Full wwPDB EM Validation Report ⓘ

May 21, 2022 – 08:30 am BST

PDB ID	:	7QP7
EMDB ID	:	EMD-14114
Title	:	Structure of the human 48S initiation complex in closed state (h48S AUG closed)
Authors	:	Yi, S.-H.; Petrychenko, V.; Schliep, J.E.; Goyal, A.; Linden, A.; Chari, A.; Urlaub, H.; Stark, H.; Rodnina, M.V.; Adio, S.; Fischer, N.
Deposited on	:	2022-01-03
Resolution	:	3.70 Å(reported)
Based on initial model	:	6ZMW

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 ⓘ symbol.

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

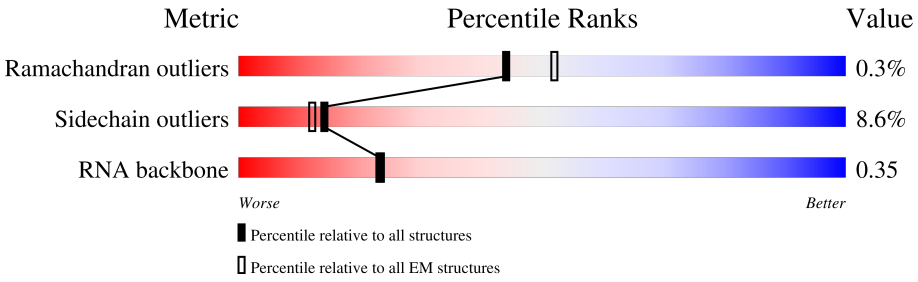
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	813	19% 55% 45%
2	3	218	64% 97%
3	4	357	15% 71% 28%
4	5	564	17% 57% 43%
5	6	374	32% 93% 6%
6	7	255	92%
7	8	352	21% 89% 10%
8	9	25	92%

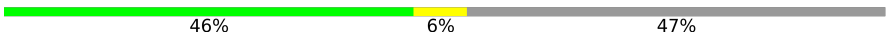
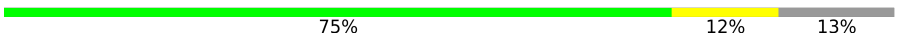
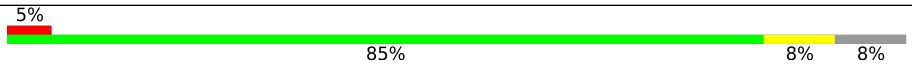
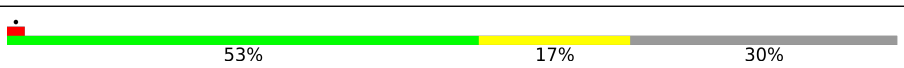
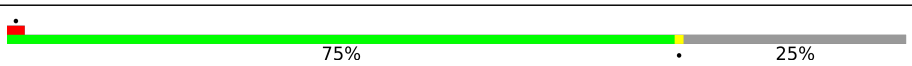
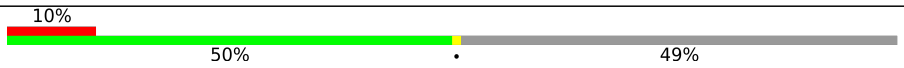
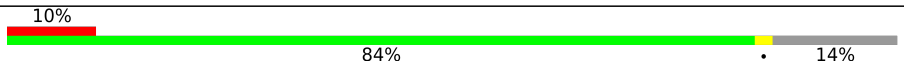
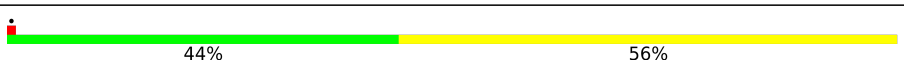
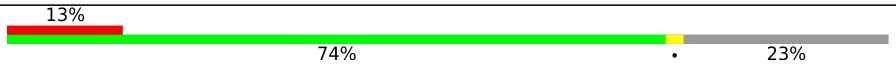
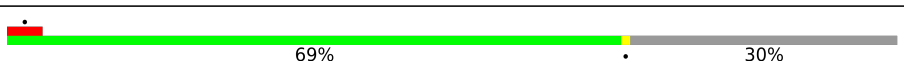
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	A	1869	63% 28% 8%
10	B	158	81% 9% 10%
11	C	263	90% 8%
12	D	194	87% 9%
13	E	143	88% 10%
14	F	59	75% 5% 20%
15	G	194	81% 10% 9%
16	H	84	83% 13%
17	I	151	97%
18	J	130	93% 5%
19	K	83	87% 11%
20	L	293	64% 11% 25%
21	M	135	82% 10% 7%
22	N	295	64% 5% 30%
23	O	264	80% 20%
24	P	151	74% 14% 12%
25	Q	115	76% 10% 14%
26	R	208	88% 8% 5%
27	S	249	81% 12% 8%
28	T	133	85% 9% 6%
29	V	204	83% 7% 10%
30	Y	146	90% 6%
31	Z	243	79% 14% 7%
32	a	165	56% 40%
33	b	145	67% 9% 24%

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 108194 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
1	1	447	Total	C	N	O	S	0	0
			2560	1570	492	493	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	213	Total	C	N	O	0	0
			1057	631	213	213		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	4	257	Total	C	N	O	0	0
			1272	757	257	258		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	5	319	Total	C	N	O	0	0
			1581	943	319	319		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	350	Total	C	N	O	S	0	0
			1917	1159	376	380	2		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	21	Total	C	N	O	P	0	0
			441	199	78	144	20		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	8	317	Total	C	N	O	0	0
			1571	936	317	318		

- Molecule 8 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 9 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1719	Total	C	N	O	P	0	0
			36668	16378	6574	11998	1718		

- Molecule 10 is a protein called 40S ribosomal protein S11.

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

- Molecule 11 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 12 is a protein called 40S ribosomal protein S9.

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

- Molecule 13 is a protein called 40S ribosomal protein S23.

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

- Molecule 14 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	47	Total	C	N	O	S	0	0
			378	231	85	61	1		

- Molecule 15 is a protein called 40S ribosomal protein S7.

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

- Molecule 16 is a protein called 40S ribosomal protein S27.

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

- Molecule 17 is a protein called 40S ribosomal protein S13.

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

- Molecule 18 is a protein called 40S ribosomal protein S15a.

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

- Molecule 19 is a protein called 40S ribosomal protein S21.

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

- Molecule 20 is a protein called 40S ribosomal protein S2.

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

- Molecule 21 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	125	Total	C	N	O	S	0	0
			1015	639	185	187	4		

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

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

- Molecule 23 is a protein called 40S ribosomal protein S3a.

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

- Molecule 24 is a protein called 40S ribosomal protein S14.

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

- Molecule 25 is a protein called 40S ribosomal protein S26.

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

- Molecule 26 is a protein called 40S ribosomal protein S8.

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

- Molecule 27 is a protein called 40S ribosomal protein S6.

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

- Molecule 28 is a protein called 40S ribosomal protein S24.

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

- Molecule 29 is a protein called 40S ribosomal protein S5.

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

- Molecule 30 is a protein called 40S ribosomal protein S16.

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

- Molecule 31 is a protein called 40S ribosomal protein S3.

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

- Molecule 32 is a protein called 40S ribosomal protein S10.

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

- Molecule 33 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	110	Total	C	N	O	S	0	0
			913	580	168	158	7		

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 35 is a protein called 40S ribosomal protein S19.

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

- Molecule 36 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	66	Total	C	N	O	S	0	0
			523	338	93	91	1		

- Molecule 37 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	142	Total	C	N	O	S	0	0
			1176	737	239	199	1		

- Molecule 38 is a protein called 40S ribosomal protein S20.

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

- Molecule 39 is a protein called 40S ribosomal protein S29.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	53	Total	C	N	O	S	0	0
			435	276	82	70	7		

- Molecule 41 is a protein called 40S ribosomal protein S12.

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

- Molecule 42 is a protein called 40S ribosomal protein S28.

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

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit G.

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

- Molecule 44 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	101	Total	C	N	O	S	0	0
			782	494	141	143	4		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	275	Total	C	N	O	S	0	0
			2215	1398	387	418	12		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	t	356	Total	C	N	O	0	0
			1750	1038	356	356		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	384	Total	C	N	O	S	0	0
			2635	1657	477	489	12		

- Molecule 49 is a RNA chain called Initiator Met-tRNA-i.

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

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	421	Total	C	N	O	S	0	0
			2831	1746	521	555	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	642	Total	C	N	O	S	0	0
			5197	3274	925	963	35		

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

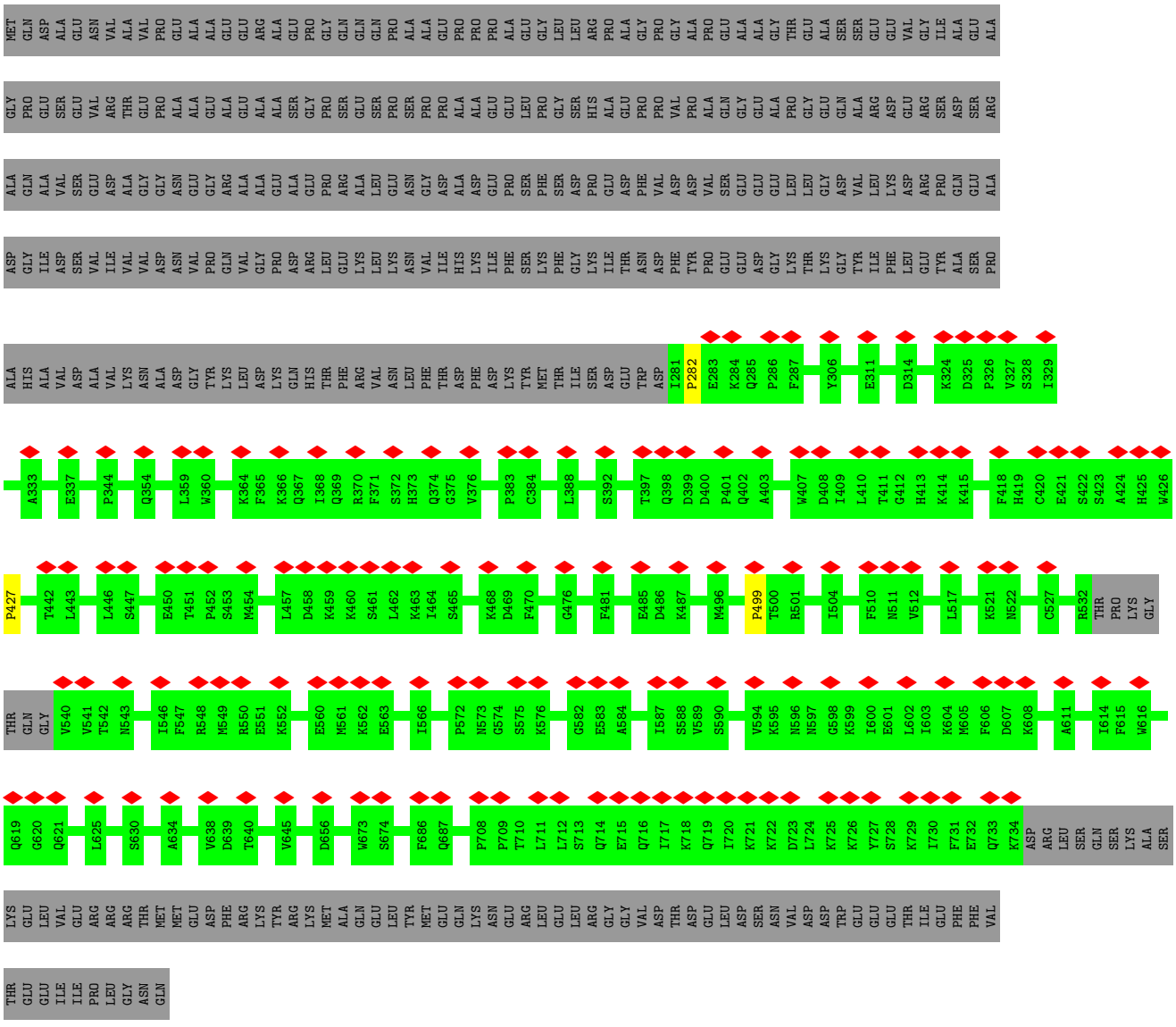
Mol	Chain	Residues	Atoms		AltConf
52	Q	1	Total	Zn	0
			1	1	
52	k	1	Total	Zn	0
			1	1	

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.

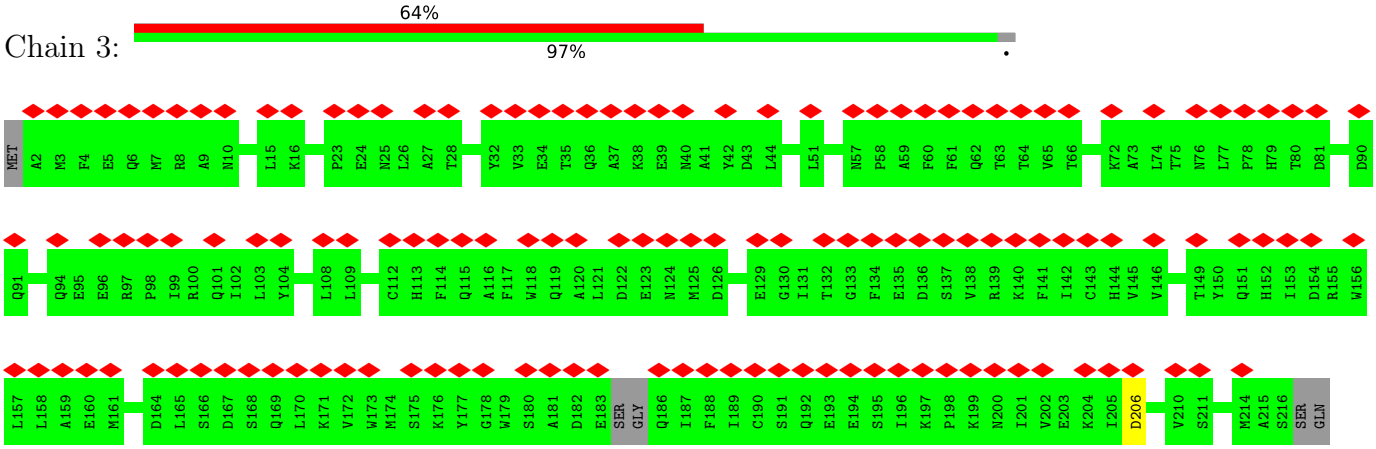
• Molecule 1: Eukaryotic translation initiation factor 3 subunit B

Chain 1:



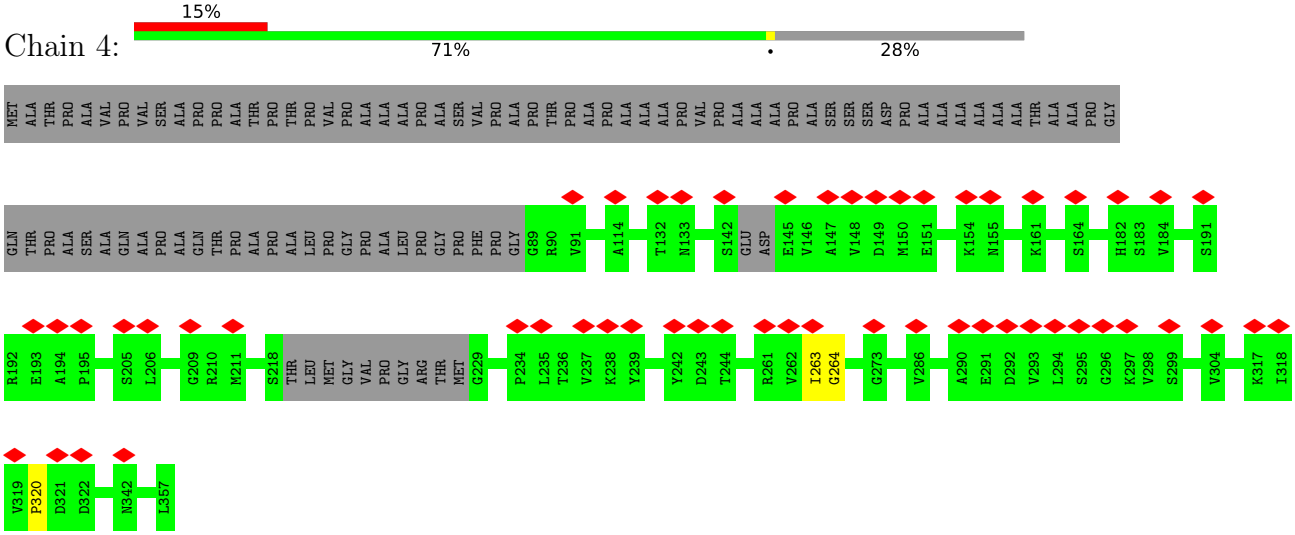
• Molecule 2: Eukaryotic translation initiation factor 3 subunit K

Chain 3:



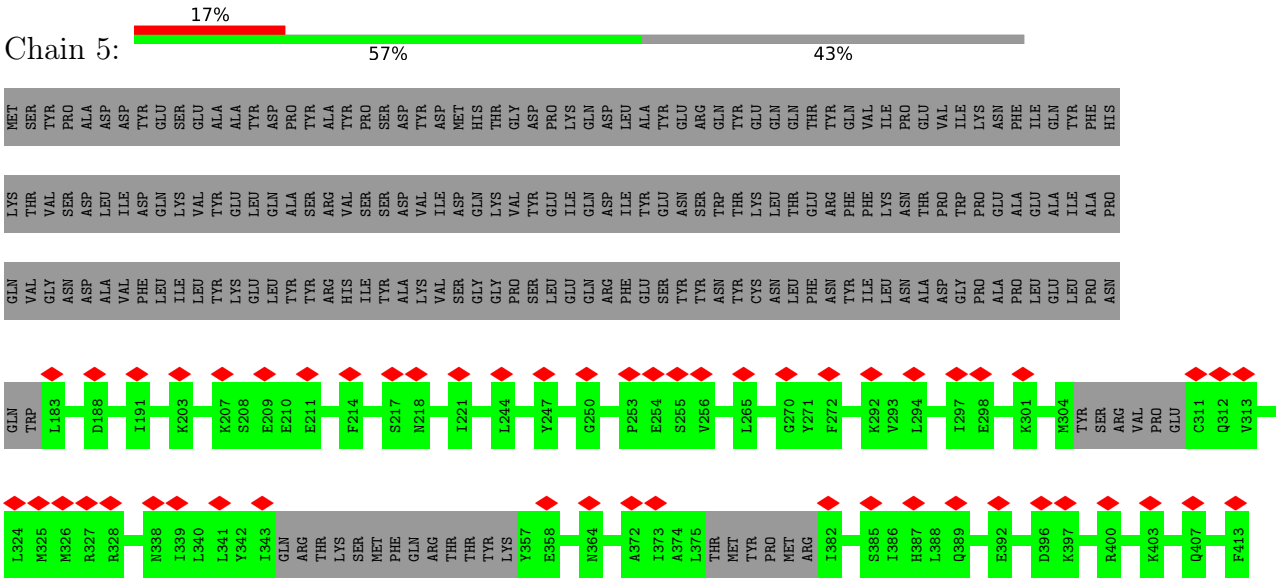
• Molecule 3: Eukaryotic translation initiation factor 3 subunit F

