



wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 02:47 PM JST

PDB ID : 8IPX / pdb_00008ipx
EMDB ID : EMD-35649
Title : human nuclear pre-60S ribosomal particle - State C'
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-03-15
Resolution : 4.30 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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

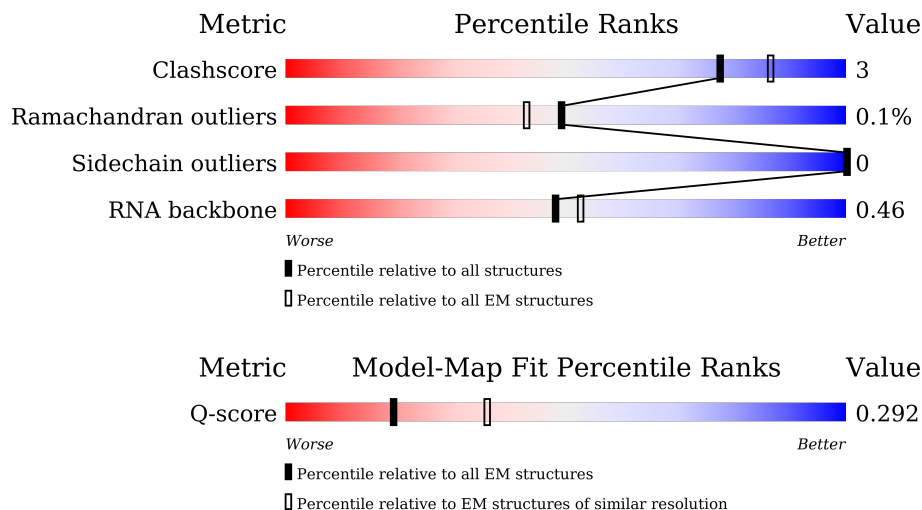
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	4585 (3.80 - 4.80)

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	2	5054	
2	6	245	
3	7	163	

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Mol	Chain	Length	Quality of chain
4	8	156	17% 77% 21%
5	9	134	64% 57% 7% 36%
6	A	159	28% 25% 72%
7	B	403	55% 89% 11%
8	D	427	36% 77% 7% 16%
9	E	115	83% 77% 9% 15%
10	G	266	78% 83% 8% 9%
11	H	123	67% 93% 6%
12	I	192	80% 92% 7%
13	J	260	82% 77% 6% 17%
14	L	148	43% 73% 24%
15	M	97	29% 81% 7% 11%
16	P	51	27% 86% 12%
17	Q	211	67% 90% 9%
18	S	215	46% 57% 6% 37%
19	U	204	49% 90% 10%
20	V	203	40% 91% 8%
21	X	92	91% 91% 8%
22	Z	188	38% 72% 8% 20%
23	a	196	61% 71% 24%
24	b	176	64% 88% 13%
25	e	140	71% 82% 11% 6%
26	h	145	50% 84% 8% 8%
27	l	137	39% 82% 9% 9%
28	m	257	95% 92%

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Mol	Chain	Length	Quality of chain
29	n	110	29% 94% 5% ..
30	o	288	65% 73% 9% 18%
31	p	248	48% 85% 6% 9%
32	r	360	23% 18% 77%
33	u	549	12% 11% 88%
34	v	239	91% 84% 7% 9%
35	w	731	59% 54% 5% 41%
36	y	165	100% 88% 12%
37	z	129	51% 40% 11% 48%
38	C	178	93% 80% 12% 7%
39	R	297	99% 82% 16% .
40	W	485	80% 72% 8% 20%
41	T	160	74% 71% 6% 22%
42	4	634	93% 85% 11% .
43	Y	184	39% 84% 7% 9%
44	k	135	37% 89% 6% .
45	j	125	53% 84% 5% 11%
46	d	128	73% 69% 12% 19%
47	t	293	38% 33% 62%
48	x	60	95% 92% 5% .
49	N	490	49% 45% 51%
50	1	255	90% 81% 9% 10%
51	K	105	85% 92% 5% .
52	F	117	76% 95% .
53	i	136	96% 86% 13% .

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Mol	Chain	Length	Quality of chain
54	O	70	<p>90%</p> <p>94%</p>
55	3	120	<p>92%</p> <p>63%</p> <p>28%</p>
56	q	588	<p>69%</p> <p>60%</p> <p>9%</p> <p>31%</p>
57	g	156	<p>67%</p> <p>83%</p> <p>10%</p> <p>7%</p>
58	f	478	<p>54%</p> <p>44%</p> <p>10%</p> <p>46%</p>

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 160786 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	3475	74602	33261	13645	24222	3474	0	0

- Molecule 2 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	6	244	1852	1149	318	372	13	0	0

- Molecule 3 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	7	135	1159	737	225	187	10	0	0

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	8	156	3315	1481	585	1094	155	0	0

- Molecule 5 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	9	86	711	433	154	121	3	0	0

- Molecule 6 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	45	352	221	76	52	3	0	0

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	402	3244	2065	609	556	14	1	0

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	358	2853	1797	570	473	13	0	0

- Molecule 9 is a protein called 60S ribosomal protein L30.

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

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	241	1927	1228	371	324	4	0	0

- Molecule 11 is a protein called 60S ribosomal protein L35.

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

- Molecule 12 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	190	1518	956	284	272	6	0	0

- Molecule 13 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	217	1772	1134	334	296	8	0	0

- Molecule 14 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	112	Total	C	N	O	S	0	0
			877	557	172	145	3		

- Molecule 15 is a protein called 60S ribosomal protein L37.

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

- Molecule 16 is a protein called 60S ribosomal protein L39.

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

- Molecule 17 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 18 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 19 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 20 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 21 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 22 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 23 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	148	Total	C	N	O	S	0	0
			1239	772	266	192	9		

- Molecule 24 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 25 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	e	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 26 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	h	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 27 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	l	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 28 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	m	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 29 is a protein called 60S ribosomal protein L35a.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	o	235	Total	C	N	O	S	0	0
			1897	1217	360	316	4		

- Molecule 31 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	p	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 32 is a protein called Coiled-coil domain-containing protein 86.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	r	82	Total	C	N	O	S	0	0
			723	442	158	121	2		

- Molecule 33 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	67	Total	C	N	O	S	0	0
			569	357	119	90	3		

- Molecule 34 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	v	217	Total	C	N	O	S	0	0
			1771	1129	311	320	11		

- Molecule 35 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	w	433	3472	2201	615	643	13	0	0

- Molecule 36 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	y	165	1250	779	232	234	5	0	0

- Molecule 37 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	z	67	581	363	128	88	2	0	0

- Molecule 38 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	C	165	1319	836	245	233	5	0	0

- Molecule 39 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	R	293	2382	1507	434	427	14	0	0

- Molecule 40 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	W	388	3018	1889	556	562	11	0	0

- Molecule 41 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	T	124	1001	632	194	171	4	0	0

- Molecule 42 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	4	611	Total	C	N	O	S	0	0
			5016	3151	918	920	27		

- Molecule 43 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Y	167	Total	C	N	O	S	0	0
			1355	848	260	238	9		

- Molecule 44 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 45 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	j	111	Total	C	N	O	S	0	0
			918	578	178	160	2		

- Molecule 46 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	d	104	Total	C	N	O	S	0	0
			850	542	149	157	2		

- Molecule 47 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	111	Total	C	N	O	S	0	0
			928	601	157	167	3		

- Molecule 48 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	57	Total	C	N	O	P	0	0
			684	285	1	341	57		

- Molecule 49 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	N	239	Total	C	N	O	S	0	0
			1924	1232	338	348	6		

- Molecule 50 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	230	Total	C	N	O	S	0	0
			1897	1226	357	310	4		

- Molecule 51 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	K	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 52 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	F	113	Total	C	N	O	S	0	0
			897	560	185	146	6		

- Molecule 53 is a protein called 60S ribosomal protein L27.

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

- Molecule 54 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	O	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 55 is a RNA chain called 5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	115	Total	C	N	O	P	0	0
			2453	1093	437	808	115		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	92	C	G	conflict	GB NR_023363
3	93	G	C	conflict	GB NR_023363
3	95	C	U	conflict	GB NR_023363
3	96	U	G	conflict	GB NR_023363

- Molecule 56 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	q	404	3317	2140	582	582	13	0	0

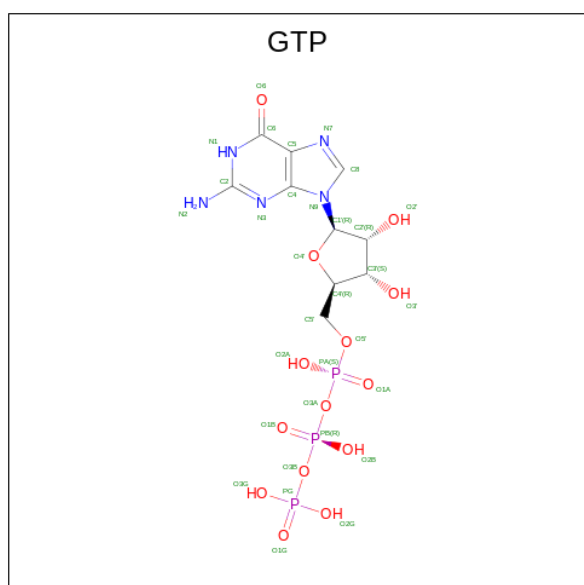
- Molecule 57 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	g	145	1170	750	222	197	1	0	0

- Molecule 58 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	f	258	2137	1326	427	382	2	0	0

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

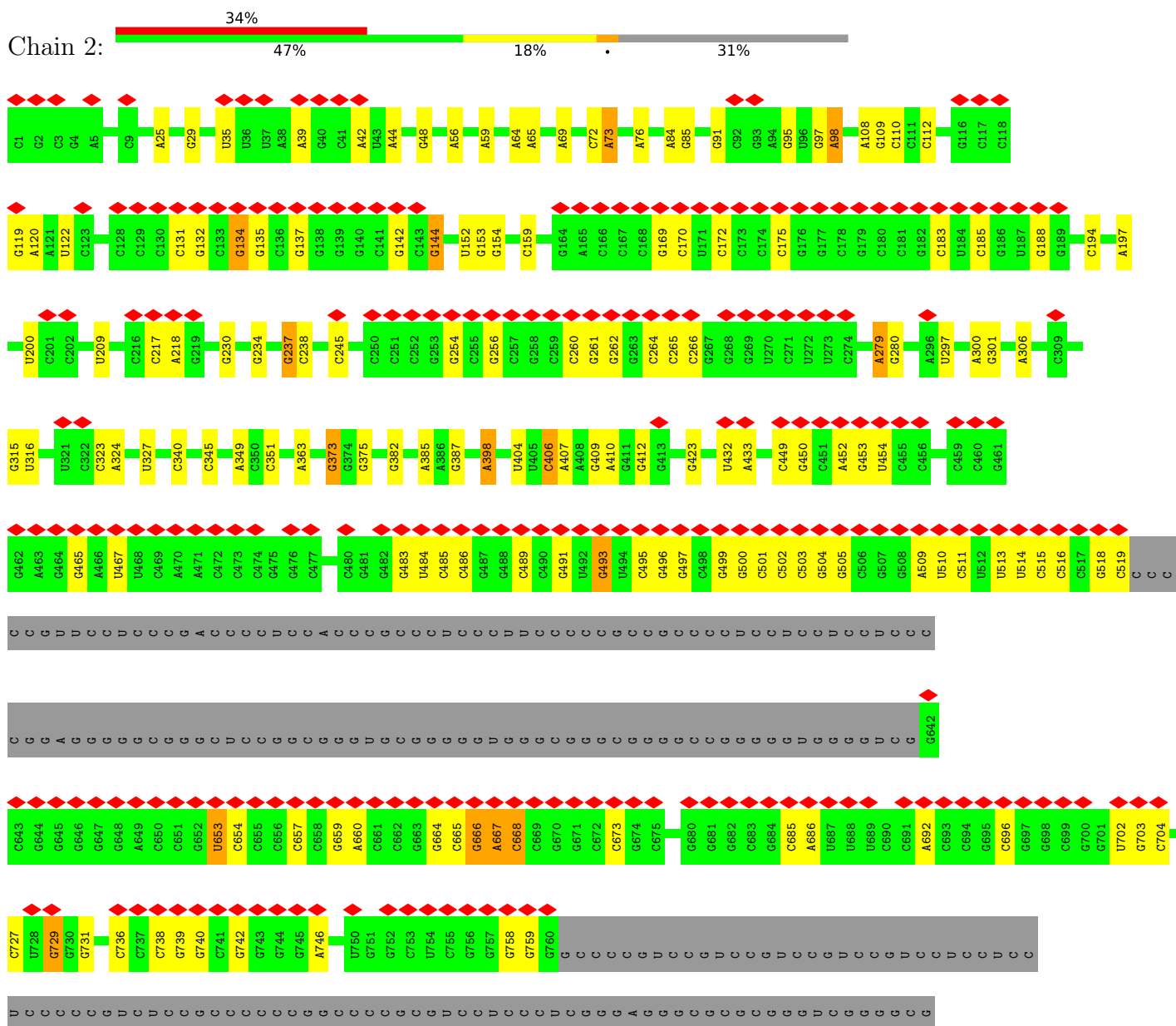
- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

