Full wwPDB EM Validation Report ⓘ

Apr 17, 2024 – 05:52 pm BST

PDB ID	:	8CGN
EMDB ID	:	EMD-16648
Title	:	Non-rotated 80S S. cerevisiae ribosome with ligands
Authors	:	Milicevic, N.; Jenner, L.; Myasnikov, A.; Yusupov, M.; Yusupova, G.
Deposited on	:	2023-02-06
Resolution	:	2.28 Å(reported)

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

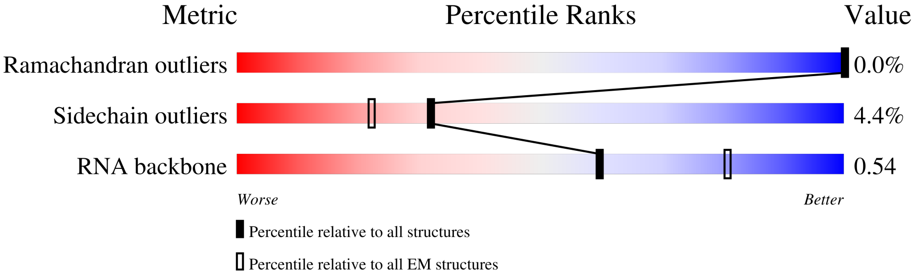
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

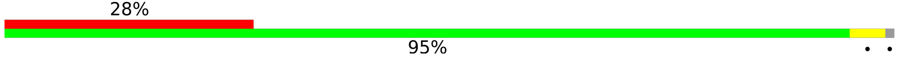
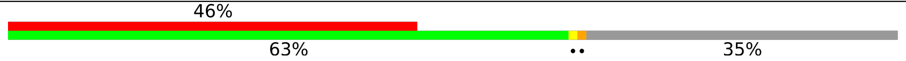
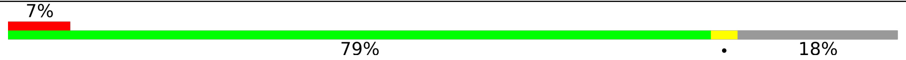
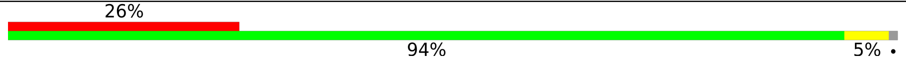
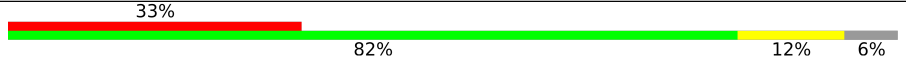
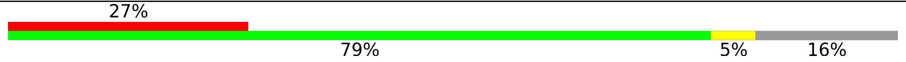
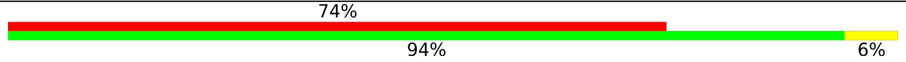
The reported resolution of this entry is 2.28 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	135	
2	1	108	
3	2	119	
4	3	82	
5	4	67	
6	5	56	
7	6	63	
8	7	319	

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Mol	Chain	Length	Quality of chain
9	8	152	24% 24% 76%
10	A	199	• 98% ••
11	AA	3396	9% 79% 15% • 6%
12	B	338	• 44% • 54%
13	BB	121	• 93% 7%
14	Bb	77	29% 71% 29%
14	Cc	77	91% 53% 42% 5%
15	C	186	• 98% ••
16	CC	158	• 85% 15%
17	D	189	8% 91% • 7%
18	DD	312	63% 59% • 37%
19	Dd	39	5% 13% • 85%
20	E	172	• 98% •
21	EE	254	• 98% • •
22	Ee	165	96% 88% 8% •
23	F	160	9% 95% • •
24	FF	387	• 98% •
25	G	121	18% 78% • 20%
26	GG	362	• 96% •
27	H	137	92% • 6%
28	HH	297	16% 98% •
29	I	155	• 41% 59%
30	II	176	6% 86% • 12%
31	J	142	5% 84% • 15%
32	JJ	244	• 89% • 9%

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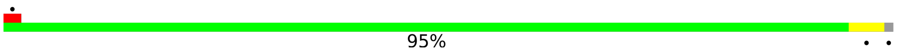
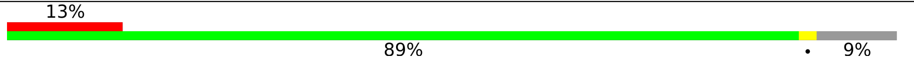
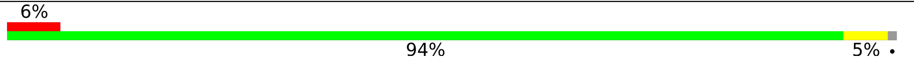
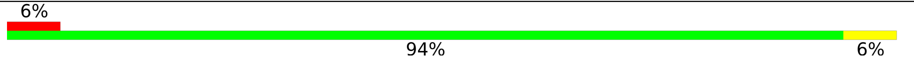
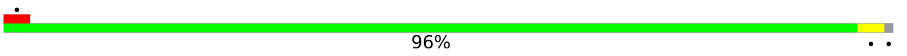
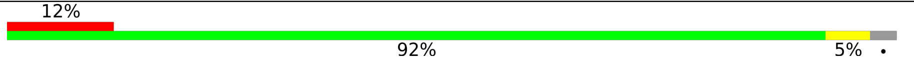
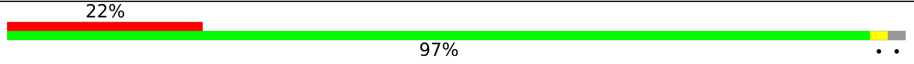
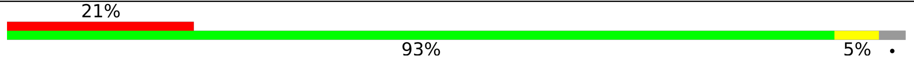
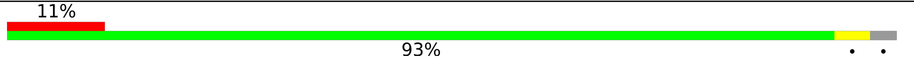
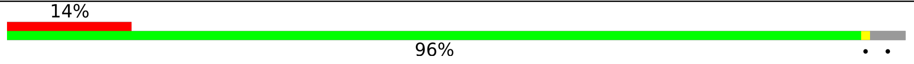
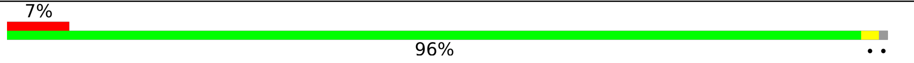
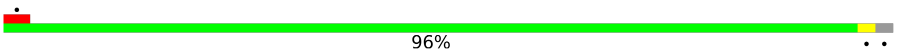
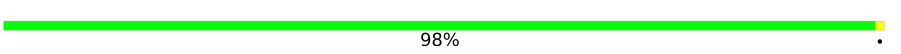
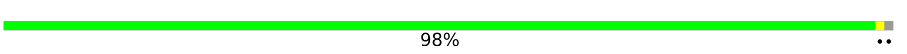
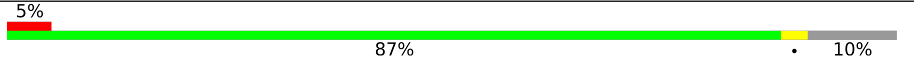
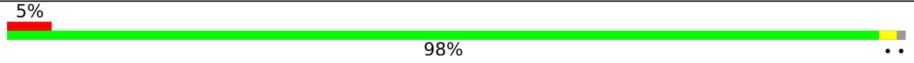
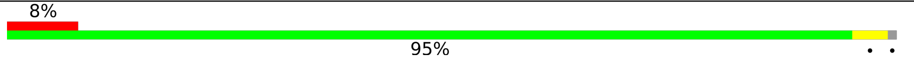
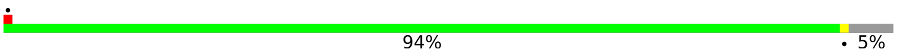
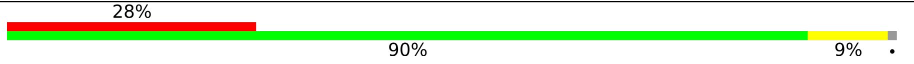
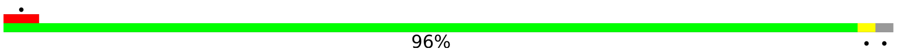
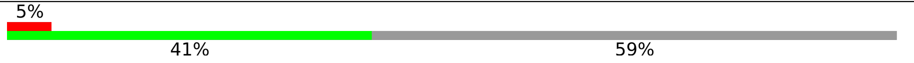
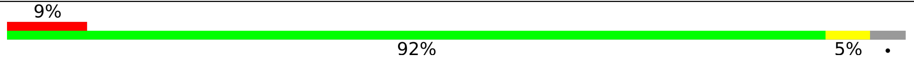
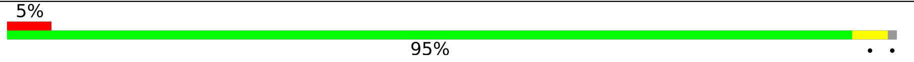
Mol	Chain	Length	Quality of chain
33	K	127	
34	KK	256	
35	L	136	
36	LL	191	
37	M	149	
38	MM	221	
39	N	59	
40	NN	174	
41	O	105	
42	OO	199	
43	P	113	
44	PP	138	
45	Q	130	
46	QQ	204	
47	R	107	
48	S	121	
49	T	120	
50	U	100	
51	V	88	
52	W	78	
53	X	51	
54	Y	128	
55	Z	25	
56	a	106	
57	b	92	

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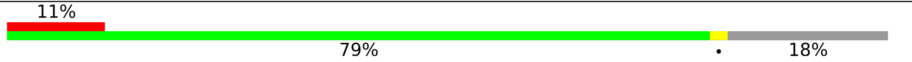
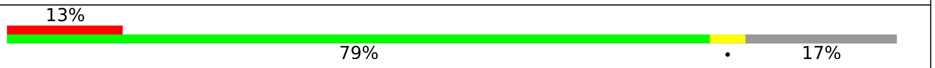
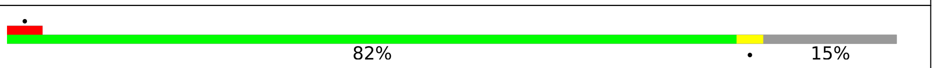
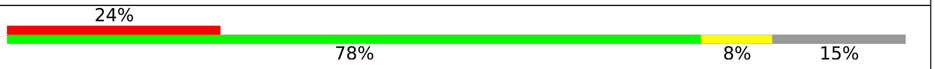
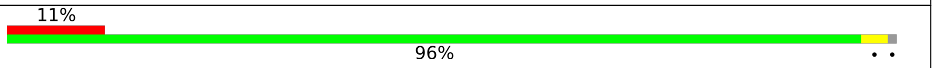
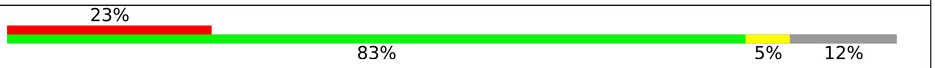
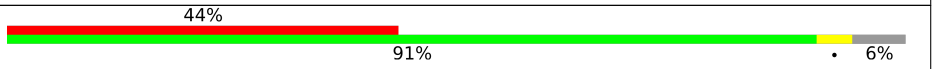
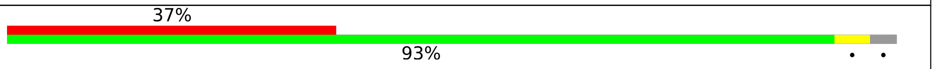
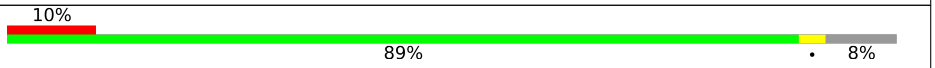
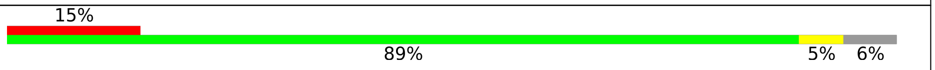
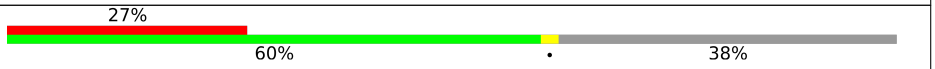
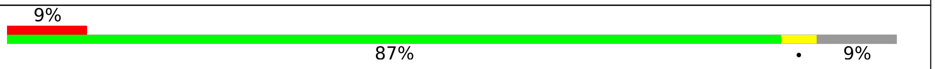
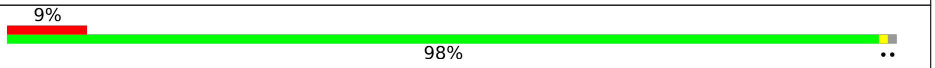
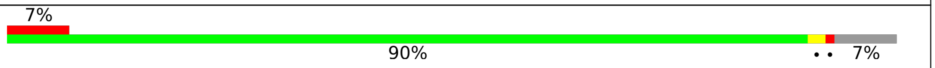
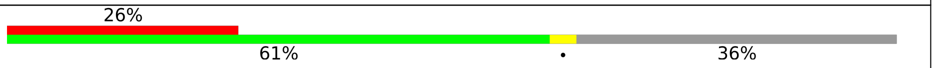
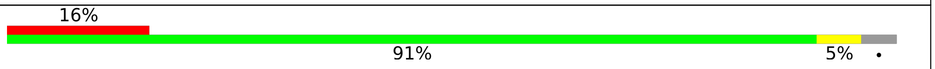
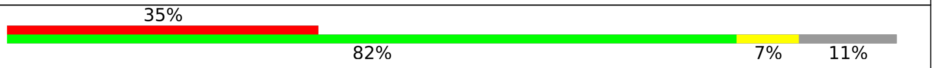
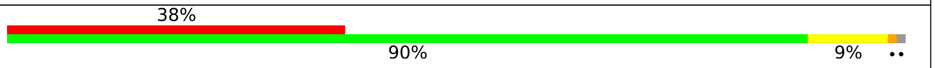
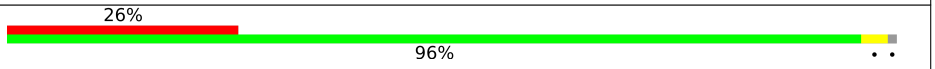
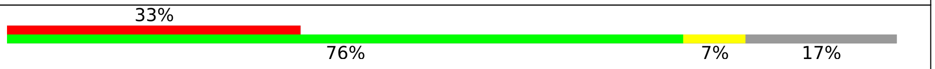
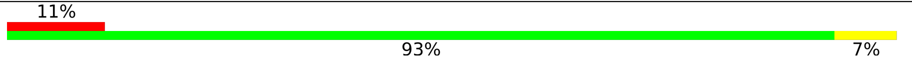
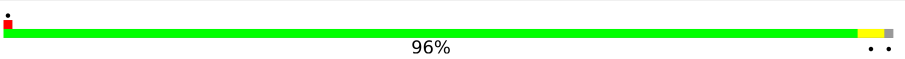
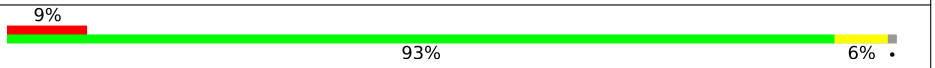
Mol	Chain	Length	Quality of chain
58	c	1800	
59	d	252	
60	e	255	
61	f	254	
62	g	240	
63	h	261	
64	i	225	
65	j	236	
66	k	190	
67	l	200	
68	m	197	
69	n	105	
70	o	156	
71	p	151	
72	q	137	
73	r	142	
74	s	143	
75	t	136	
76	u	146	
77	v	144	
78	w	121	
79	x	87	
80	y	130	
81	z	145	

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 201528 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 protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	134	1073	676	208	189	0	0

- Molecule 2 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	70	563	360	104	99	0	0

- Molecule 3 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	97	769	475	160	129	5	0	0

- Molecule 4 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	81	610	382	110	113	5	0	0

- Molecule 5 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	63	497	306	99	91	1	0	0

- Molecule 6 is a protein called HLJ1_G0030400.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	49	404	249	86	65	4	0	0

- Molecule 7 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	53	Total 427	C 269	N 88	O 69	S 1	0	0

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	318	Total 2436	C 1541	N 418	O 469	S 8	0	0

- Molecule 9 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	36	Total 276	C 173	N 54	O 45	S 4	0	0

- Molecule 10 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	197	Total 1555	C 1003	N 289	O 262	S 1	0	0

- Molecule 11 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	3197	Total 68429	C 30589	N 12334	O 22309	P 3197	0	0

- Molecule 12 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	B	154	Total 1222	C 761	N 237	O 224	0	0

- Molecule 13 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BB	121	Total 2579	C 1152	N 461	O 845	P 121	0	0

- Molecule 14 is a RNA chain called Transfer RNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Bb	77	Total 1644	C 732	N 298	O 537	P 77	0	0
14	Cc	77	Total 1644	C 732	N 298	O 537	P 77	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bb	18	C	U	conflict	GB 170517292
Cc	18	C	U	conflict	GB 170517292

- Molecule 15 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	185	Total 1441	C 908	N 290	O 241	S 2	0	0

- Molecule 16 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CC	158	Total 3353	C 1500	N 586	O 1109	P 158	0	0

- Molecule 17 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	D	176	Total 1423	C 875	N 308	O 240	0	0

- Molecule 18 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	DD	197	Total 1531	C 980	N 266	O 281	S 4	0	0

- Molecule 19 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Dd	6	Total 131	C 59	N 27	O 39	P 6	0	0

- Molecule 20 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	172	Total 1445	C 930	N 267	O 244	S 4	0	0

- Molecule 21 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	EE	252	Total 1914	C 1191	N 388	O 334	S 1	0	0

- Molecule 22 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Ee	158	Total 1196	C 750	N 216	O 228	S 2	0	0

- Molecule 23 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	F	159	Total 1276	C 805	N 246	O 221	S 4	0	0

- Molecule 24 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	FF	386	Total 3075	C 1950	N 584	O 533	S 8	0	0

- Molecule 25 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	G	97	Total 770	C 499	N 126	O 145	0	0

- Molecule 26 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	GG	361	Total 2748	C 1729	N 522	O 494	S 3	0	0

- Molecule 27 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	H	129	963	607	180	169	7	0	0

- Molecule 28 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	HH	296	2375	1501	414	458	2	0	0

- Molecule 29 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	I	63	521	336	102	82	1	0	0

- Molecule 30 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	II	155	1230	795	221	213	1	0	0

- Molecule 31 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	J	120	959	617	168	172	2	0	0

- Molecule 32 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	JJ	222	1784	1151	324	308	1	0	0

- Molecule 33 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	K	126	993	625	192	176	0	0

- Molecule 34 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	KK	233	1804	1151	323	327	3	0	0

- Molecule 35 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	L	135	1092	710	202	180	0	0

- Molecule 36 is a protein called RPL9A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	LL	191	1518	963	274	277	4	0	0

- Molecule 37 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	M	148	1173	749	231	190	3	0	0

- Molecule 38 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	MM	215	1743	1102	331	303	7	0	0

- Molecule 39 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	N	58	462	289	100	73	0	0

- Molecule 40 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	NN	169	1353	847	253	249	4	0	0

- Molecule 41 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	O	97	742	479	124	138	1	0	0

- Molecule 42 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	OO	193	1543	962	315	266	0	0

- Molecule 43 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	P	109	883	559	167	156	1	0	0

- Molecule 44 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	PP	136	1053	675	199	177	2	0	0

- Molecule 45 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Q	127	1020	647	205	167	1	0	0

- Molecule 46 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	QQ	203	1720	1077	361	281	1	0	0

- Molecule 47 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	R	106	850	540	165	144	1	0	0

- Molecule 48 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S	109	Total 861	C 533	N 175	O 149	S 4	0	0

- Molecule 49 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	T	119	Total 969	C 615	N 186	O 167	S 1	0	0

- Molecule 50 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	U	99	Total 771	C 481	N 156	O 132	S 2	0	0

- Molecule 51 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	V	84	Total 665	C 405	N 145	O 110	S 5	0	0

- Molecule 52 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	W	77	Total 612	C 391	N 115	O 106	0	0

- Molecule 53 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	50	Total 436	C 272	N 97	O 65	S 2	0	0

- Molecule 54 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Y	52	Total 417	C 259	N 86	O 67	S 5	0	0

- Molecule 55 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Z	25	233	142	63	27	1	0	0

- Molecule 56 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	a	102	819	514	166	134	5	0	0

- Molecule 57 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	b	91	694	429	138	121	6	0	0

- Molecule 58 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
58	c	1624	34663	15513	6155	11371	1624	0	0

- Molecule 59 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	d	206	1583	1017	281	283	2	0	0

- Molecule 60 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	e	212	1689	1073	303	309	4	0	0

- Molecule 61 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	f	217	1635	1047	289	297	2	0	0

- Molecule 62 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	g	205	1593	1008	293	286	6	0	0

- Molecule 63 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	h	258	2056	1308	387	358	3	0	0

- Molecule 64 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	i	199	1572	987	290	292	3	0	0

- Molecule 65 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	j	223	1798	1128	347	320	3	0	0

- Molecule 66 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
66	k	184	1481	951	265	265	0	0

- Molecule 67 is a protein called 40S ribosomal protein S8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	l	184	1457	906	291	258	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	m	185	1494	943	289	261	1	0	0

- Molecule 69 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
69	n	65	Total 556	C 361	N 90	O 105	0	0

- Molecule 70 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	o	142	Total 1146	C 735	N 217	O 191	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
71	p	150	Total 1192	C 759	N 224	O 207	S 2	0	0

- Molecule 72 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	q	127	Total 891	C 545	N 182	O 163	S 1	0	0

- Molecule 73 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	r	91	Total 732	C 469	N 138	O 120	S 5	0	0

- Molecule 74 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	s	137	Total 1080	C 692	N 199	O 189	0	0

- Molecule 75 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	t	121	Total 961	C 599	N 182	O 178	S 2	0	0

- Molecule 76 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	u	145	1192	743	237	210	2	0	0

- Molecule 77 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	v	143	1112	694	208	208	2	0	0

- Molecule 78 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	w	100	800	509	144	146	1	0	0

- Molecule 79 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	x	87	684	420	125	137	2	0	0

- Molecule 80 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	y	129	1021	650	188	180	3	0	0

- Molecule 81 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	z	144	1121	708	220	191	2	0	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
82	2	1	1	1	0
82	5	1	1	1	0
82	8	1	1	1	0

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Mol	Chain	Residues	Atoms	AltConf
82	S	1	Total Zn 1 1	0
82	V	1	Total Zn 1 1	0
82	Y	1	Total Zn 1 1	0
82	a	1	Total Zn 1 1	0
82	b	1	Total Zn 1 1	0

- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
83	AA	199	Total Mg 199 199	0
83	B	1	Total Mg 1 1	0
83	BB	5	Total Mg 5 5	0
83	Bb	2	Total Mg 2 2	0
83	CC	3	Total Mg 3 3	0
83	FF	1	Total Mg 1 1	0
83	H	1	Total Mg 1 1	0
83	MM	1	Total Mg 1 1	0
83	QQ	1	Total Mg 1 1	0
83	c	49	Total Mg 49 49	0

- Molecule 84 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
84	AA	13	Total K 13 13	0
84	EE	1	Total K 1 1	0

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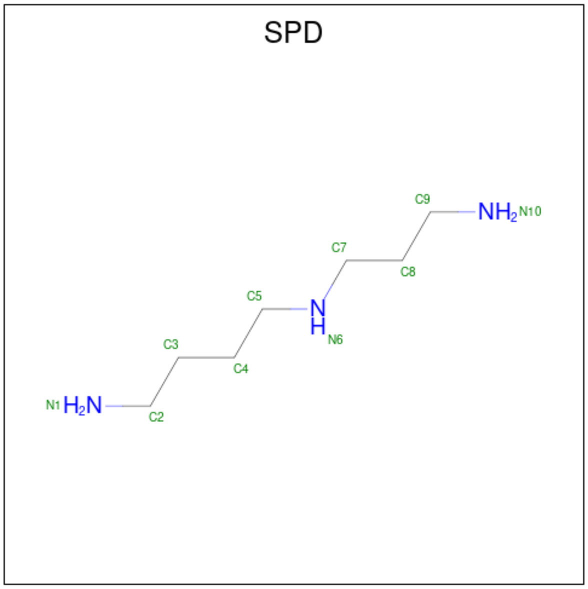
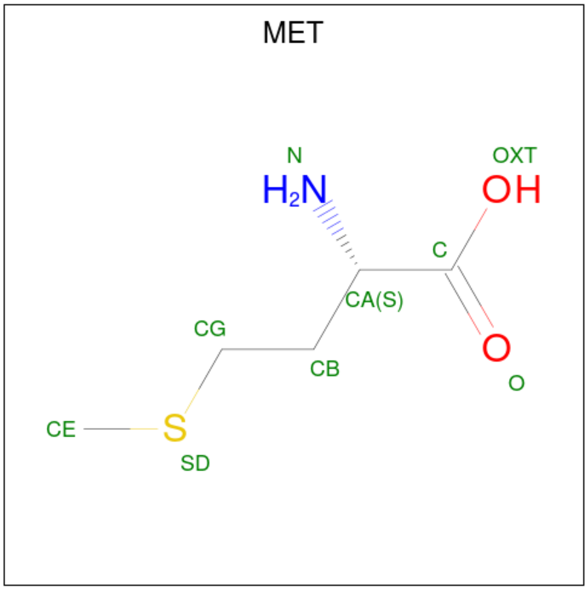
Mol	Chain	Residues	Atoms		AltConf
84	MM	1	Total 1	K 1	0
84	Q	1	Total 1	K 1	0
84	S	1	Total 1	K 1	0
84	c	1	Total 1	K 1	0
84	q	1	Total 1	K 1	0

- Molecule 85 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
85	AA	1	Total 10	C 7	N 3	0
85	AA	1	Total 10	C 7	N 3	0
85	AA	1	Total 10	C 7	N 3	0
85	c	1	Total 10	C 7	N 3	0

- Molecule 86 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



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<tr><th>Mol</th><th>Chain</th><th>Residues</th><th colspan="5">Atoms</th><th>AltConf</th></tr>
<tr><td rowspan="2">86</td><td rowspan="2">Bb</td><td rowspan="2">1</td><td>Total</td><td>C</td><td>N</td><td>O</td><td>S</td><td rowspan="2">0</td></tr>
<tr><td>8</td><td>5</td><td>1</td><td>1</td><td>1</td></tr>
</table>

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
87	2	1	1	1	0
87	A	2	2	2	0
87	AA	774	774	774	0
87	B	4	4	4	0
87	BB	13	13	13	0
87	Bb	5	5	5	0
87	CC	13	13	13	0
87	Cc	1	1	1	0
87	D	1	1	1	0
87	Dd	3	3	3	0
87	EE	11	11	11	0

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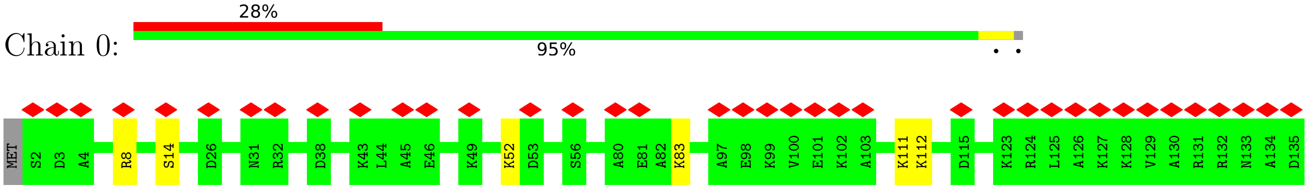
Mol	Chain	Residues	Atoms	AltConf
87	F	2	Total O 2 2	0
87	FF	4	Total O 4 4	0
87	GG	3	Total O 3 3	0
87	H	3	Total O 3 3	0
87	HH	1	Total O 1 1	0
87	J	1	Total O 1 1	0
87	JJ	1	Total O 1 1	0
87	M	2	Total O 2 2	0
87	MM	1	Total O 1 1	0
87	N	1	Total O 1 1	0
87	P	1	Total O 1 1	0
87	Q	4	Total O 4 4	0
87	QQ	7	Total O 7 7	0
87	V	4	Total O 4 4	0
87	a	1	Total O 1 1	0
87	c	122	Total O 122 122	0
87	e	1	Total O 1 1	0
87	h	2	Total O 2 2	0
87	o	2	Total O 2 2	0
87	p	1	Total O 1 1	0

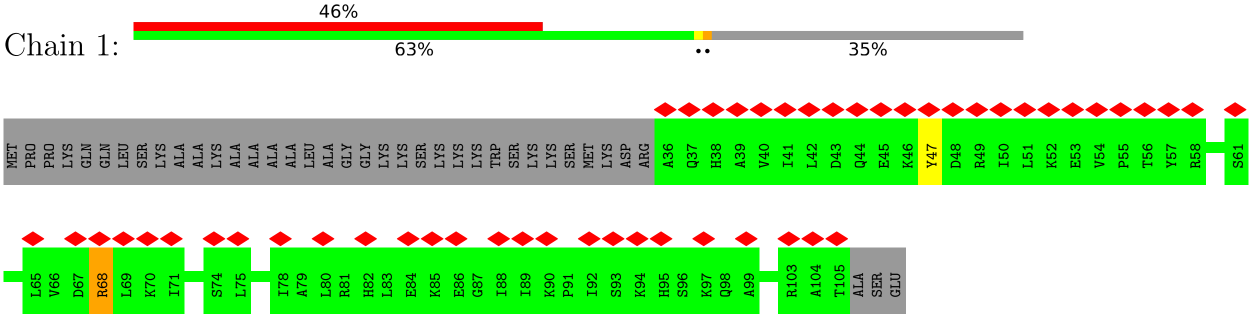
3 Residue-property plots ⓘ

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

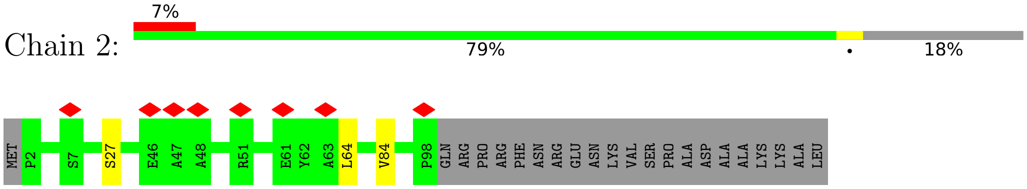
- Molecule 1: 40S ribosomal protein S24-A



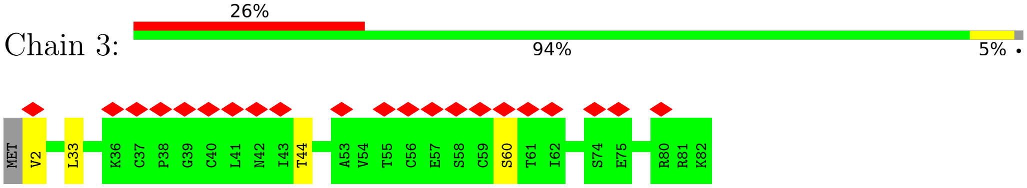
- Molecule 2: 40S ribosomal protein S25-A



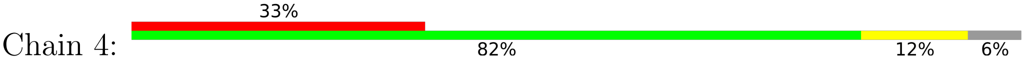
- Molecule 3: 40S ribosomal protein S26

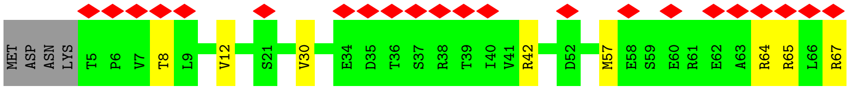


- Molecule 4: 40S ribosomal protein S27-A



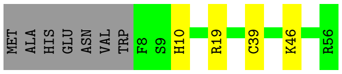
- Molecule 5: 40S ribosomal protein S28-A