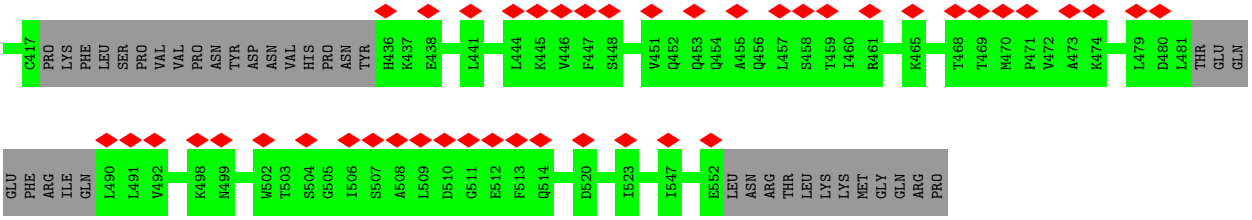
Chain 4:



• Molecule 4: Eukaryotic translation initiation factor 3 subunit L

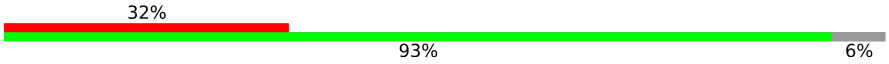
Chain 5:

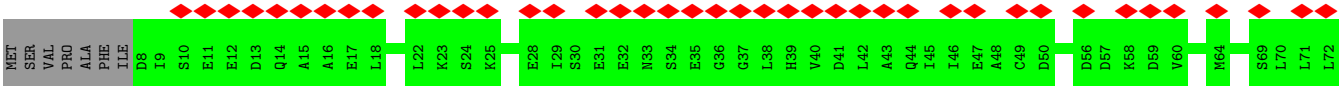


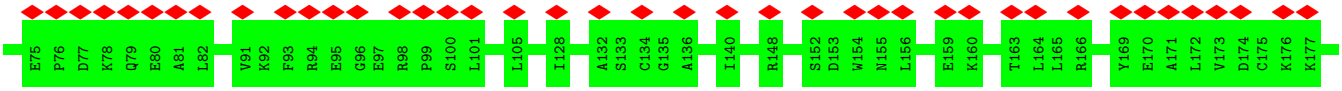


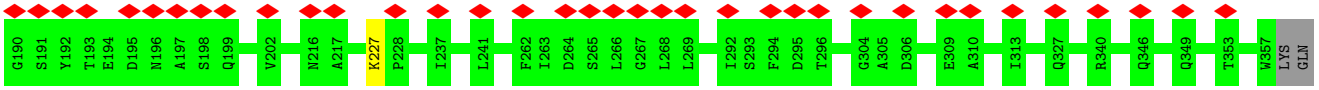
• Molecule 5: Eukaryotic translation initiation factor 3 subunit M

Chain 6:



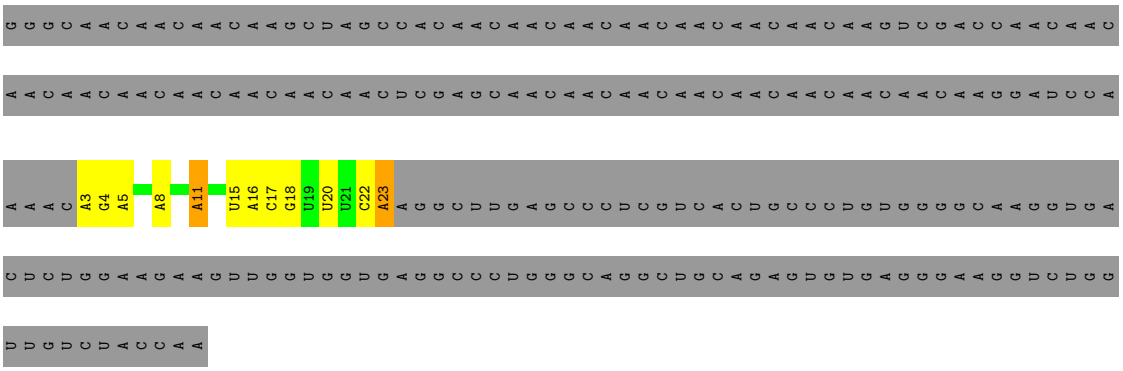






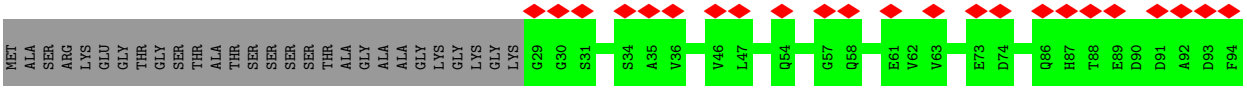
• Molecule 6: mRNA

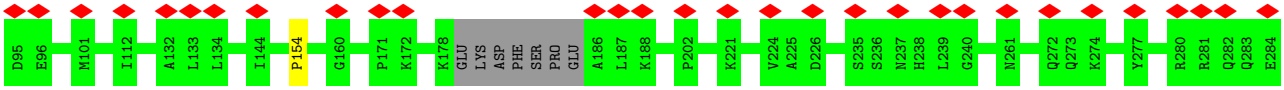
Chain 7:

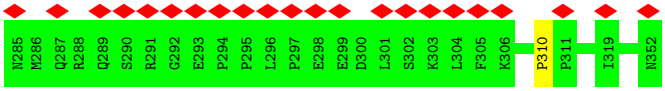


• Molecule 7: Eukaryotic translation initiation factor 3 subunit H

Chain 8:

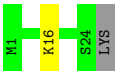






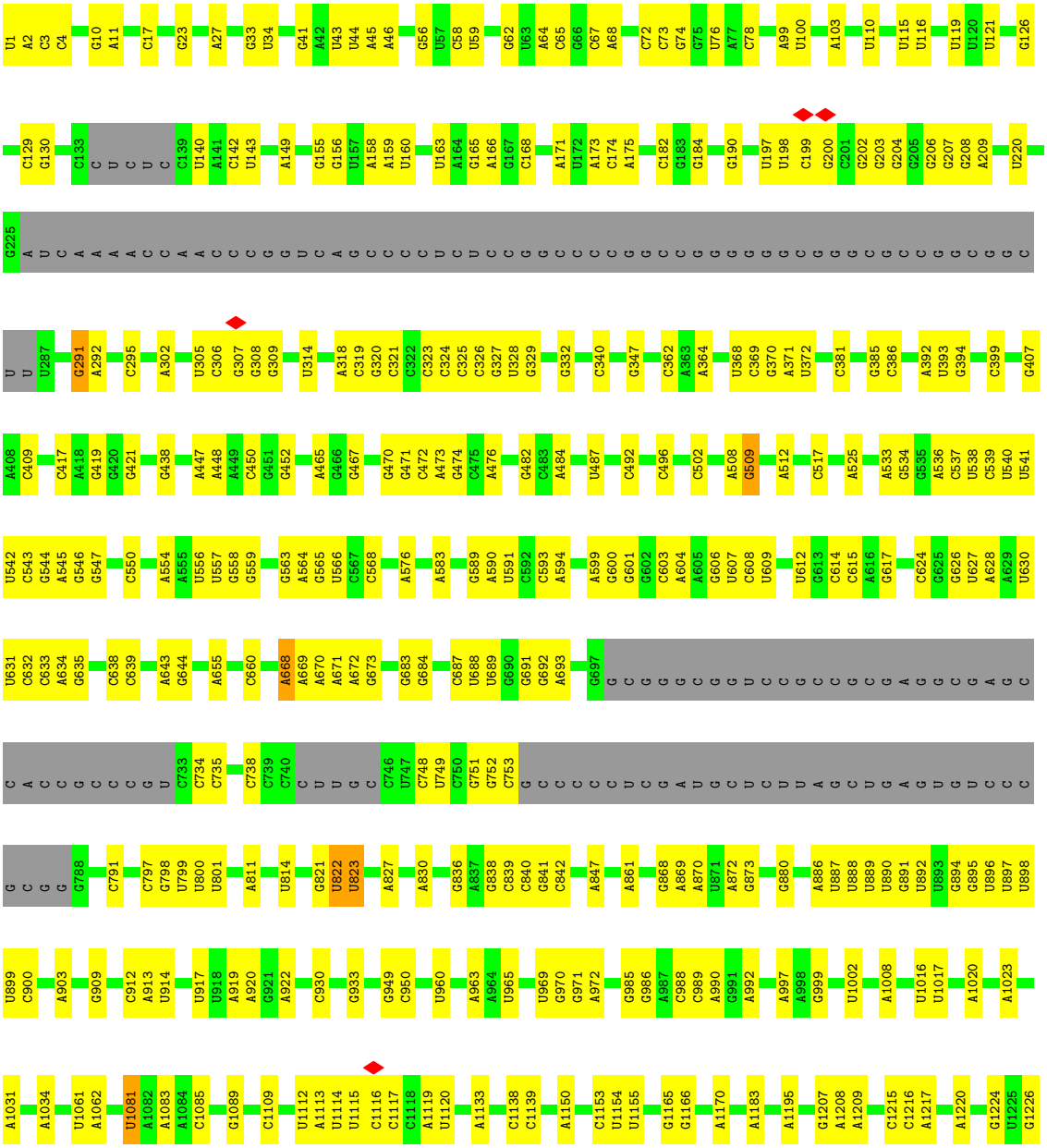
• Molecule 8: 60S ribosomal protein L41

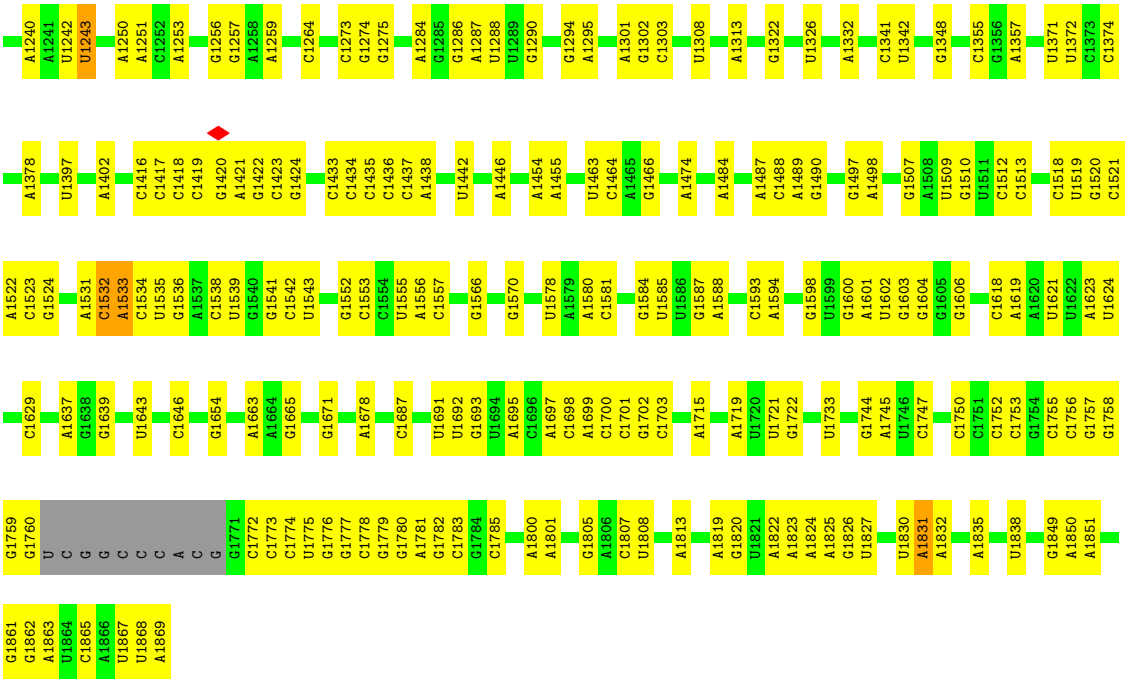
Chain 9:



• Molecule 9: 18S rRNA

Chain A:





• Molecule 10: 40S ribosomal protein S11

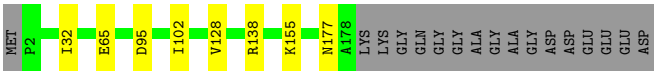
Chain B:

• Molecule 11: 40S ribosomal protein S4, X isoform

Chain C:

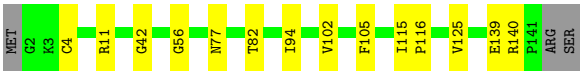
• Molecule 12: 40S ribosomal protein S9

Chain D:



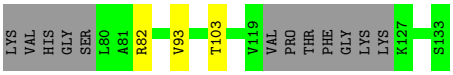
• Molecule 13: 40S ribosomal protein S23

Chain E:



• Molecule 14: 40S ribosomal protein S30

Chain F:

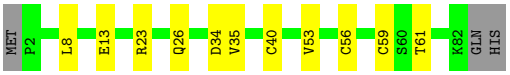


• Molecule 15: 40S ribosomal protein S7

Chain G:

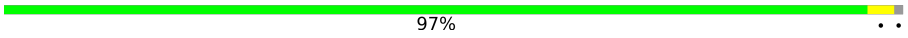
• Molecule 16: 40S ribosomal protein S27

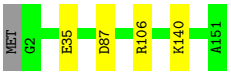
Chain H:



• Molecule 17: 40S ribosomal protein S13

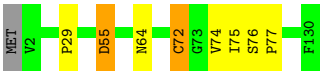
Chain I:





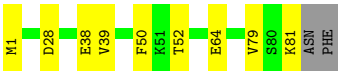
• Molecule 18: 40S ribosomal protein S15a

Chain J:



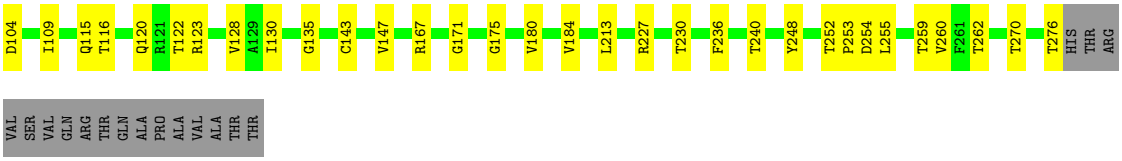
• Molecule 19: 40S ribosomal protein S21

Chain K:



• Molecule 20: 40S ribosomal protein S2

Chain L:

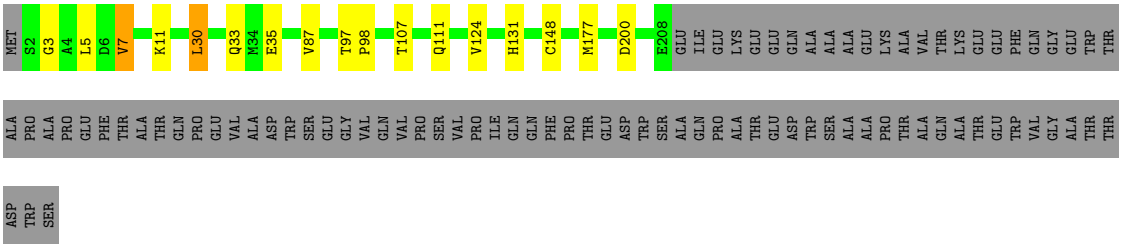


• Molecule 21: 40S ribosomal protein S17

Chain M:

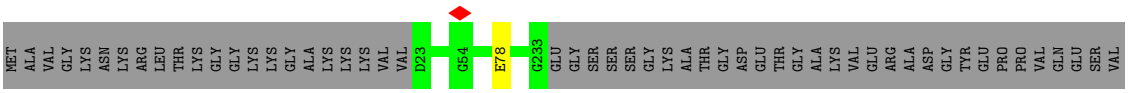
• Molecule 22: 40S ribosomal protein SA

Chain N:



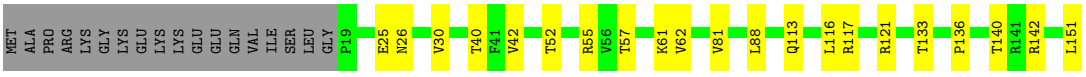
• Molecule 23: 40S ribosomal protein S3a

Chain O:



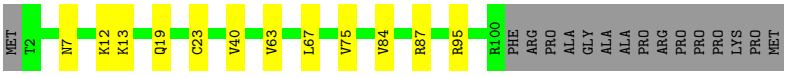
• Molecule 24: 40S ribosomal protein S14

Chain P:



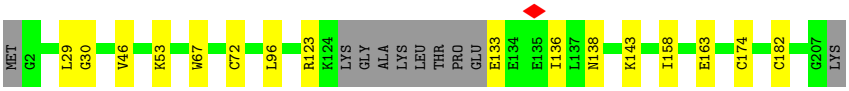
• Molecule 25: 40S ribosomal protein S26

Chain Q:

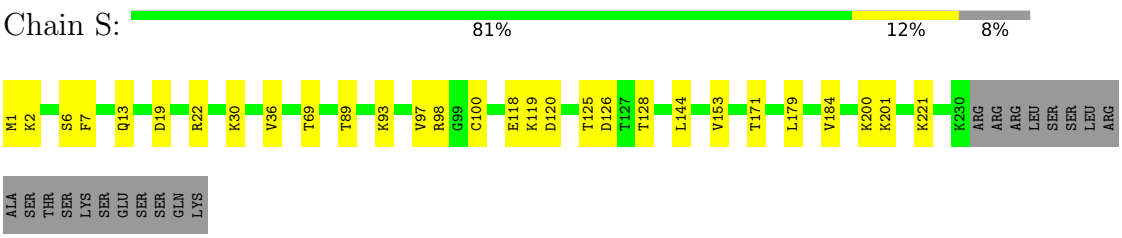


• Molecule 26: 40S ribosomal protein S8

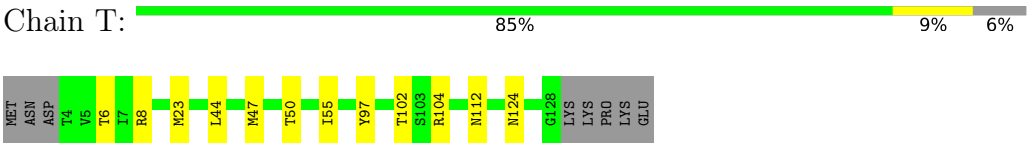
Chain R:



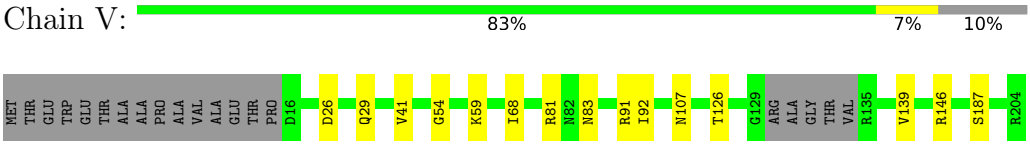
• Molecule 27: 40S ribosomal protein S6



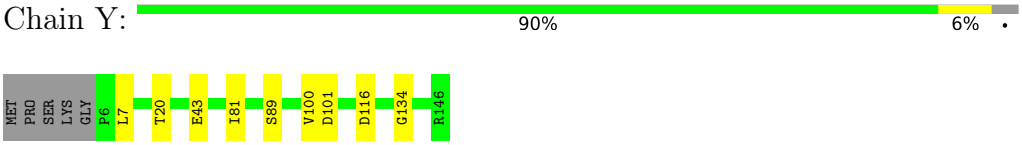
• Molecule 28: 40S ribosomal protein S24