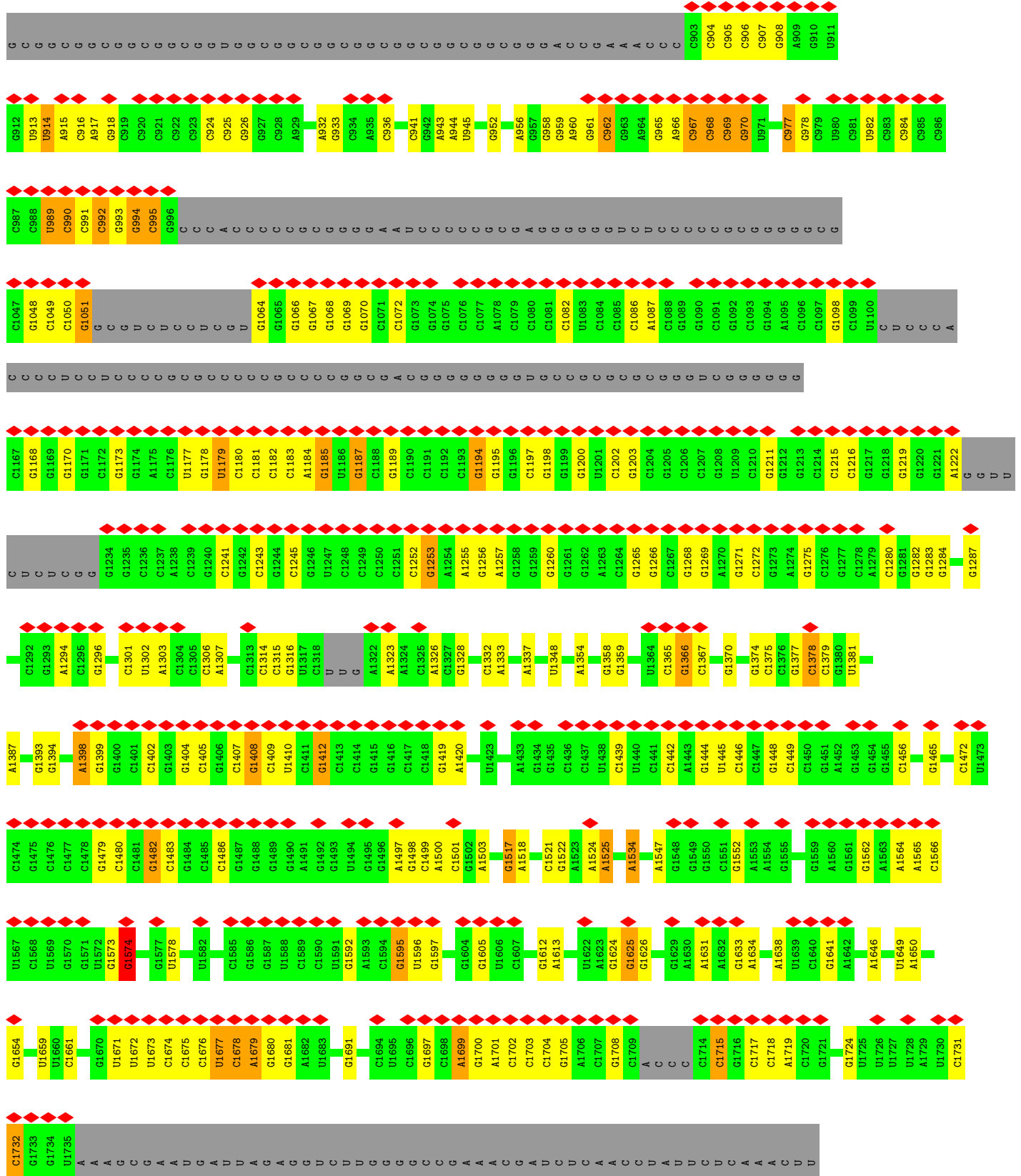
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	w	1	1	1	0

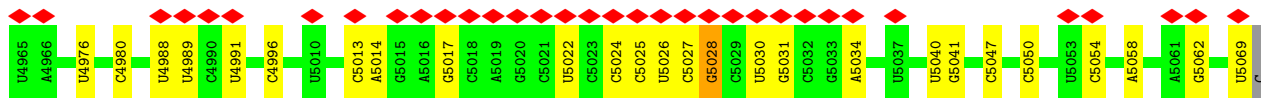
3 Residue-property plots i

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

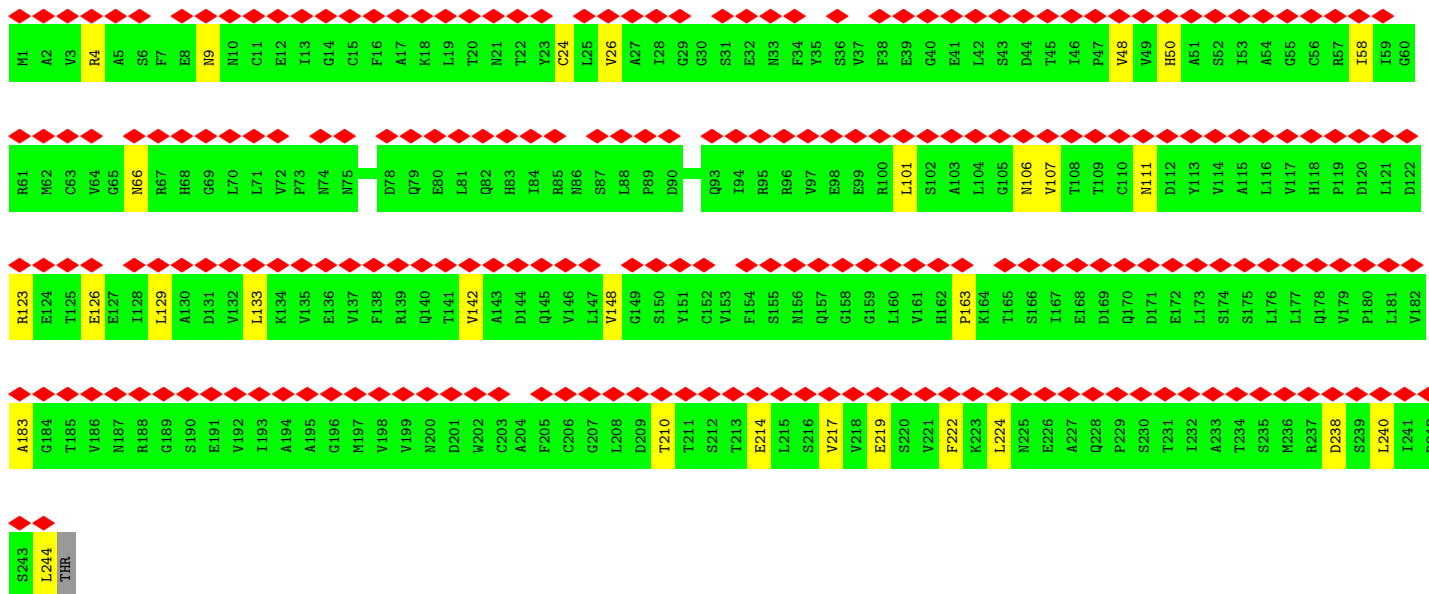
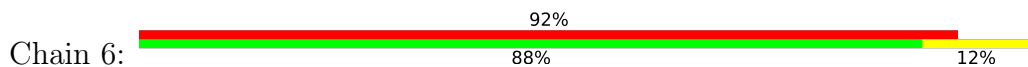
• Molecule 1: 28S rRNA



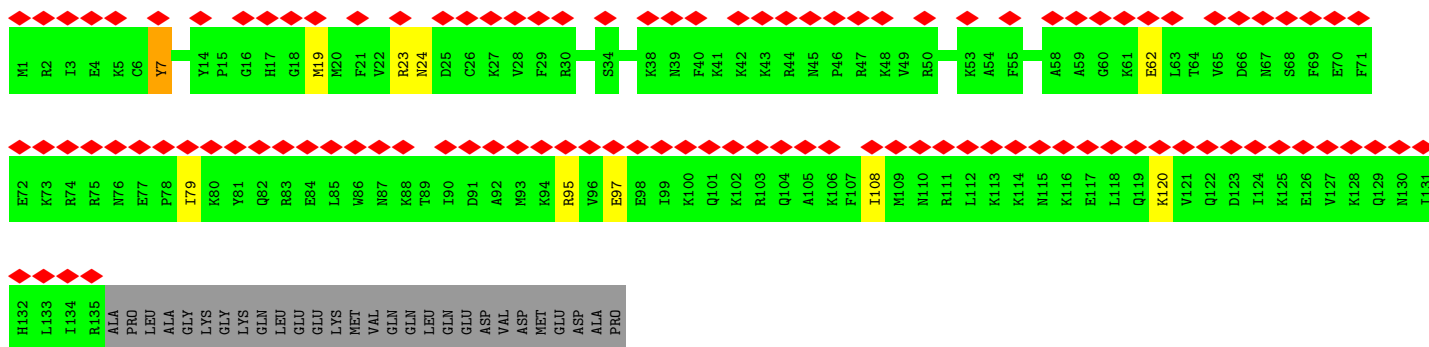
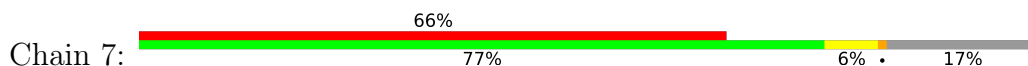




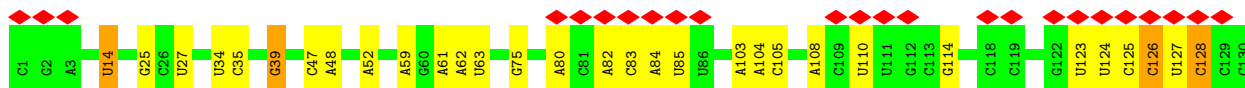
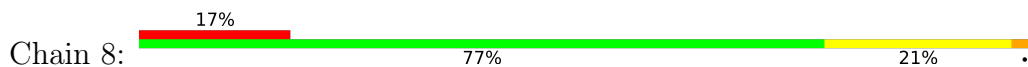
• Molecule 2: Eukaryotic translation initiation factor 6



• Molecule 3: Probable ribosome biogenesis protein RLP24

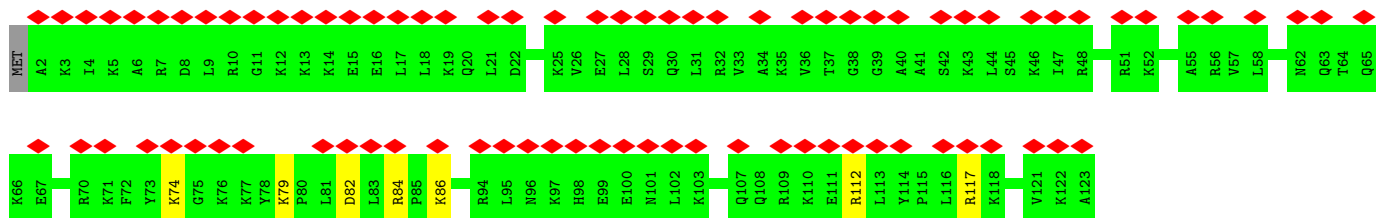
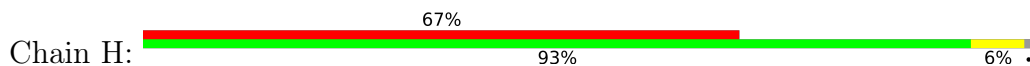


• Molecule 4: 5.8S rRNA

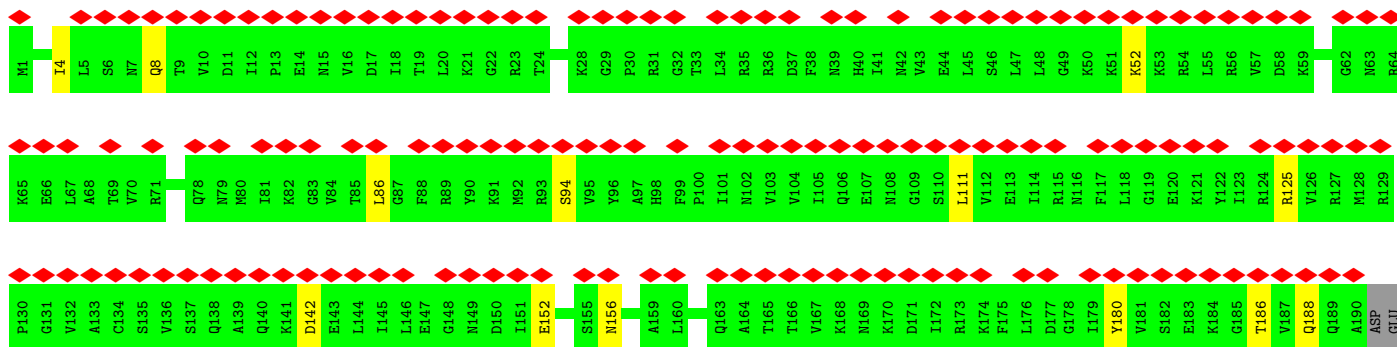
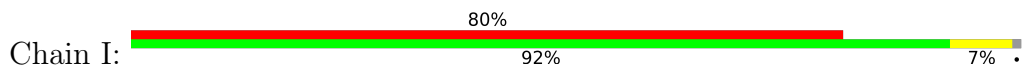




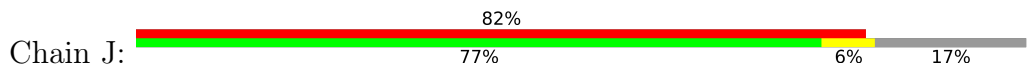
• Molecule 11: 60S ribosomal protein L35