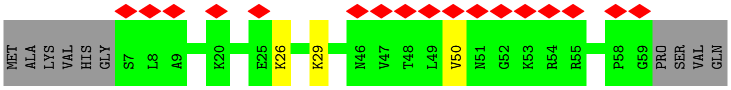
- Molecule 6: HLJ1_G0030400.mRNA.1.CDS.1

Chain 5:



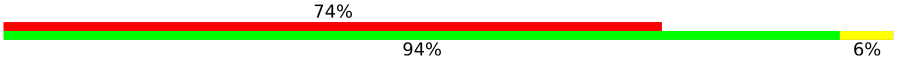
- Molecule 7: 40S ribosomal protein S30-A

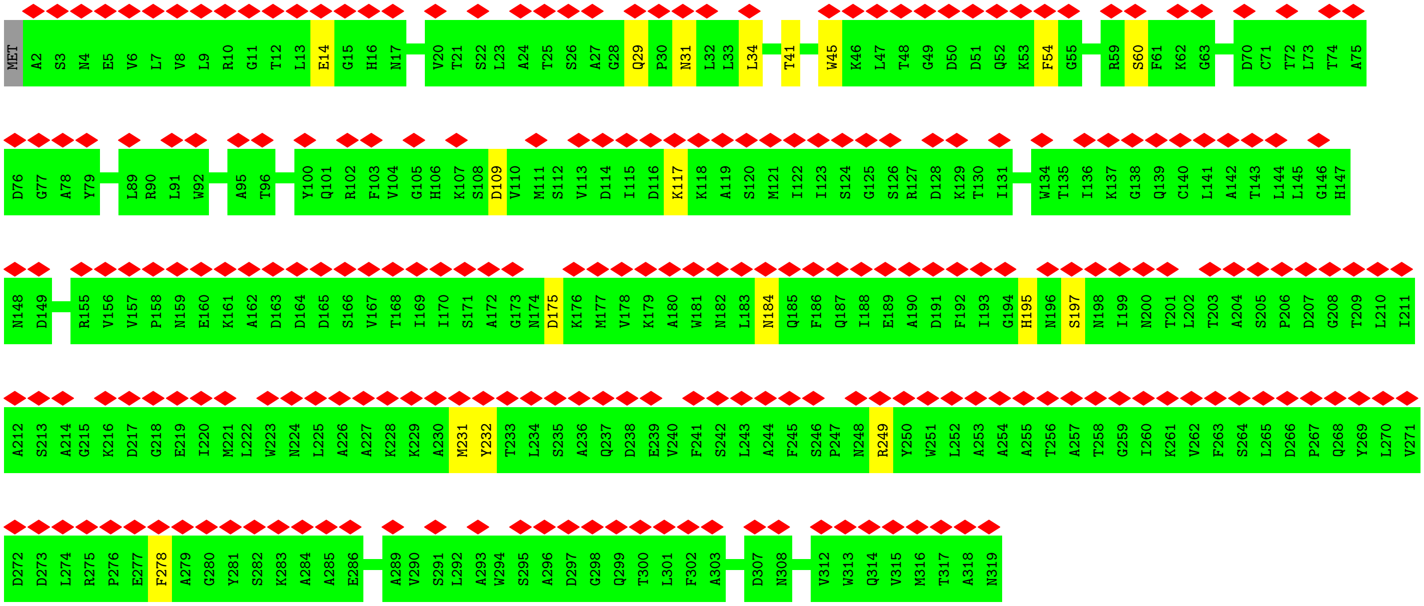
Chain 6:



- Molecule 8: Guanine nucleotide-binding protein subunit beta-like protein

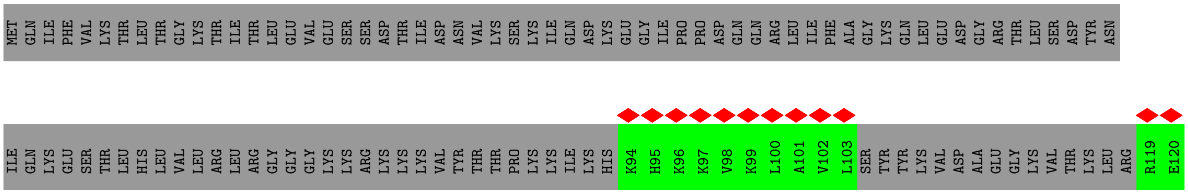
Chain 7:

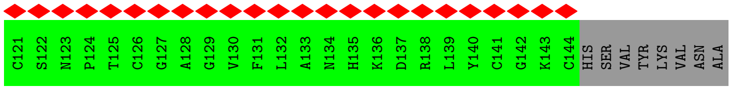




- Molecule 9: Ubiquitin-40S ribosomal protein S31

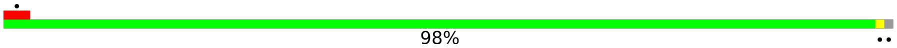
Chain 8:

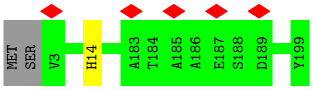




- Molecule 10: 60S ribosomal protein L16-A

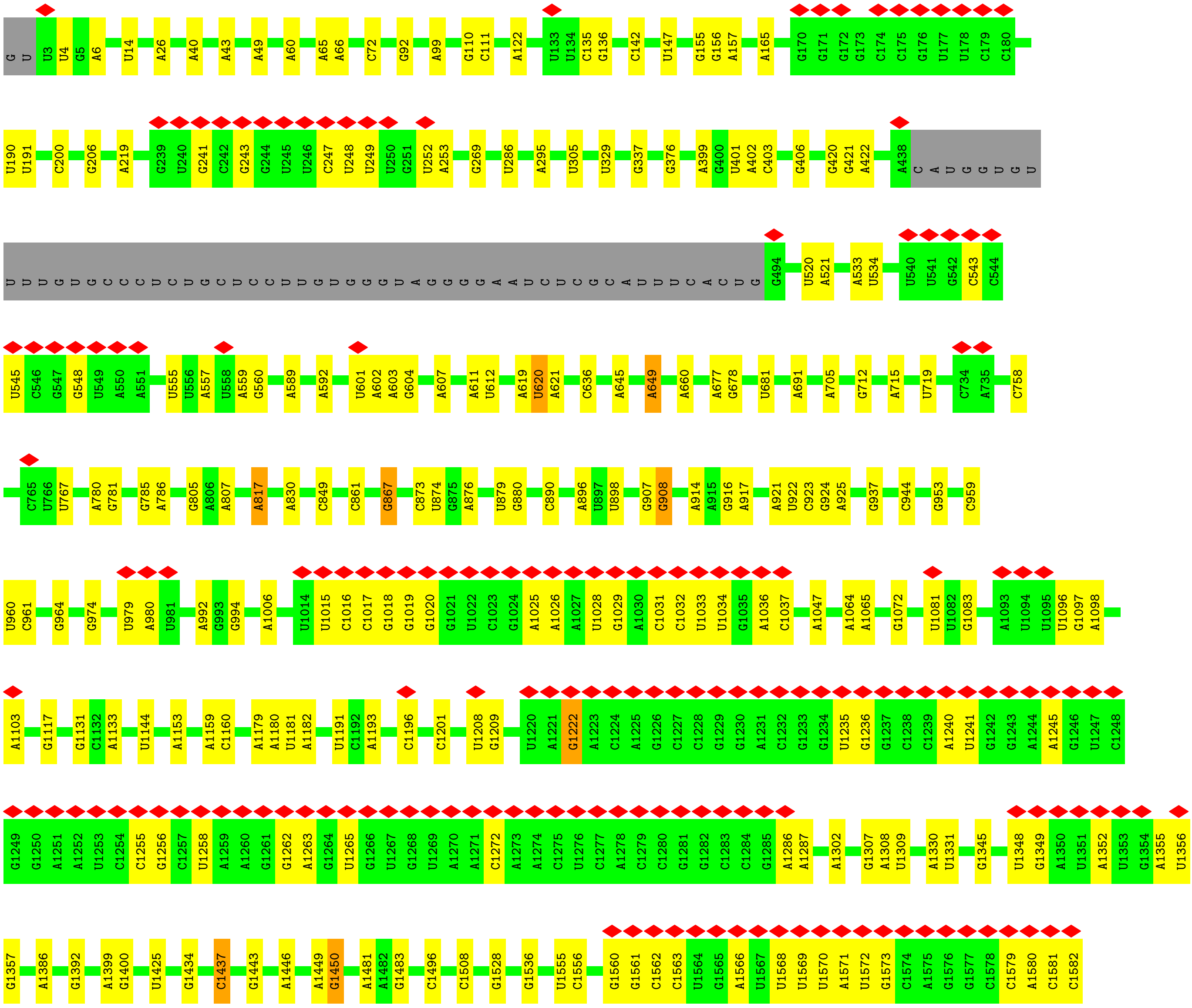
Chain A:

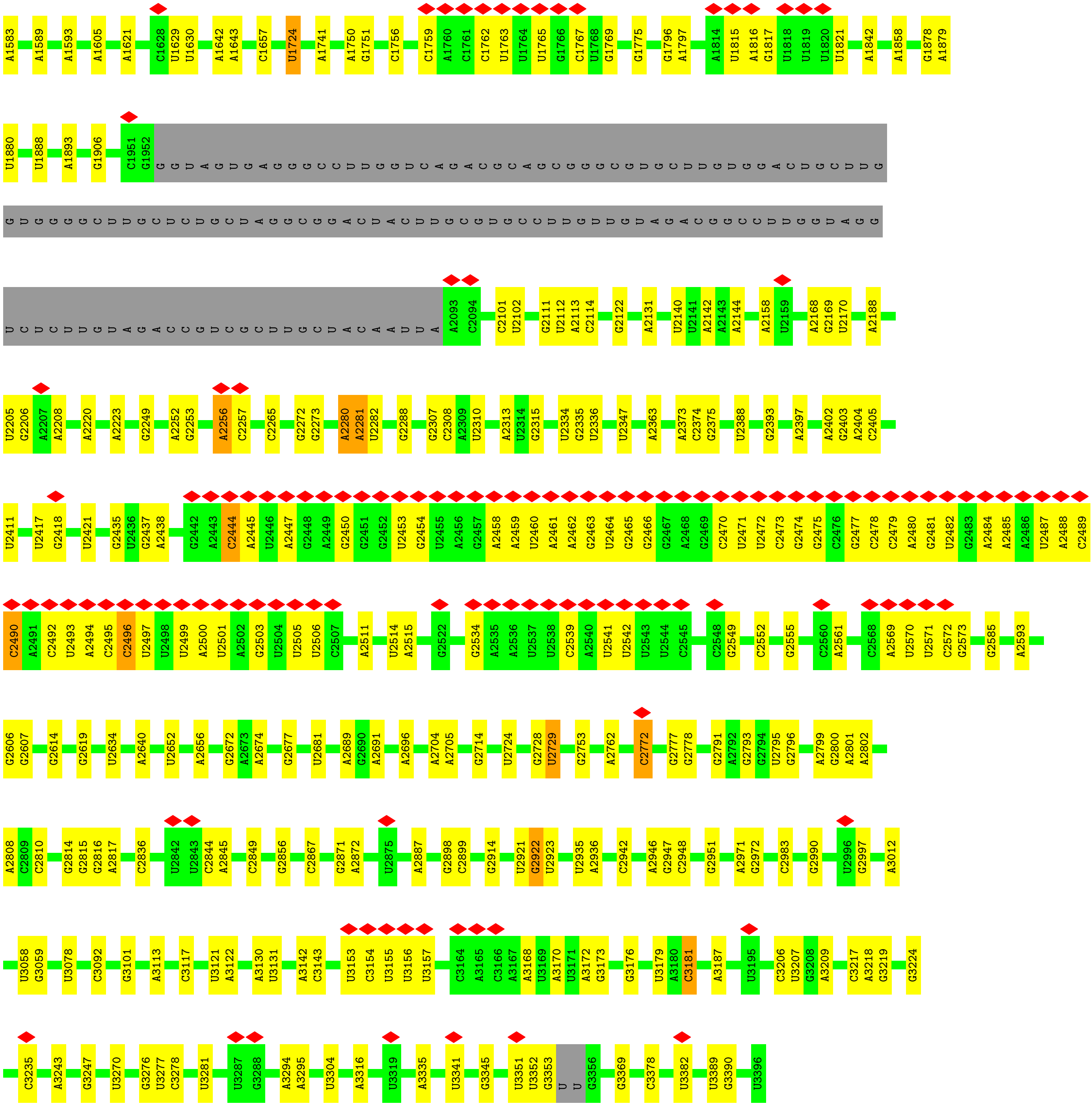




- Molecule 11: 25S ribosomal RNA

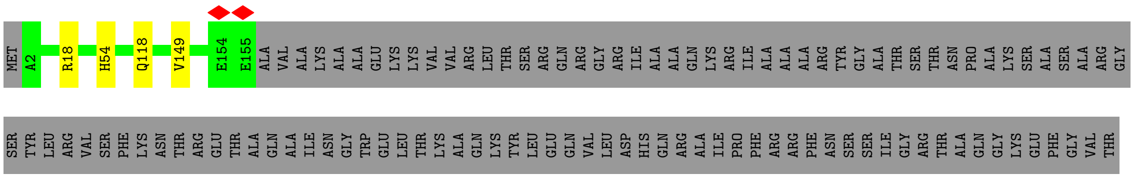
Chain AA:

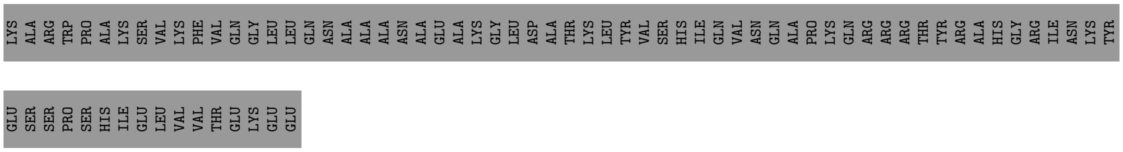




- Molecule 12: 60S ribosomal protein L17-A

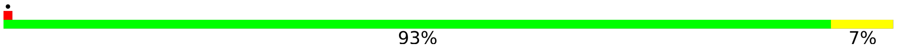
Chain B:

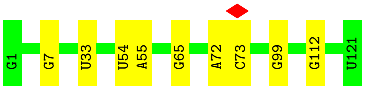




- Molecule 13: 5S ribosomal RNA

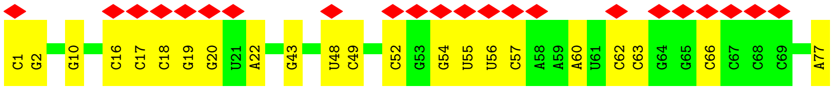
Chain BB:





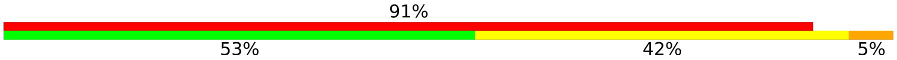
- Molecule 14: Transfer RNA fMet

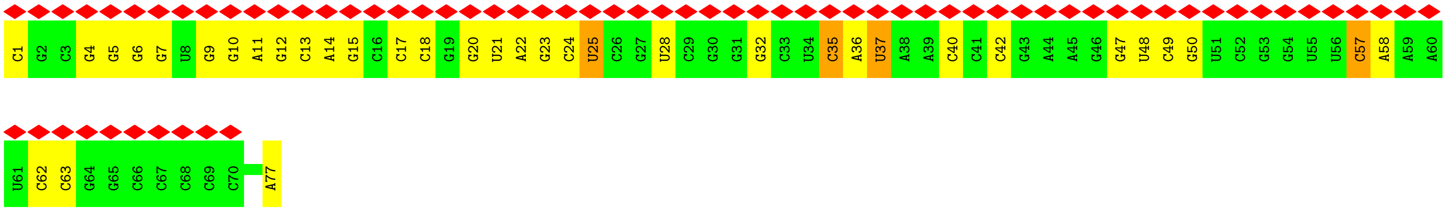
Chain Bb:



- Molecule 14: Transfer RNA fMet

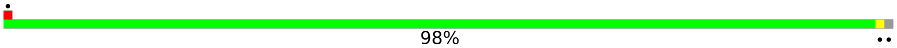
Chain Cc:

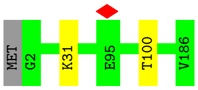




- Molecule 15: 60S ribosomal protein L18-A

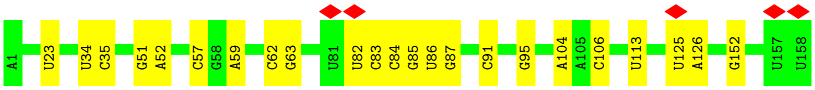
Chain C:





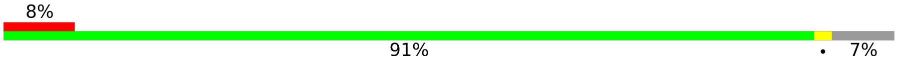
- Molecule 16: 5.8S ribosomal RNA

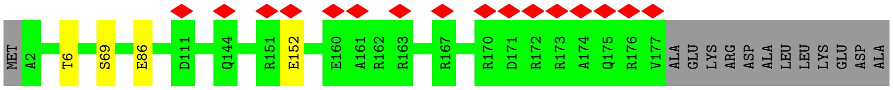
Chain CC:



- Molecule 17: 60S ribosomal protein L19-A

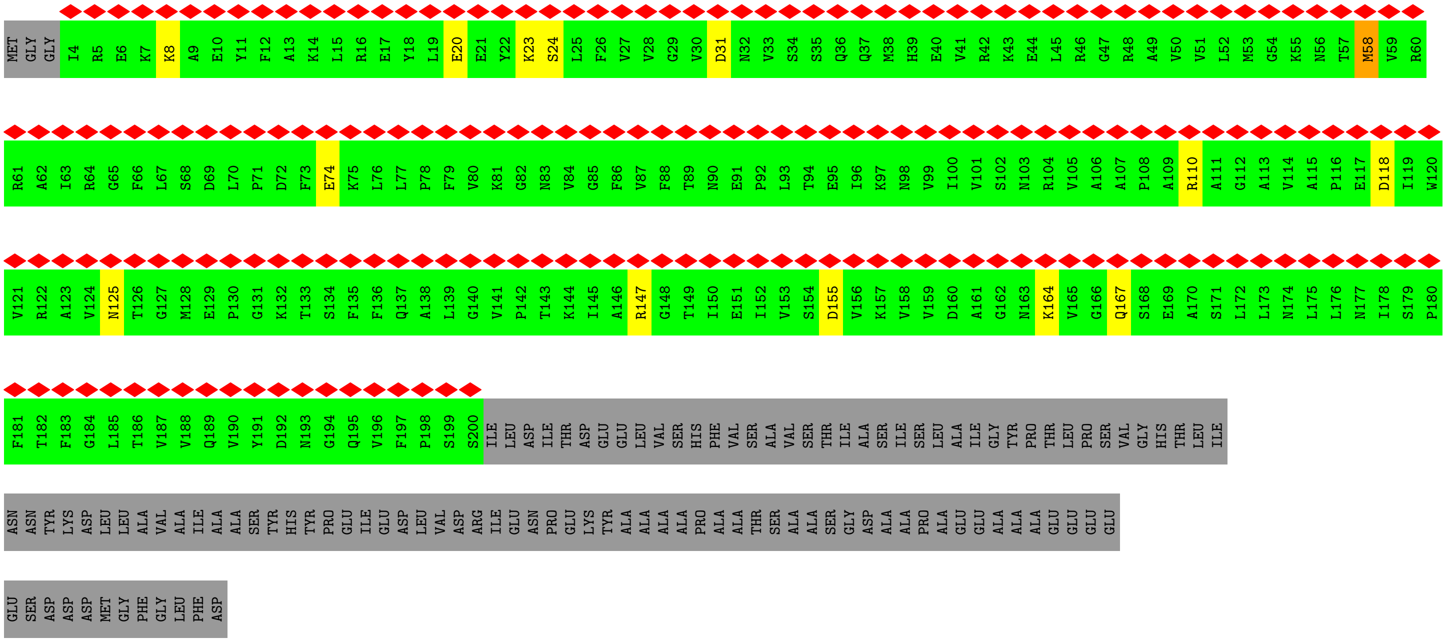
Chain D:





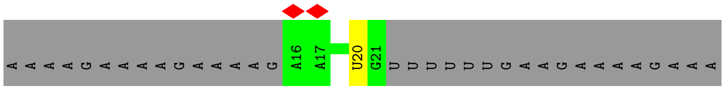
- Molecule 18: 60S acidic ribosomal protein P0

Chain DD:



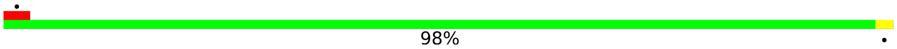
- Molecule 19: Messenger RNA

Chain Dd:



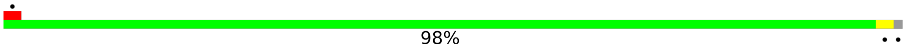
- Molecule 20: 60S ribosomal protein L20-A

Chain E:



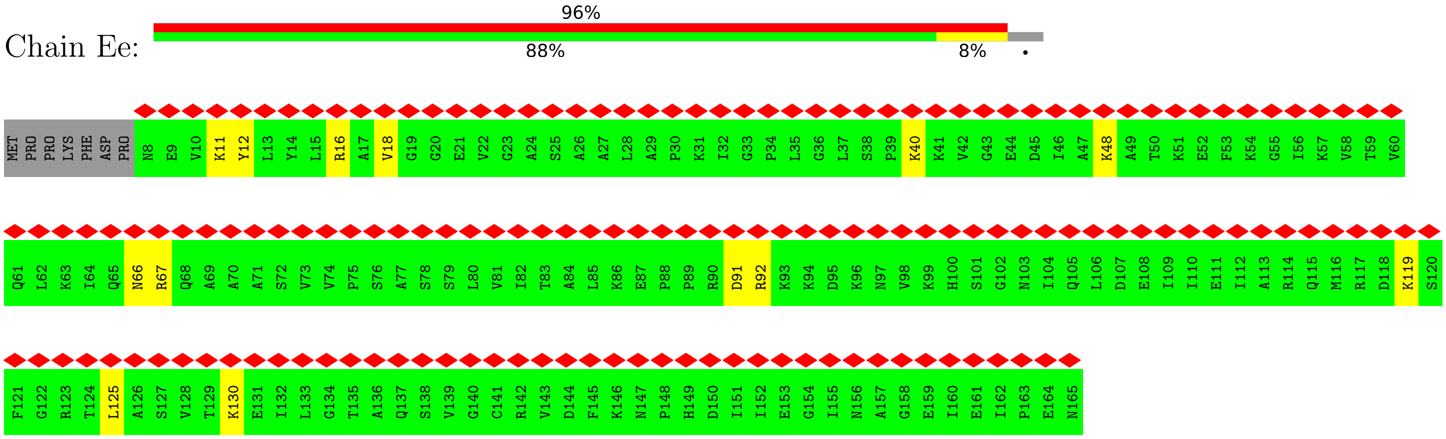
- Molecule 21: 60S ribosomal protein L2-A

Chain EE:



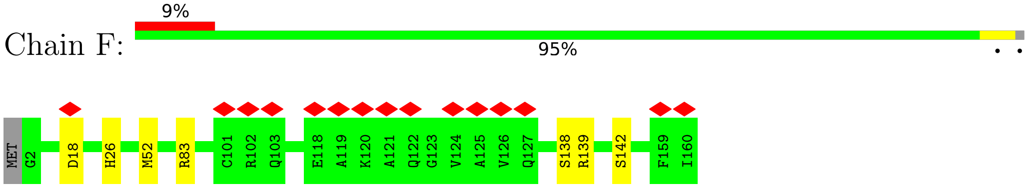
- Molecule 22: 60S ribosomal protein L12-A

Chain Ee:



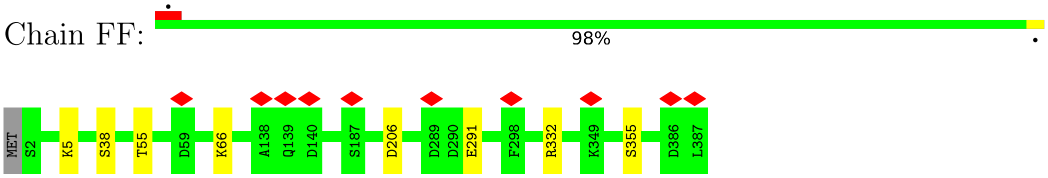
- Molecule 23: 60S ribosomal protein L21-A

Chain F:



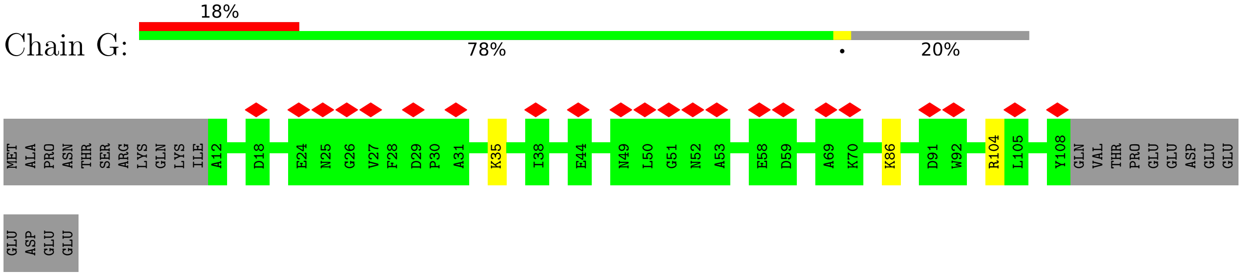
- Molecule 24: 60S ribosomal protein L3

Chain FF:



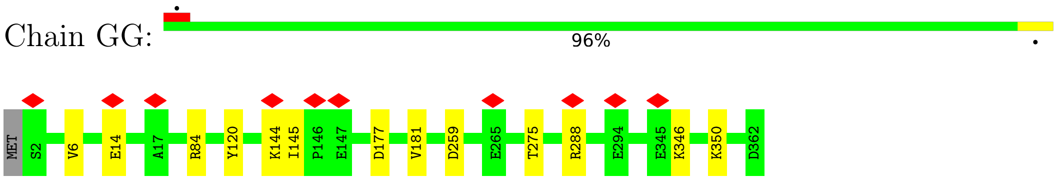
- Molecule 25: 60S ribosomal protein L22-A

Chain G:



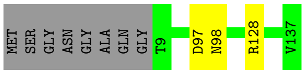
- Molecule 26: 60S ribosomal protein L4-A

Chain GG:



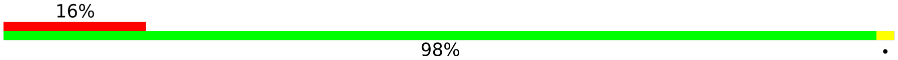
- Molecule 27: 60S ribosomal protein L23-A

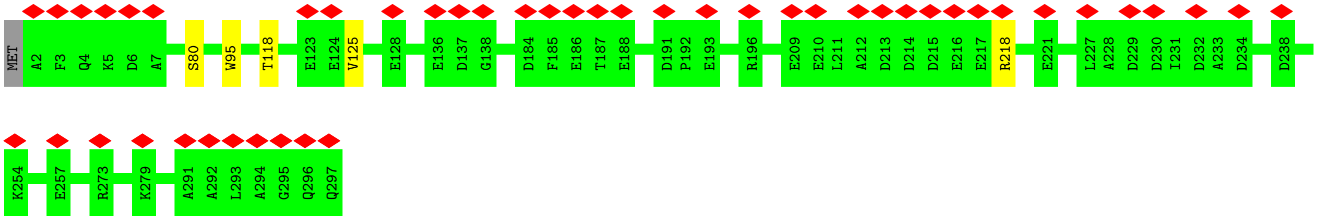
Chain H:



- Molecule 28: 60S ribosomal protein L5

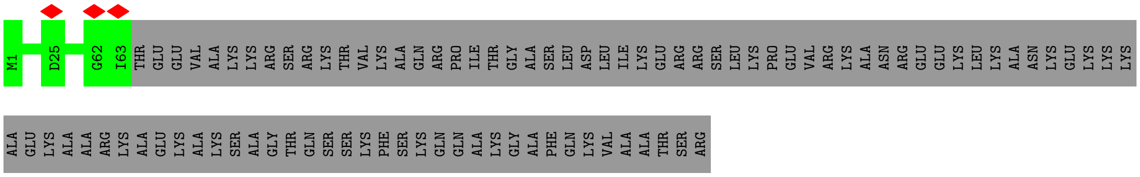
Chain HH:





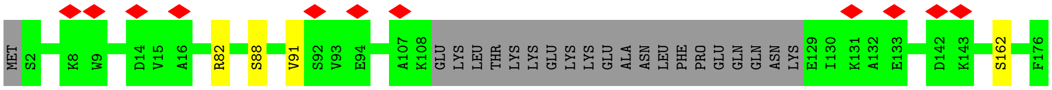
- Molecule 29: 60S ribosomal protein L24-A

Chain I:



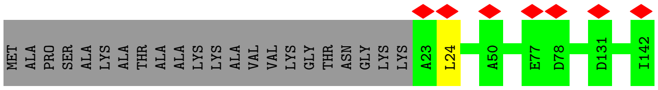
- Molecule 30: 60S ribosomal protein L6-A

Chain II:



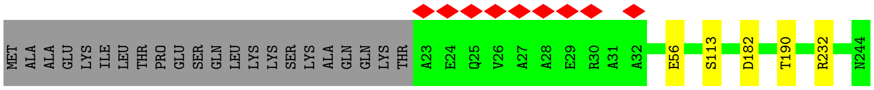
- Molecule 31: 60S ribosomal protein L25

Chain J:



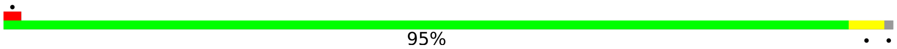
- Molecule 32: 60S ribosomal protein L7-A

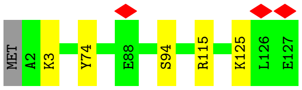
Chain JJ:



- Molecule 33: 60S ribosomal protein L26-A

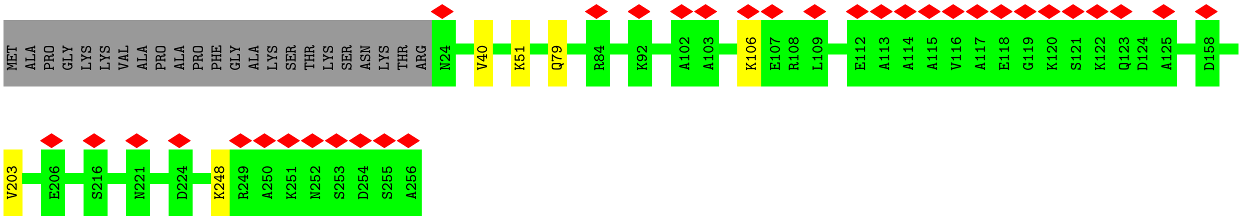
Chain K:





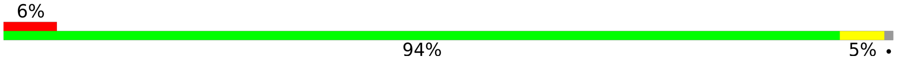
- Molecule 34: 60S ribosomal protein L8-A

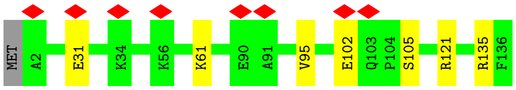
Chain KK:



- Molecule 35: 60S ribosomal protein L27-A

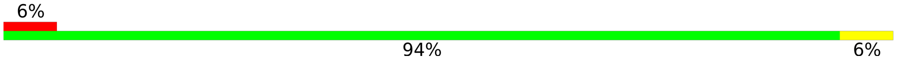
Chain L:

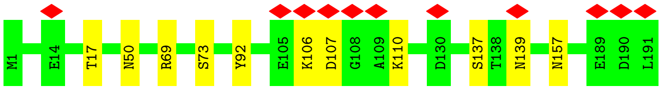




- Molecule 36: RPL9A isoform 1

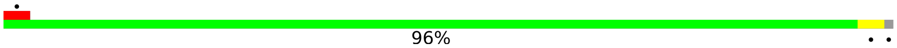
Chain LL:

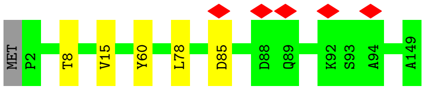




- Molecule 37: 60S ribosomal protein L28

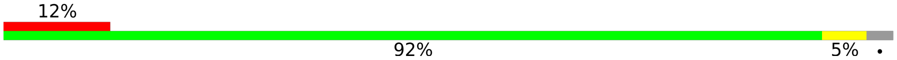
Chain M:

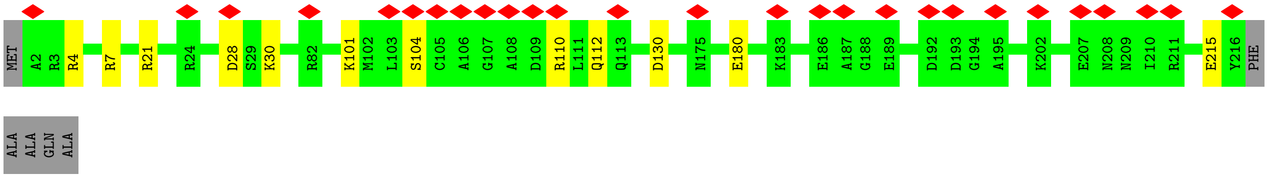




- Molecule 38: 60S ribosomal protein L10

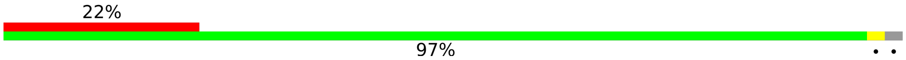
Chain MM:

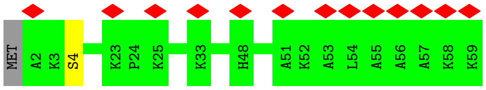




- Molecule 39: 60S ribosomal protein L29

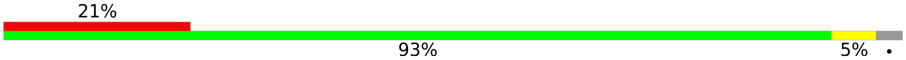
Chain N:

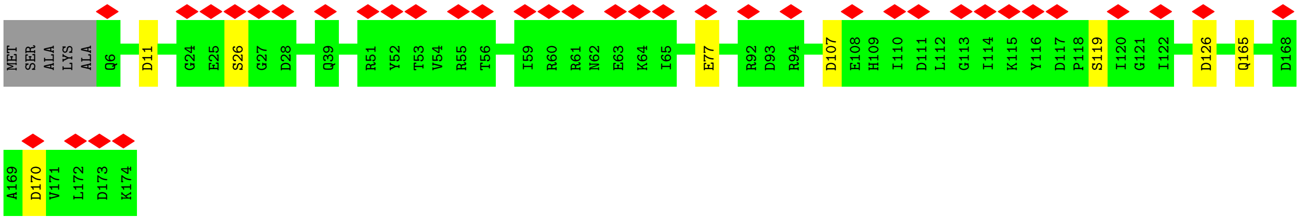




- Molecule 40: 60S ribosomal protein L11-A

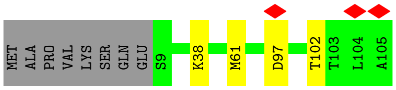
Chain NN:





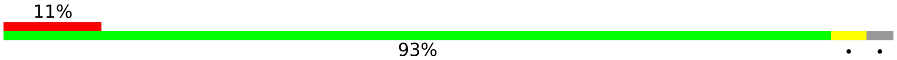
- Molecule 41: 60S ribosomal protein L30

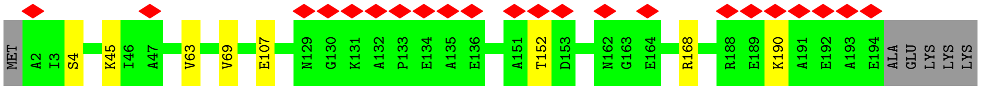
Chain O:



- Molecule 42: 60S ribosomal protein L13-A

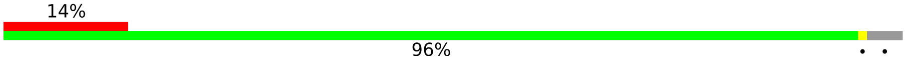
Chain OO:

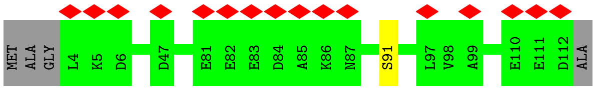




- Molecule 43: 60S ribosomal protein L31-A

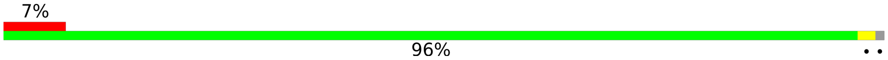
Chain P:

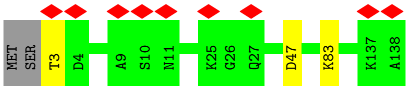




- Molecule 44: 60S ribosomal protein L14-A

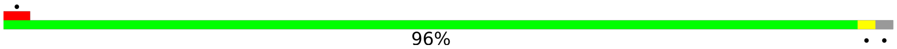
Chain PP:

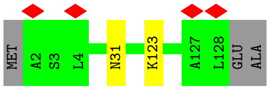




- Molecule 45: 60S ribosomal protein L32

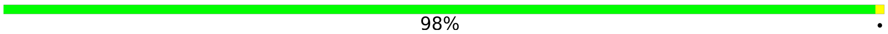
Chain Q:

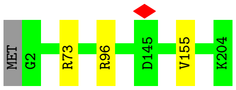




- Molecule 46: 60S ribosomal protein L15-A

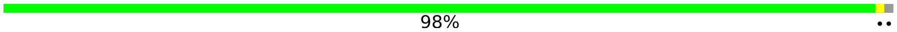
Chain QQ:

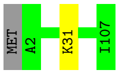




- Molecule 47: 60S ribosomal protein L33-A

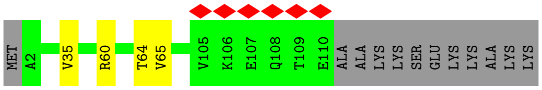
Chain R:





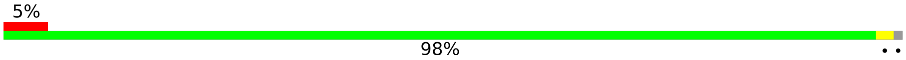
- Molecule 48: 60S ribosomal protein L34-A

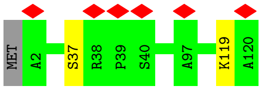
Chain S:



- Molecule 49: 60S ribosomal protein L35-A

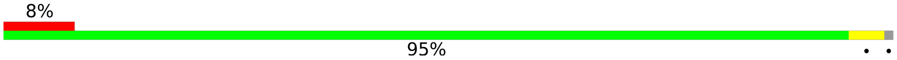
Chain T:

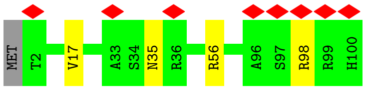




- Molecule 50: 60S ribosomal protein L36-A

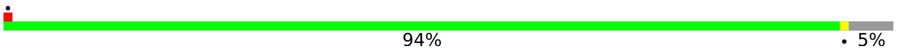
Chain U:

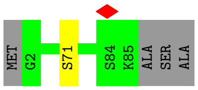




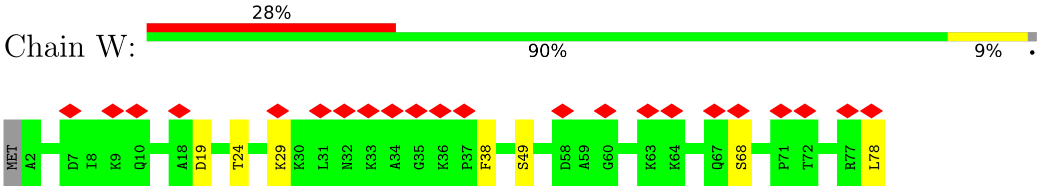
- Molecule 51: 60S ribosomal protein L37-A

Chain V:

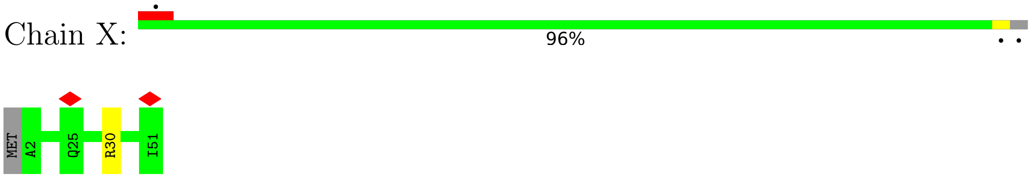




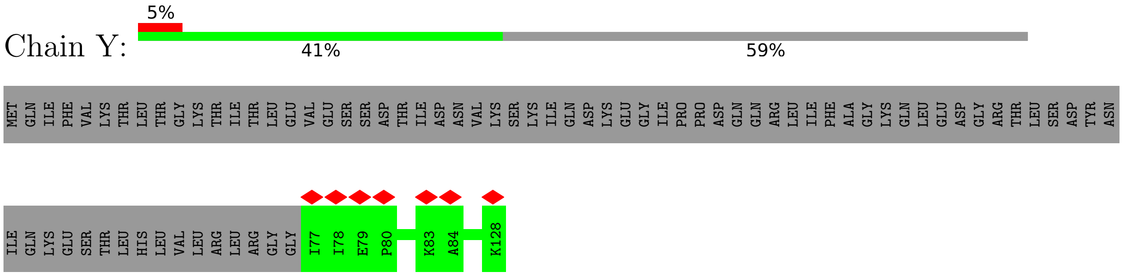
- Molecule 52: 60S ribosomal protein L38



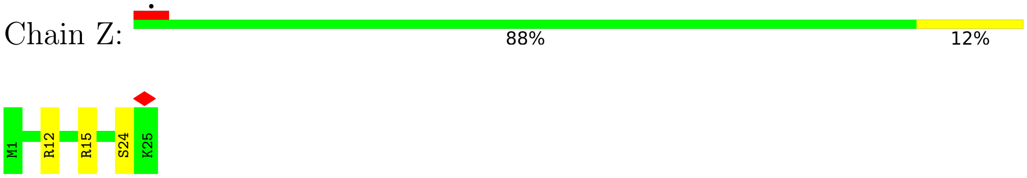
- Molecule 53: 60S ribosomal protein L39



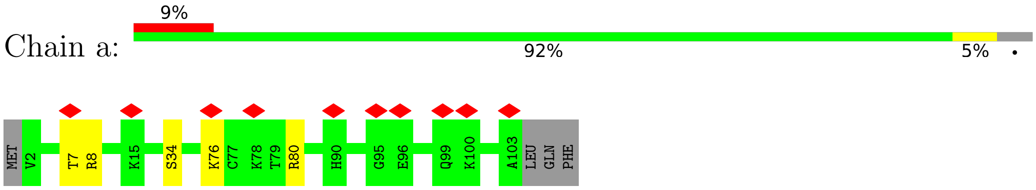
- Molecule 54: Ubiquitin-60S ribosomal protein L40



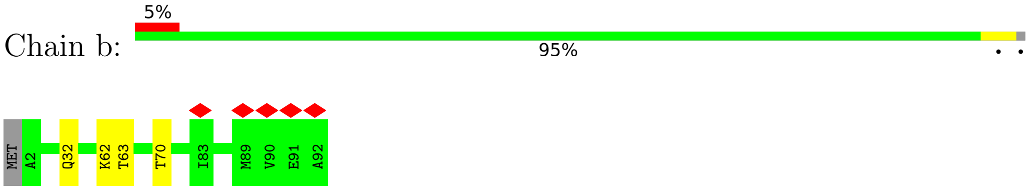
- Molecule 55: 60S ribosomal protein L41



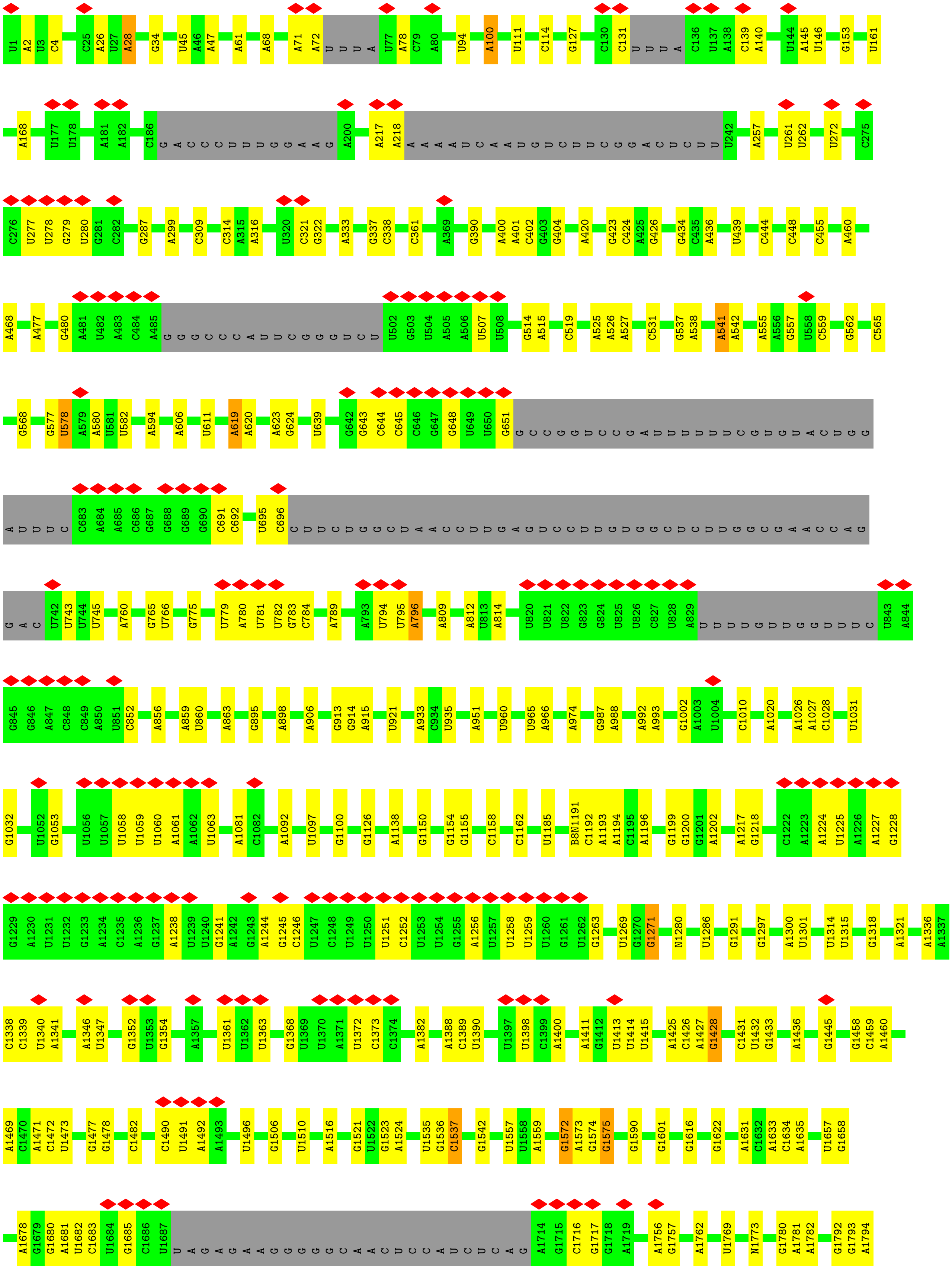
- Molecule 56: 60S ribosomal protein L42-A

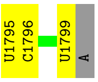


- Molecule 57: 60S ribosomal protein L43-A

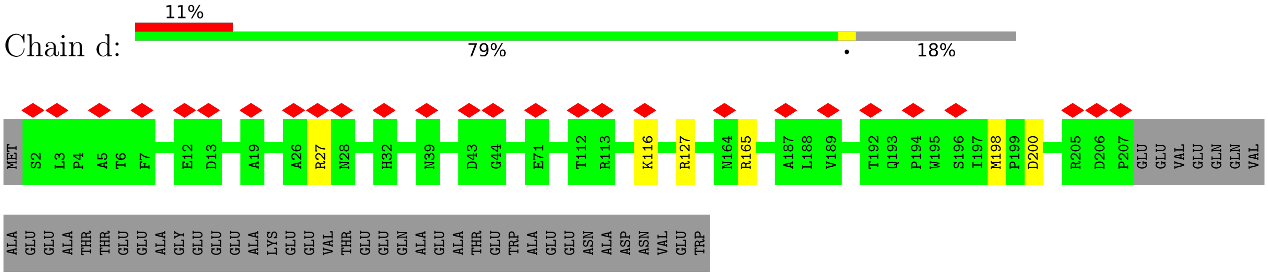


- Molecule 58: 18S ribosomal RNA

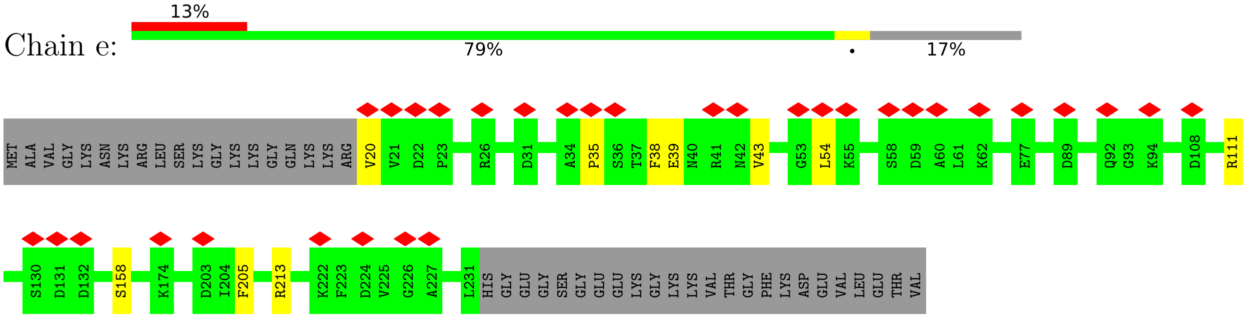

U1 A2 U3 C4 C25 A26 U27 A28 G34 U45 A46 A47 A61 A68 A71 A72 U U U A U77 A78 C79 A80 U94 A100 U111 C114 G127 C130 C131 U U U A C136 U137 A138 C139 A140 U144 A145 U146 G153 U161
A168 U177 U178 A181 A182 C186 G A C C C U U U G G A A G A200 A217 A218 A A A A U C A A U G U C U U C G G A C U C U U U242 A257 U261 U262 U272 C275
C276 U277 U278 G279 U280 G281 C282 G287 A299 C309 C314 A315 A316 U320 C321 G322 A333 G337 C338 C361 A369 G390 A400 A401 C402 G403 G404 A420 G423 C424 A425 G426 G434 C435 A436 U439 C444 C448 C455 A460
A468 A477 G480 A481 U482 A483 C484 A485 G G G C C C A U U C G G G U C U U502 G503 U504 A505 A506 U507 U508 G514 A515 C519 A525 A526 A527 C531 G537 A538 A541 A542 A555 A556 G557 U558 C559 G562 C565
G568 G577 U578 A579 A580 U581 U582 A594 A606 U611 A619 A620 A623 G624 U639 G642 G643 C644 C645 C646 G647 G648 U649 U650 G651 G C C G G U C C G A U U U U U C G U G U A C U G G
A U U U C C683 A684 A685 C686 G687 G688 G689 G690 C691 C692 U695 C696 C U U C U G G C U A A C C U U G A G U C C C U U G U G G C U C U U G G C G A A C C A G
G A C U742 U743 U744 U745 A760 G765 U766 G775 U779 A780 U781 U782 G783 C784 A789 A793 U794 U795 A796 A809 A812 U813 A814 U820 U821 U822 G823 G824 U825 U826 C827 U828 A829 U U U G U U G G U U U C U843 A844
G845 G846 A847 C848 C849 A850 U851 C852 A856 A859 U860 A863 G895 A898 A906 G913 G914 A915 U921 A933 C934 U935 A951 U960 U965 A966 A974 G987 A988 A992 A993 G1002 A1003 U1004 C1010 A1020 A1026 A1027 C1028 U1031
G1032 U1052 G1053 U1056 U1057 U1058 U1059 U1060 A1061 A1062 U1063 A1081 C1082 A1092 U1097 G1100 G1126 A1138 G1150 G1154 G1155 C1158 C1162 U1185 B8N1191 C1192 A1193 A1194 C1195 A1196 G1199 G1200 G1201 A1202 A1217 G1218 C1222 A1223 A1224 U1225 A1226 A1227 G1228
G1229 A1230 U1231 U1232 G1233 A1234 C1235 A1236 G1237 A1238 U1239 U1240 G1241 A1242 G1243 A1244 G1245 C1246 U1247 C1248 U1249 U1250 U1251 C1252 U1253 U1254 G1255 A1256 U1257 U1258 U1259 U1260 G1261 U1262 G1263 U1269 G1270 G1271 N1280 U1286 G1291 G1297 A1300 U1301 U1314 U1315 G1318 A1321 A1336 A1337
C1338 C1339 U1340 A1341 A1346 U1347 G1352 U1353 G1354 A1357 U1361 U1362 U1363 G1368 U1369 U1370 A1371 U1372 C1373 C1374 A1382 A1388 C1389 U1390 U1397 U1398 C1399 A1400 A1411 G1412 U1413 U1414 U1415 A1425 C1426 A1427 G1428 C1431 U1432 G1433 A1436 G1445 G1458 C1459 A1460
A1469 C1470 A1471 C1472 U1473 G1477 G1478 C1482 C1490 U1491 A1492 A1493 U1496 G1506 U1510 A1516 G1521 U1522 G1523 A1524 U1535 G1536 C1537 G1542 U1557 U1558 A1559 G1572 A1573 G1574 G1575 G1590 G1601 G1616 G1622 A1631 C1632 C1634 A1635 U1657 G1658
A1678 G1679 G1680 A1681 U1682 C1683 U1684 G1685 C1686 U1687 U A G A G A A G G G G G C A A C U C C A U C U C A G A1714 G1715 C1716 G1717 G1718 A1719 A1756 G1757 A1762 U1769 N1773 G1780 A1781 A1782 G1792 G1793 A1794



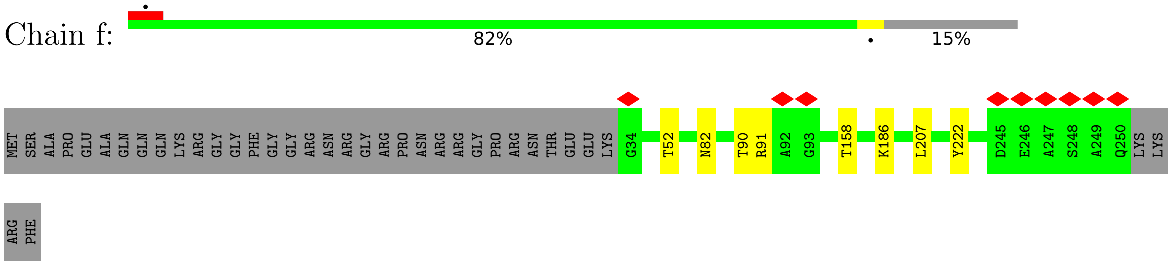
- Molecule 59: 40S ribosomal protein S0-A



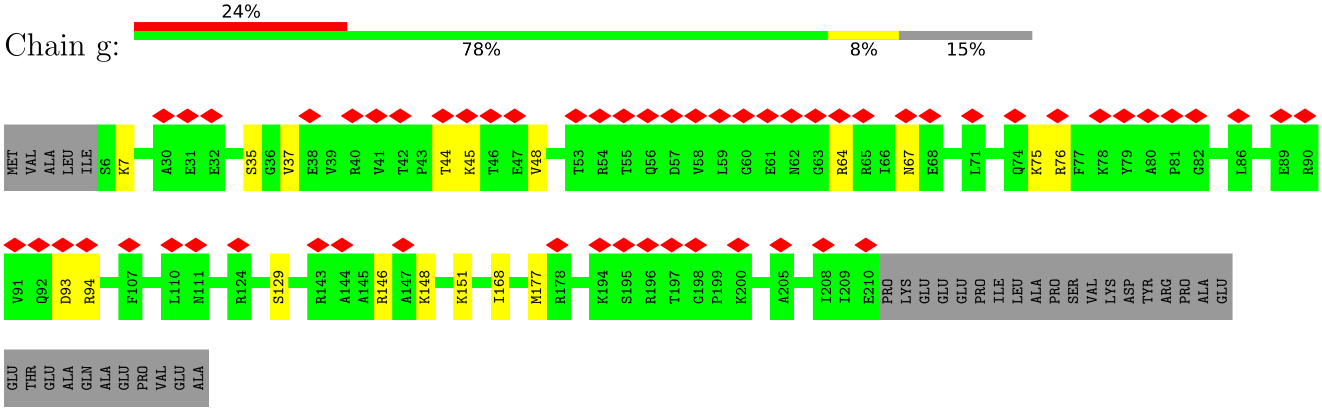
- Molecule 60: 40S ribosomal protein S1-A



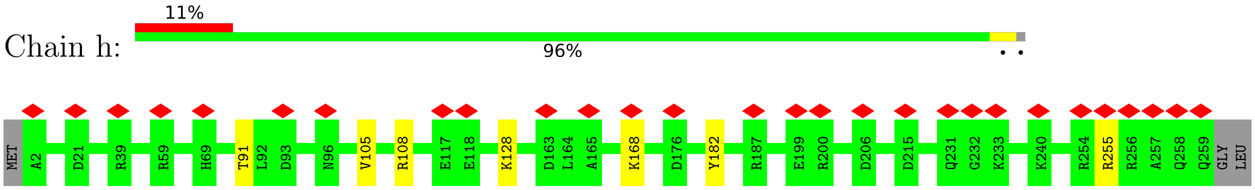
- Molecule 61: 40S ribosomal protein S2



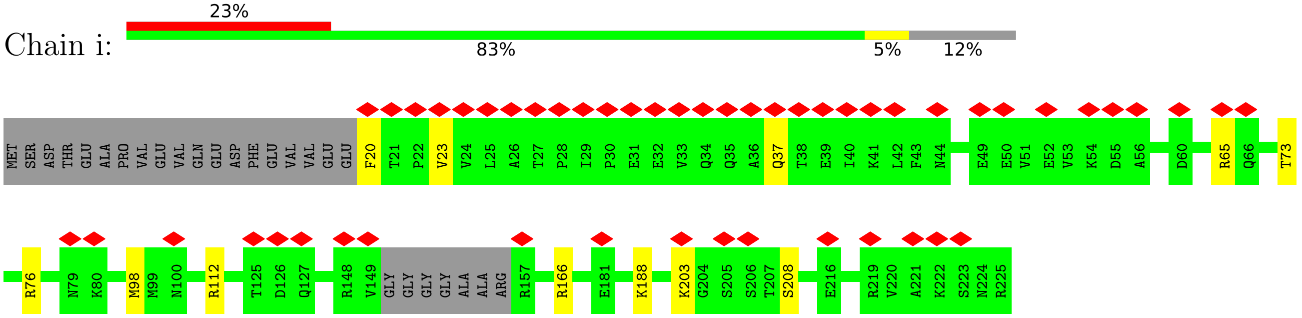
- Molecule 62: RPS3 isoform 1



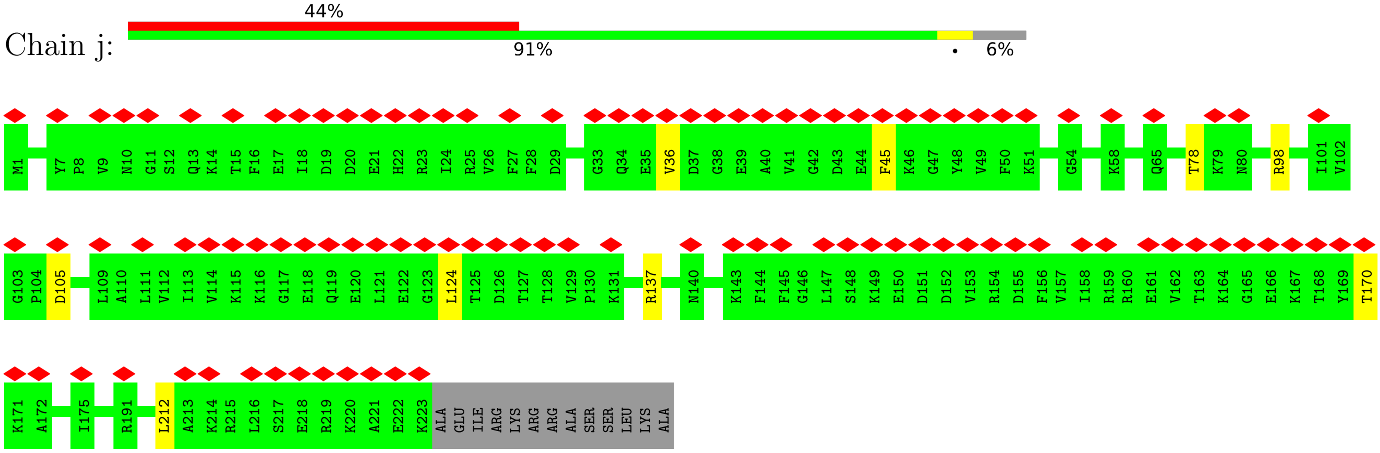
- Molecule 63: 40S ribosomal protein S4-A



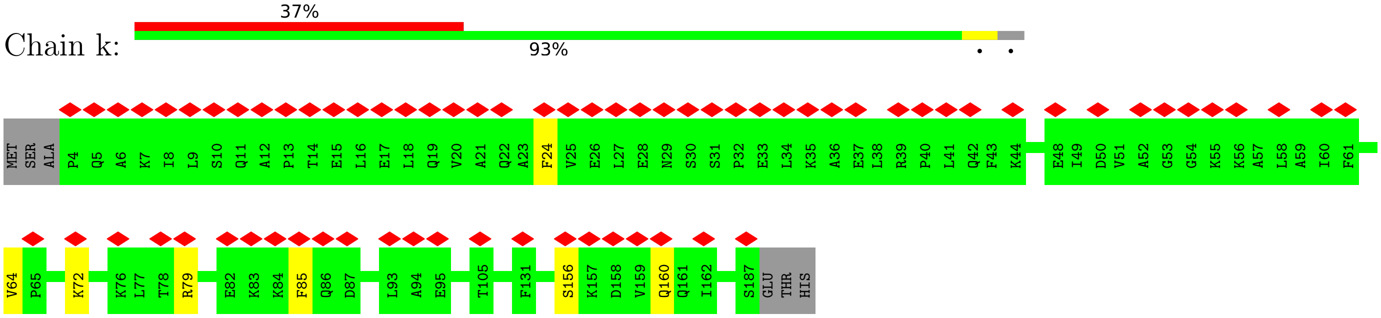
- Molecule 64: 40S ribosomal protein S5



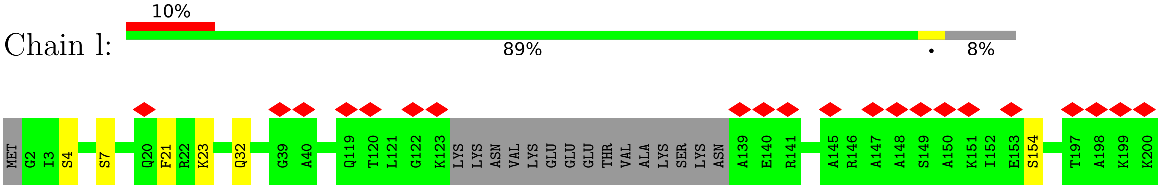
- Molecule 65: 40S ribosomal protein S6-A