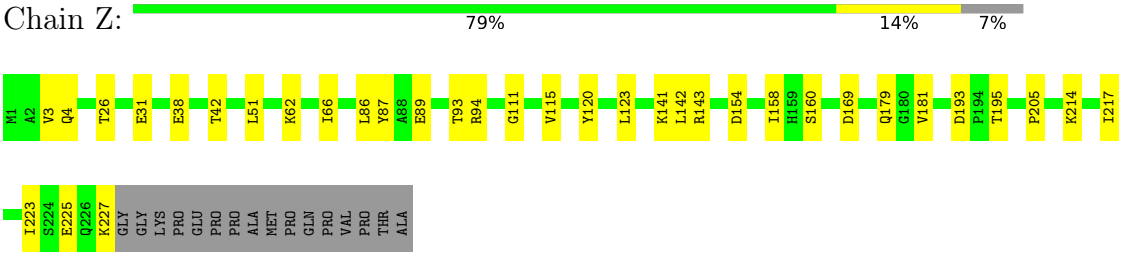
• Molecule 29: 40S ribosomal protein S5



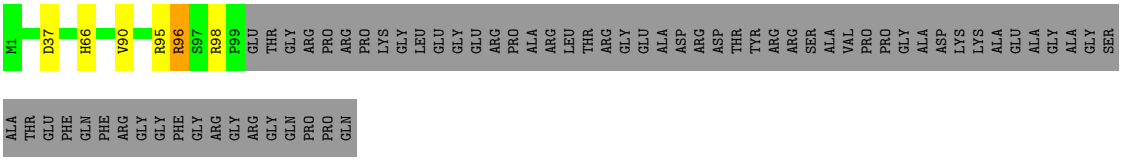
• Molecule 30: 40S ribosomal protein S16



• Molecule 31: 40S ribosomal protein S3



• Molecule 32: 40S ribosomal protein S10

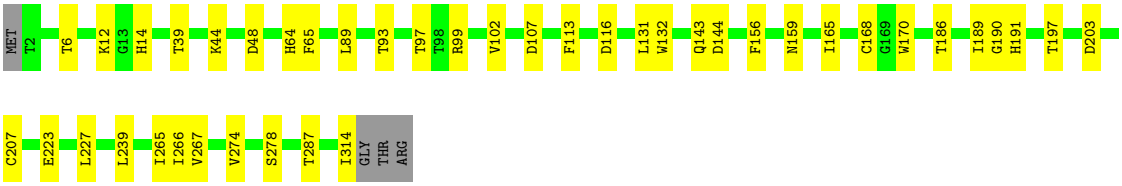


• Molecule 33: 40S ribosomal protein S15

Chain b:

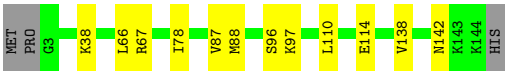
• Molecule 34: Receptor of activated protein C kinase 1

Chain c:



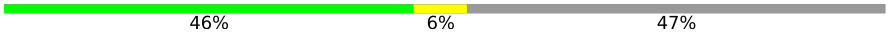
• Molecule 35: 40S ribosomal protein S19

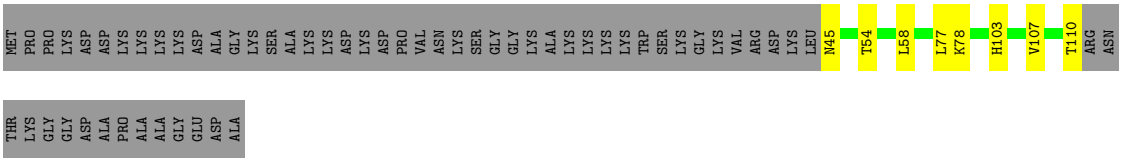
Chain d:



• Molecule 36: 40S ribosomal protein S25

Chain e:



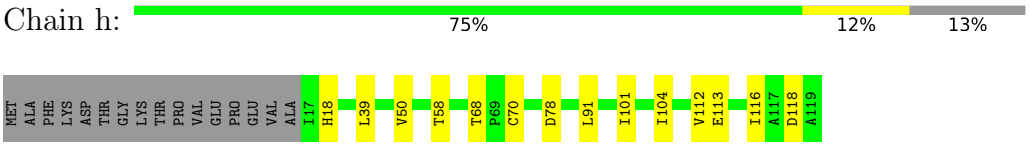


• Molecule 37: 40S ribosomal protein S18

Chain f:

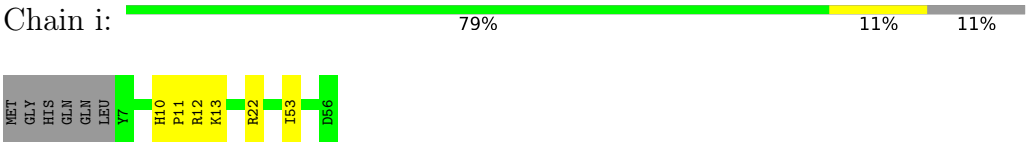
• Molecule 38: 40S ribosomal protein S20

Chain h:



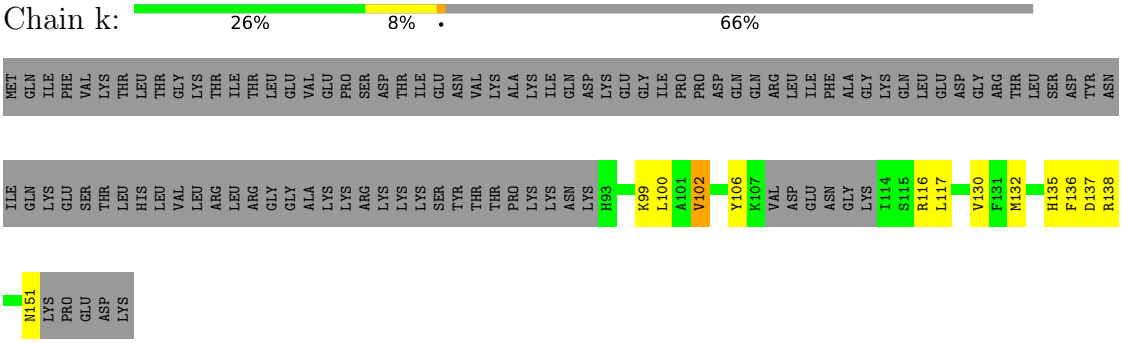
• Molecule 39: 40S ribosomal protein S29

Chain i:



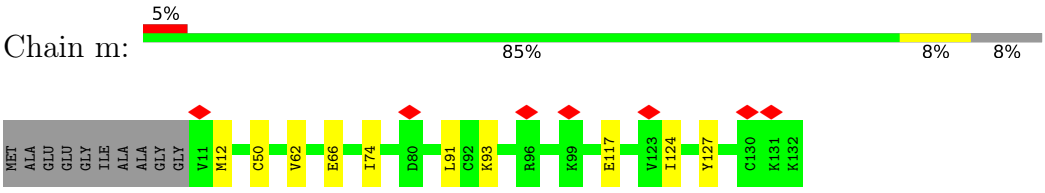
• Molecule 40: Ubiquitin-40S ribosomal protein S27a

Chain k:



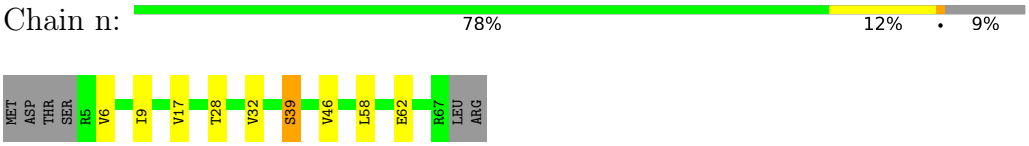
• Molecule 41: 40S ribosomal protein S12

Chain m:



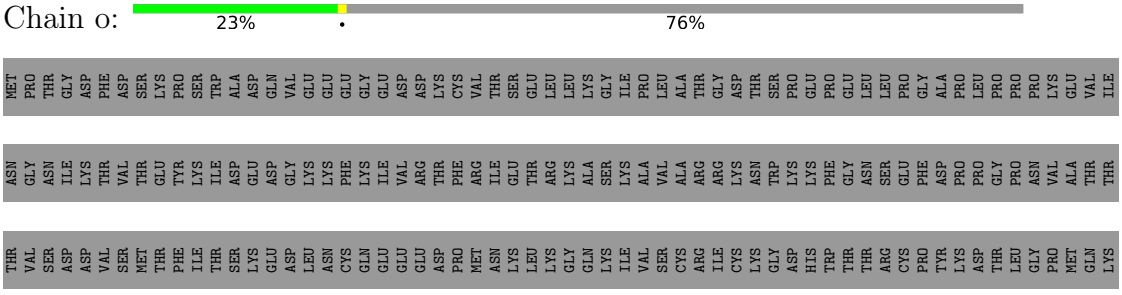
• Molecule 42: 40S ribosomal protein S28

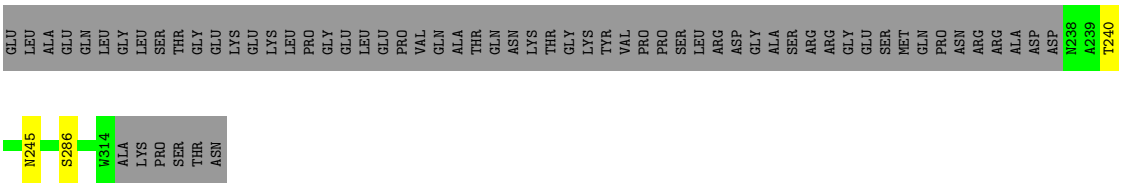
Chain n:



• Molecule 43: Eukaryotic translation initiation factor 3 subunit G

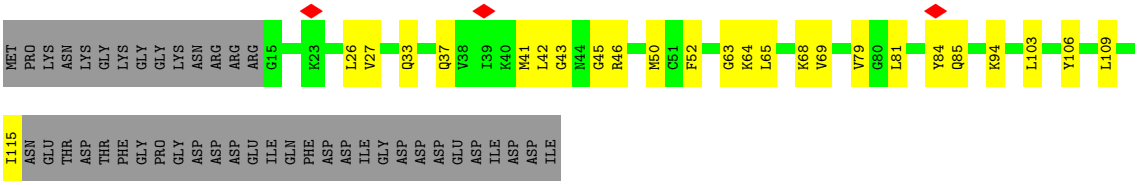
Chain o:





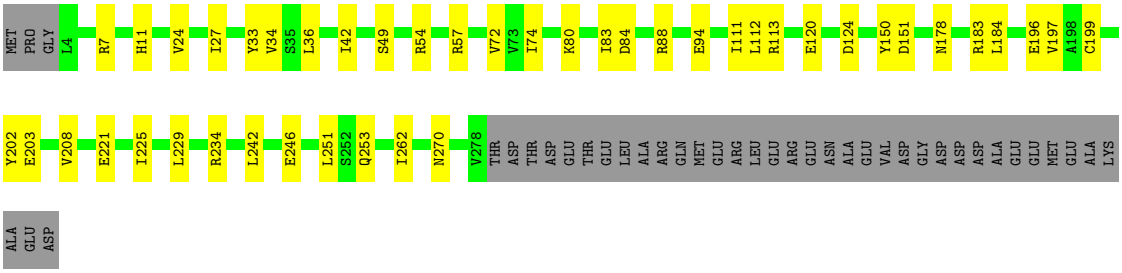
• Molecule 44: Eukaryotic translation initiation factor 1A, X-chromosomal

Chain q:



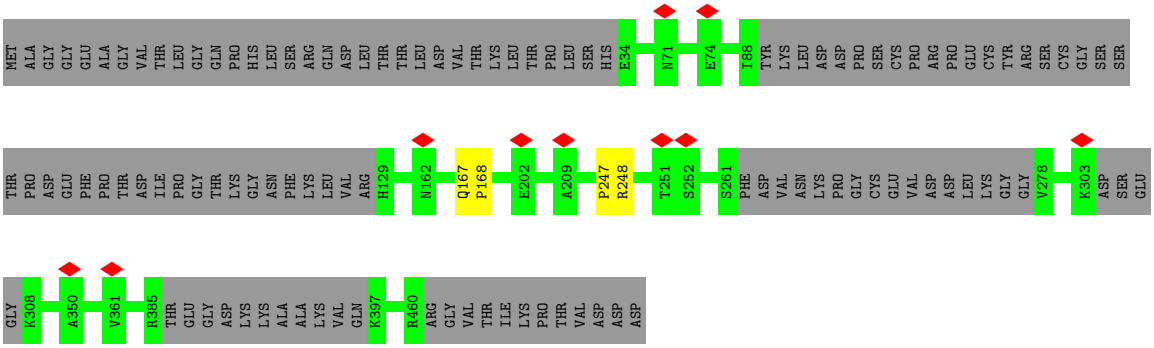
• Molecule 45: Eukaryotic translation initiation factor 2 subunit 1

Chain r:



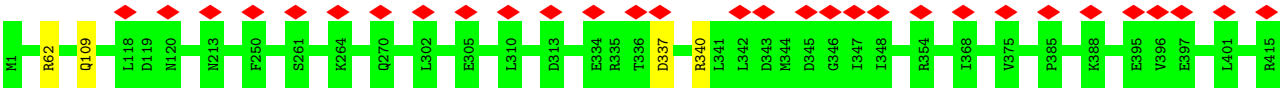
• Molecule 46: Eukaryotic translation initiation factor 2 subunit 3

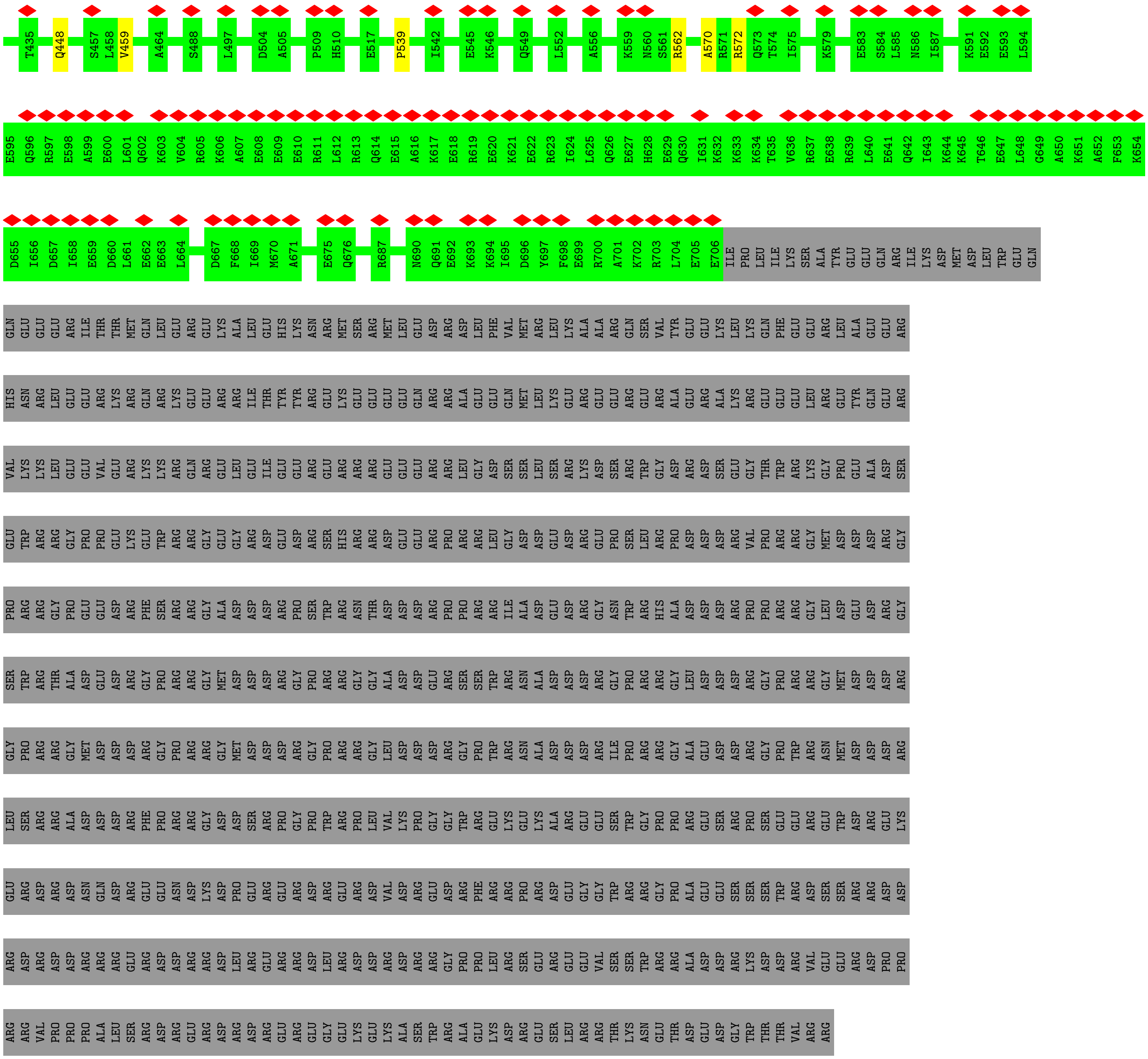
Chain t:



• Molecule 47: Eukaryotic translation initiation factor 3 subunit A

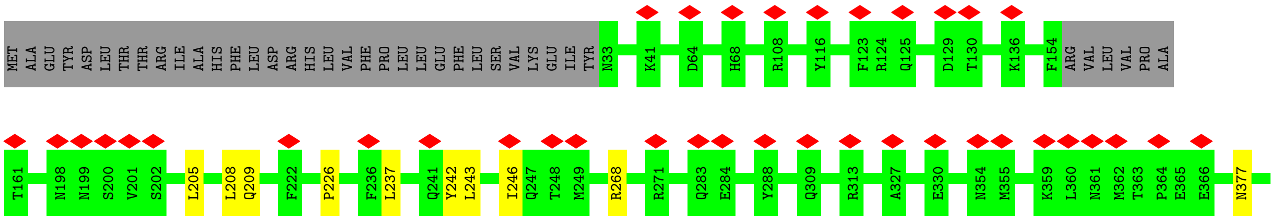
Chain u:

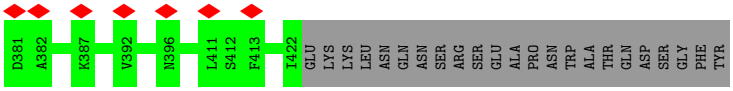




- Molecule 48: Eukaryotic translation initiation factor 3 subunit E

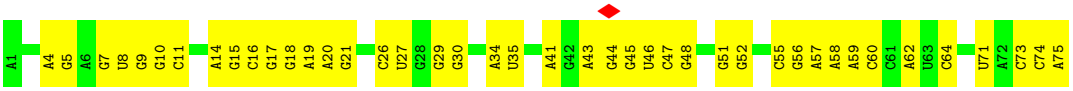
Chain v:





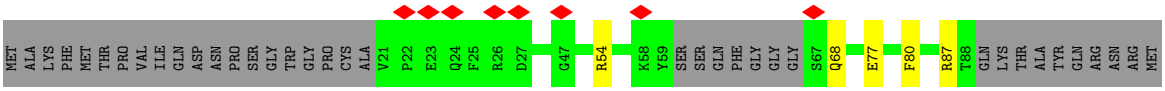
• Molecule 49: Initiator Met-tRNA-i

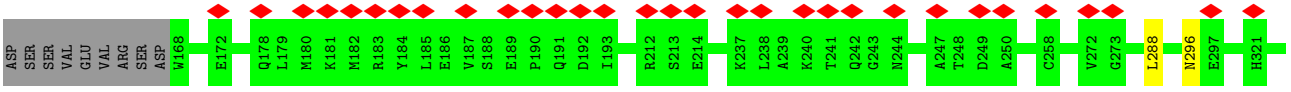
Chain w:

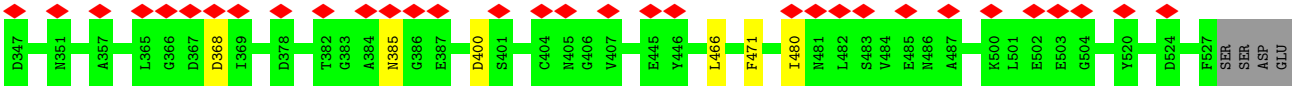


• Molecule 50: Eukaryotic translation initiation factor 3 subunit D

Chain x:

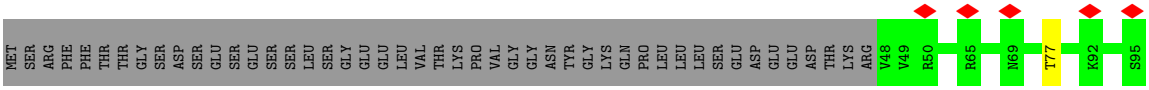


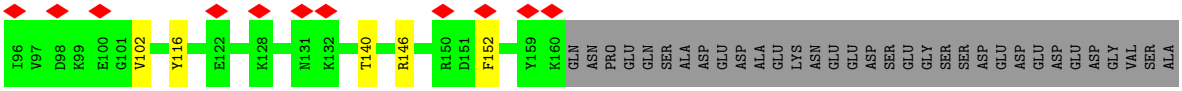


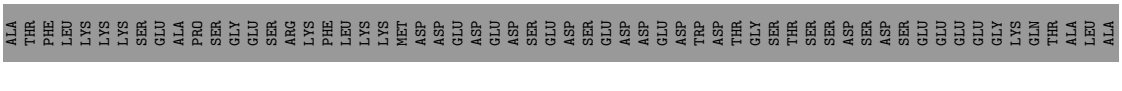


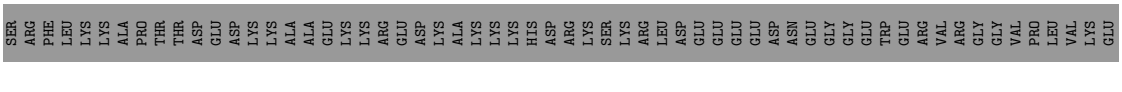
• Molecule 51: Eukaryotic translation initiation factor 3 subunit C

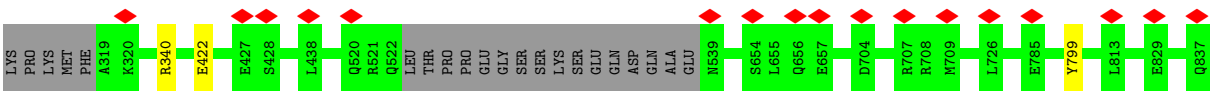
Chain y:












T841
P849
L863
GLY SER LEU VAL GLU ASN ASN GLU ARG VAL PHE ASP HIS LYS GLN GLY THR TYR GLY GLY TYR PHE ARG ASP GLN LYS ASP GLY TYR ARG LYS ASN GLU GLY TYR MET ARG ARG GLY GLY TYR ARG GLN GLN GLN SER GLN THR ALA TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	364950	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	24.271	Depositor
Minimum map value	-11.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.15	Depositor
Map size (Å)	417.59998, 417.59998, 417.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.45	0/2581	0.71	0/3561
2	3	0.35	0/1055	0.54	0/1469
3	4	0.47	0/1269	0.68	0/1762
4	5	0.36	0/1575	0.52	0/2187
5	6	0.42	0/1926	0.64	1/2669 (0.0%)
6	7	0.87	2/492 (0.4%)	1.23	3/764 (0.4%)
7	8	0.44	0/1569	0.66	0/2183
8	9	0.96	0/231	0.74	0/294
9	A	0.41	0/40362	0.69	4/62905 (0.0%)
10	B	0.84	0/1186	0.86	2/1585 (0.1%)
11	C	0.83	0/2077	0.81	1/2796 (0.0%)
12	D	0.84	0/1502	0.79	0/2008
13	E	0.96	0/1105	0.95	2/1476 (0.1%)
14	F	0.83	0/380	0.88	0/496
15	G	0.74	0/1451	0.84	0/1942
16	H	0.82	0/644	0.82	0/864
17	I	0.84	0/1232	0.82	0/1656
18	J	1.03	0/1051	0.98	5/1406 (0.4%)
19	K	0.93	0/623	0.93	1/833 (0.1%)
20	L	1.01	0/1743	0.93	2/2354 (0.1%)
21	M	0.81	0/1029	0.85	0/1383
22	N	0.94	0/1670	0.94	3/2271 (0.1%)
23	O	0.40	0/1742	0.62	0/2330
24	P	0.98	0/1010	0.99	1/1353 (0.1%)
25	Q	0.87	0/805	0.91	1/1079 (0.1%)
26	R	0.70	0/1654	0.79	2/2203 (0.1%)
27	S	0.62	0/1885	0.77	0/2510
28	T	0.80	0/1032	0.75	0/1371
29	V	0.94	0/1481	0.86	2/1988 (0.1%)
30	Y	0.93	0/1142	0.89	2/1528 (0.1%)
31	Z	0.87	0/1793	0.92	3/2414 (0.1%)
32	a	0.82	0/859	0.79	1/1159 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.73	0/929	0.78	1/1241 (0.1%)
34	c	0.73	0/2493	0.85	3/3394 (0.1%)
35	d	0.87	0/1123	0.81	1/1504 (0.1%)
36	e	0.79	0/529	0.85	2/712 (0.3%)
37	f	0.79	0/1194	0.84	1/1599 (0.1%)
38	h	0.85	0/827	0.91	1/1110 (0.1%)
39	i	0.90	0/429	0.86	0/568
40	k	0.58	0/444	0.86	2/588 (0.3%)
41	m	0.42	0/960	0.67	0/1286
42	n	0.86	0/500	0.89	0/669
43	o	0.45	0/628	0.77	0/846
44	q	0.62	0/792	0.98	4/1062 (0.4%)
45	r	0.58	0/2247	0.81	2/3029 (0.1%)
46	t	0.39	0/1745	0.61	0/2417
47	u	0.42	0/5475	0.66	1/7432 (0.0%)
48	v	0.44	0/2672	0.70	2/3647 (0.1%)
49	w	0.33	0/1795	0.66	0/2798
50	x	0.42	0/2874	0.69	1/3925 (0.0%)
51	y	0.40	0/5284	0.67	3/7123 (0.0%)
All	All	0.59	2/113096 (0.0%)	0.75	60/161749 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	7	23	A	C1'-N9	-5.25	1.39	1.46
6	7	11	A	C5-C4	-5.14	1.35	1.38

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	y	146	ARG	NE-CZ-NH2	-13.68	113.46	120.30
22	N	7	VAL	N-CA-C	-12.54	77.15	111.00
51	y	146	ARG	NE-CZ-NH1	9.22	124.91	120.30
44	q	42	LEU	N-CA-C	-9.21	86.14	111.00
10	B	53	GLY	N-CA-C	9.19	136.07	113.10
6	7	11	A	N1-C6-N6	-8.68	113.39	118.60
48	v	209	GLN	CA-CB-CG	-8.38	94.95	113.40
20	L	135	GLY	N-CA-C	8.08	133.29	113.10
38	h	104	ILE	N-CA-C	-8.01	89.37	111.00
31	Z	111	GLY	N-CA-C	-7.60	94.09	113.10
34	c	278	SER	N-CA-C	-7.55	90.61	111.00
9	A	1533	A	C5'-C4'-O4'	7.45	118.04	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	q	45	GLY	N-CA-C	-7.31	94.82	113.10
45	r	84	ASP	N-CA-C	-7.30	91.30	111.00
19	K	28	ASP	N-CA-C	-7.08	91.88	111.00
32	a	96	ARG	N-CA-C	-7.00	92.10	111.00
36	e	103	HIS	N-CA-C	-6.99	92.14	111.00
18	J	77	PRO	N-CA-C	-6.98	93.96	112.10
44	q	43	GLY	N-CA-C	-6.97	95.68	113.10
30	Y	43	GLU	N-CA-C	6.93	129.71	111.00
24	P	140	THR	N-CA-C	-6.81	92.62	111.00
13	E	56	GLY	N-CA-C	-6.70	96.35	113.10
6	7	11	A	C5-C6-N1	6.67	121.03	117.70
18	J	75	ILE	N-CA-C	-6.64	93.07	111.00
50	x	480	ILE	CG1-CB-CG2	-6.51	97.07	111.40
13	E	42	GLY	N-CA-C	-6.48	96.89	113.10
33	b	47	ARG	N-CA-C	-6.42	93.66	111.00
18	J	72	CYS	N-CA-C	-6.32	93.95	111.00
34	c	190	GLY	N-CA-C	6.27	128.78	113.10
9	A	1831	A	C2'-C3'-O3'	6.22	123.65	113.70
18	J	76	SER	N-CA-C	6.20	127.74	111.00
48	v	208	LEU	CA-CB-CG	6.14	129.43	115.30
36	e	77	LEU	N-CA-C	-6.13	94.46	111.00
29	V	54	GLY	N-CA-C	6.10	128.34	113.10
9	A	291	G	C2'-C3'-O3'	6.05	123.38	113.70
37	f	100	ALA	N-CA-C	6.04	127.32	111.00
6	7	11	A	C4-C5-C6	-5.98	114.01	117.00
35	d	78	ILE	CB-CA-C	-5.98	99.65	111.60
51	y	422	GLU	N-CA-C	-5.90	95.06	111.00
18	J	55	ASP	N-CA-C	-5.83	95.25	111.00
26	R	30	GLY	N-CA-C	-5.74	98.75	113.10
29	V	107	ASN	N-CA-C	-5.73	95.53	111.00
10	B	32	LYS	N-CA-C	-5.68	95.65	111.00
11	C	139	LEU	CA-CB-CG	5.63	128.24	115.30
30	Y	134	GLY	N-CA-C	5.61	127.12	113.10
22	N	3	GLY	N-CA-C	-5.54	99.24	113.10
40	k	130	VAL	N-CA-C	-5.50	96.16	111.00
31	Z	87	TYR	N-CA-C	5.49	125.81	111.00
5	6	227	LYS	N-CA-C	-5.46	96.25	111.00
40	k	132	MET	N-CA-C	-5.43	96.34	111.00
44	q	50	MET	N-CA-C	-5.39	96.44	111.00
45	r	203	GLU	N-CA-C	-5.38	96.48	111.00
20	L	175	GLY	N-CA-C	5.38	126.54	113.10
9	A	1532	C	C5'-C4'-C3'	-5.36	107.42	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	c	44	LYS	N-CA-C	-5.35	96.54	111.00
47	u	570	ALA	N-CA-CB	5.27	117.48	110.10
25	Q	13	LYS	N-CA-C	-5.24	96.85	111.00
22	N	30	LEU	CA-CB-CG	5.23	127.33	115.30
26	R	67	TRP	N-CA-C	-5.13	97.14	111.00
31	Z	160	SER	CB-CA-C	-5.05	100.50	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	443/813 (54%)	414 (94%)	26 (6%)	3 (1%)	22	59
2	3	209/218 (96%)	205 (98%)	3 (1%)	1 (0%)	29	66
3	4	251/357 (70%)	229 (91%)	19 (8%)	3 (1%)	13	48
4	5	307/564 (54%)	301 (98%)	6 (2%)	0	100	100
5	6	348/374 (93%)	318 (91%)	30 (9%)	0	100	100
7	8	313/352 (89%)	276 (88%)	35 (11%)	2 (1%)	25	62
8	9	22/25 (88%)	22 (100%)	0	0	100	100
10	B	138/158 (87%)	136 (99%)	2 (1%)	0	100	100
11	C	254/263 (97%)	249 (98%)	5 (2%)	0	100	100
12	D	175/194 (90%)	174 (99%)	1 (1%)	0	100	100
13	E	138/143 (96%)	134 (97%)	3 (2%)	1 (1%)	22	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	F	43/59 (73%)	43 (100%)	0	0	100	100
15	G	171/194 (88%)	163 (95%)	7 (4%)	1 (1%)	25	62
16	H	79/84 (94%)	76 (96%)	2 (2%)	1 (1%)	12	47
17	I	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
18	J	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	19	56
19	K	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
20	L	218/293 (74%)	215 (99%)	2 (1%)	1 (0%)	29	66
21	M	123/135 (91%)	121 (98%)	2 (2%)	0	100	100
22	N	205/295 (70%)	201 (98%)	3 (2%)	1 (0%)	29	66
23	O	209/264 (79%)	193 (92%)	16 (8%)	0	100	100
24	P	131/151 (87%)	123 (94%)	7 (5%)	1 (1%)	19	56
25	Q	97/115 (84%)	93 (96%)	4 (4%)	0	100	100
26	R	194/208 (93%)	194 (100%)	0	0	100	100
27	S	228/249 (92%)	223 (98%)	5 (2%)	0	100	100
28	T	123/133 (92%)	122 (99%)	1 (1%)	0	100	100
29	V	180/204 (88%)	175 (97%)	5 (3%)	0	100	100
30	Y	139/146 (95%)	136 (98%)	3 (2%)	0	100	100
31	Z	225/243 (93%)	223 (99%)	2 (1%)	0	100	100
32	a	97/165 (59%)	97 (100%)	0	0	100	100
33	b	108/145 (74%)	107 (99%)	1 (1%)	0	100	100
34	c	311/317 (98%)	301 (97%)	10 (3%)	0	100	100
35	d	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
36	e	64/125 (51%)	64 (100%)	0	0	100	100
37	f	140/152 (92%)	134 (96%)	6 (4%)	0	100	100
38	h	101/119 (85%)	97 (96%)	4 (4%)	0	100	100
39	i	48/56 (86%)	47 (98%)	0	1 (2%)	7	38
40	k	49/156 (31%)	44 (90%)	4 (8%)	1 (2%)	7	39
41	m	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
42	n	61/69 (88%)	59 (97%)	1 (2%)	1 (2%)	9	43
43	o	75/320 (23%)	73 (97%)	2 (3%)	0	100	100
44	q	99/144 (69%)	83 (84%)	12 (12%)	4 (4%)	3	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
45	r	273/315 (87%)	255 (93%)	17 (6%)	1 (0%)	34 69
46	t	346/472 (73%)	337 (97%)	5 (1%)	4 (1%)	13 48
47	u	705/1382 (51%)	672 (95%)	32 (4%)	1 (0%)	51 83
48	v	380/445 (85%)	350 (92%)	30 (8%)	0	100 100
50	x	415/548 (76%)	386 (93%)	29 (7%)	0	100 100
51	y	636/913 (70%)	610 (96%)	25 (4%)	1 (0%)	47 78
All	All	9485/12718 (75%)	9077 (96%)	378 (4%)	30 (0%)	44 74

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	282	PRO
1	1	427	PRO
3	4	264	GLY
16	H	56	CYS
24	P	136	PRO
44	q	94	LYS
45	r	54	ARG
46	t	167	GLN
46	t	168	PRO
46	t	248	ARG
7	8	154	PRO
42	n	39	SER
44	q	63	GLY
44	q	69	VAL
1	1	499	PRO
20	L	171	GLY
22	N	98	PRO
46	t	247	PRO
51	y	849	PRO
3	4	263	ILE
39	i	11	PRO
44	q	64	LYS
2	3	206	ASP
3	4	320	PRO
13	E	116	PRO
7	8	310	PRO
47	u	539	PRO
18	J	29	PRO
15	G	190	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	k	102	VAL

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	97/701 (14%)	97 (100%)	0	100 100
5	6	49/335 (15%)	49 (100%)	0	100 100
8	9	23/24 (96%)	22 (96%)	1 (4%)	29 58
10	B	129/142 (91%)	117 (91%)	12 (9%)	9 35
11	C	220/225 (98%)	201 (91%)	19 (9%)	10 39
12	D	158/168 (94%)	150 (95%)	8 (5%)	24 55
13	E	112/115 (97%)	101 (90%)	11 (10%)	8 33
14	F	38/48 (79%)	35 (92%)	3 (8%)	12 42
15	G	159/174 (91%)	141 (89%)	18 (11%)	6 28
16	H	73/76 (96%)	63 (86%)	10 (14%)	3 21
17	I	130/131 (99%)	126 (97%)	4 (3%)	40 65
18	J	112/113 (99%)	108 (96%)	4 (4%)	35 63
19	K	65/67 (97%)	57 (88%)	8 (12%)	4 24
20	L	186/225 (83%)	156 (84%)	30 (16%)	2 15
21	M	114/122 (93%)	100 (88%)	14 (12%)	4 24
22	N	173/243 (71%)	158 (91%)	15 (9%)	10 38
23	O	192/231 (83%)	191 (100%)	1 (0%)	88 94
24	P	104/119 (87%)	85 (82%)	19 (18%)	1 10
25	Q	86/98 (88%)	75 (87%)	11 (13%)	4 23
26	R	172/180 (96%)	158 (92%)	14 (8%)	11 41
27	S	200/218 (92%)	171 (86%)	29 (14%)	3 18
28	T	107/115 (93%)	95 (89%)	12 (11%)	6 28
29	V	156/170 (92%)	143 (92%)	13 (8%)	11 40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	Y	117/121 (97%)	110 (94%)	7 (6%)	19 50
31	Z	190/202 (94%)	158 (83%)	32 (17%)	2 14
32	a	90/136 (66%)	84 (93%)	6 (7%)	16 47
33	b	100/130 (77%)	88 (88%)	12 (12%)	5 25
34	c	272/275 (99%)	233 (86%)	39 (14%)	3 19
35	d	112/115 (97%)	101 (90%)	11 (10%)	8 33
36	e	58/103 (56%)	52 (90%)	6 (10%)	7 31
37	f	123/132 (93%)	111 (90%)	12 (10%)	8 33
38	h	94/107 (88%)	81 (86%)	13 (14%)	3 21
39	i	44/49 (90%)	39 (89%)	5 (11%)	5 27
40	k	47/140 (34%)	36 (77%)	11 (23%)	1 5
41	m	104/108 (96%)	94 (90%)	10 (10%)	8 34
42	n	56/62 (90%)	47 (84%)	9 (16%)	2 15
43	o	64/277 (23%)	61 (95%)	3 (5%)	26 56
44	q	77/123 (63%)	60 (78%)	17 (22%)	1 6
45	r	247/280 (88%)	206 (83%)	41 (17%)	2 14
47	u	528/1259 (42%)	520 (98%)	8 (2%)	65 81
48	v	206/406 (51%)	198 (96%)	8 (4%)	32 60
50	x	206/494 (42%)	194 (94%)	12 (6%)	20 52
51	y	563/811 (69%)	555 (99%)	8 (1%)	67 82
All	All	6153/9370 (66%)	5627 (92%)	526 (8%)	14 40

