N3	-4.26	119.99	128.15
82	BA	1933	M7G	C5-C6-N1	3.81	119.75	111.79
82	BA	1933	M7G	O6-C6-C5	-3.12	121.03	128.06
82	BA	1933	M7G	C2-N1-C6	-2.71	120.15	125.10

There are no chirality outliers.

All (1) torsion outliers are listed below:

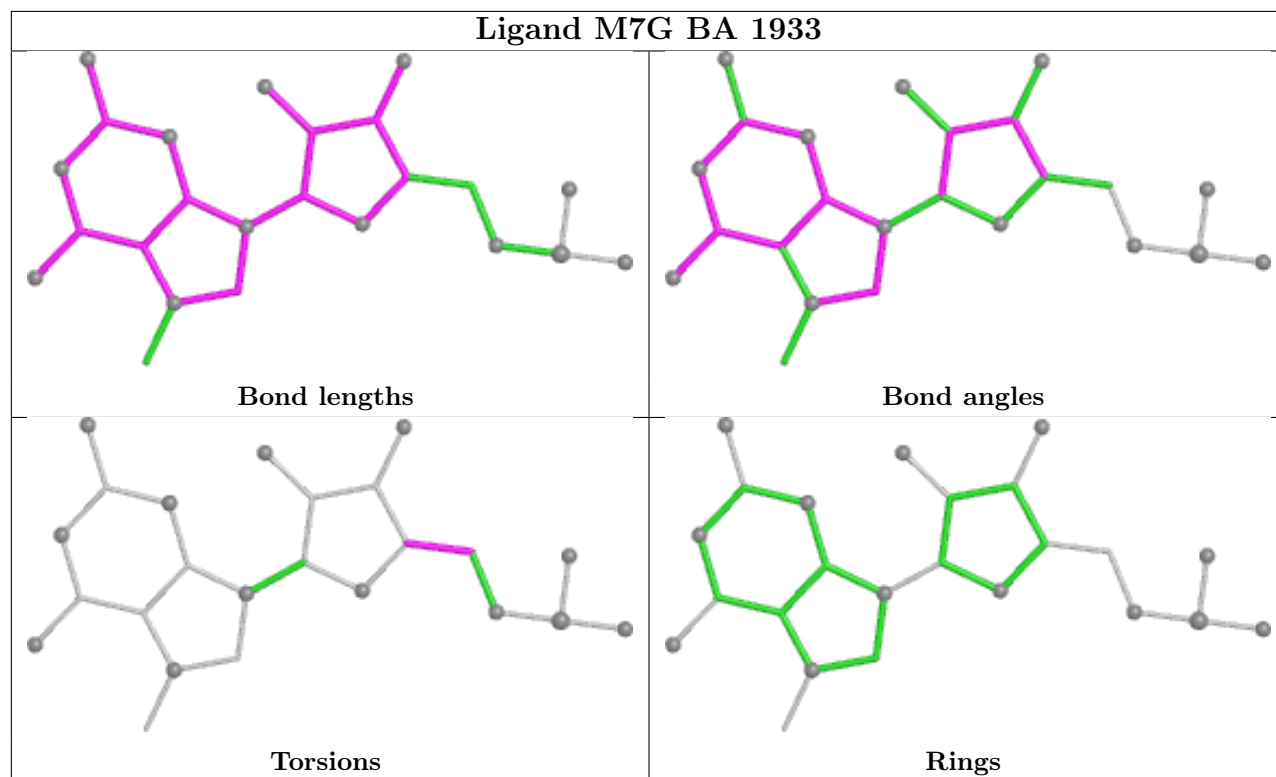
Mol	Chain	Res	Type	Atoms
82	BA	1933	M7G	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

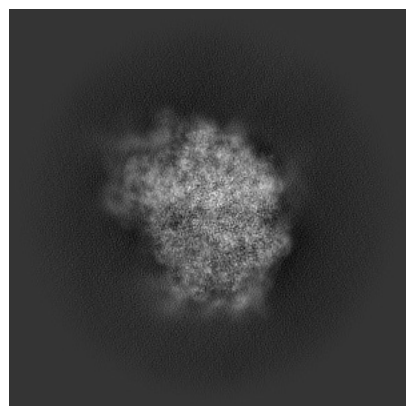
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66301. These allow visual inspection of the internal detail of the map and identification of artifacts.

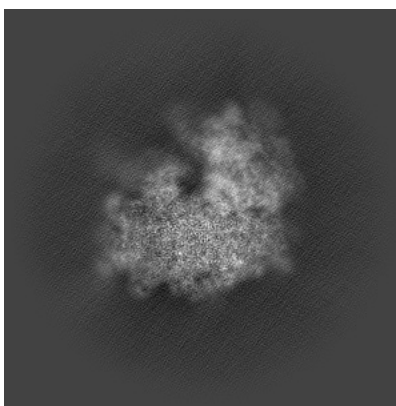
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

