Full wwPDB EM Validation Report

Aug 7, 2024 – 02:51 pm BST

PDB ID	:	8PJ2
EMDB ID	:	EMD-17697
Title	:	Structure of human 48S translation initiation complex in AUG recognition state after eIF5-induced GTP hydrolysis by eIF2 (48S-2)
Authors	:	Petrychenko, V.; Yi, S.-H.; Liedtke, D.; Peng, B.Z.; Rodnina, M.V.; Fischer, N.
Deposited on	:	2023-06-22
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

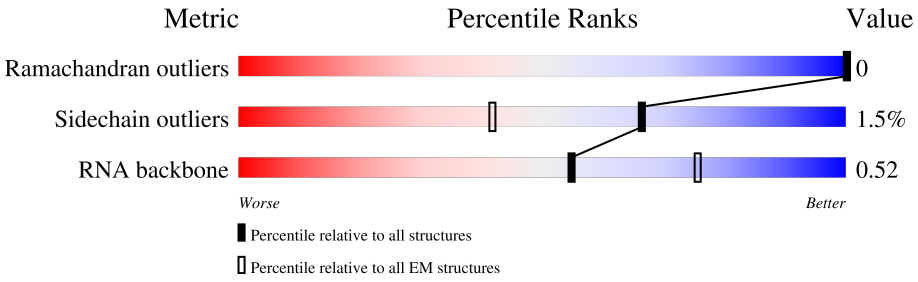
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	1	814	70% 72% 28%
2	2	325	94% 94% 6%
3	3	218	78% 98%
4	4	357	37% 72% 28%
5	5	564	65% 91% 8%
6	6	374	58% 96%
7	7	255	12% 5% 15% 78%
8	8	352	49% 90% 10%

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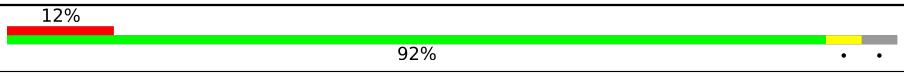
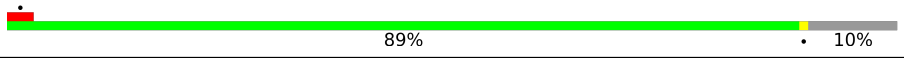
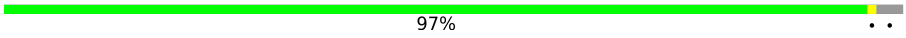
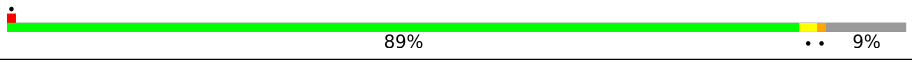
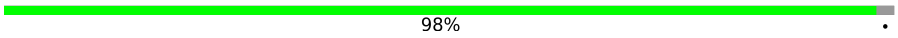
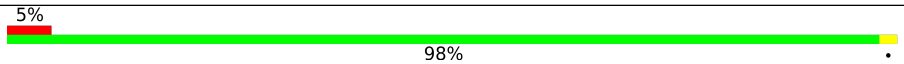
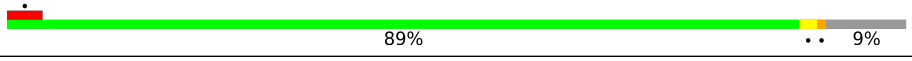
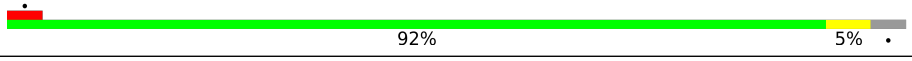
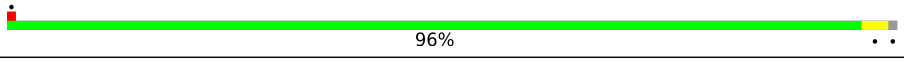
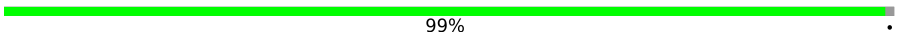
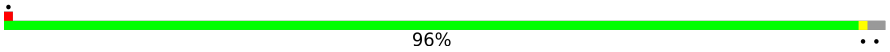
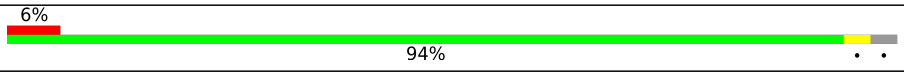
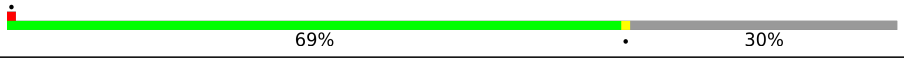
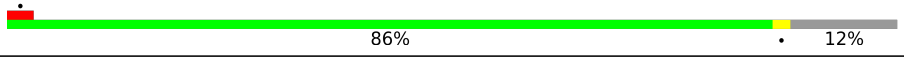
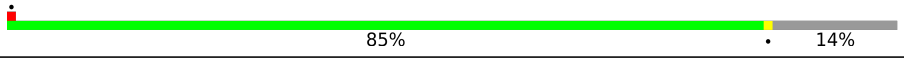
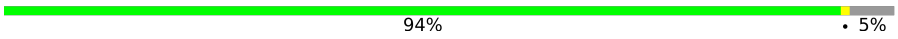
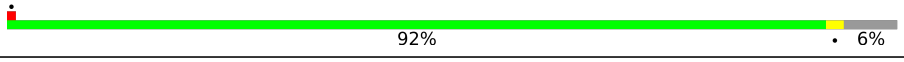
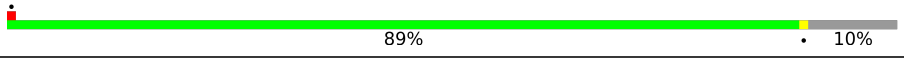
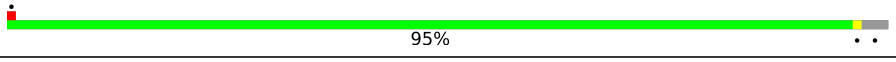
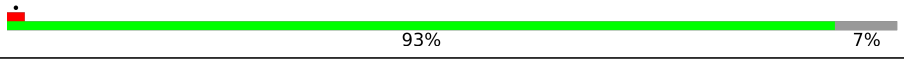
Mol	Chain	Length	Quality of chain
9	9	25	
10	A	1869	
11	B	158	
12	C	263	
13	D	194	
14	E	143	
15	F	59	
16	G	194	
17	H	84	
18	I	151	
19	J	130	
20	K	83	
21	L	293	
22	M	135	
23	N	295	
24	O	264	
25	P	151	
26	Q	115	
27	R	208	
28	S	249	
29	T	133	
30	V	204	
31	Y	146	
32	Z	243	
33	a	165	

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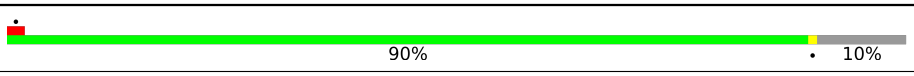
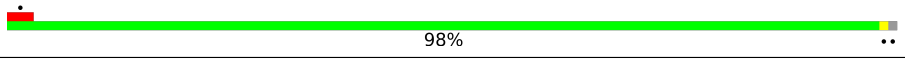
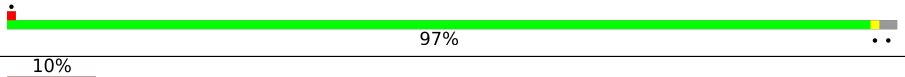
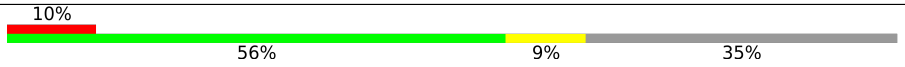
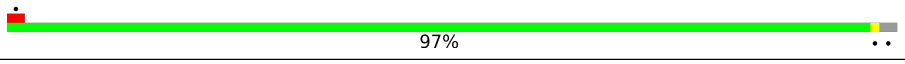
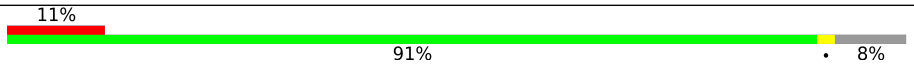
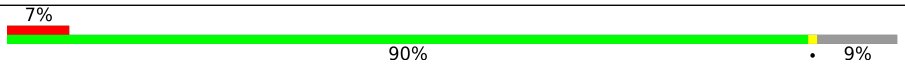
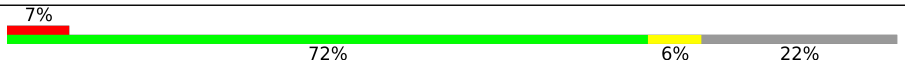
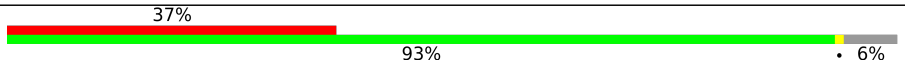
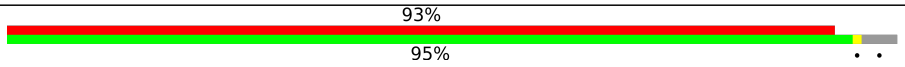
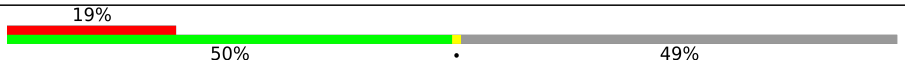
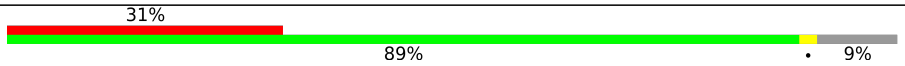
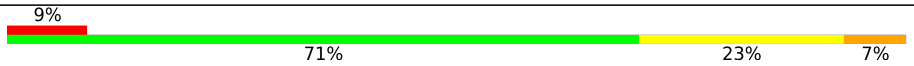
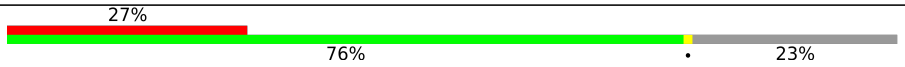
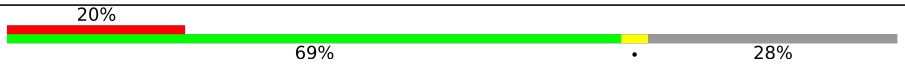
Mol	Chain	Length	Quality of chain
34	b	145	
35	c	317	
36	d	145	
37	e	125	
38	f	152	
39	h	119	
40	i	56	
41	k	156	
42	m	132	
43	n	69	
44	o	320	
45	q	144	
46	r	315	
47	t	472	
48	u	1382	
49	v	445	
50	w	75	
51	x	548	
52	y	913	
53	z	430	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 118707 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 Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	588	3258	1986	633	634	5	0	0

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	2	304	1493	885	304	304	0	0

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	3	213	1057	631	213	213	0	0

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	4	257	1272	757	257	258	0	0

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	520	4347	2814	721	793	19	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	362	2196	1348	414	427	7	0	0

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	57	Total	C	N	O	P	0	0
			1218	547	231	383	57		

- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	8	317	Total	C	N	O	0	0
			1574	937	318	319		

- Molecule 9 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 10 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1754	Total	C	N	O	P	0	0
			37429	16718	6714	12244	1753		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1248	B8N	U	conflict	GB NR_046235.3

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	142	Total	C	N	O	S	0	0
			1166	743	218	199	6		

- Molecule 12 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 13 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 14 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 15 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	59	Total	C	N	O	S	0	0
			468	290	102	75	1		

- Molecule 16 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 17 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 18 is a protein called 40S ribosomal protein S13.

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

- Molecule 19 is a protein called 40S ribosomal protein S15a.

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

- Molecule 20 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 21 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 22 is a protein called 40S ribosomal protein S17.

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

- Molecule 23 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 24 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 25 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

- Molecule 26 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 27 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 28 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 30 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 31 is a protein called 40S ribosomal protein S16.

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

- Molecule 32 is a protein called 40S ribosomal protein S3.

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

- Molecule 33 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 34 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	131	Total	C	N	O	S	0	0
			1072	682	201	182	7		

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 36 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 37 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	81	Total	C	N	O	S	0	0
			649	420	119	109	1		

- Molecule 38 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	149	Total	C	N	O	S	0	0
			1227	770	249	207	1		

- Molecule 39 is a protein called 40S ribosomal protein S20.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	50	Total	C	N	O	S	0	0
			419	262	85	67	5		

- Molecule 41 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	68	Total	C	N	O	S	0	0
			554	349	103	95	7		

- Molecule 42 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 43 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	63	Total	C	N	O	S	0	0
			498	302	101	93	2		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	o	77	Total	C	N	O	0	0
			616	389	111	116		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	112	Total	C	N	O	S	0	0
			902	560	173	165	4		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	296	Total	C	N	O	S	0	0
			2138	1342	384	404	8		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	455	Total	C	N	O	S	0	0
			3439	2179	599	643	18		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	706	Total 5383	C 3379	N 982	O 999	S 23	1	0

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	405	Total 2740	C 1720	N 498	O 510	S 12	0	0

- Molecule 50 is a RNA chain called Initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	75	Total 1604	C 717	N 298	O 515	P 74	0	0

- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	422	Total 2837	C 1749	N 522	O 556	S 10	0	0

- Molecule 52 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	656	Total 5263	C 3312	N 939	O 977	S 35	0	0

- Molecule 53 is a protein called Eukaryotic translation initiation factor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	145	Total 1146	C 723	N 203	O 209	S 11	0	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	83	Total 83	Mg 83	0
54	V	1	Total 1	Mg 1	0
54	f	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms	AltConf
54	i	2	Total Mg 2 2	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

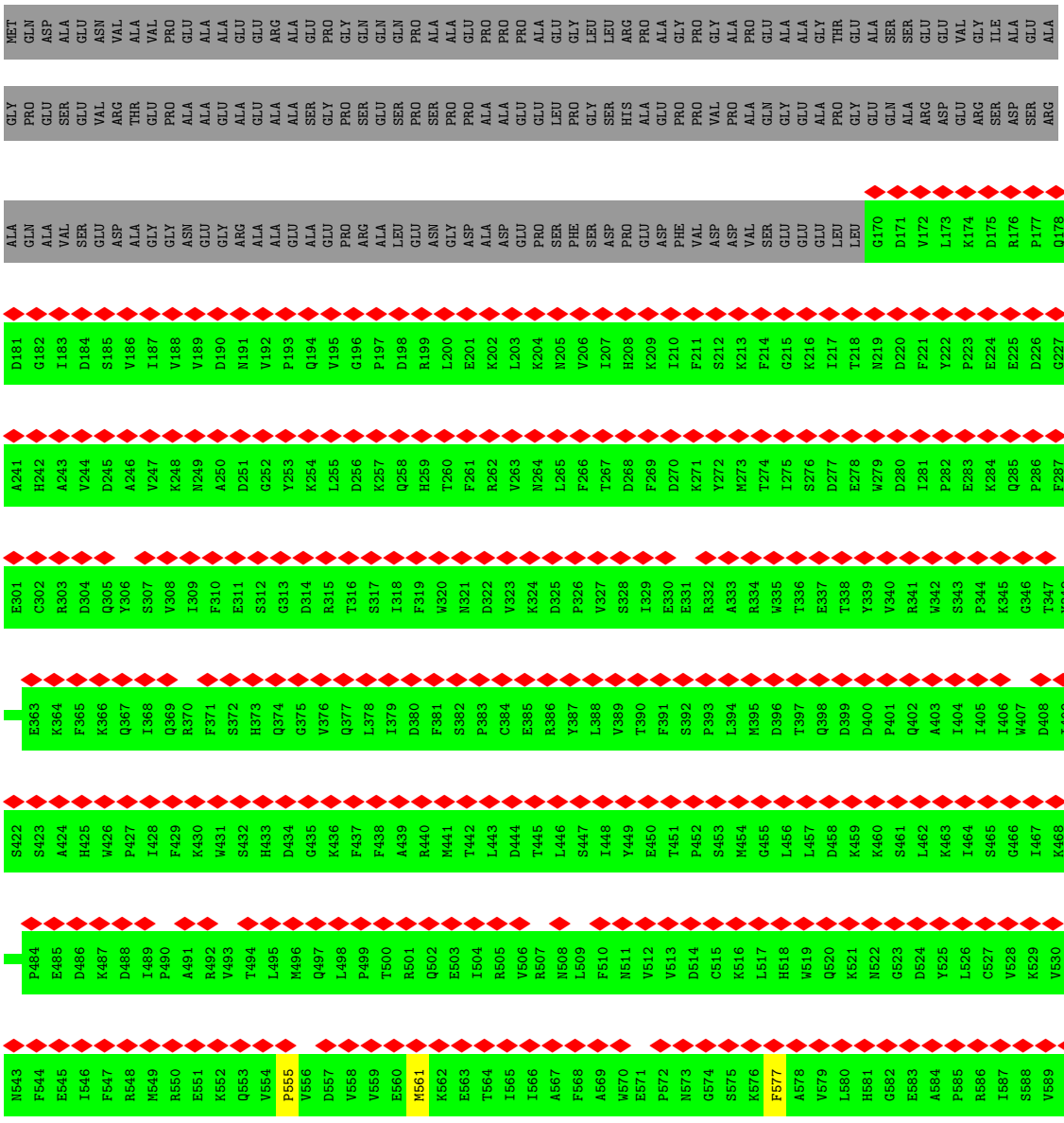
Mol	Chain	Residues	Atoms	AltConf
55	Q	1	Total Zn 1 1	0
55	k	1	Total Zn 1 1	0

3 Residue-property plots (i)

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: Eukaryotic translation initiation factor 3 subunit B

Chain 1:



I603 K604 M605 F606 D607 K608 Q609 Q610 A611 N612 T613 I614 F615 W616 S617 P618 Q619 G620 Q621 F622 V623 V624 L625 A626 G627 L628 R629 S630 M631 N632 G633 A634 L635 A636 F637 V638 D639 T640 S641 D642 C643 T644 V645 M646 N647 I648 A649 E650 H651 Y652 M653 A654 S655 D656 V657 E658 W659 D660 P661 T662

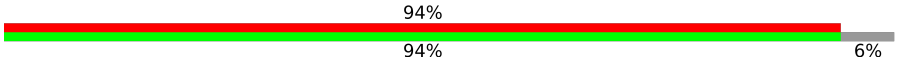
G663 R664 Y665 V666 V667 T668 S669 V670 S671 W672 W673 S674 H675 K676 V677 D678 N679 A680 Y681 W682 L683 W684 T685 F686 Q687 G688 R689 L690 L691 Q692 K693 N694 N695 K696 D697 R698 F699 C700 Q701 L702 L703 W704 R705 P706 R707 P708 P709 T710 L711 L712 S713 Q714 E715 Q716 I717 K718 Q719 I720 K721 K722

D723 L724 K725 K726 Y727 S728 K729 I730 F731 E732 Q733 K734 D735 R736 L737 S738 Q739 S740 K741 A742 S743 K744 E745 L746 V747 E748 R749 R750 R751 T752 M753 M754 E755 D756 F757 R758 K759 Y760 R761 K762 M763 A764 GLN GLU LEU TYR MET GLU GLN LYS ASN GLU ARG LEU GLU LEU ARG GLY GLY VAL

ASP THR ASP GLU LEU ASP SER ASN VAL ASP ASP TRP GLU GLU GLU THR ILE GLU PHE PHE VAL THR GLU GLU ILE ILE PRO LEU GLY ASN GLN GLU

• Molecule 2: Eukaryotic translation initiation factor 3 subunit I

Chain 2:



M1 K2 P3 I4 L5 L6 Q7 G8 H9 E10 R11 S12 I13 T14 Q15 I16 K17 Y18 N19 R20 E21 G22 D23 L24 L25 F26 T27 Y28 A29 K30 D31 P32 I33 V34 N35 V36 W37 Y38 S39 V40 N41 G42 E43 R44 L45 G46 T47 Y48 M49 G50 H51 T52 G53 A54 V55 W56 C57 V58 D59 A60

D61 W62 D63 T64 K65 H66 V67 L68 T69 G70 S71 A72 D73 N74 S75 C76 R77 L78 W79 D80 C81 E82 T83 G84 K85 Q86 L87 A88 L89 L90 K91 T92 N93 S94 A95 V96 R97 T98 C99 G100 F101 D102 F103 G104 G105 N106 I107 I108 M109 F110 S111 T112 ASP LYS GLN MET GLY TYR GLN CYS

F121 V122 S123 F124 F125 D126 L127 R128 D129 P130 S131 Q132 I133 D134 N135 N136 E137 P138 Y139 M140 K141 I142 P143 C144 N145 D146 S147 K148 I149 T150 S151 A152 V153 W154 G155 P156 L157 G158 E159 C160 I161 I162 A163 G164 H165 E166 S167 G168 E169 L170 N171 Q172 Y173 S174 A175 K176 S177 G178 E179 V180

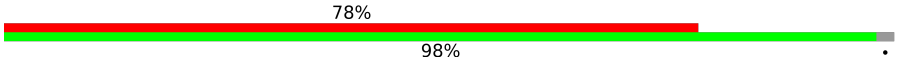
L181 V182 N183 V184 K185 E186 H187 S188 R189 Q190 I191 N192 D193 I194 Q195 L196 S197 R198 D199 M200 T201 M202 F203 V204 T205 A206 S207 K208 D209 N210 T211 A212 K213 L214 F215 D216 S217 T218 T219 L220 E221 H222 Q223 K224 T225 F226 R227 T228 E229 R230 P231 V232 N233 S234 A235 A236 L237 S238 P239 N240

Y241 D242 H243 V244 V245 L246 G247 G248 G249 Q250 E251 A252 M253 D254 V255 T256 T257 T258 S259 T260 R261 I262 G263 K264 F265 E266 A267 R268 F269 F270 H271 L272 A273 F274 E275 E276 E277 F278 G279 R280 V281 K282 G283 H284 F285 G286 P287 I288 N289 S290 V291 A292 F293 H294 P295 D296 G297 K298 S299 Y300

S301 S302 G303 G304 E305 D306 G307 Y308 V309 R310 I311 H312 TYR PHE ASP PRO GLN TYR PHE GLU PHE GLU PHE GLU ALA

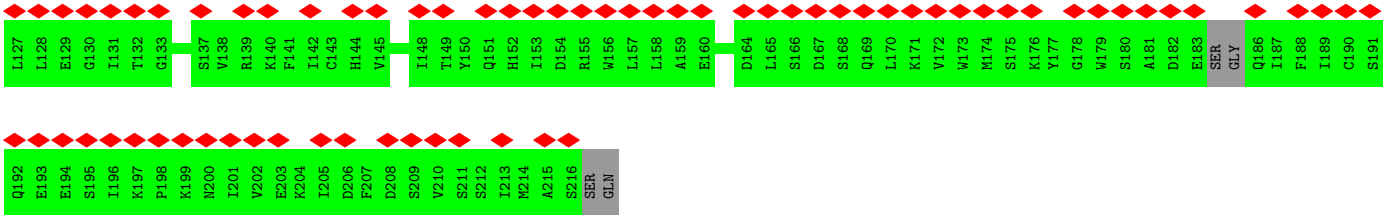
• Molecule 3: Eukaryotic translation initiation factor 3 subunit K

Chain 3:



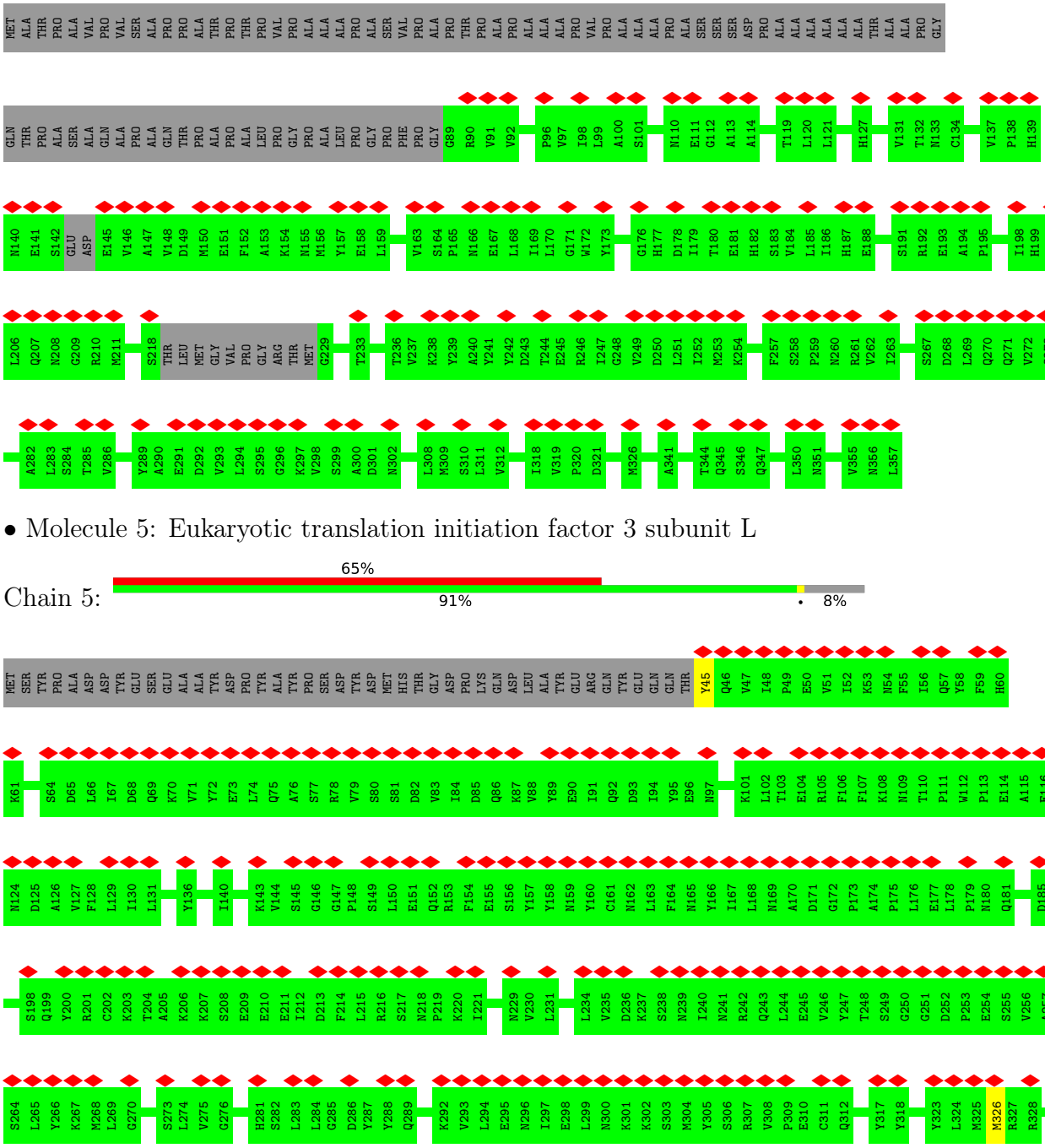
MET A2 M3 F4 E5 Q6 M7 R8 A9 N10 V11 G12 K13 L14 L15 K16 G17 I18 D19 R20 Y21 N22 P23 E24 N25 L26 A27 T28 L29 E30 R31 Y32 V33 E34 T35 Q36 A37 K38 E39 N40 A41 Y42 D43 L44 E45 A46 N47 L48 A49 V50 L51 K52 L53 Y54 Q55 F56 N57 P58 A59 F60