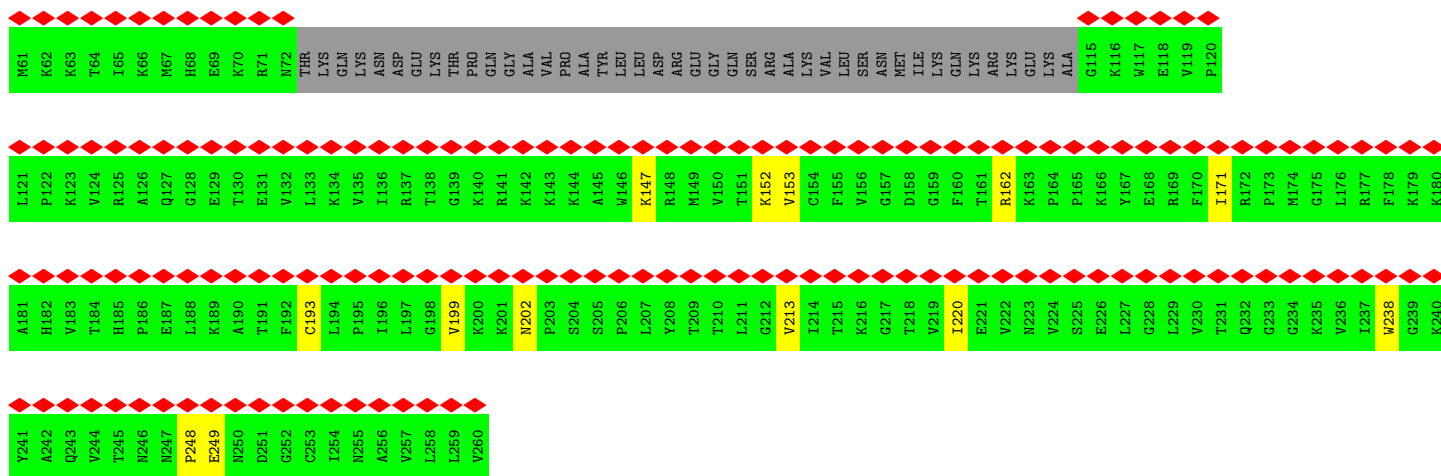


• Molecule 12: 60S ribosomal protein L9

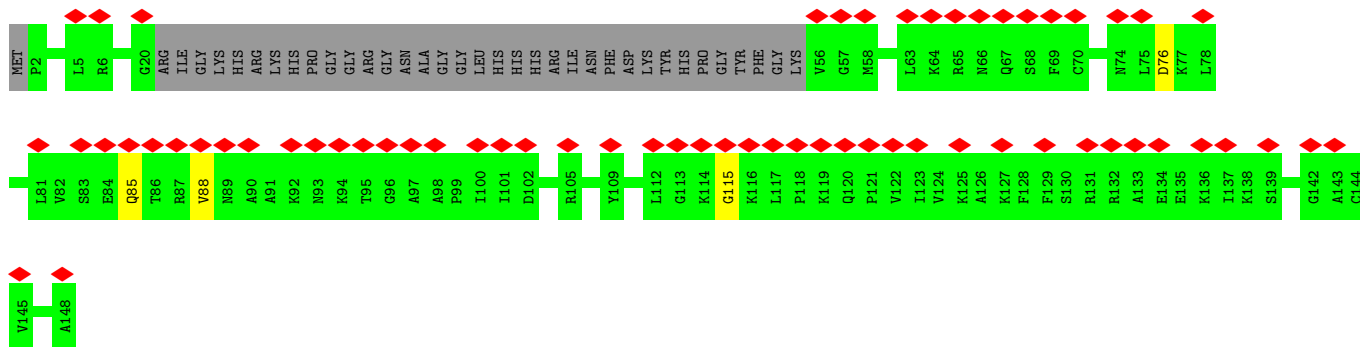
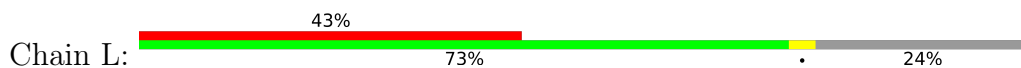


• Molecule 13: Ribosome biogenesis protein NSA2 homolog

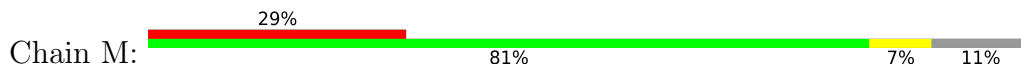




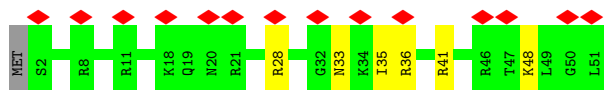
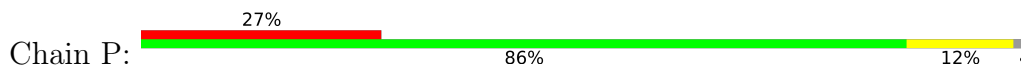
• Molecule 14: 60S ribosomal protein L27a



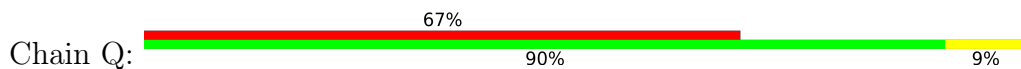
• Molecule 15: 60S ribosomal protein L37

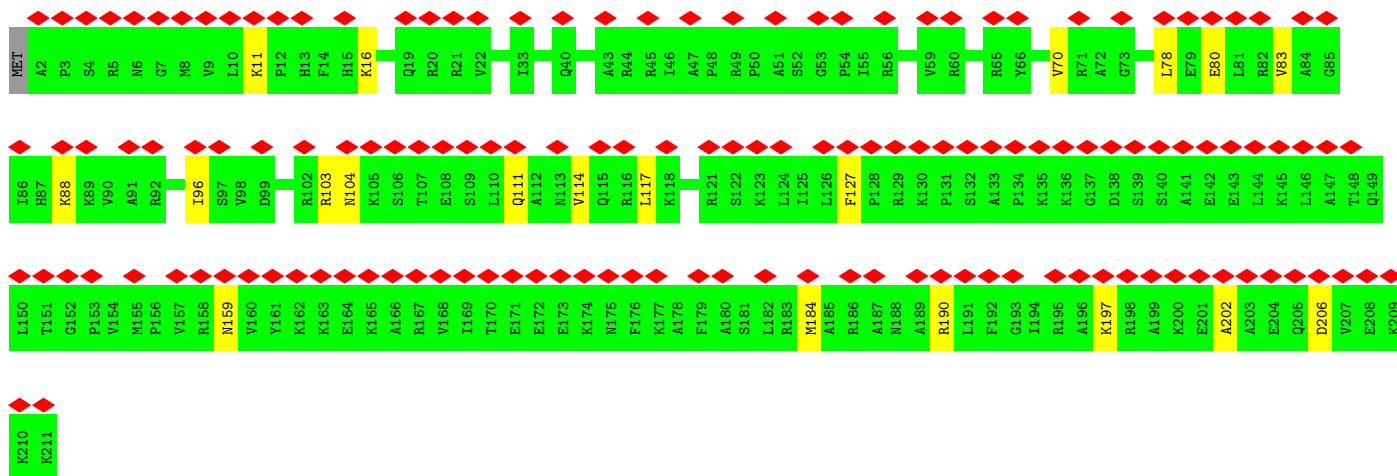


• Molecule 16: 60S ribosomal protein L39

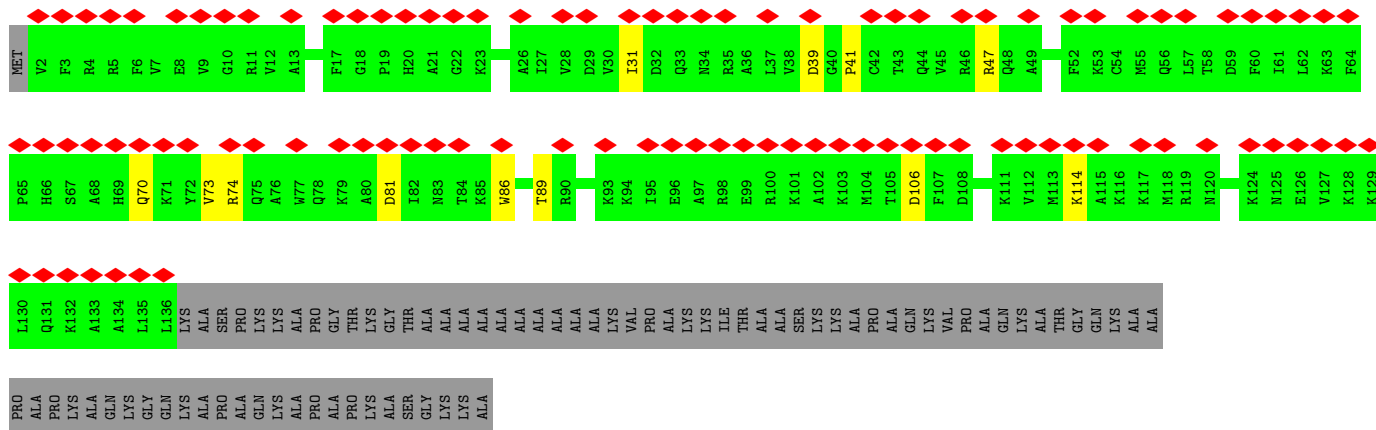


• Molecule 17: 60S ribosomal protein L13

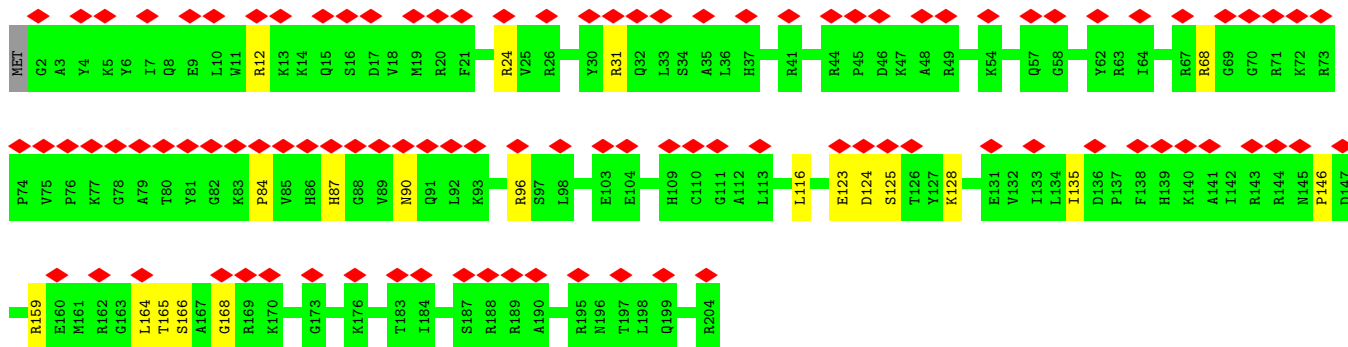
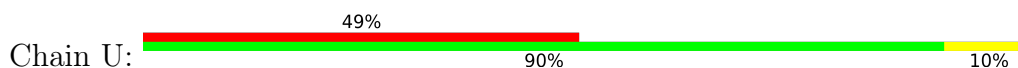




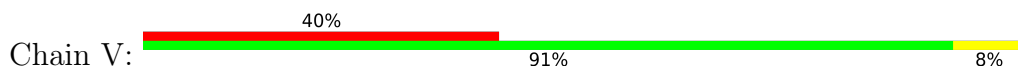
• Molecule 18: 60S ribosomal protein L14