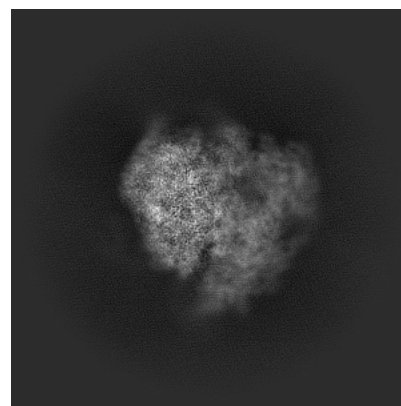
6.1.1 Primary map



X

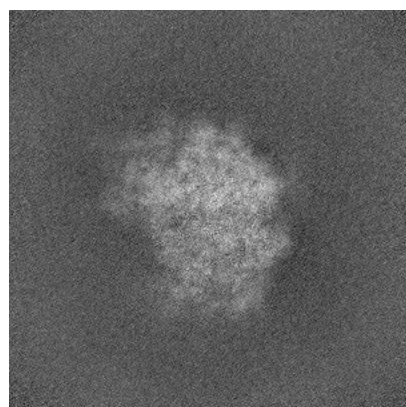


Y

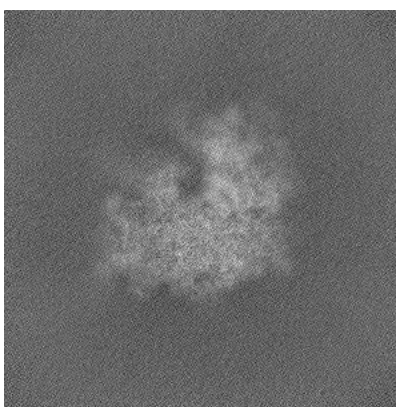


Z

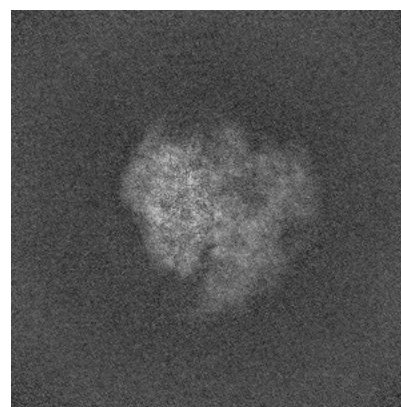
6.1.2 Raw map



X



Y

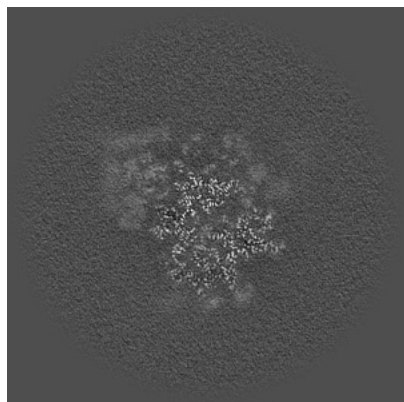


Z

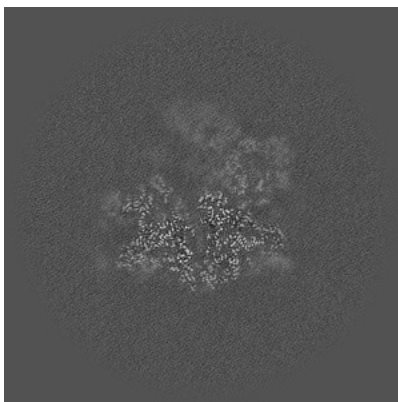
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

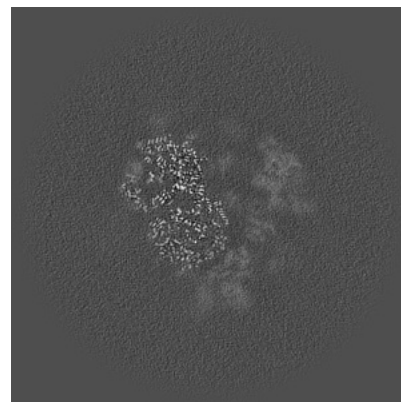
6.2.1 Primary map



X Index: 320

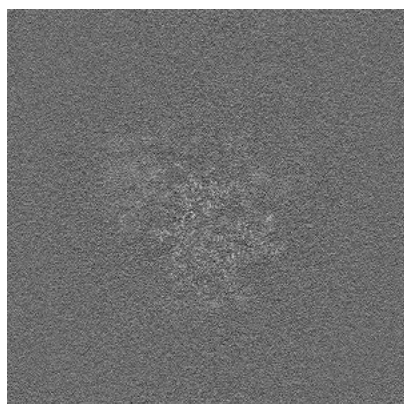


Y Index: 320

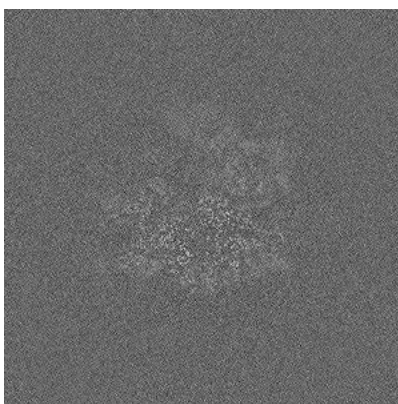


Z Index: 320

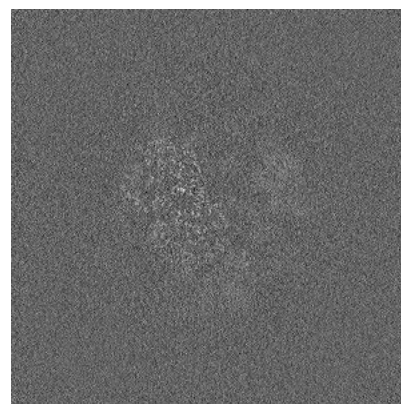
6.2.2 Raw map



X Index: 320



Y Index: 320

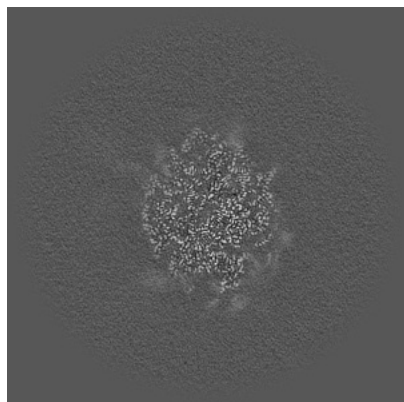


Z Index: 320

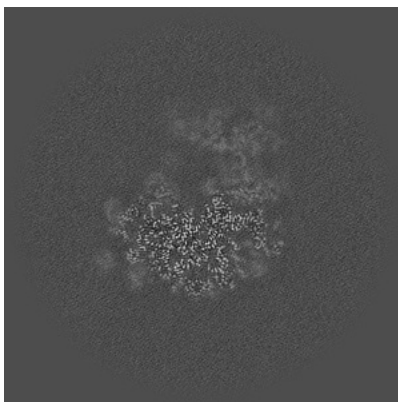
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