F61 Q62 T63 T64 V65 T66 L71 K72 A73 L74 T75 N76 H79 T80 D81 F82 C85 K86 C87 M88 I89 D90 Q91 A92 H93 Q94 E95 E96 R97 P98 I99 R100 Q101 I102 L103 Y104 L105 G106 D107 L108 T111 C112 H113 F114 Q115 A116 F117 W118 Q119 A120 L121 D122 E123 N124 M125 D126



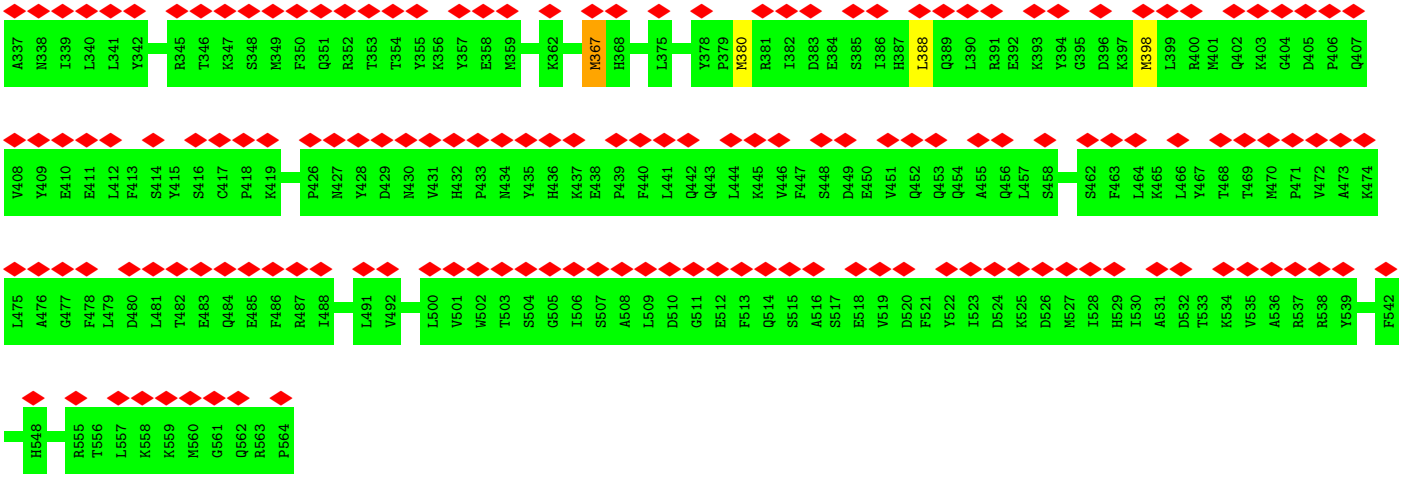
• Molecule 4: Eukaryotic translation initiation factor 3 subunit F

Chain 4:



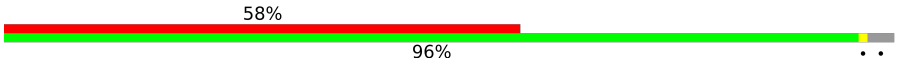
• Molecule 5: Eukaryotic translation initiation factor 3 subunit L

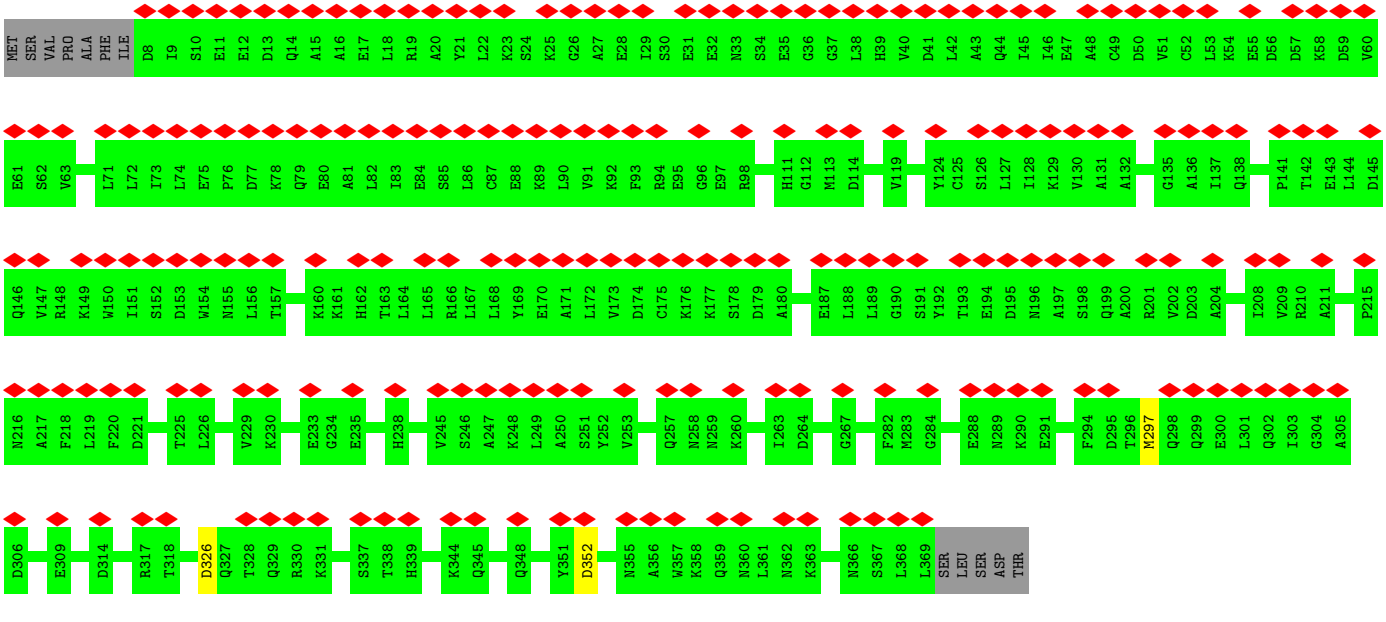
Chain 5:



• Molecule 6: Eukaryotic translation initiation factor 3 subunit M

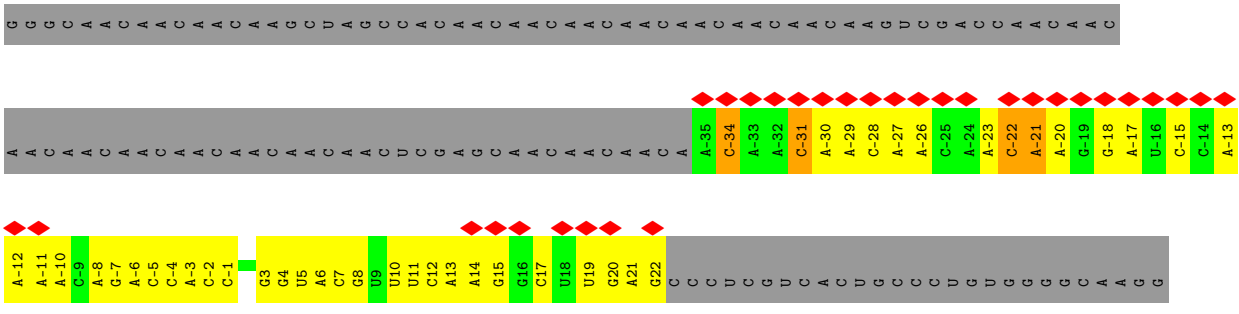
Chain 6:

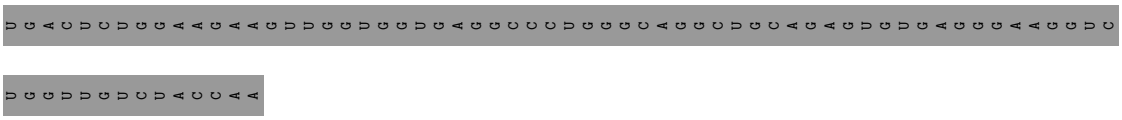




• Molecule 7: mRNA

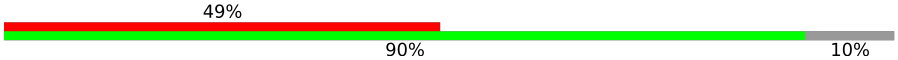
Chain 7:

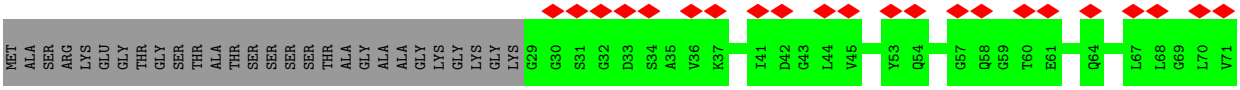


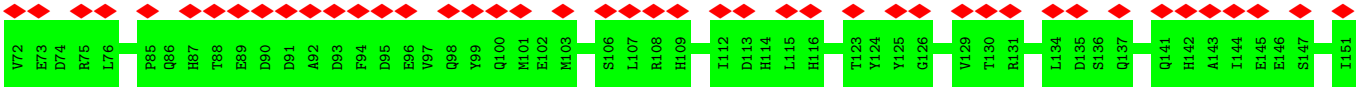


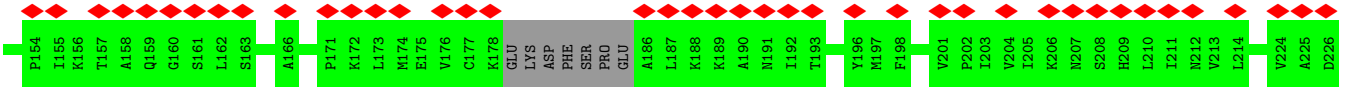
• Molecule 8: Eukaryotic translation initiation factor 3 subunit H

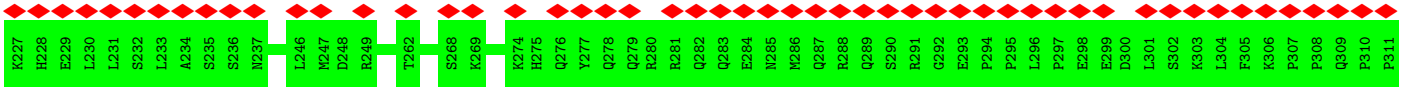
Chain 8:

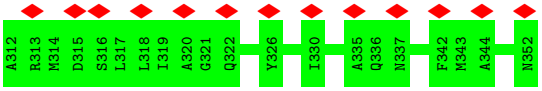






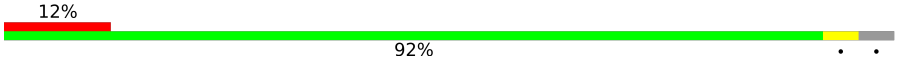


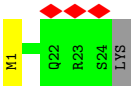




• Molecule 9: 60S ribosomal protein L41

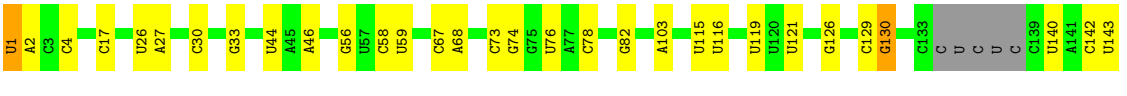
Chain 9:

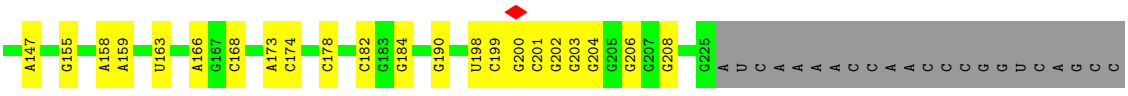


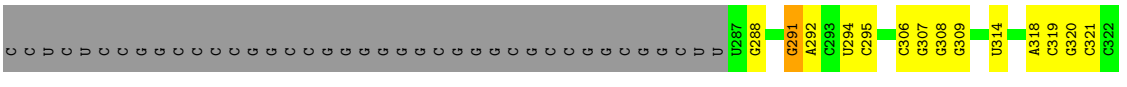


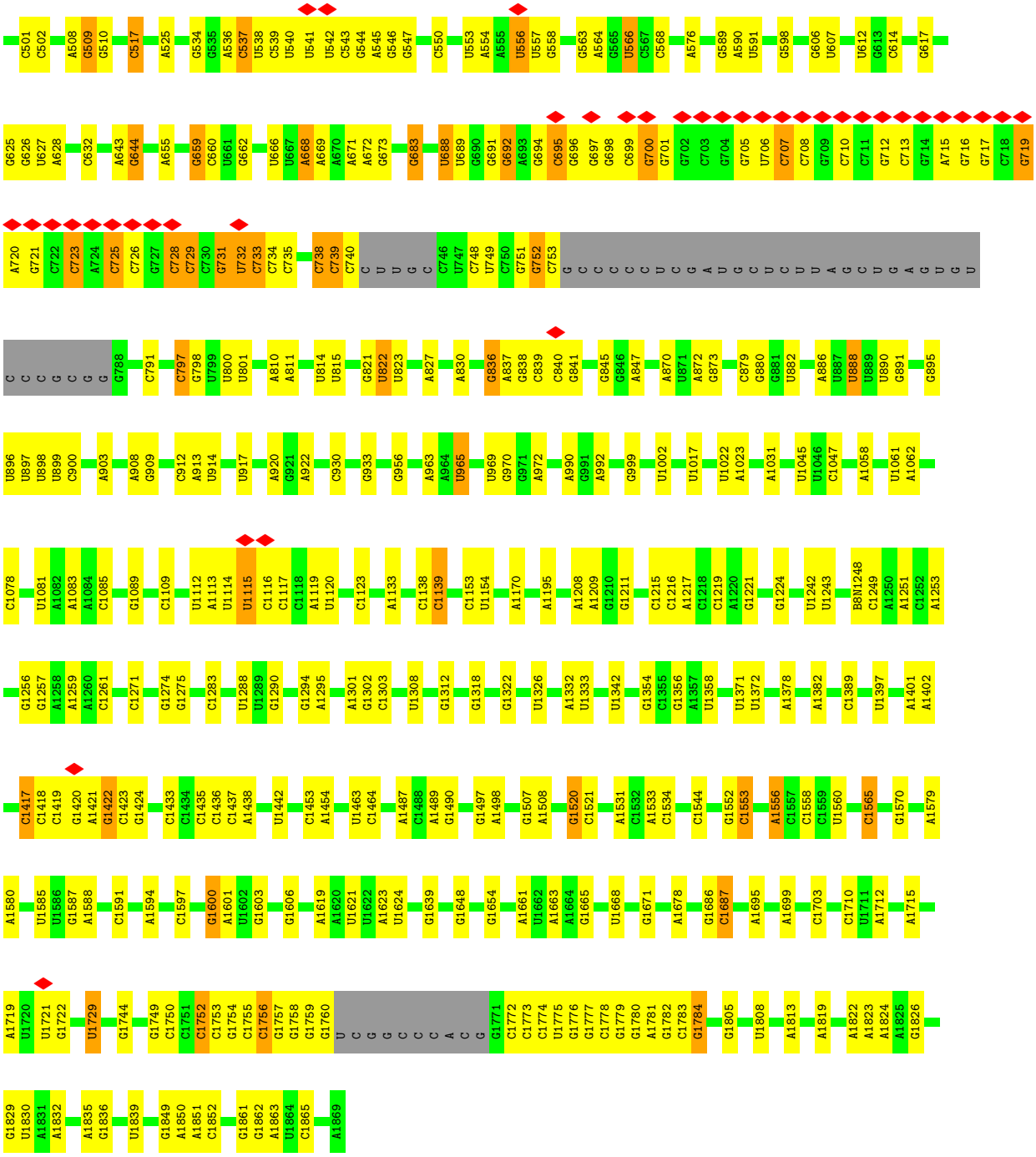
• Molecule 10: 18S rRNA

Chain A:



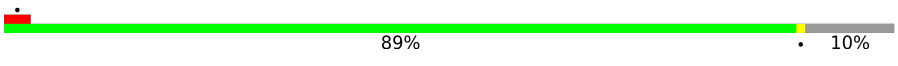


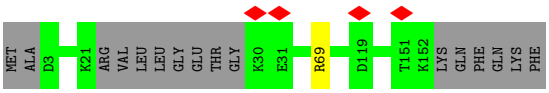




• Molecule 11: 40S ribosomal protein S11

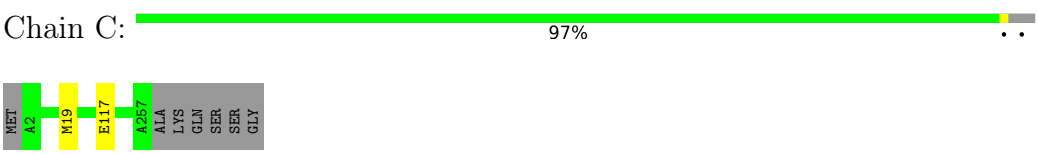
Chain B:





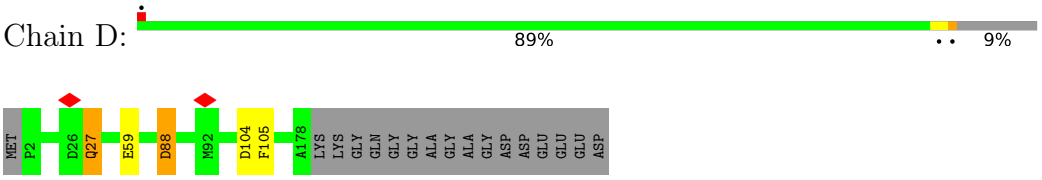
• Molecule 12: 40S ribosomal protein S4, X isoform

Chain C:



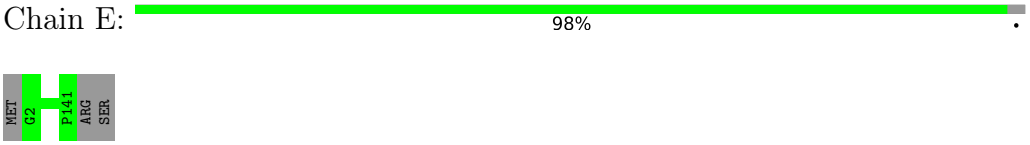
• Molecule 13: 40S ribosomal protein S9

Chain D:



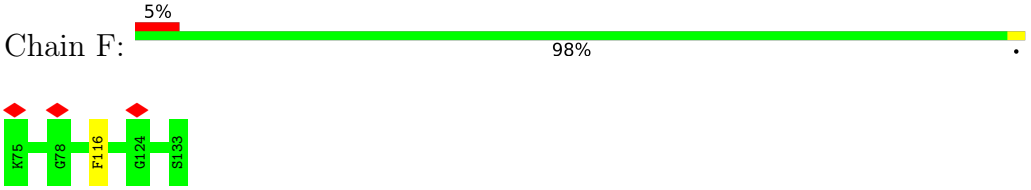
• Molecule 14: 40S ribosomal protein S23

Chain E:



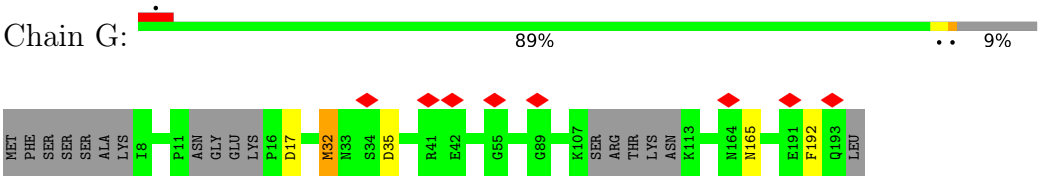
• Molecule 15: 40S ribosomal protein S30

Chain F:



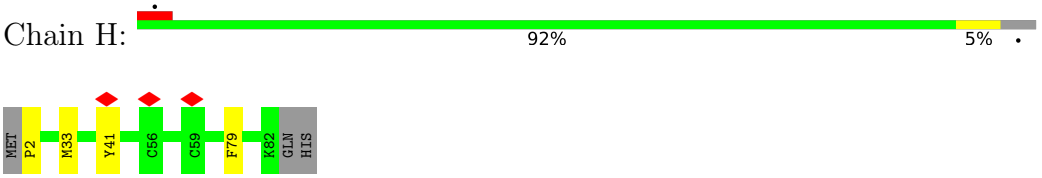
• Molecule 16: 40S ribosomal protein S7

Chain G:



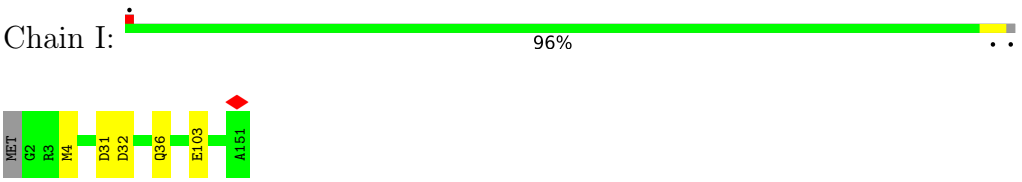
• Molecule 17: 40S ribosomal protein S27

Chain H:



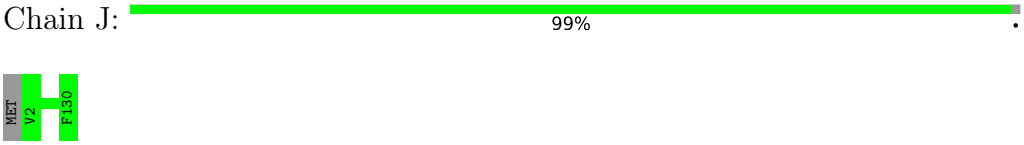
• Molecule 18: 40S ribosomal protein S13

Chain I:



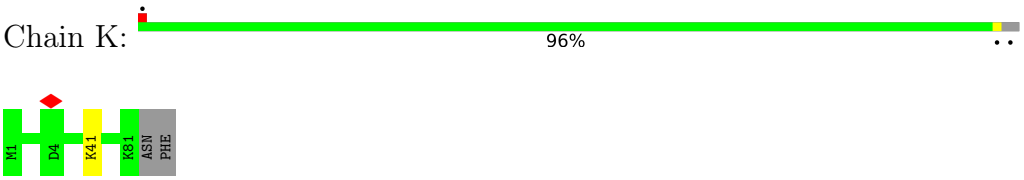
• Molecule 19: 40S ribosomal protein S15a

Chain J:



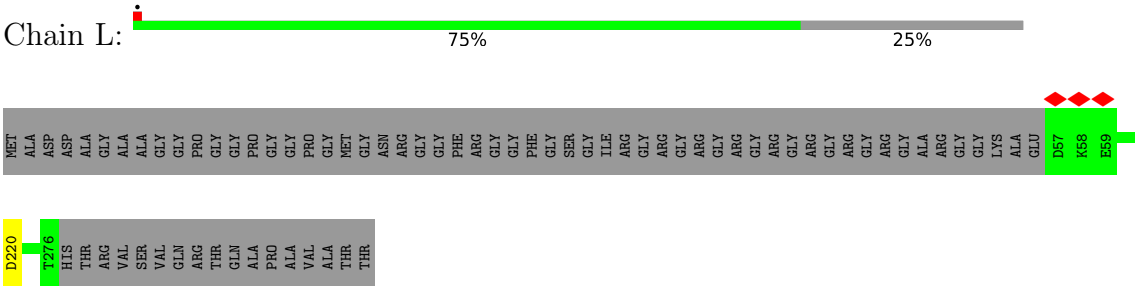
• Molecule 20: 40S ribosomal protein S21

Chain K:



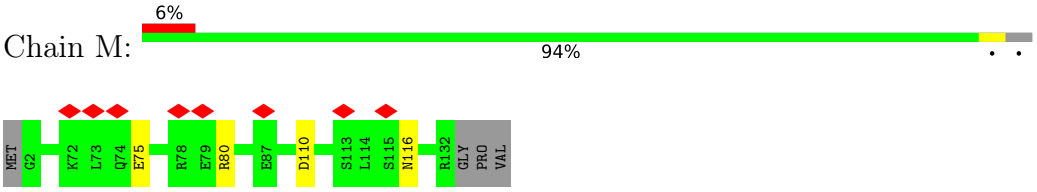
• Molecule 21: 40S ribosomal protein S2

Chain L:



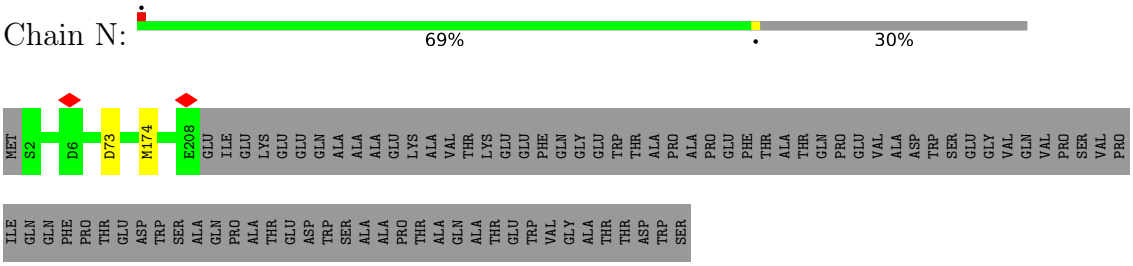
• Molecule 22: 40S ribosomal protein S17

Chain M:



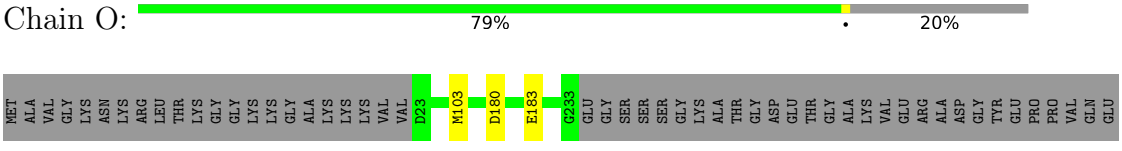
• Molecule 23: 40S ribosomal protein SA

Chain N:



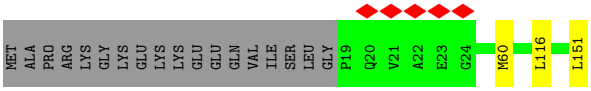
• Molecule 24: 40S ribosomal protein S3a

Chain O:



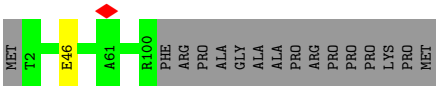
• Molecule 25: 40S ribosomal protein S14

Chain P:



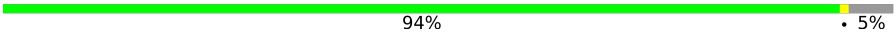
• Molecule 26: 40S ribosomal protein S26

Chain Q:



• Molecule 27: 40S ribosomal protein S8

Chain R:

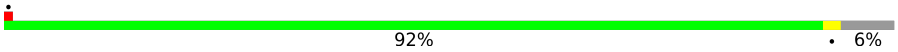


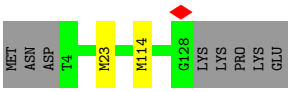
• Molecule 28: 40S ribosomal protein S6

Chain S:

• Molecule 29: 40S ribosomal protein S24

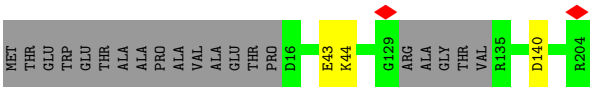
Chain T:





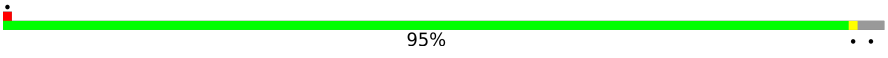
• Molecule 30: 40S ribosomal protein S5

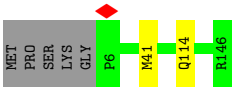
Chain V:



• Molecule 31: 40S ribosomal protein S16

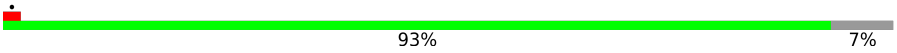
Chain Y:

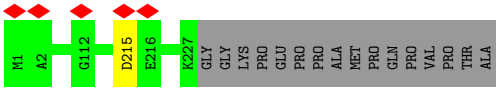




• Molecule 32: 40S ribosomal protein S3

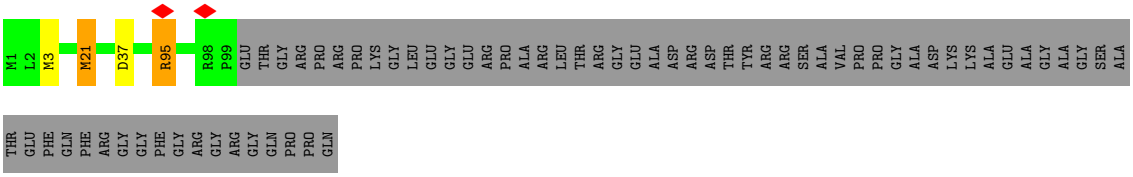
Chain Z:





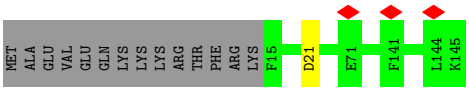
• Molecule 33: 40S ribosomal protein S10

Chain a:



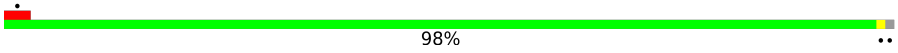
• Molecule 34: 40S ribosomal protein S15

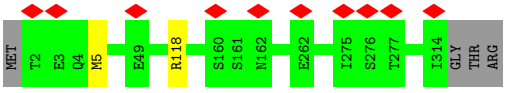
Chain b:



• Molecule 35: Receptor of activated protein C kinase 1

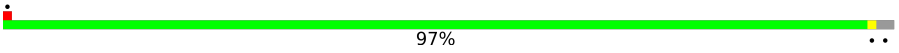
Chain c:

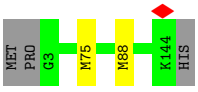




• Molecule 36: 40S ribosomal protein S19

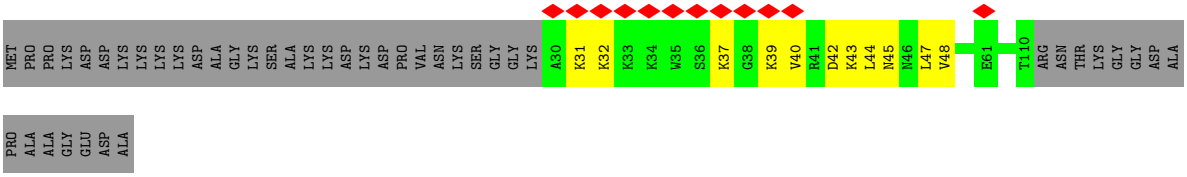
Chain d:





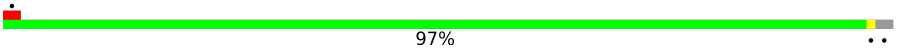
• Molecule 37: 40S ribosomal protein S25

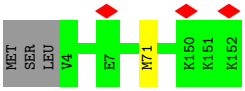
Chain e:



• Molecule 38: 40S ribosomal protein S18

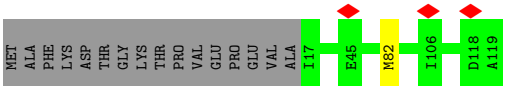
Chain f:





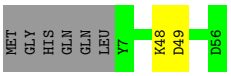
• Molecule 39: 40S ribosomal protein S20

Chain h:



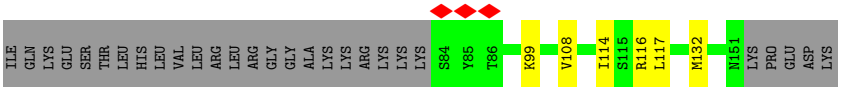
• Molecule 40: 40S ribosomal protein S29

Chain i:



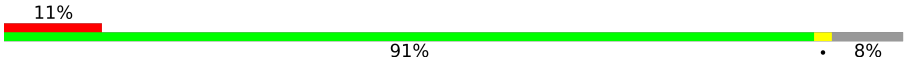
• Molecule 41: Ubiquitin

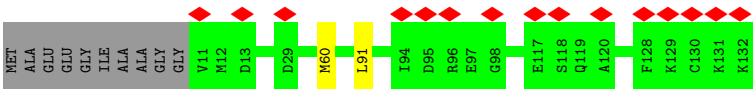
Chain k:



• Molecule 42: 40S ribosomal protein S12

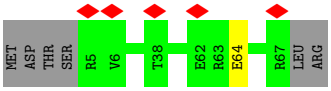
Chain m:





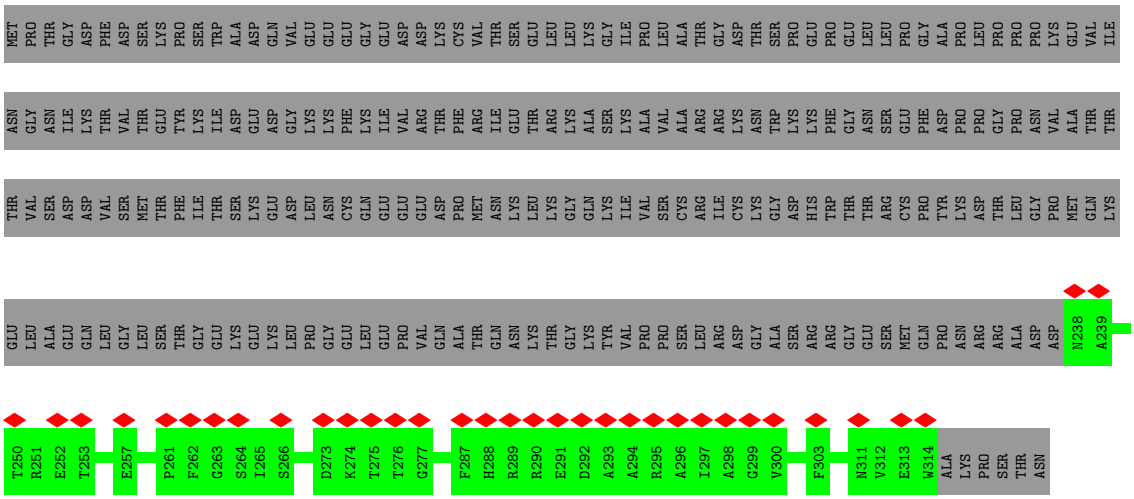
• Molecule 43: 40S ribosomal protein S28

Chain n:



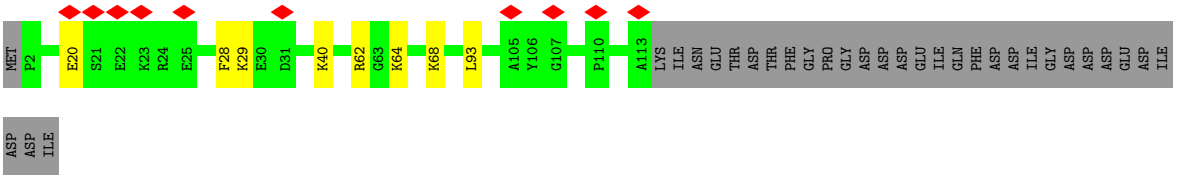
• Molecule 44: Eukaryotic translation initiation factor 3 subunit G

Chain o:



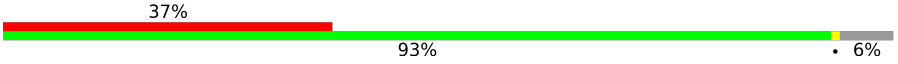
• Molecule 45: Eukaryotic translation initiation factor 1A, X-chromosomal

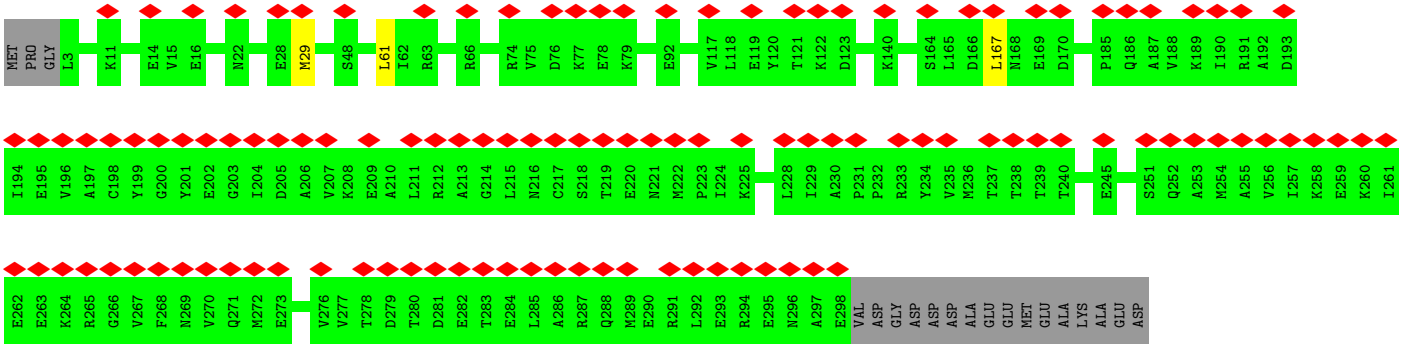
Chain q:



• Molecule 46: Eukaryotic translation initiation factor 2 subunit 1

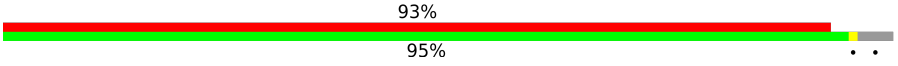
Chain r:

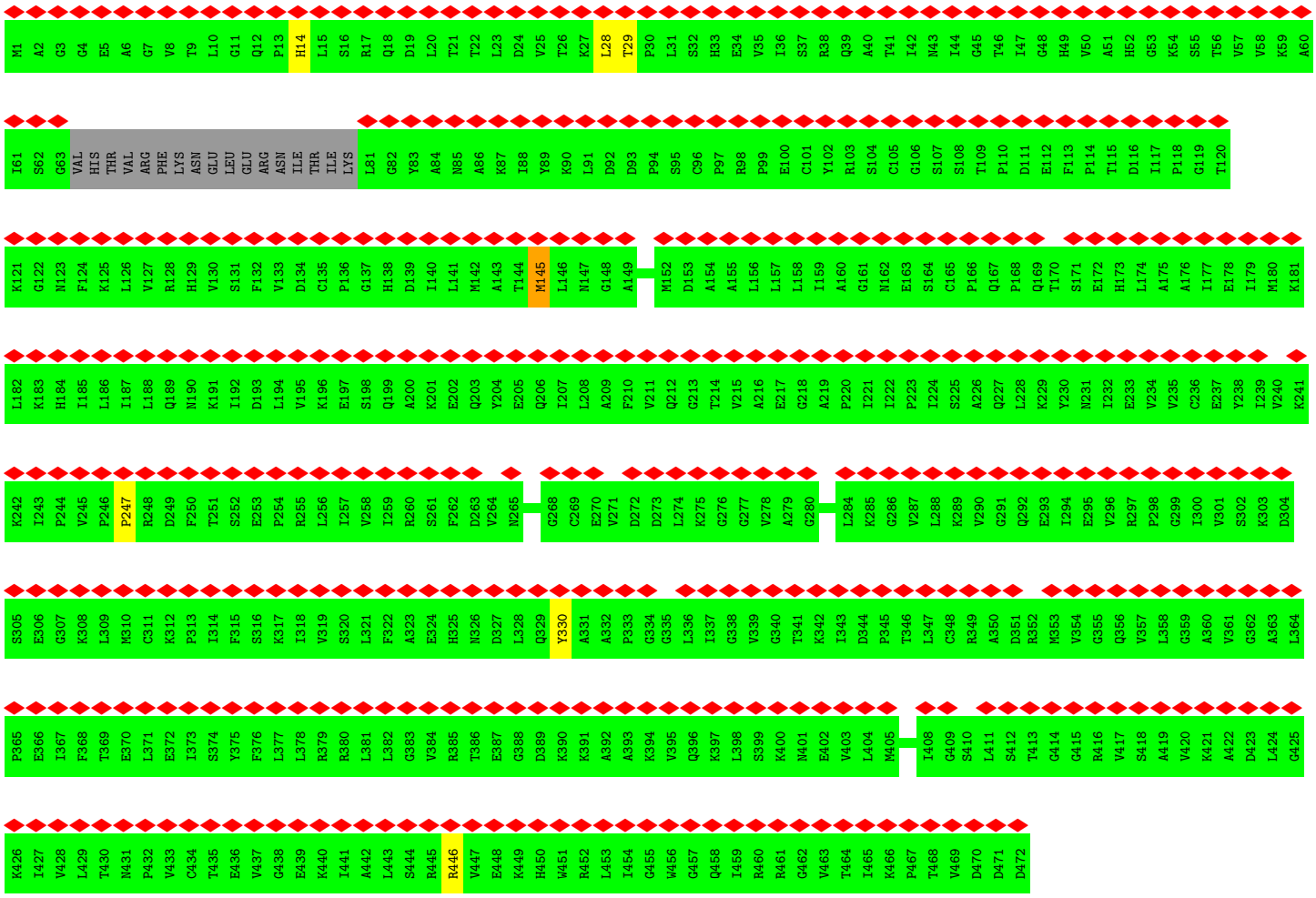




• Molecule 47: Eukaryotic translation initiation factor 2 subunit 3

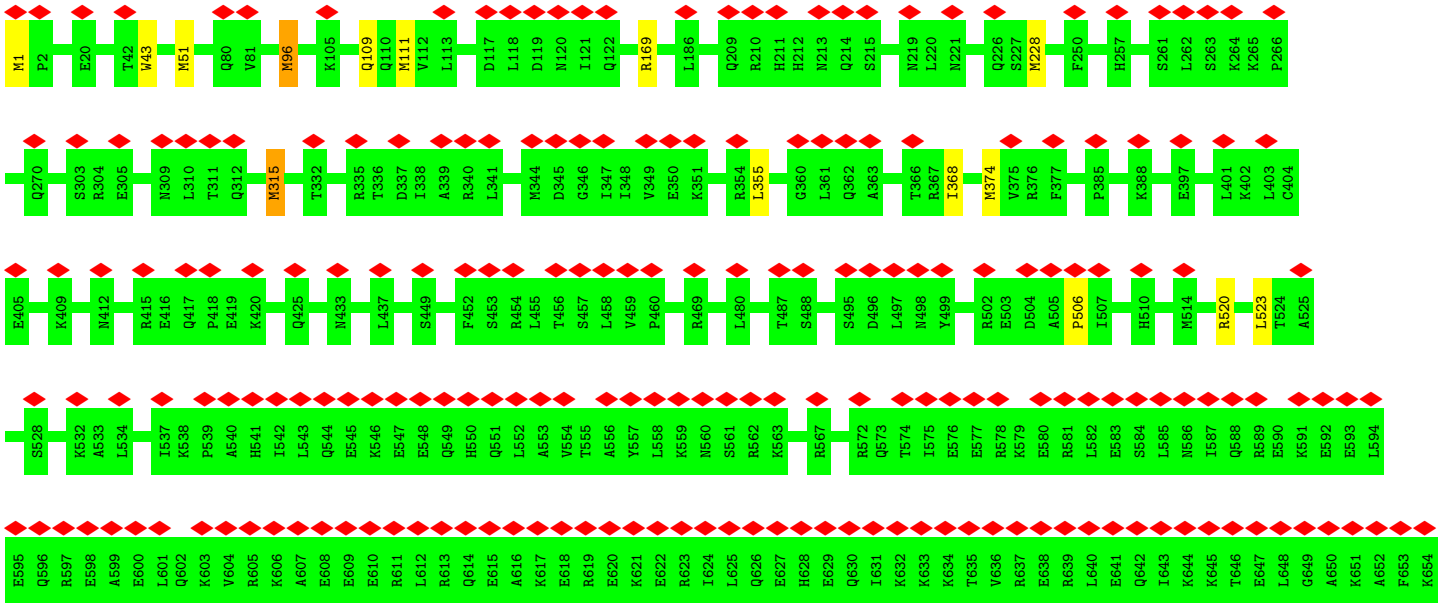
Chain t:

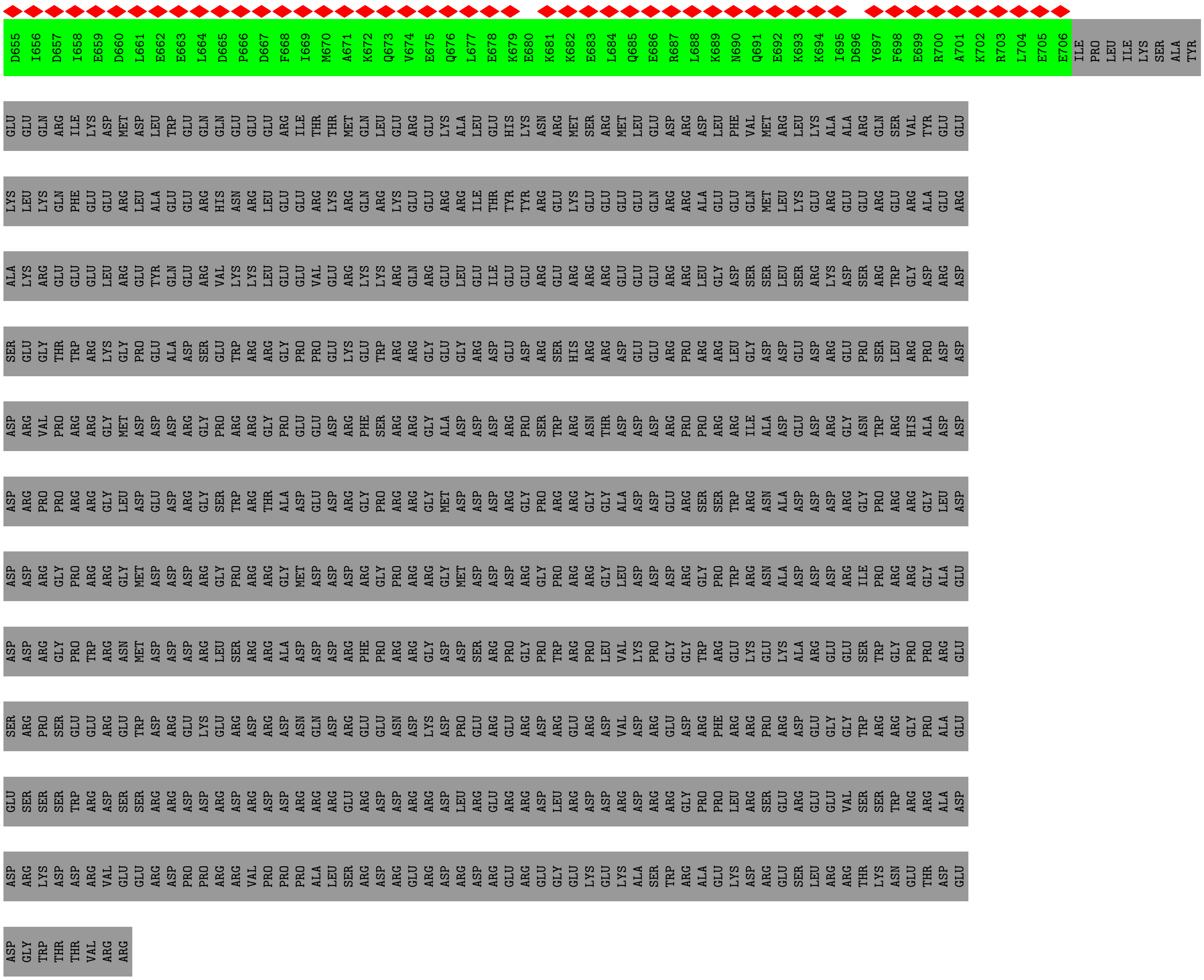




• Molecule 48: Eukaryotic translation initiation factor 3 subunit A

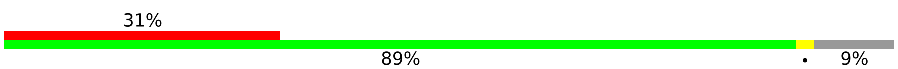
Chain u:

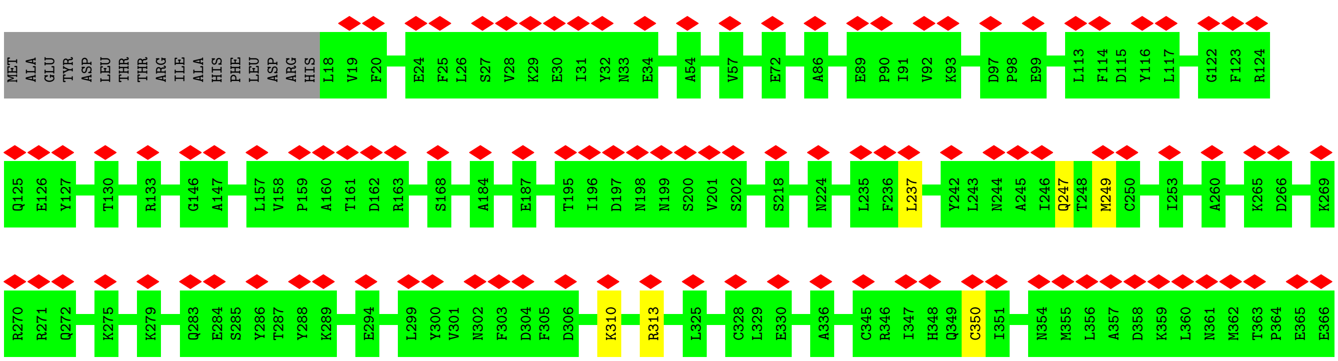


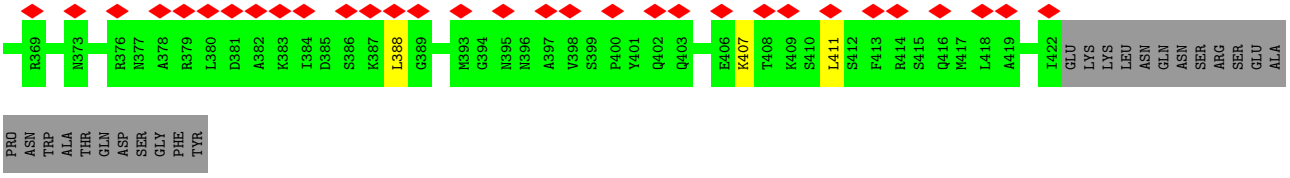


• Molecule 49: Eukaryotic translation initiation factor 3 subunit E

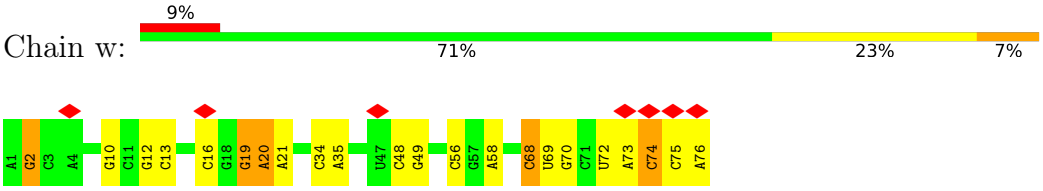
Chain v:



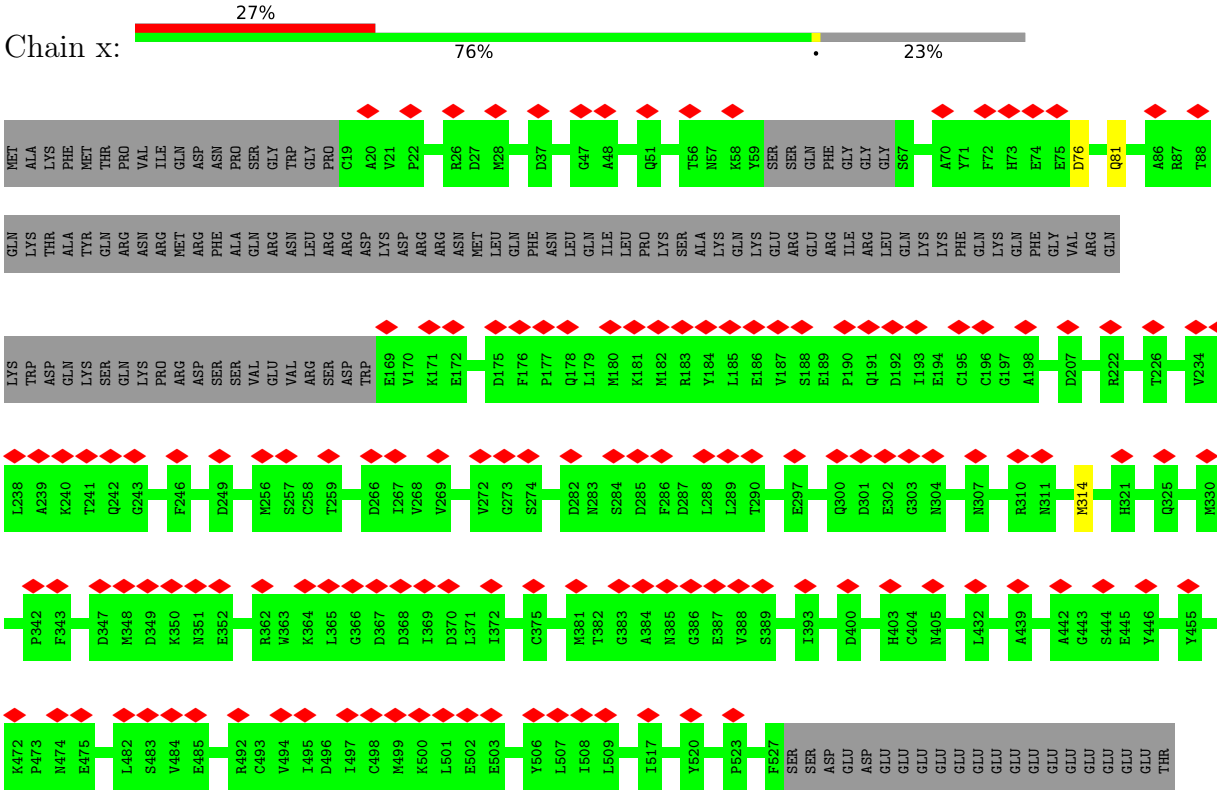




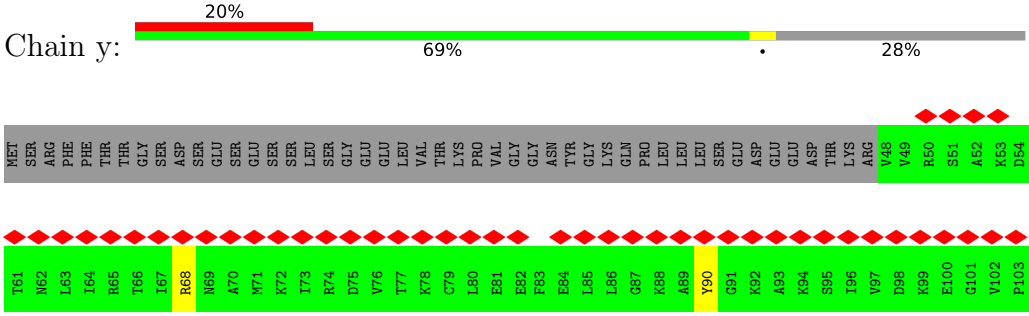
• Molecule 50: Initiator Met-tRNA-i

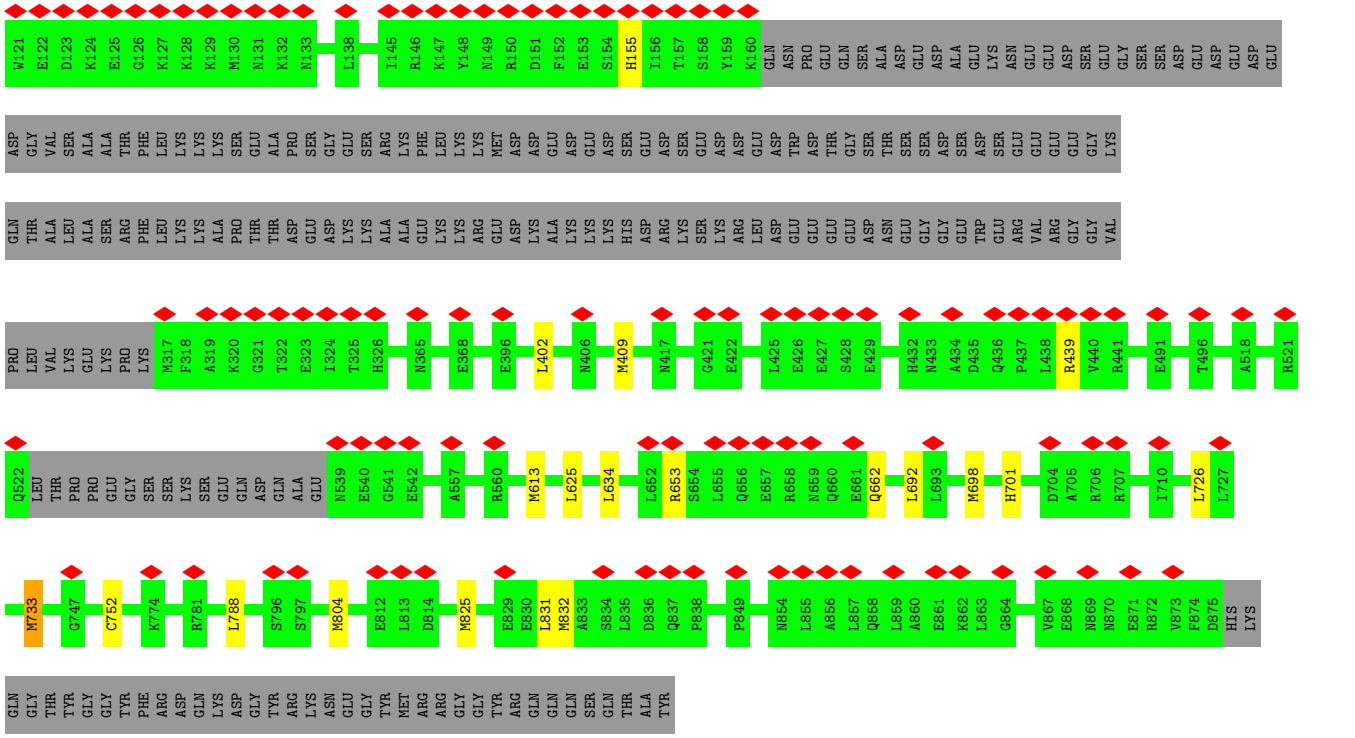


• Molecule 51: Eukaryotic translation initiation factor 3 subunit D



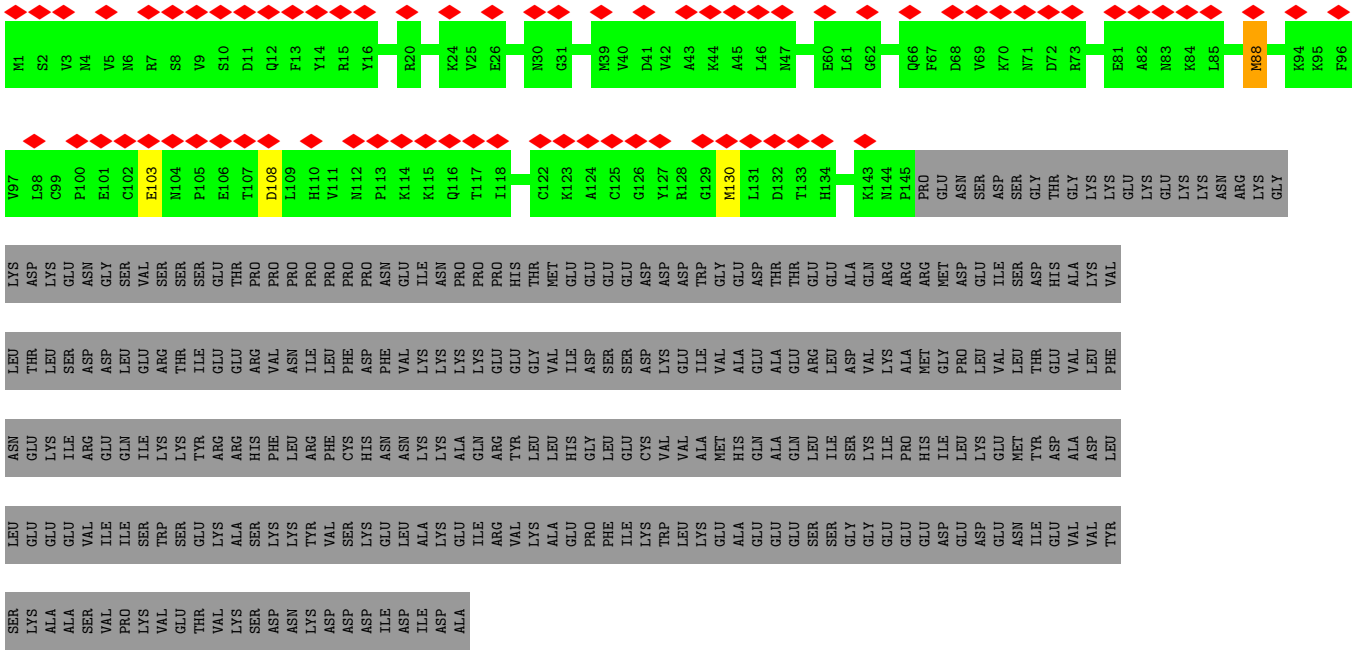
• Molecule 52: Eukaryotic translation initiation factor 3 subunit C





• Molecule 53: Eukaryotic translation initiation factor 5

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61742	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	23.548	Depositor
Minimum map value	-8.712	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	417.74402, 417.74402, 417.74402	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96700007, 0.96700007, 0.96700007	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, ZN, OMU, JMH, OMC, 5MU, 5MC, UR3, A2M, PSU, MA6, MG, OMG, B8N

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	1	0.28	0/3279	0.58	1/4534 (0.0%)
2	2	0.25	0/1491	0.48	0/2068
3	3	0.24	0/1055	0.37	0/1469
4	4	0.24	0/1269	0.39	0/1762
5	5	0.28	0/4458	0.58	4/6027 (0.1%)
6	6	0.29	0/2212	0.62	3/3034 (0.1%)
7	7	0.33	0/1365	1.05	10/2124 (0.5%)
8	8	0.25	0/1572	0.42	0/2187
9	9	0.28	0/231	0.81	0/294
10	A	0.49	0/41130	1.02	160/64100 (0.2%)
11	B	0.32	0/1186	0.59	0/1585
12	C	0.34	0/2077	0.66	2/2796 (0.1%)
13	D	0.38	0/1502	0.76	3/2008 (0.1%)
14	E	0.35	0/1105	0.65	0/1476
15	F	0.34	0/474	0.71	0/623
16	G	0.32	0/1451	0.68	2/1942 (0.1%)
17	H	0.41	0/644	0.85	4/864 (0.5%)
18	I	0.33	0/1232	0.71	3/1656 (0.2%)
19	J	0.35	0/1051	0.68	0/1406
20	K	0.33	0/623	0.68	0/833
21	L	0.37	0/1743	0.69	0/2354
22	M	0.36	0/1078	0.73	1/1447 (0.1%)
23	N	0.33	0/1670	0.63	0/2271
24	O	0.33	0/1742	0.68	0/2330
25	P	0.37	0/1010	0.79	2/1353 (0.1%)
26	Q	0.34	0/805	0.71	1/1079 (0.1%)
27	R	0.30	0/1654	0.59	0/2203
28	S	0.30	0/1885	0.64	1/2510 (0.0%)
29	T	0.32	0/1032	0.69	1/1371 (0.1%)
30	V	0.35	0/1481	0.69	1/1988 (0.1%)
31	Y	0.31	0/1142	0.68	2/1528 (0.1%)
32	Z	0.32	0/1793	0.64	1/2414 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	a	0.36	0/859	0.77	3/1159 (0.3%)
34	b	0.33	0/1094	0.74	0/1464
35	c	0.30	0/2493	0.63	1/3394 (0.0%)
36	d	0.34	0/1123	0.67	1/1504 (0.1%)
37	e	0.43	0/657	0.64	0/878
38	f	0.30	0/1245	0.64	0/1665
39	h	0.32	0/827	0.72	1/1110 (0.1%)
40	i	0.34	0/429	0.67	0/568
41	k	0.36	0/566	0.72	1/753 (0.1%)
42	m	0.28	0/960	0.61	1/1286 (0.1%)
43	n	0.36	0/500	0.76	1/669 (0.1%)
44	o	0.28	0/628	0.68	0/846
45	q	0.42	0/913	0.79	2/1213 (0.2%)
46	r	0.29	0/2167	0.60	3/2943 (0.1%)
47	t	0.30	0/3494	0.68	2/4726 (0.0%)
48	u	0.32	0/5475	0.73	10/7432 (0.1%)
49	v	0.32	0/2778	0.67	5/3797 (0.1%)
50	w	0.42	0/1795	1.07	12/2798 (0.4%)
51	x	0.28	0/2880	0.62	3/3933 (0.1%)
52	y	0.32	0/5350	0.75	15/7215 (0.2%)
53	z	0.31	0/1169	0.68	2/1575 (0.1%)
All	All	0.39	0/123844	0.82	265/176564 (0.2%)

There are no bond length outliers.

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1453	C	N1-C2-O2	10.63	125.28	118.90
10	A	882	U	N1-C2-O2	10.21	129.95	122.80
10	A	1453	C	C2-N1-C1'	9.93	129.72	118.80
10	A	888	U	C2-N1-C1'	9.77	129.42	117.70
10	A	537	C	N3-C2-O2	-9.40	115.32	121.90
10	A	501	C	C2-N1-C1'	9.29	129.02	118.80
10	A	1115	U	C2-N1-C1'	9.20	128.74	117.70
47	t	247	PRO	CA-N-CD	-9.09	98.77	111.50
10	A	1115	U	N1-C2-O2	9.08	129.16	122.80
47	t	145	MET	CA-CB-CG	9.06	128.70	113.30
25	P	151	LEU	CA-CB-CG	8.98	135.96	115.30
48	u	523	LEU	CA-CB-CG	8.84	135.63	115.30
39	h	82	MET	CA-CB-CG	8.78	128.22	113.30
10	A	501	C	N1-C2-O2	8.73	124.14	118.90
10	A	1752	C	N1-C2-O2	8.73	124.14	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	882	U	N3-C2-O2	-8.62	116.16	122.20
10	A	556	U	C2-N1-C1'	8.60	128.02	117.70
7	7	-31	C	N1-C2-O2	8.58	124.05	118.90
10	A	1115	U	N3-C2-O2	-8.49	116.26	122.20
18	I	31	ASP	CB-CG-OD1	8.43	125.89	118.30
48	u	96	MET	CB-CG-SD	8.40	137.61	112.40
10	A	1597	C	N3-C2-O2	-8.38	116.03	121.90
10	A	888	U	N3-C2-O2	-8.38	116.34	122.20
16	G	35	ASP	CB-CG-OD1	8.35	125.81	118.30
10	A	740	C	N3-C2-O2	-8.34	116.06	121.90
10	A	537	C	N1-C2-O2	8.25	123.85	118.90
10	A	168	C	N1-C2-O2	8.16	123.80	118.90
10	A	1687	C	C2-N1-C1'	8.13	127.74	118.80
10	A	556	U	N3-C2-O2	-8.12	116.51	122.20
10	A	1453	C	N3-C2-O2	-8.10	116.23	121.90
10	A	1597	C	N1-C2-O2	8.03	123.72	118.90
10	A	1752	C	C2-N1-C1'	7.95	127.54	118.80
51	x	76	ASP	CB-CG-OD1	7.91	125.42	118.30
52	y	726	LEU	CA-CB-CG	7.89	133.46	115.30
13	D	88	ASP	CB-CG-OD1	7.89	125.40	118.30
18	I	32	ASP	CB-CG-OD1	7.86	125.37	118.30
10	A	1520	G	N3-C4-N9	7.82	130.69	126.00
53	z	103	GLU	CA-CB-CG	7.79	130.53	113.40
10	A	556	U	N1-C2-O2	7.79	128.25	122.80
36	d	88	MET	CA-CB-CG	7.75	126.48	113.30
10	A	1520	G	C4-N9-C1'	7.73	136.55	126.50
10	A	1752	C	N3-C2-O2	-7.67	116.53	121.90
48	u	96	MET	CA-CB-CG	7.67	126.34	113.30
10	A	1139	C	C2-N1-C1'	7.66	127.22	118.80
10	A	1756	C	N1-C2-O2	7.65	123.49	118.90
10	A	706	U	C2-N1-C1'	7.63	126.86	117.70
12	C	19	MET	CG-SD-CE	-7.61	88.03	100.20
10	A	1520	G	C8-N9-C1'	-7.61	117.11	127.00
10	A	706	U	N1-C2-O2	7.58	128.11	122.80
10	A	710	C	C5-C6-N1	7.57	124.79	121.00
5	5	398	MET	CA-CB-CG	7.57	126.17	113.30
17	H	2	PRO	CA-N-CD	-7.54	100.94	111.50
10	A	882	U	C2-N1-C1'	7.43	126.62	117.70
52	y	110	LEU	CB-CG-CD2	7.42	123.62	111.00
10	A	729	C	C5-C6-N1	7.38	124.69	121.00
30	V	43	GLU	CA-CB-CG	7.29	129.43	113.40
10	A	1422	G	N3-C4-N9	7.29	130.37	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	41	MET	CA-CB-CG	7.28	125.68	113.30
10	A	888	U	N1-C2-O2	7.26	127.89	122.80
48	u	374	MET	CG-SD-CE	7.23	111.77	100.20
13	D	104	ASP	CB-CG-OD1	7.22	124.79	118.30
6	6	297	MET	CA-CB-CG	7.14	125.44	113.30
10	A	517	OMC	P-O3'-C3'	-7.13	111.14	119.70
50	w	20	A	C8-N9-C4	-7.12	102.95	105.80
51	x	81	GLN	CA-CB-CG	7.09	129.00	113.40
48	u	368	ILE	CG1-CB-CG2	-7.06	95.87	111.40
7	7	-31	C	N3-C2-O2	-7.05	116.96	121.90
10	A	706	U	N3-C2-O2	-6.94	117.34	122.20
10	A	731	G	P-O3'-C3'	6.91	127.99	119.70
10	A	739	C	O5'-P-OP1	-6.91	99.48	105.70
48	u	228	MET	CA-CB-CG	6.90	125.03	113.30
7	7	-21	A	P-O3'-C3'	6.89	127.97	119.70
10	A	710	C	C6-N1-C2	-6.88	117.55	120.30
10	A	510	G	C8-N9-C4	-6.87	103.65	106.40
5	5	367	MET	CA-CB-CG	6.83	124.90	113.30
10	A	1453	C	C6-N1-C1'	-6.82	112.61	120.80
10	A	1139	C	N1-C2-O2	6.82	122.99	118.90
50	w	2	G	N3-C4-C5	-6.79	125.21	128.60
10	A	706	U	C5-C6-N1	6.76	126.08	122.70
41	k	132	MET	CA-CB-CG	6.76	124.80	113.30
10	A	723	C	N1-C2-O2	6.74	122.95	118.90
10	A	739	C	N1-C2-O2	6.73	122.94	118.90
10	A	836	G	N3-C4-C5	-6.72	125.24	128.60
6	6	352	ASP	CB-CG-OD1	6.70	124.33	118.30
10	A	815	U	C5-C6-N1	6.69	126.05	122.70
10	A	707	C	C6-N1-C2	-6.65	117.64	120.30
10	A	739	C	N3-C2-O2	-6.65	117.25	121.90
10	A	537	C	C6-N1-C2	-6.64	117.64	120.30
10	A	965	U	N1-C2-O2	6.63	127.44	122.80
10	A	501	C	C6-N1-C1'	-6.63	112.85	120.80
10	A	1453	C	C6-N1-C2	-6.62	117.65	120.30
7	7	-34	C	N1-C2-O2	6.62	122.87	118.90
10	A	1756	C	C2-N1-C1'	6.61	126.07	118.80
50	w	34	C	C5-C6-N1	6.60	124.30	121.00
7	7	-31	C	C2-N1-C1'	6.59	126.05	118.80
10	A	1022	U	C2-N1-C1'	6.53	125.53	117.70
10	A	168	C	N3-C2-O2	-6.52	117.33	121.90
10	A	836	G	C4-N9-C1'	6.52	134.98	126.50
10	A	836	G	N3-C4-N9	6.52	129.91	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	37	ASP	CB-CG-OD1	6.51	124.16	118.30
10	A	1422	G	C4-N9-C1'	6.50	134.95	126.50
45	q	93	LEU	CA-CB-CG	6.47	130.19	115.30
10	A	1261	C	N1-C2-O2	6.46	122.78	118.90
10	A	728	C	C5-C6-N1	6.45	124.22	121.00
10	A	1139	C	N3-C2-O2	-6.44	117.39	121.90
10	A	501	C	N3-C2-O2	-6.40	117.42	121.90
22	M	110	ASP	CB-CG-OD1	6.39	124.05	118.30
35	c	5	MET	CB-CG-SD	6.39	131.59	112.40
10	A	739	C	C6-N1-C2	-6.36	117.76	120.30
29	T	114	MET	CA-CB-CG	6.32	124.05	113.30
42	m	91	LEU	CA-CB-CG	6.26	129.69	115.30
52	y	634	LEU	CA-CB-CG	6.25	129.68	115.30
50	w	2	G	C8-N9-C4	-6.25	103.90	106.40
10	A	1453	C	C5-C6-N1	6.24	124.12	121.00
10	A	888	U	C6-N1-C2	-6.24	117.26	121.00
10	A	707	C	C5-C6-N1	6.23	124.11	121.00
6	6	326	ASP	CB-CG-OD1	6.21	123.89	118.30
10	A	965	U	N3-C2-O2	-6.20	117.86	122.20
10	A	729	C	C6-N1-C2	-6.18	117.83	120.30
7	7	-31	C	C6-N1-C2	-6.15	117.84	120.30
10	A	688	U	P-O3'-C3'	6.15	127.08	119.70
10	A	1	U	OP1-P-O3'	6.14	118.70	105.20
48	u	355	LEU	CA-CB-CG	6.13	129.40	115.30
48	u	506	PRO	CA-N-CD	-6.10	102.96	111.50
10	A	1756	C	N3-C2-O2	-6.08	117.65	121.90
10	A	168	C	C2-N1-C1'	6.07	125.48	118.80
10	A	1271	C	N1-C2-O2	6.01	122.51	118.90
10	A	1553	C	N1-C2-O2	6.01	122.50	118.90
52	y	692	LEU	CA-CB-CG	5.99	129.07	115.30
17	H	33	MET	CB-CG-SD	5.97	130.30	112.40
10	A	1591	C	N1-C2-O2	5.93	122.46	118.90
10	A	1422	G	C8-N9-C1'	-5.90	119.33	127.00
10	A	728	C	C6-N1-C2	-5.90	117.94	120.30
10	A	178	C	N1-C2-O2	5.90	122.44	118.90
10	A	1422	G	N3-C4-C5	-5.90	125.65	128.60
10	A	1520	G	C6-C5-N7	-5.90	126.86	130.40
32	Z	215	ASP	CB-CG-OD1	5.89	123.60	118.30
43	n	64	GLU	CA-CB-CG	5.88	126.33	113.40
10	A	732	U	O5'-P-OP1	-5.87	100.42	105.70
10	A	1687	C	C6-N1-C1'	-5.86	113.77	120.80
48	u	374	MET	CA-CB-CG	5.86	123.26	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	501	C	C5-C6-N1	5.85	123.92	121.00
10	A	695	C	N3-C2-O2	-5.84	117.81	121.90
10	A	815	U	C6-N1-C2	-5.83	117.50	121.00
10	A	1115	U	C6-N1-C1'	-5.82	113.06	121.20
50	w	20	A	N7-C8-N9	5.82	116.71	113.80
49	v	411	LEU	CA-CB-CG	5.81	128.67	115.30
28	S	1	MET	N-CA-C	-5.81	95.31	111.00
10	A	644	OMG	O3'-P-O5'	5.81	115.04	104.00
5	5	388	LEU	CA-CB-CG	5.80	128.64	115.30
10	A	537	C	C2-N1-C1'	5.80	125.18	118.80
10	A	719	G	N7-C8-N9	5.79	115.99	113.10
50	w	34	C	C2-N1-C1'	5.78	125.16	118.80
25	P	60	MET	CA-CB-CG	5.78	123.12	113.30
10	A	797	C	P-O3'-C3'	5.78	126.63	119.70
10	A	659	G	C4-N9-C1'	5.77	134.00	126.50
10	A	1139	C	C6-N1-C2	-5.77	117.99	120.30
52	y	832	MET	CA-CB-CG	5.77	123.11	113.30
52	y	733	MET	CA-CB-CG	5.75	123.08	113.30
5	5	326	MET	CA-CB-CG	5.74	123.05	113.30
10	A	882	U	C5-C6-N1	5.74	125.57	122.70
33	a	21	MET	CB-CG-SD	5.74	129.60	112.40
10	A	888	U	C6-N1-C1'	-5.73	113.17	121.20
10	A	708	C	C2-N1-C1'	5.72	125.09	118.80
31	Y	41	MET	CB-CG-SD	-5.71	95.27	112.40
10	A	291	G	P-O3'-C3'	5.71	126.55	119.70
46	r	167	LEU	CA-CB-CG	5.70	128.40	115.30
10	A	740	C	N1-C2-O2	5.68	122.31	118.90
33	a	95	ARG	CA-CB-CG	5.68	125.89	113.40
10	A	708	C	C5-C6-N1	5.68	123.84	121.00
10	A	888	U	C5-C6-N1	5.65	125.53	122.70
53	z	88	MET	CA-CB-CG	5.65	122.90	113.30
10	A	725	C	C6-N1-C2	-5.64	118.04	120.30
7	7	-22	C	C6-N1-C2	-5.64	118.05	120.30
10	A	1115	U	C5-C6-N1	5.64	125.52	122.70
10	A	1389	C	C2-N1-C1'	5.61	124.97	118.80
50	w	2	G	C2-N3-C4	5.59	114.70	111.90
10	A	666	U	C2-N1-C1'	5.58	124.39	117.70
17	H	2	PRO	N-CD-CG	-5.57	94.85	103.20
10	A	501	C	C6-N1-C2	-5.56	118.08	120.30
7	7	-31	C	OP2-P-O3'	5.56	117.44	105.20
49	v	350	CYS	CA-CB-SG	5.56	124.01	114.00
52	y	804	MET	CA-CB-CG	5.55	122.74	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	r	61	LEU	CA-CB-CG	5.55	128.06	115.30
52	y	752	CYS	CA-CB-SG	-5.53	104.04	114.00
49	v	237	LEU	CA-CB-CG	5.52	128.00	115.30
10	A	879	C	C2-N1-C1'	5.52	124.87	118.80
10	A	1752	C	C6-N1-C2	-5.52	118.09	120.30
10	A	537	C	O4'-C1'-N1	5.52	112.61	108.20
10	A	1261	C	N3-C2-O2	-5.52	118.04	121.90
10	A	1600	G	N3-C4-N9	5.52	129.31	126.00
10	A	692	G	C8-N9-C4	-5.51	104.20	106.40
17	H	33	MET	CA-CB-CG	5.50	122.66	113.30
10	A	735	C	C5-C6-N1	5.50	123.75	121.00
10	A	719	G	C8-N9-C4	-5.49	104.20	106.40
10	A	738	C	N3-C2-O2	-5.48	118.06	121.90
52	y	698	MET	CA-CB-CG	5.48	122.62	113.30
10	A	700	G	N3-C4-N9	5.48	129.29	126.00
7	7	-31	C	P-O3'-C3'	5.48	126.28	119.70
10	A	710	C	C2-N1-C1'	5.47	124.82	118.80
52	y	825	MET	CA-CB-CG	5.47	122.60	113.30
10	A	731	G	OP1-P-O3'	5.44	117.16	105.20
10	A	1261	C	C2-N1-C1'	5.43	124.78	118.80
10	A	1417	C	N3-C2-O2	-5.43	118.10	121.90
52	y	831	LEU	CA-CB-CG	5.43	127.80	115.30
10	A	509	OMG	O3'-P-O5'	5.43	114.31	104.00
10	A	692	G	N1-C6-O6	-5.42	116.65	119.90
10	A	130	G	C4-N9-C1'	5.42	133.55	126.50
10	A	700	G	C6-C5-N7	-5.42	127.15	130.40
10	A	1116	C	N1-C2-O2	5.42	122.15	118.90
10	A	1520	G	N9-C4-C5	-5.40	103.24	105.40
10	A	168	C	C6-N1-C2	-5.40	118.14	120.30
10	A	723	C	N3-C2-O2	-5.39	118.12	121.90
13	D	27	GLN	CA-CB-CG	5.39	125.27	113.40
10	A	692	G	N1-C2-N2	-5.38	111.35	116.20
10	A	1784	G	C5-C6-O6	5.38	131.83	128.60
26	Q	46	GLU	CA-CB-CG	5.37	125.22	113.40
10	A	836	G	C8-N9-C1'	-5.37	120.02	127.00
1	1	561	MET	CG-SD-CE	5.37	108.79	100.20
10	A	1556	A	C2-N3-C4	5.37	113.28	110.60
10	A	494	C	N1-C2-O2	5.36	122.12	118.90
10	A	1752	C	C6-N1-C1'	-5.36	114.37	120.80
51	x	314	MET	CA-CB-CG	5.36	122.42	113.30
46	r	29	MET	CA-CB-CG	5.35	122.40	113.30
10	A	965	U	C2-N1-C1'	5.34	124.11	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	706	U	C6-N1-C2	-5.33	117.80	121.00
18	I	4	MET	CA-CB-CG	5.33	122.36	113.30
50	w	34	C	C6-N1-C2	-5.33	118.17	120.30
52	y	788	LEU	CA-CB-CG	5.33	127.55	115.30
10	A	733	C	C6-N1-C2	-5.32	118.17	120.30
10	A	1687	C	C6-N1-C2	-5.32	118.17	120.30
10	A	725	C	C5-C6-N1	5.32	123.66	121.00
10	A	30	C	C5-C6-N1	5.30	123.65	121.00
10	A	1600	G	P-O3'-C3'	5.30	126.06	119.70
10	A	1565	C	C2-N1-C1'	5.30	124.63	118.80
50	w	19	G	O4'-C1'-N9	-5.29	103.97	108.20
16	G	32	MET	CA-CB-CG	5.26	122.25	113.30
7	7	-34	C	N3-C2-O2	-5.26	118.22	121.90
10	A	30	C	C6-N1-C2	-5.25	118.20	120.30
10	A	632	C	C5-C6-N1	5.25	123.62	121.00
49	v	247	GLN	CA-CB-CG	5.21	124.87	113.40
10	A	1687	C	C5-C6-N1	5.20	123.60	121.00
49	v	388	LEU	CA-CB-CG	5.20	127.25	115.30
10	A	1687	C	N1-C2-O2	5.19	122.02	118.90
52	y	653	ARG	CA-CB-CG	5.17	124.76	113.40
10	A	556	U	C6-N1-C1'	-5.15	113.98	121.20
50	w	68	C	C6-N1-C2	-5.15	118.24	120.30
52	y	402	LEU	CA-CB-CG	5.14	127.12	115.30
10	A	368	U	P-O3'-C3'	5.13	125.86	119.70
50	w	74	C	N1-C2-O2	5.13	121.98	118.90
10	A	566	U	C2-N1-C1'	5.11	123.83	117.70
10	A	1520	G	N3-C4-C5	-5.11	126.05	128.60
10	A	1729	U	N1-C2-O2	5.09	126.37	122.80
10	A	556	U	C6-N1-C2	-5.08	117.95	121.00
48	u	315	MET	CA-CB-CG	5.08	121.93	113.30
10	A	752	G	C4-N9-C1'	5.07	133.09	126.50
50	w	69	U	C2-N1-C1'	5.06	123.78	117.70
52	y	625	LEU	CA-CB-CG	5.06	126.93	115.30
10	A	201	C	N1-C2-O2	5.03	121.92	118.90
10	A	632	C	C2-N1-C1'	5.03	124.33	118.80
12	C	19	MET	CA-CB-CG	5.03	121.85	113.30
10	A	1139	C	C6-N1-C1'	-5.03	114.77	120.80
10	A	701	G	C6-C5-N7	-5.02	127.39	130.40
45	q	29	LYS	CA-CB-CG	5.01	124.43	113.40
10	A	556	U	C5-C6-N1	5.01	125.20	122.70