• Molecule 19: 60S ribosomal protein L15

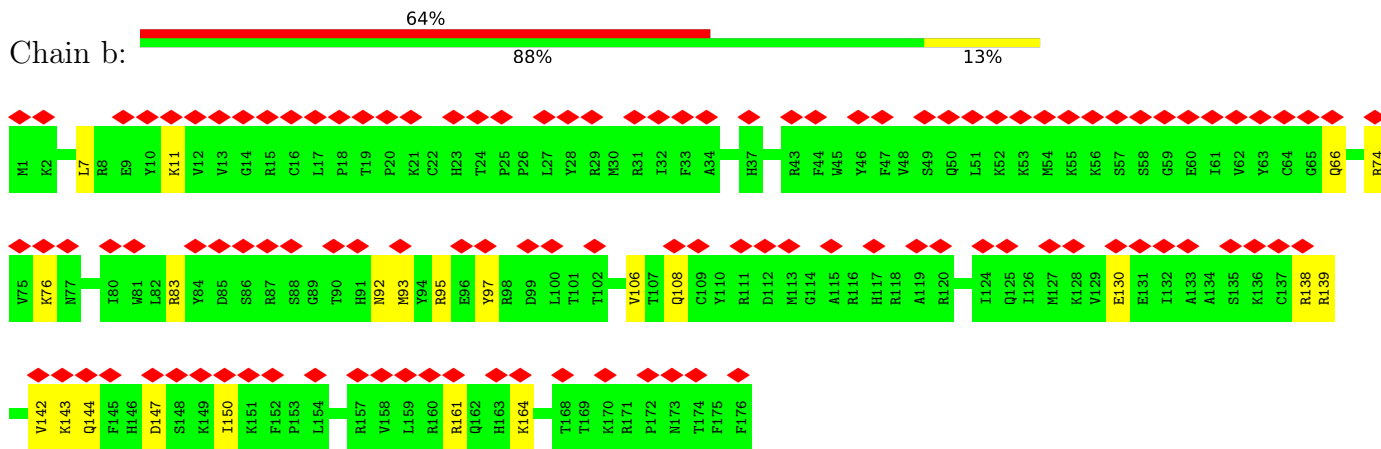


• Molecule 20: 60S ribosomal protein L13a

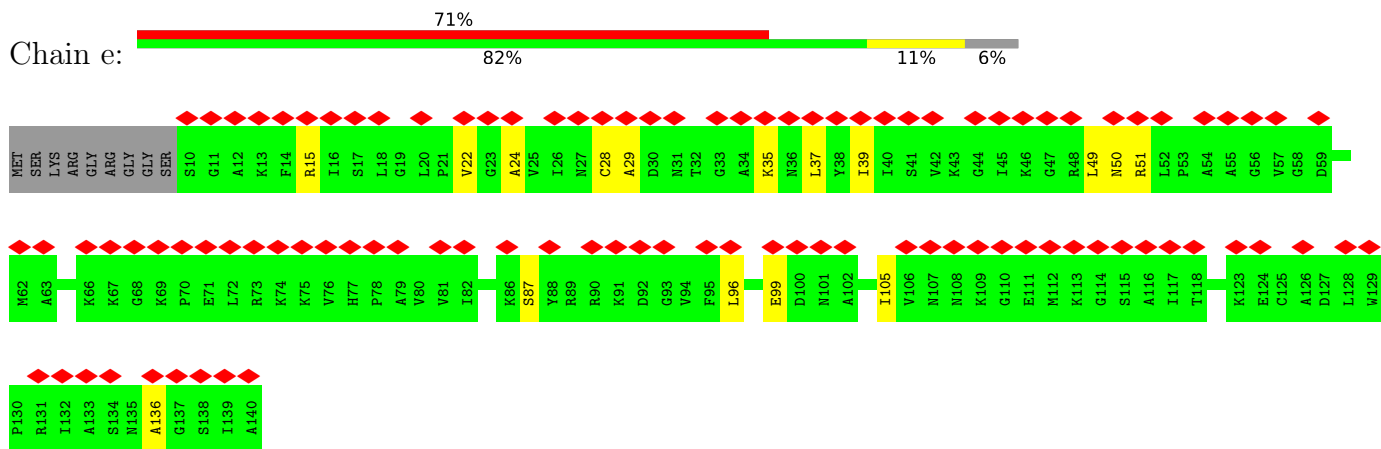


GLU
THR
LYS
LYS

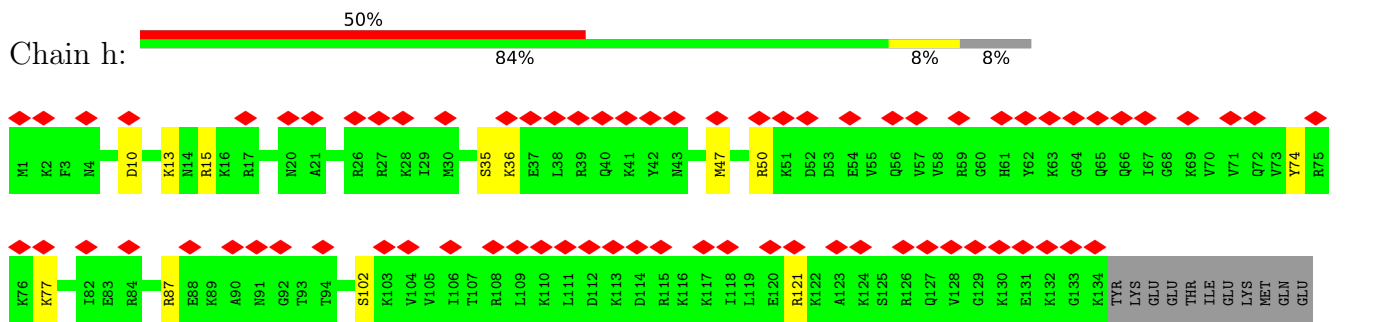
• Molecule 24: 60S ribosomal protein L18a



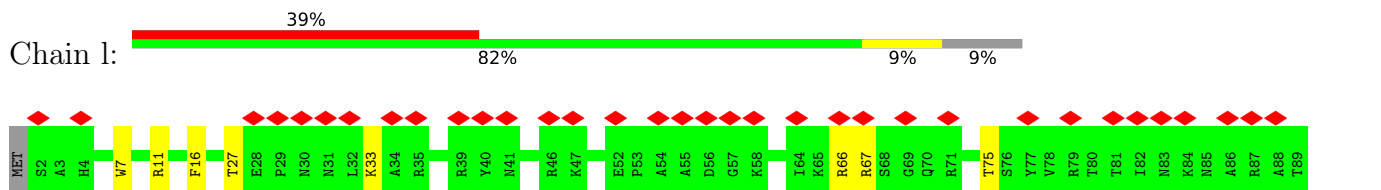
• Molecule 25: 60S ribosomal protein L23

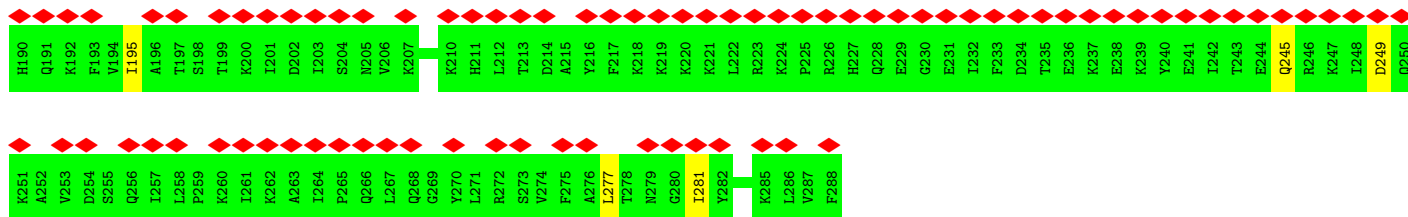


• Molecule 26: 60S ribosomal protein L26

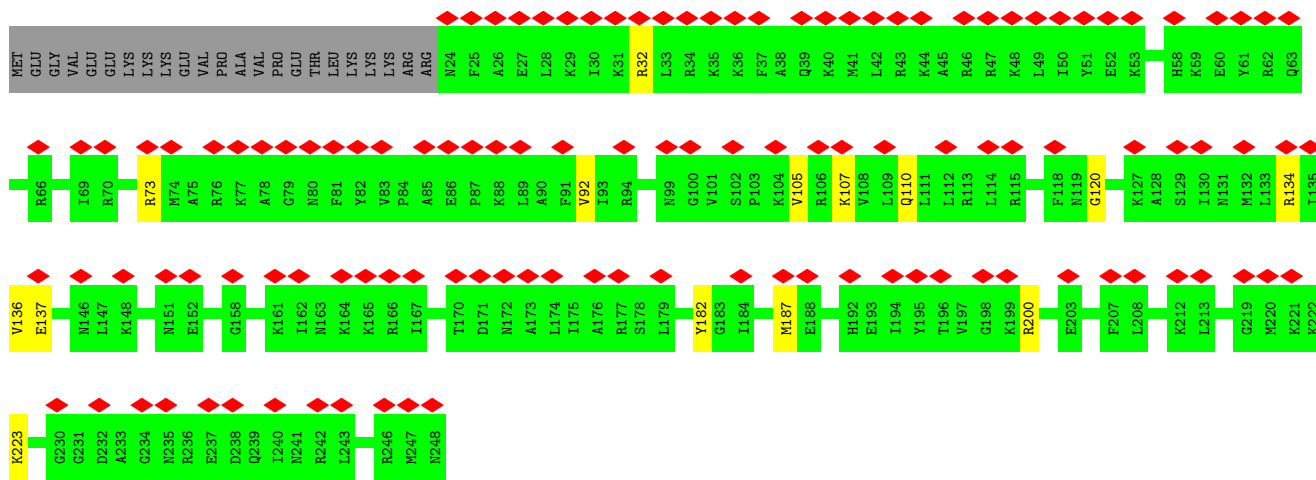
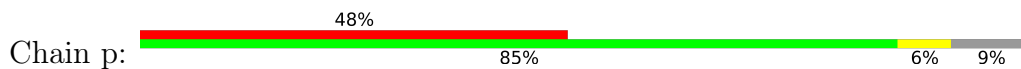


• Molecule 27: 60S ribosomal protein L28

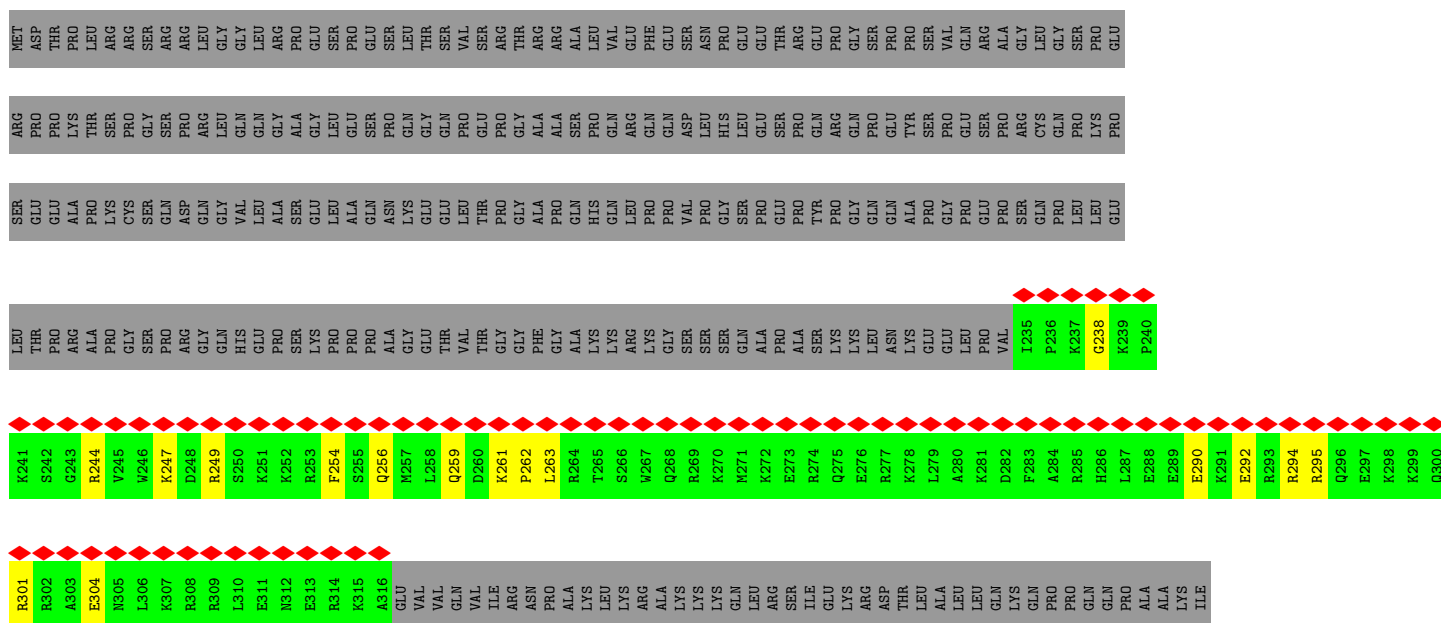




• Molecule 31: 60S ribosomal protein L7



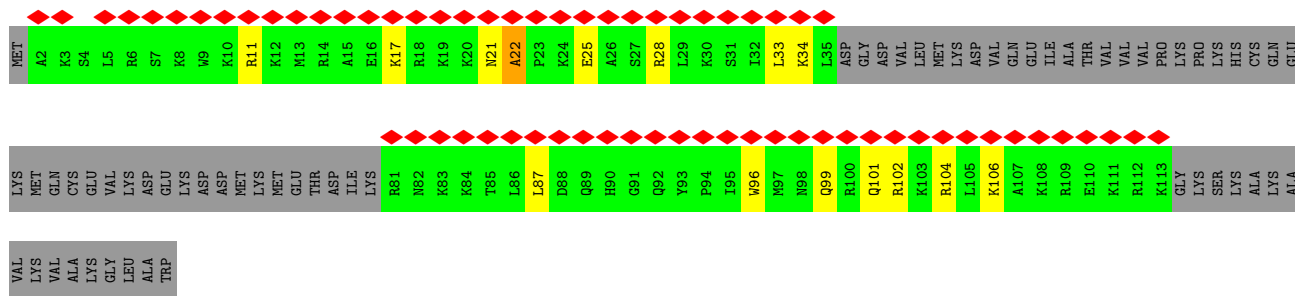
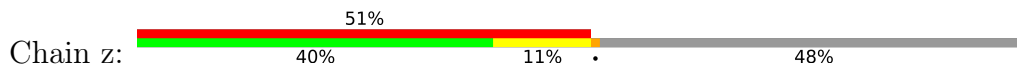
• Molecule 32: Coiled-coil domain-containing protein 86