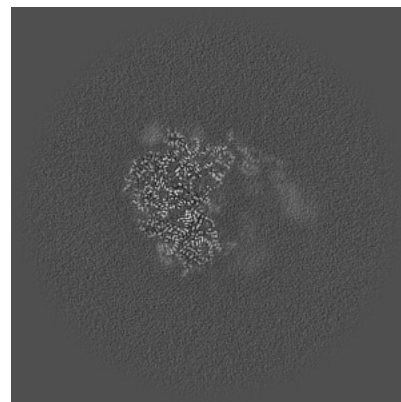
6.3.1 Primary map



X Index: 287

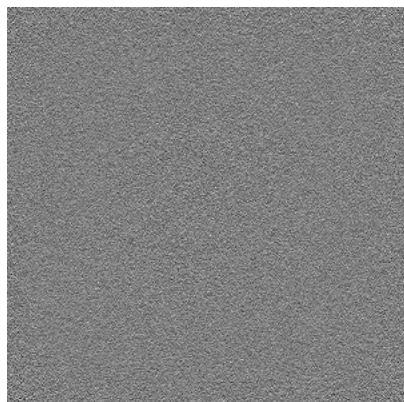


Y Index: 338

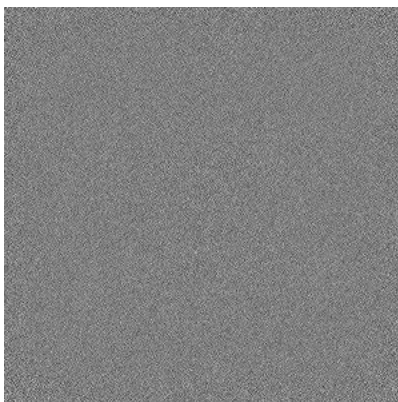


Z Index: 283

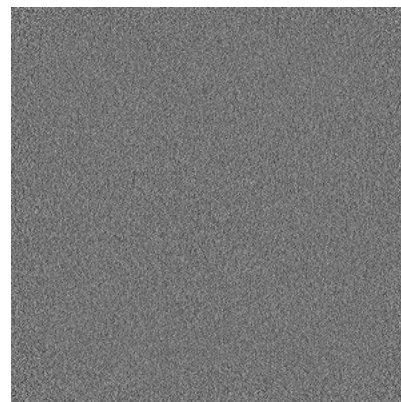
6.3.2 Raw map



X Index: 0



Y Index: 0

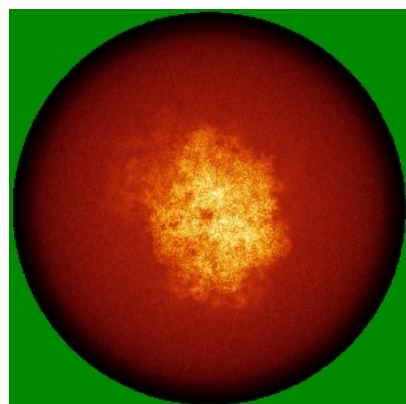


Z Index: 0

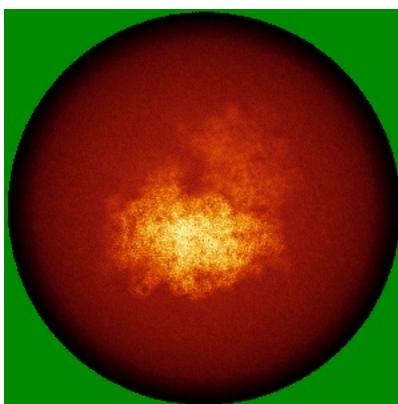
The images above show the largest variance slices of the map in three orthogonal directions.

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

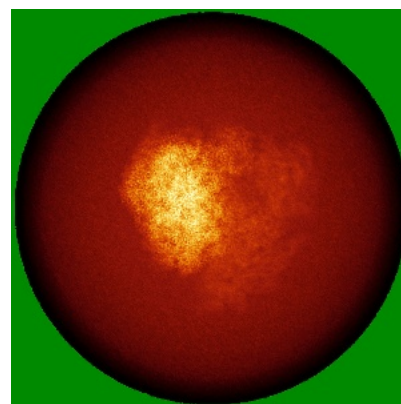
6.4.1 Primary map



X

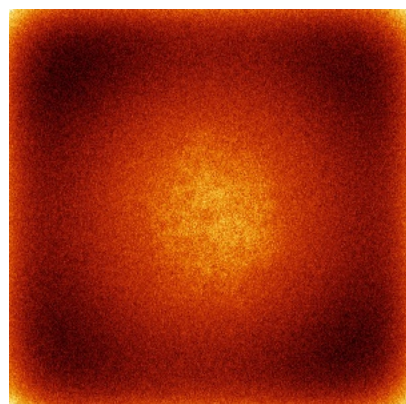


Y

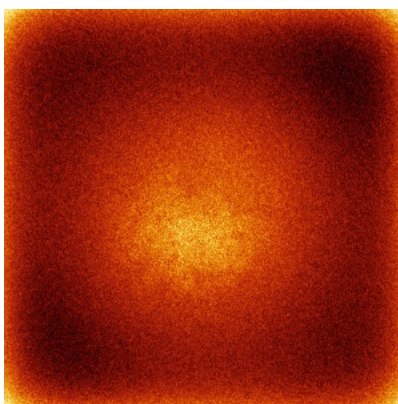


Z

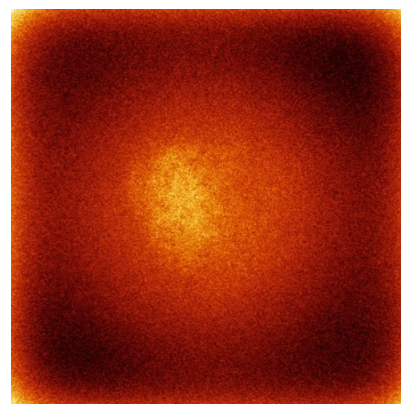
6.4.2 Raw map



X



Y

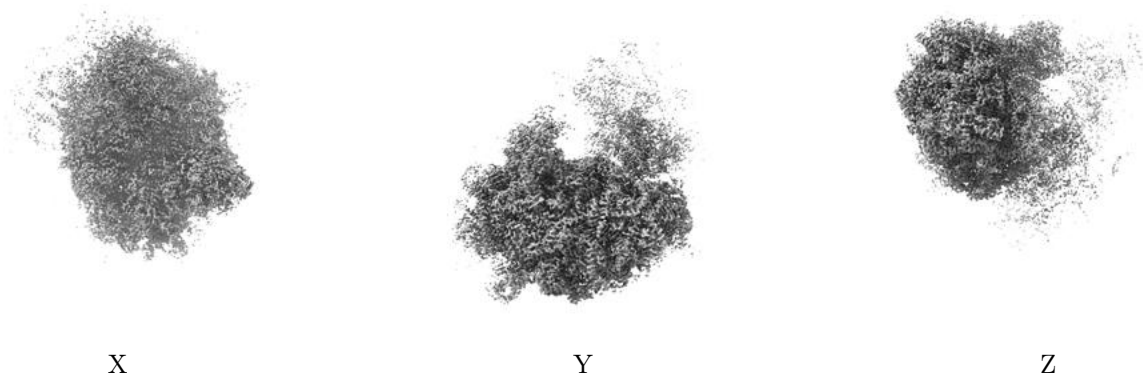


Z

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.