There are no chirality outliers.

There are no planarity outliers.

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	1	584/814 (72%)	542 (93%)	42 (7%)	0	100	100
2	2	300/325 (92%)	293 (98%)	7 (2%)	0	100	100
3	3	209/218 (96%)	201 (96%)	8 (4%)	0	100	100
4	4	251/357 (70%)	235 (94%)	16 (6%)	0	100	100
5	5	518/564 (92%)	501 (97%)	17 (3%)	0	100	100
6	6	360/374 (96%)	339 (94%)	21 (6%)	0	100	100
8	8	313/352 (89%)	290 (93%)	23 (7%)	0	100	100
9	9	22/25 (88%)	22 (100%)	0	0	100	100
11	B	138/158 (87%)	136 (99%)	2 (1%)	0	100	100
12	C	254/263 (97%)	246 (97%)	8 (3%)	0	100	100
13	D	175/194 (90%)	168 (96%)	7 (4%)	0	100	100
14	E	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
15	F	57/59 (97%)	47 (82%)	10 (18%)	0	100	100
16	G	171/194 (88%)	163 (95%)	8 (5%)	0	100	100
17	H	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
18	I	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
19	J	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
20	K	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
21	L	218/293 (74%)	215 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	M	129/135 (96%)	124 (96%)	5 (4%)	0	100	100
23	N	205/295 (70%)	195 (95%)	10 (5%)	0	100	100
24	O	209/264 (79%)	201 (96%)	8 (4%)	0	100	100
25	P	131/151 (87%)	120 (92%)	11 (8%)	0	100	100
26	Q	97/115 (84%)	92 (95%)	5 (5%)	0	100	100
27	R	194/208 (93%)	192 (99%)	2 (1%)	0	100	100
28	S	228/249 (92%)	217 (95%)	11 (5%)	0	100	100
29	T	123/133 (92%)	123 (100%)	0	0	100	100
30	V	180/204 (88%)	171 (95%)	9 (5%)	0	100	100
31	Y	139/146 (95%)	135 (97%)	4 (3%)	0	100	100
32	Z	225/243 (93%)	221 (98%)	4 (2%)	0	100	100
33	a	97/165 (59%)	94 (97%)	3 (3%)	0	100	100
34	b	129/145 (89%)	123 (95%)	6 (5%)	0	100	100
35	c	311/317 (98%)	295 (95%)	16 (5%)	0	100	100
36	d	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
37	e	79/125 (63%)	72 (91%)	7 (9%)	0	100	100
38	f	147/152 (97%)	135 (92%)	12 (8%)	0	100	100
39	h	101/119 (85%)	95 (94%)	6 (6%)	0	100	100
40	i	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
41	k	66/156 (42%)	61 (92%)	5 (8%)	0	100	100
42	m	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
43	n	61/69 (88%)	56 (92%)	5 (8%)	0	100	100
44	o	75/320 (23%)	73 (97%)	2 (3%)	0	100	100
45	q	110/144 (76%)	92 (84%)	18 (16%)	0	100	100
46	r	294/315 (93%)	269 (92%)	25 (8%)	0	100	100
47	t	451/472 (96%)	441 (98%)	10 (2%)	0	100	100
48	u	705/1382 (51%)	656 (93%)	49 (7%)	0	100	100
49	v	403/445 (91%)	367 (91%)	36 (9%)	0	100	100
51	x	416/548 (76%)	391 (94%)	25 (6%)	0	100	100
52	y	650/913 (71%)	619 (95%)	31 (5%)	0	100	100
53	z	143/430 (33%)	136 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	10547/13474 (78%)	10010 (95%)	537 (5%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	1	97/702 (14%)	95 (98%)	2 (2%)	53 76
5	5	477/515 (93%)	473 (99%)	4 (1%)	81 91
6	6	112/335 (33%)	112 (100%)	0	100 100
8	8	1/310 (0%)	1 (100%)	0	100 100
9	9	23/24 (96%)	22 (96%)	1 (4%)	29 59
11	B	129/142 (91%)	128 (99%)	1 (1%)	81 91
12	C	220/225 (98%)	219 (100%)	1 (0%)	88 94
13	D	158/168 (94%)	154 (98%)	4 (2%)	47 72
14	E	112/115 (97%)	112 (100%)	0	100 100
15	F	48/48 (100%)	47 (98%)	1 (2%)	53 76
16	G	159/174 (91%)	155 (98%)	4 (2%)	47 72
17	H	73/76 (96%)	71 (97%)	2 (3%)	44 70
18	I	130/131 (99%)	128 (98%)	2 (2%)	65 82
19	J	112/113 (99%)	112 (100%)	0	100 100
20	K	65/67 (97%)	64 (98%)	1 (2%)	65 82
21	L	186/225 (83%)	185 (100%)	1 (0%)	88 94
22	M	119/122 (98%)	116 (98%)	3 (2%)	47 72
23	N	173/243 (71%)	171 (99%)	2 (1%)	71 85
24	O	192/231 (83%)	189 (98%)	3 (2%)	62 81
25	P	104/119 (87%)	103 (99%)	1 (1%)	76 88
26	Q	86/98 (88%)	86 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	R	172/180 (96%)	170 (99%)	2 (1%)	71 85
28	S	200/218 (92%)	197 (98%)	3 (2%)	65 82
29	T	107/115 (93%)	106 (99%)	1 (1%)	78 90
30	V	156/170 (92%)	154 (99%)	2 (1%)	69 84
31	Y	117/121 (97%)	116 (99%)	1 (1%)	78 90
32	Z	190/202 (94%)	190 (100%)	0	100 100
33	a	90/136 (66%)	87 (97%)	3 (3%)	38 66
34	b	117/130 (90%)	116 (99%)	1 (1%)	78 90
35	c	272/275 (99%)	271 (100%)	1 (0%)	91 95
36	d	112/115 (97%)	111 (99%)	1 (1%)	78 90
37	e	71/103 (69%)	60 (84%)	11 (16%)	2 11
38	f	129/132 (98%)	128 (99%)	1 (1%)	81 91
39	h	94/107 (88%)	94 (100%)	0	100 100
40	i	44/49 (90%)	42 (96%)	2 (4%)	27 58
41	k	61/140 (44%)	56 (92%)	5 (8%)	11 37
42	m	104/108 (96%)	103 (99%)	1 (1%)	76 88
43	n	56/62 (90%)	56 (100%)	0	100 100
44	o	64/277 (23%)	64 (100%)	0	100 100
45	q	94/123 (76%)	88 (94%)	6 (6%)	17 47
46	r	190/280 (68%)	190 (100%)	0	100 100
47	t	380/397 (96%)	374 (98%)	6 (2%)	62 81
48	u	528/1259 (42%)	519 (98%)	9 (2%)	60 80
49	v	206/406 (51%)	202 (98%)	4 (2%)	57 78
51	x	207/494 (42%)	207 (100%)	0	100 100
52	y	562/811 (69%)	552 (98%)	10 (2%)	59 79
53	z	129/388 (33%)	126 (98%)	3 (2%)	50 74
All	All	7228/10981 (66%)	7122 (98%)	106 (2%)	66 82

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	555	PRO
1	1	577	PHE

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Mol	Chain	Res	Type
5	5	45	TYR
5	5	262	ARG
5	5	367	MET
5	5	380	MET
9	9	1	MET
11	B	69	ARG
12	C	117	GLU
13	D	27	GLN
13	D	59	GLU
13	D	88	ASP
13	D	105	PHE
15	F	116	PHE
16	G	17	ASP
16	G	32	MET
16	G	165	ASN
16	G	192	PHE
17	H	41	TYR
17	H	79	PHE
18	I	36	GLN
18	I	103	GLU
20	K	41	LYS
21	L	220	ASP
22	M	75	GLU
22	M	80	ARG
22	M	116	ASN
23	N	73	ASP
23	N	174	MET
24	O	103	MET
24	O	180	ASP
24	O	183	GLU
25	P	116	LEU
27	R	143	LYS
27	R	160	SER
28	S	39	ASP
28	S	98	ARG
28	S	120	ASP
29	T	23	MET
30	V	44	LYS
30	V	140	ASP
31	Y	114	GLN
33	a	3	MET
33	a	21	MET

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Mol	Chain	Res	Type
33	a	95	ARG
34	b	21	ASP
35	c	118	ARG
36	d	75	MET
37	e	31	LYS
37	e	32	LYS
37	e	37	LYS
37	e	39	LYS
37	e	40	VAL
37	e	42	ASP
37	e	43	LYS
37	e	44	LEU
37	e	45	ASN
37	e	47	LEU
37	e	48	VAL
38	f	71	MET
40	i	48	LYS
40	i	49	ASP
41	k	99	LYS
41	k	108	VAL
41	k	114	ILE
41	k	116	ARG
41	k	117	LEU
42	m	60	MET
45	q	20	GLU
45	q	28	PHE
45	q	40	LYS
45	q	62	ARG
45	q	64	LYS
45	q	68	LYS
47	t	14	HIS
47	t	28	LEU
47	t	29	THR
47	t	145	MET
47	t	330	TYR
47	t	446	ARG
48	u	1	MET
48	u	43	TRP
48	u	51	MET
48	u	96	MET
48	u	109	GLN
48	u	111	MET

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Mol	Chain	Res	Type
48	u	169	ARG
48	u	315	MET
48	u	520	ARG
49	v	249	MET
49	v	310	LYS
49	v	313	ARG
49	v	407	LYS
52	y	58	GLU
52	y	68	ARG
52	y	90	TYR
52	y	155	HIS
52	y	409	MET
52	y	439	ARG
52	y	613	MET
52	y	662	GLN
52	y	701	HIS
52	y	733	MET
53	z	88	MET
53	z	108	ASP
53	z	130	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
15	F	111	GLN
18	I	49	GLN
22	M	62	GLN
24	O	179	ASN
46	r	10	HIS
48	u	110	GLN
49	v	247	GLN
49	v	416	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1741/1869 (93%)	412 (23%)	13 (0%)
50	w	74/75 (98%)	20 (27%)	0
7	7	56/255 (21%)	43 (76%)	3 (5%)
All	All	1871/2199 (85%)	475 (25%)	16 (0%)

All (475) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	7	-34	C
7	7	-31	C
7	7	-30	A
7	7	-29	A
7	7	-28	C
7	7	-27	A
7	7	-26	A
7	7	-23	A
7	7	-22	C
7	7	-21	A
7	7	-20	A
7	7	-18	G
7	7	-17	A
7	7	-15	C
7	7	-13	A
7	7	-12	A
7	7	-11	A
7	7	-10	A
7	7	-8	A
7	7	-7	G
7	7	-6	A
7	7	-5	C
7	7	-4	C
7	7	-3	A
7	7	-2	C
7	7	-1	C
7	7	3	G
7	7	4	G
7	7	5	U
7	7	6	A
7	7	7	C
7	7	8	G
7	7	10	U
7	7	11	U
7	7	12	C
7	7	13	A
7	7	14	A
7	7	15	G
7	7	17	C
7	7	19	U
7	7	20	G
7	7	21	A

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Mol	Chain	Res	Type
7	7	22	G
10	A	2	A
10	A	4	C
10	A	17	C
10	A	26	U
10	A	33	G
10	A	44	U
10	A	46	A
10	A	56	G
10	A	58	C
10	A	59	U
10	A	67	C
10	A	68	A
10	A	73	C
10	A	74	G
10	A	76	U
10	A	78	C
10	A	82	G
10	A	103	A
10	A	115	U
10	A	126	G
10	A	129	C
10	A	130	G
10	A	140	U
10	A	142	C
10	A	143	U
10	A	147	A
10	A	155	G
10	A	158	A
10	A	163	U
10	A	173	A
10	A	182	C
10	A	184	G
10	A	190	G
10	A	198	U
10	A	199	C
10	A	200	G
10	A	202	G
10	A	203	G
10	A	204	G
10	A	206	G
10	A	208	G

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Mol	Chain	Res	Type
10	A	288	G
10	A	291	G
10	A	292	A
10	A	294	U
10	A	295	C
10	A	306	C
10	A	307	G
10	A	308	G
10	A	309	G
10	A	314	U
10	A	318	A
10	A	319	C
10	A	320	G
10	A	321	C
10	A	323	C
10	A	324	C
10	A	325	C
10	A	326	C
10	A	327	G
10	A	329	G
10	A	332	G
10	A	347	G
10	A	351	G
10	A	362	C
10	A	364	A
10	A	368	U
10	A	369	C
10	A	370	G
10	A	381	C
10	A	384	U
10	A	385	G
10	A	386	C
10	A	409	C
10	A	418	A
10	A	421	G
10	A	448	A
10	A	449	A
10	A	450	C
10	A	452	G
10	A	455	A
10	A	465	A
10	A	467	G

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Mol	Chain	Res	Type
10	A	471	G
10	A	472	C
10	A	473	A
10	A	474	G
10	A	482	G
10	A	487	U
10	A	492	C
10	A	502	C
10	A	508	A
10	A	509	OMG
10	A	517	OMC
10	A	525	A
10	A	534	G
10	A	536	A
10	A	537	C
10	A	538	U
10	A	539	C
10	A	540	U
10	A	541	U
10	A	542	U
10	A	543	C
10	A	544	G
10	A	545	A
10	A	546	G
10	A	547	G
10	A	550	C
10	A	553	U
10	A	554	A
10	A	556	U
10	A	557	U
10	A	558	G
10	A	563	G
10	A	564	A
10	A	566	U
10	A	568	C
10	A	576	A
10	A	589	G
10	A	590	A
10	A	591	U
10	A	598	G
10	A	606	G
10	A	607	U

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Mol	Chain	Res	Type
10	A	614	C
10	A	617	G
10	A	625	G
10	A	626	G
10	A	627	U
10	A	628	A
10	A	643	A
10	A	644	OMG
10	A	655	A
10	A	659	G
10	A	660	C
10	A	662	G
10	A	668	A2M
10	A	669	A
10	A	671	A
10	A	672	A
10	A	673	G
10	A	683	OMG
10	A	688	U
10	A	689	U
10	A	691	G
10	A	692	G
10	A	695	C
10	A	696	G
10	A	697	G
10	A	698	G
10	A	699	C
10	A	700	G
10	A	705	G
10	A	707	C
10	A	712	G
10	A	713	C
10	A	715	A
10	A	717	G
10	A	719	G
10	A	720	A
10	A	721	G
10	A	723	C
10	A	725	C
10	A	726	C
10	A	728	C
10	A	729	C

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Mol	Chain	Res	Type
10	A	731	G
10	A	732	U
10	A	733	C
10	A	734	C
10	A	738	C
10	A	739	C
10	A	748	C
10	A	749	U
10	A	751	G
10	A	752	G
10	A	753	C
10	A	791	C
10	A	798	G
10	A	800	U
10	A	801	U
10	A	810	A
10	A	811	A
10	A	821	G
10	A	822	PSU
10	A	827	A
10	A	830	A
10	A	836	G
10	A	837	A
10	A	838	G
10	A	839	C
10	A	840	C
10	A	841	G
10	A	845	G
10	A	847	A
10	A	870	A
10	A	872	A
10	A	873	G
10	A	880	G
10	A	886	A
10	A	888	U
10	A	890	U
10	A	891	G
10	A	895	G
10	A	896	U
10	A	897	U
10	A	898	U
10	A	899	U

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Mol	Chain	Res	Type
10	A	900	C
10	A	903	A
10	A	908	A
10	A	909	G
10	A	913	A
10	A	914	U
10	A	917	U
10	A	920	A
10	A	922	A
10	A	930	C
10	A	933	G
10	A	956	G
10	A	963	A
10	A	965	U
10	A	969	U
10	A	970	G
10	A	972	A
10	A	990	A
10	A	992	A
10	A	999	G
10	A	1002	U
10	A	1017	U
10	A	1023	A
10	A	1045	U
10	A	1047	C
10	A	1058	A
10	A	1061	U
10	A	1062	A
10	A	1078	C
10	A	1083	A
10	A	1085	C
10	A	1089	G
10	A	1109	C
10	A	1112	U
10	A	1113	A
10	A	1114	U
10	A	1115	U
10	A	1117	C
10	A	1119	A
10	A	1120	U
10	A	1123	C
10	A	1133	A

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Mol	Chain	Res	Type
10	A	1138	C
10	A	1139	C
10	A	1153	C
10	A	1154	U
10	A	1170	A
10	A	1195	A
10	A	1208	A
10	A	1209	A
10	A	1211	G
10	A	1215	C
10	A	1216	C
10	A	1217	A
10	A	1221	G
10	A	1224	G
10	A	1242	U
10	A	1249	C
10	A	1251	A
10	A	1253	A
10	A	1256	G
10	A	1257	G
10	A	1259	A
10	A	1274	G
10	A	1275	G
10	A	1283	C
10	A	1288	U
10	A	1290	G
10	A	1294	G
10	A	1295	A
10	A	1301	A
10	A	1302	G
10	A	1303	C
10	A	1308	U
10	A	1312	G
10	A	1318	G
10	A	1322	G
10	A	1326	U
10	A	1332	A
10	A	1333	U
10	A	1342	U
10	A	1354	G
10	A	1356	G
10	A	1358	U