All (526) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	9	16	LYS
10	B	15	THR
10	B	35	ARG
10	B	36	TYR
10	B	40	ILE
10	B	46	THR
10	B	69	ARG
10	B	86	ILE
10	B	103	GLU
10	B	114	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	B	118	ARG
10	B	128	VAL
10	B	152	LYS
11	C	12	VAL
11	C	33	THR
11	C	41	CYS
11	C	57	THR
11	C	102	ILE
11	C	105	THR
11	C	111	VAL
11	C	134	LYS
11	C	141	THR
11	C	143	ASP
11	C	166	THR
11	C	173	ILE
11	C	176	ASP
11	C	198	ARG
11	C	220	THR
11	C	227	VAL
11	C	232	ASN
11	C	236	ILE
11	C	248	ILE
12	D	32	ILE
12	D	65	GLU
12	D	95	ASP
12	D	102	ILE
12	D	128	VAL
12	D	138	ARG
12	D	155	LYS
12	D	177	ASN
13	E	4	CYS
13	E	11	ARG
13	E	77	ASN
13	E	82	THR
13	E	94	ILE
13	E	102	VAL
13	E	105	PHE
13	E	115	ILE
13	E	125	VAL
13	E	139	GLU
13	E	140	ARG
14	F	82	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	F	93	VAL
14	F	103	THR
15	G	19	PHE
15	G	25	GLN
15	G	29	GLU
15	G	30	LEU
15	G	33	ASN
15	G	46	THR
15	G	51	ILE
15	G	53	VAL
15	G	72	PHE
15	G	92	VAL
15	G	98	ARG
15	G	107	LYS
15	G	121	THR
15	G	166	VAL
15	G	171	GLU
15	G	180	LEU
15	G	183	LYS
15	G	185	VAL
16	H	8	LEU
16	H	13	GLU
16	H	23	ARG
16	H	26	GLN
16	H	34	ASP
16	H	35	VAL
16	H	40	CYS
16	H	53	VAL
16	H	59	CYS
16	H	61	THR
17	I	35	GLU
17	I	87	ASP
17	I	106	ARG
17	I	140	LYS
18	J	55	ASP
18	J	64	ASN
18	J	72	CYS
18	J	74	VAL
19	K	1	MET
19	K	38	GLU
19	K	39	VAL
19	K	50	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	K	52	THR
19	K	64	GLU
19	K	79	VAL
19	K	81	LYS
20	L	83	LEU
20	L	104	ASP
20	L	109	ILE
20	L	115	GLN
20	L	116	THR
20	L	120	GLN
20	L	122	THR
20	L	123	ARG
20	L	128	VAL
20	L	130	ILE
20	L	143	CYS
20	L	147	VAL
20	L	167	ARG
20	L	180	VAL
20	L	184	VAL
20	L	213	LEU
20	L	227	ARG
20	L	230	THR
20	L	236	PHE
20	L	240	THR
20	L	248	TYR
20	L	252	THR
20	L	253	PRO
20	L	254	ASP
20	L	255	LEU
20	L	259	THR
20	L	260	VAL
20	L	262	THR
20	L	270	THR
20	L	276	THR
21	M	8	THR
21	M	9	VAL
21	M	47	ARG
21	M	61	ILE
21	M	66	VAL
21	M	69	ILE
21	M	71	ILE
21	M	72	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	M	73	LEU
21	M	95	ILE
21	M	102	THR
21	M	108	LEU
21	M	110	ASP
21	M	127	ASN
22	N	5	LEU
22	N	7	VAL
22	N	11	LYS
22	N	30	LEU
22	N	33	GLN
22	N	35	GLU
22	N	87	VAL
22	N	97	THR
22	N	107	THR
22	N	111	GLN
22	N	124	VAL
22	N	131	HIS
22	N	148	CYS
22	N	177	MET
22	N	200	ASP
23	O	78	GLU
24	P	25	GLU
24	P	26	ASN
24	P	30	VAL
24	P	40	THR
24	P	42	VAL
24	P	52	THR
24	P	55	ARG
24	P	57	THR
24	P	61	LYS
24	P	62	VAL
24	P	81	VAL
24	P	88	LEU
24	P	113	GLN
24	P	116	LEU
24	P	117	ARG
24	P	121	ARG
24	P	133	THR
24	P	142	ARG
24	P	151	LEU
25	Q	7	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	Q	12	LYS
25	Q	19	GLN
25	Q	23	CYS
25	Q	40	VAL
25	Q	63	VAL
25	Q	67	LEU
25	Q	75	VAL
25	Q	84	VAL
25	Q	87	ARG
25	Q	95	ARG
26	R	29	LEU
26	R	46	VAL
26	R	53	LYS
26	R	72	CYS
26	R	96	LEU
26	R	123	ARG
26	R	133	GLU
26	R	136	ILE
26	R	138	ASN
26	R	143	LYS
26	R	158	ILE
26	R	163	GLU
26	R	174	CYS
26	R	182	CYS
27	S	1	MET
27	S	2	LYS
27	S	6	SER
27	S	7	PHE
27	S	13	GLN
27	S	19	ASP
27	S	22	ARG
27	S	30	LYS
27	S	36	VAL
27	S	69	THR
27	S	89	THR
27	S	93	LYS
27	S	97	VAL
27	S	98	ARG
27	S	100	CYS
27	S	118	GLU
27	S	119	LYS
27	S	120	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	S	125	THR
27	S	126	ASP
27	S	128	THR
27	S	144	LEU
27	S	153	VAL
27	S	171	THR
27	S	179	LEU
27	S	184	VAL
27	S	200	LYS
27	S	201	LYS
27	S	221	LYS
28	T	6	THR
28	T	8	ARG
28	T	23	MET
28	T	44	LEU
28	T	47	MET
28	T	50	THR
28	T	55	ILE
28	T	97	TYR
28	T	102	THR
28	T	104	ARG
28	T	112	ASN
28	T	124	ASN
29	V	26	ASP
29	V	29	GLN
29	V	41	VAL
29	V	59	LYS
29	V	68	ILE
29	V	81	ARG
29	V	83	ASN
29	V	91	ARG
29	V	92	ILE
29	V	126	THR
29	V	139	VAL
29	V	146	ARG
29	V	187	SER
30	Y	7	LEU
30	Y	20	THR
30	Y	81	ILE
30	Y	89	SER
30	Y	100	VAL
30	Y	101	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	Y	116	ASP
31	Z	3	VAL
31	Z	4	GLN
31	Z	26	THR
31	Z	31	GLU
31	Z	38	GLU
31	Z	42	THR
31	Z	51	LEU
31	Z	62	LYS
31	Z	66	ILE
31	Z	86	LEU
31	Z	89	GLU
31	Z	93	THR
31	Z	94	ARG
31	Z	115	VAL
31	Z	120	TYR
31	Z	123	LEU
31	Z	141	LYS
31	Z	142	LEU
31	Z	143	ARG
31	Z	154	ASP
31	Z	158	ILE
31	Z	169	ASP
31	Z	179	GLN
31	Z	181	VAL
31	Z	193	ASP
31	Z	195	THR
31	Z	205	PRO
31	Z	214	LYS
31	Z	217	ILE
31	Z	223	ILE
31	Z	225	GLU
31	Z	227	LYS
32	a	37	ASP
32	a	66	HIS
32	a	90	VAL
32	a	95	ARG
32	a	96	ARG
32	a	98	ARG
33	b	21	ASP
33	b	37	TYR
33	b	70	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	b	75	VAL
33	b	84	ILE
33	b	85	ILE
33	b	88	GLU
33	b	94	VAL
33	b	96	VAL
33	b	97	TYR
33	b	101	THR
33	b	103	ASN
34	c	6	THR
34	c	12	LYS
34	c	14	HIS
34	c	39	THR
34	c	48	ASP
34	c	64	HIS
34	c	65	PHE
34	c	89	LEU
34	c	93	THR
34	c	97	THR
34	c	99	ARG
34	c	102	VAL
34	c	107	ASP
34	c	113	PHE
34	c	116	ASP
34	c	131	LEU
34	c	132	TRP
34	c	143	GLN
34	c	144	ASP
34	c	156	PHE
34	c	159	ASN
34	c	165	ILE
34	c	168	CYS
34	c	170	TRP
34	c	186	THR
34	c	189	ILE
34	c	191	HIS
34	c	197	THR
34	c	203	ASP
34	c	207	CYS
34	c	223	GLU
34	c	227	LEU
34	c	239	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	c	265	ILE
34	c	266	ILE
34	c	267	VAL
34	c	274	VAL
34	c	287	THR
34	c	314	ILE
35	d	38	LYS
35	d	66	LEU
35	d	67	ARG
35	d	87	VAL
35	d	88	MET
35	d	96	SER
35	d	97	LYS
35	d	110	LEU
35	d	114	GLU
35	d	138	VAL
35	d	142	ASN
36	e	45	ASN
36	e	54	THR
36	e	58	LEU
36	e	78	LYS
36	e	107	VAL
36	e	110	THR
37	f	5	ILE
37	f	7	GLU
37	f	12	ILE
37	f	16	LEU
37	f	70	ILE
37	f	82	TRP
37	f	83	PHE
37	f	88	LYS
37	f	98	VAL
37	f	117	ILE
37	f	136	THR
37	f	145	THR
38	h	18	HIS
38	h	39	LEU
38	h	50	VAL
38	h	58	THR
38	h	68	THR
38	h	70	CYS
38	h	78	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	h	91	LEU
38	h	101	ILE
38	h	112	VAL
38	h	113	GLU
38	h	116	ILE
38	h	118	ASP
39	i	10	HIS
39	i	12	ARG
39	i	13	LYS
39	i	22	ARG
39	i	53	ILE
40	k	99	LYS
40	k	100	LEU
40	k	102	VAL
40	k	106	TYR
40	k	116	ARG
40	k	117	LEU
40	k	135	HIS
40	k	136	PHE
40	k	137	ASP
40	k	138	ARG
40	k	151	ASN
41	m	12	MET
41	m	50	CYS
41	m	62	VAL
41	m	66	GLU
41	m	74	ILE
41	m	91	LEU
41	m	93	LYS
41	m	117	GLU
41	m	124	ILE
41	m	127	TYR
42	n	6	VAL
42	n	9	ILE
42	n	17	VAL
42	n	28	THR
42	n	32	VAL
42	n	39	SER
42	n	46	VAL
42	n	58	LEU
42	n	62	GLU
43	o	240	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	o	245	ASN
43	o	286	SER
44	q	26	LEU
44	q	27	VAL
44	q	33	GLN
44	q	37	GLN
44	q	41	MET
44	q	46	ARG
44	q	52	PHE
44	q	65	LEU
44	q	68	LYS
44	q	79	VAL
44	q	81	LEU
44	q	84	TYR
44	q	85	GLN
44	q	103	LEU
44	q	106	TYR
44	q	109	LEU
44	q	115	ILE
45	r	7	ARG
45	r	11	HIS
45	r	24	VAL
45	r	27	ILE
45	r	33	TYR
45	r	34	VAL
45	r	36	LEU
45	r	42	ILE
45	r	49	SER
45	r	57	ARG
45	r	72	VAL
45	r	74	ILE
45	r	80	LYS
45	r	83	ILE
45	r	88	ARG
45	r	94	GLU
45	r	111	ILE
45	r	112	LEU
45	r	113	ARG
45	r	120	GLU
45	r	124	ASP
45	r	150	TYR
45	r	151	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	r	178	ASN
45	r	183	ARG
45	r	184	LEU
45	r	196	GLU
45	r	197	VAL
45	r	199	CYS
45	r	202	TYR
45	r	208	VAL
45	r	221	GLU
45	r	225	ILE
45	r	229	LEU
45	r	234	ARG
45	r	242	LEU
45	r	246	GLU
45	r	251	LEU
45	r	253	GLN
45	r	262	ILE
45	r	270	ASN
47	u	62	ARG
47	u	109	GLN
47	u	337	ASP
47	u	340	ARG
47	u	448	GLN
47	u	459	VAL
47	u	562	ARG
47	u	572	ARG
48	v	205	LEU
48	v	226	PRO
48	v	237	LEU
48	v	242	TYR
48	v	243	LEU
48	v	246	ILE
48	v	268	ARG
48	v	377	ASN
50	x	54	ARG
50	x	68	GLN
50	x	77	GLU
50	x	80	PHE
50	x	87	ARG
50	x	288	LEU
50	x	296	ASN
50	x	368	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	x	385	ASN
50	x	400	ASP
50	x	466	LEU
50	x	471	PHE
51	y	77	THR
51	y	102	VAL
51	y	116	TYR
51	y	140	THR
51	y	152	PHE
51	y	340	ARG
51	y	799	TYR
51	y	841	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
8	9	22	GLN
10	B	65	ASN
10	B	83	GLN
11	C	36	HIS
15	G	33	ASN
15	G	165	ASN
16	H	26	GLN
17	I	58	HIS
18	J	64	ASN
20	L	120	GLN
21	M	48	ASN
21	M	62	GLN
21	M	74	GLN
21	M	118	GLN
22	N	33	GLN
24	P	38	ASN
24	P	113	GLN
25	Q	72	HIS
26	R	84	ASN
26	R	138	ASN
26	R	168	GLN
27	S	177	GLN
28	T	89	HIS
28	T	112	ASN
28	T	124	ASN
29	V	51	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	V	83	ASN
29	V	165	ASN
29	V	186	ASN
30	Y	86	GLN
31	Z	4	GLN
31	Z	145	GLN
31	Z	179	GLN
32	a	61	GLN
33	b	79	HIS
33	b	103	ASN
34	c	143	GLN
34	c	159	ASN
34	c	162	ASN
34	c	237	ASN
35	d	51	ASN
36	e	45	ASN
37	f	10	GLN
38	h	28	ASN
38	h	92	HIS
39	i	26	ASN
43	o	245	ASN
44	q	37	GLN
44	q	85	GLN
44	q	112	HIS
45	r	60	ASN
45	r	270	ASN
48	v	209	GLN
48	v	241	GLN
48	v	283	GLN
48	v	373	ASN
48	v	402	GLN
50	x	68	GLN
50	x	73	HIS
50	x	296	ASN
50	x	416	GLN
50	x	456	HIS
50	x	479	GLN
51	y	597	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	w	74/75 (98%)	42 (56%)	0
6	7	21/255 (8%)	11 (52%)	3 (14%)
9	A	1708/1869 (91%)	506 (29%)	69 (4%)
All	All	1803/2199 (81%)	559 (31%)	72 (3%)

All (559) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	7	4	G
6	7	5	A
6	7	8	A
6	7	11	A
6	7	15	U
6	7	16	A
6	7	17	C
6	7	18	G
6	7	20	U
6	7	22	C
6	7	23	A
9	A	2	A
9	A	3	C
9	A	4	C
9	A	10	G
9	A	11	A
9	A	17	C
9	A	23	G
9	A	33	G
9	A	34	U
9	A	41	G
9	A	43	U
9	A	44	U
9	A	45	A
9	A	46	A
9	A	56	G
9	A	58	C
9	A	59	U
9	A	62	G
9	A	64	A
9	A	65	C
9	A	67	C
9	A	68	A
9	A	72	C
9	A	73	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	74	G
9	A	76	U
9	A	78	C
9	A	99	A
9	A	100	U
9	A	103	A
9	A	110	U
9	A	115	U
9	A	126	G
9	A	129	C
9	A	130	G
9	A	140	U
9	A	142	C
9	A	143	U
9	A	149	A
9	A	155	G
9	A	156	G
9	A	158	A
9	A	160	U
9	A	163	U
9	A	165	G
9	A	168	C
9	A	171	A
9	A	173	A
9	A	175	A
9	A	182	C
9	A	184	G
9	A	190	G
9	A	197	U
9	A	198	U
9	A	199	C
9	A	200	G
9	A	202	G
9	A	203	G
9	A	204	G
9	A	206	G
9	A	207	G
9	A	208	G
9	A	209	A
9	A	220	U
9	A	291	G
9	A	292	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	295	C
9	A	302	A
9	A	305	U
9	A	306	C
9	A	307	G
9	A	308	G
9	A	309	G
9	A	314	U
9	A	318	A
9	A	319	C
9	A	320	G
9	A	321	C
9	A	323	C
9	A	324	C
9	A	325	C
9	A	326	C
9	A	327	G
9	A	328	U
9	A	329	G
9	A	332	G
9	A	340	C
9	A	347	G
9	A	362	C
9	A	364	A
9	A	368	U
9	A	369	C
9	A	370	G
9	A	371	A
9	A	372	U
9	A	381	C
9	A	385	G
9	A	386	C
9	A	392	A
9	A	393	U
9	A	394	G
9	A	399	C
9	A	407	G
9	A	409	C
9	A	417	C
9	A	419	G
9	A	421	G
9	A	438	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	447	A
9	A	448	A
9	A	450	C
9	A	452	G
9	A	465	A
9	A	467	G
9	A	470	G
9	A	471	G
9	A	472	C
9	A	473	A
9	A	474	G
9	A	476	A
9	A	482	G
9	A	487	U
9	A	492	C
9	A	496	C
9	A	502	C
9	A	508	A
9	A	509	OMG
9	A	512	A
9	A	525	A
9	A	533	A
9	A	534	G
9	A	536	A
9	A	537	C
9	A	538	U
9	A	539	C
9	A	540	U
9	A	541	U
9	A	542	U
9	A	543	C
9	A	544	G
9	A	545	A
9	A	546	G
9	A	547	G
9	A	550	C
9	A	554	A
9	A	556	U
9	A	557	U
9	A	558	G
9	A	559	G
9	A	563	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	564	A
9	A	565	G
9	A	566	U
9	A	568	C
9	A	576	A
9	A	583	A
9	A	589	G
9	A	590	A
9	A	591	U
9	A	593	C
9	A	594	A
9	A	599	A
9	A	600	G
9	A	601	G
9	A	603	C
9	A	604	A
9	A	606	G
9	A	607	U
9	A	608	C
9	A	609	U
9	A	615	C
9	A	617	G
9	A	624	C
9	A	626	G
9	A	627	U
9	A	628	A
9	A	630	U
9	A	631	U
9	A	632	C
9	A	633	C
9	A	634	A
9	A	635	G
9	A	638	C
9	A	639	C
9	A	643	A
9	A	655	A
9	A	660	C
9	A	668	A2M
9	A	669	A
9	A	670	A
9	A	671	A
9	A	672	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	673	G
9	A	684	G
9	A	687	C
9	A	688	U
9	A	689	U
9	A	691	G
9	A	692	G
9	A	693	A
9	A	734	C
9	A	735	C
9	A	738	C
9	A	748	C
9	A	749	U
9	A	751	G
9	A	752	G
9	A	753	C
9	A	791	C
9	A	797	C
9	A	798	G
9	A	799	U
9	A	800	U
9	A	801	U
9	A	811	A
9	A	821	G
9	A	822	PSU
9	A	823	PSU
9	A	827	A
9	A	830	A
9	A	836	G
9	A	838	G
9	A	839	C
9	A	840	C
9	A	841	G
9	A	842	C
9	A	847	A
9	A	861	A
9	A	869	A
9	A	870	A
9	A	872	A
9	A	873	G
9	A	880	G
9	A	886	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	887	U
9	A	888	U
9	A	889	U
9	A	890	U
9	A	891	G
9	A	892	U
9	A	894	G
9	A	895	G
9	A	896	U
9	A	897	U
9	A	898	U
9	A	899	U
9	A	900	C
9	A	903	A
9	A	909	G
9	A	912	C
9	A	913	A
9	A	914	U
9	A	917	U
9	A	919	A
9	A	920	A
9	A	922	A
9	A	930	C
9	A	933	G
9	A	949	G
9	A	950	C
9	A	960	U
9	A	963	A
9	A	965	U
9	A	969	U
9	A	970	G
9	A	971	G
9	A	972	A
9	A	985	G
9	A	986	G
9	A	988	C
9	A	989	C
9	A	990	A
9	A	992	A
9	A	997	A
9	A	999	G
9	A	1002	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1008	A
9	A	1016	U
9	A	1017	U
9	A	1023	A
9	A	1034	A
9	A	1061	U
9	A	1062	A
9	A	1081	PSU
9	A	1083	A
9	A	1085	C
9	A	1089	G
9	A	1109	C
9	A	1112	U
9	A	1113	A
9	A	1114	U
9	A	1115	U
9	A	1116	C
9	A	1117	C
9	A	1120	U
9	A	1133	A
9	A	1138	C
9	A	1139	C
9	A	1150	A
9	A	1153	C
9	A	1154	U
9	A	1155	U
9	A	1165	G
9	A	1166	G
9	A	1170	A
9	A	1183	A
9	A	1195	A
9	A	1207	G
9	A	1208	A
9	A	1209	A
9	A	1215	C
9	A	1216	C
9	A	1217	A
9	A	1220	A
9	A	1224	G
9	A	1226	G
9	A	1240	A
9	A	1242	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1243	PSU
9	A	1250	A
9	A	1251	A
9	A	1253	A
9	A	1256	G
9	A	1257	G
9	A	1259	A
9	A	1264	C
9	A	1273	C
9	A	1274	G
9	A	1275	G
9	A	1284	A
9	A	1286	G
9	A	1287	A
9	A	1288	U
9	A	1290	G
9	A	1294	G
9	A	1295	A
9	A	1301	A
9	A	1302	G
9	A	1303	C
9	A	1308	U
9	A	1313	A
9	A	1322	G
9	A	1326	U
9	A	1332	A
9	A	1342	U
9	A	1348	G
9	A	1355	C
9	A	1357	A
9	A	1371	U
9	A	1372	U
9	A	1378	A
9	A	1397	U
9	A	1402	A
9	A	1416	C
9	A	1417	C
9	A	1418	C
9	A	1419	C
9	A	1420	G
9	A	1421	A
9	A	1422	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1423	C
9	A	1424	G
9	A	1433	C
9	A	1435	C
9	A	1436	C
9	A	1437	C
9	A	1438	A
9	A	1442	U
9	A	1446	A
9	A	1454	A
9	A	1455	A
9	A	1463	U
9	A	1464	C
9	A	1466	G
9	A	1474	A
9	A	1484	A
9	A	1487	A
9	A	1488	C
9	A	1489	A
9	A	1490	G
9	A	1497	G
9	A	1498	A
9	A	1507	G
9	A	1509	U
9	A	1510	G
9	A	1512	C
9	A	1513	C
9	A	1518	C
9	A	1519	U
9	A	1520	G
9	A	1521	C
9	A	1522	A
9	A	1523	C
9	A	1524	G
9	A	1531	A
9	A	1532	C
9	A	1533	A
9	A	1534	C
9	A	1535	U
9	A	1536	G
9	A	1538	C
9	A	1539	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1541	G
9	A	1542	C
9	A	1543	U
9	A	1552	G
9	A	1553	C
9	A	1555	U
9	A	1556	A
9	A	1557	C
9	A	1566	G
9	A	1570	G
9	A	1578	U
9	A	1580	A
9	A	1584	G
9	A	1585	U
9	A	1587	G
9	A	1588	A
9	A	1593	C
9	A	1594	A
9	A	1598	G
9	A	1601	A
9	A	1602	U
9	A	1603	G
9	A	1606	G
9	A	1618	C
9	A	1619	A
9	A	1621	U
9	A	1623	A
9	A	1624	U
9	A	1629	C
9	A	1637	A
9	A	1639	G
9	A	1643	U
9	A	1646	C
9	A	1654	G
9	A	1663	A
9	A	1665	G
9	A	1671	G
9	A	1687	C
9	A	1691	U
9	A	1692	U
9	A	1693	G
9	A	1695	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1697	A
9	A	1698	C
9	A	1699	A
9	A	1700	C
9	A	1701	C
9	A	1702	G
9	A	1715	A
9	A	1719	A
9	A	1721	U
9	A	1722	G
9	A	1733	U
9	A	1744	G
9	A	1745	A
9	A	1747	C
9	A	1750	C
9	A	1752	C
9	A	1753	C
9	A	1755	C
9	A	1756	C
9	A	1757	G
9	A	1758	G
9	A	1759	G
9	A	1760	G
9	A	1772	C
9	A	1773	C
9	A	1774	C
9	A	1775	U
9	A	1776	G
9	A	1777	G
9	A	1778	C
9	A	1779	G
9	A	1780	G
9	A	1781	A
9	A	1782	G
9	A	1783	C
9	A	1785	C
9	A	1800	A
9	A	1801	A
9	A	1805	G
9	A	1807	C
9	A	1808	U
9	A	1813	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1819	A
9	A	1820	G
9	A	1822	A
9	A	1823	A
9	A	1824	A
9	A	1825	A
9	A	1826	G
9	A	1827	U
9	A	1831	A
9	A	1832	A
9	A	1835	A
9	A	1838	U
9	A	1849	G
9	A	1861	G
9	A	1862	G
9	A	1863	A
9	A	1865	C
9	A	1867	U
9	A	1868	U
9	A	1869	A
49	w	4	A
49	w	5	G
49	w	7	G
49	w	8	U
49	w	9	G
49	w	10	G
49	w	11	C
49	w	14	A
49	w	15	G
49	w	16	C
49	w	17	G
49	w	18	G
49	w	19	A
49	w	20	A
49	w	21	G
49	w	26	C
49	w	27	U
49	w	29	G
49	w	30	G
49	w	34	A
49	w	35	U
49	w	41	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	w	43	A
49	w	44	G
49	w	45	G
49	w	46	U
49	w	47	C
49	w	48	G
49	w	51	G
49	w	52	G
49	w	55	C
49	w	56	G
49	w	57	A
49	w	58	A
49	w	59	A
49	w	60	C
49	w	62	A
49	w	64	C
49	w	71	U
49	w	73	C
49	w	74	C
49	w	75	A

