



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:10 AM UTC

PDB ID : 7A09 / pdb_00007a09
EMDB ID : EMD-11602
Title : Structure of a human ABCE1-bound 43S pre-initiation complex - State III
Authors : Kratzat, H.; Mackens-Kiani, T.; Ameismeier, A.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2020-08-07
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

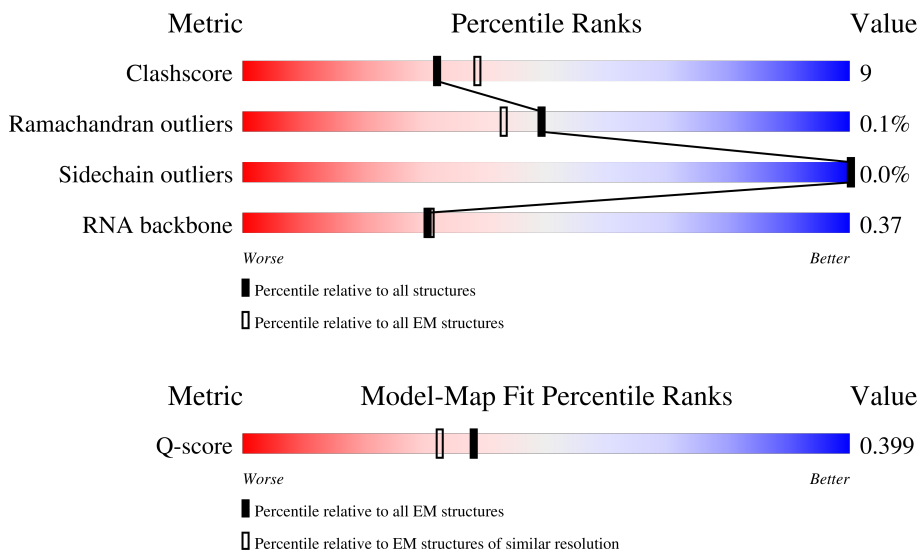
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	a	295	
2	p	264	
3	d	293	

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Mol	Chain	Length	Quality of chain
4	Q	115	77% 11% 12%
5	q	263	83% 14%
6	W	25	72% 24%
7	r	249	69% 20% 11%
8	s	194	68% 22% 11%
9	t	208	77% 18%
10	c	194	76% 16% 7%
11	n	158	73% 13% 15%
12	m	151	85% 13%
13	y	83	86% 13%
14	D	130	85% 14%
15	z	131	71% 22% 7%
16	R	84	86% 12%
17	T	59	69% 5% 25%
18	2	1721	55% 37% 8%
19	w	135	70% 24% 5%
20	b	243	70% 22% 8%
21	e	204	75% 18% 7%
22	u	165	7% 36% 22% 42%
23	v	132	36% 58% 26% 16%
24	o	145	17% 55% 27% 18%
25	g	146	73% 21% 5%
26	k	152	5% 60% 32% 8%
27	x	145	70% 27%
28	h	119	5% 54% 28% 18%


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Mol	Chain	Length	Quality of chain
29	P	125	
30	S	69	
31	l	56	
32	U	156	
33	V	317	
34	i	151	
35	j	143	
36	G	112	
37	I	325	
38	B	814	
39	A	1382	
40	C	921	
41	E	445	
42	F	357	
43	H	352	
44	K	218	
45	L	564	
46	M	374	
47	J	599	
48	N	548	
49	X	78	
50	f	75	
51	4	333	
52	O	315	
53	Y	472	

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Mol	Chain	Length	Quality of chain
54	Z	113	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '16%', a green segment in the middle labeled '75%', and a yellow segment on the right labeled '22%'. A small grey dot is visible at the far right end of the bar.</p>

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 122168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	216	1705	1083	299	315	8	0	0

- Molecule 2 is a protein called 40S ribosomal protein S3a.

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

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	216	1674	1085	287	292	10	0	0

- Molecule 4 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	Q	101	814	507	170	132	5	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	q	255	2031	1299	377	347	8	0	0

- Molecule 6 is a protein called 60S ribosomal protein L41.

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

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	r	222	1794	1123	357	308	6	0	0

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	s	173	1399	898	256	244	1	0	0

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	t	199	1638	1027	322	284	5	0	0

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	c	180	1499	955	300	242	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	n	135	1119	715	211	187	6	0	0

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	m	149	1202	770	228	203	1	0	0

- Molecule 13 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	y	82	625	384	116	120	5	0	0

- Molecule 14 is a protein called 40S ribosomal protein S15a.

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

- Molecule 15 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	z	122	Total	C	N	O	S	0	0
			999	633	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 17 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	44	Total	C	N	O	S	0	0
			354	216	81	56	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	1721	Total	C	N	O	P	0	0
			36717	16400	6603	12003	1711		

- Molecule 19 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	w	128	Total	C	N	O	S	0	0
			1011	641	182	184	4		

- Molecule 20 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	224	Total	C	N	O	S	0	0
			1745	1112	314	312	7		

- Molecule 21 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 22 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	u	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

- Molecule 23 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	v	111	Total	C	N	O	S	0	0
			861	544	151	159	7		

- Molecule 24 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	o	119	Total	C	N	O	S	0	0
			980	623	183	167	7		

- Molecule 25 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	g	138	Total	C	N	O	S	0	0
			1100	699	208	190	3		

- Molecule 26 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	k	140	Total	C	N	O	S	0	0
			1162	731	234	196	1		

- Molecule 27 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	x	141	Total	C	N	O	S	0	0
			1094	685	210	196	3		

- Molecule 28 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	h	98	780	489	148	139	4	0	0

- Molecule 29 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	P	70	557	358	101	97	1	0	0

- Molecule 30 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	S	61	479	292	95	90	2	0	0

- Molecule 31 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	l	54	450	282	93	70	5	0	0

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	U	57	465	295	89	74	7	0	0

- Molecule 33 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	V	296	2314	1464	404	434	12	0	0

- Molecule 34 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	125	939	574	187	172	6	0	0

- Molecule 35 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	G	88	Total	C	N	O	S	0	0
			712	451	129	128	4		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	I	305	Total	C	N	O	S	0	0
			1497	887	305	305			

- Molecule 38 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B	536	Total	C	N	O	S	0	0
			2966	1801	580	580	5		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A	692	Total	C	N	O	S	0	0
			5385	3379	980	1004	22		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit C, Eukaryotic translation initiation factor 3 subunit C, Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	C	633	Total	C	N	O	S	0	0
			5113	3229	907	942	35		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	E	416	Total	C	N	O	S	0	0
			3437	2202	585	630	20		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	F	269	2090	1317	356	405	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	H	295	2413	1532	417	449	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	K	217	1750	1116	288	334	12	0	0

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	L	372	3111	2011	520	563	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	M	340	2718	1734	459	508	17	0	0

- Molecule 47 is a protein called ATP-binding cassette sub-family E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	J	576	4541	2899	779	835	28	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	N	447	3617	2279	625	691	22	0	0

- Molecule 49 is a protein called RNA recognition motif.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	X	78	Total	C	N	O	0	0
			390	234	78	78		

- Molecule 50 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	f	75	Total	C	N	O	P	0	0
			1603	717	298	514	74		

- Molecule 51 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	144	Total	C	N	O	S	0	0
			1080	679	202	192	7		

- Molecule 52 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

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

- Molecule 53 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Y	414	Total	C	N	O	0	0
			2156	1296	433	427		

- Molecule 54 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Z	110	Total	C	N	O	S	0	0
			830	524	150	154	2		

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

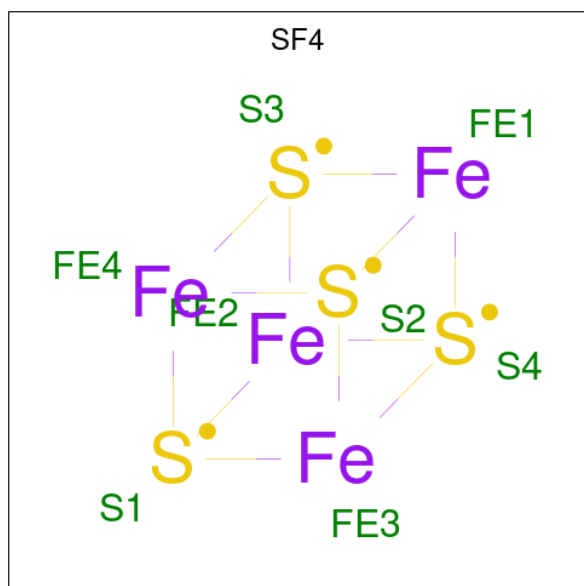
Mol	Chain	Residues	Atoms		AltConf
55	Q	1	Total	Zn	0
			1	1	
55	l	1	Total	Zn	0
			1	1	
55	U	1	Total	Zn	0
			1	1	

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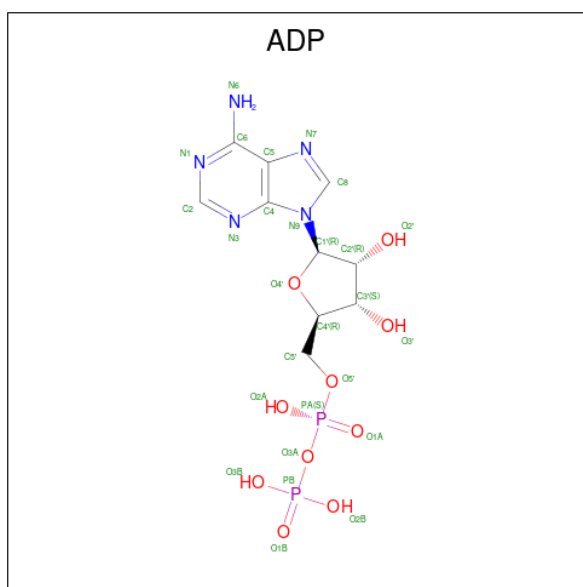
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	4	1	1	1	0

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
56	J	1	8	4	4	0
56	J	1	Total	Fe	S	0
			8	4	4	

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

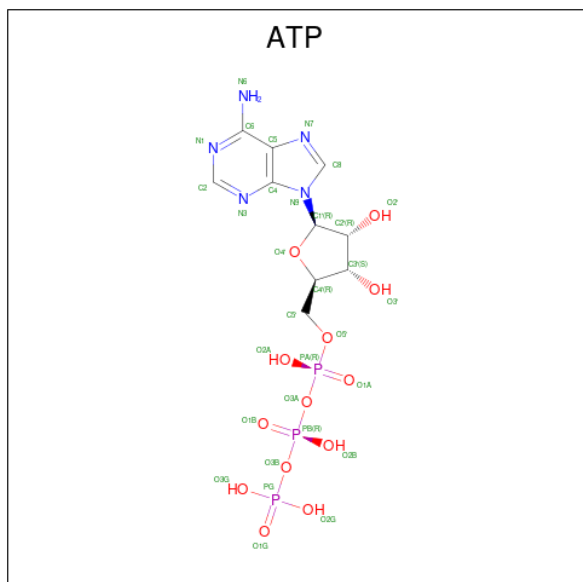


Mol	Chain	Residues	Atoms					AltConf
57	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

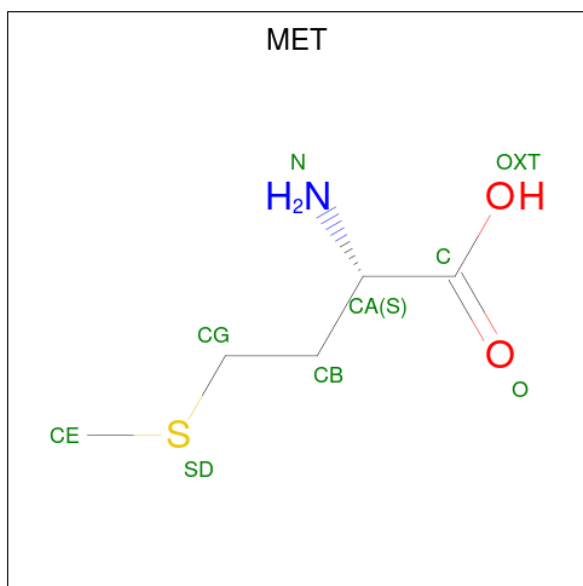
Mol	Chain	Residues	Atoms		AltConf
58	J	2	Total	Mg	0
			2	2	
58	Y	1	Total	Mg	0
			1	1	

- Molecule 59 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



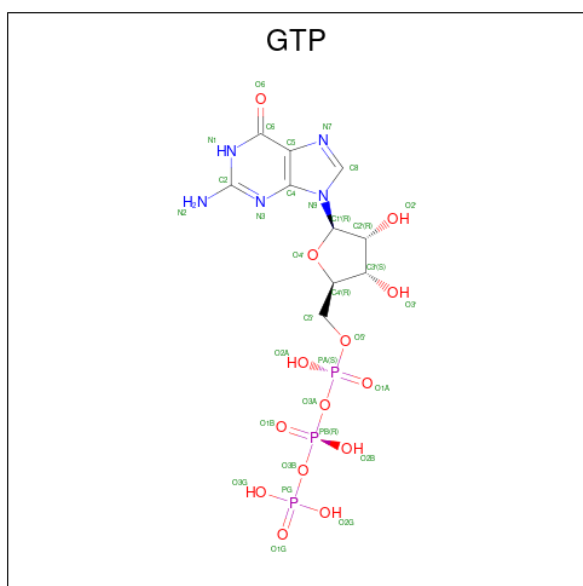
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	J	1	31	10	5	13	3	0

- Molecule 60 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).