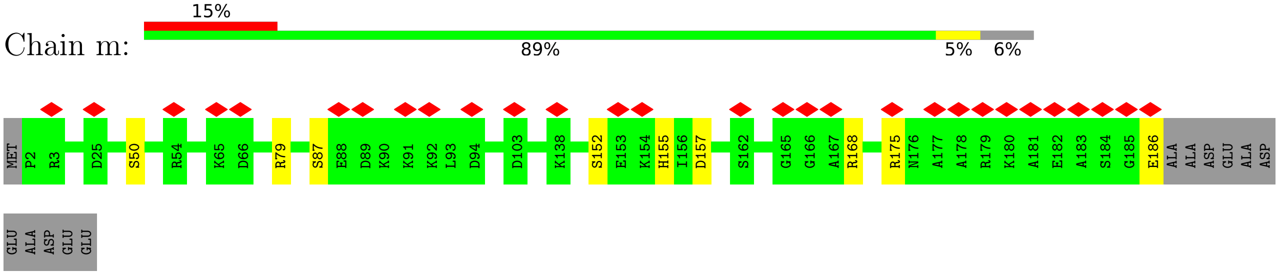
- Molecule 66: 40S ribosomal protein S7-A



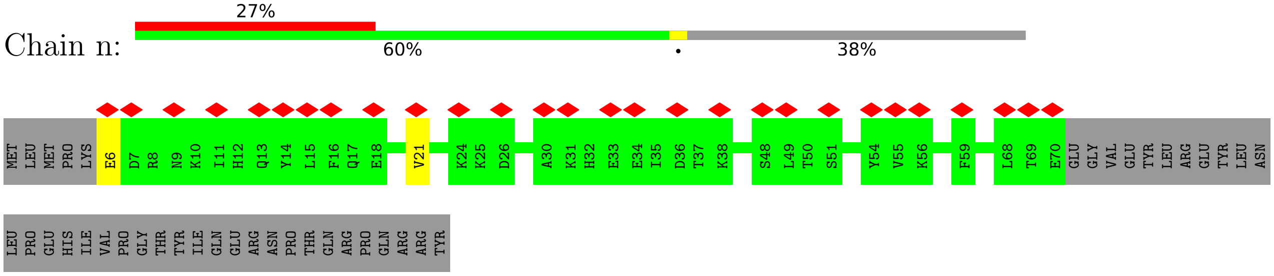
- Molecule 67: 40S ribosomal protein S8-B



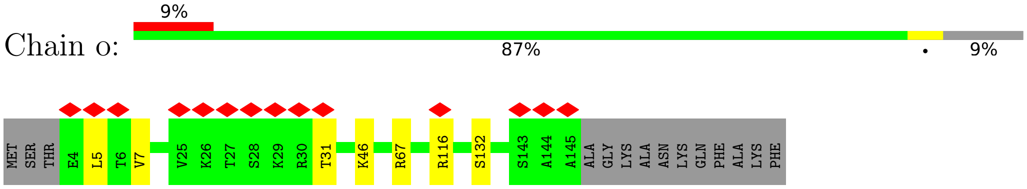
- Molecule 68: 40S ribosomal protein S9-A



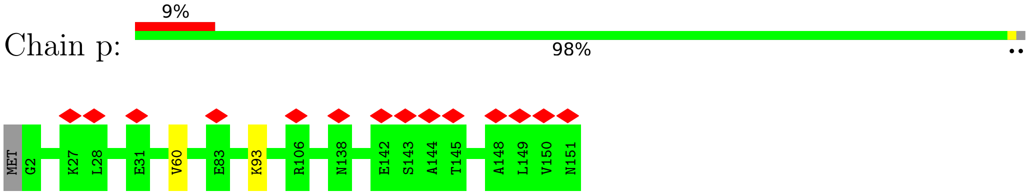
- Molecule 69: 40S ribosomal protein S10-A



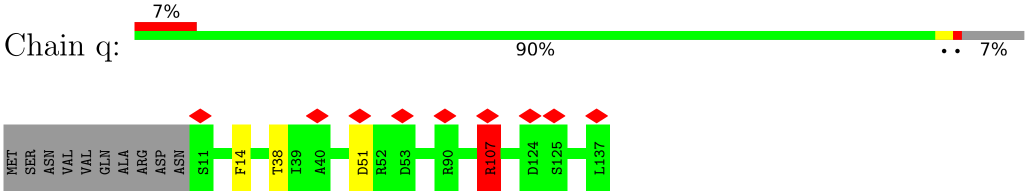
- Molecule 70: 40S ribosomal protein S11-A



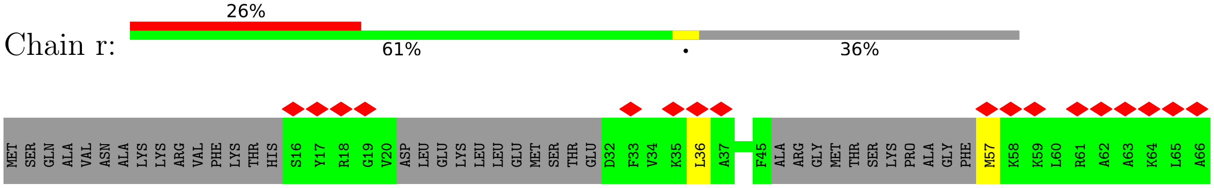
- Molecule 71: 40S ribosomal protein S13

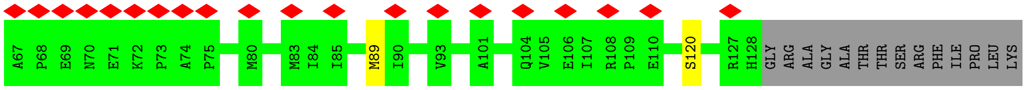


- Molecule 72: 40S ribosomal protein S14-A



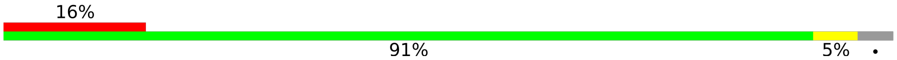
- Molecule 73: 40S ribosomal protein S15

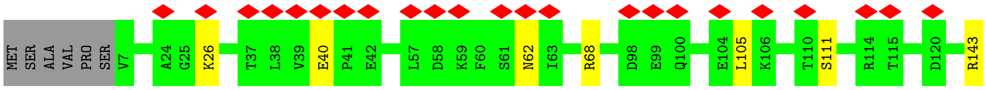




- Molecule 74: 40S ribosomal protein S16-A

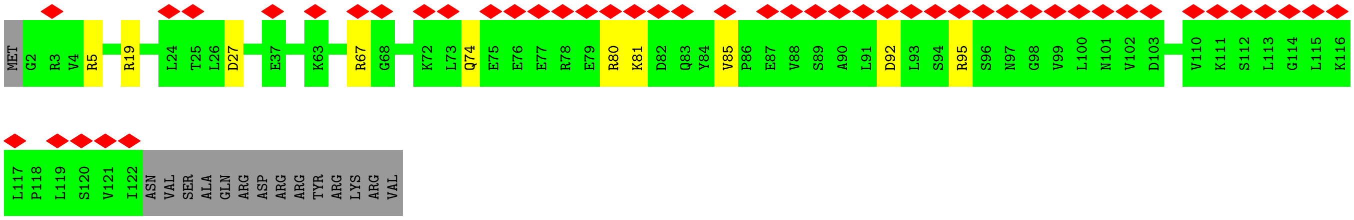
Chain s:





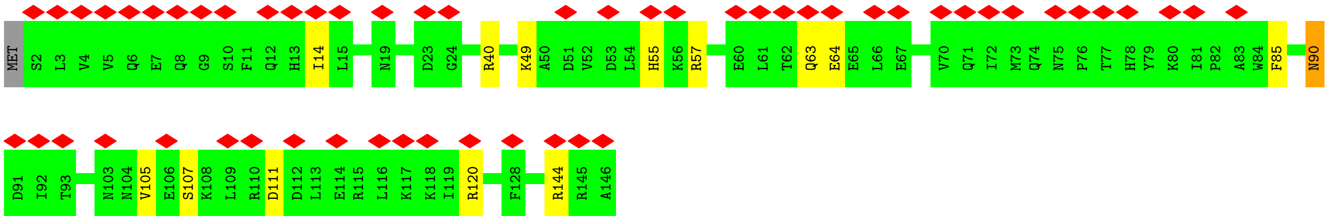
- Molecule 75: 40S ribosomal protein S17-A

Chain t:



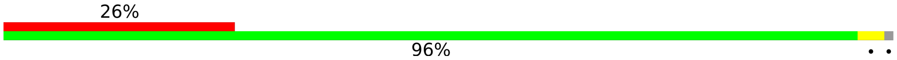
- Molecule 76: 40S ribosomal protein S18-A

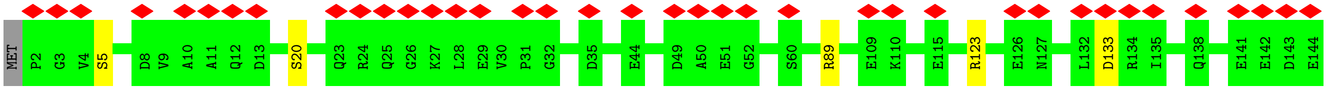
Chain u:



- Molecule 77: 40S ribosomal protein S19-A

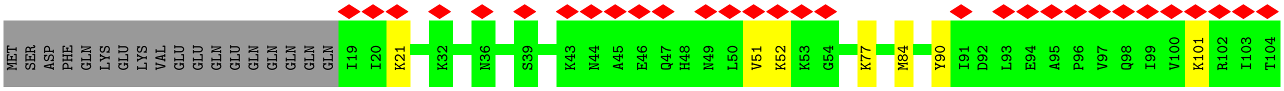
Chain v:

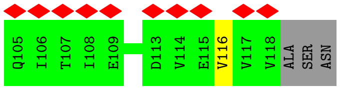




- Molecule 78: 40S ribosomal protein S20

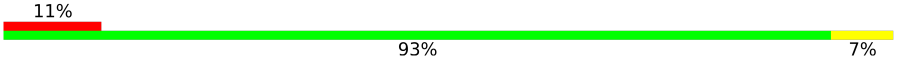
Chain w:

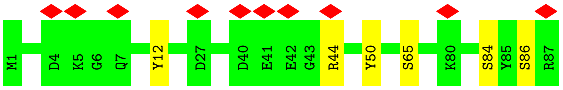




- Molecule 79: 40S ribosomal protein S21-A

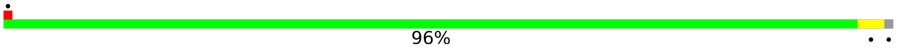
Chain x:

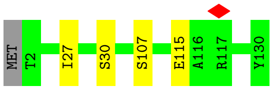




- Molecule 80: 40S ribosomal protein S22-A

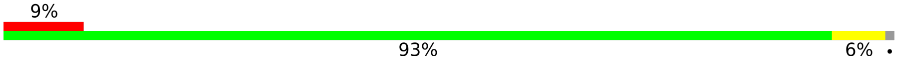
Chain y:

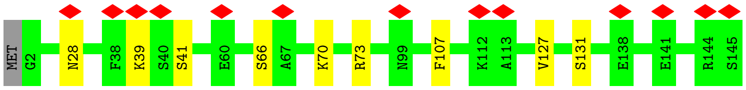




- Molecule 81: 40S ribosomal protein S23-A

Chain z:





4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21458	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	270000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.688	Depositor
Minimum map value	-0.693	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.249	Depositor
Map size (Å)	540.0, 540.0, 540.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9, 0.9, 0.9	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, K, UR3, ZN, OMG, 1MA, OMU, MA6, B8N, A2M, 5MC, G7M, MG, OMC, 4AC

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	0	0.26	0/1087	0.54	0/1449
2	1	0.29	0/571	0.64	1/768 (0.1%)
3	2	0.24	0/782	0.56	0/1047
4	3	0.24	0/620	0.54	0/838
5	4	0.26	0/499	0.65	0/670
6	5	0.25	0/412	0.57	0/544
7	6	0.25	0/433	0.62	0/575
8	7	0.26	0/2489	0.58	1/3389 (0.0%)
9	8	0.23	0/279	0.51	0/369
10	A	0.26	0/1585	0.51	0/2128
11	AA	0.23	0/75545	0.80	24/117782 (0.0%)
12	B	0.25	0/1245	0.52	0/1676
13	BB	0.20	0/2883	0.76	0/4491
14	Bb	0.32	1/1836 (0.1%)	0.78	0/2859
14	Cc	0.52	5/1836 (0.3%)	0.86	1/2859 (0.0%)
15	C	0.25	0/1465	0.54	0/1965
16	CC	0.22	0/3746	0.78	0/5832
17	D	0.24	0/1440	0.55	0/1921
18	DD	0.27	0/1558	0.59	1/2107 (0.0%)
19	Dd	0.29	0/147	0.84	0/227
20	E	0.26	0/1481	0.55	0/1990
21	EE	0.25	0/1948	0.56	0/2617
22	Ee	0.28	0/1210	0.57	1/1627 (0.1%)
23	F	0.26	0/1300	0.52	0/1743
24	FF	0.25	0/3146	0.54	0/4228
25	G	0.26	0/786	0.50	0/1065
26	GG	0.24	0/2800	0.51	0/3790
27	H	0.26	0/978	0.53	0/1316
28	HH	0.25	0/2425	0.50	0/3271
29	I	0.26	0/533	0.52	0/707
30	II	0.26	0/1251	0.50	0/1682
31	J	0.25	0/974	0.50	0/1314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	JJ	0.26	0/1821	0.49	0/2451
33	K	0.25	0/1004	0.53	0/1341
34	KK	0.25	0/1836	0.48	0/2481
35	L	0.26	0/1118	0.49	0/1497
36	LL	0.26	0/1539	0.52	0/2073
37	M	0.25	0/1204	0.53	0/1612
38	MM	0.25	0/1779	0.53	0/2386
39	N	0.25	0/473	0.48	0/629
40	NN	0.25	0/1374	0.57	0/1842
41	O	0.25	0/750	0.45	0/1008
42	OO	0.26	0/1568	0.57	0/2106
43	P	0.24	0/897	0.54	0/1205
44	PP	0.24	0/1068	0.49	0/1438
45	Q	0.24	0/1041	0.51	0/1394
46	QQ	0.25	0/1757	0.58	0/2354
47	R	0.27	0/868	0.54	0/1168
48	S	0.24	0/871	0.55	0/1164
49	T	0.24	0/978	0.51	0/1301
50	U	0.24	0/778	0.55	0/1034
51	V	0.26	0/680	0.59	0/901
52	W	0.26	0/618	0.57	0/826
53	X	0.24	0/443	0.62	0/588
54	Y	0.24	0/423	0.53	0/562
55	Z	0.24	0/234	0.71	0/300
56	a	0.26	0/831	0.56	0/1097
57	b	0.25	0/701	0.58	0/934
58	c	0.22	0/38143	0.81	18/59408 (0.0%)
59	d	0.25	0/1623	0.52	0/2222
60	e	0.25	0/1714	0.54	0/2308
61	f	0.25	0/1665	0.52	0/2263
62	g	0.27	0/1614	0.58	0/2169
63	h	0.25	0/2097	0.53	0/2823
64	i	0.24	0/1591	0.54	0/2151
65	j	0.25	0/1822	0.56	0/2434
66	k	0.25	0/1506	0.55	0/2028
67	l	0.28	0/1482	0.56	0/1980
68	m	0.25	0/1519	0.54	0/2035
69	n	0.26	0/569	0.54	0/767
70	o	0.25	0/1172	0.54	0/1580
71	p	0.25	0/1215	0.52	0/1638
72	q	0.26	0/901	0.64	1/1217 (0.1%)
73	r	0.27	0/747	0.59	0/1002
74	s	0.29	0/1099	0.61	1/1473 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	t	0.24	0/971	0.58	0/1303
76	u	0.25	0/1211	0.61	0/1628
77	v	0.26	0/1130	0.52	0/1517
78	w	0.25	0/810	0.55	0/1095
79	x	0.25	0/693	0.58	0/935
80	y	0.26	0/1038	0.53	0/1395
81	z	0.25	0/1139	0.54	0/1518
All	All	0.24	6/213415 (0.0%)	0.72	49/313427 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1	0	1
18	DD	0	1
32	JJ	0	1
35	L	0	1
56	a	0	1
60	e	0	2
64	i	0	1
66	k	0	1
72	q	0	1
74	s	0	1
76	u	0	1
All	All	0	12

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Bb	1	C	OP3-P	-10.59	1.48	1.61
14	Cc	1	C	OP3-P	-10.42	1.48	1.61
14	Cc	37	U	C1'-N1	5.99	1.57	1.48
14	Cc	25	U	C1'-N1	5.78	1.57	1.48
14	Cc	24	C	C1'-N1	5.53	1.57	1.48
14	Cc	35	C	C1'-N1	5.43	1.56	1.48

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	c	94	U	C2-N3-C4	14.44	135.66	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	c	1537	C	C2-N1-C1’	8.46	128.11	118.80
58	c	1537	C	N1-C2-O2	8.12	123.77	118.90
11	AA	3278	C	N1-C2-O2	7.33	123.30	118.90
58	c	94	U	N3-C4-C5	7.32	118.99	114.60
11	AA	3278	C	C2-N1-C1’	6.96	126.45	118.80
58	c	1389	C	C2-N1-C1’	6.79	126.27	118.80
58	c	965	U	C2-N1-C1’	6.64	125.67	117.70
11	AA	406	G	O4’-C1’-N9	6.62	113.50	108.20
18	DD	58	MET	CA-CB-CG	6.56	124.44	113.30
11	AA	620	U	C2-N1-C1’	6.55	125.56	117.70
11	AA	1222	G	O4’-C1’-N9	6.50	113.40	108.20
58	c	1537	C	N3-C2-O2	-6.50	117.35	121.90
11	AA	922	U	C2-N1-C1’	6.46	125.45	117.70
58	c	1473	U	C2-N1-C1’	6.44	125.42	117.70
14	Cc	57	C	O4’-C1’-C2’	-6.43	99.37	105.80
11	AA	1496	C	C2-N1-C1’	6.22	125.64	118.80
11	AA	3278	C	N3-C2-O2	-5.97	117.72	121.90
11	AA	620	U	N1-C2-O2	5.92	126.94	122.80
58	c	531	C	C2-N1-C1’	5.80	125.18	118.80
58	c	1537	C	C6-N1-C1’	-5.79	113.85	120.80
58	c	1537	C	C6-N1-C2	-5.74	118.00	120.30
58	c	94	U	N1-C2-N3	5.72	118.33	114.90
8	7	34	LEU	CA-CB-CG	5.71	128.44	115.30
58	c	139	C	N1-C2-O2	5.66	122.30	118.90
11	AA	620	U	N3-C2-O2	-5.62	118.26	122.20
11	AA	2836	C	C6-N1-C2	-5.60	118.06	120.30
58	c	139	C	C2-N1-C1’	5.50	124.85	118.80
58	c	1458	G	C4-N9-C1’	5.47	133.61	126.50
11	AA	2836	C	C2-N1-C1’	5.45	124.80	118.80
58	c	1473	U	N1-C2-O2	5.45	126.61	122.80
11	AA	2444	C	C2-N1-C1’	5.40	124.74	118.80
58	c	1458	G	N3-C4-N9	5.29	129.17	126.00
11	AA	1767	C	C2-N1-C1’	5.28	124.61	118.80
11	AA	3058	U	C2-N1-C1’	5.28	124.03	117.70
58	c	1389	C	C6-N1-C2	-5.25	118.20	120.30
11	AA	2772	C	N1-C2-O2	5.24	122.04	118.90
2	1	68	ARG	CG-CD-NE	-5.21	100.85	111.80
11	AA	2836	C	N3-C2-O2	-5.18	118.27	121.90
11	AA	2490	C	C2-N1-C1’	5.17	124.48	118.80
72	q	107	ARG	CG-CD-NE	-5.15	100.98	111.80
11	AA	1031	C	N1-C2-O2	5.15	121.99	118.90
22	Ee	130	LYS	CD-CE-NZ	5.15	123.54	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	3181	C	N1-C2-O2	5.11	121.97	118.90
74	s	105	LEU	CA-CB-CG	5.09	127.02	115.30
11	AA	3181	C	C2-N1-C1’	5.07	124.37	118.80
11	AA	2496	C	C2-N1-C1’	5.06	124.37	118.80
11	AA	922	U	N1-C2-O2	5.03	126.32	122.80
11	AA	1724	U	O4’-C1’-N1	5.01	112.21	108.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	68	ARG	Sidechain
18	DD	20	GLU	Peptide
32	JJ	232	ARG	Peptide
35	L	102	GLU	Peptide
56	a	7	THR	Peptide
60	e	35	PRO	Peptide
60	e	38	PHE	Peptide
64	i	65	ARG	Peptide
66	k	64	VAL	Peptide
72	q	107	ARG	Sidechain
74	s	40	GLU	Peptide
76	u	90	ASN	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	132/135 (98%)	127 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	68/108 (63%)	62 (91%)	6 (9%)	0	100	100
3	2	95/119 (80%)	89 (94%)	6 (6%)	0	100	100
4	3	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
5	4	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
6	5	47/56 (84%)	47 (100%)	0	0	100	100
7	6	51/63 (81%)	49 (96%)	2 (4%)	0	100	100
8	7	316/319 (99%)	297 (94%)	19 (6%)	0	100	100
9	8	32/152 (21%)	25 (78%)	7 (22%)	0	100	100
10	A	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
12	B	152/338 (45%)	150 (99%)	2 (1%)	0	100	100
15	C	183/186 (98%)	182 (100%)	1 (0%)	0	100	100
17	D	174/189 (92%)	170 (98%)	4 (2%)	0	100	100
18	DD	195/312 (62%)	189 (97%)	6 (3%)	0	100	100
20	E	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
21	EE	250/254 (98%)	247 (99%)	3 (1%)	0	100	100
22	Ee	156/165 (94%)	150 (96%)	6 (4%)	0	100	100
23	F	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
24	FF	384/387 (99%)	373 (97%)	11 (3%)	0	100	100
25	G	95/121 (78%)	92 (97%)	3 (3%)	0	100	100
26	GG	359/362 (99%)	345 (96%)	14 (4%)	0	100	100
27	H	127/137 (93%)	126 (99%)	1 (1%)	0	100	100
28	HH	294/297 (99%)	288 (98%)	6 (2%)	0	100	100
29	I	61/155 (39%)	61 (100%)	0	0	100	100
30	II	151/176 (86%)	148 (98%)	3 (2%)	0	100	100
31	J	118/142 (83%)	115 (98%)	3 (2%)	0	100	100
32	JJ	220/244 (90%)	217 (99%)	3 (1%)	0	100	100
33	K	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
34	KK	231/256 (90%)	227 (98%)	4 (2%)	0	100	100
35	L	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
36	LL	189/191 (99%)	181 (96%)	8 (4%)	0	100	100
37	M	146/149 (98%)	141 (97%)	4 (3%)	1 (1%)	22	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	MM	213/221 (96%)	208 (98%)	5 (2%)	0	100	100
39	N	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
40	NN	167/174 (96%)	161 (96%)	6 (4%)	0	100	100
41	O	95/105 (90%)	95 (100%)	0	0	100	100
42	OO	191/199 (96%)	178 (93%)	12 (6%)	1 (0%)	29	34
43	P	107/113 (95%)	103 (96%)	4 (4%)	0	100	100
44	PP	134/138 (97%)	133 (99%)	1 (1%)	0	100	100
45	Q	125/130 (96%)	125 (100%)	0	0	100	100
46	QQ	201/204 (98%)	194 (96%)	7 (4%)	0	100	100
47	R	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
48	S	107/121 (88%)	107 (100%)	0	0	100	100
49	T	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
50	U	97/100 (97%)	90 (93%)	7 (7%)	0	100	100
51	V	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
52	W	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
53	X	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
54	Y	50/128 (39%)	50 (100%)	0	0	100	100
55	Z	23/25 (92%)	23 (100%)	0	0	100	100
56	a	100/106 (94%)	96 (96%)	4 (4%)	0	100	100
57	b	89/92 (97%)	89 (100%)	0	0	100	100
59	d	204/252 (81%)	194 (95%)	10 (5%)	0	100	100
60	e	210/255 (82%)	195 (93%)	15 (7%)	0	100	100
61	f	215/254 (85%)	203 (94%)	12 (6%)	0	100	100
62	g	203/240 (85%)	196 (97%)	7 (3%)	0	100	100
63	h	256/261 (98%)	248 (97%)	8 (3%)	0	100	100
64	i	195/225 (87%)	186 (95%)	9 (5%)	0	100	100
65	j	221/236 (94%)	215 (97%)	6 (3%)	0	100	100
66	k	182/190 (96%)	175 (96%)	7 (4%)	0	100	100
67	l	180/200 (90%)	164 (91%)	16 (9%)	0	100	100
68	m	183/197 (93%)	178 (97%)	5 (3%)	0	100	100
69	n	63/105 (60%)	58 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	o	140/156 (90%)	132 (94%)	8 (6%)	0	100	100
71	p	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
72	q	125/137 (91%)	118 (94%)	7 (6%)	0	100	100
73	r	85/142 (60%)	82 (96%)	3 (4%)	0	100	100
74	s	135/143 (94%)	125 (93%)	10 (7%)	0	100	100
75	t	119/136 (88%)	111 (93%)	8 (7%)	0	100	100
76	u	143/146 (98%)	132 (92%)	11 (8%)	0	100	100
77	v	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
78	w	98/121 (81%)	98 (100%)	0	0	100	100
79	x	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
80	y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
81	z	142/145 (98%)	129 (91%)	13 (9%)	0	100	100
All	All	10926/12368 (88%)	10539 (96%)	385 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	OO	63	VAL
37	M	78	LEU

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	
1	0	112/113 (99%)	106 (95%)	6 (5%)	22	28
2	1	61/89 (68%)	60 (98%)	1 (2%)	62	76
3	2	83/101 (82%)	80 (96%)	3 (4%)	35	47
4	3	70/71 (99%)	66 (94%)	4 (6%)	20	26
5	4	56/60 (93%)	48 (86%)	8 (14%)	3	3
6	5	43/49 (88%)	39 (91%)	4 (9%)	9	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	6	46/54 (85%)	43 (94%)	3 (6%)	17	21
8	7	259/262 (99%)	242 (93%)	17 (7%)	16	20
9	8	30/135 (22%)	30 (100%)	0	100	100
10	A	160/162 (99%)	159 (99%)	1 (1%)	86	93
12	B	125/271 (46%)	121 (97%)	4 (3%)	39	52
15	C	150/151 (99%)	148 (99%)	2 (1%)	69	80
17	D	143/154 (93%)	139 (97%)	4 (3%)	43	57
18	DD	167/254 (66%)	154 (92%)	13 (8%)	12	14
20	E	156/156 (100%)	152 (97%)	4 (3%)	46	60
21	EE	193/196 (98%)	189 (98%)	4 (2%)	53	68
22	Ee	129/136 (95%)	117 (91%)	12 (9%)	9	9
23	F	136/137 (99%)	129 (95%)	7 (5%)	24	31
24	FF	320/323 (99%)	312 (98%)	8 (2%)	47	62
25	G	84/107 (78%)	81 (96%)	3 (4%)	35	47
26	GG	288/289 (100%)	275 (96%)	13 (4%)	27	36
27	H	101/105 (96%)	98 (97%)	3 (3%)	41	54
28	HH	244/245 (100%)	239 (98%)	5 (2%)	55	70
29	I	55/129 (43%)	55 (100%)	0	100	100
30	II	133/153 (87%)	129 (97%)	4 (3%)	41	54
31	J	104/118 (88%)	103 (99%)	1 (1%)	76	86
32	JJ	186/205 (91%)	182 (98%)	4 (2%)	52	66
33	K	109/110 (99%)	104 (95%)	5 (5%)	27	35
34	KK	187/208 (90%)	181 (97%)	6 (3%)	39	52
35	L	115/116 (99%)	109 (95%)	6 (5%)	23	30
36	LL	171/171 (100%)	160 (94%)	11 (6%)	17	21
37	M	118/119 (99%)	114 (97%)	4 (3%)	37	49
38	MM	184/187 (98%)	172 (94%)	12 (6%)	17	21
39	N	46/47 (98%)	45 (98%)	1 (2%)	52	66
40	NN	147/150 (98%)	139 (95%)	8 (5%)	22	28
41	O	81/88 (92%)	77 (95%)	4 (5%)	25	33
42	OO	154/159 (97%)	147 (96%)	7 (4%)	27	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	P	94/97 (97%)	93 (99%)	1 (1%)	73	84
44	PP	107/109 (98%)	104 (97%)	3 (3%)	43	57
45	Q	109/111 (98%)	107 (98%)	2 (2%)	59	72
46	QQ	175/176 (99%)	172 (98%)	3 (2%)	60	74
47	R	90/91 (99%)	89 (99%)	1 (1%)	73	84
48	S	94/103 (91%)	90 (96%)	4 (4%)	29	38
49	T	104/105 (99%)	102 (98%)	2 (2%)	57	71
50	U	81/82 (99%)	77 (95%)	4 (5%)	25	33
51	V	69/71 (97%)	68 (99%)	1 (1%)	67	79
52	W	68/69 (99%)	61 (90%)	7 (10%)	7	7
53	X	45/46 (98%)	44 (98%)	1 (2%)	52	66
54	Y	47/116 (40%)	47 (100%)	0	100	100
55	Z	23/23 (100%)	20 (87%)	3 (13%)	4	4
56	a	87/91 (96%)	83 (95%)	4 (5%)	27	35
57	b	71/72 (99%)	67 (94%)	4 (6%)	21	27
59	d	165/210 (79%)	159 (96%)	6 (4%)	35	47
60	e	189/224 (84%)	181 (96%)	8 (4%)	30	39
61	f	176/205 (86%)	168 (96%)	8 (4%)	27	36
62	g	166/195 (85%)	148 (89%)	18 (11%)	6	6
63	h	220/222 (99%)	213 (97%)	7 (3%)	39	52
64	i	172/191 (90%)	161 (94%)	11 (6%)	17	21
65	j	191/201 (95%)	182 (95%)	9 (5%)	26	34
66	k	165/170 (97%)	159 (96%)	6 (4%)	35	47
67	l	146/161 (91%)	140 (96%)	6 (4%)	30	41
68	m	158/166 (95%)	149 (94%)	9 (6%)	20	26
69	n	60/98 (61%)	58 (97%)	2 (3%)	38	51
70	o	127/137 (93%)	120 (94%)	7 (6%)	21	27
71	p	127/128 (99%)	125 (98%)	2 (2%)	62	76
72	q	81/105 (77%)	77 (95%)	4 (5%)	25	33
73	r	77/118 (65%)	73 (95%)	4 (5%)	23	30
74	s	114/119 (96%)	109 (96%)	5 (4%)	28	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	t	105/124 (85%)	95 (90%)	10 (10%)	8	9
76	u	128/129 (99%)	114 (89%)	14 (11%)	6	6
77	v	115/116 (99%)	110 (96%)	5 (4%)	29	38
78	w	94/114 (82%)	86 (92%)	8 (8%)	10	12
79	x	74/74 (100%)	68 (92%)	6 (8%)	11	13
80	y	110/111 (99%)	106 (96%)	4 (4%)	35	47
81	z	119/120 (99%)	110 (92%)	9 (8%)	13	15
All	All	9289/10380 (90%)	8879 (96%)	410 (4%)	32	37