All (72) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	7	3	A
6	7	4	G
6	7	17	C
9	A	1	U
9	A	43	U
9	A	72	C
9	A	203	G
9	A	291	G
9	A	306	C
9	A	307	G
9	A	368	U
9	A	369	C
9	A	371	A
9	A	392	A
9	A	557	U
9	A	563	G
9	A	589	G
9	A	593	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	606	G
9	A	614	C
9	A	630	U
9	A	670	A
9	A	797	C
9	A	838	G
9	A	839	C
9	A	840	C
9	A	861	A
9	A	868	G
9	A	912	C
9	A	985	G
9	A	1016	U
9	A	1020	A
9	A	1081	PSU
9	A	1112	U
9	A	1114	U
9	A	1119	A
9	A	1138	C
9	A	1165	G
9	A	1302	G
9	A	1341	C
9	A	1355	C
9	A	1371	U
9	A	1434	C
9	A	1488	C
9	A	1497	G
9	A	1509	U
9	A	1519	U
9	A	1520	G
9	A	1521	C
9	A	1522	A
9	A	1533	A
9	A	1542	C
9	A	1556	A
9	A	1580	A
9	A	1581	C
9	A	1587	G
9	A	1598	G
9	A	1600	G
9	A	1604	G
9	A	1637	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	A	1695	A
9	A	1700	C
9	A	1701	C
9	A	1744	G
9	A	1756	C
9	A	1757	G
9	A	1775	U
9	A	1777	G
9	A	1778	C
9	A	1781	A
9	A	1825	A
9	A	1831	A

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

26 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	$\#\|Z\| > 2$
9	PSU	A	1081	9	17,21,22	2.06	5 (29%)	20,30,33	3.67	8 (40%)
9	PSU	A	823	9	17,21,22	2.10	5 (29%)	20,30,33	3.42	7 (35%)
9	A2M	A	166	9	18,25,26	1.05	1 (5%)	18,36,39	1.26	2 (11%)
9	A2M	A	1678	9	18,25,26	1.04	0	18,36,39	1.48	3 (16%)
9	A2M	A	27	9	18,25,26	0.99	1 (5%)	18,36,39	1.30	2 (11%)
9	PSU	A	1243	9	17,21,22	2.01	5 (29%)	20,30,33	3.34	7 (35%)
9	A2M	A	159	9	18,25,26	0.95	1 (5%)	18,36,39	1.23	2 (11%)
9	MA6	A	1851	9	19,26,27	1.23	2 (10%)	18,38,41	1.93	6 (33%)
9	UR3	A	1830	9	14,22,23	1.13	2 (14%)	15,32,35	1.44	3 (20%)
9	A2M	A	668	9	18,25,26	0.98	0	18,36,39	1.54	2 (11%)
9	OMG	A	644	9	18,26,27	1.10	2 (11%)	20,38,41	2.22	8 (40%)
9	A2M	A	1031	9	18,25,26	0.98	1 (5%)	18,36,39	1.31	2 (11%)
9	PSU	A	822	9	17,21,22	1.88	5 (29%)	20,30,33	3.20	7 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	OMU	A	121	9	14,22,23	1.21	2 (14%)	14,31,34	0.85	0
9	5MU	A	814	9	15,22,23	1.31	2 (13%)	16,32,35	2.34	6 (37%)
9	PSU	A	119	9	17,21,22	2.01	5 (29%)	20,30,33	3.44	7 (35%)
9	OMC	A	517	9	15,22,23	1.08	0	17,31,34	1.46	1 (5%)
9	OMC	A	1703	9	15,22,23	1.17	2 (13%)	17,31,34	1.33	1 (5%)
9	OMG	A	509	9	18,26,27	1.14	2 (11%)	20,38,41	2.06	6 (30%)
9	OMC	A	174	9	15,22,23	1.03	0	17,31,34	1.27	1 (5%)
9	OMU	A	116	9	14,22,23	1.03	1 (7%)	14,31,34	0.78	0
9	PSU	A	612	9	17,21,22	1.95	5 (29%)	20,30,33	3.26	7 (35%)
9	MA6	A	1850	9	19,26,27	1.26	1 (5%)	18,38,41	2.01	5 (27%)
9	OMG	A	683	9	18,26,27	1.17	1 (5%)	20,38,41	2.32	6 (30%)
9	5MC	A	1374	9	15,22,23	1.56	2 (13%)	19,32,35	1.54	4 (21%)
9	A2M	A	484	9	18,25,26	1.00	1 (5%)	18,36,39	1.20	2 (11%)

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
9	PSU	A	1081	9	-	2/7/25/26	0/2/2/2
9	PSU	A	823	9	-	0/7/25/26	0/2/2/2
9	A2M	A	166	9	-	0/5/27/28	0/3/3/3
9	A2M	A	1678	9	-	0/5/27/28	0/3/3/3
9	A2M	A	27	9	-	1/5/27/28	0/3/3/3
9	PSU	A	1243	9	-	0/7/25/26	0/2/2/2
9	A2M	A	159	9	-	1/5/27/28	0/3/3/3
9	MA6	A	1851	9	-	4/7/29/30	0/3/3/3
9	UR3	A	1830	9	-	0/5/25/26	0/2/2/2
9	A2M	A	668	9	-	2/5/27/28	0/3/3/3
9	OMG	A	644	9	-	2/5/27/28	0/3/3/3
9	A2M	A	1031	9	-	1/5/27/28	0/3/3/3
9	PSU	A	822	9	-	0/7/25/26	0/2/2/2
9	OMU	A	121	9	-	0/7/27/28	0/2/2/2
9	5MU	A	814	9	-	0/5/25/26	0/2/2/2
9	PSU	A	119	9	-	1/7/25/26	0/2/2/2
9	OMC	A	517	9	-	1/7/27/28	0/2/2/2
9	OMC	A	1703	9	-	2/7/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	OMG	A	509	9	-	2/5/27/28	0/3/3/3
9	OMC	A	174	9	-	0/7/27/28	0/2/2/2
9	OMU	A	116	9	-	1/7/27/28	0/2/2/2
9	PSU	A	612	9	-	1/7/25/26	0/2/2/2
9	MA6	A	1850	9	-	1/7/29/30	0/3/3/3
9	OMG	A	683	9	-	1/5/27/28	0/3/3/3
9	5MC	A	1374	9	-	0/5/25/26	0/2/2/2
9	A2M	A	484	9	-	1/5/27/28	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	823	PSU	C5-C1'	-6.74	1.46	1.52
9	A	119	PSU	C5-C1'	-6.24	1.46	1.52
9	A	1243	PSU	C5-C1'	-6.00	1.47	1.52
9	A	612	PSU	C5-C1'	-5.72	1.47	1.52
9	A	1081	PSU	C5-C1'	-5.65	1.47	1.52
9	A	822	PSU	C5-C1'	-5.43	1.47	1.52
9	A	1374	5MC	C5-C4	4.66	1.48	1.41
9	A	683	OMG	C5-C6	3.62	1.47	1.41
9	A	509	OMG	C5-C6	3.42	1.47	1.41
9	A	644	OMG	C5-C6	3.27	1.47	1.41
9	A	1081	PSU	C5-C4	3.20	1.48	1.41
9	A	1850	MA6	C2'-C1'	-3.12	1.49	1.53
9	A	1243	PSU	C5-C4	2.98	1.47	1.41
9	A	612	PSU	C5-C4	2.97	1.47	1.41
9	A	822	PSU	C5-C4	2.97	1.47	1.41
9	A	119	PSU	C5-C4	2.93	1.47	1.41
9	A	1081	PSU	C2-N3	-2.88	1.32	1.38
9	A	1243	PSU	C2'-C1'	-2.88	1.50	1.54
9	A	612	PSU	C2'-C1'	-2.78	1.50	1.54
9	A	823	PSU	C2'-C1'	-2.76	1.50	1.54
9	A	121	OMU	C2-N3	-2.74	1.32	1.38
9	A	814	5MU	C5-C4	2.71	1.47	1.41
9	A	1081	PSU	C2'-C1'	-2.70	1.50	1.54
9	A	1081	PSU	C2-N1	-2.62	1.33	1.38
9	A	1851	MA6	C2'-C1'	-2.53	1.49	1.53
9	A	814	5MU	C2-N3	-2.51	1.33	1.38
9	A	822	PSU	C2'-C1'	-2.47	1.51	1.54
9	A	823	PSU	C2-N3	-2.46	1.33	1.38
9	A	116	OMU	C2-N3	-2.43	1.33	1.38
9	A	822	PSU	C2-N3	-2.41	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1374	5MC	C2'-C1'	-2.39	1.50	1.53
9	A	612	PSU	C2-N1	-2.38	1.33	1.38
9	A	1243	PSU	C2-N1	-2.38	1.33	1.38
9	A	159	A2M	C5-C4	2.36	1.47	1.40
9	A	119	PSU	C2'-C1'	-2.34	1.51	1.54
9	A	119	PSU	C2-N3	-2.31	1.33	1.38
9	A	822	PSU	C2-N1	-2.31	1.33	1.38
9	A	166	A2M	C5-C4	2.31	1.47	1.40
9	A	612	PSU	C2-N3	-2.30	1.33	1.38
9	A	119	PSU	C2-N1	-2.29	1.33	1.38
9	A	823	PSU	C5-C4	2.22	1.46	1.41
9	A	121	OMU	C6-N1	-2.21	1.33	1.35
9	A	509	OMG	C5-C4	2.21	1.46	1.40
9	A	1243	PSU	C2-N3	-2.21	1.33	1.38
9	A	823	PSU	C2-N1	-2.18	1.33	1.38
9	A	1703	OMC	C6-N1	-2.18	1.33	1.35
9	A	1703	OMC	C2-N3	-2.16	1.33	1.38
9	A	484	A2M	C5-C4	2.15	1.46	1.40
9	A	1830	UR3	C6-N1	-2.13	1.33	1.35
9	A	1830	UR3	C2'-C1'	-2.13	1.50	1.53
9	A	1031	A2M	C5-C4	2.13	1.46	1.40
9	A	1851	MA6	C5-C4	2.12	1.46	1.40
9	A	644	OMG	C5-C4	2.05	1.46	1.40
9	A	27	A2M	C5-C4	2.01	1.46	1.40