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Mol	Chain	Res	Type
10	A	1371	U
10	A	1372	U
10	A	1378	A
10	A	1382	A
10	A	1397	U
10	A	1401	A
10	A	1402	A
10	A	1417	C
10	A	1418	C
10	A	1419	C
10	A	1420	G
10	A	1421	A
10	A	1422	G
10	A	1423	C
10	A	1424	G
10	A	1433	C
10	A	1435	C
10	A	1436	C
10	A	1437	C
10	A	1438	A
10	A	1442	U
10	A	1454	A
10	A	1463	U
10	A	1464	C
10	A	1487	A
10	A	1489	A
10	A	1490	G
10	A	1497	G
10	A	1498	A
10	A	1507	G
10	A	1508	A
10	A	1520	G
10	A	1521	C
10	A	1531	A
10	A	1533	A
10	A	1534	C
10	A	1544	C
10	A	1552	G
10	A	1553	C
10	A	1556	A
10	A	1558	C
10	A	1560	U

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Mol	Chain	Res	Type
10	A	1565	C
10	A	1570	G
10	A	1579	A
10	A	1580	A
10	A	1585	U
10	A	1587	G
10	A	1588	A
10	A	1594	A
10	A	1600	G
10	A	1601	A
10	A	1603	G
10	A	1606	G
10	A	1619	A
10	A	1621	U
10	A	1623	A
10	A	1624	U
10	A	1639	G
10	A	1648	G
10	A	1654	G
10	A	1661	A
10	A	1663	A
10	A	1665	G
10	A	1668	U
10	A	1671	G
10	A	1686	G
10	A	1687	C
10	A	1695	A
10	A	1699	A
10	A	1710	C
10	A	1712	A
10	A	1715	A
10	A	1719	A
10	A	1721	U
10	A	1722	G
10	A	1729	U
10	A	1744	G
10	A	1749	G
10	A	1750	C
10	A	1752	C
10	A	1753	C
10	A	1754	G
10	A	1755	C

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Mol	Chain	Res	Type
10	A	1756	C
10	A	1757	G
10	A	1758	G
10	A	1759	G
10	A	1760	G
10	A	1772	C
10	A	1773	C
10	A	1774	C
10	A	1775	U
10	A	1776	G
10	A	1777	G
10	A	1778	C
10	A	1779	G
10	A	1780	G
10	A	1781	A
10	A	1782	G
10	A	1783	C
10	A	1784	G
10	A	1805	G
10	A	1808	U
10	A	1813	A
10	A	1819	A
10	A	1822	A
10	A	1823	A
10	A	1824	A
10	A	1826	G
10	A	1829	G
10	A	1835	A
10	A	1839	U
10	A	1849	G
10	A	1852	C
10	A	1861	G
10	A	1862	G
10	A	1863	A
10	A	1865	C
50	w	2	G
50	w	10	G
50	w	12	G
50	w	13	C
50	w	16	C
50	w	19	G
50	w	20	A

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Mol	Chain	Res	Type
50	w	21	A
50	w	35	A
50	w	48	C
50	w	49	G
50	w	56	C
50	w	58	A
50	w	68	C
50	w	70	G
50	w	72	U
50	w	73	A
50	w	74	C
50	w	75	C
50	w	76	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	7	-31	C
7	7	-21	A
7	7	13	A
10	A	1	U
10	A	291	G
10	A	368	U
10	A	606	G
10	A	644	OMG
10	A	688	U
10	A	694	G
10	A	716	G
10	A	731	G
10	A	797	C
10	A	912	C
10	A	1600	G
10	A	1836	G

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

29 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	$\#\|Z\| > 2$
10	5MC	A	1374	10	18,22,23	0.62	0	26,32,35	0.56	0
10	OMC	A	517	10	19,22,23	2.95	8 (42%)	26,31,34	3.28	8 (30%)
10	PSU	A	612	10	18,21,22	1.00	1 (5%)	22,30,33	1.82	5 (22%)
10	PSU	A	1243	10	18,21,22	1.07	1 (5%)	22,30,33	1.81	4 (18%)
10	A2M	A	484	10	18,25,26	4.23	9 (50%)	18,36,39	3.91	5 (27%)
10	B8N	A	1248	10	24,29,30	3.02	6 (25%)	29,42,45	2.29	7 (24%)
10	A2M	A	1031	10	18,25,26	4.37	7 (38%)	18,36,39	3.81	4 (22%)
10	PSU	A	823	10	18,21,22	1.12	1 (5%)	22,30,33	1.78	5 (22%)
10	A2M	A	668	10,54	18,25,26	4.20	7 (38%)	18,36,39	3.84	5 (27%)
10	MA6	A	1851	10	18,26,27	1.33	2 (11%)	19,38,41	3.27	2 (10%)
10	6MZ	A	1832	10,54	18,25,26	1.75	4 (22%)	16,36,39	2.23	3 (18%)
10	A2M	A	27	10,54	18,25,26	4.27	8 (44%)	18,36,39	3.75	5 (27%)
10	A2M	A	1678	10,54	18,25,26	4.34	8 (44%)	18,36,39	3.82	4 (22%)
10	OMC	A	1703	10	19,22,23	3.23	8 (42%)	26,31,34	2.83	9 (34%)
10	OMG	A	683	10	18,26,27	1.03	1 (5%)	19,38,41	1.27	2 (10%)
10	PSU	A	119	10	18,21,22	1.00	1 (5%)	22,30,33	1.64	4 (18%)
10	OMU	A	116	10	19,22,23	2.98	6 (31%)	26,31,34	1.64	4 (15%)
10	OMC	A	174	10,54	19,22,23	3.20	8 (42%)	26,31,34	2.79	9 (34%)
10	5MU	A	814	10	19,22,23	7.25	10 (52%)	28,32,35	3.91	19 (67%)
10	PSU	A	1081	10	18,21,22	1.00	1 (5%)	22,30,33	1.74	3 (13%)
10	A2M	A	166	10	18,25,26	4.27	8 (44%)	18,36,39	3.73	4 (22%)
10	OMG	A	644	10	18,26,27	2.35	7 (38%)	19,38,41	2.58	9 (47%)
10	A2M	A	159	10	18,25,26	4.28	8 (44%)	18,36,39	3.81	4 (22%)
10	UR3	A	1830	10	19,22,23	2.77	8 (42%)	26,32,35	1.45	4 (15%)
10	PSU	A	822	10	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
10	MA6	A	1850	10	18,26,27	1.37	2 (11%)	19,38,41	3.07	2 (10%)
10	OMU	A	121	10	19,22,23	2.97	6 (31%)	26,31,34	1.73	5 (19%)
10	JMH	A	1219	10	18,22,23	2.87	6 (33%)	21,32,35	1.62	4 (19%)
10	OMG	A	509	10,54	18,26,27	2.65	9 (50%)	19,38,41	2.55	9 (47%)

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
10	5MC	A	1374	10	-	0/7/25/26	0/2/2/2
10	OMC	A	517	10	-	3/9/27/28	0/2/2/2
10	PSU	A	612	10	-	0/7/25/26	0/2/2/2
10	PSU	A	1243	10	-	0/7/25/26	0/2/2/2
10	A2M	A	484	10	-	1/5/27/28	0/3/3/3
10	B8N	A	1248	10	-	5/16/34/35	0/2/2/2
10	A2M	A	1031	10	-	1/5/27/28	0/3/3/3
10	PSU	A	823	10	-	2/7/25/26	0/2/2/2
10	A2M	A	668	10,54	-	2/5/27/28	0/3/3/3
10	MA6	A	1851	10	-	3/7/29/30	0/3/3/3
10	6MZ	A	1832	10,54	-	2/5/27/28	0/3/3/3
10	A2M	A	27	10,54	-	1/5/27/28	0/3/3/3
10	A2M	A	1678	10,54	-	1/5/27/28	0/3/3/3
10	OMC	A	1703	10	-	2/9/27/28	0/2/2/2
10	OMG	A	683	10	-	2/5/27/28	0/3/3/3
10	PSU	A	119	10	-	0/7/25/26	0/2/2/2
10	OMU	A	116	10	-	1/9/27/28	0/2/2/2
10	OMC	A	174	10,54	-	1/9/27/28	0/2/2/2
10	5MU	A	814	10	-	0/7/25/26	0/2/2/2
10	PSU	A	1081	10	-	1/7/25/26	0/2/2/2
10	A2M	A	166	10	-	1/5/27/28	0/3/3/3
10	OMG	A	644	10	-	4/5/27/28	0/3/3/3
10	A2M	A	159	10	-	3/5/27/28	0/3/3/3
10	UR3	A	1830	10	-	2/7/25/26	0/2/2/2
10	PSU	A	822	10	-	2/7/25/26	0/2/2/2
10	MA6	A	1850	10	-	1/7/29/30	0/3/3/3
10	OMU	A	121	10	-	0/9/27/28	0/2/2/2
10	JMH	A	1219	10	-	2/7/25/26	0/2/2/2
10	OMG	A	509	10,54	-	3/5/27/28	0/3/3/3

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	814	5MU	C4-C5	20.88	1.79	1.44
10	A	814	5MU	C6-N1	15.31	1.64	1.38
10	A	1031	A2M	C3'-C2'	-13.11	1.23	1.52
10	A	1678	A2M	C3'-C2'	-12.88	1.24	1.52
10	A	27	A2M	C3'-C2'	-12.84	1.24	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	166	A2M	C3'-C2'	-12.76	1.24	1.52
10	A	159	A2M	C3'-C2'	-12.68	1.24	1.52
10	A	484	A2M	C3'-C2'	-12.47	1.25	1.52
10	A	668	A2M	C3'-C2'	-12.42	1.25	1.52
10	A	814	5MU	C6-C5	-12.32	1.14	1.34
10	A	814	5MU	C4-N3	-11.30	1.17	1.38
10	A	1219	JMH	C2-N1	8.12	1.50	1.38
10	A	1248	B8N	C4-N3	-8.06	1.25	1.40
10	A	1031	A2M	O4'-C1'	7.60	1.51	1.41
10	A	159	A2M	O4'-C1'	7.53	1.51	1.41
10	A	1678	A2M	O4'-C1'	7.41	1.51	1.41
10	A	1248	B8N	C6-N1	7.40	1.54	1.36
10	A	1830	UR3	C2-N1	7.38	1.49	1.38
10	A	27	A2M	O4'-C1'	7.37	1.51	1.41
10	A	166	A2M	O4'-C1'	7.37	1.51	1.41
10	A	484	A2M	O4'-C1'	7.34	1.51	1.41
10	A	116	OMU	C2-N1	7.05	1.49	1.38
10	A	116	OMU	C2-N3	6.97	1.50	1.38
10	A	668	A2M	O4'-C4'	-6.95	1.29	1.45
10	A	121	OMU	C2-N3	6.95	1.50	1.38
10	A	121	OMU	C2-N1	6.85	1.49	1.38
10	A	1678	A2M	O4'-C4'	-6.74	1.29	1.45
10	A	668	A2M	O4'-C1'	6.73	1.50	1.41
10	A	1031	A2M	O4'-C4'	-6.59	1.30	1.45
10	A	159	A2M	O4'-C4'	-6.52	1.30	1.45
10	A	166	A2M	O4'-C4'	-6.40	1.30	1.45
10	A	484	A2M	O4'-C4'	-6.34	1.30	1.45
10	A	1703	OMC	C4-N4	6.30	1.48	1.33
10	A	27	A2M	O4'-C4'	-6.26	1.31	1.45
10	A	174	OMC	C4-N4	6.18	1.48	1.33
10	A	121	OMU	C6-C5	6.13	1.49	1.35
10	A	116	OMU	C6-C5	6.05	1.49	1.35
10	A	1830	UR3	C6-C5	6.01	1.49	1.35
10	A	1219	JMH	C6-C5	5.90	1.48	1.35
10	A	174	OMC	C2-N3	5.82	1.48	1.36
10	A	1703	OMC	C2-N3	5.63	1.47	1.36
10	A	517	OMC	C2-N3	5.47	1.47	1.36
10	A	1248	B8N	C6-C5	5.30	1.42	1.34
10	A	509	OMG	C4-N3	5.28	1.50	1.37
10	A	1832	6MZ	C6-N6	5.22	1.43	1.35
10	A	1219	JMH	C2-N3	5.17	1.49	1.39
10	A	1678	A2M	C3'-C4'	5.14	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	174	OMC	C2-N1	5.14	1.51	1.40
10	A	1703	OMC	C6-C5	5.12	1.46	1.35
10	A	509	OMG	C2-N3	5.10	1.45	1.33
10	A	174	OMC	C6-C5	5.10	1.46	1.35
10	A	517	OMC	C4-N4	5.08	1.45	1.33
10	A	484	A2M	C3'-C4'	5.08	1.66	1.53
10	A	1248	B8N	C2-N1	5.05	1.54	1.39
10	A	1830	UR3	C2-N3	5.03	1.48	1.39
10	A	509	OMG	C2-N2	5.01	1.46	1.34
10	A	1703	OMC	O2-C2	-4.99	1.14	1.23
10	A	1031	A2M	C3'-C4'	4.96	1.65	1.53
10	A	159	A2M	C3'-C4'	4.95	1.65	1.53
10	A	668	A2M	C3'-C4'	4.88	1.65	1.53
10	A	166	A2M	C3'-C4'	4.86	1.65	1.53
10	A	27	A2M	C3'-C4'	4.85	1.65	1.53
10	A	1703	OMC	C2-N1	4.82	1.50	1.40
10	A	517	OMC	C2-N1	4.77	1.50	1.40
10	A	517	OMC	C4-N3	4.74	1.44	1.34
10	A	174	OMC	O2-C2	-4.72	1.15	1.23
10	A	644	OMG	C4-N3	4.68	1.48	1.37
10	A	644	OMG	C2-N2	4.60	1.45	1.34
10	A	174	OMC	C4-N3	4.57	1.43	1.34
10	A	644	OMG	C2-N3	4.50	1.44	1.33
10	A	1703	OMC	C4-N3	4.33	1.43	1.34
10	A	517	OMC	O2-C2	-4.31	1.15	1.23
10	A	517	OMC	C6-C5	4.11	1.44	1.35
10	A	814	5MU	C2-N3	4.07	1.45	1.38
10	A	116	OMU	C4-N3	4.01	1.45	1.38
10	A	121	OMU	C4-N3	4.00	1.45	1.38
10	A	1248	B8N	C1'-C5	3.77	1.58	1.50
10	A	1248	B8N	O2-C2	-3.50	1.16	1.22
10	A	484	A2M	O2'-C2'	3.45	1.51	1.42
10	A	1243	PSU	C6-C5	3.40	1.39	1.35
10	A	159	A2M	O2'-C2'	3.38	1.51	1.42
10	A	27	A2M	O2'-C2'	3.38	1.51	1.42
10	A	823	PSU	C6-C5	3.37	1.39	1.35
10	A	1678	A2M	O2'-C2'	3.35	1.51	1.42
10	A	668	A2M	O2'-C2'	3.32	1.51	1.42
10	A	119	PSU	C6-C5	3.31	1.39	1.35
10	A	166	A2M	O2'-C2'	3.31	1.51	1.42
10	A	1031	A2M	O2'-C2'	3.28	1.51	1.42
10	A	1850	MA6	C2-N3	3.12	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1678	A2M	C6-N6	3.12	1.45	1.34
10	A	166	A2M	C6-N6	3.10	1.45	1.34
10	A	159	A2M	C6-N6	3.10	1.45	1.34
10	A	1031	A2M	C6-N6	3.10	1.45	1.34
10	A	484	A2M	C6-N6	3.10	1.45	1.34
10	A	27	A2M	C6-N6	3.08	1.45	1.34
10	A	822	PSU	C6-C5	3.07	1.38	1.35
10	A	668	A2M	C6-N6	3.07	1.45	1.34
10	A	1081	PSU	C6-C5	3.04	1.38	1.35
10	A	509	OMG	C6-N1	3.02	1.42	1.37
10	A	1851	MA6	C2-N3	3.00	1.36	1.32
10	A	644	OMG	C6-N1	2.98	1.42	1.37
10	A	509	OMG	C5-C6	2.96	1.53	1.47
10	A	1830	UR3	C6-N1	2.95	1.45	1.38
10	A	1851	MA6	C5-C4	-2.94	1.33	1.40
10	A	1850	MA6	C5-C4	-2.91	1.33	1.40
10	A	668	A2M	C5-C4	-2.90	1.33	1.40
10	A	27	A2M	C5-C4	-2.88	1.33	1.40
10	A	1031	A2M	C5-C4	-2.88	1.33	1.40
10	A	1703	OMC	C5-C4	2.86	1.49	1.42
10	A	166	A2M	C5-C4	-2.86	1.33	1.40
10	A	1678	A2M	C5-C4	-2.85	1.33	1.40
10	A	174	OMC	C6-N1	2.83	1.44	1.38
10	A	612	PSU	C6-C5	2.82	1.38	1.35
10	A	509	OMG	O6-C6	-2.81	1.17	1.23
10	A	1219	JMH	C6-N1	2.76	1.44	1.38
10	A	1703	OMC	C6-N1	2.76	1.44	1.38
10	A	683	OMG	C6-N1	-2.73	1.33	1.37
10	A	159	A2M	C5-C4	-2.73	1.33	1.40
10	A	174	OMC	C5-C4	2.71	1.49	1.42
10	A	484	A2M	C5-C4	-2.70	1.33	1.40
10	A	517	OMC	C6-N1	2.57	1.44	1.38
10	A	121	OMU	C6-N1	2.56	1.44	1.38
10	A	1832	6MZ	C5-C4	-2.54	1.34	1.40
10	A	644	OMG	O6-C6	-2.49	1.18	1.23
10	A	116	OMU	C6-N1	2.49	1.44	1.38
10	A	1219	JMH	C5-C4	2.47	1.48	1.42
10	A	644	OMG	C5-C6	2.46	1.52	1.47
10	A	644	OMG	C5-C4	-2.41	1.36	1.43
10	A	814	5MU	O2-C2	-2.40	1.18	1.23
10	A	509	OMG	C5-C4	-2.40	1.37	1.43
10	A	1832	6MZ	C9-N6	-2.38	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	814	5MU	O4-C4	-2.36	1.19	1.23
10	A	1830	UR3	O4-C4	-2.24	1.18	1.23
10	A	121	OMU	C5-C4	2.22	1.48	1.43
10	A	509	OMG	O2'-C2'	-2.20	1.37	1.42
10	A	517	OMC	C5-C4	2.20	1.48	1.42
10	A	484	A2M	C2-N3	2.20	1.35	1.32
10	A	1830	UR3	C5-C4	2.18	1.49	1.43
10	A	1830	UR3	O2-C2	-2.18	1.18	1.22
10	A	1832	6MZ	C6-N1	-2.16	1.30	1.34
10	A	484	A2M	O3'-C3'	2.16	1.48	1.43
10	A	116	OMU	C5-C4	2.12	1.48	1.43
10	A	166	A2M	O3'-C3'	2.10	1.47	1.43
10	A	1830	UR3	C4-N3	2.08	1.45	1.40
10	A	814	5MU	C2-N1	2.08	1.41	1.38
10	A	159	A2M	C2-N3	2.07	1.35	1.32
10	A	509	OMG	C2-N1	2.06	1.42	1.37
10	A	27	A2M	C2-N3	2.05	1.35	1.32
10	A	1219	JMH	O2-C2	-2.05	1.18	1.22
10	A	814	5MU	C2'-C1'	-2.02	1.47	1.53
10	A	1678	A2M	O3'-C3'	2.02	1.47	1.43
10	A	814	5MU	O2'-C2'	-2.00	1.38	1.43

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1851	MA6	N1-C6-N6	-12.87	103.51	117.06
10	A	1850	MA6	N1-C6-N6	-12.03	104.40	117.06
10	A	484	A2M	C1'-N9-C4	10.54	145.17	126.64
10	A	814	5MU	C5-C4-N3	10.31	124.11	115.31
10	A	1678	A2M	C1'-N9-C4	10.23	144.61	126.64
10	A	1031	A2M	C1'-N9-C4	10.02	144.25	126.64
10	A	668	A2M	C1'-N9-C4	9.93	144.09	126.64
10	A	159	A2M	C1'-N9-C4	9.93	144.09	126.64
10	A	27	A2M	C1'-N9-C4	9.84	143.93	126.64
10	A	166	A2M	C1'-N9-C4	9.53	143.39	126.64
10	A	668	A2M	C5-C6-N6	9.09	134.16	120.35
10	A	1031	A2M	C5-C6-N6	9.03	134.07	120.35
10	A	484	A2M	C5-C6-N6	8.89	133.86	120.35
10	A	166	A2M	C5-C6-N6	8.89	133.86	120.35
10	A	159	A2M	C5-C6-N6	8.87	133.83	120.35
10	A	1678	A2M	C5-C6-N6	8.85	133.81	120.35
10	A	27	A2M	C5-C6-N6	8.59	133.41	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	814	5MU	C5-C6-N1	-8.54	114.55	123.34
10	A	517	OMC	C1'-N1-C6	-7.97	103.46	120.84
10	A	517	OMC	C1'-N1-C2	7.54	135.24	118.42
10	A	1703	OMC	CM2-O2'-C2'	6.93	132.71	114.52
10	A	814	5MU	C4-N3-C2	-6.92	118.39	127.35
10	A	174	OMC	O2'-C2'-C1'	6.81	122.37	109.08
10	A	517	OMC	O2'-C2'-C1'	6.80	122.35	109.08
10	A	1248	B8N	C32-C31-N3	6.40	123.99	112.00
10	A	517	OMC	O3'-C3'-C4'	6.14	128.80	111.05
10	A	174	OMC	C1'-N1-C2	6.14	132.11	118.42
10	A	668	A2M	N6-C6-N1	-6.12	105.88	118.57
10	A	1031	A2M	N6-C6-N1	-6.08	105.95	118.57
10	A	1703	OMC	O2'-C2'-C1'	6.06	120.89	109.08
10	A	484	A2M	N6-C6-N1	-6.00	106.12	118.57
10	A	159	A2M	N6-C6-N1	-5.94	106.25	118.57
10	A	1678	A2M	N6-C6-N1	-5.93	106.26	118.57
10	A	166	A2M	N6-C6-N1	-5.92	106.28	118.57
10	A	166	A2M	N3-C2-N1	-5.86	119.51	128.68
10	A	27	A2M	N6-C6-N1	-5.85	106.42	118.57
10	A	1832	6MZ	N3-C2-N1	-5.85	119.53	128.68
10	A	27	A2M	N3-C2-N1	-5.73	119.72	128.68
10	A	1678	A2M	N3-C2-N1	-5.73	119.72	128.68
10	A	644	OMG	O3'-C3'-C4'	5.72	127.59	111.05
10	A	159	A2M	N3-C2-N1	-5.72	119.74	128.68
10	A	1703	OMC	C1'-N1-C2	5.63	130.97	118.42
10	A	644	OMG	O2'-C2'-C1'	5.61	120.21	109.09
10	A	1031	A2M	N3-C2-N1	-5.60	119.92	128.68
10	A	1851	MA6	N3-C2-N1	-5.58	119.96	128.68
10	A	484	A2M	N3-C2-N1	-5.53	120.03	128.68
10	A	668	A2M	N3-C2-N1	-5.48	120.11	128.68
10	A	121	OMU	C4-N3-C2	-5.36	119.51	126.58
10	A	1850	MA6	N3-C2-N1	-5.35	120.32	128.68
10	A	509	OMG	O2'-C2'-C1'	5.33	119.66	109.09
10	A	1248	B8N	C5-C4-N3	5.28	125.95	116.17
10	A	814	5MU	O3'-C3'-C4'	5.18	126.03	111.05
10	A	1248	B8N	C4-N3-C2	-5.14	118.96	125.46
10	A	517	OMC	CM2-O2'-C2'	5.07	127.83	114.52
10	A	116	OMU	C4-N3-C2	-5.00	119.99	126.58
10	A	174	OMC	O3'-C3'-C4'	4.94	125.34	111.05
10	A	174	OMC	C1'-N1-C6	-4.88	110.21	120.84
10	A	1219	JMH	C1'-N1-C2	4.86	125.20	116.99
10	A	814	5MU	C5M-C5-C6	-4.83	116.41	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	823	PSU	C4-N3-C2	-4.75	119.49	126.34
10	A	1832	6MZ	C2-N1-C6	4.74	120.65	116.59
10	A	1243	PSU	N1-C2-N3	4.73	120.49	115.13
10	A	822	PSU	C4-N3-C2	-4.71	119.55	126.34
10	A	509	OMG	O3'-C3'-C4'	4.69	124.61	111.05
10	A	822	PSU	N1-C2-N3	4.61	120.36	115.13
10	A	1703	OMC	O3'-C3'-C4'	4.58	124.30	111.05
10	A	1081	PSU	C4-N3-C2	-4.58	119.74	126.34
10	A	612	PSU	C4-N3-C2	-4.57	119.76	126.34
10	A	1243	PSU	C4-N3-C2	-4.56	119.77	126.34
10	A	612	PSU	N1-C2-N3	4.54	120.27	115.13
10	A	1830	UR3	C4-N3-C2	-4.50	120.33	124.56
10	A	823	PSU	N1-C2-N3	4.47	120.19	115.13
10	A	1081	PSU	N1-C2-N3	4.41	120.12	115.13
10	A	814	5MU	O4'-C1'-N1	4.31	118.21	108.36
10	A	119	PSU	N1-C2-N3	4.26	119.96	115.13
10	A	1832	6MZ	C1'-N9-C4	-4.26	119.16	126.64
10	A	1703	OMC	C1'-N1-C6	-4.24	111.60	120.84
10	A	814	5MU	C5M-C5-C4	4.18	123.37	118.77
10	A	119	PSU	C4-N3-C2	-4.11	120.41	126.34
10	A	509	OMG	C5-C6-N1	3.98	120.98	113.95
10	A	121	OMU	N3-C2-N1	3.89	120.05	114.89
10	A	814	5MU	O4-C4-C5	-3.83	120.47	124.90
10	A	814	5MU	N3-C2-N1	3.80	119.93	114.89
10	A	116	OMU	N3-C2-N1	3.71	119.82	114.89
10	A	174	OMC	CM2-O2'-C2'	3.70	124.24	114.52
10	A	1248	B8N	C31-N3-C4	3.67	122.72	117.31
10	A	814	5MU	O2-C2-N1	-3.57	118.04	122.79
10	A	1219	JMH	C6-N1-C2	-3.49	118.66	121.79
10	A	509	OMG	O3'-C3'-C2'	3.49	121.08	111.17
10	A	1248	B8N	N3-C2-N1	3.47	121.66	116.76
10	A	644	OMG	O3'-C3'-C2'	3.39	120.80	111.17
10	A	121	OMU	C5-C4-N3	3.38	119.90	114.84
10	A	1703	OMC	C5'-C4'-C3'	3.38	127.85	115.18
10	A	1830	UR3	C1'-N1-C2	3.33	122.60	116.99
10	A	174	OMC	C2'-C1'-N1	3.32	120.67	114.22
10	A	1703	OMC	O2-C2-N3	-3.24	117.06	122.33
10	A	116	OMU	C5-C4-N3	3.22	119.66	114.84
10	A	1219	JMH	O2-C2-N3	-3.21	116.82	121.34
10	A	509	OMG	C2-N1-C6	-3.21	119.19	125.10
10	A	174	OMC	C5'-C4'-C3'	3.14	126.95	115.18
10	A	517	OMC	C5-C4-N4	-3.13	115.64	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	509	OMG	C5'-C4'-C3'	3.13	126.91	115.18
10	A	612	PSU	O2-C2-N1	-2.95	119.54	122.79
10	A	814	5MU	C1'-N1-C6	-2.93	116.25	121.12
10	A	1248	B8N	O4-C4-N3	-2.91	115.03	119.98
10	A	644	OMG	O5'-C5'-C4'	2.91	118.89	108.99
10	A	517	OMC	C5'-C4'-C3'	2.90	126.04	115.18
10	A	814	5MU	O2'-C2'-C3'	2.90	121.19	111.82
10	A	174	OMC	O3'-C3'-C2'	2.87	119.33	111.17
10	A	644	OMG	C5-C6-N1	2.86	119.00	113.95
10	A	1703	OMC	C2'-C1'-N1	2.77	119.61	114.22
10	A	121	OMU	O4-C4-C5	-2.76	120.30	125.16
10	A	174	OMC	O2-C2-N3	-2.76	117.84	122.33
10	A	116	OMU	O4-C4-C5	-2.74	120.34	125.16
10	A	517	OMC	O2-C2-N1	2.71	124.50	118.89
10	A	814	5MU	O3'-C3'-C2'	2.68	120.50	111.82
10	A	822	PSU	O2-C2-N1	-2.68	119.84	122.79
10	A	814	5MU	C5'-C4'-C3'	2.60	124.92	115.18
10	A	814	5MU	C6-C5-C4	2.57	120.18	118.03
10	A	1243	PSU	O2-C2-N1	-2.52	120.02	122.79
10	A	119	PSU	O2-C2-N1	-2.51	120.03	122.79
10	A	814	5MU	O2'-C2'-C1'	2.50	118.37	110.02
10	A	119	PSU	C6-N1-C2	-2.48	120.15	122.68
10	A	814	5MU	O4-C4-N3	-2.45	115.42	120.12
10	A	683	OMG	C5-C6-N1	2.44	118.25	113.95
10	A	668	A2M	C3'-C2'-C1'	2.43	107.45	102.89
10	A	823	PSU	O2-C2-N1	-2.42	120.13	122.79
10	A	1830	UR3	C6-N1-C2	-2.39	119.65	121.79
10	A	644	OMG	C2-N1-C6	-2.35	120.77	125.10
10	A	484	A2M	C3'-C2'-C1'	2.34	107.29	102.89
10	A	27	A2M	O4'-C1'-C2'	-2.34	102.53	106.59
10	A	822	PSU	O4'-C1'-C2'	2.30	108.39	105.14
10	A	121	OMU	O2-C2-N1	-2.30	119.73	122.79
10	A	683	OMG	C8-N7-C5	2.30	107.37	102.99
10	A	1243	PSU	C6-N1-C2	-2.29	120.34	122.68
10	A	612	PSU	C6-N1-C2	-2.28	120.35	122.68
10	A	509	OMG	N1-C2-N3	-2.28	119.06	123.32
10	A	1081	PSU	O2-C2-N1	-2.28	120.29	122.79
10	A	509	OMG	C8-N7-C5	2.27	107.32	102.99
10	A	1703	OMC	O3'-C3'-C2'	2.26	117.57	111.17
10	A	1248	B8N	C32-C33-C34	-2.23	104.99	110.30
10	A	823	PSU	C6-N1-C2	-2.22	120.41	122.68
10	A	644	OMG	N1-C2-N3	-2.19	119.23	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	644	OMG	N2-C2-N1	2.18	121.35	116.71
10	A	822	PSU	C6-N1-C2	-2.17	120.47	122.68
10	A	814	5MU	C3'-C2'-C1'	2.17	105.55	101.43
10	A	814	5MU	O5'-C5'-C4'	-2.17	101.63	108.99
10	A	1219	JMH	C1'-N1-C6	-2.16	116.14	120.84
10	A	612	PSU	O4'-C1'-C2'	2.13	108.15	105.14
10	A	509	OMG	O6-C6-N1	-2.12	118.14	120.65
10	A	1830	UR3	O2-C2-N3	-2.10	118.39	121.34
10	A	644	OMG	C5'-C4'-C3'	2.05	122.88	115.18
10	A	823	PSU	O4'-C1'-C2'	2.05	108.04	105.14