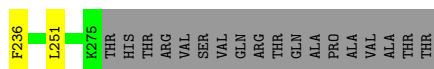


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	f	1	8	5	1	1	1	0

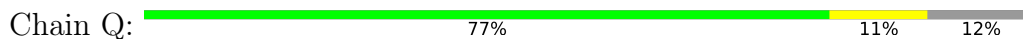
- Molecule 61 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



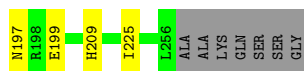
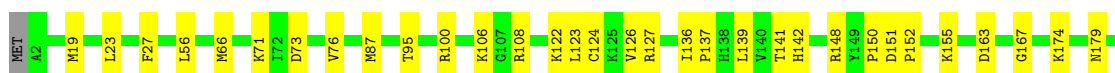
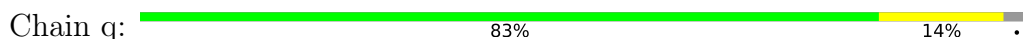
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
61	Y	1	32	10	5	14	3	0



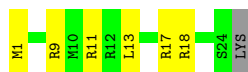
- Molecule 4: 40S ribosomal protein S26



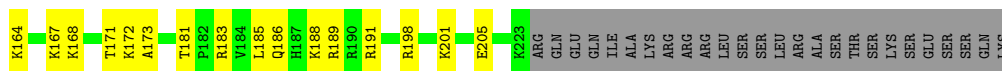
- Molecule 5: 40S ribosomal protein S4, X isoform



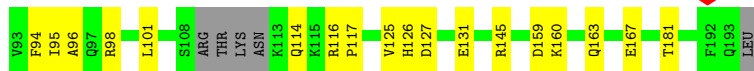
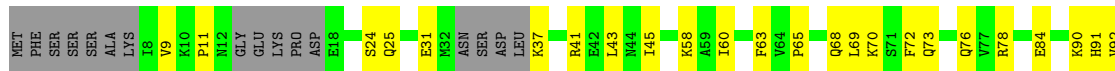
- Molecule 6: 60S ribosomal protein L41




- Molecule 7: 40S ribosomal protein S6

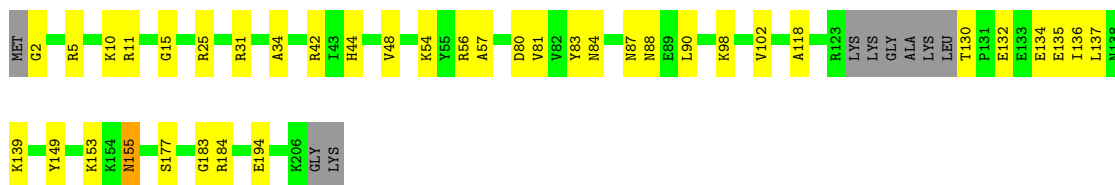


- Molecule 8: 40S ribosomal protein S7




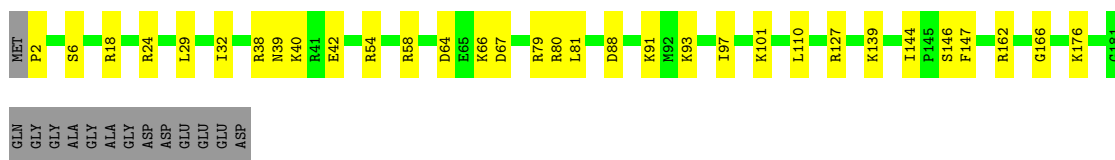
- Molecule 9: 40S ribosomal protein S8

Chain t:  77% 18%



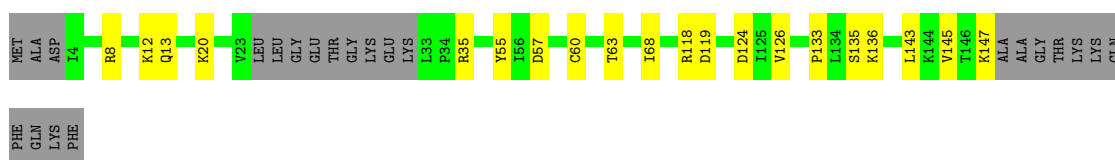
• Molecule 10: 40S ribosomal protein S9

Chain c:  76% 16% 7%




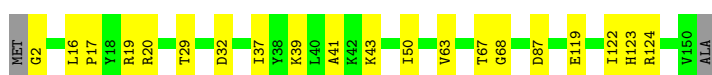
• Molecule 11: 40S ribosomal protein S11

Chain n:  73% 13% 15%




• Molecule 12: 40S ribosomal protein S13

Chain m:  85% 13%



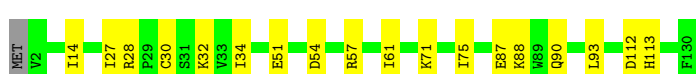
• Molecule 13: 40S ribosomal protein S21

Chain y:  86% 13%



• Molecule 14: 40S ribosomal protein S15a

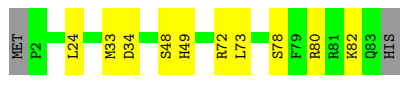
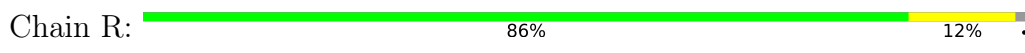
Chain D:  85% 14%



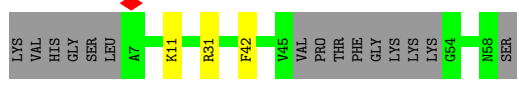
• Molecule 15: 40S ribosomal protein S24



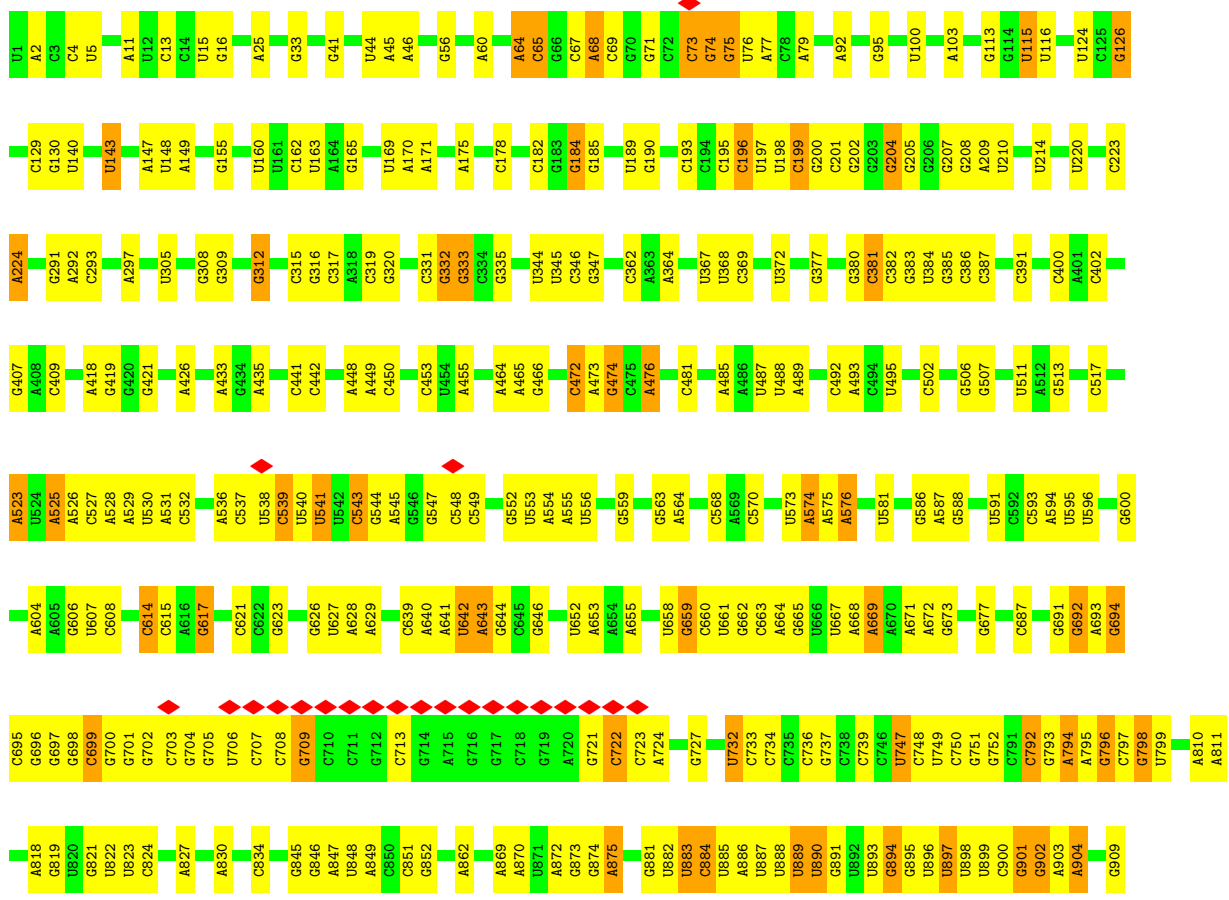
• Molecule 16: 40S ribosomal protein S27

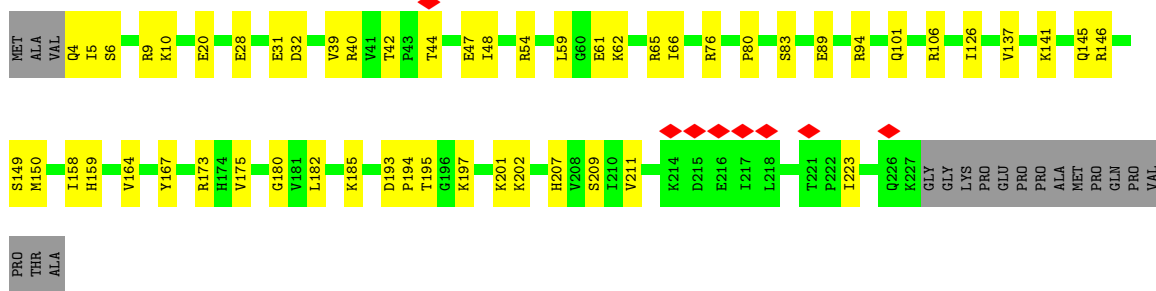


• Molecule 17: 40S ribosomal protein S30

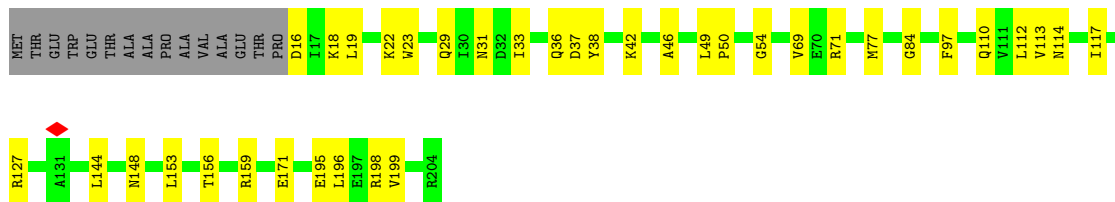


• Molecule 18: 18S ribosomal RNA

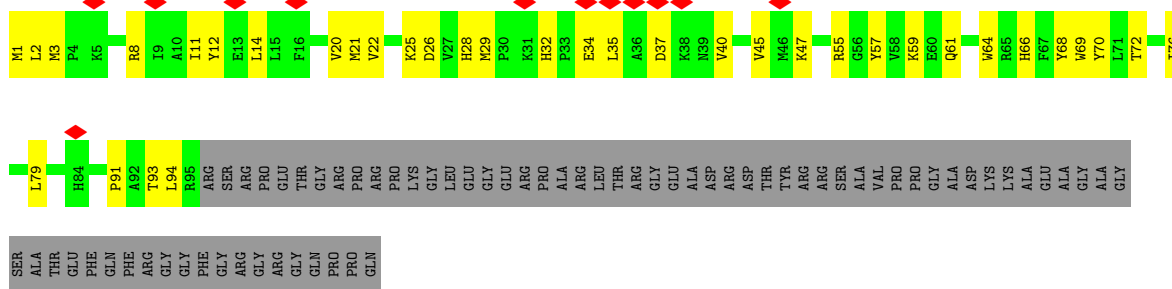
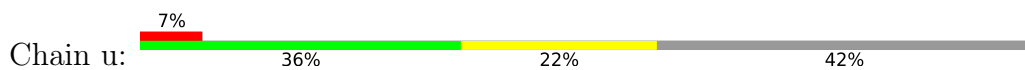




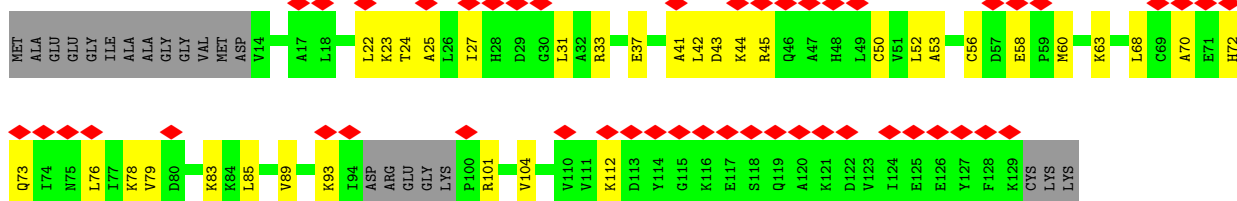
- Molecule 21: 40S ribosomal protein S5



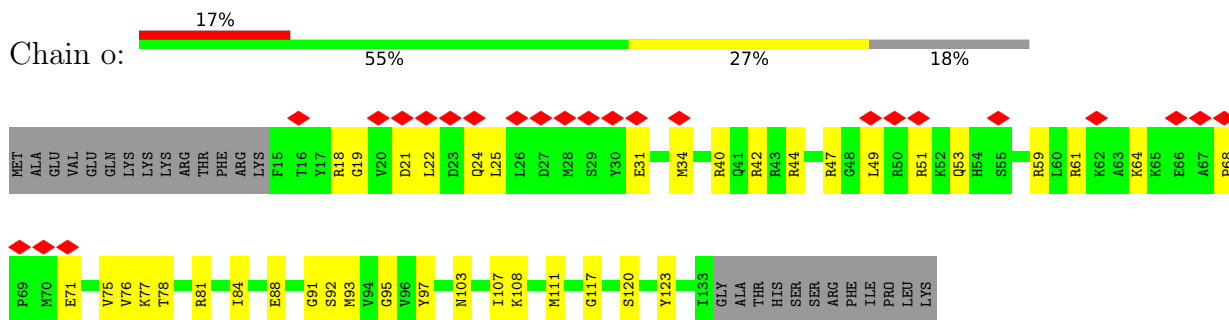
- Molecule 22: 40S ribosomal protein S10



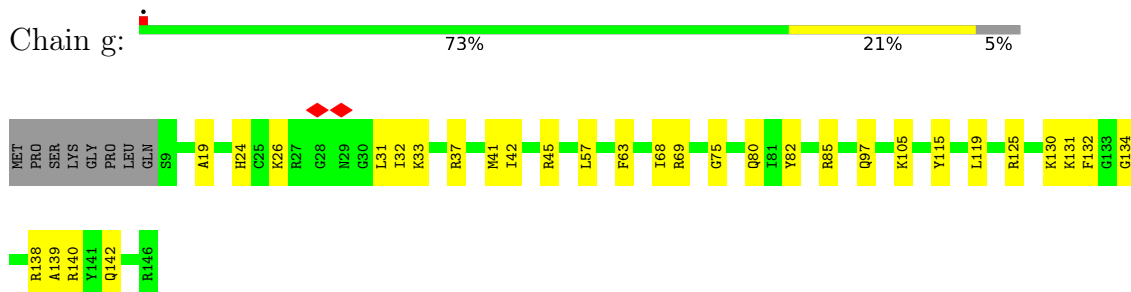
- Molecule 23: 40S ribosomal protein S12



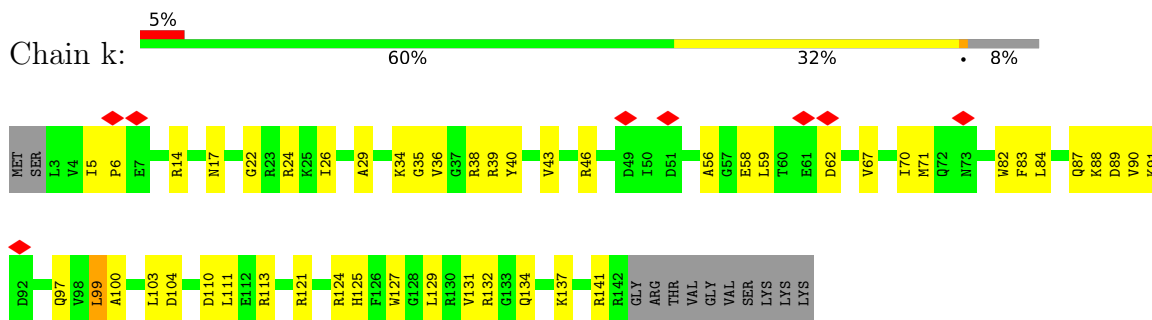
- Molecule 24: 40S ribosomal protein S15