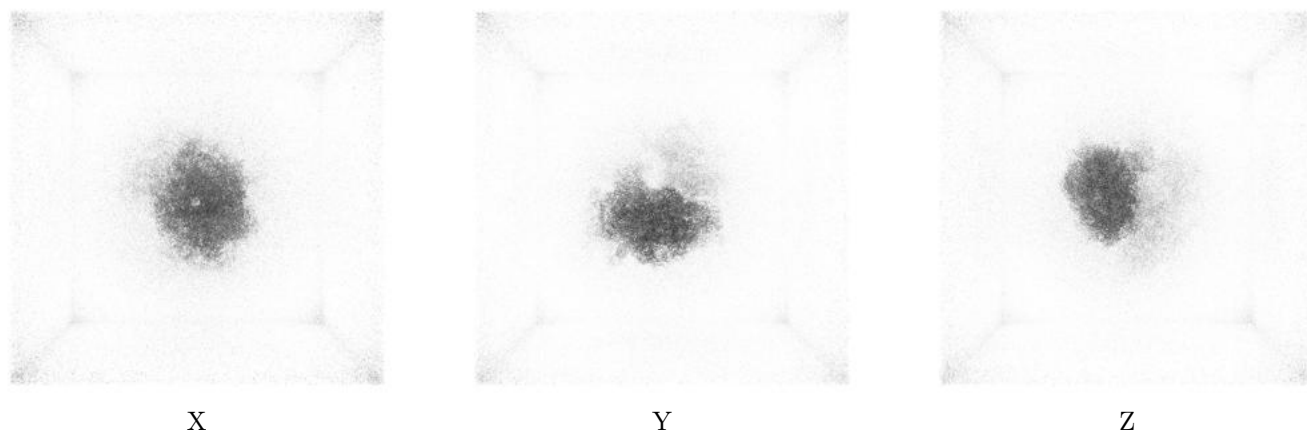
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

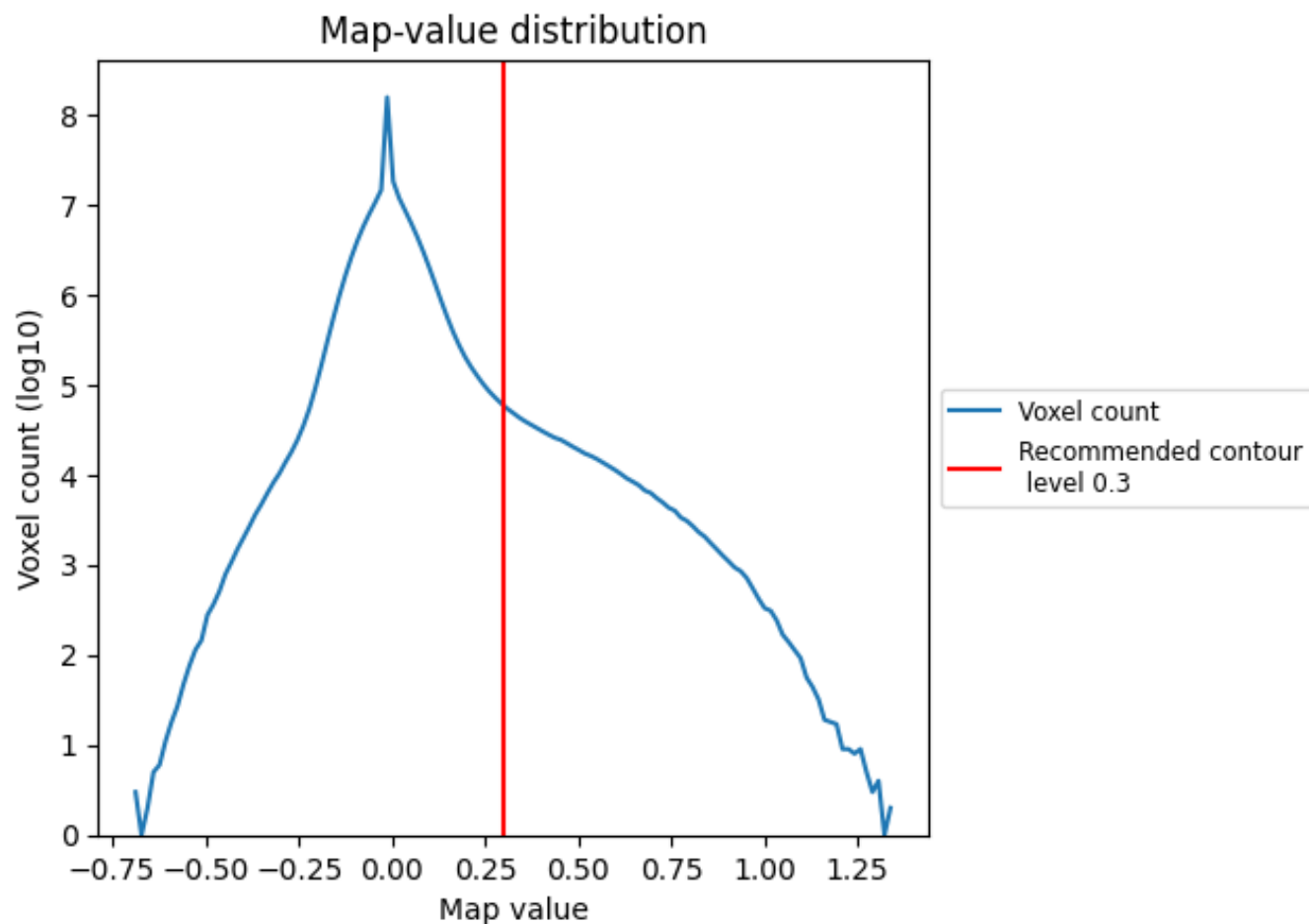
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