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	27	A2M	C1'-C2'-O2'-CM'
10	A	116	OMU	C1'-C2'-O2'-CM2
10	A	159	A2M	C1'-C2'-O2'-CM'
10	A	166	A2M	C1'-C2'-O2'-CM'
10	A	174	OMC	C1'-C2'-O2'-CM2
10	A	484	A2M	C1'-C2'-O2'-CM'
10	A	509	OMG	C1'-C2'-O2'-CM2
10	A	517	OMC	C1'-C2'-O2'-CM2
10	A	644	OMG	C3'-C4'-C5'-O5'
10	A	644	OMG	C1'-C2'-O2'-CM2
10	A	1031	A2M	C1'-C2'-O2'-CM'
10	A	1678	A2M	C1'-C2'-O2'-CM'
10	A	1832	6MZ	N1-C6-N6-C9
10	A	1851	MA6	O4'-C4'-C5'-O5'
10	A	1248	B8N	N34-C33-C34-O35
10	A	1248	B8N	C31-C32-C33-C34
10	A	1248	B8N	C31-C32-C33-N34
10	A	1830	UR3	O4'-C1'-N1-C2
10	A	668	A2M	O4'-C4'-C5'-O5'
10	A	668	A2M	C3'-C4'-C5'-O5'
10	A	683	OMG	O4'-C4'-C5'-O5'
10	A	1851	MA6	C3'-C4'-C5'-O5'
10	A	159	A2M	C3'-C4'-C5'-O5'
10	A	517	OMC	C3'-C4'-C5'-O5'
10	A	517	OMC	O4'-C4'-C5'-O5'
10	A	644	OMG	O4'-C4'-C5'-O5'
10	A	683	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
10	A	1830	UR3	O4'-C1'-N1-C6
10	A	1248	B8N	N34-C33-C34-O36
10	A	1703	OMC	C3'-C4'-C5'-O5'
10	A	822	PSU	C3'-C4'-C5'-O5'
10	A	644	OMG	C4'-C5'-O5'-P
10	A	509	OMG	C3'-C4'-C5'-O5'
10	A	822	PSU	O4'-C4'-C5'-O5'
10	A	1703	OMC	O4'-C4'-C5'-O5'
10	A	1850	MA6	C5-C6-N6-C10
10	A	1832	6MZ	C5-C6-N6-C9
10	A	1081	PSU	C4'-C5'-O5'-P
10	A	1851	MA6	C4'-C5'-O5'-P
10	A	823	PSU	O4'-C1'-C5-C4
10	A	159	A2M	O4'-C4'-C5'-O5'
10	A	509	OMG	O4'-C4'-C5'-O5'
10	A	1248	B8N	C32-C33-C34-O36
10	A	823	PSU	O4'-C1'-C5-C6
10	A	1219	JMH	C2'-C1'-N1-C2
10	A	1219	JMH	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 89 ligands modelled in this entry, 89 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

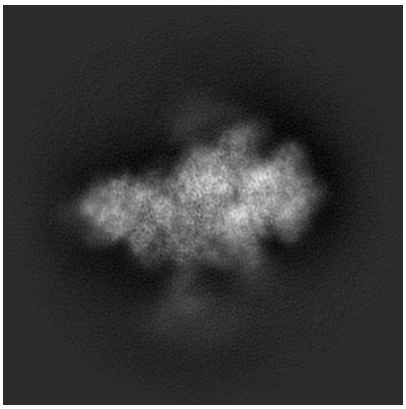
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17697. These allow visual inspection of the internal detail of the map and identification of artifacts.

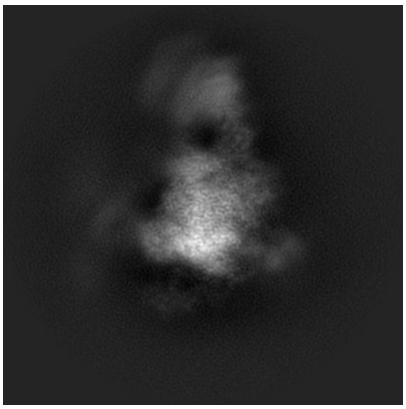
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

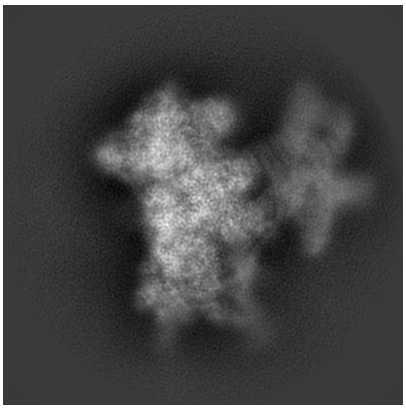
6.1.1 Primary map



X

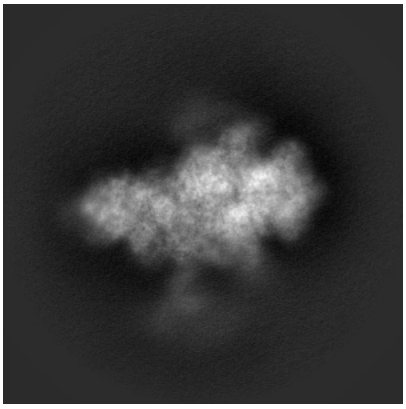


Y

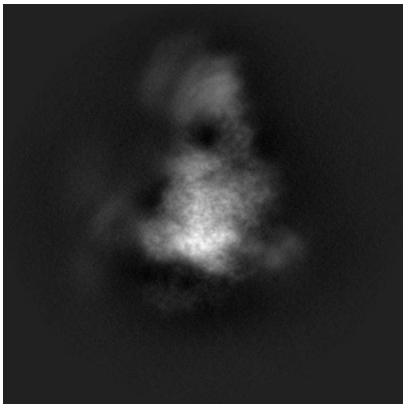


Z

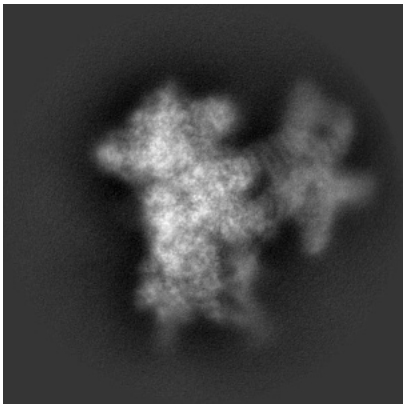
6.1.2 Raw map



X



Y

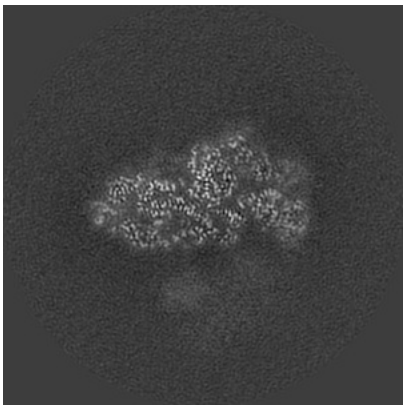


Z

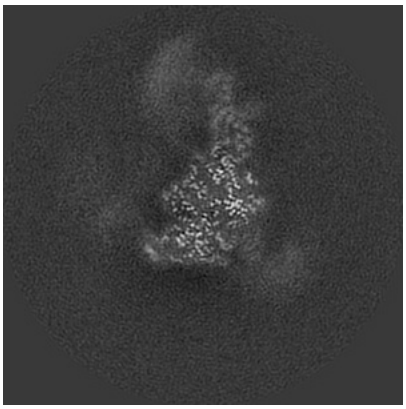
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

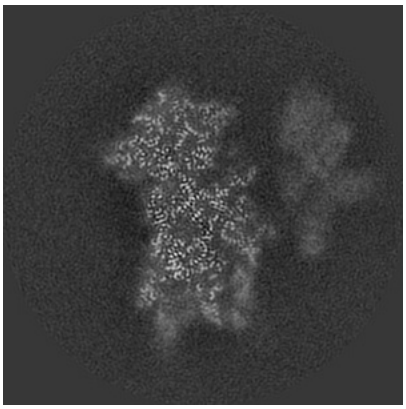
6.2.1 Primary map



X Index: 216

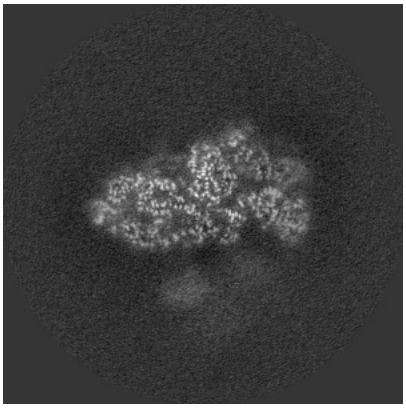


Y Index: 216

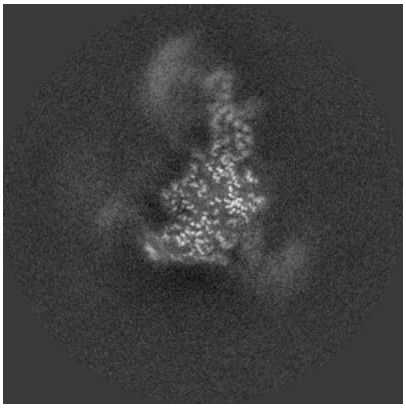


Z Index: 216

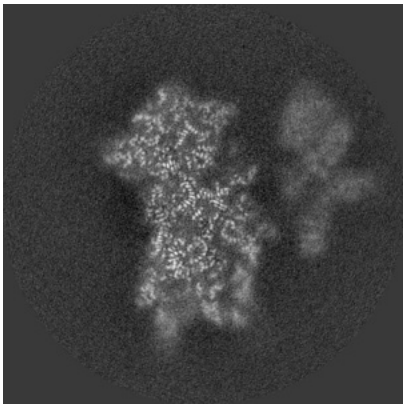
6.2.2 Raw map



X Index: 180



Y Index: 180

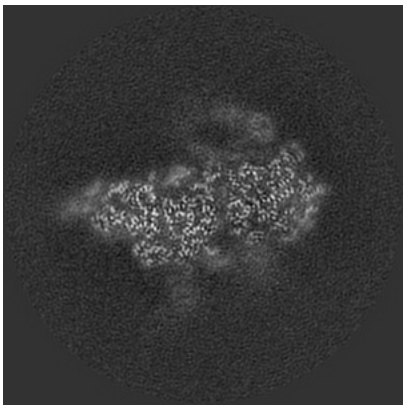


Z Index: 180

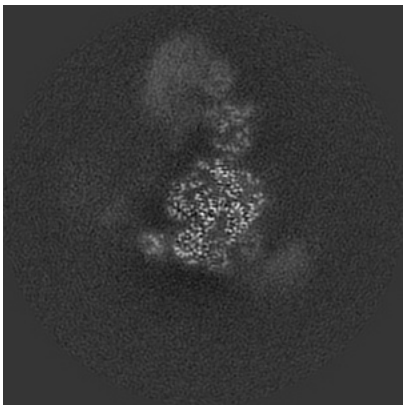
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

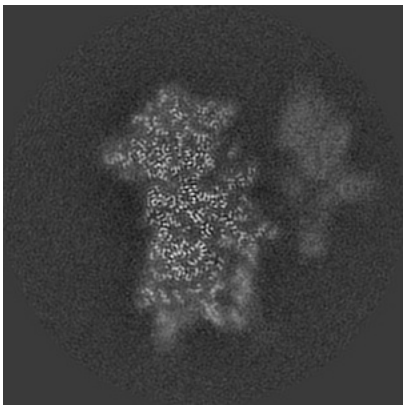
6.3.1 Primary map



X Index: 176

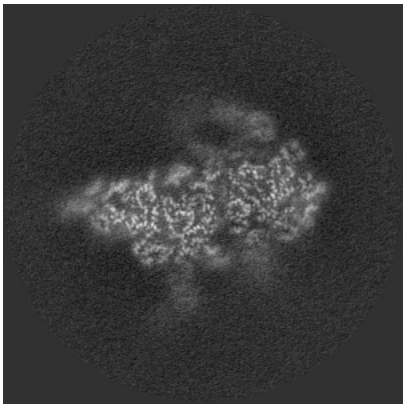


Y Index: 222

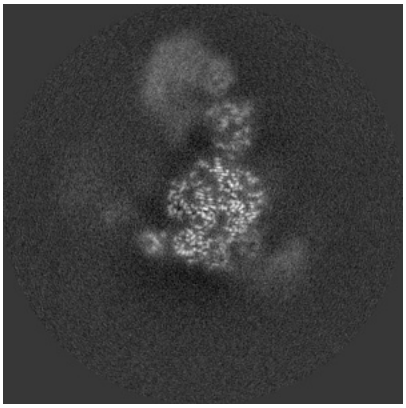


Z Index: 214

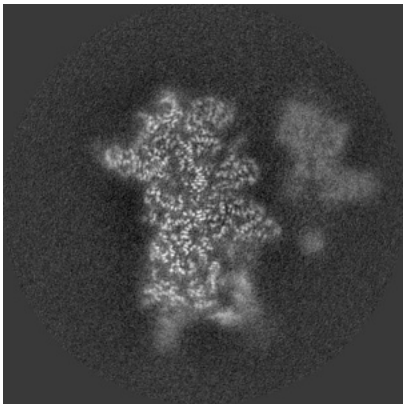
6.3.2 Raw map



X Index: 147



Y Index: 186

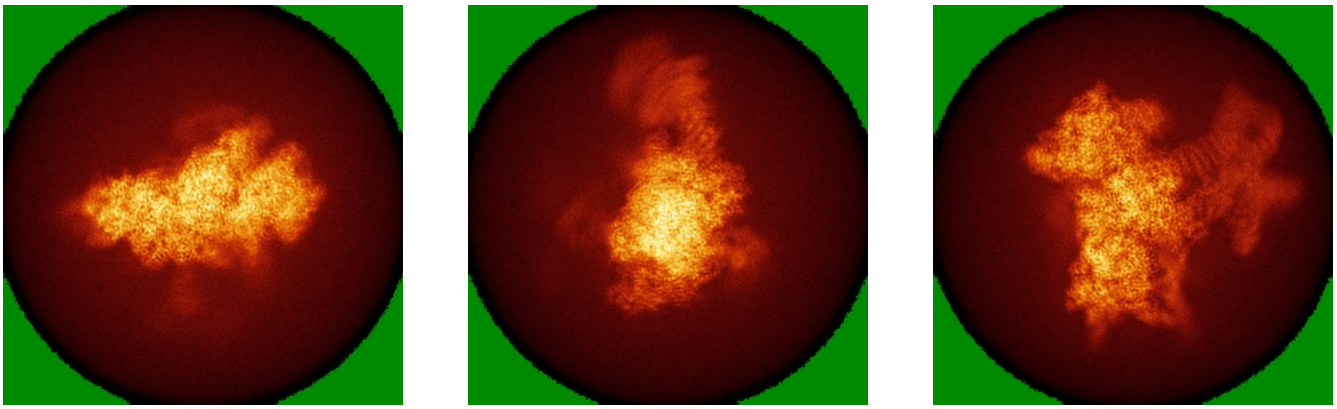


Z Index: 173

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

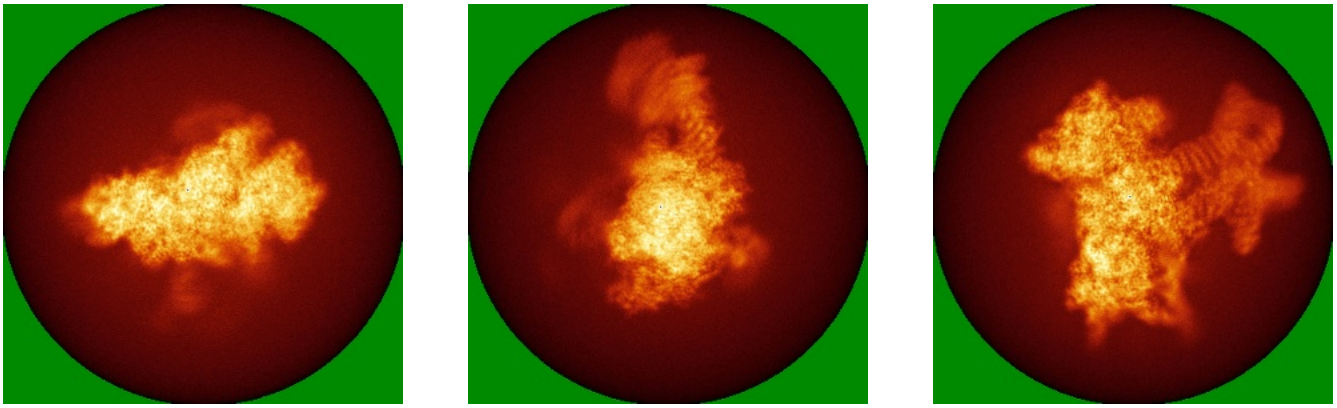
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

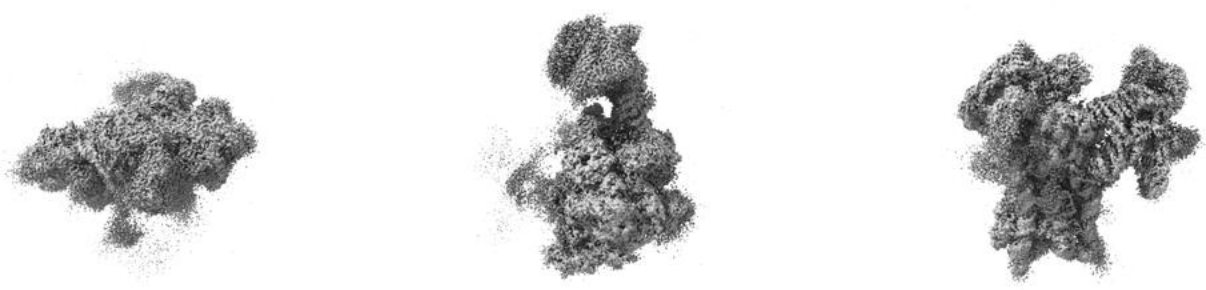


X Y Z

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

6.5 Orthogonal surface views (i)

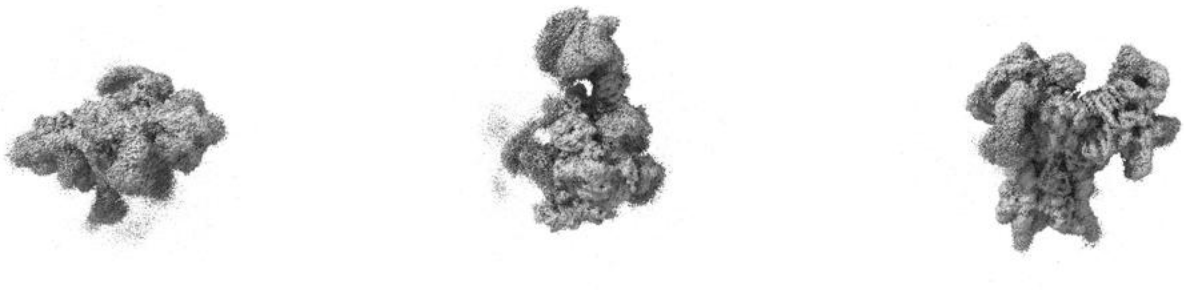
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. 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.