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	612	PSU	N3-C2-N1	-8.21	121.91	128.43
9	A	1243	PSU	N3-C2-N1	-8.14	121.96	128.43
9	A	823	PSU	N3-C2-N1	-8.05	122.03	128.43
9	A	119	PSU	N3-C2-N1	-8.00	122.07	128.43
9	A	1081	PSU	N3-C2-N1	-7.50	122.47	128.43
9	A	119	PSU	C5-C1'-C2'	-7.44	102.05	115.32
9	A	822	PSU	N3-C2-N1	-7.36	122.58	128.43
9	A	823	PSU	C2-N3-C4	7.01	121.06	115.14
9	A	1081	PSU	C5-C1'-C2'	-7.00	102.83	115.32
9	A	1081	PSU	C2-N3-C4	6.88	120.95	115.14
9	A	1243	PSU	C2-N3-C4	6.75	120.84	115.14
9	A	612	PSU	C2-N3-C4	6.65	120.75	115.14
9	A	814	5MU	C2-N3-C4	6.49	120.62	115.14
9	A	823	PSU	C5-C1'-C2'	-6.31	104.06	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	822	PSU	C2-N3-C4	5.93	120.15	115.14
9	A	119	PSU	C2-N3-C4	5.78	120.02	115.14
9	A	1081	PSU	C3'-C2'-C1'	5.74	108.54	101.93
9	A	1081	PSU	C5-C4-N3	-5.61	118.14	125.36
9	A	1243	PSU	C5-C1'-C2'	-5.54	105.43	115.32
9	A	612	PSU	C5-C4-N3	-5.46	118.33	125.36
9	A	823	PSU	C5-C4-N3	-5.44	118.35	125.36
9	A	1243	PSU	C5-C4-N3	-5.43	118.36	125.36
9	A	822	PSU	C5-C4-N3	-5.16	118.71	125.36
9	A	822	PSU	C5-C1'-C2'	-5.15	106.13	115.32
9	A	683	OMG	C2-N3-C4	5.02	121.09	115.36
9	A	119	PSU	C5-C4-N3	-4.90	119.05	125.36
9	A	644	OMG	C2-N3-C4	4.72	120.74	115.36
9	A	822	PSU	C5-C6-N1	-4.62	118.76	124.44
9	A	119	PSU	C5-C6-N1	-4.54	118.86	124.44
9	A	1081	PSU	C5-C6-N1	-4.53	118.87	124.44
9	A	509	OMG	C2-N3-C4	4.32	120.30	115.36
9	A	612	PSU	C5-C1'-C2'	-4.32	107.61	115.32
9	A	119	PSU	C6-N1-C2	4.32	122.49	115.36
9	A	509	OMG	C5-C6-N1	-4.27	117.58	123.43
9	A	1850	MA6	C9-N6-C6	-4.25	106.64	119.51
9	A	683	OMG	C5-C6-N1	-4.19	117.70	123.43
9	A	517	OMC	C4-N3-C2	4.11	120.51	116.34
9	A	823	PSU	C5-C6-N1	-4.10	119.40	124.44
9	A	822	PSU	C6-N1-C2	4.06	122.06	115.36
9	A	1243	PSU	C5-C6-N1	-4.03	119.48	124.44
9	A	1081	PSU	C6-N1-C2	4.01	121.97	115.36
9	A	612	PSU	C6-N1-C2	3.99	121.95	115.36
9	A	644	OMG	C2-N1-C6	3.99	122.27	115.93
9	A	644	OMG	C5-C6-N1	-3.99	117.98	123.43
9	A	1243	PSU	C6-N1-C2	3.97	121.90	115.36
9	A	683	OMG	C2-N1-C6	3.95	122.20	115.93
9	A	612	PSU	C5-C6-N1	-3.89	119.66	124.44
9	A	1243	PSU	C3'-C2'-C1'	3.79	106.31	101.93
9	A	119	PSU	C3'-C2'-C1'	3.77	106.28	101.93
9	A	509	OMG	C2-N1-C6	3.74	121.87	115.93
9	A	683	OMG	C4-C5-C6	-3.69	117.28	120.80
9	A	644	OMG	C4-C5-C6	-3.62	117.34	120.80
9	A	1703	OMC	C4-N3-C2	3.62	120.01	116.34
9	A	823	PSU	C6-N1-C2	3.61	121.31	115.36
9	A	174	OMC	C4-N3-C2	3.57	119.96	116.34
9	A	822	PSU	C3'-C2'-C1'	3.56	106.04	101.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1830	UR3	O3'-C3'-C2'	-3.55	100.35	111.82
9	A	612	PSU	C3'-C2'-C1'	3.54	106.02	101.93
9	A	1850	MA6	N3-C2-N1	-3.46	123.27	128.68
9	A	1851	MA6	C9-N6-C6	-3.37	109.32	119.51
9	A	1851	MA6	N1-C6-N6	3.34	120.57	117.06
9	A	166	A2M	N3-C2-N1	-3.26	123.58	128.68
9	A	683	OMG	N3-C2-N1	-3.22	122.92	127.22
9	A	1678	A2M	N3-C2-N1	-3.22	123.64	128.68
9	A	644	OMG	N3-C2-N1	-3.21	122.94	127.22
9	A	1851	MA6	C10-N6-C6	-3.19	109.85	119.51
9	A	1850	MA6	N1-C6-N6	3.19	120.41	117.06
9	A	814	5MU	C3'-C2'-C1'	3.18	105.77	100.98
9	A	668	A2M	N3-C2-N1	-3.16	123.74	128.68
9	A	1850	MA6	C10-N6-C6	-3.12	110.05	119.51
9	A	683	OMG	C4-C5-N7	-3.08	106.19	109.40
9	A	27	A2M	C4-C5-N7	-3.06	106.21	109.40
9	A	1374	5MC	C5-C6-N1	-3.06	118.90	122.19
9	A	1850	MA6	C3'-C2'-C1'	3.03	105.54	100.98
9	A	27	A2M	N3-C2-N1	-3.01	123.98	128.68
9	A	1374	5MC	C3'-C2'-C1'	3.00	105.50	100.98
9	A	1851	MA6	N3-C2-N1	-3.00	123.99	128.68
9	A	1031	A2M	N3-C2-N1	-2.99	124.00	128.68
9	A	509	OMG	C4-C5-C6	-2.96	117.97	120.80
9	A	823	PSU	C3'-C2'-C1'	2.92	105.30	101.93
9	A	1031	A2M	C4-C5-N7	-2.90	106.38	109.40
9	A	1374	5MC	C4-N3-C2	2.87	119.48	116.02
9	A	159	A2M	N3-C2-N1	-2.84	124.23	128.68
9	A	668	A2M	C4-C5-N7	-2.84	106.44	109.40
9	A	814	5MU	O4'-C1'-C2'	-2.76	102.89	106.93
9	A	509	OMG	C4-C5-N7	-2.71	106.57	109.40
9	A	814	5MU	O2'-C2'-C3'	-2.67	103.17	111.82
9	A	166	A2M	C4-C5-N7	-2.66	106.62	109.40
9	A	1678	A2M	C4-C5-N7	-2.64	106.65	109.40
9	A	644	OMG	C4-C5-N7	-2.55	106.74	109.40
9	A	159	A2M	C4-C5-N7	-2.48	106.82	109.40
9	A	1081	PSU	O4'-C1'-C5	2.45	113.72	109.93
9	A	484	A2M	N3-C2-N1	-2.44	124.86	128.68
9	A	1374	5MC	N4-C4-N3	2.42	120.45	117.03
9	A	484	A2M	C4-C5-N7	-2.42	106.88	109.40
9	A	509	OMG	N3-C2-N1	-2.39	124.03	127.22
9	A	814	5MU	C5-C6-N1	-2.33	119.68	122.19
9	A	644	OMG	O2'-C2'-C1'	-2.28	104.56	109.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1851	MA6	C4-C5-N7	-2.25	107.06	109.40
9	A	1678	A2M	O2'-C2'-C1'	-2.22	104.70	109.09
9	A	1830	UR3	O4'-C1'-C2'	-2.19	103.72	106.93
9	A	814	5MU	C2'-C3'-C4'	-2.19	98.40	102.64
9	A	644	OMG	CM2-O2'-C2'	-2.12	108.97	114.52
9	A	1851	MA6	C1'-N9-C4	-2.12	122.92	126.64
9	A	1830	UR3	C3U-N3-C4	2.10	120.90	118.12

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	27	A2M	C1'-C2'-O2'-CM'
9	A	116	OMU	C1'-C2'-O2'-CM2
9	A	159	A2M	C1'-C2'-O2'-CM'
9	A	484	A2M	C1'-C2'-O2'-CM'
9	A	517	OMC	C1'-C2'-O2'-CM2
9	A	644	OMG	C1'-C2'-O2'-CM2
9	A	668	A2M	O4'-C4'-C5'-O5'
9	A	668	A2M	C3'-C4'-C5'-O5'
9	A	1031	A2M	C1'-C2'-O2'-CM'
9	A	1703	OMC	C1'-C2'-O2'-CM2
9	A	1851	MA6	O4'-C4'-C5'-O5'
9	A	1851	MA6	C3'-C4'-C5'-O5'
9	A	683	OMG	C1'-C2'-O2'-CM2
9	A	509	OMG	O4'-C4'-C5'-O5'
9	A	1851	MA6	C5-C6-N6-C9
9	A	509	OMG	C3'-C4'-C5'-O5'
9	A	1850	MA6	C5-C6-N6-C9
9	A	1851	MA6	C4'-C5'-O5'-P
9	A	1081	PSU	C4'-C5'-O5'-P
9	A	612	PSU	O4'-C4'-C5'-O5'
9	A	119	PSU	O4'-C4'-C5'-O5'
9	A	1703	OMC	O4'-C4'-C5'-O5'
9	A	1081	PSU	O4'-C4'-C5'-O5'
9	A	644	OMG	C4'-C5'-O5'-P

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 2 ligands modelled in this entry, 2 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.

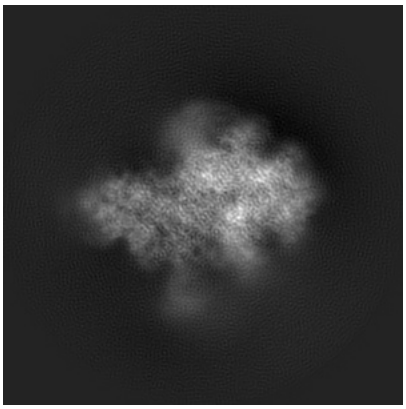
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14114. These allow visual inspection of the internal detail of the map and identification of artifacts.

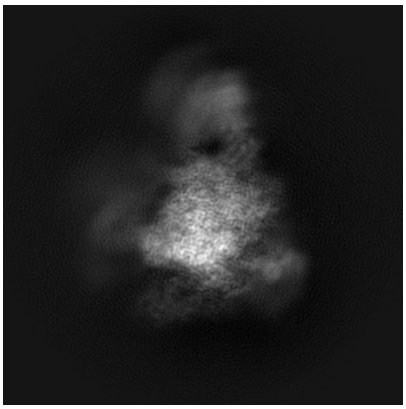
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

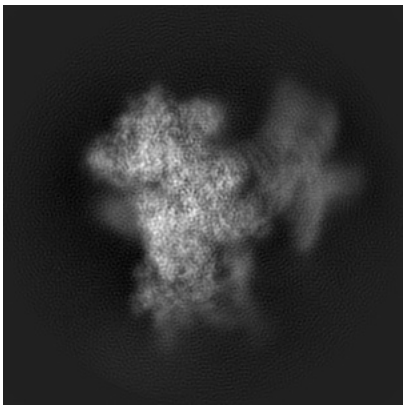
6.1.1 Primary map



X

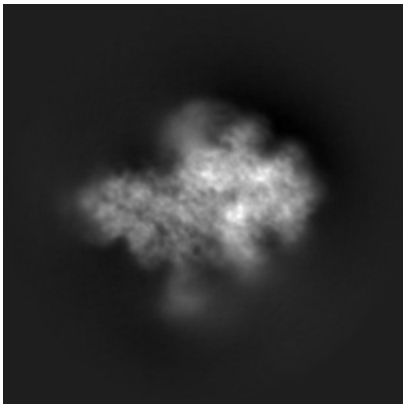


Y

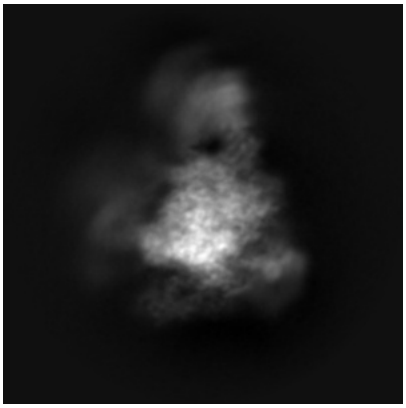


Z

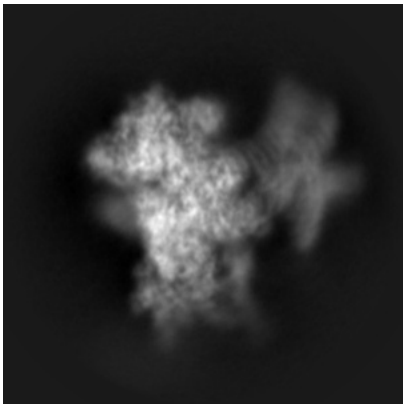
6.1.2 Raw map



X



Y

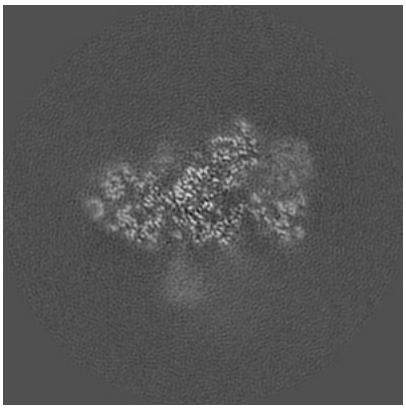


Z

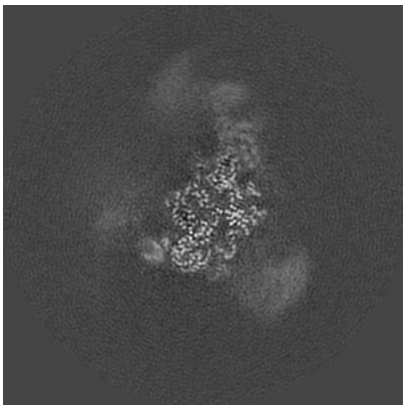
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

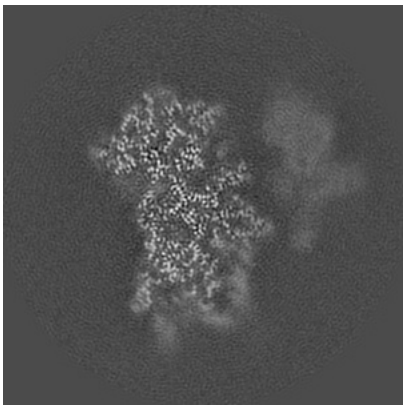
6.2.1 Primary map



X Index: 180

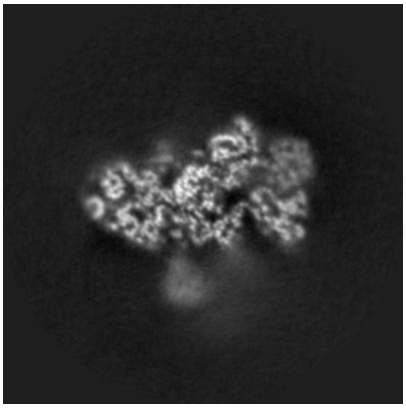


Y Index: 180

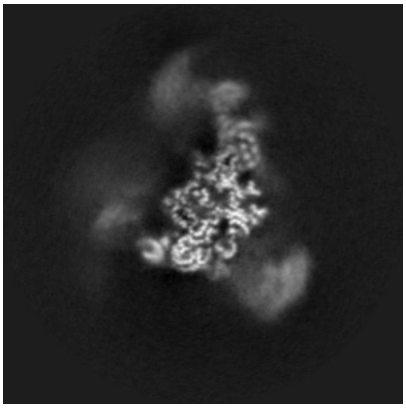


Z Index: 180

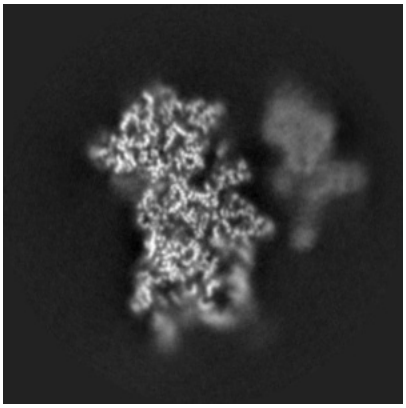
6.2.2 Raw map



X Index: 180



Y Index: 180

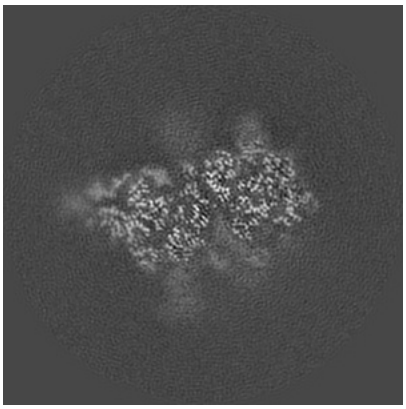


Z Index: 180

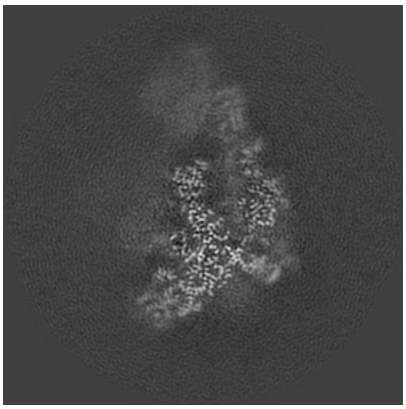
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

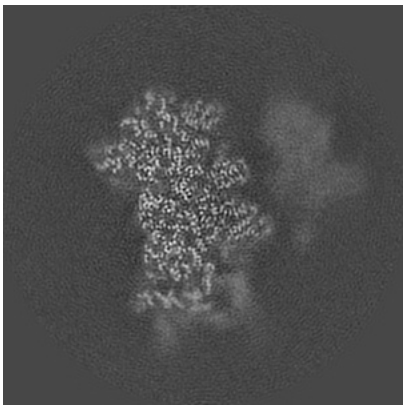
6.3.1 Primary map



X Index: 149

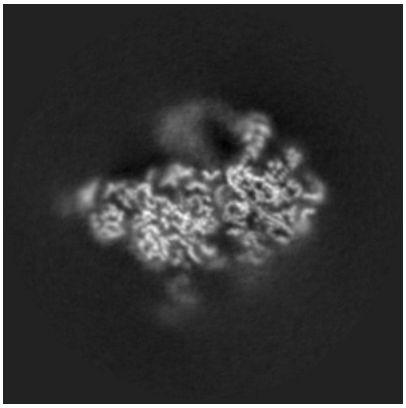


Y Index: 213

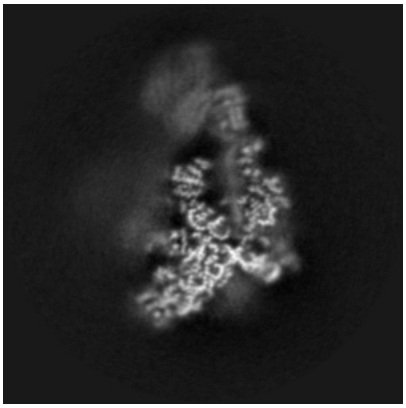


Z Index: 176

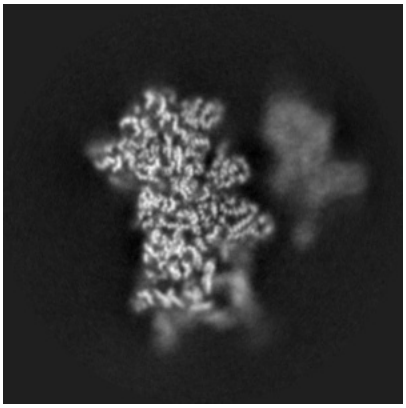
6.3.2 Raw map



X Index: 139



Y Index: 213



Z Index: 176

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

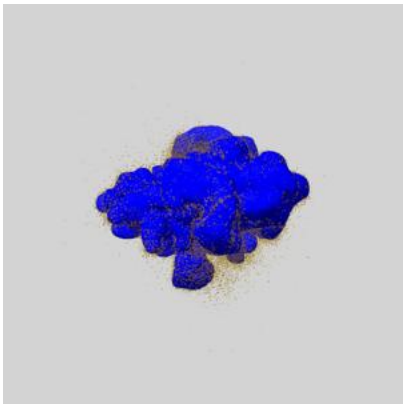
6.5 Mask visualisation (i)

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

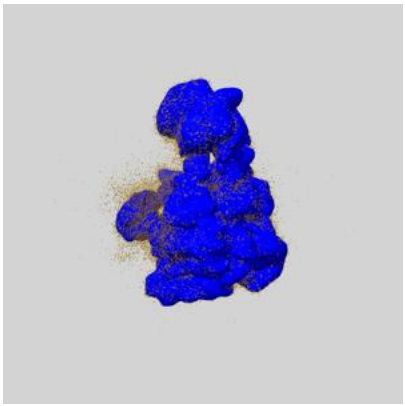
A mask typically either:

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

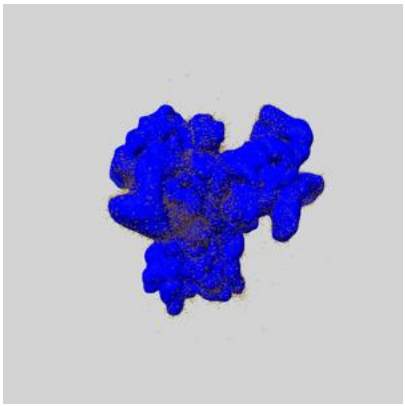
6.5.1 emd_14114_msk_1.map (i)