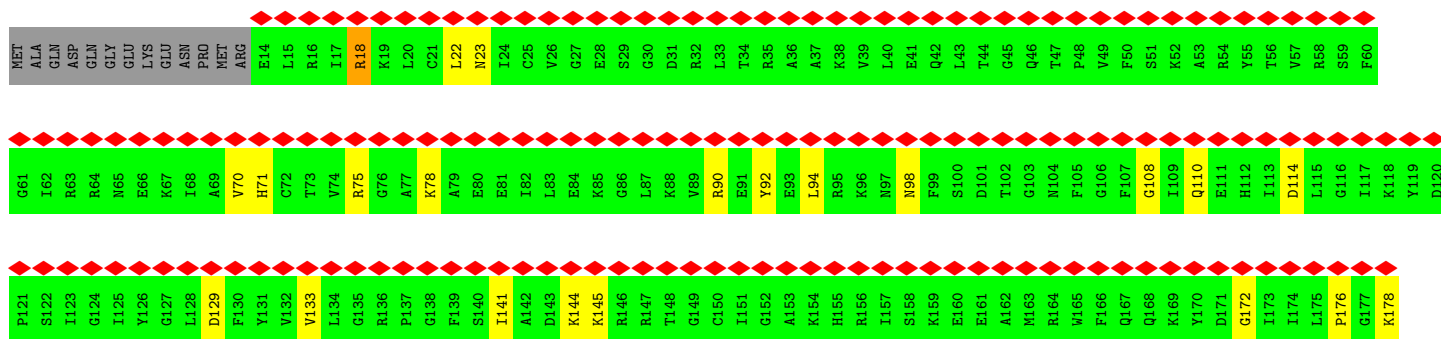
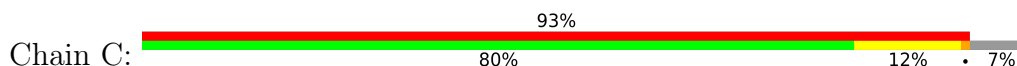
• Molecule 33: Guanine nucleotide-binding protein-like 3



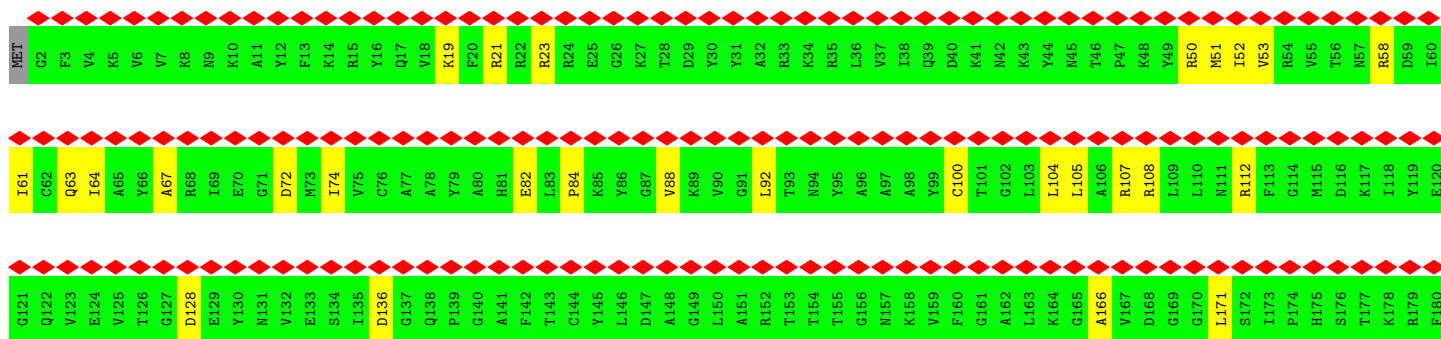
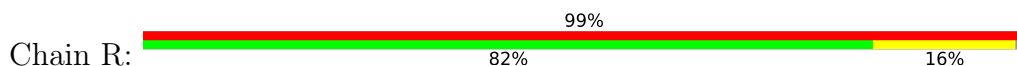
• Molecule 37: Protein LLP homolog



• Molecule 38: 60S ribosomal protein L11

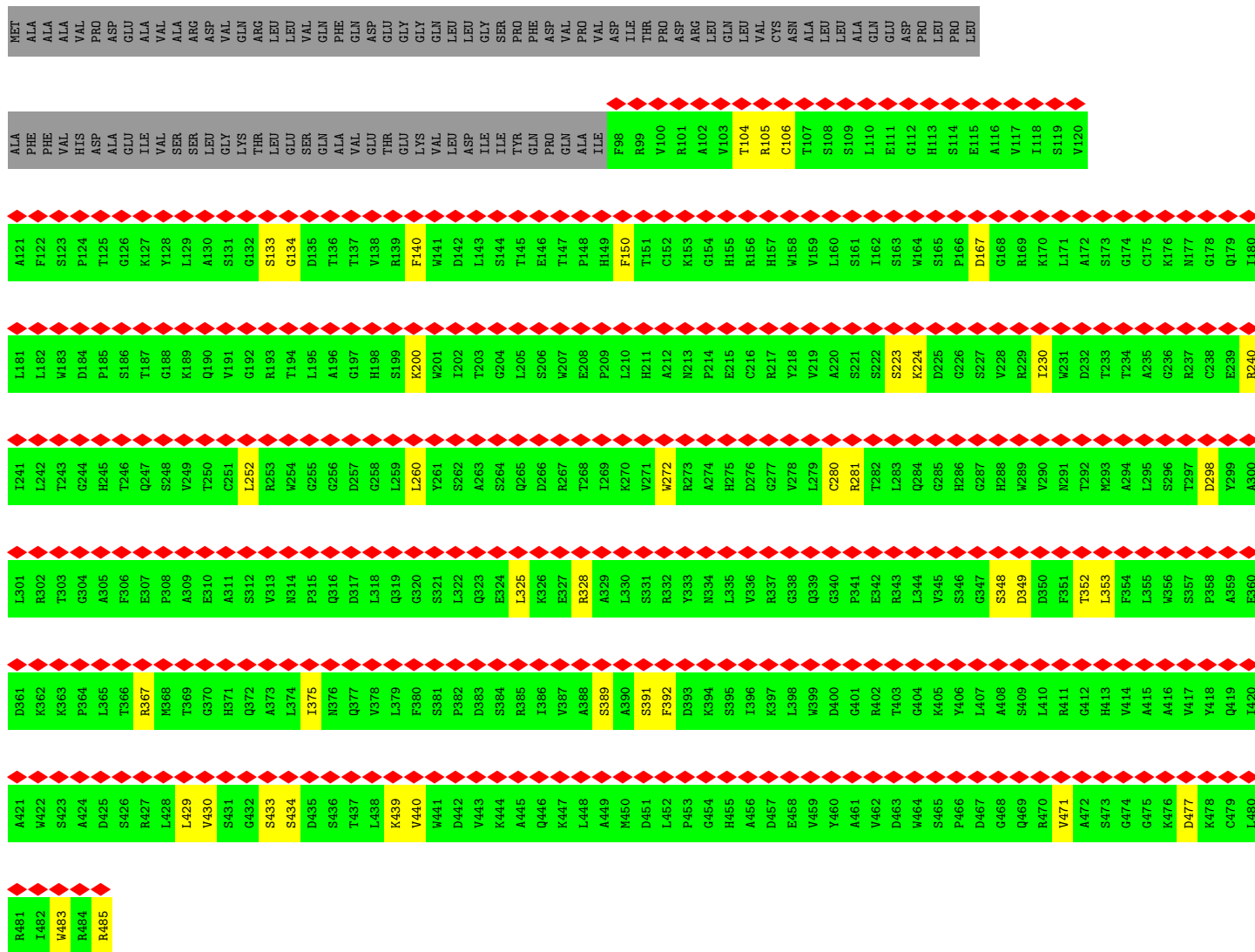
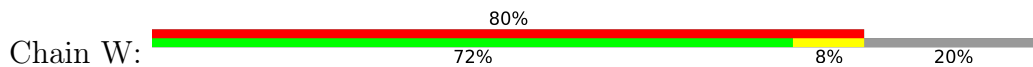


• Molecule 39: 60S ribosomal protein L5

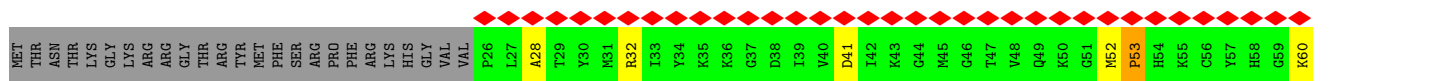
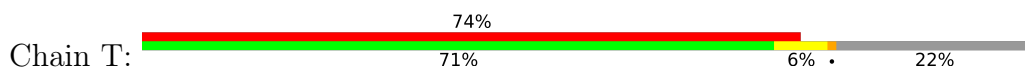


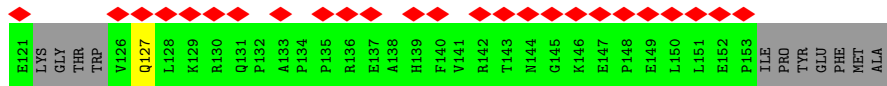
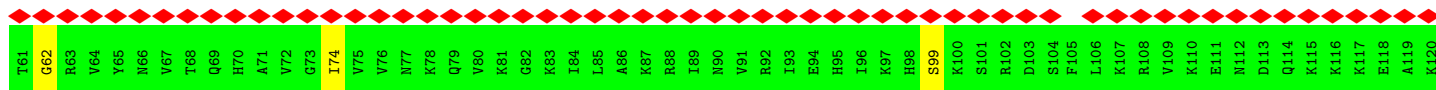


• Molecule 40: Notchless protein homolog 1

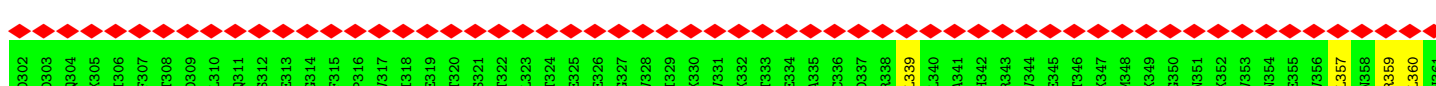
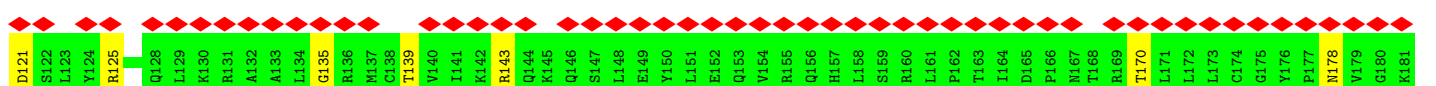
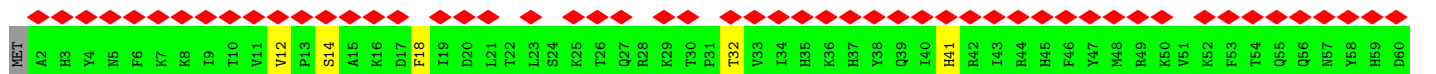
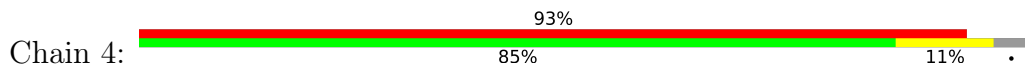


• Molecule 41: 60S ribosomal protein L21

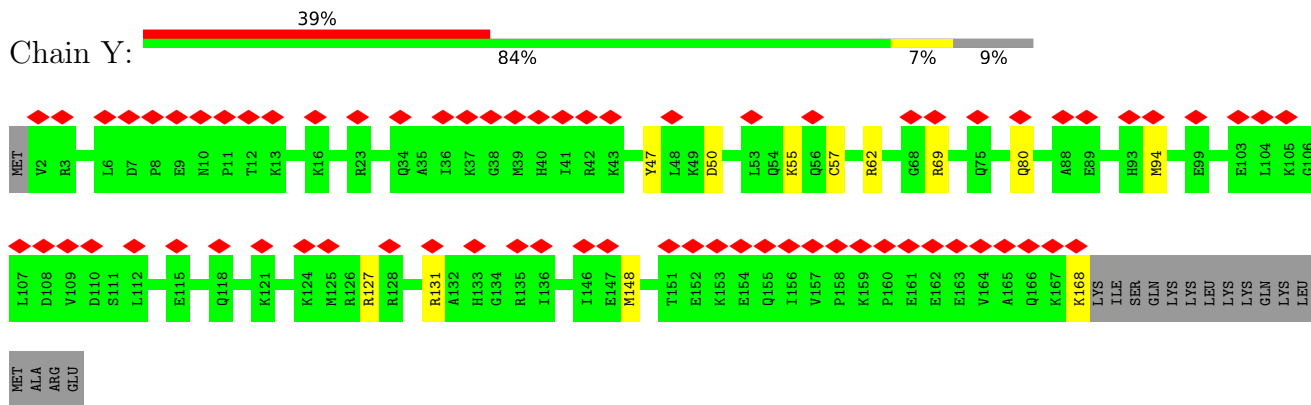




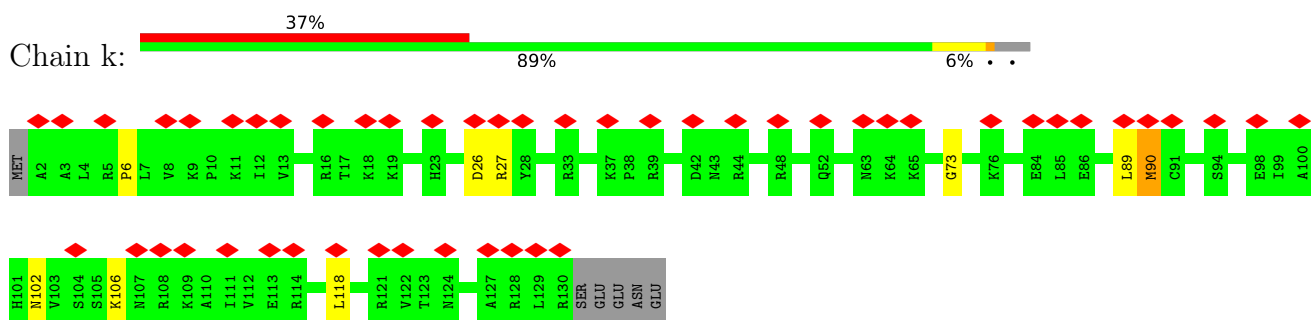
• Molecule 42: GTP-binding protein 4



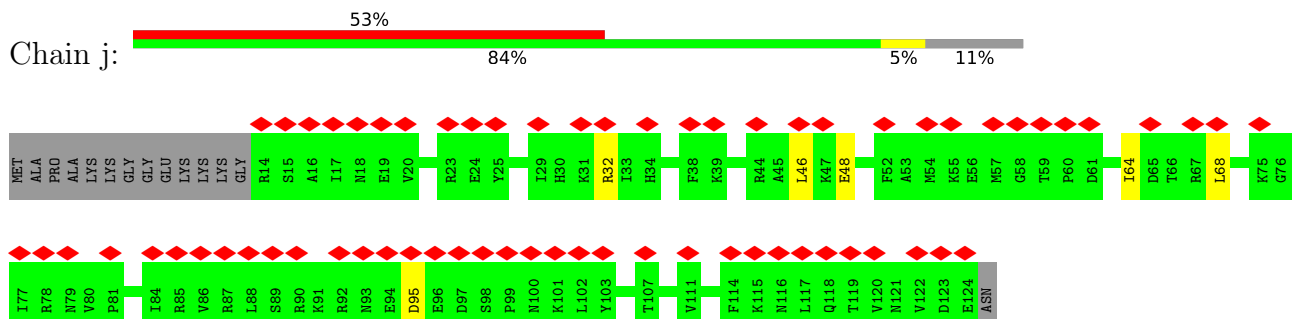
• Molecule 43: 60S ribosomal protein L17