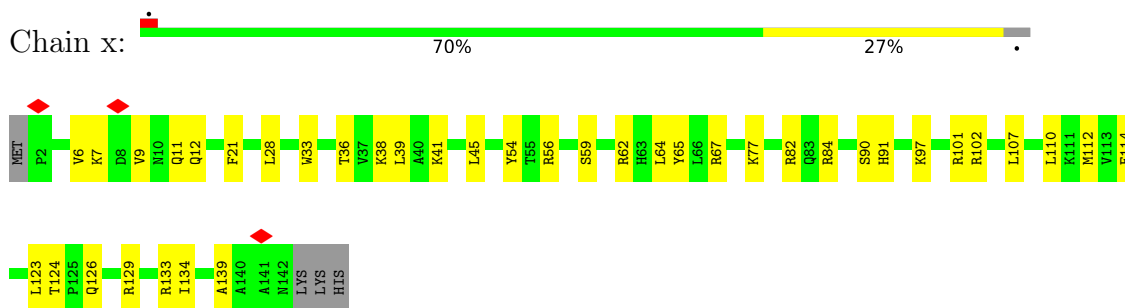
• Molecule 25: 40S ribosomal protein S16



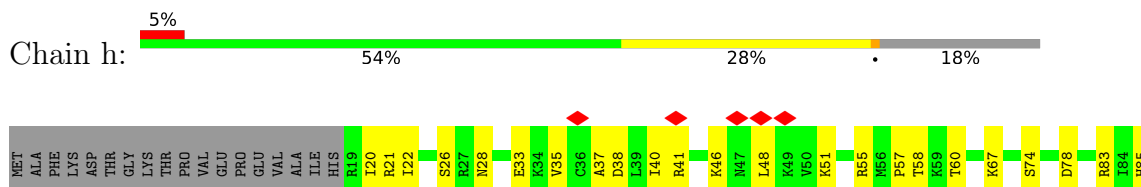
• Molecule 26: 40S ribosomal protein S18

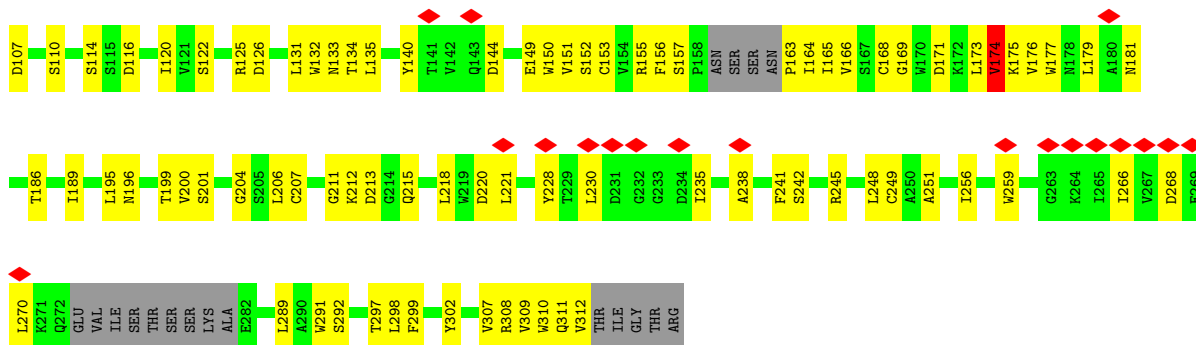


• Molecule 27: 40S ribosomal protein S19

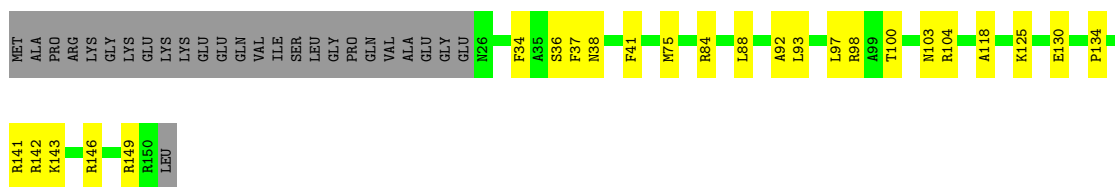


• Molecule 28: 40S ribosomal protein S20

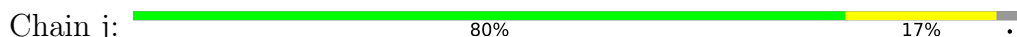




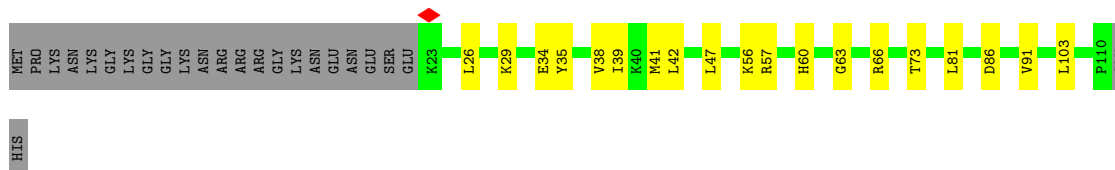
• Molecule 34: 40S ribosomal protein S14



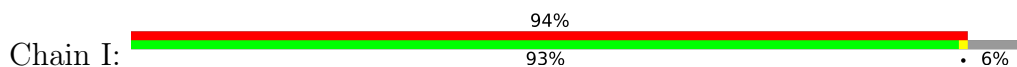
• Molecule 35: 40S ribosomal protein S23

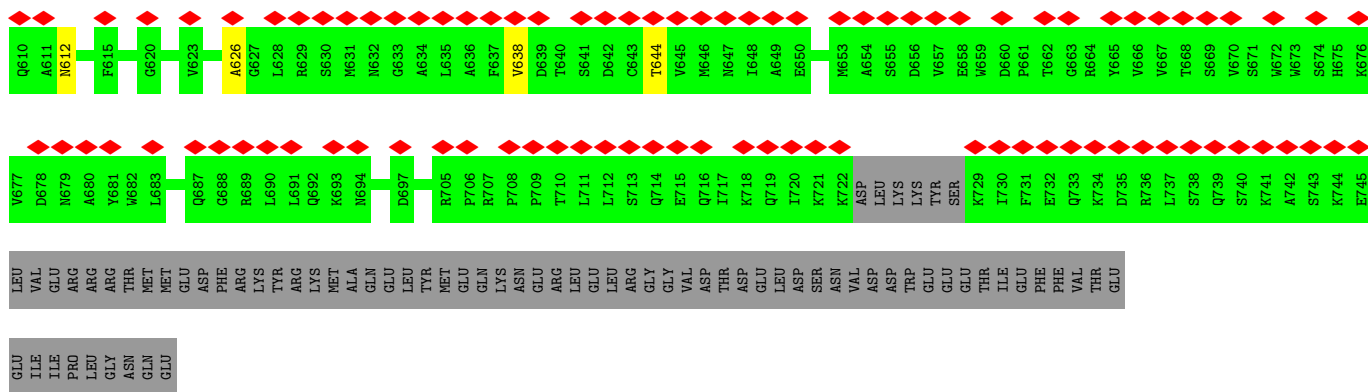


• Molecule 36: Eukaryotic translation initiation factor 1A, X-chromosomal

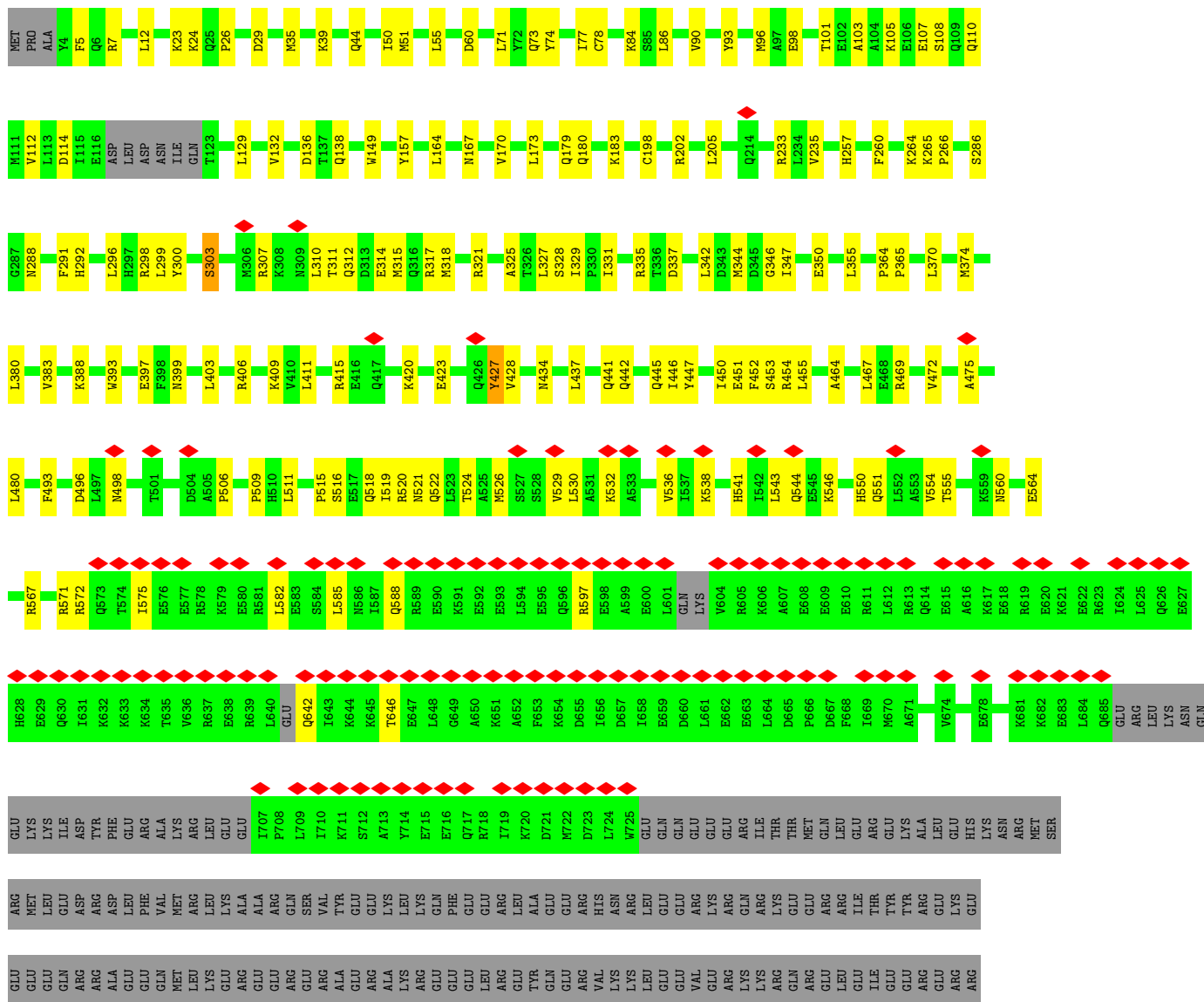
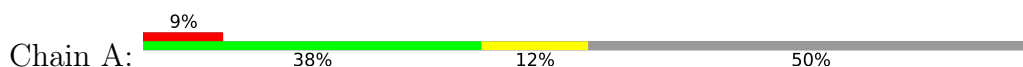


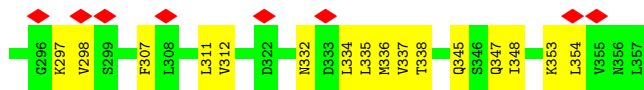
• Molecule 37: Eukaryotic translation initiation factor 3 subunit I



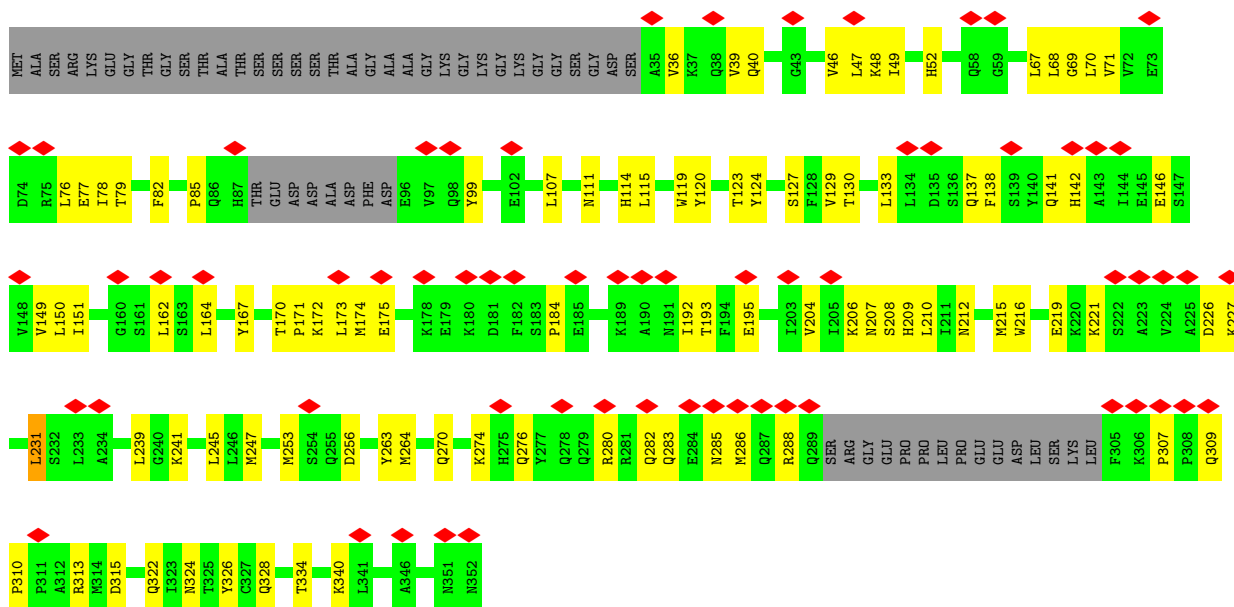


● Molecule 39: Eukaryotic translation initiation factor 3 subunit A

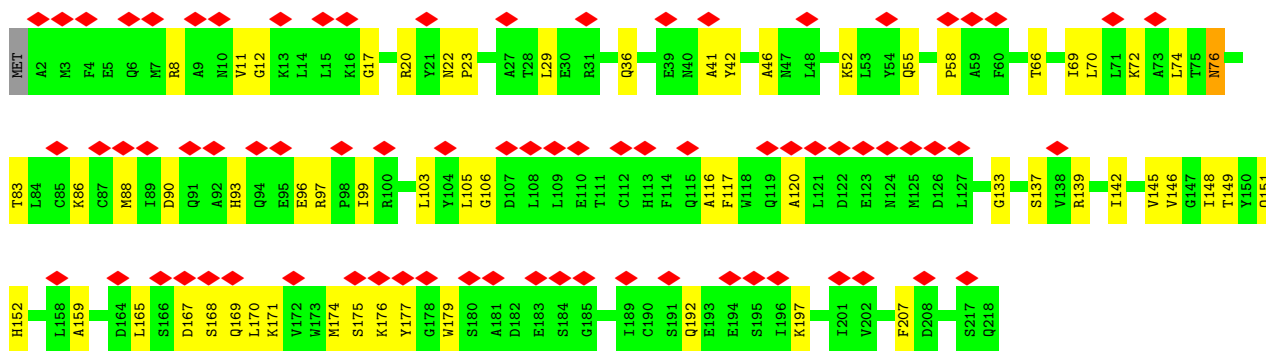
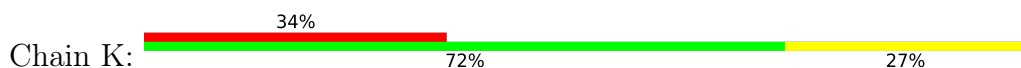