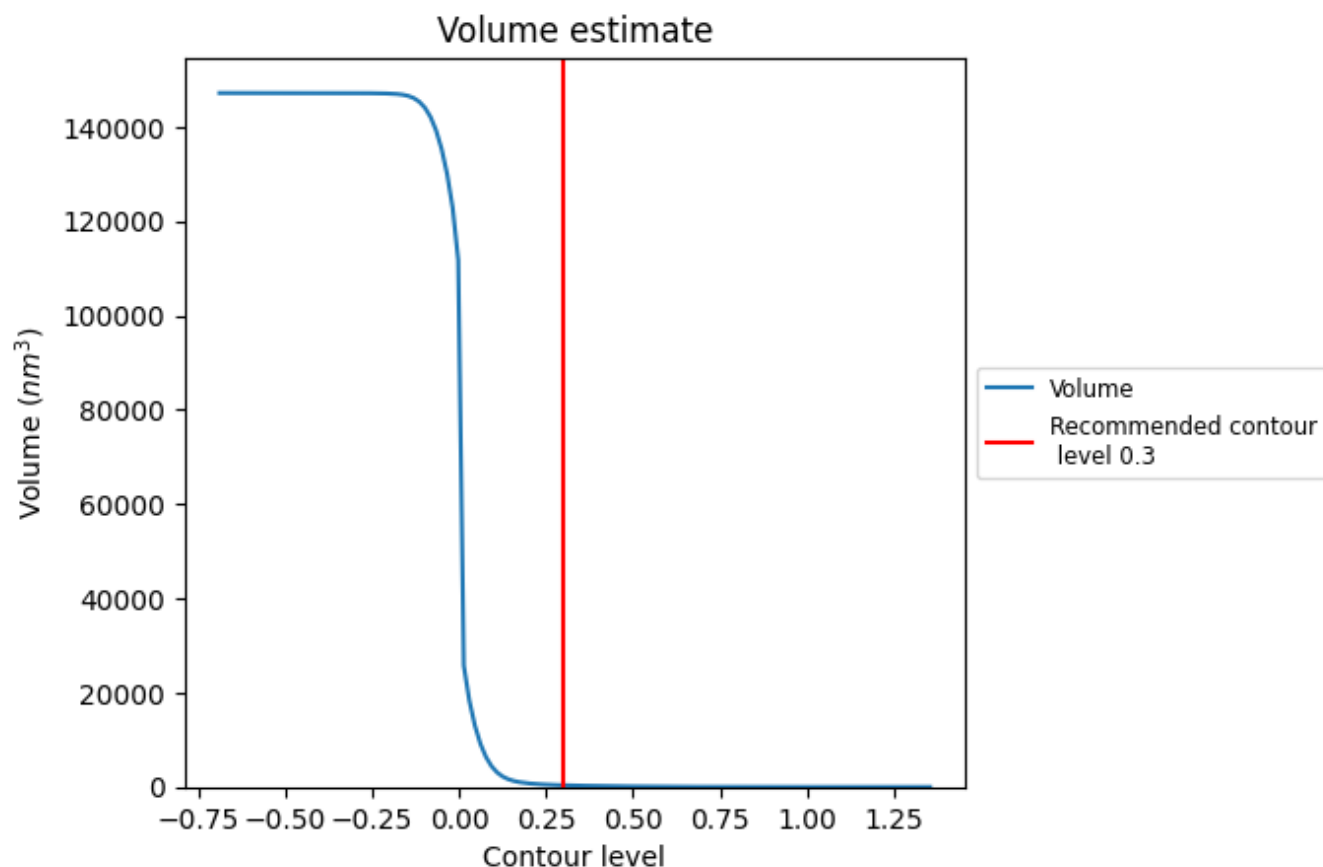
This section contains the results of statistical analysis of the map.

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.