All (410) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	8	ARG
1	0	14	SER
1	0	52	LYS
1	0	83	LYS
1	0	111	LYS
1	0	112	LYS
2	1	47	TYR
3	2	27	SER
3	2	64	LEU
3	2	84	VAL
4	3	2	VAL
4	3	33	LEU
4	3	44	THR
4	3	60	SER
5	4	8	THR
5	4	12	VAL
5	4	30	VAL
5	4	42	ARG
5	4	57	MET
5	4	64	ARG
5	4	65	ARG
5	4	67	ARG
6	5	10	HIS
6	5	19	ARG
6	5	39	CYS
6	5	46	LYS
7	6	26	LYS
7	6	29	LYS

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Mol	Chain	Res	Type
7	6	50	VAL
8	7	14	GLU
8	7	29	GLN
8	7	31	ASN
8	7	41	THR
8	7	45	TRP
8	7	54	PHE
8	7	60	SER
8	7	109	ASP
8	7	117	LYS
8	7	175	ASP
8	7	184	ASN
8	7	195	HIS
8	7	197	SER
8	7	231	MET
8	7	232	TYR
8	7	249	ARG
8	7	278	PHE
10	A	14	HIS
12	B	18	ARG
12	B	54	HIS
12	B	118	GLN
12	B	149	VAL
15	C	31	LYS
15	C	100	THR
17	D	6	THR
17	D	69	SER
17	D	86	GLU
17	D	152	GLU
18	DD	8	LYS
18	DD	23	LYS
18	DD	24	SER
18	DD	31	ASP
18	DD	58	MET
18	DD	74	GLU
18	DD	110	ARG
18	DD	118	ASP
18	DD	125	ASN
18	DD	147	ARG
18	DD	155	ASP
18	DD	164	LYS
18	DD	167	GLN

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Mol	Chain	Res	Type
20	E	45	LEU
20	E	74	ASN
20	E	96	ASP
20	E	172	TYR
21	EE	70	ARG
21	EE	72	ARG
21	EE	191	LEU
21	EE	202	VAL
22	Ee	11	LYS
22	Ee	12	TYR
22	Ee	16	ARG
22	Ee	18	VAL
22	Ee	40	LYS
22	Ee	48	LYS
22	Ee	66	ASN
22	Ee	67	ARG
22	Ee	91	ASP
22	Ee	92	ARG
22	Ee	119	LYS
22	Ee	125	LEU
23	F	18	ASP
23	F	26	HIS
23	F	52	MET
23	F	83	ARG
23	F	138	SER
23	F	139	ARG
23	F	142	SER
24	FF	5	LYS
24	FF	38	SER
24	FF	55	THR
24	FF	66	LYS
24	FF	206	ASP
24	FF	291	GLU
24	FF	332	ARG
24	FF	355	SER
25	G	35	LYS
25	G	86	LYS
25	G	104	ARG
26	GG	6	VAL
26	GG	14	GLU
26	GG	84	ARG
26	GG	120	TYR

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Mol	Chain	Res	Type
26	GG	144	LYS
26	GG	145	ILE
26	GG	177	ASP
26	GG	181	VAL
26	GG	259	ASP
26	GG	275	THR
26	GG	288	ARG
26	GG	346	LYS
26	GG	350	LYS
27	H	97	ASP
27	H	98	ASN
27	H	128	ARG
28	HH	80	SER
28	HH	95	TRP
28	HH	118	THR
28	HH	125	VAL
28	HH	218	ARG
30	II	82	ARG
30	II	88	SER
30	II	91	VAL
30	II	162	SER
31	J	24	LEU
32	JJ	56	GLU
32	JJ	113	SER
32	JJ	182	ASP
32	JJ	190	THR
33	K	3	LYS
33	K	74	TYR
33	K	94	SER
33	K	115	ARG
33	K	125	LYS
34	KK	40	VAL
34	KK	51	LYS
34	KK	79	GLN
34	KK	106	LYS
34	KK	203	VAL
34	KK	248	LYS
35	L	31	GLU
35	L	61	LYS
35	L	95	VAL
35	L	105	SER
35	L	121	ARG

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Mol	Chain	Res	Type
35	L	135	ARG
36	LL	17	THR
36	LL	50	ASN
36	LL	69	ARG
36	LL	73	SER
36	LL	92	TYR
36	LL	106	LYS
36	LL	107	ASP
36	LL	110	LYS
36	LL	137	SER
36	LL	139	ASN
36	LL	157	ASN
37	M	8	THR
37	M	15	VAL
37	M	60	TYR
37	M	85	ASP
38	MM	4	ARG
38	MM	7	ARG
38	MM	21	ARG
38	MM	28	ASP
38	MM	30	LYS
38	MM	101	LYS
38	MM	104	SER
38	MM	110	ARG
38	MM	112	GLN
38	MM	130	ASP
38	MM	180	GLU
38	MM	215	GLU
39	N	4	SER
40	NN	11	ASP
40	NN	26	SER
40	NN	77	GLU
40	NN	107	ASP
40	NN	119	SER
40	NN	126	ASP
40	NN	165	GLN
40	NN	170	ASP
41	O	38	LYS
41	O	61	MET
41	O	97	ASP
41	O	102	THR
42	OO	4	SER

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Mol	Chain	Res	Type
42	OO	45	LYS
42	OO	69	VAL
42	OO	107	GLU
42	OO	152	THR
42	OO	168	ARG
42	OO	190	LYS
43	P	91	SER
44	PP	3	THR
44	PP	47	ASP
44	PP	83	LYS
45	Q	31	ASN
45	Q	123	LYS
46	QQ	73	ARG
46	QQ	96	ARG
46	QQ	155	VAL
47	R	31	LYS
48	S	35	VAL
48	S	60	ARG
48	S	64	THR
48	S	65	VAL
49	T	37	SER
49	T	119	LYS
50	U	17	VAL
50	U	35	ASN
50	U	56	ARG
50	U	98	ARG
51	V	71	SER
52	W	19	ASP
52	W	24	THR
52	W	29	LYS
52	W	38	PHE
52	W	49	SER
52	W	68	SER
52	W	78	LEU
53	X	30	ARG
55	Z	12	ARG
55	Z	15	ARG
55	Z	24	SER
56	a	8	ARG
56	a	34	SER
56	a	76	LYS
56	a	80	ARG

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Mol	Chain	Res	Type
57	b	32	GLN
57	b	62	LYS
57	b	63	THR
57	b	70	THR
59	d	27	ARG
59	d	116	LYS
59	d	127	ARG
59	d	165	ARG
59	d	198	MET
59	d	200	ASP
60	e	20	VAL
60	e	39	GLU
60	e	43	VAL
60	e	54	LEU
60	e	111	ARG
60	e	158	SER
60	e	205	PHE
60	e	213	ARG
61	f	52	THR
61	f	82	ASN
61	f	90	THR
61	f	91	ARG
61	f	158	THR
61	f	186	LYS
61	f	207	LEU
61	f	222	TYR
62	g	7	LYS
62	g	35	SER
62	g	37	VAL
62	g	44	THR
62	g	45	LYS
62	g	48	VAL
62	g	64	ARG
62	g	67	ASN
62	g	75	LYS
62	g	76	ARG
62	g	93	ASP
62	g	94	ARG
62	g	129	SER
62	g	146	ARG
62	g	148	LYS
62	g	151	LYS

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Mol	Chain	Res	Type
62	g	168	ILE
62	g	177	MET
63	h	91	THR
63	h	105	VAL
63	h	108	ARG
63	h	128	LYS
63	h	168	LYS
63	h	182	TYR
63	h	255	ARG
64	i	20	PHE
64	i	23	VAL
64	i	37	GLN
64	i	73	THR
64	i	76	ARG
64	i	98	MET
64	i	112	ARG
64	i	166	ARG
64	i	188	LYS
64	i	203	LYS
64	i	208	SER
65	j	36	VAL
65	j	45	PHE
65	j	78	THR
65	j	98	ARG
65	j	105	ASP
65	j	124	LEU
65	j	137	ARG
65	j	170	THR
65	j	212	LEU
66	k	24	PHE
66	k	72	LYS
66	k	79	ARG
66	k	85	PHE
66	k	156	SER
66	k	160	GLN
67	l	4	SER
67	l	7	SER
67	l	21	PHE
67	l	23	LYS
67	l	32	GLN
67	l	154	SER
68	m	50	SER

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Mol	Chain	Res	Type
68	m	79	ARG
68	m	87	SER
68	m	152	SER
68	m	155	HIS
68	m	157	ASP
68	m	168	ARG
68	m	175	ARG
68	m	186	GLU
69	n	6	GLU
69	n	21	VAL
70	o	5	LEU
70	o	7	VAL
70	o	31	THR
70	o	46	LYS
70	o	67	ARG
70	o	116	ARG
70	o	132	SER
71	p	60	VAL
71	p	93	LYS
72	q	14	PHE
72	q	38	THR
72	q	51	ASP
72	q	107	ARG
73	r	36	LEU
73	r	57	MET
73	r	89	MET
73	r	120	SER
74	s	26	LYS
74	s	62	ASN
74	s	68	ARG
74	s	111	SER
74	s	143	ARG
75	t	5	ARG
75	t	19	ARG
75	t	27	ASP
75	t	67	ARG
75	t	74	GLN
75	t	80	ARG
75	t	81	LYS
75	t	85	VAL
75	t	92	ASP
75	t	95	ARG

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Mol	Chain	Res	Type
76	u	14	ILE
76	u	40	ARG
76	u	49	LYS
76	u	55	HIS
76	u	57	ARG
76	u	63	GLN
76	u	64	GLU
76	u	85	PHE
76	u	90	ASN
76	u	105	VAL
76	u	107	SER
76	u	111	ASP
76	u	120	ARG
76	u	144	ARG
77	v	5	SER
77	v	20	SER
77	v	89	ARG
77	v	123	ARG
77	v	133	ASP
78	w	21	LYS
78	w	51	VAL
78	w	52	LYS
78	w	77	LYS
78	w	84	MET
78	w	90	TYR
78	w	101	LYS
78	w	116	VAL
79	x	12	TYR
79	x	44	ARG
79	x	50	TYR
79	x	65	SER
79	x	84	SER
79	x	86	SER
80	y	27	ILE
80	y	30	SER
80	y	107	SER
80	y	115	GLU
81	z	28	ASN
81	z	39	LYS
81	z	41	SER
81	z	66	SER
81	z	70	LYS

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Mol	Chain	Res	Type
81	z	73	ARG
81	z	107	PHE
81	z	127	VAL
81	z	131	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	95	HIS
6	5	48	ASN
8	7	29	GLN
8	7	182	ASN
8	7	185	GLN
10	A	122	GLN
22	Ee	156	ASN
24	FF	269	GLN
27	H	98	ASN
30	II	157	GLN
31	J	111	ASN
53	X	33	ASN
56	a	22	GLN
59	d	131	GLN
60	e	49	ASN
64	i	79	ASN
66	k	19	GLN
75	t	31	ASN
78	w	44	ASN
78	w	47	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	3193/3396 (94%)	478 (14%)	16 (0%)
13	BB	120/121 (99%)	8 (6%)	1 (0%)
14	Bb	76/77 (98%)	21 (27%)	0
14	Cc	76/77 (98%)	34 (44%)	0
16	CC	157/158 (99%)	22 (14%)	1 (0%)
19	Dd	5/39 (12%)	1 (20%)	0
58	c	1609/1800 (89%)	286 (17%)	0
All	All	5236/5668 (92%)	850 (16%)	18 (0%)

All (850) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	AA	4	U
11	AA	6	A
11	AA	14	U
11	AA	26	A
11	AA	40	A
11	AA	43	A
11	AA	49	A
11	AA	60	A
11	AA	65	A
11	AA	66	A
11	AA	72	C
11	AA	92	G
11	AA	99	A
11	AA	110	G
11	AA	111	C
11	AA	122	A
11	AA	135	C
11	AA	136	G
11	AA	142	C
11	AA	147	U
11	AA	155	G
11	AA	156	G
11	AA	157	A
11	AA	165	A
11	AA	190	U
11	AA	191	U
11	AA	200	C
11	AA	206	G
11	AA	219	A
11	AA	241	G
11	AA	243	G
11	AA	247	C
11	AA	248	U
11	AA	249	U
11	AA	252	U
11	AA	253	A
11	AA	269	G
11	AA	286	U
11	AA	295	A
11	AA	305	U
11	AA	329	U
11	AA	337	G

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Mol	Chain	Res	Type
11	AA	376	G
11	AA	399	A
11	AA	401	U
11	AA	402	A
11	AA	403	C
11	AA	420	G
11	AA	421	G
11	AA	422	A
11	AA	520	U
11	AA	521	A
11	AA	533	A
11	AA	534	U
11	AA	543	C
11	AA	545	U
11	AA	548	G
11	AA	555	U
11	AA	557	A
11	AA	559	A
11	AA	560	G
11	AA	589	A
11	AA	592	A
11	AA	602	A
11	AA	603	A
11	AA	604	G
11	AA	607	A
11	AA	611	A
11	AA	612	U
11	AA	620	U
11	AA	621	A
11	AA	636	C
11	AA	649	A2M
11	AA	660	A
11	AA	677	A
11	AA	678	G
11	AA	681	U
11	AA	691	A
11	AA	705	A
11	AA	712	G
11	AA	715	A
11	AA	719	U
11	AA	758	C
11	AA	767	U

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Mol	Chain	Res	Type
11	AA	780	A
11	AA	781	G
11	AA	785	G
11	AA	786	A
11	AA	817	A2M
11	AA	830	A
11	AA	849	C
11	AA	861	C
11	AA	867	OMG
11	AA	874	U
11	AA	879	U
11	AA	880	G
11	AA	890	C
11	AA	896	A
11	AA	907	G
11	AA	908	OMG
11	AA	914	A
11	AA	916	G
11	AA	917	A
11	AA	921	A
11	AA	923	C
11	AA	924	G
11	AA	925	A
11	AA	937	G
11	AA	944	C
11	AA	953	G
11	AA	959	C
11	AA	960	U
11	AA	961	C
11	AA	964	G
11	AA	974	G
11	AA	979	U
11	AA	980	A
11	AA	992	A
11	AA	994	G
11	AA	1006	A
11	AA	1015	U
11	AA	1016	C
11	AA	1017	C
11	AA	1018	G
11	AA	1019	G
11	AA	1020	G

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Mol	Chain	Res	Type
11	AA	1025	A
11	AA	1026	A
11	AA	1028	U
11	AA	1029	G
11	AA	1032	C
11	AA	1034	U
11	AA	1036	A
11	AA	1037	C
11	AA	1047	A
11	AA	1064	A
11	AA	1065	A
11	AA	1072	G
11	AA	1081	U
11	AA	1083	G
11	AA	1096	U
11	AA	1097	G
11	AA	1098	A
11	AA	1103	A
11	AA	1117	G
11	AA	1131	G
11	AA	1144	U
11	AA	1153	A
11	AA	1159	A
11	AA	1160	C
11	AA	1179	A
11	AA	1180	A
11	AA	1181	U
11	AA	1182	A
11	AA	1191	U
11	AA	1193	A
11	AA	1196	C
11	AA	1201	C
11	AA	1208	U
11	AA	1209	G
11	AA	1222	G
11	AA	1235	U
11	AA	1236	G
11	AA	1240	A
11	AA	1241	U
11	AA	1245	A
11	AA	1255	C
11	AA	1256	G

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Mol	Chain	Res	Type
11	AA	1258	U
11	AA	1262	G
11	AA	1263	A
11	AA	1265	U
11	AA	1272	C
11	AA	1286	A
11	AA	1287	A
11	AA	1302	A
11	AA	1307	G
11	AA	1308	A
11	AA	1309	U
11	AA	1330	A
11	AA	1331	U
11	AA	1345	G
11	AA	1348	U
11	AA	1349	G
11	AA	1352	A
11	AA	1355	A
11	AA	1356	U
11	AA	1357	G
11	AA	1386	A
11	AA	1392	G
11	AA	1399	A
11	AA	1400	G
11	AA	1425	U
11	AA	1434	G
11	AA	1437	OMC
11	AA	1443	G
11	AA	1446	A
11	AA	1450	OMG
11	AA	1481	A
11	AA	1483	G
11	AA	1508	C
11	AA	1528	G
11	AA	1536	G
11	AA	1555	U
11	AA	1556	C
11	AA	1560	G
11	AA	1561	G
11	AA	1562	C
11	AA	1563	C
11	AA	1566	A

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Mol	Chain	Res	Type
11	AA	1568	U
11	AA	1569	U
11	AA	1570	U
11	AA	1571	A
11	AA	1572	U
11	AA	1573	G
11	AA	1579	C
11	AA	1580	A
11	AA	1581	C
11	AA	1582	C
11	AA	1583	A
11	AA	1589	A
11	AA	1593	A
11	AA	1605	A
11	AA	1621	A
11	AA	1629	U
11	AA	1630	U
11	AA	1642	A
11	AA	1643	A
11	AA	1657	C
11	AA	1724	U
11	AA	1741	A
11	AA	1750	A
11	AA	1751	G
11	AA	1756	C
11	AA	1759	C
11	AA	1762	C
11	AA	1763	U
11	AA	1765	U
11	AA	1769	G
11	AA	1775	G
11	AA	1796	G
11	AA	1797	A
11	AA	1815	U
11	AA	1816	A
11	AA	1817	G
11	AA	1821	U
11	AA	1842	A
11	AA	1858	A
11	AA	1878	G
11	AA	1879	A
11	AA	1880	U

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Mol	Chain	Res	Type
11	AA	1893	A
11	AA	1906	G
11	AA	2102	U
11	AA	2111	G
11	AA	2112	U
11	AA	2113	A
11	AA	2114	C
11	AA	2122	G
11	AA	2131	A
11	AA	2140	U
11	AA	2144	A
11	AA	2158	A
11	AA	2168	A
11	AA	2169	G
11	AA	2170	U
11	AA	2188	A
11	AA	2205	U
11	AA	2206	G
11	AA	2208	A
11	AA	2223	A
11	AA	2249	G
11	AA	2252	A
11	AA	2253	G
11	AA	2256	A2M
11	AA	2257	C
11	AA	2265	C
11	AA	2272	G
11	AA	2273	G
11	AA	2280	A2M
11	AA	2281	A2M
11	AA	2282	U
11	AA	2307	G
11	AA	2308	C
11	AA	2310	U
11	AA	2313	A
11	AA	2315	G
11	AA	2334	U
11	AA	2335	G
11	AA	2336	U
11	AA	2363	A
11	AA	2373	A
11	AA	2374	C

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Mol	Chain	Res	Type
11	AA	2375	G
11	AA	2388	U
11	AA	2393	G
11	AA	2397	A
11	AA	2402	A
11	AA	2403	G
11	AA	2404	A
11	AA	2405	C
11	AA	2411	U
11	AA	2418	G
11	AA	2435	G
11	AA	2437	G
11	AA	2438	A
11	AA	2444	C
11	AA	2445	A
11	AA	2447	A
11	AA	2450	G
11	AA	2453	U
11	AA	2454	G
11	AA	2459	A
11	AA	2460	U
11	AA	2461	A
11	AA	2462	A
11	AA	2463	G
11	AA	2464	U
11	AA	2465	G
11	AA	2466	G
11	AA	2470	C
11	AA	2471	U
11	AA	2472	U
11	AA	2473	C
11	AA	2474	G
11	AA	2475	G
11	AA	2477	G
11	AA	2478	C
11	AA	2479	C
11	AA	2480	A
11	AA	2481	G
11	AA	2482	U
11	AA	2484	A
11	AA	2485	A
11	AA	2487	U

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Mol	Chain	Res	Type
11	AA	2488	A
11	AA	2489	C
11	AA	2490	C
11	AA	2492	C
11	AA	2493	U
11	AA	2494	A
11	AA	2495	C
11	AA	2496	C
11	AA	2497	U
11	AA	2499	U
11	AA	2500	A
11	AA	2501	U
11	AA	2503	G
11	AA	2505	U
11	AA	2506	U
11	AA	2511	A
11	AA	2514	U
11	AA	2515	A
11	AA	2534	G
11	AA	2539	C
11	AA	2541	U
11	AA	2542	U
11	AA	2549	G
11	AA	2552	C
11	AA	2555	G
11	AA	2561	A
11	AA	2569	A
11	AA	2570	U
11	AA	2571	U
11	AA	2572	C
11	AA	2573	G
11	AA	2585	G
11	AA	2593	A
11	AA	2606	G
11	AA	2607	G
11	AA	2614	G
11	AA	2652	U
11	AA	2656	A
11	AA	2672	G
11	AA	2674	A
11	AA	2677	G
11	AA	2681	U

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Mol	Chain	Res	Type
11	AA	2689	A
11	AA	2691	A
11	AA	2696	A
11	AA	2704	A
11	AA	2705	A
11	AA	2714	G
11	AA	2728	G
11	AA	2729	OMU
11	AA	2753	G
11	AA	2762	A
11	AA	2772	C
11	AA	2777	G
11	AA	2778	G
11	AA	2795	U
11	AA	2796	G
11	AA	2799	A
11	AA	2800	G
11	AA	2801	A
11	AA	2802	A
11	AA	2808	A
11	AA	2810	C
11	AA	2814	G
11	AA	2816	G
11	AA	2817	A
11	AA	2844	C
11	AA	2845	A
11	AA	2849	C
11	AA	2856	G
11	AA	2867	C
11	AA	2871	G
11	AA	2872	A
11	AA	2887	A
11	AA	2898	G
11	AA	2899	C
11	AA	2914	G
11	AA	2922	OMG
11	AA	2923	U
11	AA	2935	U
11	AA	2936	A
11	AA	2942	C
11	AA	2947	G
11	AA	2951	G

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Mol	Chain	Res	Type
11	AA	2971	A
11	AA	2972	G
11	AA	2983	C
11	AA	2990	G
11	AA	2997	G
11	AA	3012	A
11	AA	3059	G
11	AA	3078	U
11	AA	3092	C
11	AA	3101	G
11	AA	3113	A
11	AA	3117	C
11	AA	3122	A
11	AA	3130	A
11	AA	3131	U
11	AA	3142	A
11	AA	3143	C
11	AA	3153	U
11	AA	3154	C
11	AA	3155	U
11	AA	3156	U
11	AA	3157	U
11	AA	3168	A
11	AA	3170	A
11	AA	3172	A
11	AA	3173	G
11	AA	3176	G
11	AA	3179	U
11	AA	3181	C
11	AA	3187	A
11	AA	3207	U
11	AA	3209	A
11	AA	3217	C
11	AA	3218	A
11	AA	3219	G
11	AA	3224	G
11	AA	3235	C
11	AA	3243	A
11	AA	3247	G
11	AA	3270	U
11	AA	3276	G
11	AA	3277	U

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Mol	Chain	Res	Type
11	AA	3281	U
11	AA	3294	A
11	AA	3295	A
11	AA	3304	U
11	AA	3316	A
11	AA	3335	A
11	AA	3341	U
11	AA	3345	G
11	AA	3351	U
11	AA	3352	U
11	AA	3353	G
11	AA	3369	G
11	AA	3378	C
11	AA	3382	U
11	AA	3389	U
11	AA	3390	G
13	BB	7	G
13	BB	33	U
13	BB	54	U
13	BB	55	A
13	BB	65	G
13	BB	73	C
13	BB	99	G
13	BB	112	G
14	Bb	2	G
14	Bb	10	G
14	Bb	16	C
14	Bb	17	C
14	Bb	18	C
14	Bb	19	G
14	Bb	20	G
14	Bb	22	A
14	Bb	43	G
14	Bb	48	U
14	Bb	49	C
14	Bb	52	C
14	Bb	54	G
14	Bb	55	U
14	Bb	56	U
14	Bb	57	C
14	Bb	60	A
14	Bb	62	C

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Mol	Chain	Res	Type
14	Bb	63	C
14	Bb	66	C
14	Bb	77	A
16	CC	23	U
16	CC	34	U
16	CC	35	C
16	CC	51	G
16	CC	52	A
16	CC	59	A
16	CC	62	C
16	CC	63	G
16	CC	82	U
16	CC	83	C
16	CC	84	C
16	CC	85	G
16	CC	86	U
16	CC	87	G
16	CC	91	C
16	CC	95	G
16	CC	104	A
16	CC	106	C
16	CC	113	U
16	CC	125	U
16	CC	126	A
16	CC	152	G
14	Cc	4	G
14	Cc	5	G
14	Cc	6	G
14	Cc	7	G
14	Cc	9	G
14	Cc	10	G
14	Cc	11	A
14	Cc	12	G
14	Cc	13	C
14	Cc	14	A
14	Cc	15	G
14	Cc	17	C
14	Cc	18	C
14	Cc	20	G
14	Cc	21	U
14	Cc	22	A
14	Cc	23	G

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Mol	Chain	Res	Type
14	Cc	25	U
14	Cc	28	U
14	Cc	32	G
14	Cc	35	C
14	Cc	36	A
14	Cc	37	U
14	Cc	40	C
14	Cc	42	C
14	Cc	47	G
14	Cc	48	U
14	Cc	49	C
14	Cc	50	G
14	Cc	57	C
14	Cc	58	A
14	Cc	62	C
14	Cc	63	C
14	Cc	77	A
19	Dd	20	U
58	c	2	A
58	c	4	C
58	c	26	A
58	c	28	A2M
58	c	34	G
58	c	45	U
58	c	47	A
58	c	61	A
58	c	68	A
58	c	71	A
58	c	72	A
58	c	78	A
58	c	100	A2M
58	c	111	U
58	c	114	C
58	c	127	G
58	c	131	C
58	c	140	A
58	c	145	A
58	c	146	U
58	c	153	G
58	c	161	U
58	c	168	A
58	c	217	A

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Mol	Chain	Res	Type
58	c	218	A
58	c	257	A
58	c	261	U
58	c	262	U
58	c	272	U
58	c	277	U
58	c	278	U
58	c	279	G
58	c	280	U
58	c	287	G
58	c	299	A
58	c	309	C
58	c	314	C
58	c	316	A
58	c	321	C
58	c	322	G
58	c	333	A
58	c	337	G
58	c	338	C
58	c	361	C
58	c	390	G
58	c	400	A
58	c	401	A
58	c	402	C
58	c	404	G
58	c	423	G
58	c	424	C
58	c	426	G
58	c	434	G
58	c	439	U
58	c	444	C
58	c	448	C
58	c	455	C
58	c	460	A
58	c	468	A
58	c	477	A
58	c	480	G
58	c	507	U
58	c	514	G
58	c	515	A
58	c	519	C
58	c	525	A

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Mol	Chain	Res	Type
58	c	526	A
58	c	527	A
58	c	537	G
58	c	538	A
58	c	541	A2M
58	c	542	A
58	c	555	A
58	c	557	G
58	c	559	C
58	c	565	C
58	c	568	G
58	c	577	G
58	c	578	OMU
58	c	580	A
58	c	582	U
58	c	594	A
58	c	606	A
58	c	611	U
58	c	619	A2M
58	c	620	A
58	c	623	A
58	c	624	G
58	c	639	U
58	c	643	G
58	c	644	C
58	c	645	C
58	c	648	G
58	c	651	G
58	c	691	C
58	c	692	C
58	c	695	U
58	c	696	C
58	c	743	U
58	c	745	U
58	c	760	A
58	c	765	G
58	c	766	U
58	c	775	G
58	c	779	U
58	c	780	A
58	c	781	U
58	c	782	U

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Mol	Chain	Res	Type
58	c	783	G
58	c	784	C
58	c	789	A
58	c	794	U
58	c	795	U
58	c	796	A2M
58	c	809	A
58	c	812	A
58	c	814	A
58	c	852	C
58	c	856	A
58	c	859	A
58	c	860	U
58	c	863	A
58	c	895	G
58	c	898	A
58	c	906	A
58	c	913	G
58	c	914	G
58	c	915	A
58	c	921	U
58	c	933	A
58	c	935	U
58	c	951	A
58	c	960	U
58	c	966	A
58	c	987	G
58	c	988	A
58	c	992	A
58	c	993	A
58	c	1002	G
58	c	1010	C
58	c	1020	A
58	c	1026	A
58	c	1027	A
58	c	1028	C
58	c	1031	U
58	c	1032	G
58	c	1053	G
58	c	1058	U
58	c	1059	U
58	c	1060	U

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Mol	Chain	Res	Type
58	c	1061	A
58	c	1063	U
58	c	1081	A
58	c	1092	A
58	c	1097	U
58	c	1100	G
58	c	1138	A
58	c	1150	G
58	c	1154	G
58	c	1155	G
58	c	1158	C
58	c	1162	C
58	c	1185	U
58	c	1192	C
58	c	1193	A
58	c	1194	A
58	c	1196	A
58	c	1199	G
58	c	1200	G
58	c	1202	A
58	c	1217	A
58	c	1218	G
58	c	1224	A
58	c	1225	U
58	c	1227	A
58	c	1228	G
58	c	1238	A
58	c	1241	G
58	c	1244	A
58	c	1245	G
58	c	1246	C
58	c	1251	U
58	c	1252	C
58	c	1256	A
58	c	1258	U
58	c	1259	U
58	c	1263	G
58	c	1271	OMG
58	c	1286	U
58	c	1291	G
58	c	1297	G
58	c	1300	A

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Mol	Chain	Res	Type
58	c	1301	U
58	c	1314	U
58	c	1315	U
58	c	1318	G
58	c	1321	A
58	c	1336	A
58	c	1338	C
58	c	1339	C
58	c	1340	U
58	c	1341	A
58	c	1346	A
58	c	1347	U
58	c	1352	G
58	c	1354	G
58	c	1361	U
58	c	1363	U
58	c	1368	G
58	c	1372	U
58	c	1373	C
58	c	1382	A
58	c	1388	A
58	c	1390	U
58	c	1398	U
58	c	1400	A
58	c	1411	A
58	c	1413	U
58	c	1414	U
58	c	1415	U
58	c	1425	A
58	c	1426	C
58	c	1427	A
58	c	1428	OMG
58	c	1431	C
58	c	1432	U
58	c	1433	G
58	c	1436	A
58	c	1445	G
58	c	1459	C
58	c	1460	A
58	c	1469	A
58	c	1471	A
58	c	1472	C

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Mol	Chain	Res	Type
58	c	1477	G
58	c	1478	G
58	c	1482	C
58	c	1490	C
58	c	1491	U
58	c	1492	A
58	c	1496	U
58	c	1506	G
58	c	1510	U
58	c	1516	A
58	c	1521	G
58	c	1523	G
58	c	1524	A
58	c	1535	U
58	c	1536	G
58	c	1537	C
58	c	1542	G
58	c	1557	U
58	c	1559	A
58	c	1572	OMG
58	c	1573	A
58	c	1574	G
58	c	1575	G7M
58	c	1590	G
58	c	1601	G
58	c	1616	G
58	c	1622	G
58	c	1631	A
58	c	1633	A
58	c	1634	C
58	c	1635	A
58	c	1657	U
58	c	1658	G
58	c	1678	A
58	c	1680	G
58	c	1681	A
58	c	1682	U
58	c	1683	C
58	c	1685	G
58	c	1716	C
58	c	1717	G
58	c	1756	A

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Mol	Chain	Res	Type
58	c	1757	G
58	c	1762	A
58	c	1769	U
58	c	1780	G
58	c	1792	G
58	c	1793	G
58	c	1794	A
58	c	1795	U
58	c	1796	C
58	c	1799	U

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	AA	601	U
11	AA	619	A
11	AA	873	C
11	AA	916	G
11	AA	1028	U
11	AA	1033	U
11	AA	1562	C
11	AA	2101	C
11	AA	2458	A
11	AA	2464	U
11	AA	2477	G
11	AA	2487	U
11	AA	2500	A
11	AA	2971	A
11	AA	3121	U
11	AA	3206	C
13	BB	72	A
16	CC	57	C