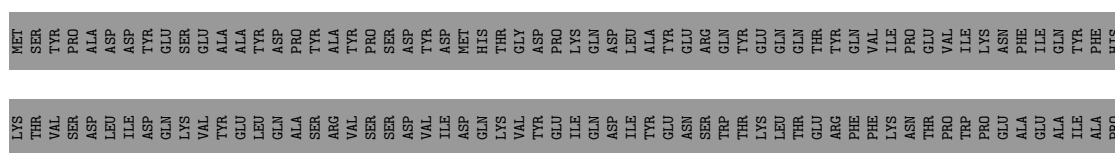
• Molecule 43: Eukaryotic translation initiation factor 3 subunit H

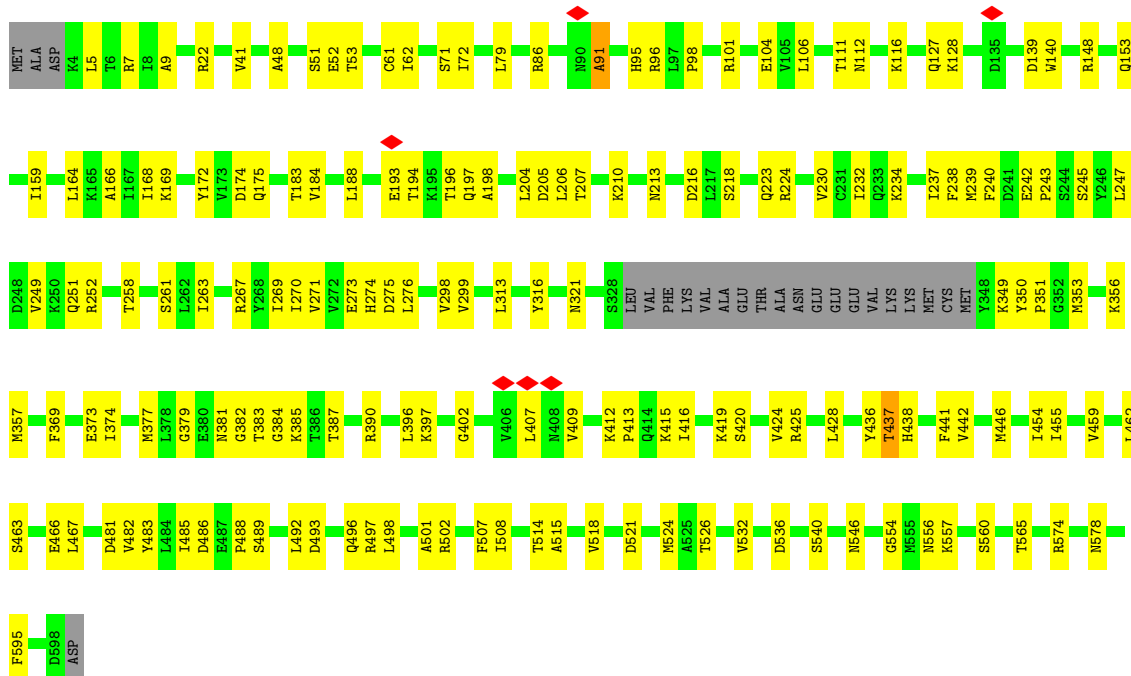


• Molecule 44: Eukaryotic translation initiation factor 3 subunit K

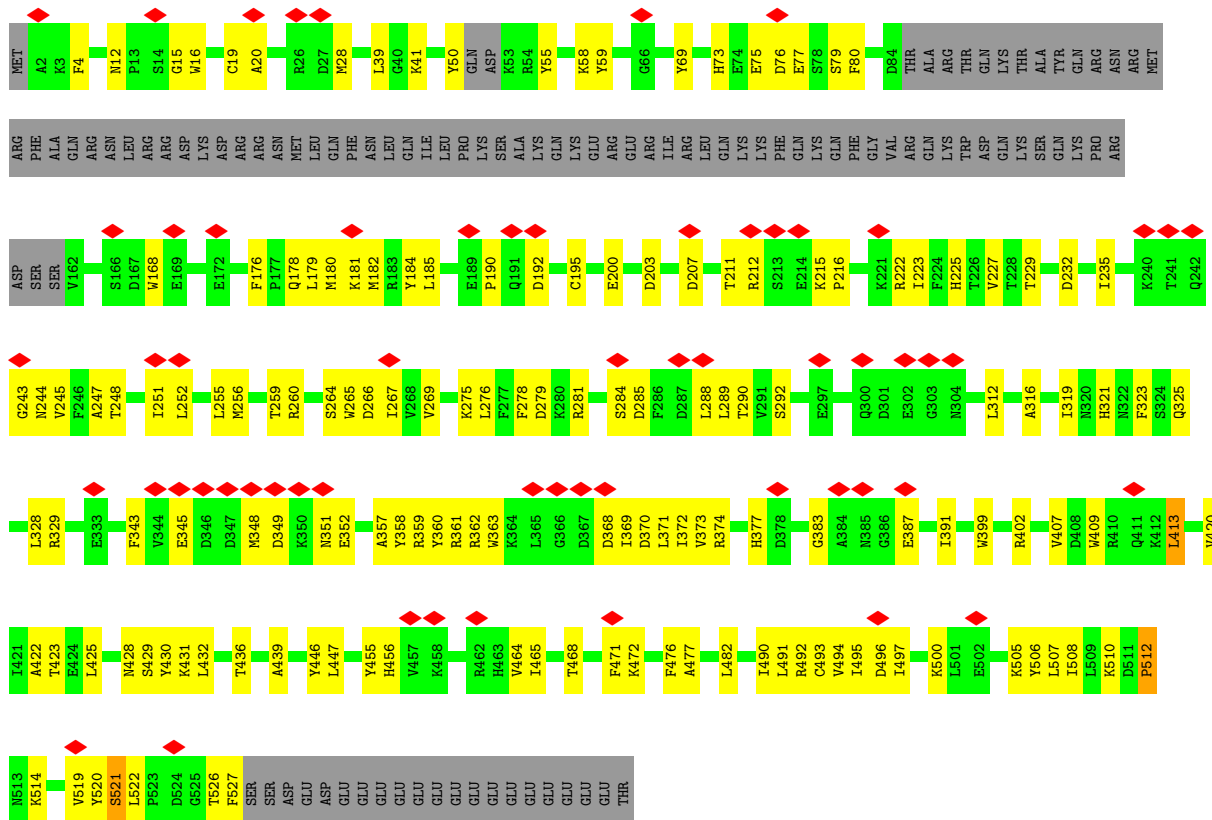


• Molecule 45: Eukaryotic translation initiation factor 3 subunit L

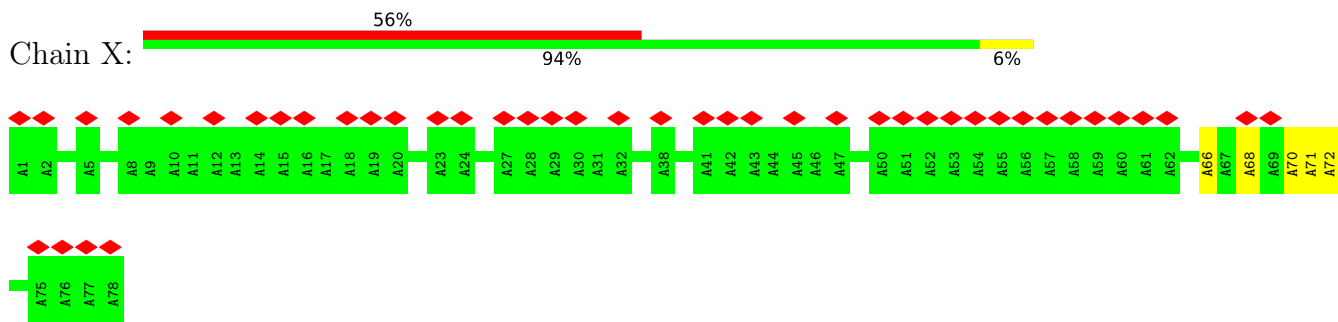




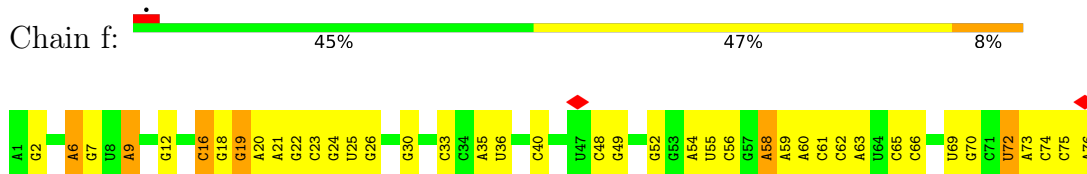
• Molecule 48: Eukaryotic translation initiation factor 3 subunit D



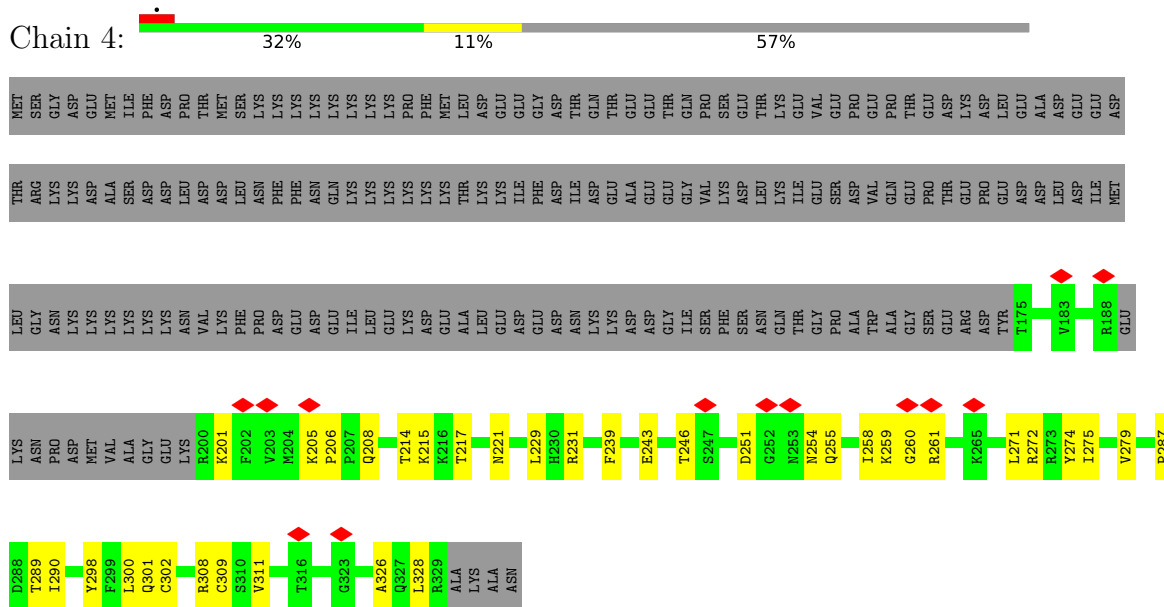
• Molecule 49: RNA recognition motif



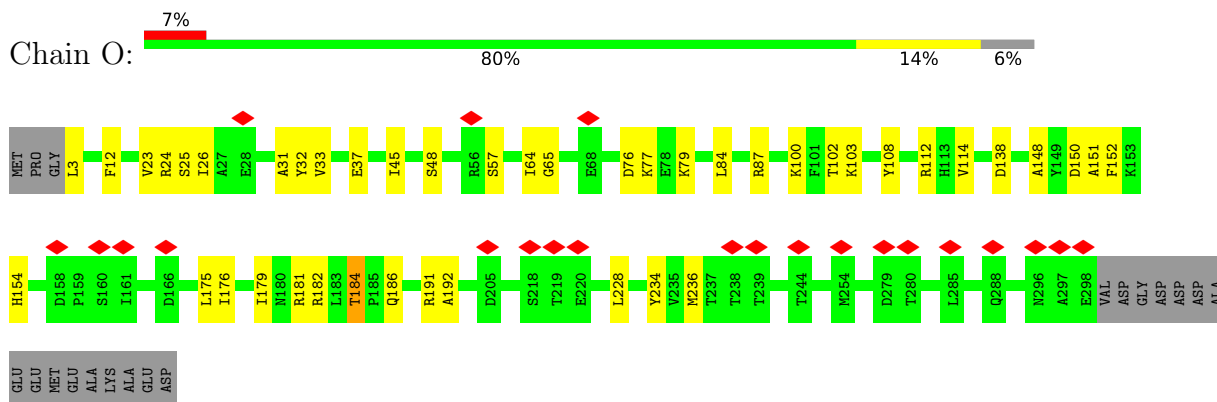
• Molecule 50: tRNA



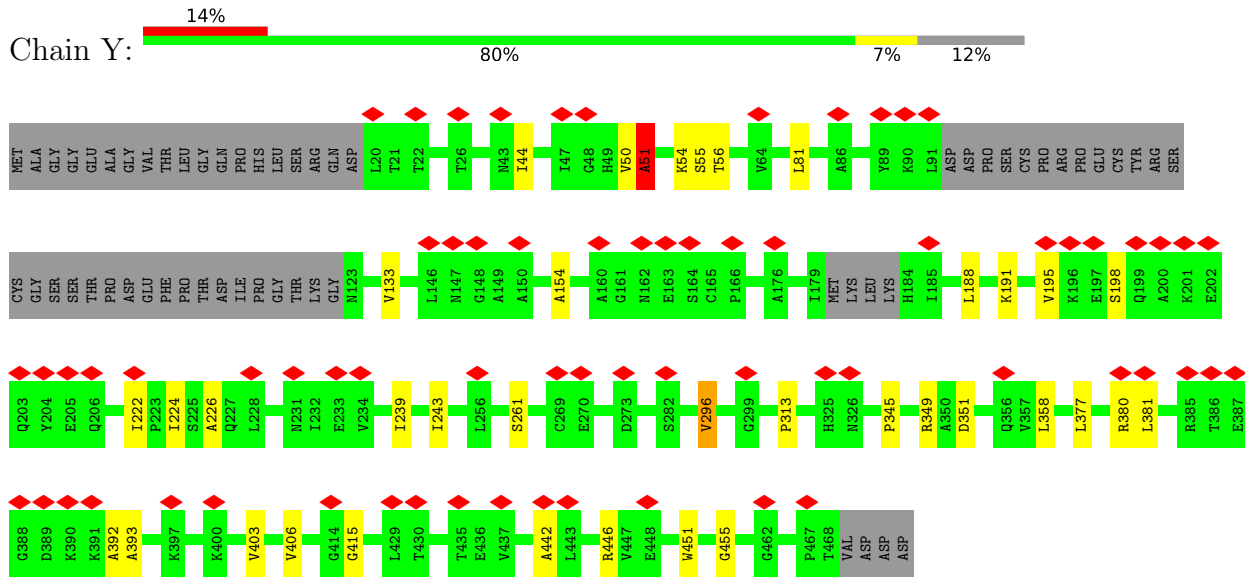
• Molecule 51: Eukaryotic translation initiation factor 2 subunit 2