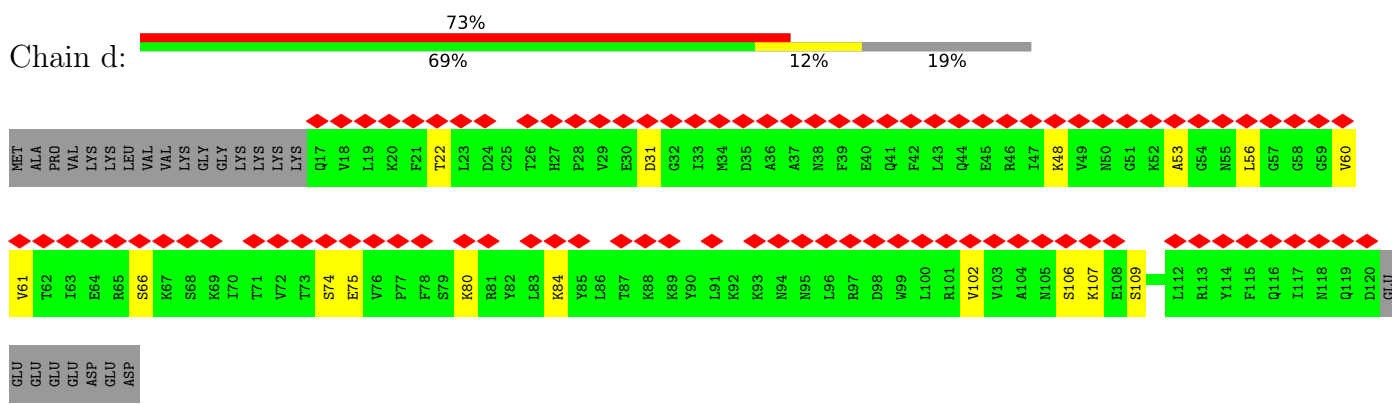
• Molecule 44: 60S ribosomal protein L32



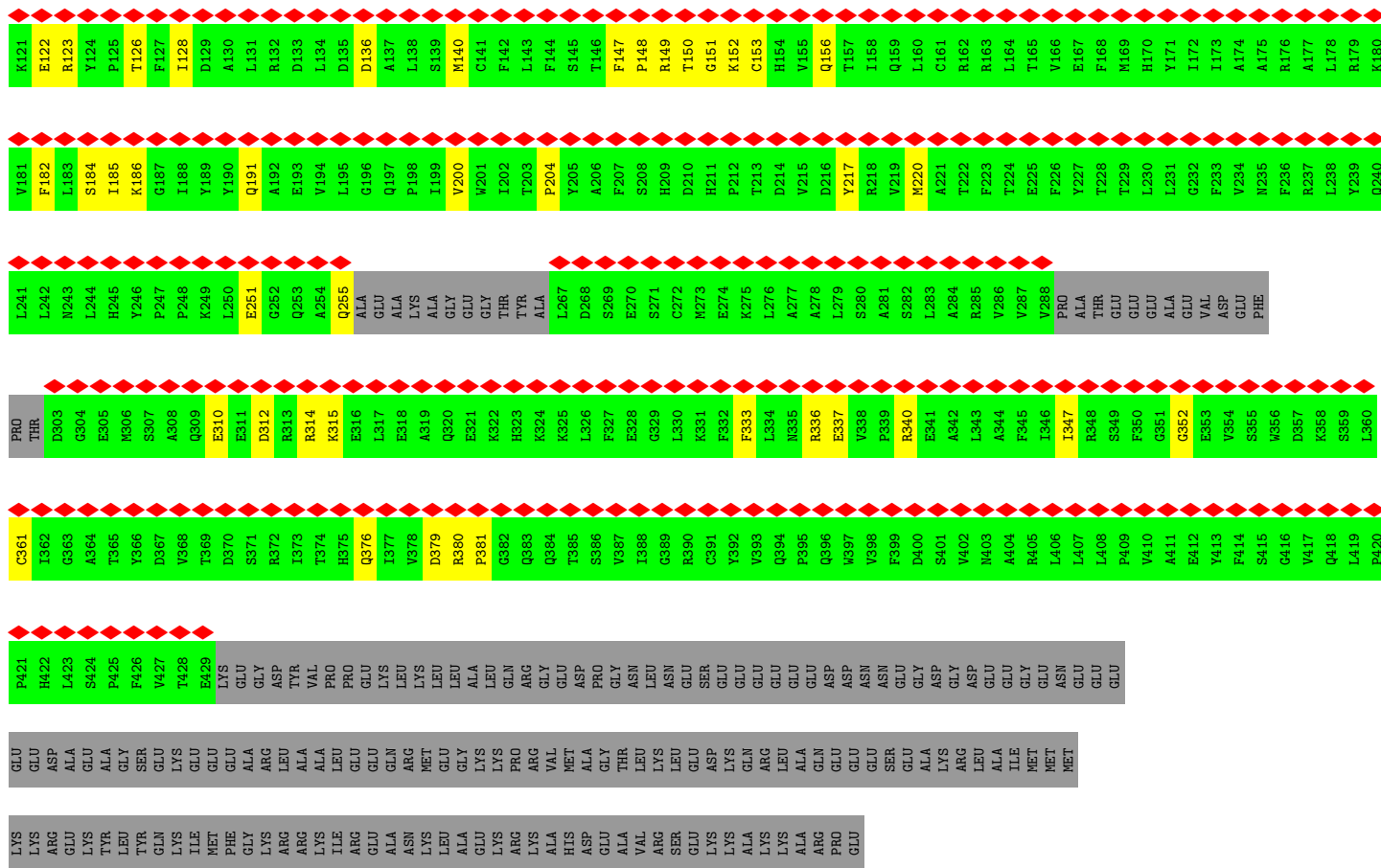
• Molecule 45: 60S ribosomal protein L31



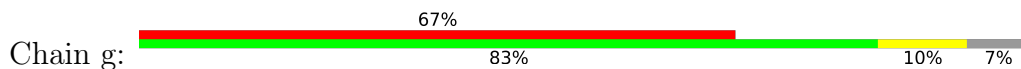
• Molecule 46: 60S ribosomal protein L22



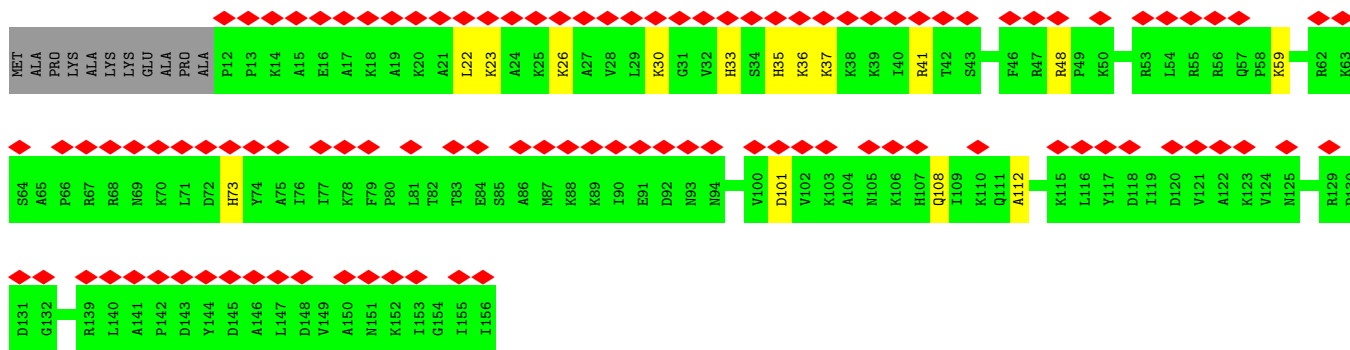
• Molecule 47: MKI67 FHA domain-interacting nucleolar phosphoprotein



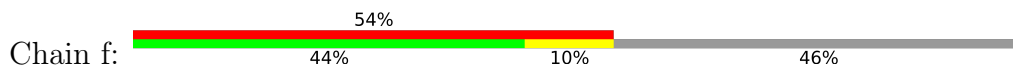
• Molecule 57: 60S ribosomal protein L23a



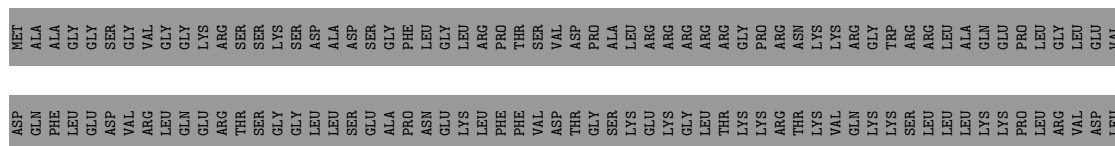
Chain g:



• Molecule 58: Ribosome biogenesis protein NOP53



Chain f:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4919	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	548.0, 548.0, 548.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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: B9B, OMG, GTP, B8W, 5MU, B9H, P4U, 2MG, M7A, OMU, 7MG, BGH, B8Q, A2M, OMC, B8K, P7G, MG, UR3, B8T, I4U, E7G

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	2	0.23	0/81689	0.44	21/127350 (0.0%)
2	6	0.26	0/1877	0.65	1/2554 (0.0%)
3	7	0.32	0/1181	0.64	2/1563 (0.1%)
4	8	0.23	0/3679	0.41	0/5732
5	9	0.29	0/723	0.75	3/961 (0.3%)
6	A	0.24	0/354	0.63	0/465
7	B	0.26	0/3315	0.63	4/4435 (0.1%)
8	D	0.25	0/2907	0.61	4/3905 (0.1%)
9	E	0.28	0/774	0.69	0/1038
10	G	0.31	0/1960	0.74	4/2637 (0.2%)
11	H	0.27	0/1023	0.57	0/1351
12	I	0.28	0/1537	0.66	1/2066 (0.0%)
13	J	0.20	0/1808	0.48	0/2414
14	L	0.21	0/893	0.52	0/1193
15	M	0.27	0/720	0.61	0/952
16	P	0.27	0/454	0.50	0/599
17	Q	0.28	0/1732	0.58	0/2315
18	S	0.31	0/1133	0.69	2/1516 (0.1%)
19	U	0.23	0/1746	0.55	2/2338 (0.1%)
20	V	0.29	0/1682	0.62	2/2250 (0.1%)
21	X	0.28	0/718	0.69	0/953
22	Z	0.24	0/1239	0.52	0/1658
23	a	0.28	0/1255	0.69	4/1662 (0.2%)
24	b	0.21	0/1501	0.46	0/2013
25	e	0.23	0/993	0.60	0/1332
26	h	0.25	0/1132	0.59	0/1504
27	l	0.26	0/1017	0.57	0/1364
28	m	0.26	0/1936	0.64	0/2596
29	n	0.25	0/895	0.66	3/1198 (0.3%)
30	o	0.27	0/1935	0.67	2/2596 (0.1%)
31	p	0.31	0/1916	0.60	0/2553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	r	0.37	0/732	0.82	1/960 (0.1%)
33	u	0.30	0/576	0.71	2/755 (0.3%)
34	v	0.26	0/1806	0.62	0/2420
35	w	0.26	0/3541	0.59	0/4775
36	y	0.30	0/1269	0.71	0/1712
37	z	0.35	1/587 (0.2%)	0.68	0/767
38	C	0.30	0/1341	0.73	2/1793 (0.1%)
39	R	0.30	0/2428	0.74	3/3252 (0.1%)
40	W	0.25	0/3093	0.63	0/4196
41	T	0.27	0/1018	0.67	1/1357 (0.1%)
42	4	0.33	0/5099	0.80	15/6840 (0.2%)
43	Y	0.25	0/1383	0.57	0/1856
44	k	0.23	0/1082	0.62	1/1443 (0.1%)
45	j	0.25	0/933	0.56	0/1256
46	d	0.27	0/864	0.75	2/1160 (0.2%)
47	t	0.29	0/955	0.68	0/1290
49	N	0.25	0/1956	0.58	1/2631 (0.0%)
50	1	0.28	1/1933 (0.1%)	0.65	2/2591 (0.1%)
51	K	0.29	0/843	0.67	0/1115
52	F	0.25	0/907	0.55	0/1209
53	i	0.27	0/1130	0.61	0/1507
54	O	0.32	0/575	0.79	0/761
55	3	0.24	0/2739	0.49	1/4266 (0.0%)
56	q	0.31	0/3395	0.69	0/4578
57	g	0.29	0/1191	0.61	0/1595
58	f	0.26	0/2169	0.65	2/2902 (0.1%)
All	All	0.25	2/169269 (0.0%)	0.54	88/246050 (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
6	A	0	1
7	B	0	1
10	G	0	2
29	n	0	1
32	r	0	1
33	u	0	1
41	T	0	1
42	4	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	Y	0	1
47	t	0	1
50	1	0	1
58	f	0	1
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	z	22	ALA	C-N	5.64	1.40	1.34
50	1	152	PRO	CG-CD	-5.28	1.32	1.50