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

66 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	$\#\|Z\| > 2$
11	A2M	AA	2280	11	18,25,26	3.59	8 (44%)	18,36,39	3.38	3 (16%)
11	A2M	AA	1449	11,83	18,25,26	3.59	8 (44%)	18,36,39	3.38	4 (22%)
11	5MC	AA	2870	11,84	18,22,23	0.66	0	26,32,35	0.61	0
58	OMG	c	1428	58	18,26,27	1.12	2 (11%)	19,38,41	0.89	2 (10%)
11	A2M	AA	1133	11,83	18,25,26	3.59	8 (44%)	18,36,39	3.40	3 (16%)
11	OMU	AA	1888	11	19,22,23	3.07	8 (42%)	26,31,34	1.75	5 (19%)
58	A2M	c	796	58	18,25,26	3.60	8 (44%)	18,36,39	3.36	4 (22%)
11	A2M	AA	2220	11	18,25,26	3.57	8 (44%)	18,36,39	3.36	3 (16%)
11	OMG	AA	2922	11	18,26,27	1.16	2 (11%)	19,38,41	0.92	1 (5%)
58	B8N	c	1191	58	24,29,30	3.07	7 (29%)	29,42,45	1.72	5 (17%)
11	OMU	AA	2421	11	19,22,23	3.07	8 (42%)	26,31,34	1.70	4 (15%)
11	OMG	AA	2619	11,14	18,26,27	1.13	2 (11%)	19,38,41	0.83	1 (5%)
58	A2M	c	28	58	18,25,26	3.61	9 (50%)	18,36,39	3.38	4 (22%)
11	OMG	AA	2815	11	18,26,27	1.10	2 (11%)	19,38,41	0.84	1 (5%)
58	G7M	c	1575	58,14	20,26,27	2.43	7 (35%)	17,39,42	1.17	1 (5%)
58	A2M	c	974	58	18,25,26	3.57	8 (44%)	18,36,39	3.38	3 (16%)
11	OMC	AA	2197	11,84	19,22,23	0.51	0	26,31,34	0.60	0
11	5MC	AA	2278	11,83	18,22,23	0.54	0	26,32,35	0.60	0
58	A2M	c	541	58	18,25,26	3.57	8 (44%)	18,36,39	3.37	4 (22%)
11	OMC	AA	650	11	19,22,23	0.52	0	26,31,34	0.69	0
11	OMC	AA	2959	11,83	19,22,23	0.53	0	26,31,34	0.68	0
58	MA6	c	1781	58	18,26,27	1.03	2 (11%)	19,38,41	3.37	2 (10%)
11	A2M	AA	2256	11,58	18,25,26	3.59	8 (44%)	18,36,39	3.43	4 (22%)
11	1MA	AA	645	11,83	16,25,26	0.92	2 (12%)	18,37,40	1.08	2 (11%)
58	OMC	c	1007	58	19,22,23	0.52	0	26,31,34	0.67	0
11	A2M	AA	2281	11	18,25,26	3.63	8 (44%)	18,36,39	3.42	4 (22%)
11	OMU	AA	2724	11	19,22,23	3.07	8 (42%)	26,31,34	1.68	5 (19%)
58	OMU	c	1269	58	19,22,23	3.08	8 (42%)	26,31,34	1.73	5 (19%)
58	4AC	c	1280	58	21,24,25	3.54	10 (47%)	29,34,37	1.60	5 (17%)
11	A2M	AA	817	11,83	18,25,26	3.56	8 (44%)	18,36,39	3.44	3 (16%)
11	UR3	AA	2634	11	19,22,23	2.91	6 (31%)	26,32,35	1.31	2 (7%)
58	A2M	c	100	83,58	18,25,26	3.58	8 (44%)	18,36,39	3.36	4 (22%)
58	OMC	c	414	58	19,22,23	0.51	0	26,31,34	0.70	0
11	OMG	AA	867	11,84	18,26,27	1.12	2 (11%)	19,38,41	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
58	OMG	c	1126	58	18,26,27	1.13	2 (11%)	19,38,41	0.87	1 (5%)
11	A2M	AA	807	11	18,25,26	3.59	8 (44%)	18,36,39	3.40	4 (22%)
58	OMU	c	578	58	19,22,23	3.08	8 (42%)	26,31,34	1.66	5 (19%)
11	A2M	AA	876	11	18,25,26	3.59	8 (44%)	18,36,39	3.38	4 (22%)
11	OMU	AA	2347	11	19,22,23	3.08	8 (42%)	26,31,34	1.69	5 (19%)
11	OMC	AA	2337	11	19,22,23	0.51	0	26,31,34	0.67	0
11	OMG	AA	2791	11	18,26,27	1.13	2 (11%)	19,38,41	0.84	1 (5%)
11	A2M	AA	2946	11,83	18,25,26	3.58	8 (44%)	18,36,39	3.34	3 (16%)
11	OMC	AA	1437	11,83	19,22,23	0.53	0	26,31,34	0.80	1 (3%)
11	OMU	AA	2729	11	19,22,23	3.05	8 (42%)	26,31,34	1.68	5 (19%)
11	1MA	AA	2142	11,83	16,25,26	0.94	2 (12%)	18,37,40	1.07	2 (11%)
58	A2M	c	619	83,58	18,25,26	3.60	7 (38%)	18,36,39	3.43	3 (16%)
58	OMC	c	1639	83,58	19,22,23	0.53	0	26,31,34	0.63	0
11	A2M	AA	2640	11	18,25,26	3.58	8 (44%)	18,36,39	3.34	4 (22%)
11	OMU	AA	2417	11	19,22,23	3.05	8 (42%)	26,31,34	1.68	5 (19%)
11	OMG	AA	908	11	18,26,27	1.13	2 (11%)	19,38,41	0.84	1 (5%)
58	OMG	c	562	58	18,26,27	1.10	2 (11%)	19,38,41	0.84	1 (5%)
11	A2M	AA	649	11	18,25,26	3.58	8 (44%)	18,36,39	3.36	4 (22%)
11	OMG	AA	2793	11	18,26,27	1.13	2 (11%)	19,38,41	0.85	1 (5%)
58	OMG	c	1572	58	18,26,27	1.12	2 (11%)	19,38,41	0.88	1 (5%)
58	OMG	c	1271	58	18,26,27	1.10	2 (11%)	19,38,41	0.88	1 (5%)
58	A2M	c	436	58	18,25,26	3.61	8 (44%)	18,36,39	3.38	4 (22%)
11	OMC	AA	2948	11	19,22,23	0.53	0	26,31,34	0.85	1 (3%)
11	OMC	AA	663	11	19,22,23	0.53	0	26,31,34	0.77	0
58	4AC	c	1773	58	21,24,25	3.54	10 (47%)	29,34,37	1.58	5 (17%)
11	OMU	AA	898	11	19,22,23	3.07	8 (42%)	26,31,34	1.68	5 (19%)
58	A2M	c	420	58	18,25,26	3.58	8 (44%)	18,36,39	3.34	3 (16%)
11	OMU	AA	2921	11,83	19,22,23	3.07	8 (42%)	26,31,34	1.70	5 (19%)
11	OMG	AA	2288	11	18,26,27	1.10	2 (11%)	19,38,41	0.81	1 (5%)
11	OMG	AA	1450	11	18,26,27	1.10	2 (11%)	19,38,41	0.80	1 (5%)
11	OMG	AA	805	11	18,26,27	1.10	2 (11%)	19,38,41	0.88	1 (5%)
58	MA6	c	1782	58	18,26,27	1.02	2 (11%)	19,38,41	3.49	2 (10%)

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
11	A2M	AA	2280	11	-	2/5/27/28	0/3/3/3
11	A2M	AA	1449	11,83	-	0/5/27/28	0/3/3/3
11	5MC	AA	2870	11,84	-	4/7/25/26	0/2/2/2
58	OMG	c	1428	58	-	2/5/27/28	0/3/3/3
11	A2M	AA	1133	11,83	-	0/5/27/28	0/3/3/3
11	OMU	AA	1888	11	-	0/9/27/28	0/2/2/2
58	A2M	c	796	58	-	2/5/27/28	0/3/3/3
11	A2M	AA	2220	11	-	1/5/27/28	0/3/3/3
11	OMG	AA	2922	11	-	2/5/27/28	0/3/3/3
58	B8N	c	1191	58	-	4/16/34/35	0/2/2/2
11	OMU	AA	2421	11	-	1/9/27/28	0/2/2/2
11	OMG	AA	2619	11,14	-	1/5/27/28	0/3/3/3
58	A2M	c	28	58	-	2/5/27/28	0/3/3/3
11	OMG	AA	2815	11	-	0/5/27/28	0/3/3/3
58	G7M	c	1575	58,14	-	3/3/25/26	0/3/3/3
58	A2M	c	974	58	-	0/5/27/28	0/3/3/3
11	OMC	AA	2197	11,84	-	4/9/27/28	0/2/2/2
11	5MC	AA	2278	11,83	-	0/7/25/26	0/2/2/2
58	A2M	c	541	58	-	1/5/27/28	0/3/3/3
11	OMC	AA	650	11	-	0/9/27/28	0/2/2/2
11	OMC	AA	2959	11,83	-	0/9/27/28	0/2/2/2
58	MA6	c	1781	58	-	0/7/29/30	0/3/3/3
11	A2M	AA	2256	11,58	-	1/5/27/28	0/3/3/3
11	1MA	AA	645	11,83	-	0/3/25/26	0/3/3/3
58	OMC	c	1007	58	-	0/9/27/28	0/2/2/2
11	A2M	AA	2281	11	-	1/5/27/28	0/3/3/3
11	OMU	AA	2724	11	-	1/9/27/28	0/2/2/2
58	OMU	c	1269	58	-	2/9/27/28	0/2/2/2
58	4AC	c	1280	58	-	2/11/29/30	0/2/2/2
11	A2M	AA	817	11,83	-	2/5/27/28	0/3/3/3
11	UR3	AA	2634	11	-	0/7/25/26	0/2/2/2
58	A2M	c	100	83,58	-	2/5/27/28	0/3/3/3
58	OMC	c	414	58	-	1/9/27/28	0/2/2/2
11	OMG	AA	867	11,84	-	2/5/27/28	0/3/3/3
58	OMG	c	1126	58	-	0/5/27/28	0/3/3/3
11	A2M	AA	807	11	-	2/5/27/28	0/3/3/3
58	OMU	c	578	58	-	1/9/27/28	0/2/2/2
11	A2M	AA	876	11	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMU	AA	2347	11	-	0/9/27/28	0/2/2/2
11	OMC	AA	2337	11	-	0/9/27/28	0/2/2/2
11	OMG	AA	2791	11	-	0/5/27/28	0/3/3/3
11	A2M	AA	2946	11,83	-	1/5/27/28	0/3/3/3
11	OMC	AA	1437	11,83	-	2/9/27/28	0/2/2/2
11	OMU	AA	2729	11	-	0/9/27/28	0/2/2/2
11	1MA	AA	2142	11,83	-	0/3/25/26	0/3/3/3
58	A2M	c	619	83,58	-	3/5/27/28	0/3/3/3
58	OMC	c	1639	83,58	-	0/9/27/28	0/2/2/2
11	A2M	AA	2640	11	-	1/5/27/28	0/3/3/3
11	OMU	AA	2417	11	-	1/9/27/28	0/2/2/2
11	OMG	AA	908	11	-	3/5/27/28	0/3/3/3
58	OMG	c	562	58	-	0/5/27/28	0/3/3/3
11	A2M	AA	649	11	-	2/5/27/28	0/3/3/3
11	OMG	AA	2793	11	-	0/5/27/28	0/3/3/3
58	OMG	c	1572	58	-	2/5/27/28	0/3/3/3
58	OMG	c	1271	58	-	4/5/27/28	0/3/3/3
58	A2M	c	436	58	-	0/5/27/28	0/3/3/3
11	OMC	AA	2948	11	-	0/9/27/28	0/2/2/2
11	OMC	AA	663	11	-	1/9/27/28	0/2/2/2
58	4AC	c	1773	58	-	2/11/29/30	0/2/2/2
11	OMU	AA	898	11	-	0/9/27/28	0/2/2/2
58	A2M	c	420	58	-	1/5/27/28	0/3/3/3
11	OMU	AA	2921	11,83	-	0/9/27/28	0/2/2/2
11	OMG	AA	2288	11	-	0/5/27/28	0/3/3/3
11	OMG	AA	1450	11	-	2/5/27/28	0/3/3/3
11	OMG	AA	805	11	-	0/5/27/28	0/3/3/3
58	MA6	c	1782	58	-	1/7/29/30	0/3/3/3

All (318) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	c	28	A2M	C3'-C4'	-8.97	1.30	1.53
11	AA	807	A2M	C3'-C4'	-8.90	1.30	1.53
58	c	541	A2M	C3'-C4'	-8.83	1.30	1.53
11	AA	2220	A2M	C3'-C4'	-8.80	1.30	1.53
11	AA	1133	A2M	C3'-C4'	-8.79	1.30	1.53
58	c	100	A2M	C3'-C4'	-8.75	1.30	1.53
58	c	619	A2M	C3'-C4'	-8.75	1.30	1.53
11	AA	817	A2M	C3'-C4'	-8.75	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	c	796	A2M	C3'-C4'	-8.74	1.30	1.53
58	c	974	A2M	C3'-C4'	-8.73	1.30	1.53
11	AA	2946	A2M	C3'-C4'	-8.73	1.30	1.53
58	c	420	A2M	C3'-C4'	-8.70	1.30	1.53
11	AA	1449	A2M	C3'-C4'	-8.70	1.30	1.53
58	c	436	A2M	C3'-C4'	-8.70	1.30	1.53
11	AA	2640	A2M	C3'-C4'	-8.69	1.30	1.53
11	AA	876	A2M	C3'-C4'	-8.67	1.30	1.53
11	AA	2280	A2M	C3'-C4'	-8.64	1.30	1.53
11	AA	649	A2M	C3'-C4'	-8.58	1.31	1.53
11	AA	2256	A2M	C3'-C4'	-8.49	1.31	1.53
11	AA	2281	A2M	C3'-C4'	-8.34	1.31	1.53
58	c	1191	B8N	C6-N1	7.89	1.56	1.36
11	AA	2946	A2M	O4'-C4'	7.79	1.62	1.45
11	AA	1133	A2M	O4'-C4'	7.78	1.62	1.45
58	c	796	A2M	O4'-C4'	7.77	1.62	1.45
58	c	100	A2M	O4'-C4'	7.77	1.62	1.45
58	c	436	A2M	O4'-C4'	7.76	1.62	1.45
11	AA	2281	A2M	O4'-C1'	-7.76	1.30	1.41
58	c	420	A2M	O4'-C4'	7.74	1.62	1.45
11	AA	2640	A2M	O4'-C4'	7.72	1.62	1.45
58	c	1191	B8N	C4-N3	-7.72	1.26	1.40
58	c	974	A2M	O4'-C4'	7.72	1.62	1.45
11	AA	2281	A2M	O4'-C4'	7.71	1.62	1.45
11	AA	876	A2M	O4'-C4'	7.70	1.62	1.45
11	AA	1449	A2M	O4'-C4'	7.70	1.62	1.45
11	AA	649	A2M	O4'-C4'	7.68	1.62	1.45
11	AA	2220	A2M	O4'-C4'	7.67	1.62	1.45
11	AA	2256	A2M	O4'-C4'	7.66	1.62	1.45
58	c	28	A2M	O4'-C4'	7.65	1.62	1.45
11	AA	2280	A2M	O4'-C4'	7.64	1.62	1.45
58	c	541	A2M	O4'-C4'	7.60	1.62	1.45
11	AA	817	A2M	O4'-C4'	7.53	1.61	1.45
11	AA	807	A2M	O4'-C4'	7.52	1.61	1.45
58	c	619	A2M	O4'-C1'	-7.42	1.30	1.41
11	AA	2256	A2M	O4'-C1'	-7.39	1.30	1.41
58	c	1280	4AC	C4-N3	7.37	1.45	1.32
58	c	619	A2M	O4'-C4'	7.36	1.61	1.45
11	AA	2347	OMU	C2-N1	7.29	1.50	1.38
58	c	1773	4AC	C4-N3	7.29	1.45	1.32
58	c	1269	OMU	C2-N1	7.28	1.50	1.38
11	AA	2421	OMU	C2-N1	7.23	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2724	OMU	C2-N1	7.23	1.50	1.38
58	c	436	A2M	O4'-C1'	-7.21	1.31	1.41
11	AA	649	A2M	O4'-C1'	-7.21	1.31	1.41
58	c	578	OMU	C2-N1	7.20	1.50	1.38
11	AA	1888	OMU	C2-N1	7.18	1.50	1.38
11	AA	2921	OMU	C2-N1	7.15	1.49	1.38
11	AA	2280	A2M	O4'-C1'	-7.14	1.31	1.41
11	AA	898	OMU	C2-N1	7.10	1.49	1.38
11	AA	876	A2M	O4'-C1'	-7.08	1.31	1.41
11	AA	2417	OMU	C2-N1	7.05	1.49	1.38
11	AA	1449	A2M	O4'-C1'	-7.04	1.31	1.41
11	AA	2729	OMU	C2-N1	7.03	1.49	1.38
11	AA	807	A2M	O4'-C1'	-7.03	1.31	1.41
58	c	1773	4AC	C6-C5	7.03	1.51	1.35
11	AA	2640	A2M	O4'-C1'	-7.02	1.31	1.41
11	AA	817	A2M	O4'-C1'	-7.02	1.31	1.41
58	c	420	A2M	O4'-C1'	-7.00	1.31	1.41
58	c	796	A2M	O4'-C1'	-6.97	1.31	1.41
11	AA	2634	UR3	C2-N1	6.95	1.48	1.38
58	c	541	A2M	O4'-C1'	-6.91	1.31	1.41
58	c	28	A2M	O4'-C1'	-6.91	1.31	1.41
11	AA	2220	A2M	O4'-C1'	-6.89	1.31	1.41
58	c	974	A2M	O4'-C1'	-6.89	1.31	1.41
11	AA	1133	A2M	O4'-C1'	-6.88	1.31	1.41
58	c	578	OMU	C2-N3	6.87	1.50	1.38
11	AA	898	OMU	C2-N3	6.87	1.50	1.38
11	AA	2946	A2M	O4'-C1'	-6.87	1.31	1.41
58	c	1269	OMU	C2-N3	6.86	1.50	1.38
58	c	100	A2M	O4'-C1'	-6.86	1.31	1.41
58	c	1280	4AC	C6-C5	6.86	1.51	1.35
11	AA	2724	OMU	C2-N3	6.86	1.50	1.38
11	AA	2634	UR3	C6-C5	6.83	1.50	1.35
11	AA	2421	OMU	C2-N3	6.82	1.50	1.38
11	AA	2417	OMU	C2-N3	6.80	1.50	1.38
11	AA	2921	OMU	C2-N3	6.80	1.50	1.38
11	AA	2347	OMU	C2-N3	6.79	1.50	1.38
11	AA	1888	OMU	C2-N3	6.78	1.50	1.38
11	AA	2729	OMU	C2-N3	6.76	1.50	1.38
58	c	1191	B8N	C2-N1	5.87	1.56	1.39
11	AA	2634	UR3	C2-N3	5.87	1.50	1.39
11	AA	1888	OMU	C6-C5	5.75	1.48	1.35
11	AA	2729	OMU	C6-C5	5.74	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	c	578	OMU	C6-C5	5.73	1.48	1.35
11	AA	2921	OMU	C6-C5	5.73	1.48	1.35
11	AA	898	OMU	C6-C5	5.72	1.48	1.35
58	c	1269	OMU	C6-C5	5.70	1.48	1.35
58	c	1280	4AC	C7-N4	5.70	1.47	1.37
11	AA	2421	OMU	C6-C5	5.69	1.48	1.35
11	AA	2417	OMU	C6-C5	5.69	1.48	1.35
11	AA	2724	OMU	C6-C5	5.68	1.48	1.35
58	c	1773	4AC	C7-N4	5.67	1.47	1.37
11	AA	2347	OMU	C6-C5	5.65	1.48	1.35
58	c	1191	B8N	C6-C5	5.55	1.42	1.34
58	c	1773	4AC	C4-N4	5.37	1.47	1.39
58	c	1575	G7M	C2-N3	5.36	1.46	1.33
58	c	1280	4AC	C4-N4	5.28	1.47	1.39
58	c	1280	4AC	C2-N3	5.09	1.46	1.36
58	c	1280	4AC	C2-N1	5.02	1.50	1.40
58	c	1773	4AC	C2-N1	5.01	1.50	1.40
58	c	1773	4AC	C2-N3	5.00	1.46	1.36
58	c	1575	G7M	C4-N3	4.94	1.49	1.37
58	c	1575	G7M	C2-N2	4.67	1.45	1.34
58	c	578	OMU	C4-N3	4.34	1.46	1.38
11	AA	898	OMU	C4-N3	4.29	1.46	1.38
11	AA	2724	OMU	C4-N3	4.28	1.46	1.38
11	AA	2729	OMU	C4-N3	4.27	1.46	1.38
11	AA	2417	OMU	C4-N3	4.26	1.46	1.38
58	c	1269	OMU	C4-N3	4.26	1.46	1.38
11	AA	2921	OMU	C4-N3	4.26	1.46	1.38
11	AA	2347	OMU	C4-N3	4.22	1.46	1.38
11	AA	2421	OMU	C4-N3	4.22	1.46	1.38
58	c	1280	4AC	CM7-C7	4.19	1.59	1.50
11	AA	1888	OMU	C4-N3	4.18	1.46	1.38
58	c	1773	4AC	C5-C4	4.12	1.49	1.40
58	c	1280	4AC	C5-C4	4.12	1.49	1.40
58	c	1773	4AC	CM7-C7	3.97	1.58	1.50
58	c	1191	B8N	C1'-C5	3.79	1.58	1.50
58	c	1575	G7M	C6-N1	3.77	1.43	1.37
11	AA	2634	UR3	C6-N1	3.40	1.46	1.38
58	c	1575	G7M	C5-C6	3.29	1.53	1.45
11	AA	2256	A2M	C6-N6	3.17	1.45	1.34
58	c	28	A2M	C6-N6	3.17	1.45	1.34
58	c	436	A2M	C6-N6	3.15	1.45	1.34
58	c	420	A2M	C6-N6	3.15	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	c	796	A2M	C6-N6	3.15	1.45	1.34
11	AA	1449	A2M	C6-N6	3.14	1.45	1.34
11	AA	2280	A2M	C6-N6	3.14	1.45	1.34
58	c	541	A2M	C6-N6	3.14	1.45	1.34
11	AA	876	A2M	C6-N6	3.14	1.45	1.34
11	AA	2640	A2M	C6-N6	3.14	1.45	1.34
58	c	619	A2M	C6-N6	3.13	1.45	1.34
11	AA	807	A2M	C6-N6	3.13	1.45	1.34
11	AA	2220	A2M	C6-N6	3.13	1.45	1.34
58	c	974	A2M	C6-N6	3.12	1.45	1.34
11	AA	2946	A2M	C6-N6	3.12	1.45	1.34
58	c	100	A2M	C6-N6	3.12	1.45	1.34
11	AA	1133	A2M	C6-N6	3.11	1.45	1.34
11	AA	817	A2M	C6-N6	3.11	1.45	1.34
11	AA	649	A2M	C6-N6	3.10	1.45	1.34
11	AA	1449	A2M	O3'-C3'	3.02	1.50	1.43
58	c	436	A2M	O3'-C3'	3.00	1.50	1.43
11	AA	2281	A2M	C6-N6	3.00	1.45	1.34
11	AA	2280	A2M	O3'-C3'	2.99	1.50	1.43
58	c	619	A2M	O3'-C3'	2.98	1.50	1.43
11	AA	2347	OMU	C6-N1	2.96	1.45	1.38
11	AA	898	OMU	O4-C4	-2.95	1.18	1.24
11	AA	2921	OMU	C6-N1	2.94	1.45	1.38
11	AA	1888	OMU	O4-C4	-2.94	1.18	1.24
11	AA	2281	A2M	O3'-C3'	2.93	1.49	1.43
11	AA	876	A2M	O3'-C3'	2.93	1.49	1.43
11	AA	1888	OMU	C6-N1	2.93	1.45	1.38
58	c	578	OMU	C6-N1	2.93	1.45	1.38
11	AA	2347	OMU	O4-C4	-2.92	1.18	1.24
11	AA	2417	OMU	C6-N1	2.92	1.45	1.38
11	AA	2256	A2M	O3'-C3'	2.92	1.49	1.43
11	AA	2921	OMU	O4-C4	-2.92	1.18	1.24
58	c	420	A2M	O3'-C3'	2.91	1.49	1.43
11	AA	2729	OMU	C6-N1	2.91	1.45	1.38
11	AA	2421	OMU	C6-N1	2.91	1.45	1.38
58	c	796	A2M	O3'-C3'	2.91	1.49	1.43
11	AA	2729	OMU	O4-C4	-2.91	1.18	1.24
58	c	1269	OMU	C6-N1	2.90	1.45	1.38
58	c	1269	OMU	O4-C4	-2.90	1.18	1.24
58	c	100	A2M	O3'-C3'	2.90	1.49	1.43
11	AA	2640	A2M	O3'-C3'	2.90	1.49	1.43
11	AA	1133	A2M	O3'-C3'	2.90	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	c	578	OMU	O4-C4	-2.90	1.18	1.24
11	AA	2417	OMU	O4-C4	-2.89	1.18	1.24
11	AA	908	OMG	C8-N7	-2.89	1.30	1.35
11	AA	2724	OMU	O4-C4	-2.88	1.18	1.24
11	AA	2724	OMU	C6-N1	2.88	1.44	1.38
11	AA	898	OMU	C6-N1	2.88	1.44	1.38
11	AA	2220	A2M	O3'-C3'	2.87	1.49	1.43
11	AA	2922	OMG	C8-N7	-2.87	1.30	1.35
58	c	541	A2M	O3'-C3'	2.87	1.49	1.43
11	AA	2946	A2M	O3'-C3'	2.87	1.49	1.43
11	AA	2421	OMU	O4-C4	-2.86	1.18	1.24
11	AA	807	A2M	O3'-C3'	2.86	1.49	1.43
11	AA	649	A2M	O3'-C3'	2.85	1.49	1.43
58	c	974	A2M	O3'-C3'	2.84	1.49	1.43
11	AA	2288	OMG	C8-N7	-2.84	1.30	1.35
58	c	28	A2M	O3'-C3'	2.83	1.49	1.43
11	AA	2619	OMG	C8-N7	-2.82	1.30	1.35
11	AA	2281	A2M	C5-C4	-2.81	1.33	1.40
11	AA	817	A2M	O3'-C3'	2.81	1.49	1.43
11	AA	2791	OMG	C8-N7	-2.78	1.30	1.35
11	AA	2793	OMG	C8-N7	-2.74	1.30	1.35
11	AA	867	OMG	C8-N7	-2.73	1.30	1.35
58	c	562	OMG	C8-N7	-2.73	1.30	1.35
11	AA	1450	OMG	C8-N7	-2.71	1.30	1.35
58	c	1575	G7M	C2-N1	2.71	1.44	1.37
58	c	1126	OMG	C8-N7	-2.70	1.30	1.35
11	AA	2815	OMG	C8-N7	-2.70	1.30	1.35
58	c	1428	OMG	C8-N7	-2.70	1.30	1.35
58	c	619	A2M	C5-C4	-2.68	1.33	1.40
58	c	28	A2M	O2'-C2'	-2.66	1.35	1.42
58	c	1271	OMG	C8-N7	-2.66	1.30	1.35
58	c	100	A2M	C5-C4	-2.65	1.33	1.40
58	c	796	A2M	C5-C4	-2.65	1.33	1.40
11	AA	649	A2M	C5-C4	-2.65	1.33	1.40
58	c	1773	4AC	C6-N1	2.65	1.44	1.38
11	AA	2946	A2M	C5-C4	-2.64	1.33	1.40
11	AA	2280	A2M	C5-C4	-2.64	1.33	1.40
11	AA	807	A2M	C5-C4	-2.64	1.33	1.40
11	AA	1133	A2M	C5-C4	-2.64	1.33	1.40
11	AA	2220	A2M	C5-C4	-2.64	1.33	1.40
58	c	1782	MA6	C5-C4	-2.64	1.33	1.40
11	AA	817	A2M	C5-C4	-2.64	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	805	OMG	C8-N7	-2.64	1.30	1.35
58	c	974	A2M	C5-C4	-2.63	1.34	1.40
58	c	796	A2M	O2'-C2'	-2.63	1.35	1.42
11	AA	1449	A2M	C5-C4	-2.63	1.34	1.40
11	AA	2640	A2M	C5-C4	-2.62	1.34	1.40
11	AA	2256	A2M	C5-C4	-2.61	1.34	1.40
11	AA	807	A2M	O2'-C2'	-2.61	1.35	1.42
11	AA	1449	A2M	O2'-C2'	-2.61	1.35	1.42
58	c	28	A2M	C5-C4	-2.60	1.34	1.40
58	c	436	A2M	C5-C4	-2.60	1.34	1.40
11	AA	876	A2M	C5-C4	-2.60	1.34	1.40
58	c	420	A2M	C5-C4	-2.59	1.34	1.40
11	AA	2281	A2M	O2'-C2'	-2.59	1.36	1.42
11	AA	817	A2M	O2'-C2'	-2.58	1.36	1.42
11	AA	876	A2M	O2'-C2'	-2.57	1.36	1.42
11	AA	1133	A2M	O2'-C2'	-2.57	1.36	1.42
58	c	974	A2M	O2'-C2'	-2.57	1.36	1.42
58	c	1572	OMG	C8-N7	-2.57	1.30	1.35
58	c	541	A2M	O2'-C2'	-2.57	1.36	1.42
58	c	1781	MA6	C5-C4	-2.57	1.34	1.40
58	c	541	A2M	C5-C4	-2.56	1.34	1.40
11	AA	2256	A2M	O2'-C2'	-2.56	1.36	1.42
58	c	619	A2M	O2'-C2'	-2.55	1.36	1.42
11	AA	2946	A2M	O2'-C2'	-2.54	1.36	1.42
58	c	436	A2M	O2'-C2'	-2.54	1.36	1.42
58	c	1280	4AC	C6-N1	2.53	1.44	1.38
11	AA	2280	A2M	O2'-C2'	-2.52	1.36	1.42
58	c	100	A2M	O2'-C2'	-2.52	1.36	1.42
58	c	1781	MA6	C2-N3	2.52	1.36	1.32
11	AA	2142	1MA	C8-N7	-2.51	1.30	1.35
11	AA	2220	A2M	O2'-C2'	-2.51	1.36	1.42
11	AA	2640	A2M	O2'-C2'	-2.50	1.36	1.42
11	AA	649	A2M	O2'-C2'	-2.47	1.36	1.42
58	c	420	A2M	O2'-C2'	-2.46	1.36	1.42
11	AA	1888	OMU	C5-C4	2.46	1.49	1.43
58	c	578	OMU	C5-C4	2.45	1.49	1.43
11	AA	2347	OMU	O2-C2	-2.45	1.18	1.23
58	c	1269	OMU	O2-C2	-2.45	1.18	1.23
11	AA	2921	OMU	C5-C4	2.44	1.49	1.43
11	AA	645	1MA	C8-N7	-2.44	1.30	1.35
11	AA	2421	OMU	C5-C4	2.41	1.49	1.43
11	AA	898	OMU	C5-C4	2.41	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2729	OMU	C5-C4	2.40	1.48	1.43
11	AA	2417	OMU	C5-C4	2.40	1.48	1.43
58	c	1269	OMU	C5-C4	2.39	1.48	1.43
11	AA	2347	OMU	C5-C4	2.39	1.48	1.43
11	AA	898	OMU	O2-C2	-2.39	1.18	1.23
11	AA	2417	OMU	O2-C2	-2.39	1.18	1.23
11	AA	2724	OMU	O2-C2	-2.39	1.18	1.23
11	AA	908	OMG	C5-C6	-2.38	1.42	1.47
58	c	1782	MA6	C2-N3	2.37	1.35	1.32
58	c	1428	OMG	C5-C6	-2.36	1.42	1.47
11	AA	1888	OMU	O2-C2	-2.36	1.18	1.23
11	AA	2729	OMU	O2-C2	-2.35	1.18	1.23
11	AA	2922	OMG	C5-C6	-2.35	1.42	1.47
11	AA	2421	OMU	O2-C2	-2.35	1.18	1.23
11	AA	2619	OMG	C5-C6	-2.34	1.42	1.47
11	AA	2921	OMU	O2-C2	-2.34	1.18	1.23
11	AA	2793	OMG	C5-C6	-2.32	1.42	1.47
11	AA	1450	OMG	C5-C6	-2.31	1.42	1.47
11	AA	867	OMG	C5-C6	-2.30	1.42	1.47
11	AA	2724	OMU	C5-C4	2.29	1.48	1.43
11	AA	2634	UR3	C4-N3	2.29	1.45	1.40
58	c	1126	OMG	C5-C6	-2.29	1.42	1.47
11	AA	2791	OMG	C5-C6	-2.28	1.42	1.47
11	AA	2815	OMG	C5-C6	-2.28	1.42	1.47
58	c	578	OMU	O2-C2	-2.27	1.18	1.23
58	c	562	OMG	C5-C6	-2.27	1.42	1.47
58	c	1271	OMG	C5-C6	-2.26	1.42	1.47
58	c	1572	OMG	C5-C6	-2.26	1.42	1.47
58	c	1575	G7M	O6-C6	-2.25	1.18	1.23
11	AA	2288	OMG	C5-C6	-2.25	1.42	1.47
11	AA	805	OMG	C5-C6	-2.24	1.42	1.47
58	c	100	A2M	C2-N3	2.24	1.35	1.32
58	c	1773	4AC	O7-C7	-2.24	1.18	1.23
11	AA	2634	UR3	C5-C4	2.24	1.49	1.43
58	c	541	A2M	C2-N3	2.23	1.35	1.32
11	AA	645	1MA	C5-C4	-2.23	1.37	1.43
11	AA	2640	A2M	C2-N3	2.23	1.35	1.32
58	c	28	A2M	C2-N3	2.23	1.35	1.32
58	c	1280	4AC	O7-C7	-2.22	1.18	1.23
11	AA	2142	1MA	C5-C4	-2.22	1.37	1.43
58	c	796	A2M	C2-N3	2.20	1.35	1.32
11	AA	2256	A2M	C2-N3	2.20	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	2281	A2M	C2-N3	2.19	1.35	1.32
11	AA	2280	A2M	C2-N3	2.19	1.35	1.32
11	AA	876	A2M	C2-N3	2.17	1.35	1.32
11	AA	2946	A2M	C2-N3	2.16	1.35	1.32
11	AA	2220	A2M	C2-N3	2.16	1.35	1.32
58	c	436	A2M	C2-N3	2.16	1.35	1.32
11	AA	1449	A2M	C2-N3	2.14	1.35	1.32
11	AA	649	A2M	C2-N3	2.12	1.35	1.32
58	c	420	A2M	C2-N3	2.11	1.35	1.32
11	AA	817	A2M	C2-N3	2.10	1.35	1.32
58	c	974	A2M	C2-N3	2.09	1.35	1.32
58	c	1191	B8N	O4-C4	-2.07	1.18	1.23
11	AA	1133	A2M	C2-N3	2.05	1.35	1.32
58	c	28	A2M	O5'-C5'	-2.01	1.39	1.44
11	AA	807	A2M	C2-N3	2.01	1.35	1.32
58	c	1191	B8N	O2-C2	-2.00	1.18	1.22