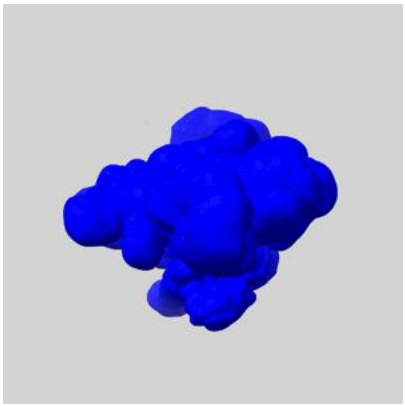
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

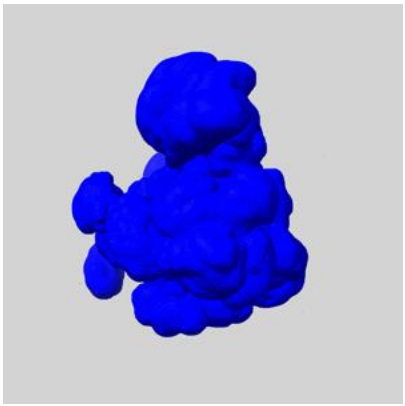
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

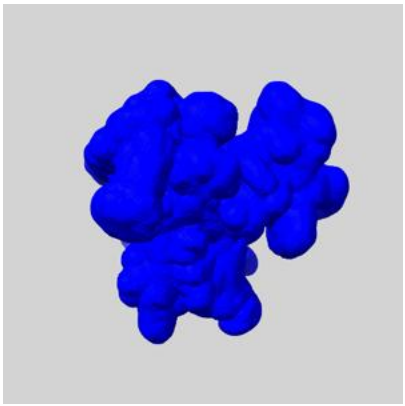
6.6.1 emd_17697_msk_1.map (i)



X



Y

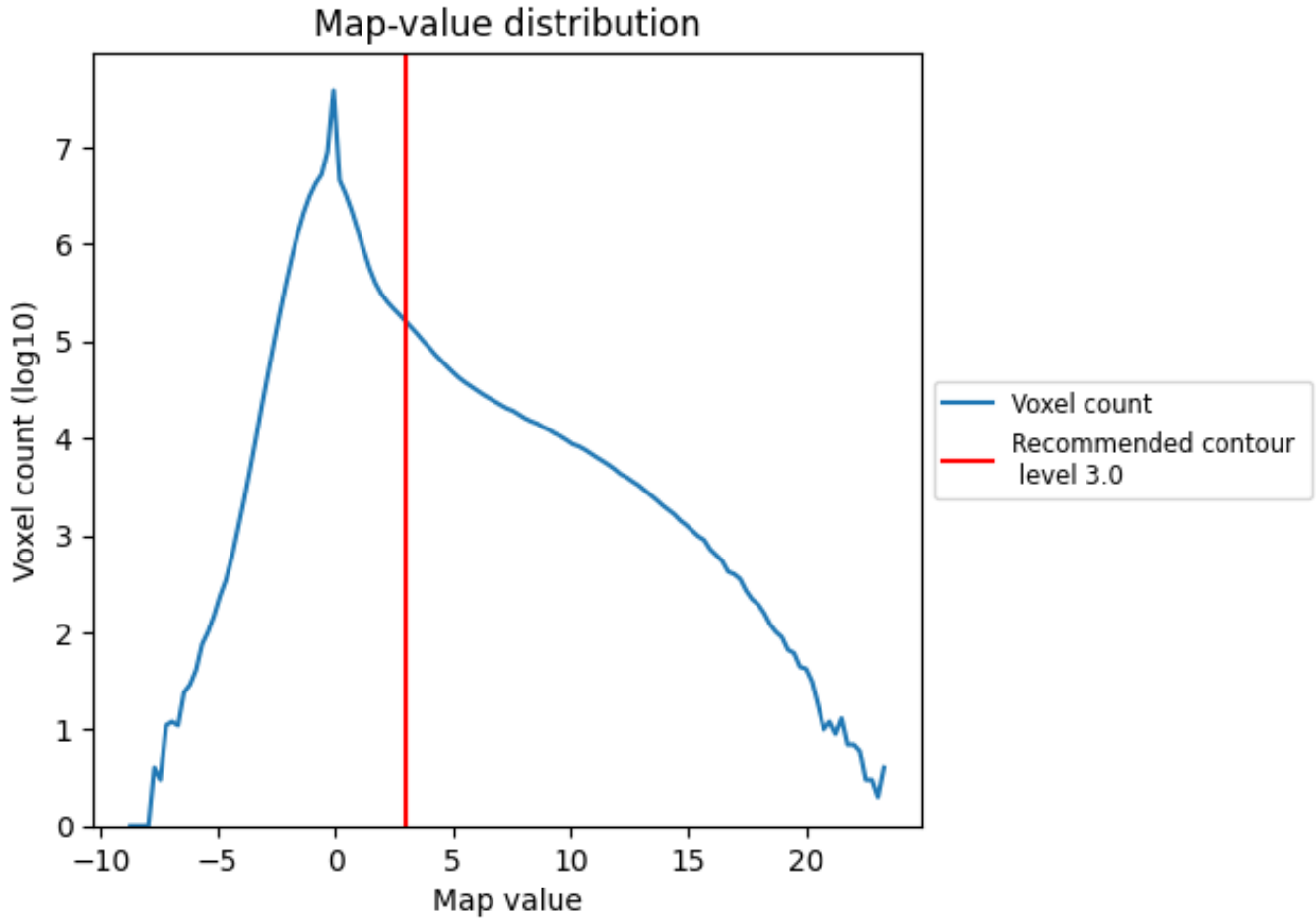


Z

7 Map analysis

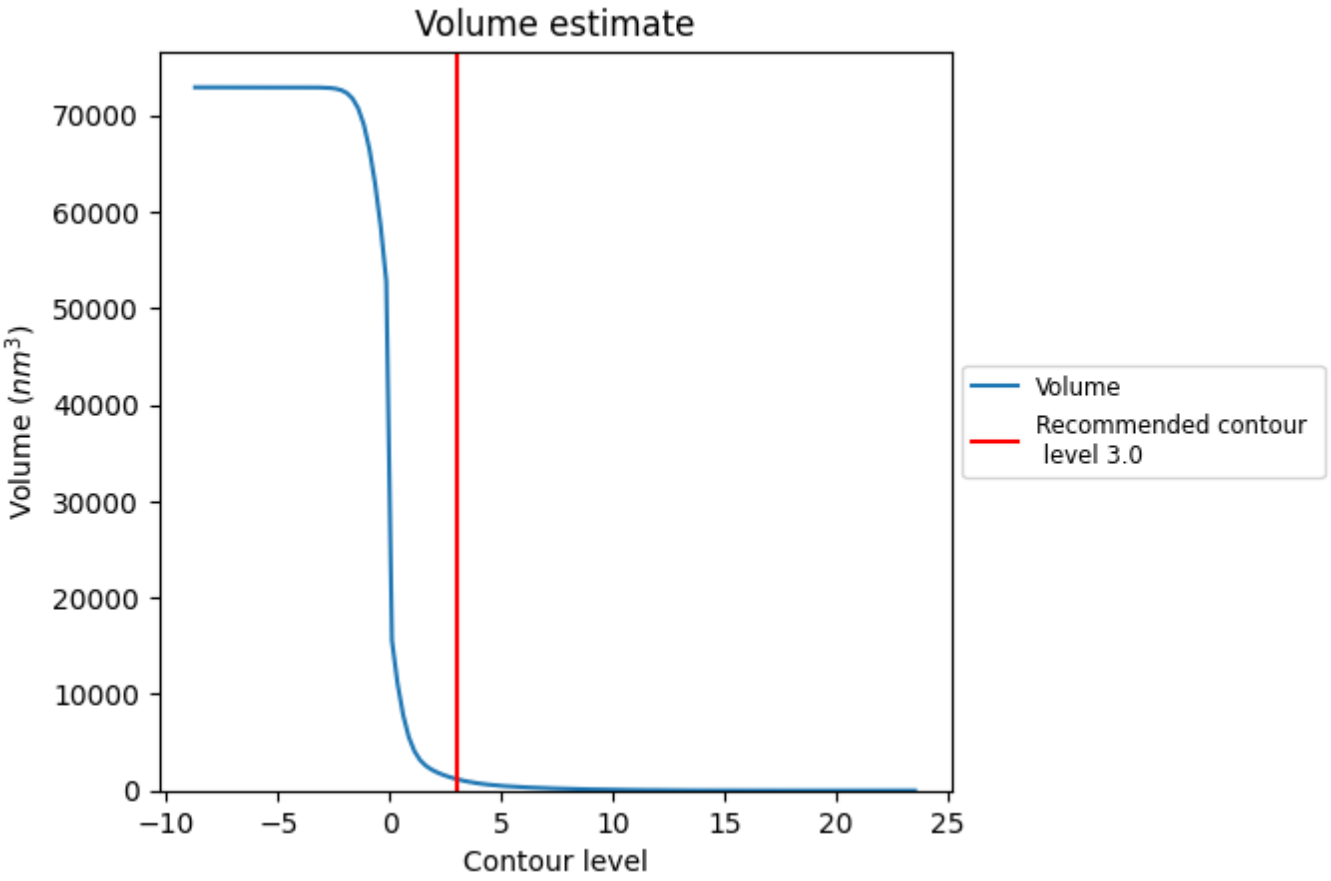
This section contains the results of statistical analysis of the map.

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.

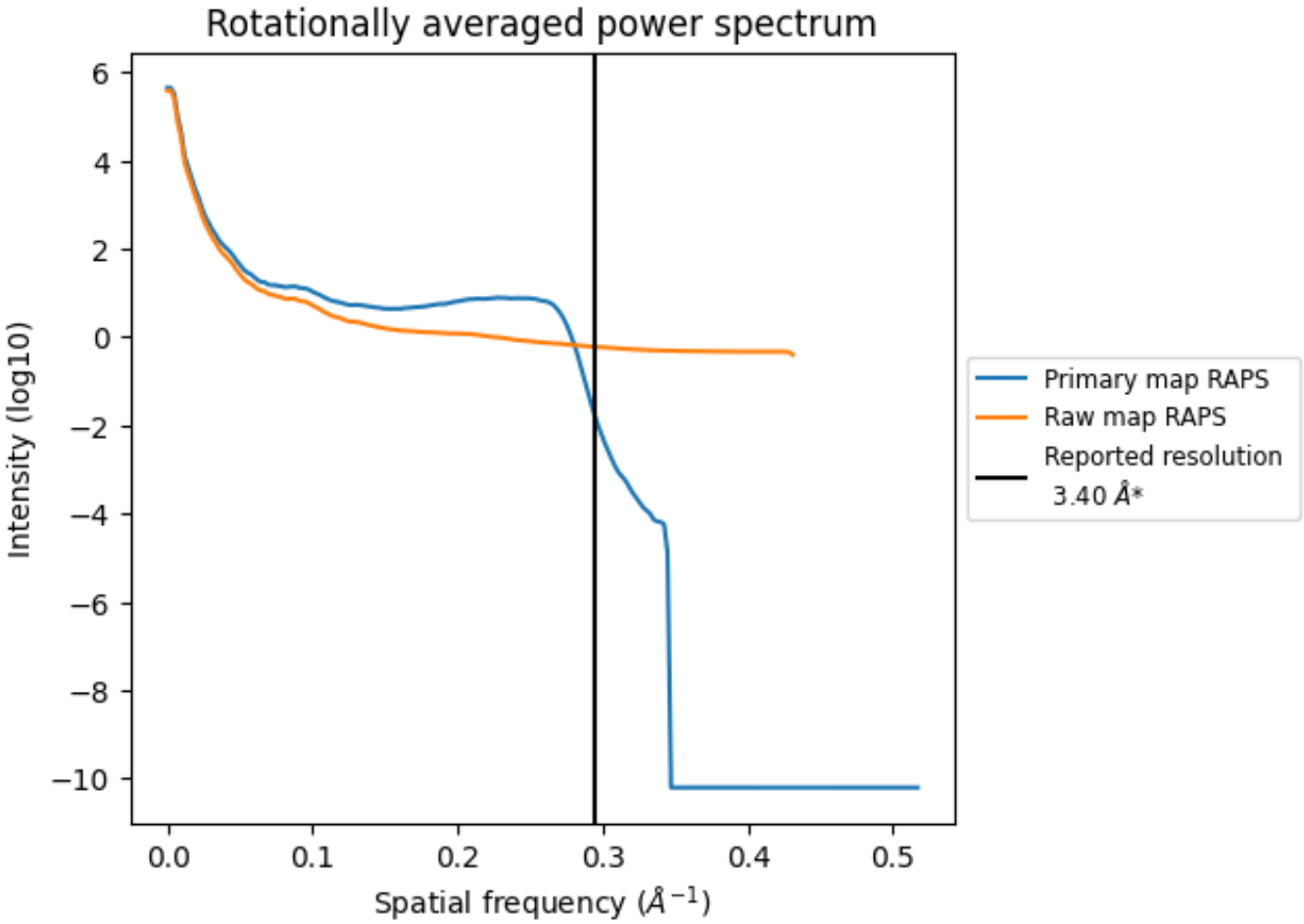
7.2 Volume estimate



The volume at the recommended contour level is 1196 nm^3; this corresponds to an approximate mass of 1081 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 (i)

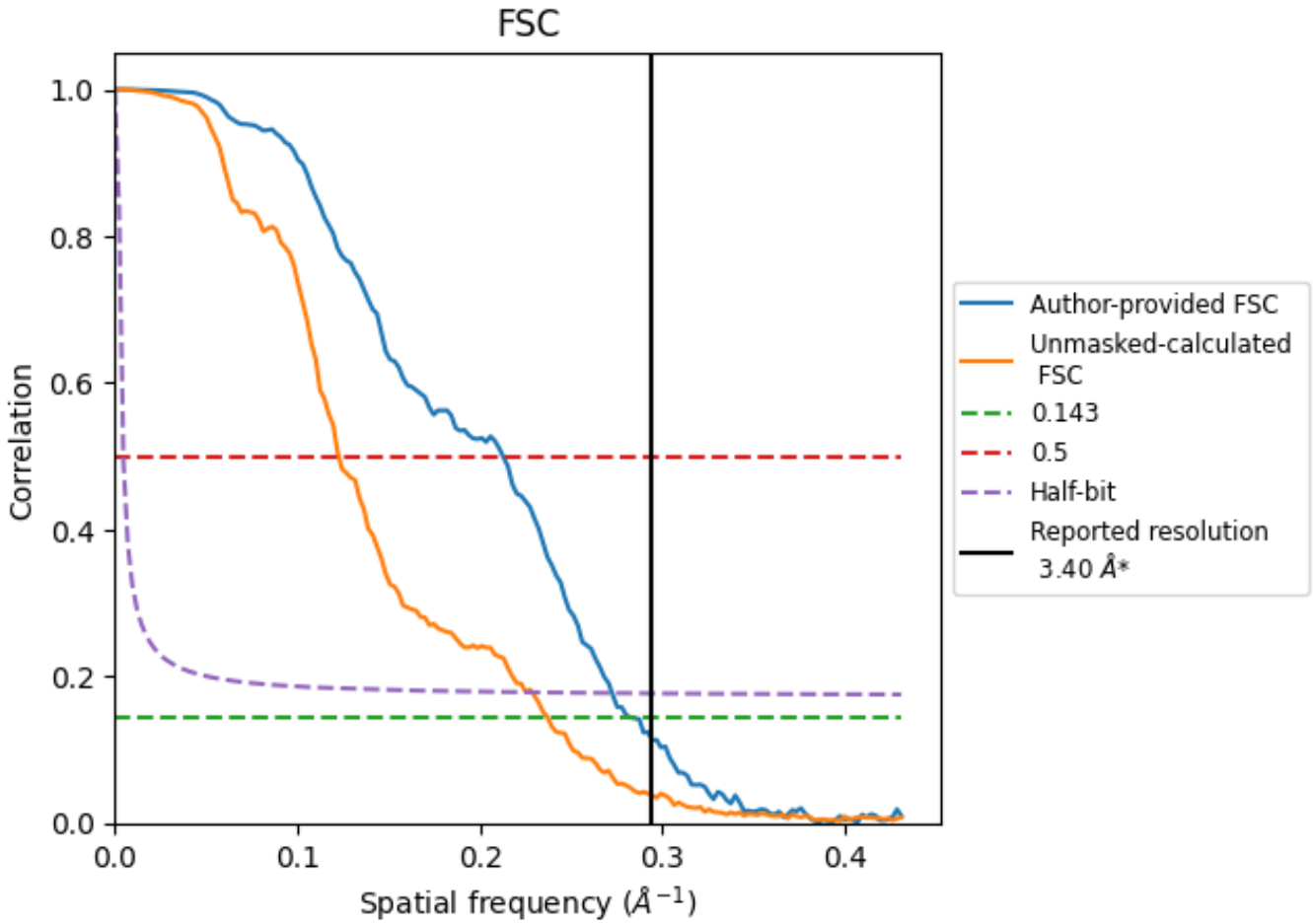


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

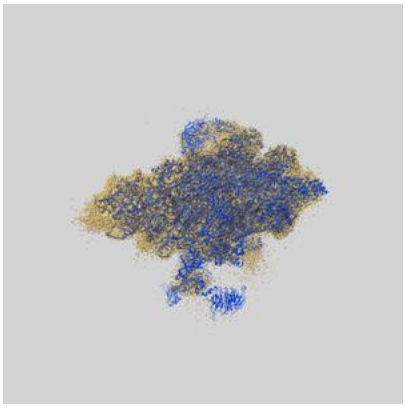
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.53	4.70	3.67
Unmasked-calculated*	4.22	8.15	4.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.4 by more than 10 %

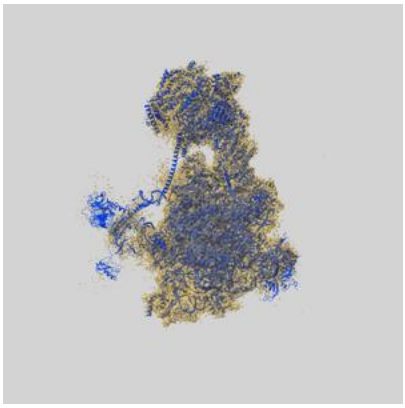
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17697 and PDB model 8PJ2. Per-residue inclusion information can be found in section 3 on page 14.

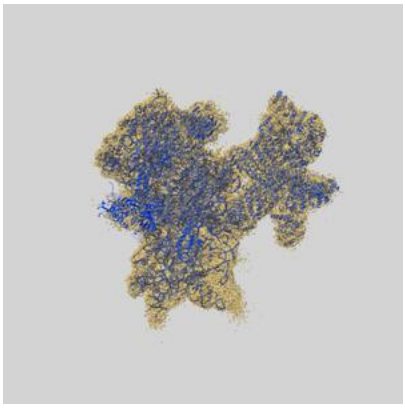
9.1 Map-model overlay



X



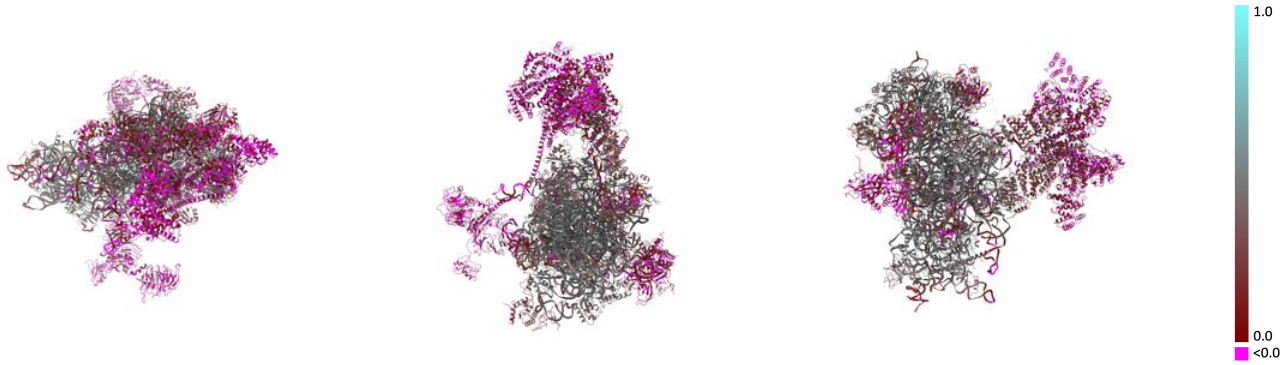
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

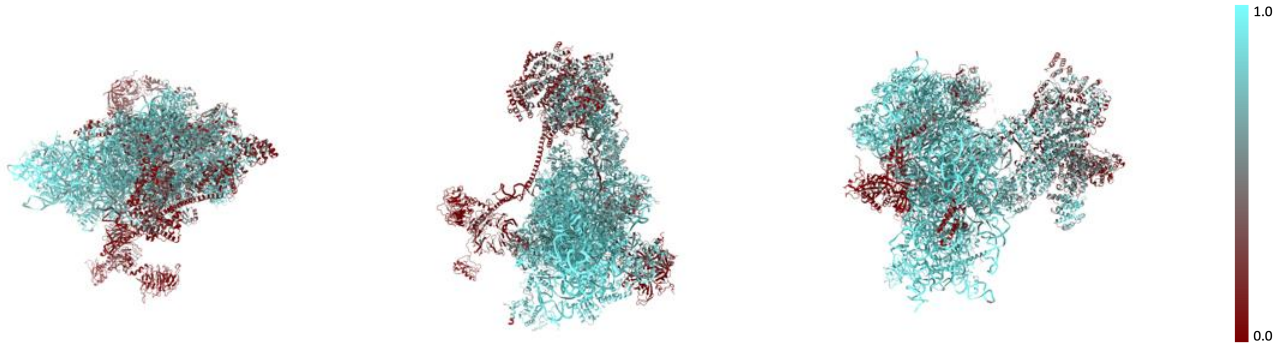
9.2 Q-score mapped to coordinate model (i)



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.

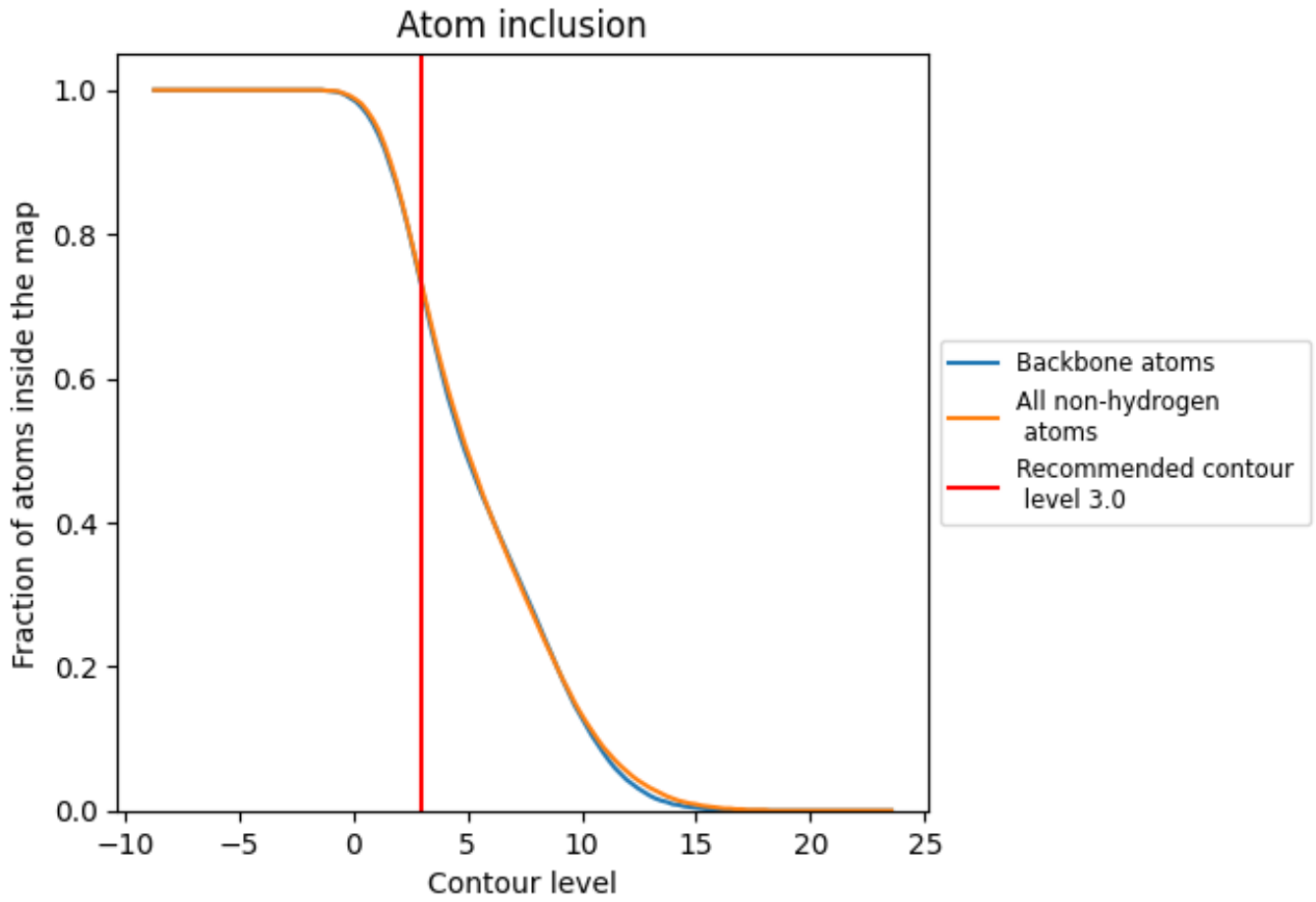
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.0).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7290	0.3200
1	0.0660	0.0560
2	0.0030	0.0270
3	0.2680	0.0420
4	0.4680	0.0680
5	0.2880	0.0140
6	0.4120	0.0450
7	0.4450	0.1710
8	0.4440	0.0950
9	0.8130	0.3960
A	0.9550	0.4200
B	0.8770	0.4630
C	0.9170	0.4800
D	0.8830	0.4620
E	0.9000	0.4850
F	0.7810	0.4060
G	0.7900	0.3880
H	0.8420	0.4310
I	0.8670	0.4410
J	0.8900	0.4870
K	0.8230	0.4450
L	0.8350	0.4600
M	0.7810	0.3970
N	0.8590	0.4560
O	0.8670	0.4260
P	0.8470	0.4250
Q	0.9070	0.4720
R	0.9160	0.4400
S	0.9250	0.4050
T	0.9210	0.4370
V	0.8450	0.4470
Y	0.9070	0.4670
Z	0.8020	0.4310
a	0.8630	0.4190
b	0.8600	0.4060

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	0.8720	0.4070
d	0.9250	0.4570
e	0.7370	0.3520
f	0.8570	0.4140
h	0.8220	0.4070
i	0.9350	0.4950
k	0.7930	0.2220
m	0.7210	0.2450
n	0.7590	0.4100
o	0.4240	0.1700
q	0.7200	0.3750
r	0.5210	0.2030
t	0.0590	0.0420
u	0.5390	0.1820
v	0.5470	0.1060
w	0.8120	0.2070
x	0.5380	0.2200
y	0.5820	0.2390
z	0.3610	0.2520