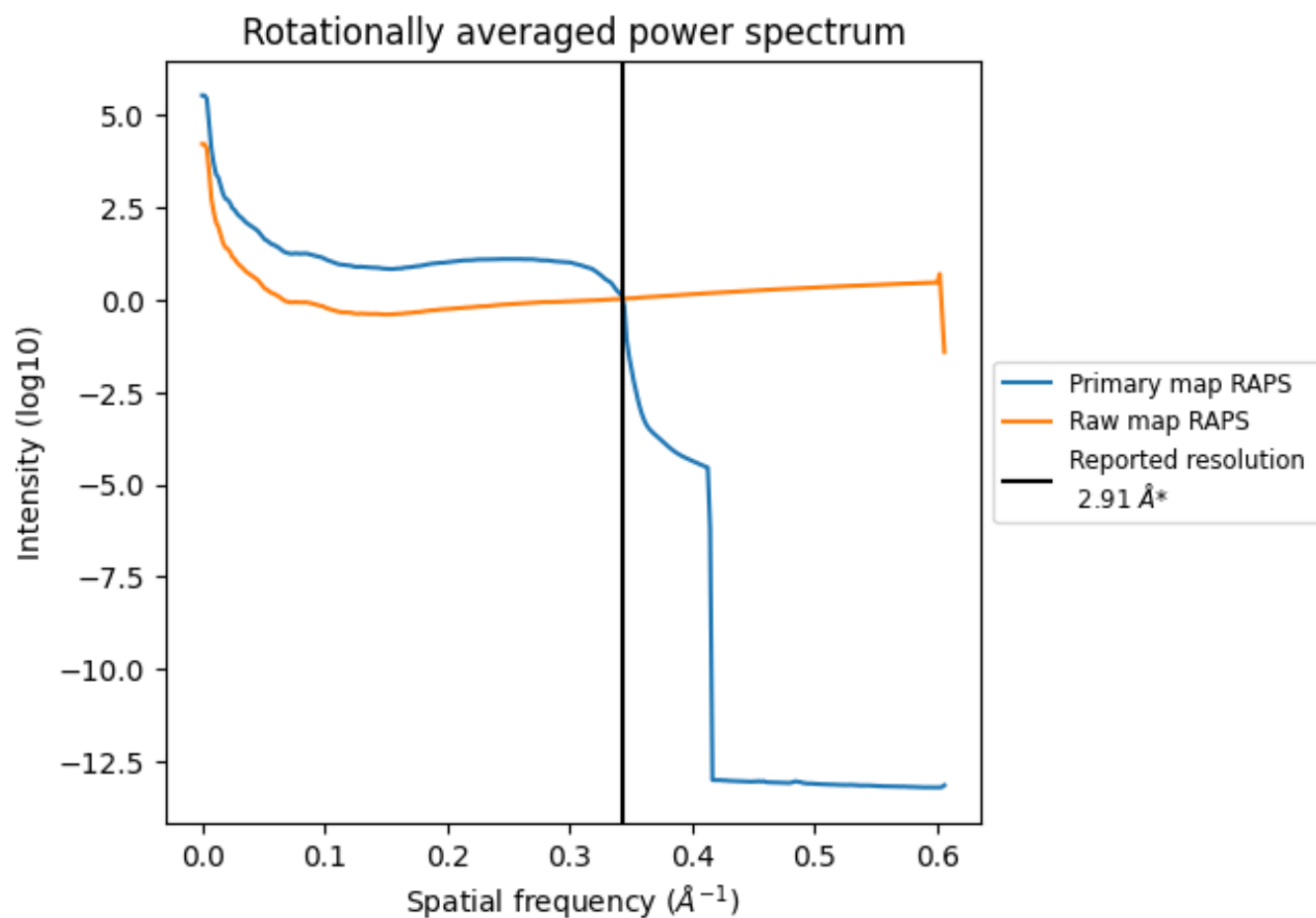
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm³; this corresponds to an approximate mass of 322 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 ⓘ