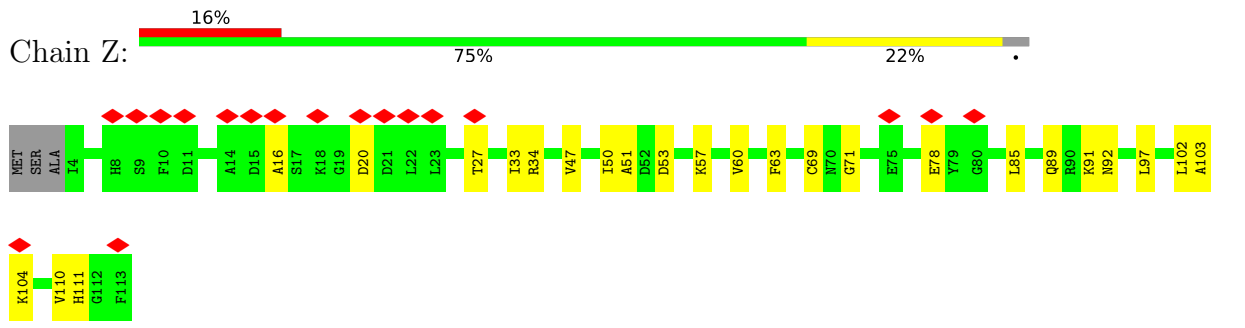
• Molecule 52: Eukaryotic translation initiation factor 2 subunit 1



• Molecule 53: Eukaryotic translation initiation factor 2 subunit 3



• Molecule 54: Eukaryotic translation initiation factor 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.059, 1.059, 1.059	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: ATP, ZN, GTP, ADP, MG, SF4

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	a	0.62	0/1742	0.71	0/2367
2	p	0.58	0/1742	0.68	0/2330
3	d	0.65	0/1710	0.75	0/2310
4	Q	0.64	0/828	0.74	0/1109
5	q	0.62	0/2073	0.67	0/2791
6	W	0.59	0/231	0.81	0/294
7	r	0.48	0/1817	0.68	1/2421 (0.0%)
8	s	0.49	0/1418	0.69	0/1895
9	t	0.56	0/1666	0.70	0/2223
10	c	0.62	0/1524	0.71	0/2035
11	n	0.64	0/1139	0.67	0/1524
12	m	0.59	0/1226	0.64	0/1649
13	y	0.55	0/631	0.70	0/844
14	D	0.73	1/1051 (0.1%)	0.75	0/1406
15	z	0.55	0/1016	0.73	0/1349
16	R	0.60	0/653	0.75	0/876
17	T	0.56	0/356	0.69	0/466
18	2	0.56	0/41057	0.53	0/63987
19	w	0.43	0/1024	0.74	0/1377
20	b	0.37	0/1773	0.66	0/2387
21	e	0.37	0/1516	0.72	0/2037
22	u	0.39	0/823	0.75	0/1111
23	v	0.28	0/870	0.68	2/1168 (0.2%)
24	o	0.33	0/999	0.73	0/1336
25	g	0.40	0/1117	0.67	0/1494
26	k	0.36	0/1180	0.71	0/1581
27	x	0.34	0/1113	0.64	0/1493
28	h	0.37	0/789	0.76	0/1059
29	P	0.33	0/563	0.69	0/758
30	S	0.44	0/481	0.80	0/643
31	l	0.39	0/461	0.73	0/612
32	U	0.29	0/474	0.75	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	V	0.38	0/2369	0.78	3/3221 (0.1%)
34	i	0.54	0/951	0.70	0/1275
35	j	0.61	0/1097	0.75	1/1464 (0.1%)
36	G	0.41	0/721	0.62	0/963
37	I	0.13	0/1495	0.39	0/2073
38	B	0.26	0/2981	0.63	0/4115
39	A	0.35	0/5469	0.70	3/7403 (0.0%)
40	C	0.39	0/5157	0.76	1/6946 (0.0%)
41	E	0.33	0/3503	0.74	1/4728 (0.0%)
42	F	0.33	0/2126	0.77	1/2890 (0.0%)
43	H	0.34	0/2458	0.77	1/3313 (0.0%)
44	K	0.37	1/1785 (0.1%)	0.82	0/2414
45	L	0.31	0/3187	0.79	10/4299 (0.2%)
46	M	0.32	0/2756	0.82	3/3714 (0.1%)
47	J	0.42	0/4626	0.74	2/6247 (0.0%)
48	N	0.42	3/3699 (0.1%)	0.85	8/5001 (0.2%)
49	X	0.16	0/389	0.50	0/543
50	f	0.29	0/1794	0.47	0/2796
51	4	0.35	0/1095	0.83	0/1477
52	O	0.30	0/2167	0.68	0/2943
53	Y	0.27	0/2161	0.69	2/2985 (0.1%)
54	Z	0.40	0/843	0.75	0/1134
All	All	0.48	5/127892 (0.0%)	0.66	39/181502 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	y	0	1
14	D	0	1
15	z	0	1
19	w	0	1
21	e	0	1
24	o	0	1
25	g	0	1
26	k	0	1
28	h	0	1
33	V	0	3
37	I	0	1
39	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	C	0	2
41	E	0	2
42	F	0	1
43	H	0	1
44	K	0	1
45	L	0	1
46	M	0	1
47	J	0	1
48	N	0	3
52	O	0	1
53	Y	0	3
54	Z	0	2
All	All	0	33

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	N	512	PRO	CG-CD	-11.77	1.10	1.50
14	D	93	LEU	C-N	-8.05	1.21	1.33
44	K	76	ASN	C-N	-6.57	1.25	1.33
48	N	512	PRO	CB-CG	-6.55	1.16	1.49
48	N	521	SER	C-N	6.22	1.42	1.33

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N	512	PRO	N-CD-CG	-17.68	76.69	103.20
48	N	512	PRO	CB-CG-CD	13.13	148.11	106.10
48	N	512	PRO	CA-CB-CG	-12.84	80.10	104.50
45	L	379	PRO	CA-C-N	8.42	136.86	121.70
45	L	379	PRO	C-N-CA	8.42	136.86	121.70

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	D	54	ASP	Peptide
21	e	77	MET	Peptide
19	w	115	SER	Peptide
13	y	50	PHE	Peptide
15	z	29	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1705	0	1706	20	0
2	p	1715	0	1785	29	0
3	d	1674	0	1764	25	0
4	Q	814	0	863	12	0
5	q	2031	0	2133	26	0
6	W	230	0	276	7	0
7	r	1794	0	1942	37	0
8	s	1399	0	1492	30	0
9	t	1638	0	1710	30	0
10	c	1499	0	1618	26	0
11	n	1119	0	1186	14	0
12	m	1202	0	1289	15	0
13	y	625	0	628	8	0
14	D	1034	0	1080	13	0
15	z	999	0	1071	19	0
16	R	640	0	665	10	0
17	T	354	0	388	3	0
18	2	36717	0	18572	345	0
19	w	1011	0	1053	24	0
20	b	1745	0	1839	37	0
21	e	1495	0	1549	26	0
22	u	799	0	823	29	0
23	v	861	0	895	23	0
24	o	980	0	1025	30	0
25	g	1100	0	1166	22	0
26	k	1162	0	1221	37	0
27	x	1094	0	1120	31	0
28	h	780	0	850	22	0
29	P	557	0	610	12	0
30	S	479	0	507	9	0
31	l	450	0	448	9	0
32	U	465	0	482	15	0
33	V	2314	0	2273	76	0
34	i	939	0	965	17	0
35	j	1080	0	1147	17	0
36	G	712	0	736	14	0
37	I	1497	0	676	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	B	2966	0	1764	31	0
39	A	5385	0	5173	111	0
40	C	5113	0	5124	126	0
41	E	3437	0	3433	100	0
42	F	2090	0	2092	66	0
43	H	2413	0	2411	76	0
44	K	1750	0	1717	43	0
45	L	3111	0	3085	63	0
46	M	2718	0	2768	66	0
47	J	4541	0	4658	110	0
48	N	3617	0	3495	115	0
49	X	390	0	392	4	0
50	f	1603	0	816	16	0
51	4	1080	0	1047	25	0
52	O	2138	0	1930	29	0
53	Y	2156	0	1161	19	0
54	Z	830	0	793	15	0
55	4	1	0	0	0	0
55	Q	1	0	0	0	0
55	U	1	0	0	0	0
55	l	1	0	0	0	0
56	J	16	0	0	1	0
57	J	27	0	12	1	0
58	J	2	0	0	0	0
58	Y	1	0	0	0	0
59	J	31	0	11	4	0
60	f	8	0	8	0	0
61	Y	32	0	12	2	0
All	All	122168	0	101455	1874	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1874 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:E:132:TYR:CE2	41:E:164:ASN:ND2	1.93	1.36
41:E:132:TYR:CD2	41:E:164:ASN:ND2	2.01	1.28
47:J:493:ASP:O	47:J:497:ARG:HB2	1.61	1.01
40:C:697:TYR:HH	40:C:708:ARG:N	1.60	0.98
18:2:1533:A:H62	18:2:1602:U:H3	1.01	0.97

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	214/295 (72%)	205 (96%)	9 (4%)	0	100	100
2	p	209/264 (79%)	194 (93%)	15 (7%)	0	100	100
3	d	214/293 (73%)	196 (92%)	18 (8%)	0	100	100
4	Q	99/115 (86%)	95 (96%)	4 (4%)	0	100	100
5	q	253/263 (96%)	231 (91%)	22 (9%)	0	100	100
6	W	22/25 (88%)	22 (100%)	0	0	100	100
7	r	220/249 (88%)	203 (92%)	17 (8%)	0	100	100
8	s	165/194 (85%)	151 (92%)	14 (8%)	0	100	100
9	t	195/208 (94%)	177 (91%)	18 (9%)	0	100	100
10	c	178/194 (92%)	165 (93%)	13 (7%)	0	100	100
11	n	131/158 (83%)	119 (91%)	12 (9%)	0	100	100
12	m	147/151 (97%)	140 (95%)	7 (5%)	0	100	100
13	y	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
14	D	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
15	z	120/131 (92%)	111 (92%)	9 (8%)	0	100	100
16	R	80/84 (95%)	76 (95%)	4 (5%)	0	100	100
17	T	40/59 (68%)	37 (92%)	3 (8%)	0	100	100
19	w	124/135 (92%)	109 (88%)	15 (12%)	0	100	100
20	b	222/243 (91%)	203 (91%)	19 (9%)	0	100	100
21	e	187/204 (92%)	172 (92%)	15 (8%)	0	100	100
22	u	93/165 (56%)	84 (90%)	9 (10%)	0	100	100
23	v	107/132 (81%)	99 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	o	117/145 (81%)	113 (97%)	4 (3%)	0	100	100
25	g	136/146 (93%)	129 (95%)	7 (5%)	0	100	100
26	k	138/152 (91%)	129 (94%)	9 (6%)	0	100	100
27	x	139/145 (96%)	132 (95%)	7 (5%)	0	100	100
28	h	96/119 (81%)	88 (92%)	8 (8%)	0	100	100
29	P	68/125 (54%)	61 (90%)	7 (10%)	0	100	100
30	S	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
31	l	52/56 (93%)	48 (92%)	4 (8%)	0	100	100
32	U	53/156 (34%)	46 (87%)	7 (13%)	0	100	100
33	V	290/317 (92%)	248 (86%)	40 (14%)	2 (1%)	18	51
34	i	123/151 (82%)	108 (88%)	15 (12%)	0	100	100
35	j	137/143 (96%)	128 (93%)	8 (6%)	1 (1%)	18	51
36	G	86/112 (77%)	81 (94%)	5 (6%)	0	100	100
37	I	301/325 (93%)	292 (97%)	9 (3%)	0	100	100
38	B	528/814 (65%)	468 (89%)	60 (11%)	0	100	100
39	A	682/1382 (49%)	646 (95%)	36 (5%)	0	100	100
40	C	615/921 (67%)	571 (93%)	44 (7%)	0	100	100
41	E	406/445 (91%)	386 (95%)	20 (5%)	0	100	100
42	F	267/357 (75%)	237 (89%)	30 (11%)	0	100	100
43	H	289/352 (82%)	262 (91%)	27 (9%)	0	100	100
44	K	215/218 (99%)	195 (91%)	20 (9%)	0	100	100
45	L	370/564 (66%)	325 (88%)	45 (12%)	0	100	100
46	M	328/374 (88%)	302 (92%)	26 (8%)	0	100	100
47	J	572/599 (96%)	506 (88%)	65 (11%)	1 (0%)	43	74
48	N	441/548 (80%)	385 (87%)	56 (13%)	0	100	100
49	X	76/78 (97%)	72 (95%)	4 (5%)	0	100	100
51	4	140/333 (42%)	119 (85%)	21 (15%)	0	100	100
52	O	294/315 (93%)	264 (90%)	30 (10%)	0	100	100
53	Y	408/472 (86%)	312 (76%)	94 (23%)	2 (0%)	24	57
54	Z	108/113 (96%)	94 (87%)	14 (13%)	0	100	100
All	All	10761/13821 (78%)	9789 (91%)	966 (9%)	6 (0%)	49	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	V	175	LYS
53	Y	224	ILE
35	j	86	PRO
53	Y	51	ALA
47	J	193	GLU

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	a	180/243 (74%)	180 (100%)	0	100	100
2	p	192/231 (83%)	192 (100%)	0	100	100
3	d	182/225 (81%)	182 (100%)	0	100	100
4	Q	88/98 (90%)	88 (100%)	0	100	100
5	q	220/225 (98%)	220 (100%)	0	100	100
6	W	23/24 (96%)	23 (100%)	0	100	100
7	r	193/218 (88%)	193 (100%)	0	100	100
8	s	155/174 (89%)	155 (100%)	0	100	100
9	t	174/180 (97%)	173 (99%)	1 (1%)	78	79
10	c	160/168 (95%)	160 (100%)	0	100	100
11	n	125/142 (88%)	125 (100%)	0	100	100
12	m	130/131 (99%)	130 (100%)	0	100	100
13	y	66/67 (98%)	66 (100%)	0	100	100
14	D	112/113 (99%)	112 (100%)	0	100	100
15	z	106/113 (94%)	106 (100%)	0	100	100
16	R	74/76 (97%)	74 (100%)	0	100	100
17	T	35/48 (73%)	35 (100%)	0	100	100
19	w	111/122 (91%)	111 (100%)	0	100	100
20	b	188/202 (93%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	e	159/170 (94%)	159 (100%)	0	100	100
22	u	86/136 (63%)	86 (100%)	0	100	100
23	v	94/108 (87%)	94 (100%)	0	100	100
24	o	107/130 (82%)	107 (100%)	0	100	100
25	g	114/121 (94%)	114 (100%)	0	100	100
26	k	122/132 (92%)	122 (100%)	0	100	100
27	x	111/115 (96%)	111 (100%)	0	100	100
28	h	91/107 (85%)	91 (100%)	0	100	100
29	P	62/103 (60%)	62 (100%)	0	100	100
30	S	54/62 (87%)	54 (100%)	0	100	100
31	l	47/49 (96%)	47 (100%)	0	100	100
32	U	51/140 (36%)	51 (100%)	0	100	100
33	V	256/275 (93%)	256 (100%)	0	100	100
34	i	98/119 (82%)	98 (100%)	0	100	100
35	j	111/115 (96%)	111 (100%)	0	100	100
36	G	75/95 (79%)	75 (100%)	0	100	100
38	B	90/702 (13%)	90 (100%)	0	100	100
39	A	546/1259 (43%)	546 (100%)	0	100	100
40	C	554/811 (68%)	554 (100%)	0	100	100
41	E	380/406 (94%)	379 (100%)	1 (0%)	86	83
42	F	237/289 (82%)	237 (100%)	0	100	100
43	H	269/310 (87%)	269 (100%)	0	100	100
44	K	192/193 (100%)	192 (100%)	0	100	100
45	L	342/515 (66%)	342 (100%)	0	100	100
46	M	305/335 (91%)	305 (100%)	0	100	100
47	J	506/526 (96%)	506 (100%)	0	100	100
48	N	398/494 (81%)	398 (100%)	0	100	100
51	4	109/304 (36%)	109 (100%)	0	100	100
52	O	190/280 (68%)	190 (100%)	0	100	100
53	Y	33/397 (8%)	33 (100%)	0	100	100
54	Z	79/96 (82%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8382/11694 (72%)	8380 (100%)	2 (0%)	100 100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	t	155	ASN
41	E	132	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
42	F	288	GLN
44	K	151	GLN
43	H	58	GLN
43	H	336	GLN
45	L	243	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	2	1710/1721 (99%)	514 (30%)	7 (0%)
50	f	74/75 (98%)	24 (32%)	0
All	All	1784/1796 (99%)	538 (30%)	7 (0%)