X



Y

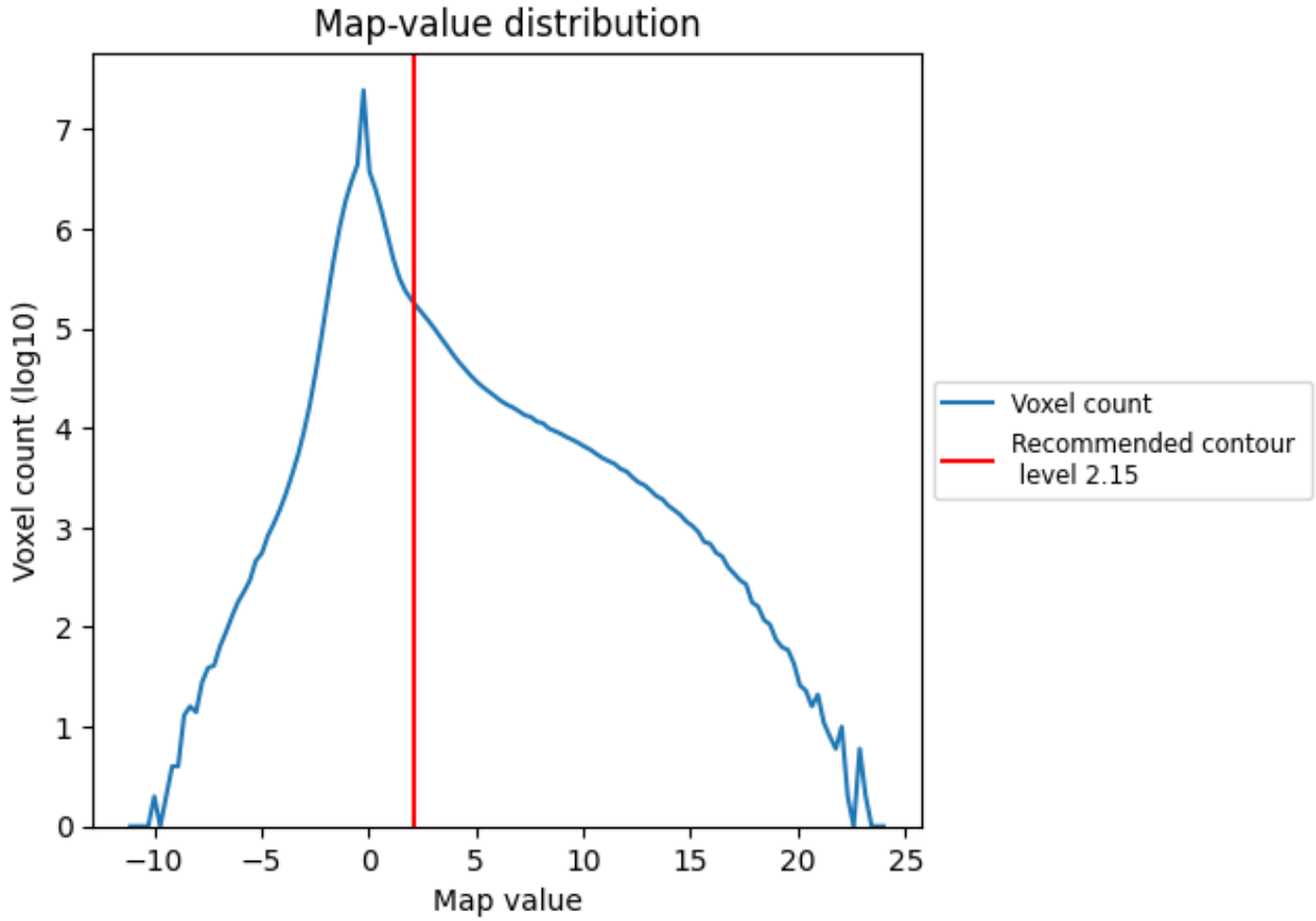


Z

7 Map analysis

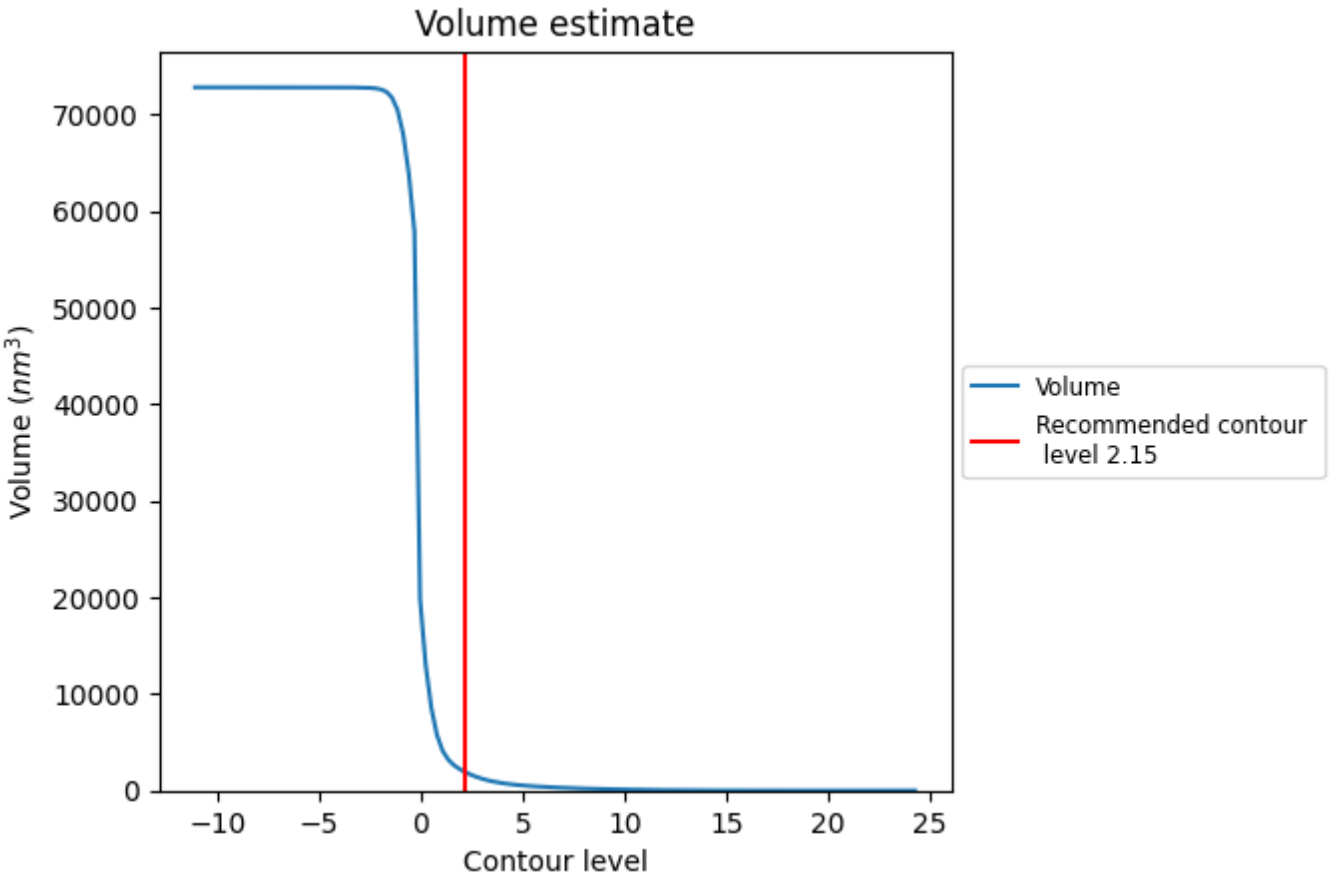
This section contains the results of statistical analysis of the map.

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.

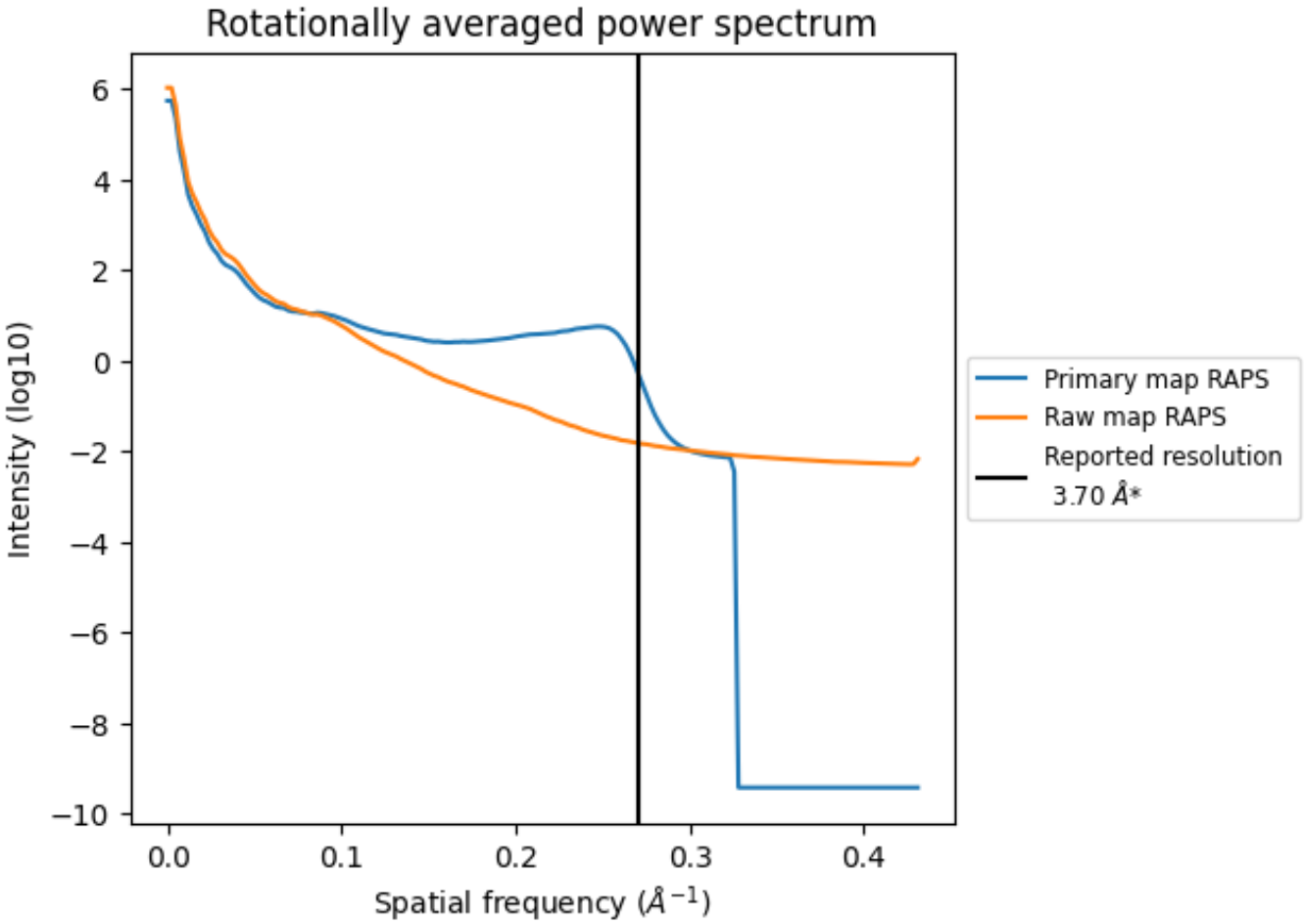
7.2 Volume estimate



The volume at the recommended contour level is 1935 nm^3; this corresponds to an approximate mass of 1748 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)

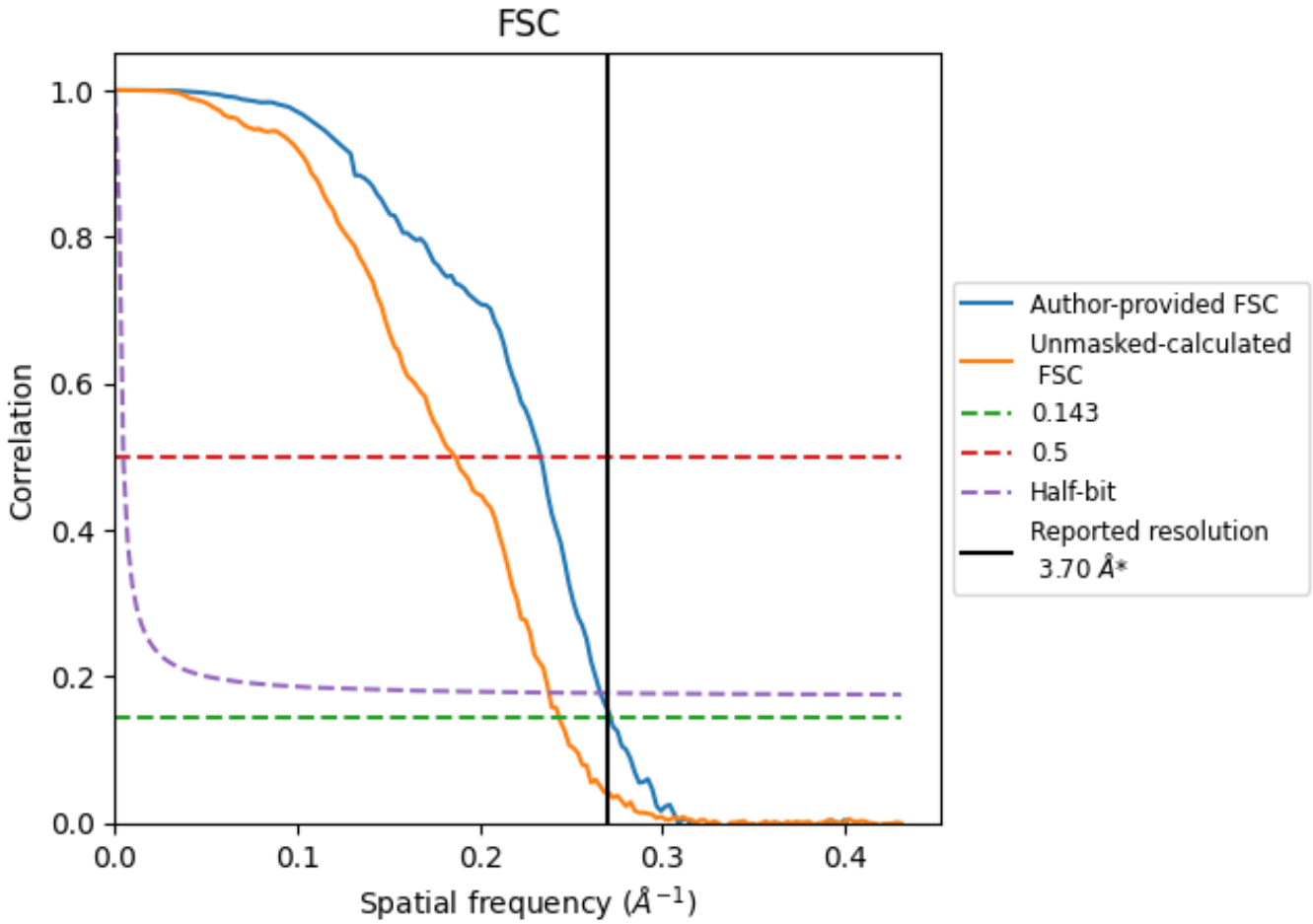


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

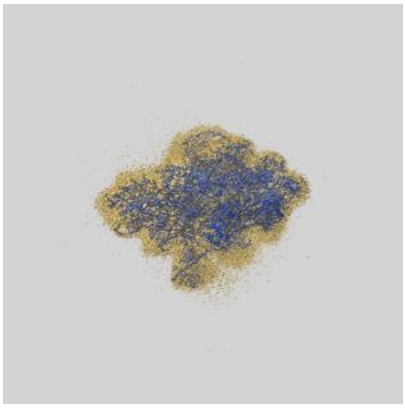
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.29	3.76
Unmasked-calculated*	4.11	5.36	4.20

*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 4.11 differs from the reported value 3.7 by more than 10 %

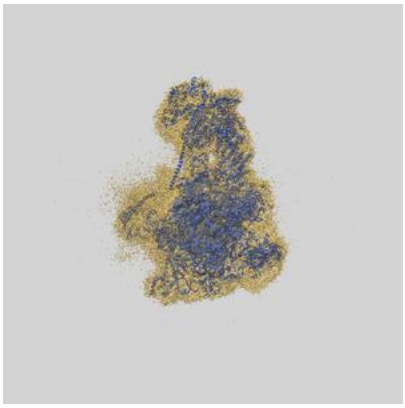
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14114 and PDB model 7QP7. Per-residue inclusion information can be found in section 3 on page 13.

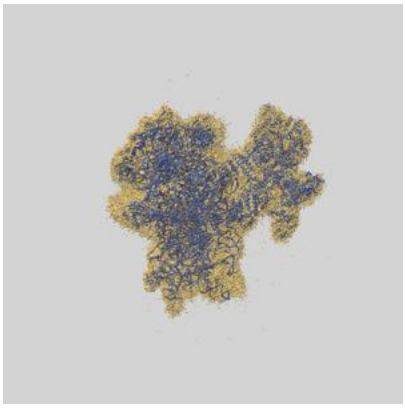
9.1 Map-model overlay



X



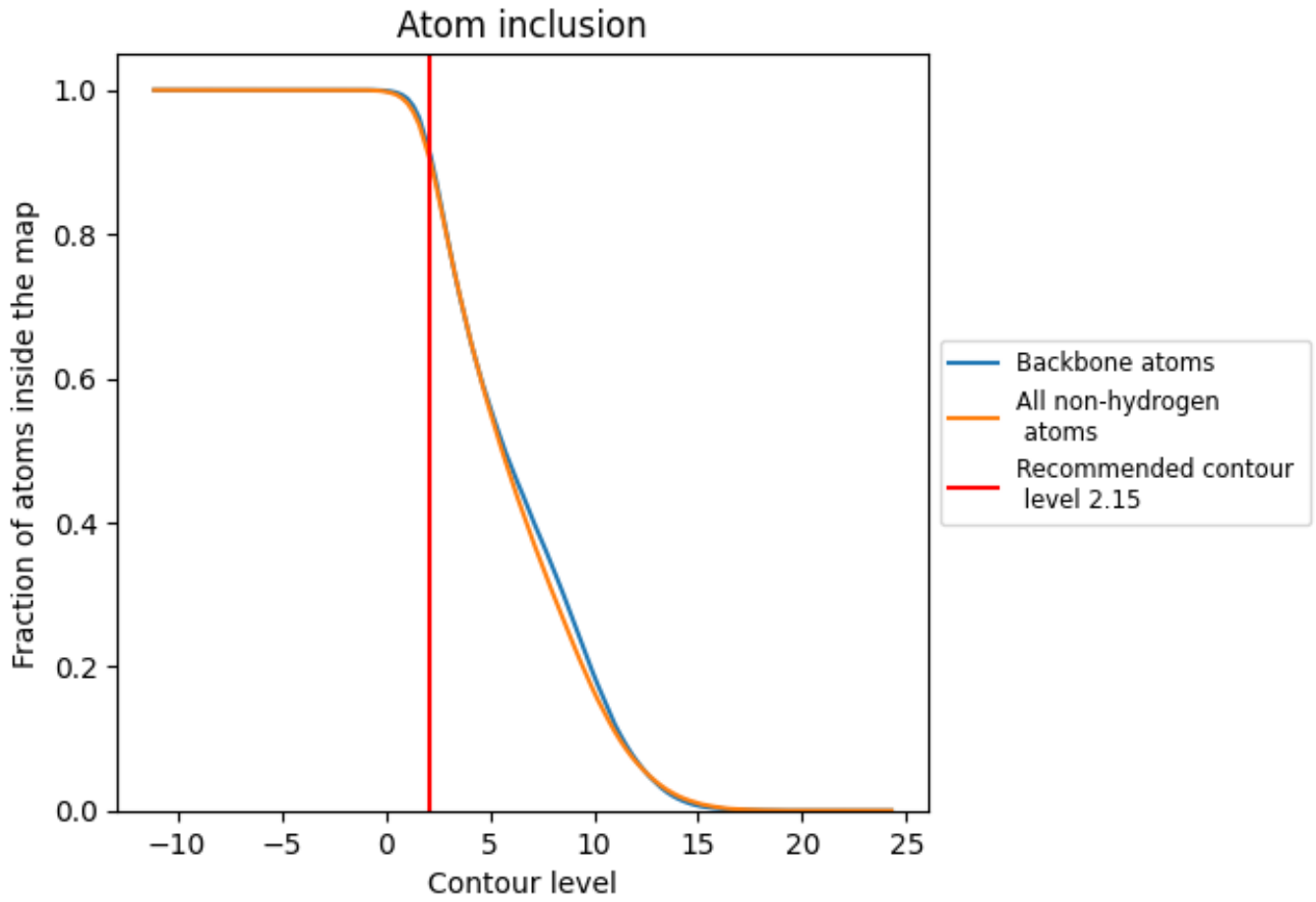
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.15 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 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.