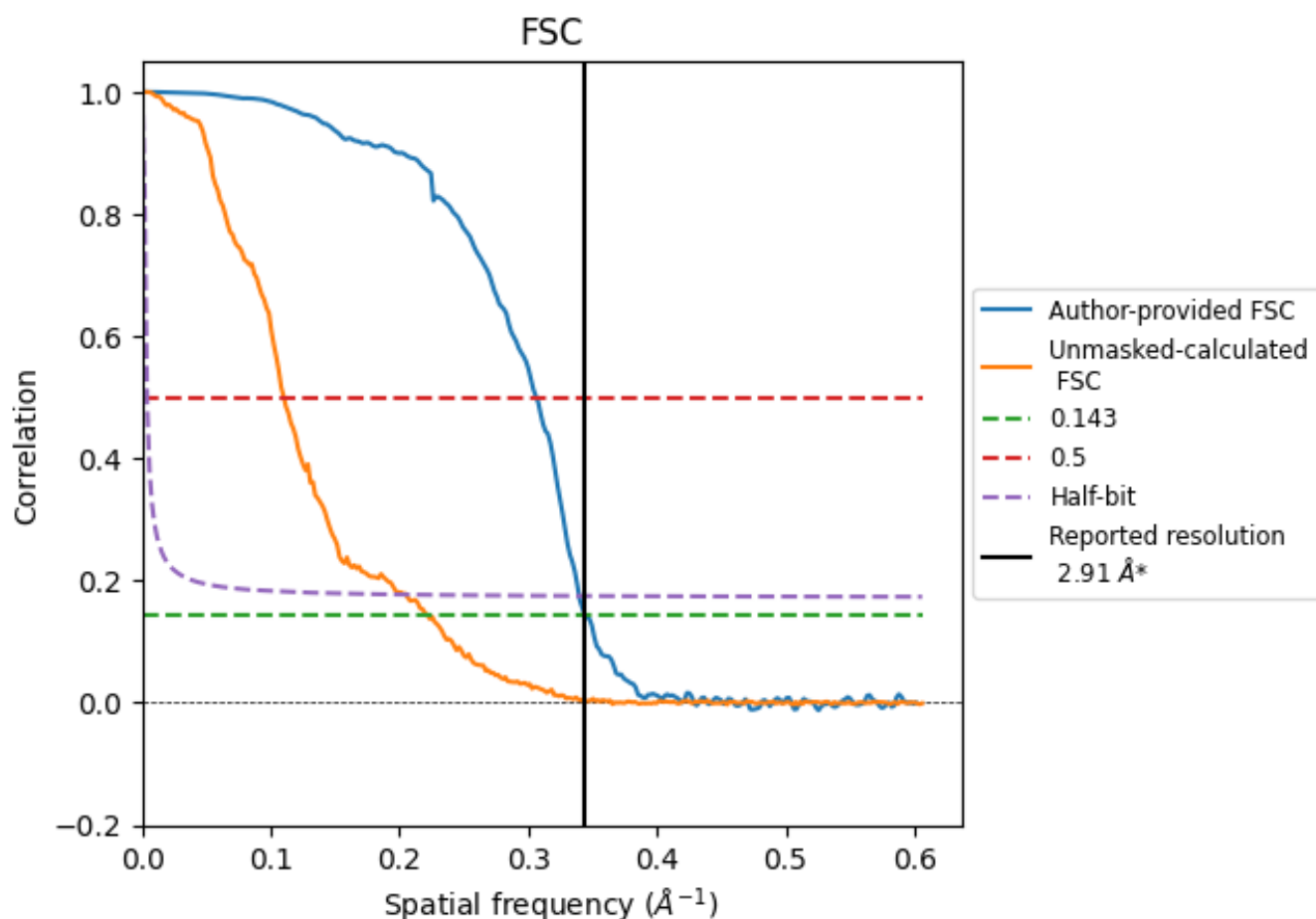


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

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 0.344 Å⁻¹

8.2 Resolution estimates [i](#)

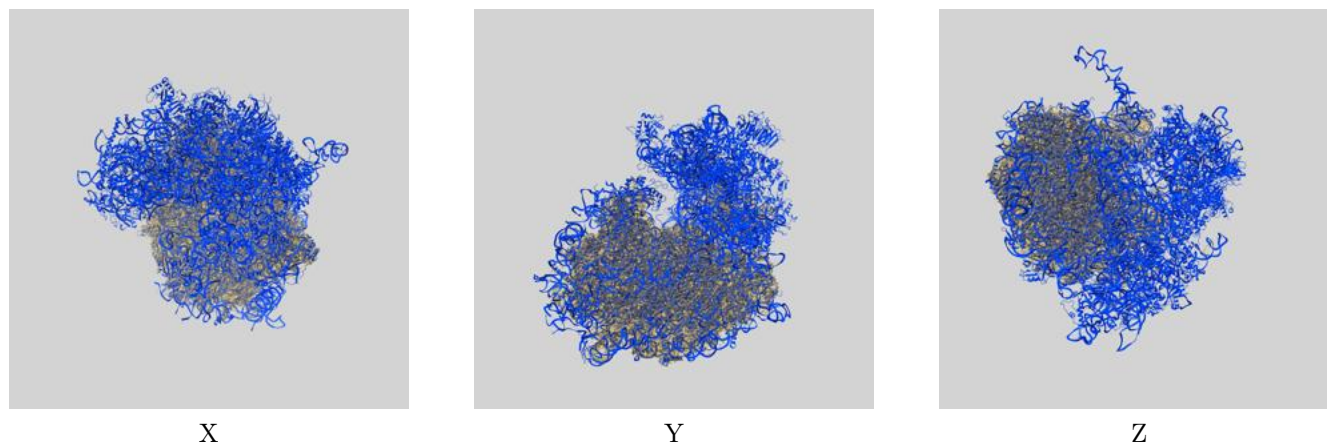
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.91	3.27	2.95
Unmasked-calculated*	4.51	9.08	4.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

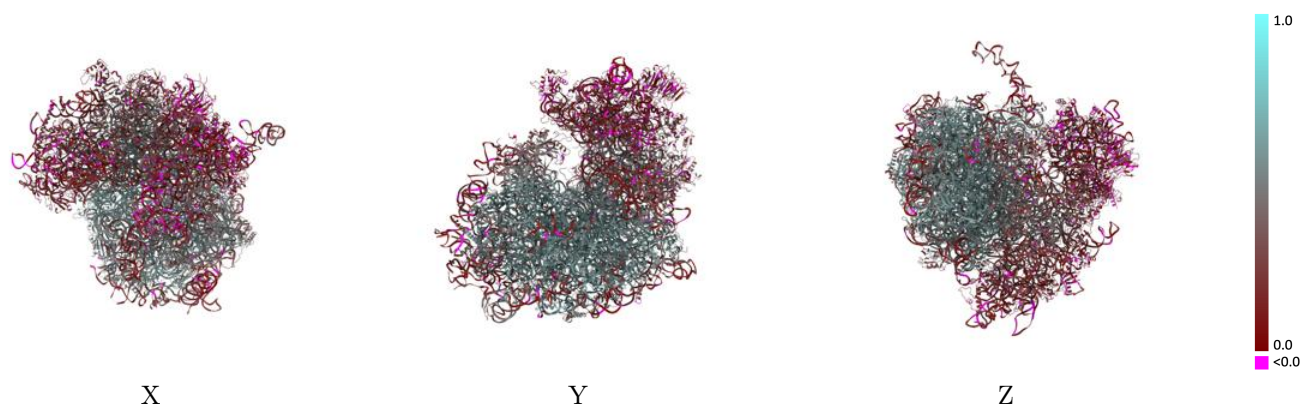
This section contains information regarding the fit between EMDB map EMD-66301 and PDB model 9WW7. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



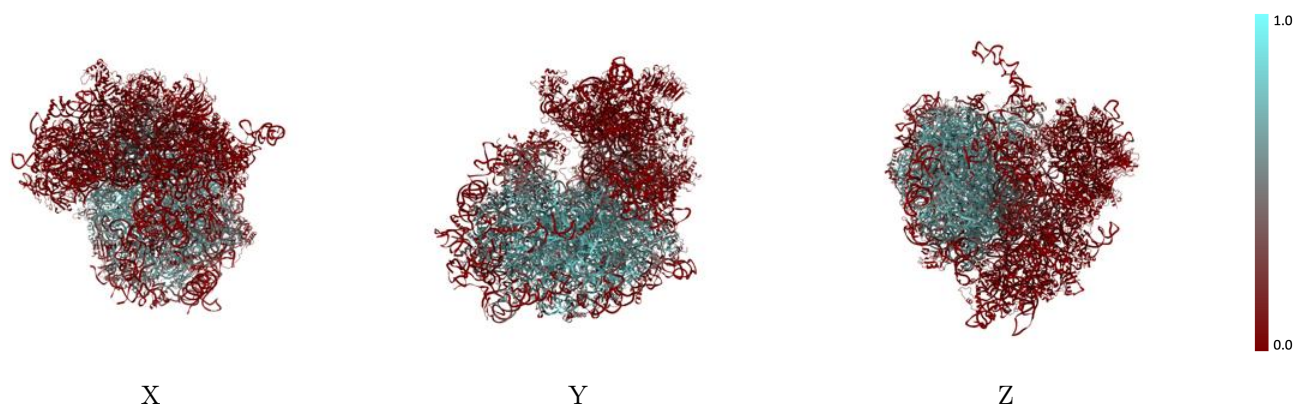
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