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1871	A2M	OP2-P-O3'	-15.92	70.18	105.20
1	2	1871	A2M	OP1-P-O3'	14.70	137.55	105.20
1	2	1872	G	OP1-P-OP2	-13.63	78.71	119.60
1	2	1872	G	O5'-P-OP1	-9.23	80.30	108.00
50	1	152	PRO	N-CD-CG	-8.68	90.18	103.20

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	107	ARG	Sidechain
7	B	241	PRO	Peptide
10	G	162	ASP	Peptide
10	G	189	ARG	Sidechain
29	n	106	TYR	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	2	74602	0	37551	265	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6	1852	0	1828	17	0
3	7	1159	0	1224	9	0
4	8	3315	0	1684	8	0
5	9	711	0	724	7	0
6	A	352	0	398	3	0
7	B	3244	0	3389	28	0
8	D	2853	0	3028	22	0
9	E	764	0	804	5	0
10	G	1927	0	2074	13	0
11	H	1015	0	1148	6	0
12	I	1518	0	1601	8	0
13	J	1772	0	1892	11	0
14	L	877	0	938	3	0
15	M	705	0	741	5	0
16	P	444	0	483	5	0
17	Q	1701	0	1818	16	0
18	S	1111	0	1174	8	0
19	U	1701	0	1749	13	0
20	V	1650	0	1794	8	0
21	X	708	0	760	6	0
22	Z	1223	0	1330	10	0
23	a	1239	0	1363	10	0
24	b	1461	0	1502	17	0
25	e	979	0	1039	12	0
26	h	1115	0	1205	10	0
27	l	1002	0	1068	9	0
28	m	1898	0	1993	8	0
29	n	876	0	912	3	0
30	o	1897	0	2046	19	0
31	p	1878	0	2009	9	0
32	r	723	0	770	9	0
33	u	569	0	635	2	0
34	v	1771	0	1810	12	0
35	w	3472	0	3527	23	0
36	y	1250	0	1305	12	0
37	z	581	0	656	10	0
38	C	1319	0	1358	14	0
39	R	2382	0	2410	31	0
40	W	3018	0	2959	24	0
41	T	1001	0	1064	5	0
42	4	5016	0	5153	45	0
43	Y	1355	0	1389	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	k	1064	0	1160	7	0
45	j	918	0	964	5	0
46	d	850	0	868	9	0
47	t	928	0	906	9	0
48	x	684	0	456	2	0
49	N	1924	0	2027	12	0
50	1	1897	0	2029	12	0
51	K	832	0	917	3	0
52	F	897	0	989	2	0
53	i	1107	0	1182	19	0
54	O	569	0	635	5	0
55	3	2453	0	1243	15	0
56	q	3317	0	3368	62	0
57	g	1170	0	1283	36	0
58	f	2137	0	2201	111	0
59	w	32	0	12	0	0
60	w	1	0	0	0	0
All	All	160786	0	124545	799	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 3.

The worst 5 of 799 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)
57:g:30:LYS:HE3	58:f:473:PHE:CE1	1.24	1.70
1:2:4083:5MU:C5	1:2:4083:5MU:C4	1.79	1.68
56:q:186:LYS:NZ	58:f:417:ASP:HB2	1.41	1.34
57:g:37:LYS:HE2	58:f:465:VAL:CG2	1.59	1.33
57:g:33:HIS:HB2	58:f:473:PHE:CZ	1.63	1.32

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	
2	6	242/245 (99%)	227 (94%)	15 (6%)	0	100	100
3	7	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
5	9	82/134 (61%)	71 (87%)	11 (13%)	0	100	100
6	A	41/159 (26%)	39 (95%)	2 (5%)	0	100	100
7	B	401/403 (100%)	382 (95%)	18 (4%)	1 (0%)	43	77
8	D	356/427 (83%)	334 (94%)	22 (6%)	0	100	100
9	E	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
10	G	239/266 (90%)	225 (94%)	14 (6%)	0	100	100
11	H	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
12	I	188/192 (98%)	179 (95%)	9 (5%)	0	100	100
13	J	213/260 (82%)	207 (97%)	6 (3%)	0	100	100
14	L	108/148 (73%)	101 (94%)	7 (6%)	0	100	100
15	M	84/97 (87%)	80 (95%)	4 (5%)	0	100	100
16	P	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
17	Q	208/211 (99%)	200 (96%)	8 (4%)	0	100	100
18	S	133/215 (62%)	127 (96%)	6 (4%)	0	100	100
19	U	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
20	V	199/203 (98%)	192 (96%)	7 (4%)	0	100	100
21	X	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
22	Z	149/188 (79%)	147 (99%)	2 (1%)	0	100	100
23	a	146/196 (74%)	142 (97%)	4 (3%)	0	100	100
24	b	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
25	e	129/140 (92%)	118 (92%)	11 (8%)	0	100	100
26	h	132/145 (91%)	126 (96%)	6 (4%)	0	100	100
27	l	123/137 (90%)	115 (94%)	8 (6%)	0	100	100
28	m	246/257 (96%)	221 (90%)	25 (10%)	0	100	100
29	n	107/110 (97%)	102 (95%)	5 (5%)	0	100	100
30	o	231/288 (80%)	220 (95%)	11 (5%)	0	100	100
31	p	224/248 (90%)	216 (96%)	8 (4%)	0	100	100
32	r	80/360 (22%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	u	63/549 (12%)	58 (92%)	4 (6%)	1 (2%)	7	37
34	v	215/239 (90%)	206 (96%)	9 (4%)	0	100	100
35	w	427/731 (58%)	406 (95%)	19 (4%)	2 (0%)	24	62
36	y	163/165 (99%)	155 (95%)	8 (5%)	0	100	100
37	z	63/129 (49%)	60 (95%)	3 (5%)	0	100	100
38	C	163/178 (92%)	145 (89%)	18 (11%)	0	100	100
39	R	291/297 (98%)	273 (94%)	17 (6%)	1 (0%)	36	71
40	W	386/485 (80%)	365 (95%)	21 (5%)	0	100	100
41	T	120/160 (75%)	112 (93%)	8 (7%)	0	100	100
42	4	607/634 (96%)	555 (91%)	47 (8%)	5 (1%)	16	52
43	Y	165/184 (90%)	158 (96%)	7 (4%)	0	100	100
44	k	127/135 (94%)	120 (94%)	7 (6%)	0	100	100
45	j	109/125 (87%)	103 (94%)	6 (6%)	0	100	100
46	d	102/128 (80%)	95 (93%)	7 (7%)	0	100	100
47	t	109/293 (37%)	105 (96%)	4 (4%)	0	100	100
49	N	237/490 (48%)	231 (98%)	6 (2%)	0	100	100
50	1	224/255 (88%)	216 (96%)	7 (3%)	1 (0%)	30	66
51	K	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
52	F	111/117 (95%)	109 (98%)	2 (2%)	0	100	100
53	i	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
54	O	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
56	q	398/588 (68%)	382 (96%)	16 (4%)	0	100	100
57	g	143/156 (92%)	135 (94%)	8 (6%)	0	100	100
58	f	254/478 (53%)	236 (93%)	17 (7%)	1 (0%)	30	66
All	All	9699/12780 (76%)	9184 (95%)	503 (5%)	12 (0%)	49	83

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	u	55	PRO
50	1	24	ASN
58	f	203	ASP
39	R	270	LYS
42	4	88	ASP

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	
2	6	212/213 (100%)	212 (100%)	0	100	100
3	7	126/149 (85%)	126 (100%)	0	100	100
5	9	74/114 (65%)	74 (100%)	0	100	100
6	A	34/126 (27%)	34 (100%)	0	100	100
7	B	349/349 (100%)	349 (100%)	0	100	100
8	D	298/348 (86%)	298 (100%)	0	100	100
9	E	83/97 (86%)	83 (100%)	0	100	100
10	G	203/223 (91%)	203 (100%)	0	100	100
11	H	109/110 (99%)	109 (100%)	0	100	100
12	I	169/171 (99%)	169 (100%)	0	100	100
13	J	191/228 (84%)	191 (100%)	0	100	100
14	L	94/121 (78%)	94 (100%)	0	100	100
15	M	73/80 (91%)	73 (100%)	0	100	100
16	P	47/48 (98%)	47 (100%)	0	100	100
17	Q	176/177 (99%)	176 (100%)	0	100	100
18	S	115/161 (71%)	115 (100%)	0	100	100
19	U	171/172 (99%)	171 (100%)	0	100	100
20	V	173/174 (99%)	173 (100%)	0	100	100
21	X	74/75 (99%)	74 (100%)	0	100	100
22	Z	136/165 (82%)	136 (100%)	0	100	100
23	a	133/175 (76%)	133 (100%)	0	100	100
24	b	157/157 (100%)	157 (100%)	0	100	100
25	e	101/107 (94%)	101 (100%)	0	100	100
26	h	124/135 (92%)	124 (100%)	0	100	100
27	l	109/121 (90%)	109 (100%)	0	100	100
28	m	190/199 (96%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	n	88/89 (99%)	88 (100%)	0	100	100
30	o	208/252 (82%)	208 (100%)	0	100	100
31	p	195/215 (91%)	195 (100%)	0	100	100
32	r	76/312 (24%)	76 (100%)	0	100	100
33	u	61/485 (13%)	61 (100%)	0	100	100
34	v	194/214 (91%)	194 (100%)	0	100	100
35	w	385/654 (59%)	385 (100%)	0	100	100
36	y	137/137 (100%)	137 (100%)	0	100	100
37	z	61/115 (53%)	61 (100%)	0	100	100
38	C	138/149 (93%)	138 (100%)	0	100	100
39	R	246/250 (98%)	246 (100%)	0	100	100
40	W	322/404 (80%)	322 (100%)	0	100	100
41	T	109/140 (78%)	109 (100%)	0	100	100
42	4	554/574 (96%)	554 (100%)	0	100	100
43	Y	147/163 (90%)	147 (100%)	0	100	100
44	k	115/121 (95%)	115 (100%)	0	100	100
45	j	101/110 (92%)	101 (100%)	0	100	100
46	d	94/115 (82%)	94 (100%)	0	100	100
47	t	103/274 (38%)	103 (100%)	0	100	100
49	N	222/437 (51%)	222 (100%)	0	100	100
50	l	206/228 (90%)	206 (100%)	0	100	100
51	K	86/89 (97%)	86 (100%)	0	100	100
52	F	97/100 (97%)	97 (100%)	0	100	100
53	i	117/118 (99%)	117 (100%)	0	100	100
54	O	64/65 (98%)	64 (100%)	0	100	100
56	q	359/509 (70%)	359 (100%)	0	100	100
57	g	126/133 (95%)	126 (100%)	0	100	100
58	f	222/402 (55%)	222 (100%)	0	100	100
All	All	8554/11049 (77%)	8554 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89

such sidechains are listed below:

Mol	Chain	Res	Type
37	z	89	GLN
44	k	63	ASN
37	z	98	ASN
41	T	77	ASN
50	1	185	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	3451/5054 (68%)	818 (23%)	21 (0%)
4	8	155/156 (99%)	29 (18%)	0
48	x	0/60	-	-
55	3	113/120 (94%)	23 (20%)	2 (1%)
All	All	3719/5390 (68%)	870 (23%)	23 (0%)

5 of 870 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	25	A
1	2	39	A
1	2	42	A
1	2	44	A
1	2	48	G

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	3774	A
1	2	4228	G
1	2	3905	A
1	2	4555	U
1	2	1931	C