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	c	1782	MA6	N1-C6-N6	-13.91	102.42	117.06
58	c	1781	MA6	N1-C6-N6	-13.44	102.91	117.06
11	AA	817	A2M	C5-C6-N6	10.80	136.76	120.35
11	AA	807	A2M	C5-C6-N6	10.77	136.72	120.35
11	AA	1133	A2M	C5-C6-N6	10.73	136.66	120.35
58	c	619	A2M	C5-C6-N6	10.70	136.61	120.35
58	c	974	A2M	C5-C6-N6	10.64	136.53	120.35
11	AA	1449	A2M	C5-C6-N6	10.64	136.52	120.35
11	AA	2220	A2M	C5-C6-N6	10.59	136.44	120.35
58	c	436	A2M	C5-C6-N6	10.58	136.43	120.35
58	c	420	A2M	C5-C6-N6	10.58	136.43	120.35
11	AA	876	A2M	C5-C6-N6	10.58	136.43	120.35
58	c	28	A2M	C5-C6-N6	10.57	136.42	120.35
58	c	100	A2M	C5-C6-N6	10.56	136.40	120.35
58	c	796	A2M	C5-C6-N6	10.56	136.39	120.35
11	AA	2256	A2M	C5-C6-N6	10.55	136.38	120.35
11	AA	649	A2M	C5-C6-N6	10.55	136.38	120.35
11	AA	2946	A2M	C5-C6-N6	10.51	136.32	120.35
11	AA	2280	A2M	C5-C6-N6	10.50	136.31	120.35
58	c	541	A2M	C5-C6-N6	10.45	136.24	120.35
11	AA	2640	A2M	C5-C6-N6	10.45	136.23	120.35
11	AA	2281	A2M	C5-C6-N6	10.35	136.09	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	817	A2M	N6-C6-N1	-7.43	103.16	118.57
11	AA	1449	A2M	N6-C6-N1	-7.28	103.46	118.57
11	AA	807	A2M	N6-C6-N1	-7.26	103.51	118.57
11	AA	2281	A2M	N6-C6-N1	-7.25	103.53	118.57
58	c	619	A2M	N6-C6-N1	-7.23	103.58	118.57
11	AA	2280	A2M	N6-C6-N1	-7.21	103.60	118.57
58	c	436	A2M	N6-C6-N1	-7.21	103.61	118.57
58	c	974	A2M	N6-C6-N1	-7.21	103.61	118.57
58	c	28	A2M	N6-C6-N1	-7.21	103.61	118.57
58	c	100	A2M	N6-C6-N1	-7.20	103.63	118.57
11	AA	1133	A2M	N6-C6-N1	-7.20	103.63	118.57
11	AA	649	A2M	N6-C6-N1	-7.19	103.64	118.57
58	c	541	A2M	N6-C6-N1	-7.19	103.65	118.57
11	AA	876	A2M	N6-C6-N1	-7.19	103.65	118.57
58	c	796	A2M	N6-C6-N1	-7.19	103.65	118.57
11	AA	2220	A2M	N6-C6-N1	-7.18	103.67	118.57
11	AA	2256	A2M	N6-C6-N1	-7.17	103.70	118.57
58	c	420	A2M	N6-C6-N1	-7.16	103.72	118.57
11	AA	2946	A2M	N6-C6-N1	-7.12	103.80	118.57
11	AA	2640	A2M	N6-C6-N1	-7.12	103.81	118.57
58	c	619	A2M	N3-C2-N1	-5.70	119.77	128.68
11	AA	1133	A2M	N3-C2-N1	-5.67	119.82	128.68
11	AA	2281	A2M	N3-C2-N1	-5.62	119.90	128.68
58	c	974	A2M	N3-C2-N1	-5.60	119.92	128.68
11	AA	2256	A2M	N3-C2-N1	-5.58	119.96	128.68
11	AA	2220	A2M	N3-C2-N1	-5.56	119.99	128.68
58	c	1280	4AC	CM7-C7-N4	5.55	124.90	115.29
11	AA	817	A2M	N3-C2-N1	-5.55	120.01	128.68
11	AA	649	A2M	N3-C2-N1	-5.52	120.05	128.68
58	c	100	A2M	N3-C2-N1	-5.51	120.06	128.68
58	c	28	A2M	N3-C2-N1	-5.50	120.08	128.68
58	c	1773	4AC	CM7-C7-N4	5.50	124.81	115.29
11	AA	1449	A2M	N3-C2-N1	-5.49	120.09	128.68
58	c	420	A2M	N3-C2-N1	-5.48	120.11	128.68
11	AA	2280	A2M	N3-C2-N1	-5.48	120.11	128.68
58	c	436	A2M	N3-C2-N1	-5.48	120.12	128.68
11	AA	2640	A2M	N3-C2-N1	-5.47	120.13	128.68
58	c	1782	MA6	N3-C2-N1	-5.46	120.14	128.68
11	AA	876	A2M	N3-C2-N1	-5.46	120.14	128.68
11	AA	2946	A2M	N3-C2-N1	-5.44	120.18	128.68
58	c	541	A2M	N3-C2-N1	-5.44	120.18	128.68
58	c	1781	MA6	N3-C2-N1	-5.42	120.21	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
58	c	796	A2M	N3-C2-N1	-5.36	120.29	128.68
11	AA	1888	OMU	C4-N3-C2	-5.23	119.69	126.58
11	AA	807	A2M	N3-C2-N1	-5.23	120.51	128.68
11	AA	2421	OMU	C4-N3-C2	-5.19	119.74	126.58
11	AA	2921	OMU	C4-N3-C2	-5.14	119.80	126.58
58	c	578	OMU	C4-N3-C2	-5.14	119.80	126.58
11	AA	2417	OMU	C4-N3-C2	-5.11	119.84	126.58
11	AA	2729	OMU	C4-N3-C2	-5.08	119.88	126.58
11	AA	898	OMU	C4-N3-C2	-5.06	119.90	126.58
11	AA	2347	OMU	C4-N3-C2	-5.01	119.97	126.58
58	c	1191	B8N	C5-C4-N3	5.00	125.43	116.17
11	AA	2724	OMU	C4-N3-C2	-4.99	120.00	126.58
58	c	1269	OMU	C4-N3-C2	-4.98	120.01	126.58
11	AA	2634	UR3	C4-N3-C2	-4.93	119.92	124.56
58	c	1191	B8N	C4-N3-C2	-4.03	120.36	125.46
11	AA	1888	OMU	N3-C2-N1	3.91	120.08	114.89
11	AA	2921	OMU	N3-C2-N1	3.91	120.07	114.89
11	AA	2347	OMU	N3-C2-N1	3.87	120.03	114.89
11	AA	2421	OMU	N3-C2-N1	3.82	119.96	114.89
11	AA	2417	OMU	N3-C2-N1	3.81	119.94	114.89
11	AA	898	OMU	N3-C2-N1	3.80	119.94	114.89
11	AA	2729	OMU	N3-C2-N1	3.74	119.86	114.89
11	AA	2724	OMU	N3-C2-N1	3.74	119.86	114.89
58	c	1269	OMU	N3-C2-N1	3.67	119.77	114.89
58	c	578	OMU	N3-C2-N1	3.62	119.69	114.89
58	c	578	OMU	C5-C4-N3	3.35	119.85	114.84
11	AA	1888	OMU	C5-C4-N3	3.29	119.76	114.84
11	AA	2417	OMU	C5-C4-N3	3.25	119.70	114.84
11	AA	2421	OMU	C5-C4-N3	3.24	119.69	114.84
11	AA	2921	OMU	C5-C4-N3	3.24	119.68	114.84
58	c	1269	OMU	C5-C4-N3	3.22	119.66	114.84
11	AA	2729	OMU	C5-C4-N3	3.22	119.65	114.84
11	AA	898	OMU	C5-C4-N3	3.20	119.63	114.84
11	AA	2724	OMU	C5-C4-N3	3.20	119.63	114.84
11	AA	2347	OMU	C5-C4-N3	3.14	119.53	114.84
58	c	1575	G7M	C2-N1-C6	-2.97	119.62	125.10
58	c	1280	4AC	C6-C5-C4	2.96	120.58	116.96
11	AA	2724	OMU	O4-C4-C5	-2.95	119.98	125.16
11	AA	898	OMU	O4-C4-C5	-2.93	120.00	125.16
58	c	578	OMU	O4-C4-C5	-2.93	120.01	125.16
58	c	1191	B8N	N3-C2-N1	2.92	120.88	116.76
11	AA	2417	OMU	O4-C4-C5	-2.90	120.06	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AA	2921	OMU	O4-C4-C5	-2.88	120.09	125.16
58	c	1269	OMU	O4-C4-C5	-2.87	120.11	125.16
11	AA	2729	OMU	O4-C4-C5	-2.86	120.12	125.16
11	AA	1888	OMU	O4-C4-C5	-2.86	120.12	125.16
11	AA	2347	OMU	O4-C4-C5	-2.86	120.13	125.16
11	AA	2421	OMU	O4-C4-C5	-2.85	120.14	125.16
58	c	1773	4AC	C5-C4-N3	-2.84	118.02	122.59
58	c	1280	4AC	O7-C7-N4	-2.71	117.43	121.82
58	c	1191	B8N	O4-C4-N3	-2.67	115.44	119.98
11	AA	2281	A2M	O4'-C1'-C2'	-2.67	101.96	106.59
58	c	541	A2M	C1'-N9-C4	2.65	131.31	126.64
58	c	1280	4AC	C5-C4-N3	-2.65	118.33	122.59
11	AA	2948	OMC	C1'-N1-C2	2.57	124.15	118.42
58	c	1773	4AC	O7-C7-CM7	-2.54	117.33	122.06
58	c	1269	OMU	C1'-N1-C2	2.54	122.17	117.57
58	c	1773	4AC	C6-C5-C4	2.52	120.04	116.96
11	AA	876	A2M	C1'-N9-C4	2.51	131.05	126.64
11	AA	2142	1MA	N1-C6-N6	2.46	126.03	119.77
58	c	1773	4AC	O7-C7-N4	-2.44	117.86	121.82
58	c	1428	OMG	O6-C6-C5	2.42	129.09	124.37
58	c	1271	OMG	O6-C6-C5	2.38	129.03	124.37
11	AA	2815	OMG	O6-C6-C5	2.38	129.03	124.37
11	AA	2640	A2M	C1'-N9-C4	2.37	130.80	126.64
11	AA	867	OMG	O6-C6-C5	2.36	128.99	124.37
58	c	1280	4AC	O7-C7-CM7	-2.36	117.67	122.06
11	AA	2619	OMG	O6-C6-C5	2.36	128.98	124.37
11	AA	1437	OMC	C1'-N1-C2	2.35	123.67	118.42
58	c	1572	OMG	O6-C6-C5	2.35	128.95	124.37
11	AA	805	OMG	O6-C6-C5	2.34	128.94	124.37
11	AA	2793	OMG	O6-C6-C5	2.33	128.93	124.37
58	c	1126	OMG	O6-C6-C5	2.32	128.91	124.37
58	c	562	OMG	O6-C6-C5	2.32	128.91	124.37
58	c	28	A2M	C1'-N9-C4	2.32	130.72	126.64
11	AA	2922	OMG	O6-C6-C5	2.31	128.88	124.37
11	AA	645	1MA	N1-C6-N6	2.31	125.63	119.77
58	c	1191	B8N	O4'-C1'-C2'	2.31	108.39	105.14
11	AA	2791	OMG	O6-C6-C5	2.30	128.86	124.37
11	AA	1450	OMG	O6-C6-C5	2.30	128.86	124.37
11	AA	2288	OMG	O6-C6-C5	2.29	128.85	124.37
11	AA	908	OMG	O6-C6-C5	2.25	128.76	124.37
11	AA	2256	A2M	C2'-C3'-C4'	2.19	106.75	101.99
11	AA	1888	OMU	O2-C2-N1	-2.17	119.90	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AA	2347	OMU	C1’-N1-C2	2.17	121.50	117.57
11	AA	898	OMU	O2-C2-N1	-2.16	119.92	122.79
11	AA	1449	A2M	C1’-N9-C4	2.15	130.41	126.64
11	AA	2417	OMU	O2-C2-N1	-2.14	119.94	122.79
11	AA	2729	OMU	O2-C2-N1	-2.13	119.96	122.79
11	AA	2634	UR3	C6-N1-C2	-2.12	119.89	121.79
11	AA	645	1MA	C5-C6-N1	-2.11	110.75	113.90
11	AA	2921	OMU	O2-C2-N1	-2.10	119.99	122.79
11	AA	2142	1MA	C5-C6-N1	-2.09	110.78	113.90
58	c	100	A2M	C1’-N9-C4	2.08	130.29	126.64
11	AA	2724	OMU	O2-C2-N1	-2.05	120.06	122.79
58	c	436	A2M	C1’-N9-C4	2.03	130.21	126.64
58	c	796	A2M	C1’-N9-C4	2.02	130.19	126.64
11	AA	807	A2M	C1’-N9-C4	2.02	130.19	126.64
58	c	1428	OMG	C5-C6-N1	-2.02	110.39	113.95
58	c	578	OMU	O2-C2-N1	-2.01	120.11	122.79
11	AA	649	A2M	C1’-N9-C4	2.01	130.18	126.64

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AA	649	A2M	C1’-C2’-O2’-CM’
11	AA	663	OMC	C1’-C2’-O2’-CM2
11	AA	867	OMG	C3’-C4’-C5’-O5’
11	AA	908	OMG	O4’-C4’-C5’-O5’
11	AA	1437	OMC	C1’-C2’-O2’-CM2
11	AA	1450	OMG	O4’-C4’-C5’-O5’
11	AA	2197	OMC	C2’-C1’-N1-C6
11	AA	2220	A2M	C1’-C2’-O2’-CM’
11	AA	2417	OMU	C1’-C2’-O2’-CM2
11	AA	2421	OMU	C1’-C2’-O2’-CM2
11	AA	2619	OMG	C1’-C2’-O2’-CM2
11	AA	2640	A2M	C1’-C2’-O2’-CM’
11	AA	2724	OMU	C1’-C2’-O2’-CM2
58	c	28	A2M	C3’-C4’-C5’-O5’
58	c	414	OMC	C1’-C2’-O2’-CM2
58	c	420	A2M	C1’-C2’-O2’-CM’
58	c	578	OMU	C4’-C5’-O5’-P
58	c	619	A2M	C1’-C2’-O2’-CM’
58	c	1271	OMG	C1’-C2’-O2’-CM2
58	c	1572	OMG	O4’-C4’-C5’-O5’

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Mol	Chain	Res	Type	Atoms
58	c	1575	G7M	O4'-C4'-C5'-O5'
11	AA	908	OMG	C3'-C4'-C5'-O5'
11	AA	1450	OMG	C3'-C4'-C5'-O5'
11	AA	2256	A2M	O4'-C4'-C5'-O5'
11	AA	2922	OMG	C3'-C4'-C5'-O5'
58	c	28	A2M	O4'-C4'-C5'-O5'
58	c	619	A2M	O4'-C4'-C5'-O5'
58	c	619	A2M	C3'-C4'-C5'-O5'
58	c	796	A2M	C3'-C4'-C5'-O5'
58	c	1575	G7M	C3'-C4'-C5'-O5'
58	c	1191	B8N	N34-C33-C34-O36
11	AA	2197	OMC	C2'-C1'-N1-C2
11	AA	2280	A2M	O4'-C4'-C5'-O5'
11	AA	2280	A2M	C3'-C4'-C5'-O5'
58	c	796	A2M	O4'-C4'-C5'-O5'
58	c	1271	OMG	O4'-C4'-C5'-O5'
58	c	1271	OMG	C3'-C4'-C5'-O5'
58	c	1572	OMG	C3'-C4'-C5'-O5'
11	AA	908	OMG	C3'-C2'-O2'-CM2
58	c	1191	B8N	C32-C33-C34-O36
58	c	1191	B8N	C32-C33-C34-O35
11	AA	867	OMG	O4'-C4'-C5'-O5'
11	AA	2922	OMG	O4'-C4'-C5'-O5'
58	c	1428	OMG	O4'-C4'-C5'-O5'
58	c	541	A2M	C4'-C5'-O5'-P
58	c	100	A2M	O4'-C4'-C5'-O5'
58	c	1269	OMU	O4'-C1'-N1-C6
11	AA	2870	5MC	C2'-C1'-N1-C6
58	c	1269	OMU	O4'-C1'-N1-C2
58	c	1191	B8N	N34-C33-C34-O35
58	c	1280	4AC	O7-C7-N4-C4
58	c	1280	4AC	CM7-C7-N4-C4
58	c	1773	4AC	O7-C7-N4-C4
58	c	1773	4AC	CM7-C7-N4-C4
11	AA	2946	A2M	C1'-C2'-O2'-CM'
58	c	1575	G7M	C4'-C5'-O5'-P
11	AA	2197	OMC	O4'-C1'-N1-C6
11	AA	817	A2M	C4'-C5'-O5'-P
11	AA	2870	5MC	O4'-C1'-N1-C6
11	AA	2197	OMC	O4'-C1'-N1-C2
58	c	1428	OMG	C4'-C5'-O5'-P
58	c	1782	MA6	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
11	AA	807	A2M	C3'-C4'-C5'-O5'
11	AA	1437	OMC	O4'-C4'-C5'-O5'
11	AA	2870	5MC	O4'-C1'-N1-C2
11	AA	2870	5MC	C2'-C1'-N1-C2
58	c	1271	OMG	C4'-C5'-O5'-P
11	AA	817	A2M	O4'-C4'-C5'-O5'
11	AA	2281	A2M	O4'-C4'-C5'-O5'
11	AA	807	A2M	C3'-C2'-O2'-CM'
58	c	100	A2M	C3'-C4'-C5'-O5'
11	AA	649	A2M	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 295 ligands modelled in this entry, 290 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
85	SPD	c	1951	-	9,9,9	0.32	0	8,8,8	0.83	0
85	SPD	AA	3610	-	9,9,9	0.32	0	8,8,8	0.83	0
86	MET	Bb	103	14	6,7,8	0.46	0	2,7,9	0.15	0
85	SPD	AA	3608	-	9,9,9	0.34	0	8,8,8	0.79	0
85	SPD	AA	3611	-	9,9,9	0.33	0	8,8,8	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	c	1951	-	-	1/7/7/7	-
85	SPD	AA	3610	-	-	0/7/7/7	-
86	MET	Bb	103	14	-	2/5/6/8	-
85	SPD	AA	3608	-	-	5/7/7/7	-
85	SPD	AA	3611	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	Bb	103	MET	C-CA-CB-CG
85	AA	3608	SPD	C3-C4-C5-N6
85	AA	3608	SPD	C4-C5-N6-C7
86	Bb	103	MET	CB-CG-SD-CE
85	AA	3608	SPD	C2-C3-C4-C5
85	AA	3608	SPD	C7-C8-C9-N10
85	c	1951	SPD	C4-C5-N6-C7
85	AA	3608	SPD	N6-C7-C8-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

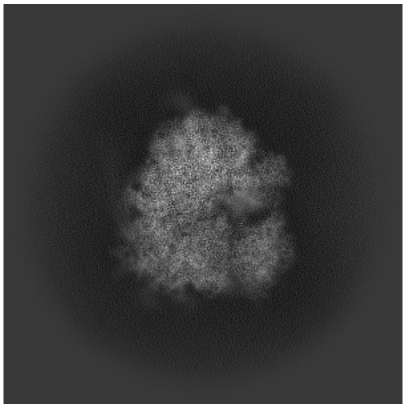
6 Map visualisation ⓘ

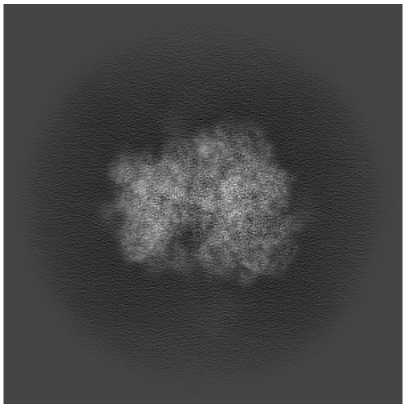
This section contains visualisations of the EMDB entry EMD-16648. These allow visual inspection of the internal detail of the map and identification of artifacts.

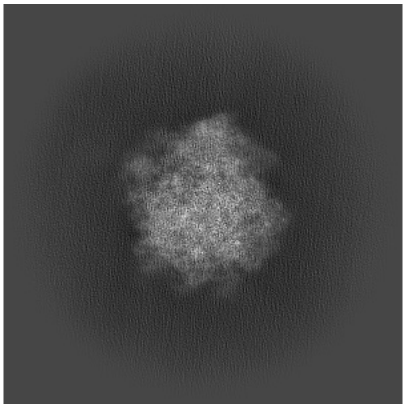
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

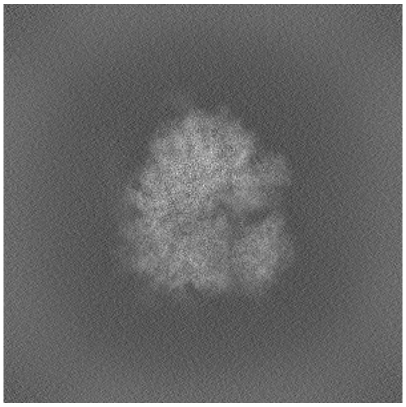
6.1.1 Primary map

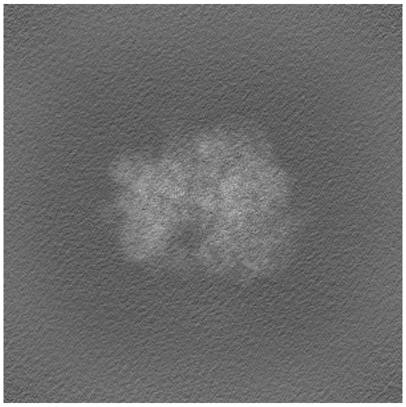

X

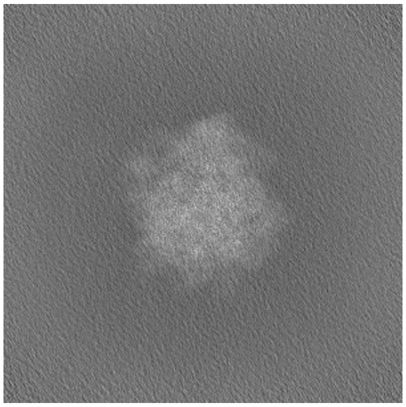

Y


Z

6.1.2 Raw map


X

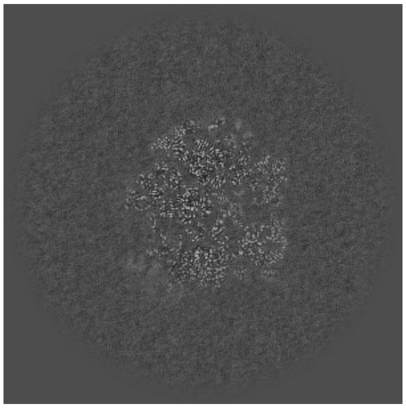

Y


Z

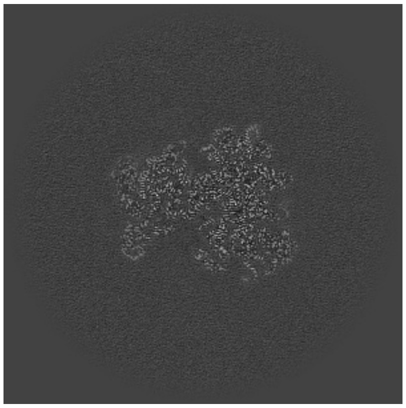
The images above show the map projected in three orthogonal directions.

6.2 Central slices

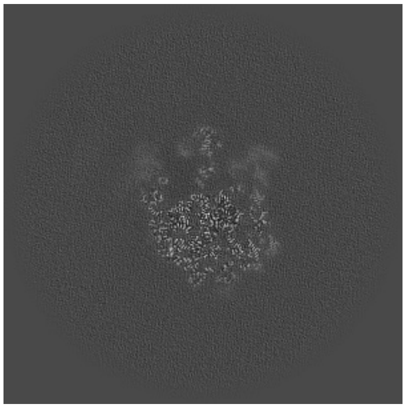
6.2.1 Primary map



X Index: 300

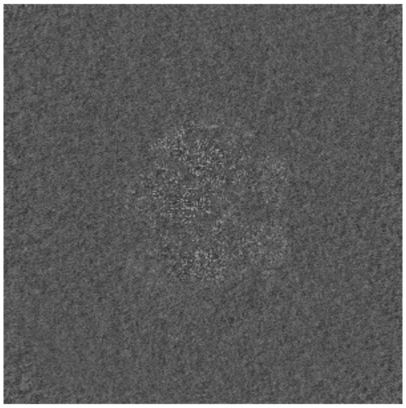


Y Index: 300

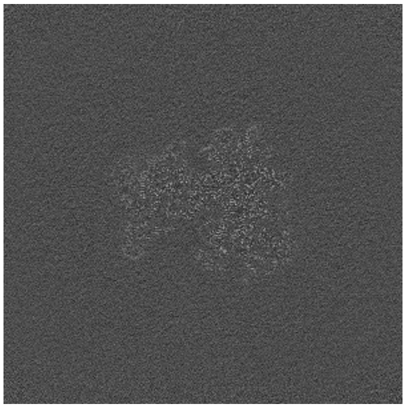


Z Index: 300

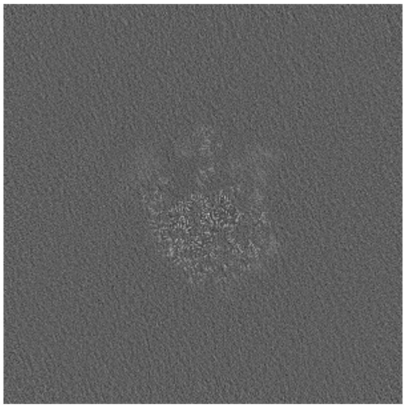
6.2.2 Raw map



X Index: 300



Y Index: 300

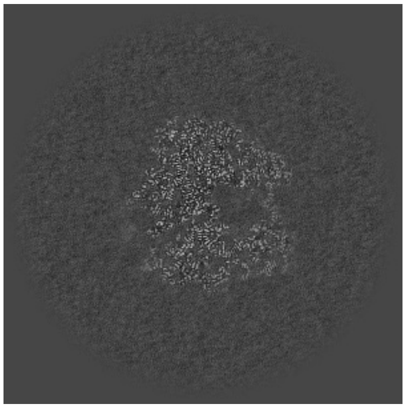


Z Index: 300

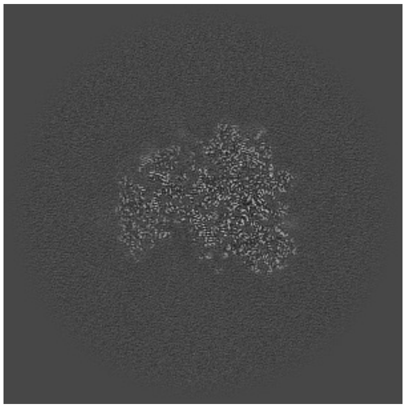
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

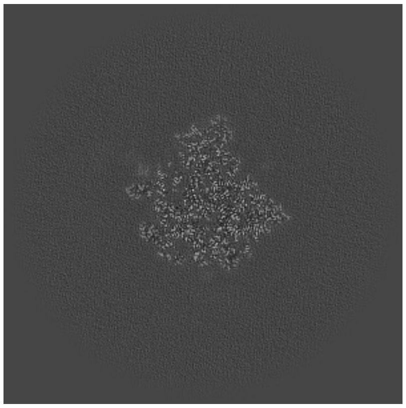
6.3.1 Primary map



X Index: 324

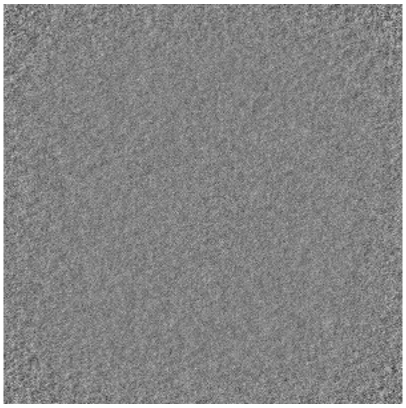


Y Index: 291

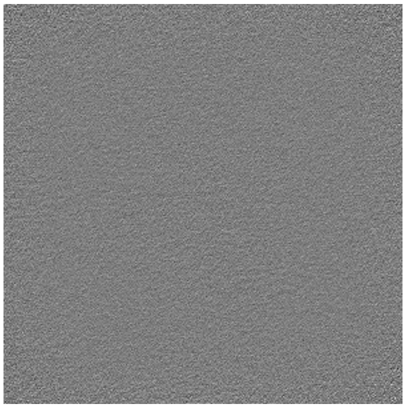


Z Index: 345

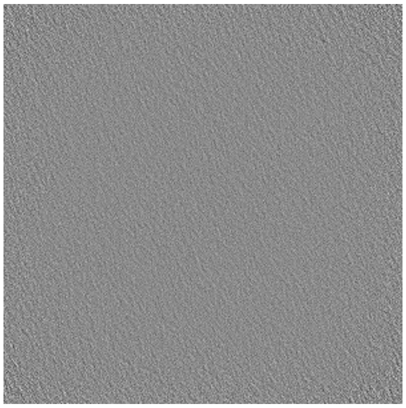
6.3.2 Raw map



X Index: 0



Y Index: 0

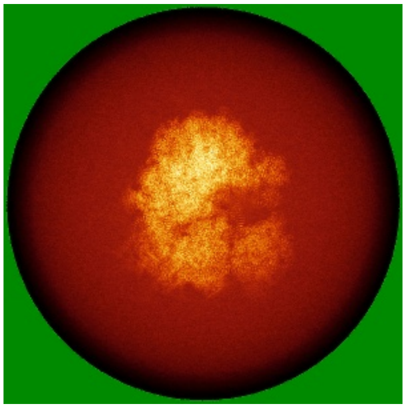


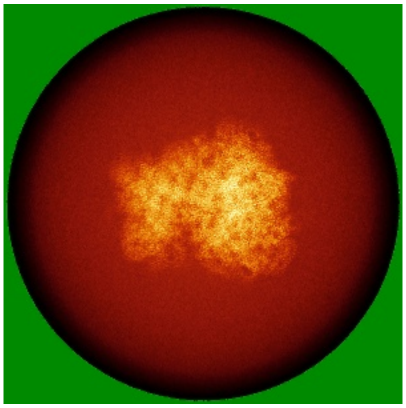
Z Index: 0

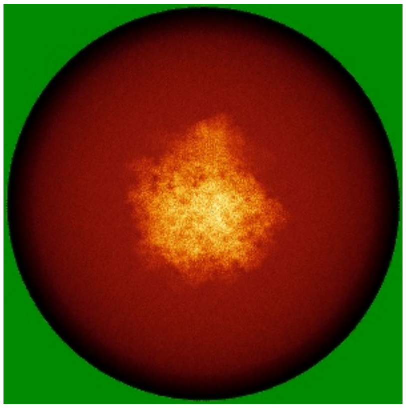
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