5 of 538 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	2	2	A
18	2	4	C
18	2	5	U
18	2	11	A
18	2	25	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	2	1292	C
18	2	1474	A
18	2	1698	C

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Mol	Chain	Res	Type
18	2	1621	U
18	2	1060	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	SF4	J	602	47	0,12,12	-	-	-		
56	SF4	J	601	47	0,12,12	-	-	-		
60	MET	f	701	-	6,7,8	0.57	0	2,7,9	0.66	0
61	GTP	Y	501	58	33,34,34	0.93	1 (3%)	50,54,54	1.80	8 (16%)
59	ATP	J	605	58	32,33,33	3.45	12 (37%)	48,52,52	2.17	14 (29%)
57	ADP	J	603	58	28,29,29	3.37	11 (39%)	43,45,45	2.95	14 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SF4	J	602	47	-	-	0/6/5/5
56	SF4	J	601	47	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	MET	f	701	-	-	0/5/6/8	-
61	GTP	Y	501	58	-	3/22/38/38	0/3/3/3
59	ATP	J	605	58	-	7/22/38/38	0/3/3/3
57	ADP	J	603	58	-	8/16/32/32	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	J	603	ADP	C2'-C3'	-10.67	1.24	1.53
59	J	605	ATP	C3'-C4'	-9.87	1.28	1.53
59	J	605	ATP	C2'-C1'	-8.43	1.27	1.53
57	J	603	ADP	O4'-C4'	-6.56	1.30	1.45
59	J	605	ATP	O4'-C1'	6.42	1.56	1.42

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	J	603	ADP	C1'-N9-C8	-10.31	104.20	127.09
57	J	603	ADP	C4-N9-C1'	9.98	149.97	126.63
61	Y	501	GTP	C5-C4-N3	-6.08	118.72	128.39
57	J	603	ADP	N3-C2-N1	-5.83	119.75	128.58
59	J	605	ATP	C1'-N9-C8	-5.58	114.72	127.09

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	J	603	ADP	C5'-O5'-PA-O2A
57	J	603	ADP	C5'-O5'-PA-O3A
59	J	605	ATP	C5'-O5'-PA-O2A
59	J	605	ATP	C5'-O5'-PA-O3A
61	Y	501	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

4 monomers are involved in 8 short contacts:

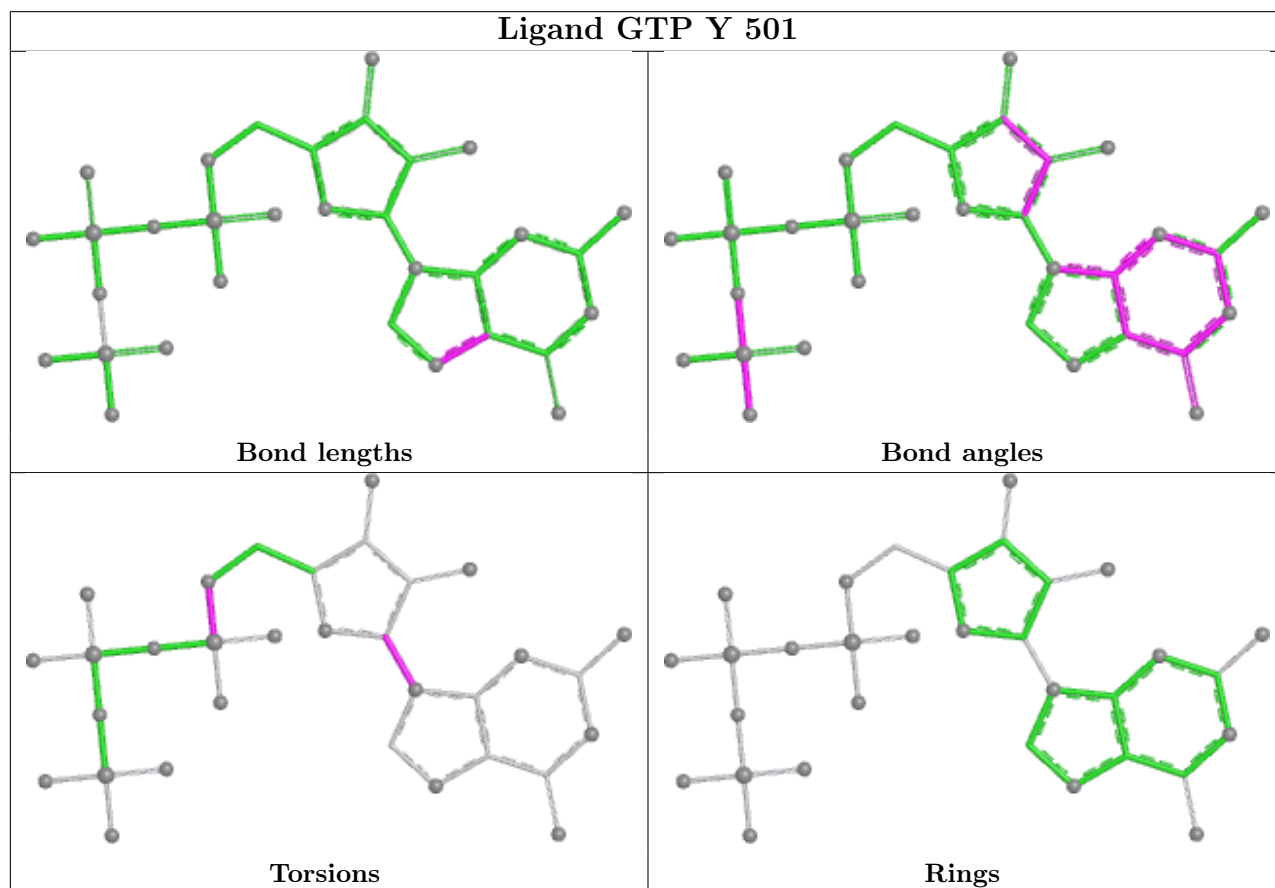
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	J	601	SF4	1	0
61	Y	501	GTP	2	0
59	J	605	ATP	4	0

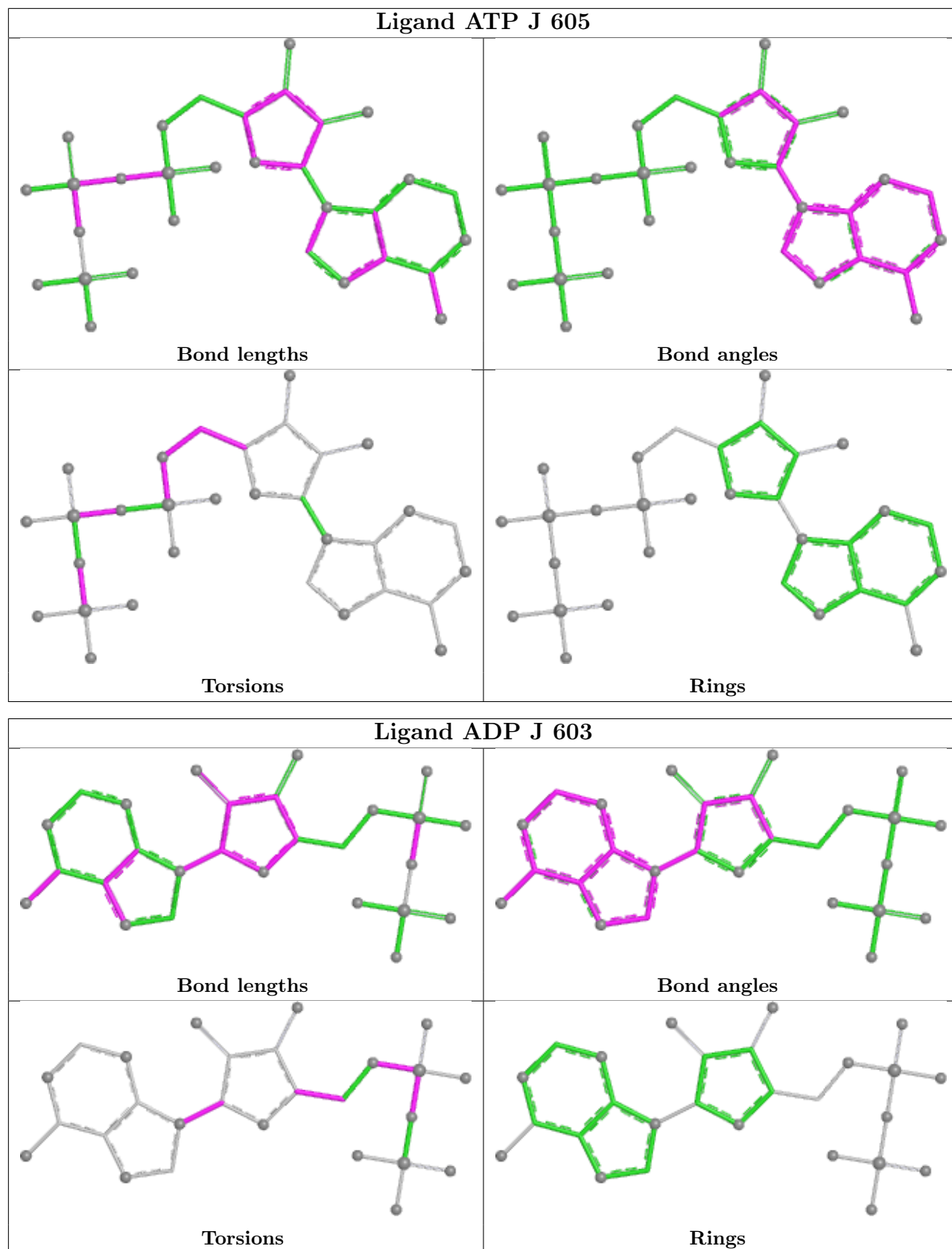
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	J	603	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	2	3
46	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	96:GLY	C	97:GLU	N	10.75
1	2	1207:G	O3'	1208:A	P	4.50
1	2	368:U	O3'	369:C	P	3.24
1	2	1682:C	O3'	1683:C	P	3.13

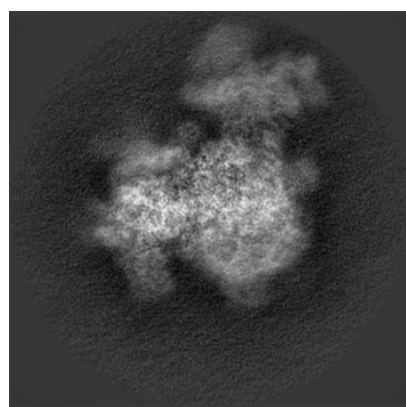
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11602. These allow visual inspection of the internal detail of the map and identification of artifacts.

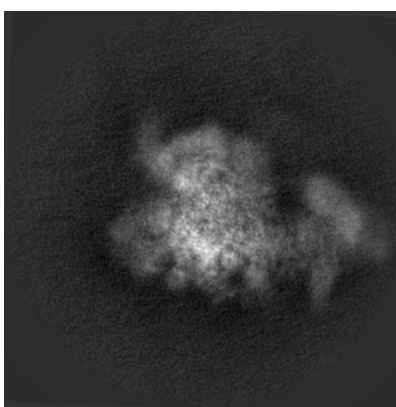
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

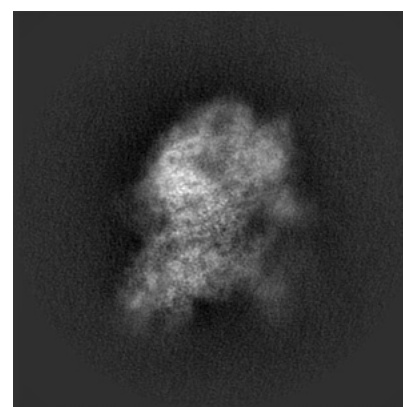
6.1.1 Primary map



X



Y

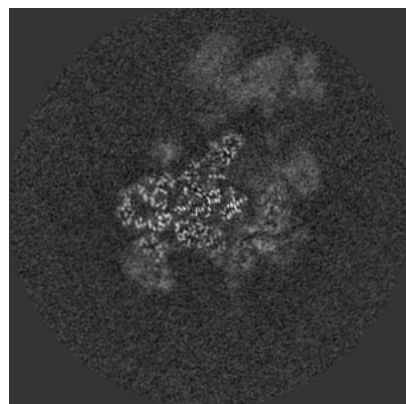


Z

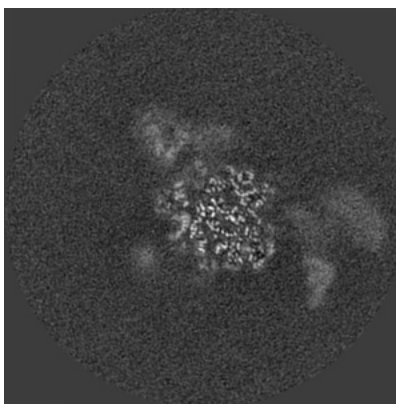
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

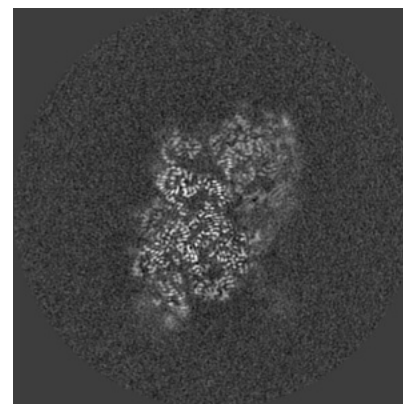
6.2.1 Primary map



X Index: 200



Y Index: 200

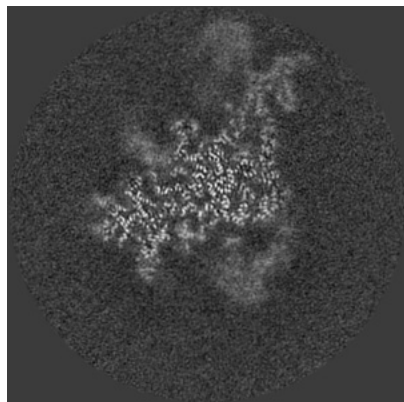


Z Index: 200

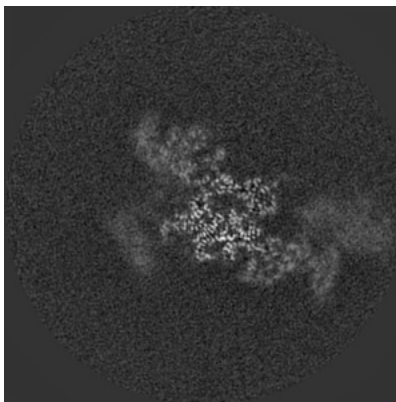
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

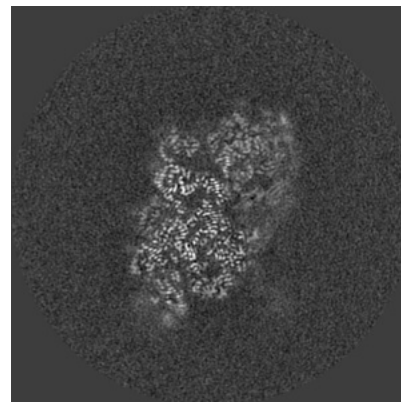
6.3.1 Primary map



X Index: 165



Y Index: 218

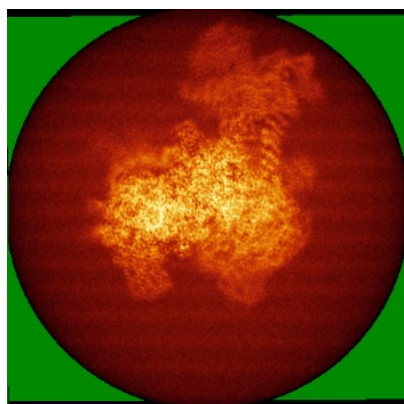


Z Index: 200

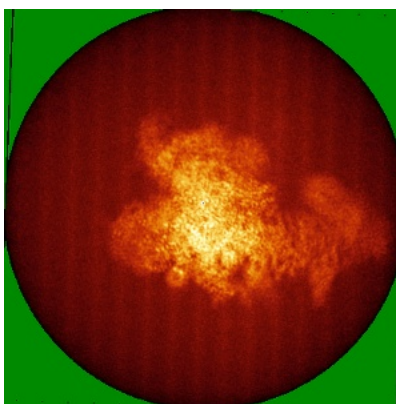
The images above show the largest variance slices of the map in three orthogonal directions.