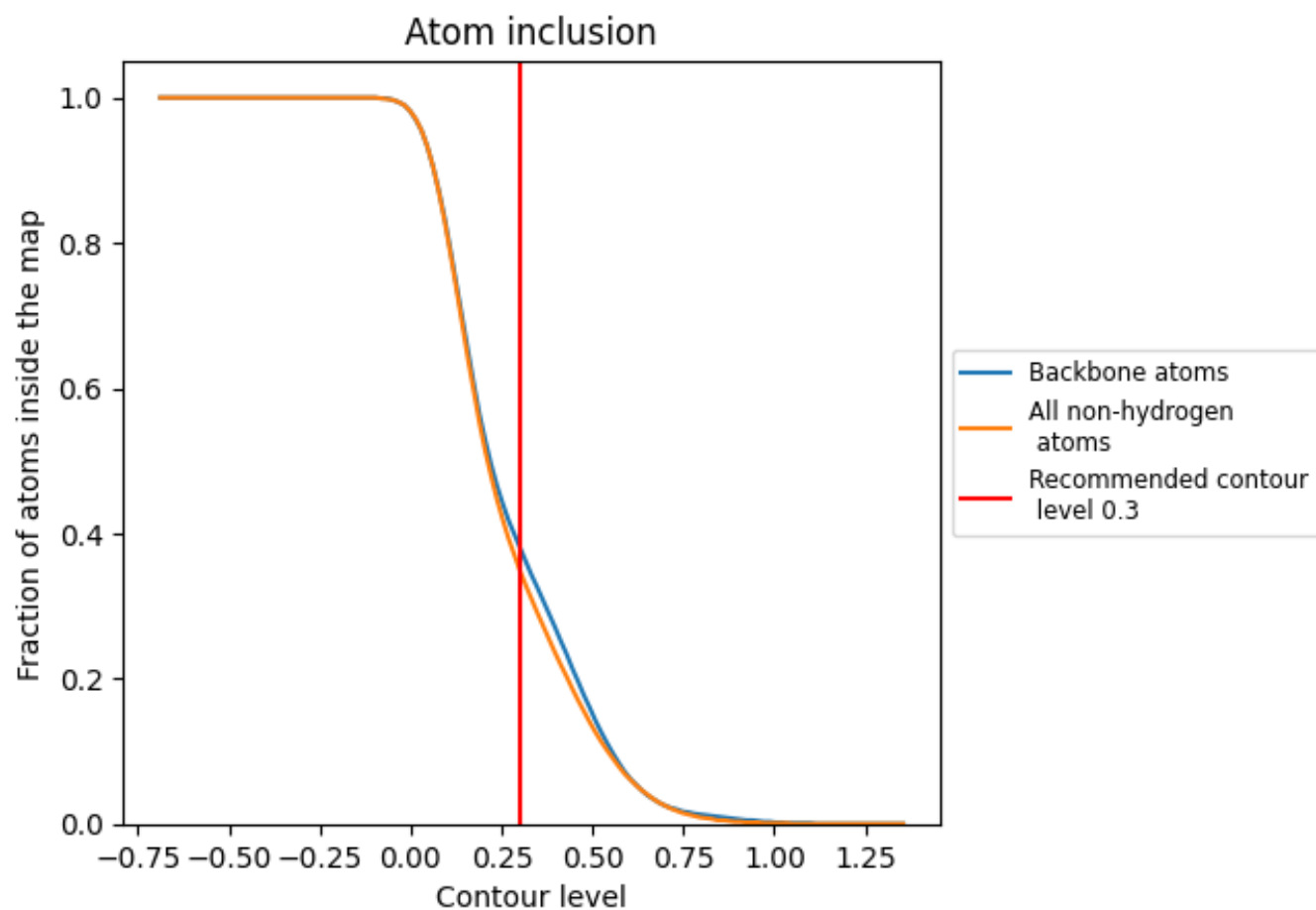
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 35% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3500	 0.4050
AA	 0.5290	 0.4560
AB	 0.5150	 0.4980
AC	 0.6540	 0.5310
AD	 0.7060	 0.6100
AE	 0.5740	 0.5720
AF	 0.6530	 0.5810
AG	 0.2980	 0.4600
AH	 0.3690	 0.4870
AI	 0.6350	 0.5800
AJ	 0.4530	 0.5090
AK	 0.2880	 0.5000
AL	 0.0500	 0.3800
AM	 0.0860	 0.3880
AN	 0.5030	 0.5390
AO	 0.4190	 0.5340
AP	 0.7480	 0.6170
AQ	 0.5970	 0.5750
AR	 0.6450	 0.5920
AS	 0.7020	 0.6080
AT	 0.4360	 0.5200
AU	 0.5250	 0.5680
AV	 0.5450	 0.5720
AW	 0.0250	 0.3420
AX	 0.5910	 0.5900
AY	 0.4860	 0.5770
AZ	 0.5740	 0.5770
Aa	 0.5690	 0.5580
Ab	 0.4560	 0.5380
Ac	 0.6770	 0.5980
Ad	 0.2950	 0.4740
Ae	 0.4140	 0.5000
Af	 0.5570	 0.5520
Ag	 0.6590	 0.5980
Ah	 0.6780	 0.6090



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Chain	Atom inclusion	Q-score
Ai	 0.6190	 0.5820
Aj	 0.5450	 0.5620
Ak	 0.3810	 0.5160
Al	 0.7220	 0.6120
Am	 0.2160	 0.4710
An	 0.5700	 0.5840
Ao	 0.0030	 0.1970
Aq	 0.4520	 0.5440
Ar	 0.6210	 0.5950
As	 0.6000	 0.5750
BA	 0.0690	 0.2600
BB	 0.0020	 0.2720
BC	 0.0060	 0.2830
BD	 0.0110	 0.3310
BE	 0.0010	 0.2190
BF	 0.0010	 0.1610
BG	 0.0050	 0.2550
BH	 0.0050	 0.2590
BI	 0.0000	 0.0910
BJ	 0.0260	 0.3470
BK	 0.0010	 0.2050
BL	 0.0000	 0.1990
BM	 0.0020	 0.2220
BN	 0.0000	 0.1700
BO	 0.0010	 0.2030
BP	 0.0060	 0.3140
BQ	 0.0170	 0.3550
BR	 0.0080	 0.2740
BS	 0.0000	 0.1510
BT	 0.0070	 0.1380
BU	 0.0000	 0.1460
BV	 0.0130	 0.2820
BW	 0.0000	 0.1840
BX	 0.0030	 0.1950
BY	 0.0000	 0.1210
BZ	 0.0500	 0.3990
Ba	 0.0100	 0.3140
Bb	 0.0310	 0.4230
Bc	 0.0000	 0.1510
Bd	 0.0020	 0.1470
Be	 0.0050	 0.3070
Bf	 0.0000	 0.2130

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Chain	Atom inclusion	Q-score
Bg	 0.0020	 0.0760
Bh	 0.0000	 0.1790