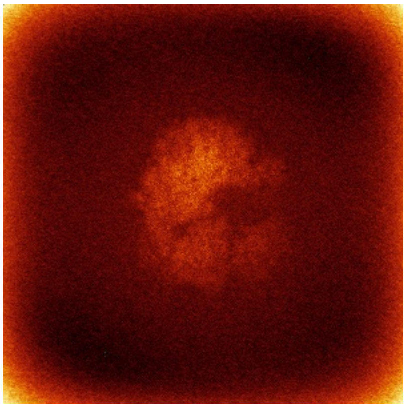
6.4.1 Primary map

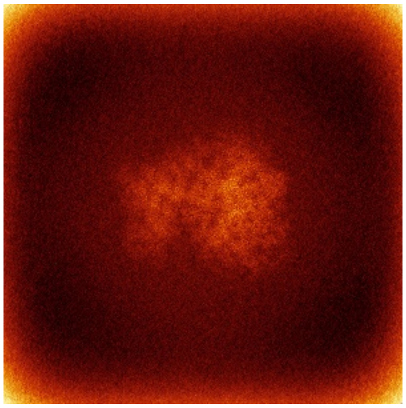

X

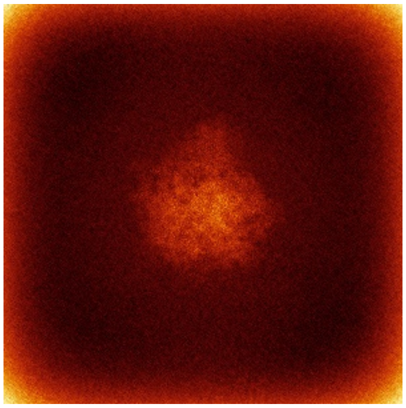

Y


Z

6.4.2 Raw map


X

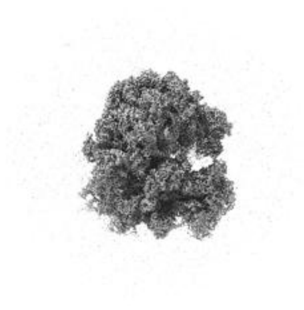

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



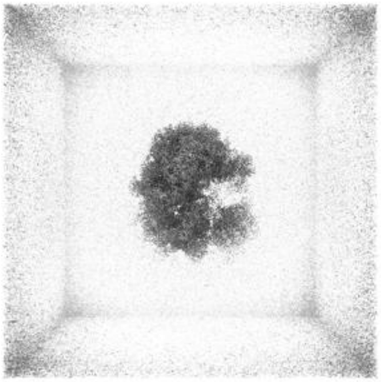
X

Y

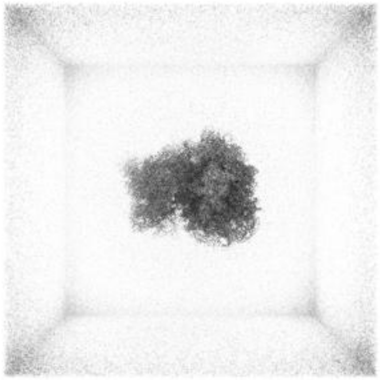
Z

The images above show the 3D surface view of the map at the recommended contour level 0.249. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

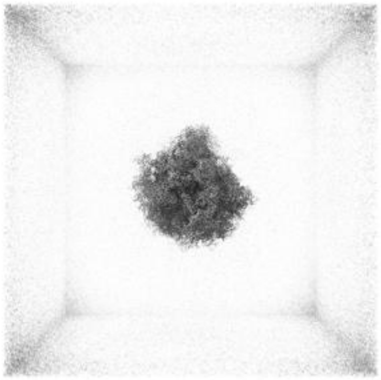
6.5.2 Raw map



X



Y



Z

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

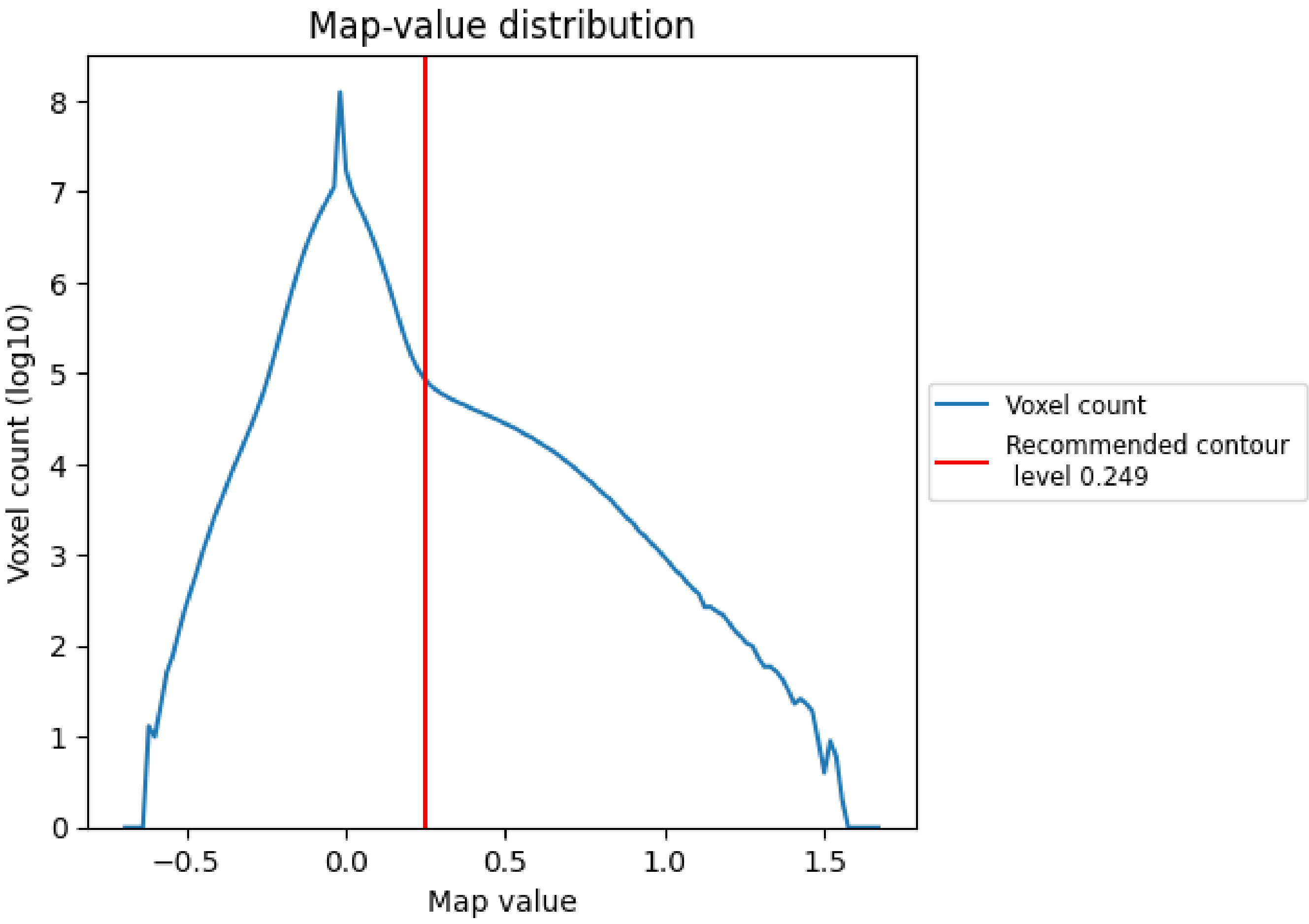
6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

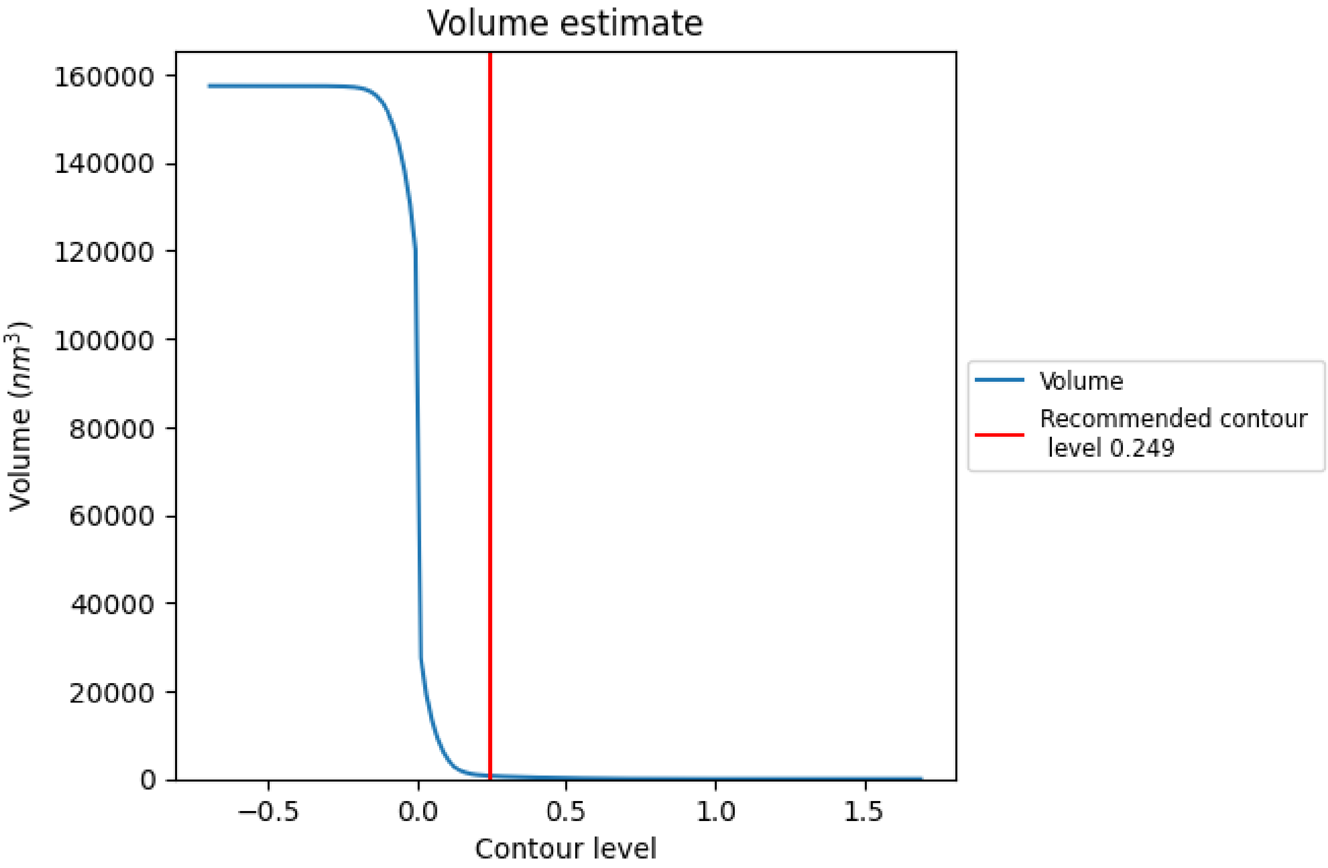
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

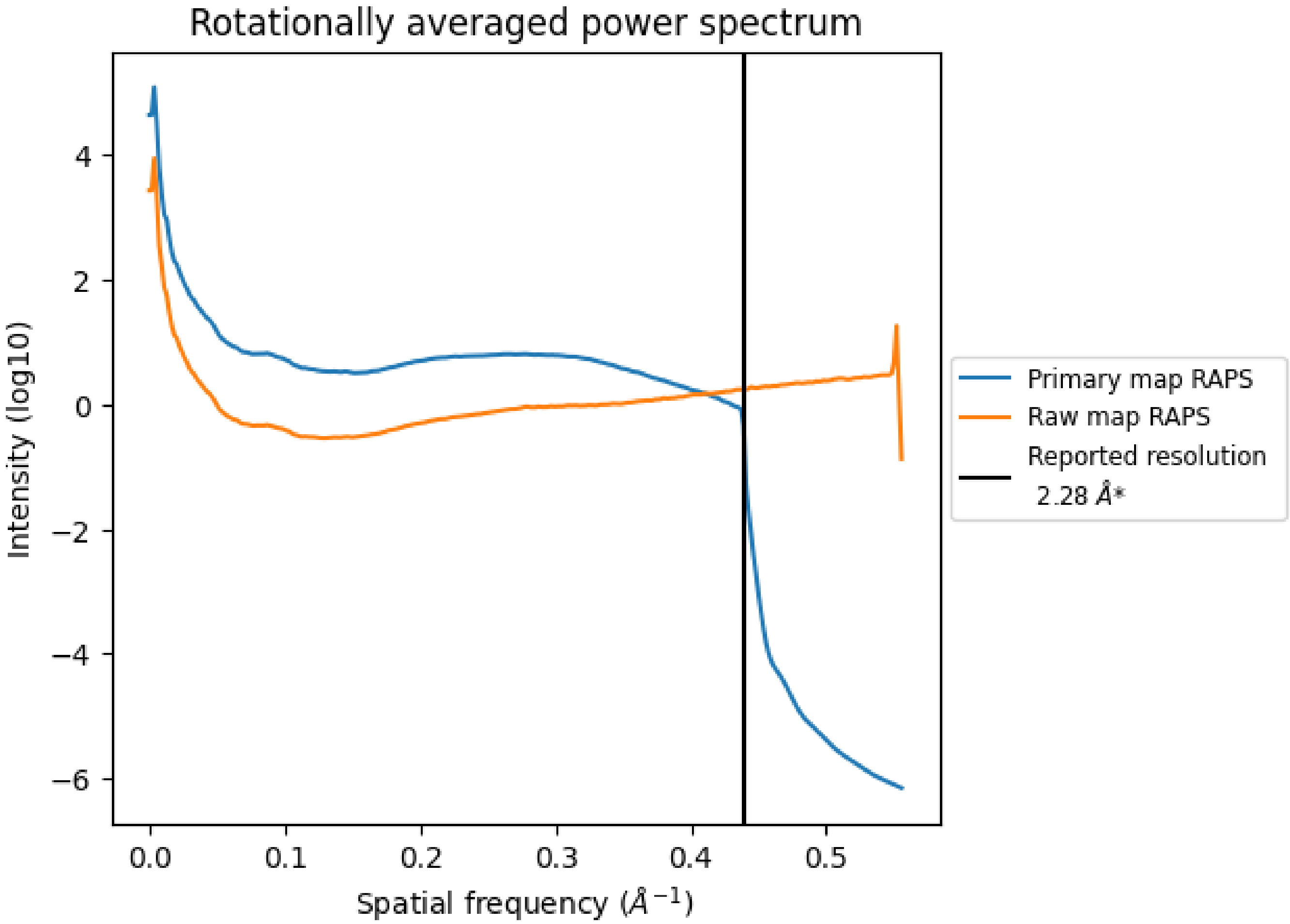
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 688 nm^3; this corresponds to an approximate mass of 621 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 ⓘ

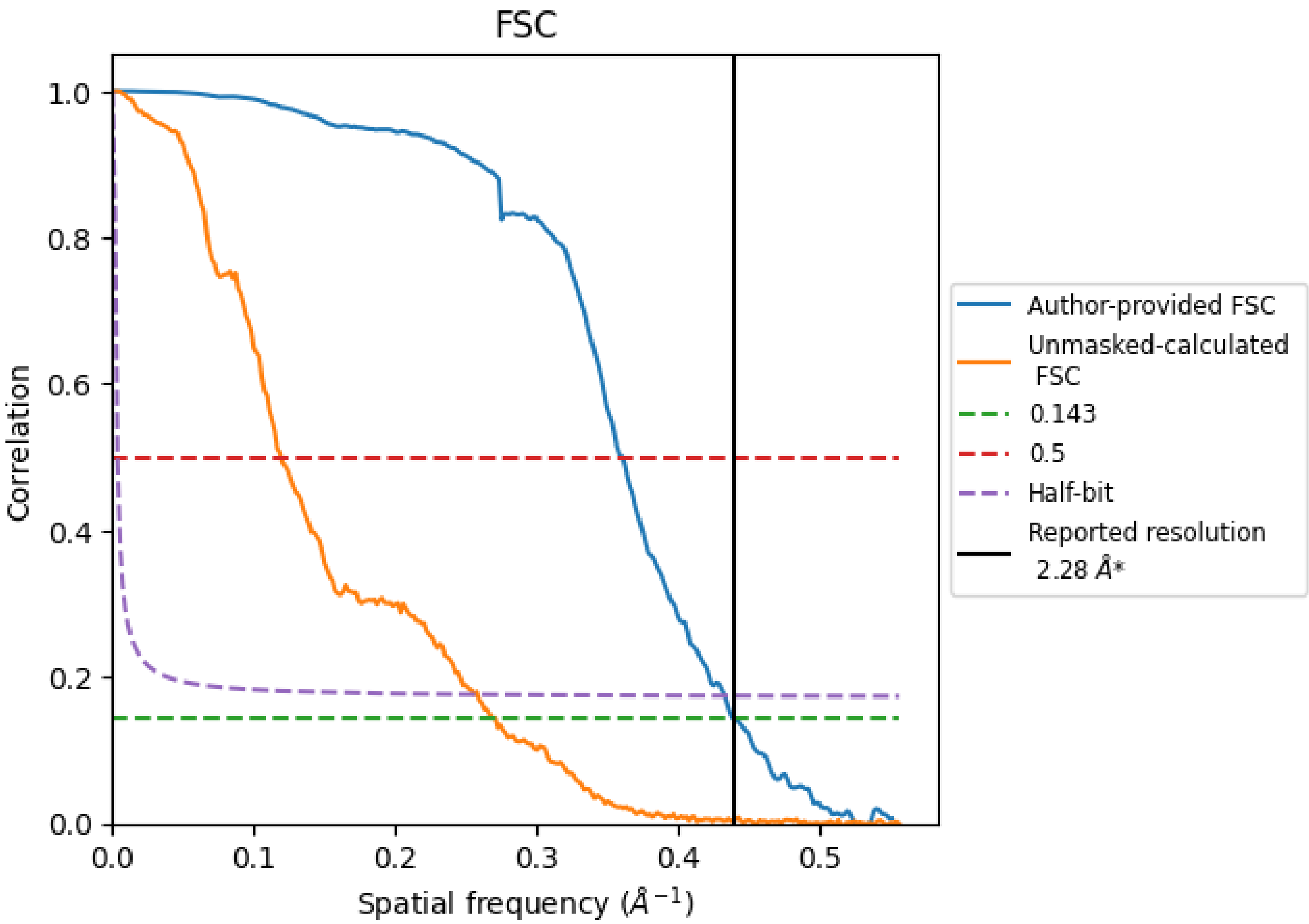


*Reported resolution corresponds to spatial frequency of 0.439 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.439 $Å^{-1}$

8.2 Resolution estimates ⓘ

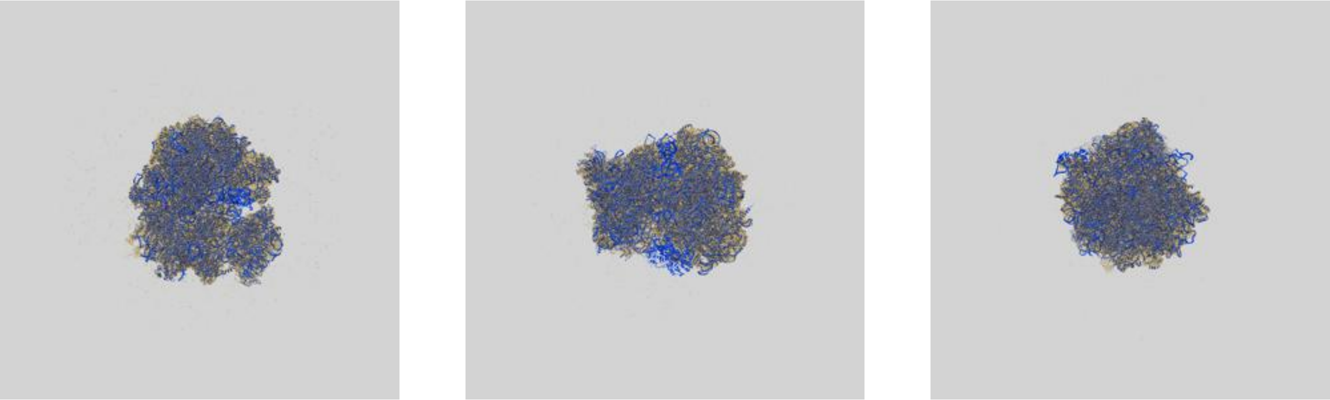
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.28	-	-
Author-provided FSC curve	2.28	2.78	2.31
Unmasked-calculated*	3.70	8.38	3.88

*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 3.70 differs from the reported value 2.28 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16648 and PDB model 8CGN. Per-residue inclusion information can be found in section 3 on page 22.

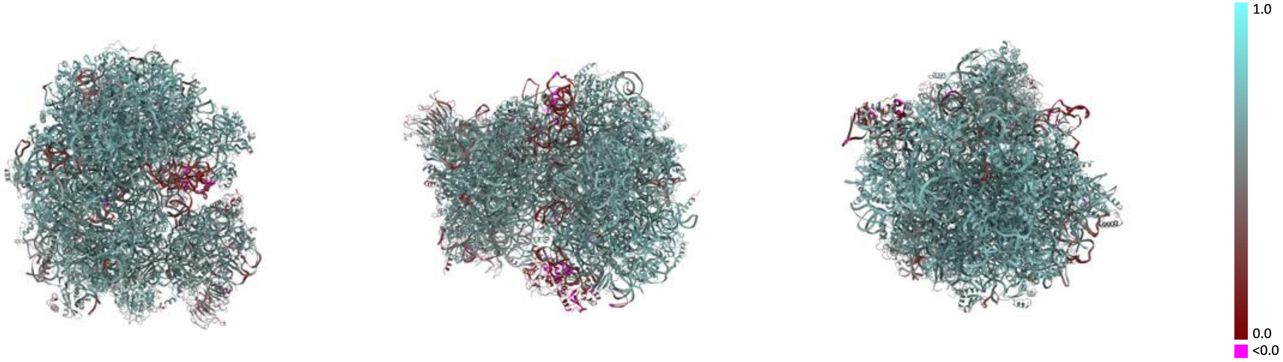
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.249 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.

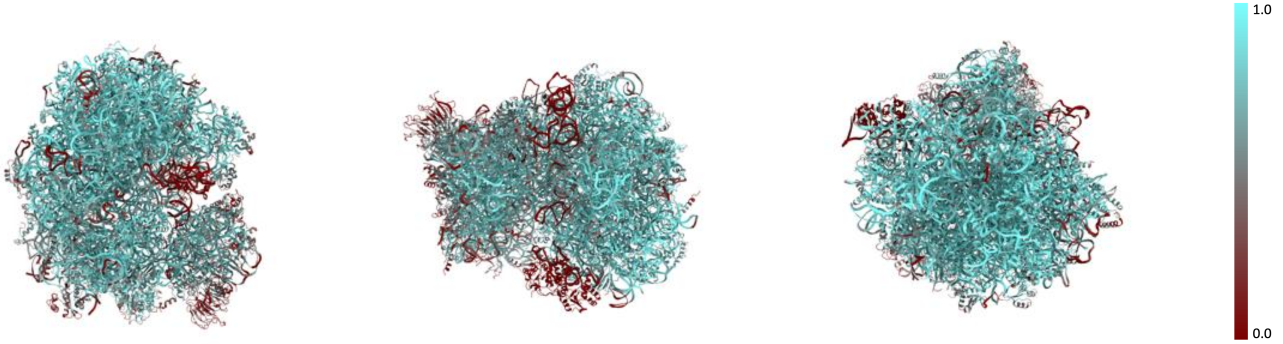
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

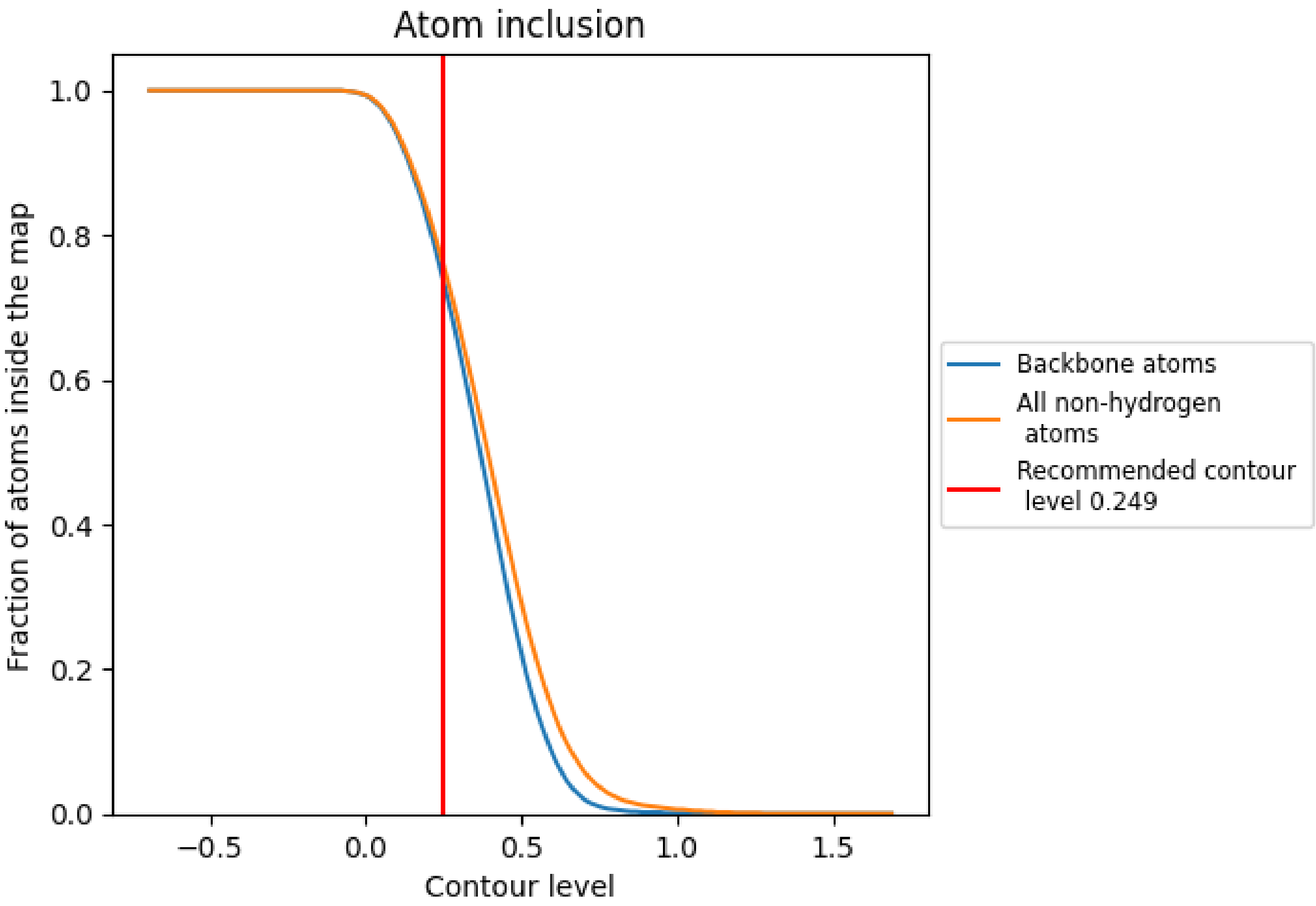
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.249).

9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 76% 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 (0.249) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7600	0.6110
0	0.5440	0.5690
1	0.2650	0.3850
2	0.7770	0.6370
3	0.6310	0.5740
4	0.4950	0.5660
5	0.8110	0.6460
6	0.5280	0.5300
7	0.2620	0.4430
8	0.0590	0.3080
A	0.8640	0.6720
AA	0.8420	0.6230
B	0.8950	0.6880
BB	0.9060	0.6450
Bb	0.5910	0.5460
C	0.8840	0.6810
CC	0.9120	0.6520
Cc	0.0990	0.2980
D	0.7890	0.6410
DD	0.0030	0.2590
Dd	0.6490	0.6000
E	0.8560	0.6710
EE	0.8810	0.6860
Ee	0.0010	0.1550
F	0.8070	0.6540
FF	0.8590	0.6710
G	0.6090	0.5880
GG	0.8620	0.6730
H	0.8610	0.6820
HH	0.6790	0.6110
I	0.8240	0.6780
II	0.7560	0.6480
J	0.7950	0.6540
JJ	0.8590	0.6760
K	0.8280	0.6650

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Chain	Atom inclusion	Q-score
KK	0.6990	0.6240
L	0.7560	0.6330
LL	0.7260	0.6390
M	0.8790	0.6770
MM	0.7610	0.6600
N	0.7060	0.6130
NN	0.6070	0.5840
O	0.8030	0.6630
OO	0.7870	0.6420
P	0.7400	0.6310
PP	0.7940	0.6580
Q	0.8760	0.6840
QQ	0.9240	0.6900
R	0.9260	0.6940
S	0.8390	0.6620
T	0.7930	0.6450
U	0.7170	0.6220
V	0.9190	0.6880
W	0.5930	0.5890
X	0.8510	0.6550
Y	0.7050	0.6560
Z	0.8020	0.6610
a	0.7780	0.6600
b	0.7970	0.6610
c	0.7890	0.6040
d	0.6830	0.6020
e	0.6800	0.6180
f	0.7750	0.6430
g	0.5330	0.5740
h	0.6870	0.6210
i	0.5580	0.5640
j	0.4070	0.5200
k	0.4750	0.5400
l	0.7320	0.6200
m	0.6670	0.6040
n	0.4470	0.5270
o	0.7660	0.6360
p	0.7610	0.6480
q	0.7790	0.6330
r	0.4530	0.5400
s	0.6280	0.5760
t	0.4940	0.5290

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Chain	Atom inclusion	Q-score
u	0.5030	0.5370
v	0.5720	0.5600
w	0.4590	0.5460
x	0.7210	0.6210
y	0.8580	0.6750
z	0.7050	0.6310