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

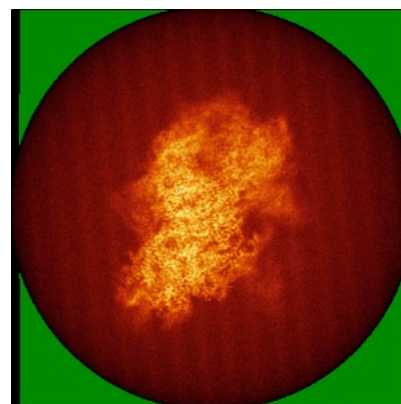
6.4.1 Primary map



X



Y

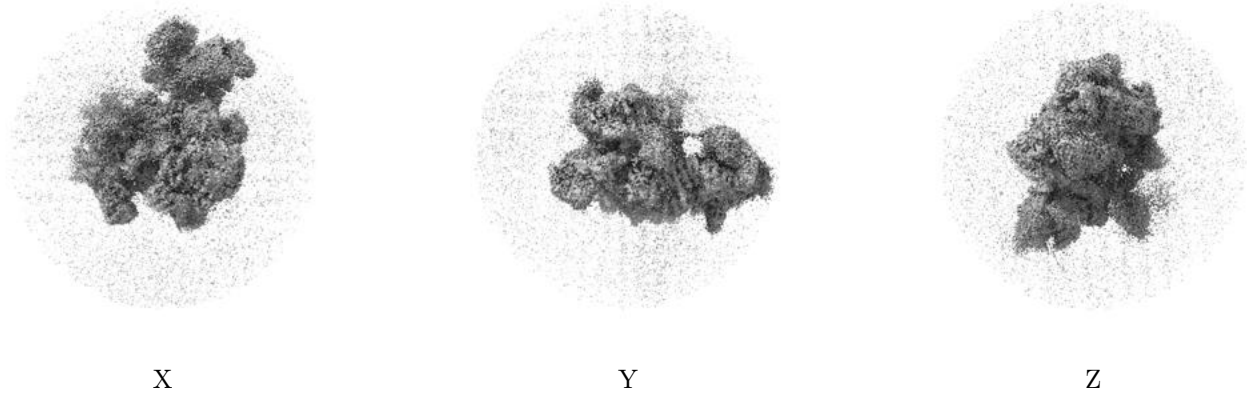


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

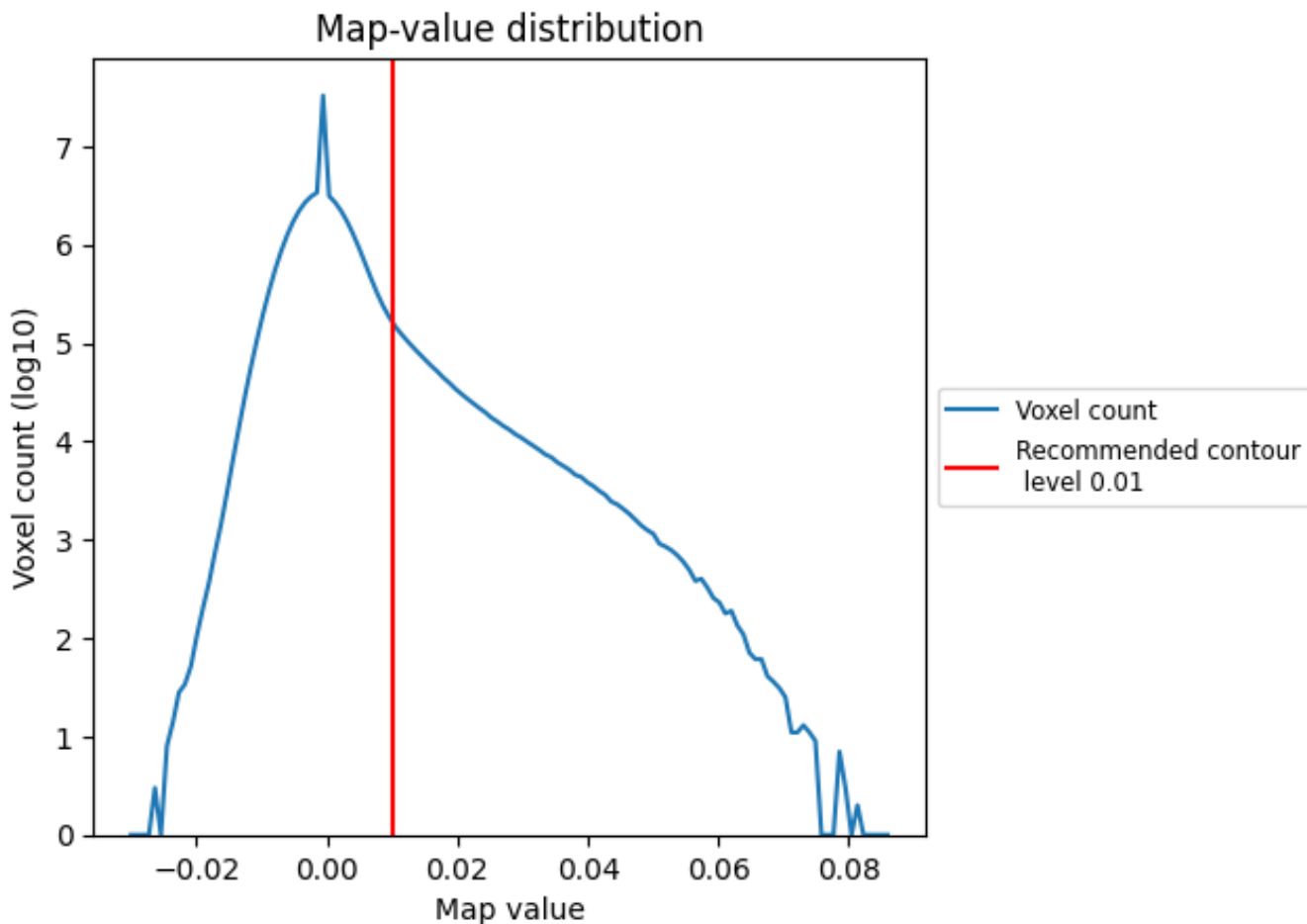
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

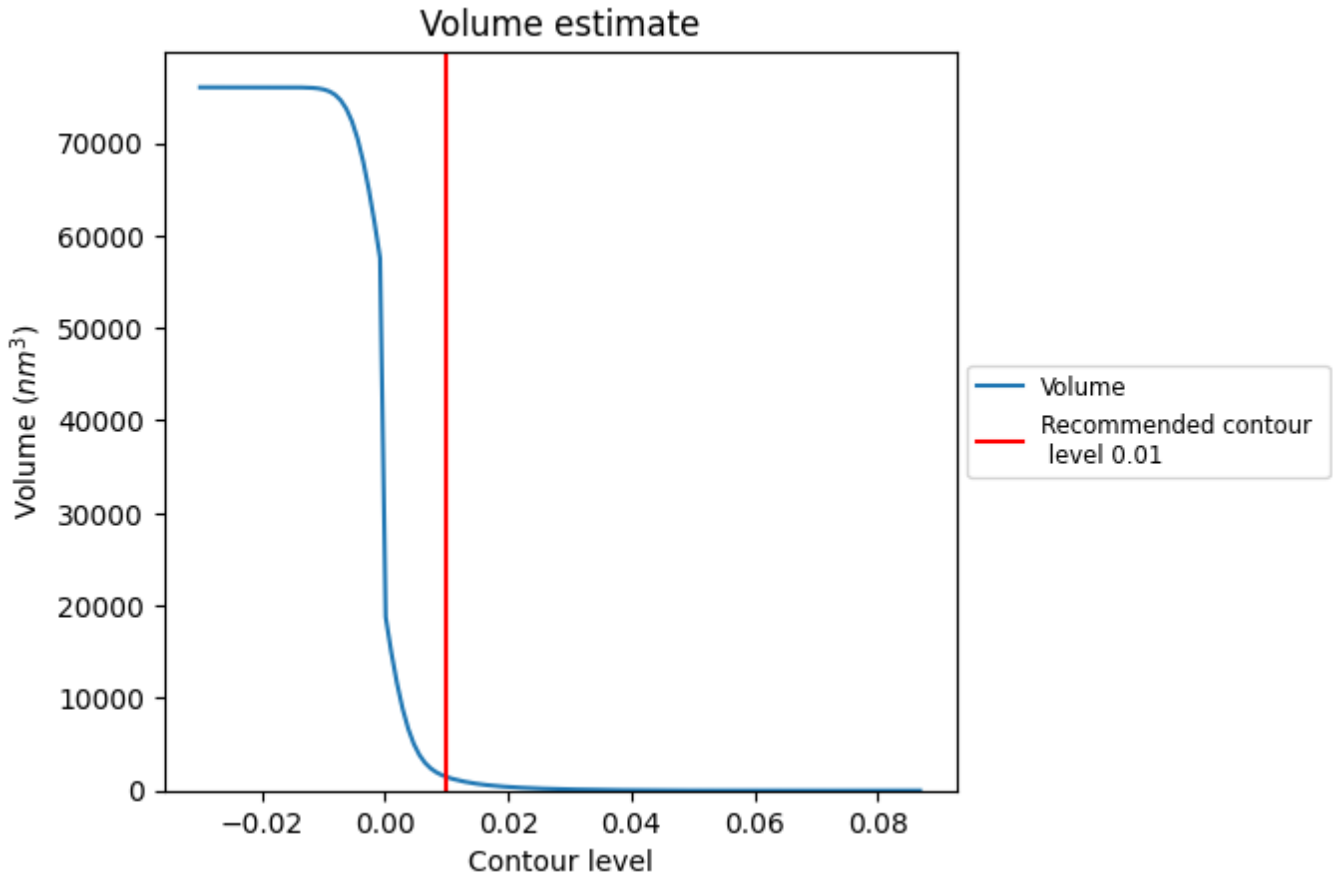
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

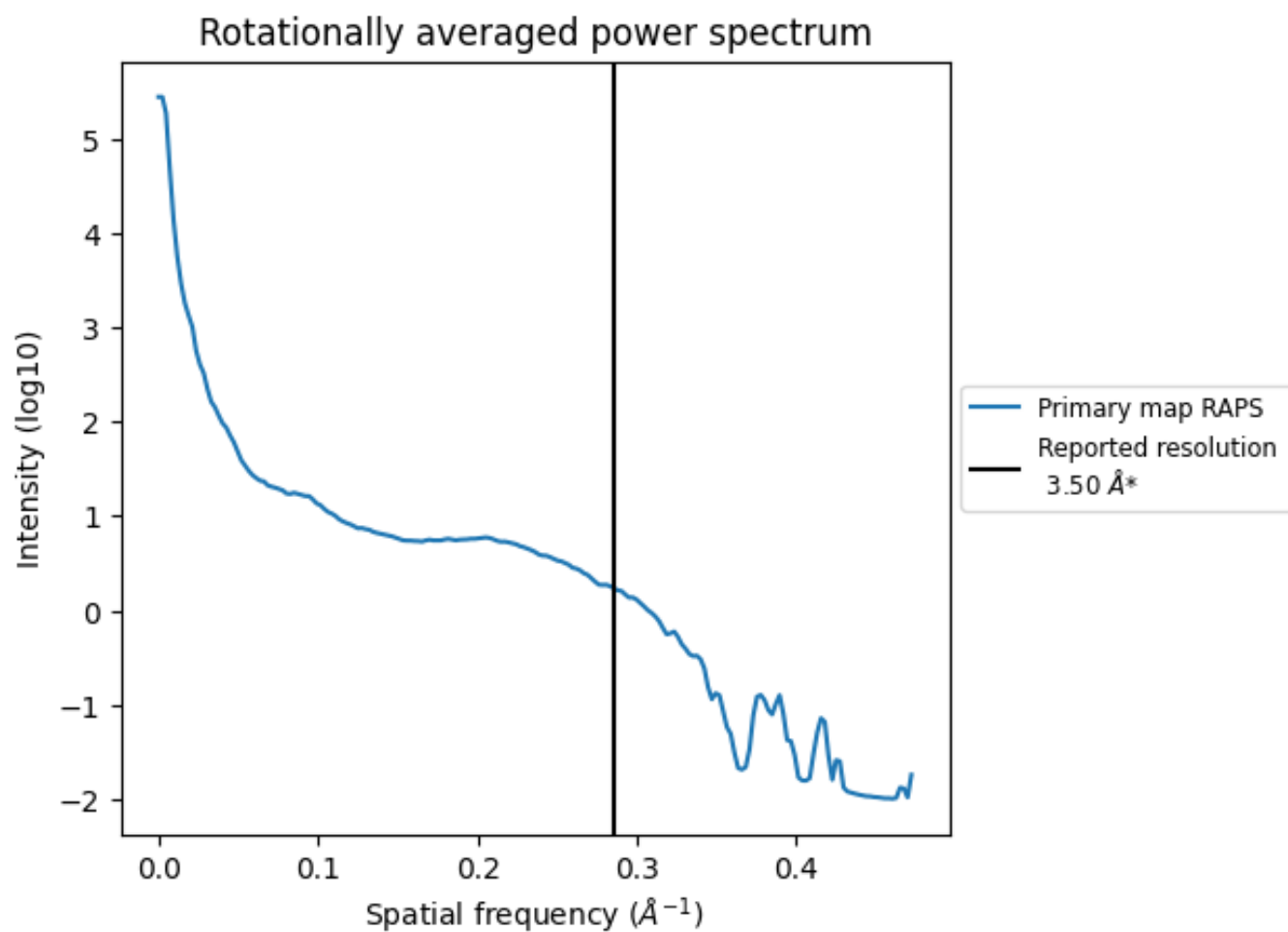
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1473 nm^3 ; this corresponds to an approximate mass of 1330 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](#)

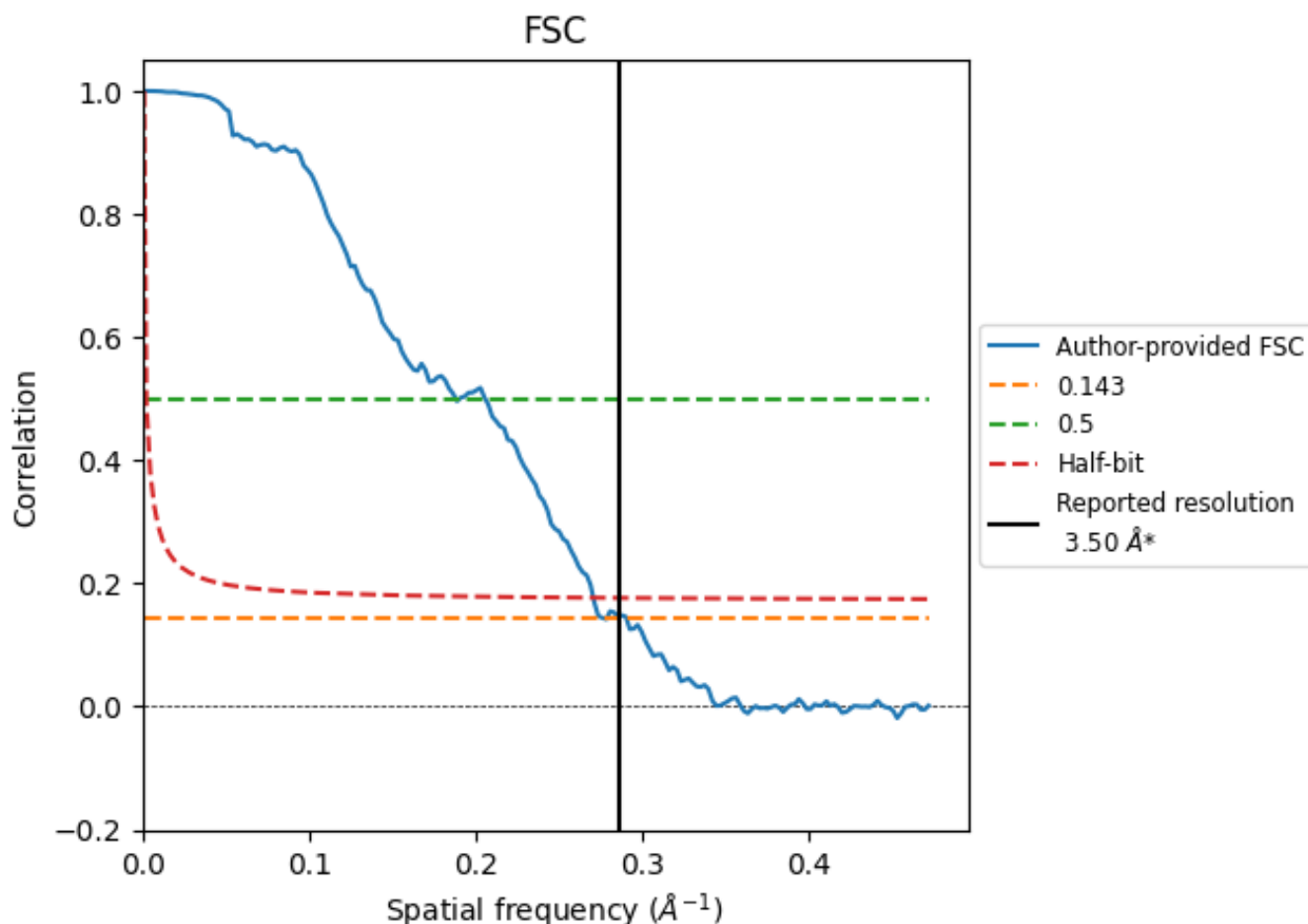


*Reported resolution corresponds to spatial frequency of 0.286\AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

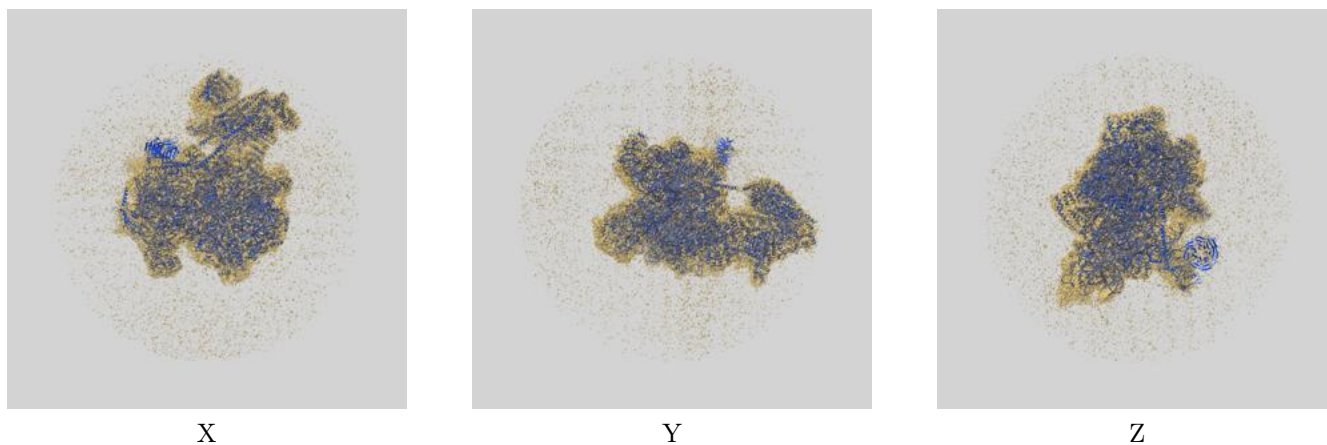
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.60	5.32	3.69
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

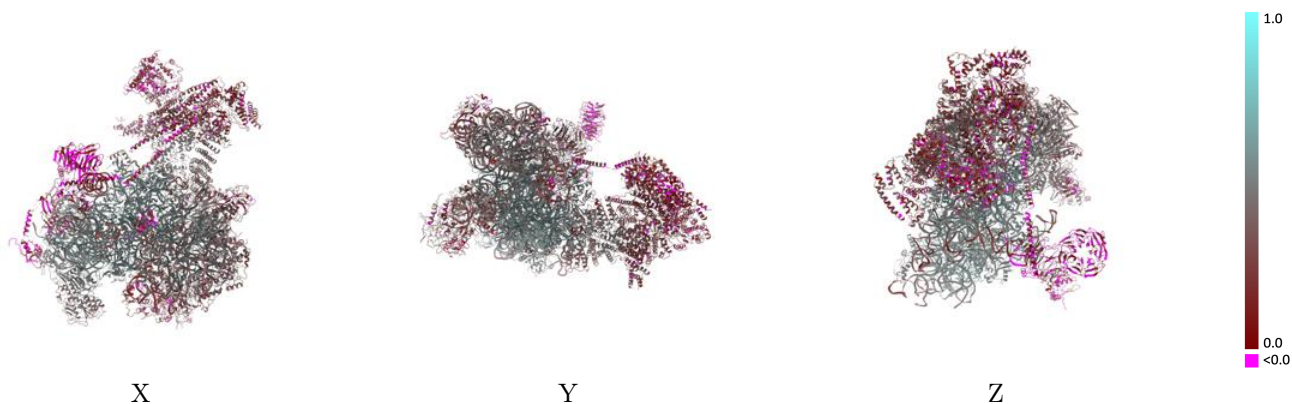
This section contains information regarding the fit between EMDB map EMD-11602 and PDB model 7A09. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



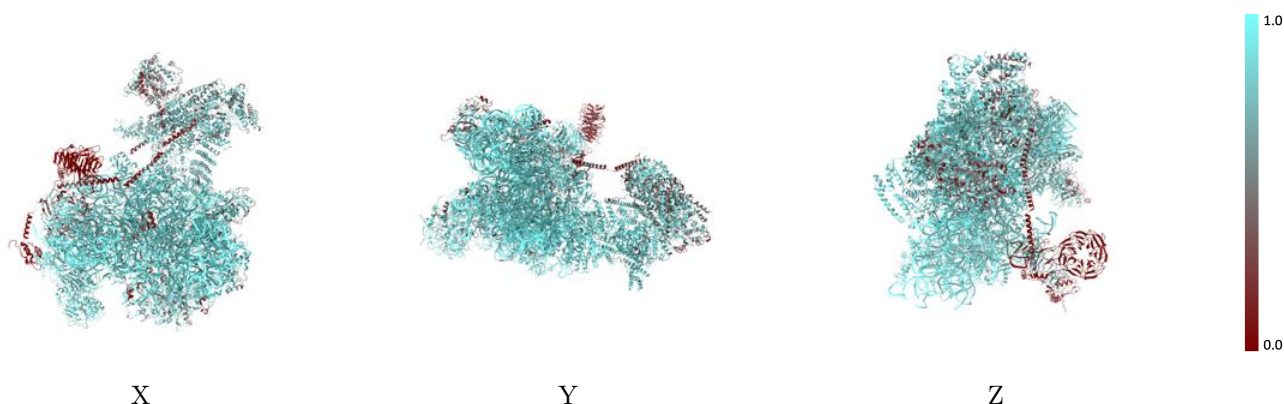
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



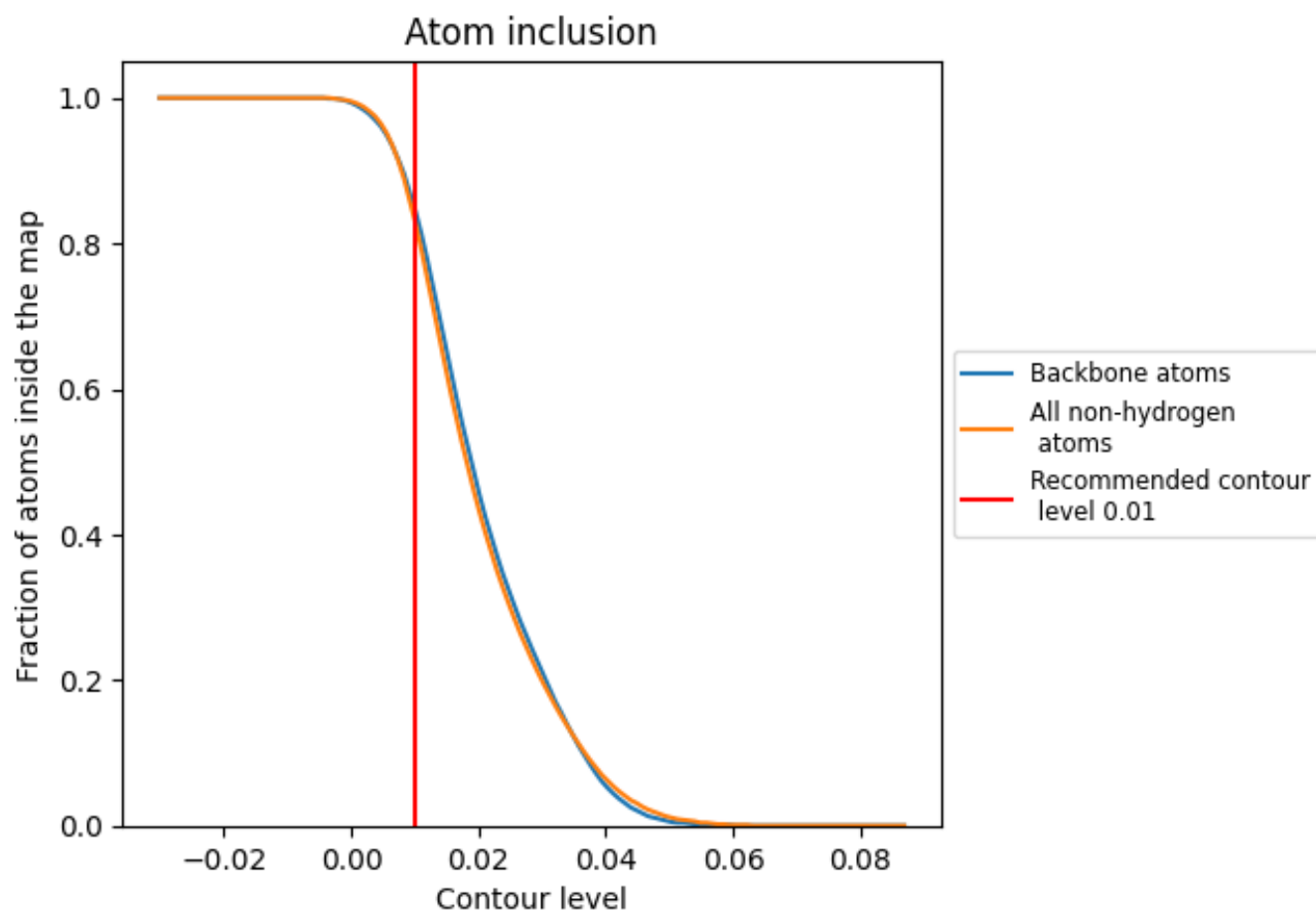
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary









































The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.3990
2	 0.9680	 0.4800
4	 0.7780	 0.3780
A	 0.7280	 0.3030
B	 0.3860	 0.1700
C	 0.8430	 0.3840
D	 0.9370	 0.5480
E	 0.7770	 0.2550
F	 0.6330	 0.2030
G	 0.8460	 0.4710
H	 0.6510	 0.2120
I	 0.0130	 0.0160
J	 0.8730	 0.4370
K	 0.5400	 0.1930
L	 0.4400	 0.1530
M	 0.6990	 0.2230
N	 0.7120	 0.2910
O	 0.7870	 0.3250
P	 0.8490	 0.3750
Q	 0.9260	 0.5360
R	 0.9250	 0.5260
S	 0.8440	 0.4400
T	 0.9410	 0.5160
U	 0.6040	 0.2410
V	 0.8270	 0.3880
W	 0.9380	 0.5250
X	 0.4280	 0.1410
Y	 0.7720	 0.2760
Z	 0.7590	 0.4040
a	 0.9260	 0.5140
b	 0.8100	 0.4000
c	 0.9320	 0.5300
d	 0.9370	 0.5420
e	 0.8760	 0.4380
f	 0.9320	 0.3740



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Chain	Atom inclusion	Q-score
g	 0.8530	 0.4370
h	 0.7900	 0.4100
i	 0.9340	 0.5180
j	 0.9300	 0.5520
k	 0.8000	 0.3770
l	 0.8480	 0.4420
m	 0.9410	 0.5280
n	 0.9460	 0.5440
o	 0.6790	 0.3310
p	 0.9440	 0.5270
q	 0.9510	 0.5420
r	 0.9350	 0.4860
s	 0.9040	 0.4810
t	 0.9420	 0.5080
u	 0.7620	 0.3280
v	 0.5050	 0.2240
w	 0.8710	 0.4640
x	 0.8940	 0.4100
y	 0.9380	 0.5280
z	 0.9270	 0.5150