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

67 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	2	398	1	22,25,26	3.20	9 (40%)	31,36,39	2.94	10 (32%)
1	B8T	2	4483	1	19,22,23	3.66	8 (42%)	26,31,34	1.37	6 (23%)
1	UR3	2	4597	1	19,22,23	2.82	6 (31%)	26,32,35	1.88	3 (11%)
1	B8Q	2	1456	1	17,22,23	2.96	5 (29%)	22,32,35	2.21	6 (27%)
1	B8T	2	4671	1	19,22,23	3.61	8 (42%)	26,31,34	0.93	1 (3%)
1	OMG	2	2050	1	23,26,27	2.65	8 (34%)	33,38,41	2.72	11 (33%)
1	7MG	2	2522	1	22,26,27	3.76	10 (45%)	29,39,42	1.97	10 (34%)
1	OMC	2	3909	1	19,22,23	3.13	8 (42%)	26,31,34	1.85	7 (26%)
1	A2M	2	3718	1	22,25,26	3.20	9 (40%)	31,36,39	2.92	10 (32%)
1	BGH	2	3899	1	25,29,30	4.60	17 (68%)	31,43,46	2.58	11 (35%)
1	7MG	2	4550	1	22,26,27	3.85	10 (45%)	29,39,42	1.98	7 (24%)
1	OMG	2	2424	1	23,26,27	2.72	8 (34%)	33,38,41	2.91	10 (30%)
1	M7A	2	4564	1	20,25,26	2.02	3 (15%)	28,37,40	3.91	7 (25%)
1	A2M	2	1534	1	22,25,26	3.18	9 (40%)	31,36,39	2.99	10 (32%)
1	OMU	2	4620	1	19,22,23	2.97	8 (42%)	26,31,34	1.74	5 (19%)
1	B9B	2	1574	1	25,28,29	1.73	5 (20%)	35,40,43	5.15	11 (31%)
1	A2M	2	4523	1	22,25,26	3.16	9 (40%)	31,36,39	3.00	10 (32%)
1	OMG	2	2364	1	23,26,27	2.66	8 (34%)	33,38,41	2.73	11 (33%)
1	A2M	2	3723	1	22,25,26	3.17	9 (40%)	31,36,39	3.01	10 (32%)
1	A2M	2	3867	1	22,25,26	3.16	9 (40%)	31,36,39	2.98	10 (32%)
1	7MG	2	1605	1	22,26,27	3.87	10 (45%)	29,39,42	2.00	8 (27%)
1	P4U	2	1348	1	21,24,25	3.61	8 (38%)	27,33,36	1.06	2 (7%)
1	A2M	2	2401	1	22,25,26	3.20	9 (40%)	31,36,39	3.03	11 (35%)
1	A2M	2	1871	1	22,25,26	3.19	10 (45%)	31,36,39	2.97	11 (35%)
1	OMG	2	1625	1	23,26,27	2.71	8 (34%)	33,38,41	2.76	10 (30%)
1	OMC	2	3887	1	19,22,23	3.05	8 (42%)	26,31,34	1.01	1 (3%)
1	B8W	2	4472	1	23,26,27	2.74	5 (21%)	33,38,41	2.47	15 (45%)
1	2MG	2	1517	1	23,26,27	2.99	8 (34%)	32,38,41	2.35	8 (25%)
1	P7G	2	1909	1	24,28,29	4.09	11 (45%)	27,41,44	1.55	3 (11%)
1	A2M	2	2363	1	22,25,26	3.19	9 (40%)	31,36,39	2.98	11 (35%)
1	OMC	2	2422	1	19,22,23	3.03	8 (42%)	26,31,34	1.00	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	2	4494	1	23,26,27	2.71	8 (34%)	33,38,41	2.81	10 (30%)
1	B8W	2	4185	1	23,26,27	2.75	6 (26%)	33,38,41	2.61	13 (39%)
1	B8W	2	4529	1	23,26,27	2.78	5 (21%)	33,38,41	2.58	13 (39%)
1	A2M	2	1524	1	22,25,26	3.20	9 (40%)	31,36,39	2.99	11 (35%)
1	OMG	2	4637	1	23,26,27	2.66	8 (34%)	33,38,41	2.74	11 (33%)
1	OMG	2	1522	1	23,26,27	2.68	8 (34%)	33,38,41	2.81	10 (30%)
1	B8K	2	4690	1	24,28,29	3.30	12 (50%)	30,42,45	2.67	11 (36%)
1	OMG	2	4870	1	23,26,27	2.70	8 (34%)	33,38,41	3.00	10 (30%)
1	A2M	2	3825	1	22,25,26	3.19	9 (40%)	31,36,39	3.01	10 (32%)
1	E7G	2	2297	1	24,27,28	4.04	11 (45%)	30,40,43	2.12	9 (30%)
1	B8W	2	2380	1	23,26,27	2.71	5 (21%)	33,38,41	2.57	14 (42%)
1	OMG	2	1316	1	23,26,27	2.68	8 (34%)	33,38,41	2.74	11 (33%)
1	2MG	2	978	1	23,26,27	3.03	8 (34%)	32,38,41	2.20	9 (28%)
1	2MG	2	729	1	23,26,27	2.97	8 (34%)	32,38,41	2.31	8 (25%)
1	OMG	2	373	1	23,26,27	2.68	8 (34%)	33,38,41	2.71	13 (39%)
1	OMC	2	4536	1	19,22,23	3.04	8 (42%)	26,31,34	1.12	3 (11%)
1	B9B	2	237	1	25,28,29	1.74	6 (24%)	35,40,43	5.18	12 (34%)
1	B8K	2	3897	1	24,28,29	3.44	11 (45%)	30,42,45	2.53	11 (36%)
1	A2M	2	4571	1	22,25,26	3.16	9 (40%)	31,36,39	2.94	11 (35%)
1	OMG	2	2773	1	23,26,27	2.70	8 (34%)	33,38,41	2.78	9 (27%)
1	2MG	2	4872	1	23,26,27	2.93	8 (34%)	32,38,41	2.27	11 (34%)
1	OMC	2	2365	1	19,22,23	2.99	8 (42%)	26,31,34	0.74	0
4	OMU	8	14	1,4	19,22,23	2.96	8 (42%)	26,31,34	1.79	6 (23%)
1	OMC	2	3701	1	19,22,23	3.01	8 (42%)	26,31,34	0.74	0
1	5MU	2	4083	1	19,22,23	7.22	8 (42%)	28,32,35	3.37	10 (35%)
1	B9H	2	2786	1	20,25,26	3.24	3 (15%)	22,35,38	1.95	5 (22%)
1	OMC	2	2804	1	19,22,23	2.98	8 (42%)	26,31,34	0.76	0
1	A2M	2	1326	1	22,25,26	3.18	9 (40%)	31,36,39	2.95	10 (32%)
1	OMC	2	3869	1	19,22,23	3.02	8 (42%)	26,31,34	0.90	1 (3%)
1	I4U	2	1659	1	21,24,25	3.56	9 (42%)	27,34,37	1.11	2 (7%)
1	B9B	2	2754	1	25,28,29	1.73	5 (20%)	35,40,43	5.23	11 (31%)
1	UR3	2	4530	1	19,22,23	2.89	6 (31%)	26,32,35	1.26	2 (7%)
1	P7G	2	3880	1	24,28,29	4.19	11 (45%)	27,41,44	1.37	2 (7%)
1	OMC	2	2861	1	19,22,23	3.04	8 (42%)	26,31,34	1.10	3 (11%)
1	OMG	2	4623	1	23,26,27	2.67	8 (34%)	33,38,41	2.76	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	2	1883	1	23,26,27	2.72	8 (34%)	33,38,41	2.75	11 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	2	398	1	-	2/9/27/28	0/3/3/3
1	B8T	2	4483	1	-	0/7/27/28	0/2/2/2
1	UR3	2	4597	1	-	0/7/25/26	0/2/2/2
1	B8Q	2	1456	1	-	0/7/42/43	0/2/2/2
1	B8T	2	4671	1	-	0/7/27/28	0/2/2/2
1	OMG	2	2050	1	-	0/9/27/28	0/3/3/3
1	7MG	2	2522	1	-	0/7/37/38	0/3/3/3
1	OMC	2	3909	1	-	2/9/27/28	0/2/2/2
1	A2M	2	3718	1	-	0/9/27/28	0/3/3/3
1	BGH	2	3899	1	-	1/13/43/44	0/3/3/3
1	7MG	2	4550	1	-	2/7/37/38	0/3/3/3
1	OMG	2	2424	1	-	2/9/27/28	0/3/3/3
1	M7A	2	4564	1	-	0/7/37/38	0/3/3/3
1	A2M	2	1534	1	-	2/9/27/28	0/3/3/3
1	OMU	2	4620	1	-	0/9/27/28	0/2/2/2
1	B9B	2	1574	1	-	3/11/29/30	0/3/3/3
1	A2M	2	4523	1	-	1/9/27/28	0/3/3/3
1	OMG	2	2364	1	-	3/9/27/28	0/3/3/3
1	A2M	2	3723	1	-	0/9/27/28	0/3/3/3
1	A2M	2	3867	1	-	3/9/27/28	0/3/3/3
1	7MG	2	1605	1	-	0/7/37/38	0/3/3/3
1	P4U	2	1348	1	-	1/10/29/30	0/2/2/2
1	A2M	2	2401	1	-	0/9/27/28	0/3/3/3
1	A2M	2	1871	1	-	2/9/27/28	0/3/3/3
1	OMG	2	1625	1	-	3/9/27/28	0/3/3/3
1	OMC	2	3887	1	-	1/9/27/28	0/2/2/2
1	B8W	2	4472	1	-	2/9/27/28	0/3/3/3
1	2MG	2	1517	1	-	1/9/27/28	0/3/3/3
1	P7G	2	1909	1	-	3/10/40/41	0/3/3/3
1	A2M	2	2363	1	-	0/9/27/28	0/3/3/3
1	OMC	2	2422	1	-	1/9/27/28	0/2/2/2
1	OMG	2	4494	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	B8W	2	4185	1	-	2/9/27/28	0/3/3/3
1	B8W	2	4529	1	-	2/9/27/28	0/3/3/3
1	A2M	2	1524	1	-	2/9/27/28	0/3/3/3
1	OMG	2	4637	1	-	4/9/27/28	0/3/3/3
1	OMG	2	1522	1	-	0/9/27/28	0/3/3/3
1	B8K	2	4690	1	-	0/11/41/42	0/3/3/3
1	OMG	2	4870	1	-	3/9/27/28	0/3/3/3
1	A2M	2	3825	1	-	0/9/27/28	0/3/3/3
1	E7G	2	2297	1	-	1/9/39/40	0/3/3/3
1	B8W	2	2380	1	-	2/9/27/28	0/3/3/3
1	OMG	2	1316	1	-	0/9/27/28	0/3/3/3
1	2MG	2	978	1	-	0/9/27/28	0/3/3/3
1	2MG	2	729	1	-	1/9/27/28	0/3/3/3
1	OMG	2	373	1	-	1/9/27/28	0/3/3/3
1	OMC	2	4536	1	-	0/9/27/28	0/2/2/2
1	B9B	2	237	1	-	6/11/29/30	0/3/3/3
1	B8K	2	3897	1	-	3/11/41/42	0/3/3/3
1	A2M	2	4571	1	-	0/9/27/28	0/3/3/3
1	OMG	2	2773	1	-	0/9/27/28	0/3/3/3
1	2MG	2	4872	1	-	2/9/27/28	0/3/3/3
1	OMC	2	2365	1	-	0/9/27/28	0/2/2/2
4	OMU	8	14	1,4	-	1/9/27/28	0/2/2/2
1	OMC	2	3701	1	-	2/9/27/28	0/2/2/2
1	5MU	2	4083	1	-	0/7/25/26	0/2/2/2
1	B9H	2	2786	1	-	1/12/47/48	0/2/2/2
1	OMC	2	2804	1	-	0/9/27/28	0/2/2/2
1	A2M	2	1326	1	-	0/9/27/28	0/3/3/3
1	OMC	2	3869	1	-	0/9/27/28	0/2/2/2
1	I4U	2	1659	1	-	1/9/29/30	0/2/2/2
1	B9B	2	2754	1	-	4/11/29/30	0/3/3/3
1	UR3	2	4530	1	-	0/7/25/26	0/2/2/2
1	P7G	2	3880	1	-	2/10/40/41	0/3/3/3
1	OMC	2	2861	1	-	0/9/27/28	0/2/2/2
1	OMG	2	4623	1	-	0/9/27/28	0/3/3/3
1	OMG	2	1883	1	-	2/9/27/28	0/3/3/3

The worst 5 of 546 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	4083	5MU	C4-C5	20.78	1.79	1.44
1	2	4083	5MU	C6-N1	16.00	1.65	1.38
1	2	4083	5MU	C6-C5	-11.45	1.15	1.34
1	2	4083	5MU	C4-N3	-11.05	1.18	1.38
1	2	1659	I4U	C4-N3	10.65	1.45	1.31

The worst 5 of 543 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	2754	B9B	O6-C6-C5	21.33	143.58	116.57
1	2	1574	B9B	O6-C6-C5	21.25	143.47	116.57
1	2	237	B9B	O6-C6-C5	20.95	143.10	116.57
1	2	2754	B9B	O6-C6-N1	-18.29	94.52	120.00
1	2	1574	B9B	O6-C6-N1	-18.08	94.82	120.00

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	8	14	OMU	C1'-C2'-O2'-CM2
1	2	237	B9B	C5-C6-O6-C61
1	2	237	B9B	N1-C6-O6-C61
1	2	237	B9B	C3'-C4'-C5'-O5'
1	2	237	B9B	O4'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	4483	B8T	1	0
1	2	2522	7MG	1	0
1	2	3718	A2M	1	0
1	2	4620	OMU	1	0
1	2	1574	B9B	1	0
1	2	3723	A2M	1	0
1	2	1871	A2M	1	0
1	2	4472	B8W	1	0
1	2	1517	2MG	1	0
1	2	2363	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	4494	OMG	1	0
1	2	729	2MG	1	0
1	2	4571	A2M	1	0
4	8	14	OMU	1	0
1	2	4083	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	GTP	w	801	60	30,34,34	0.83	1 (3%)	46,54,54	1.77	11 (23%)

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
59	GTP	w	801	60	-	5/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	w	801	GTP	C2-N3	2.13	1.38	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	w	801	GTP	C5-C4-N3	-5.20	120.02	128.46
59	w	801	GTP	C2-N3-C4	4.68	120.63	112.30
59	w	801	GTP	N9-C4-N3	3.39	132.76	125.94
59	w	801	GTP	PA-O3A-PB	-3.29	121.53	132.83
59	w	801	GTP	C2-N1-C6	-2.95	119.73	125.10

There are no chirality outliers.

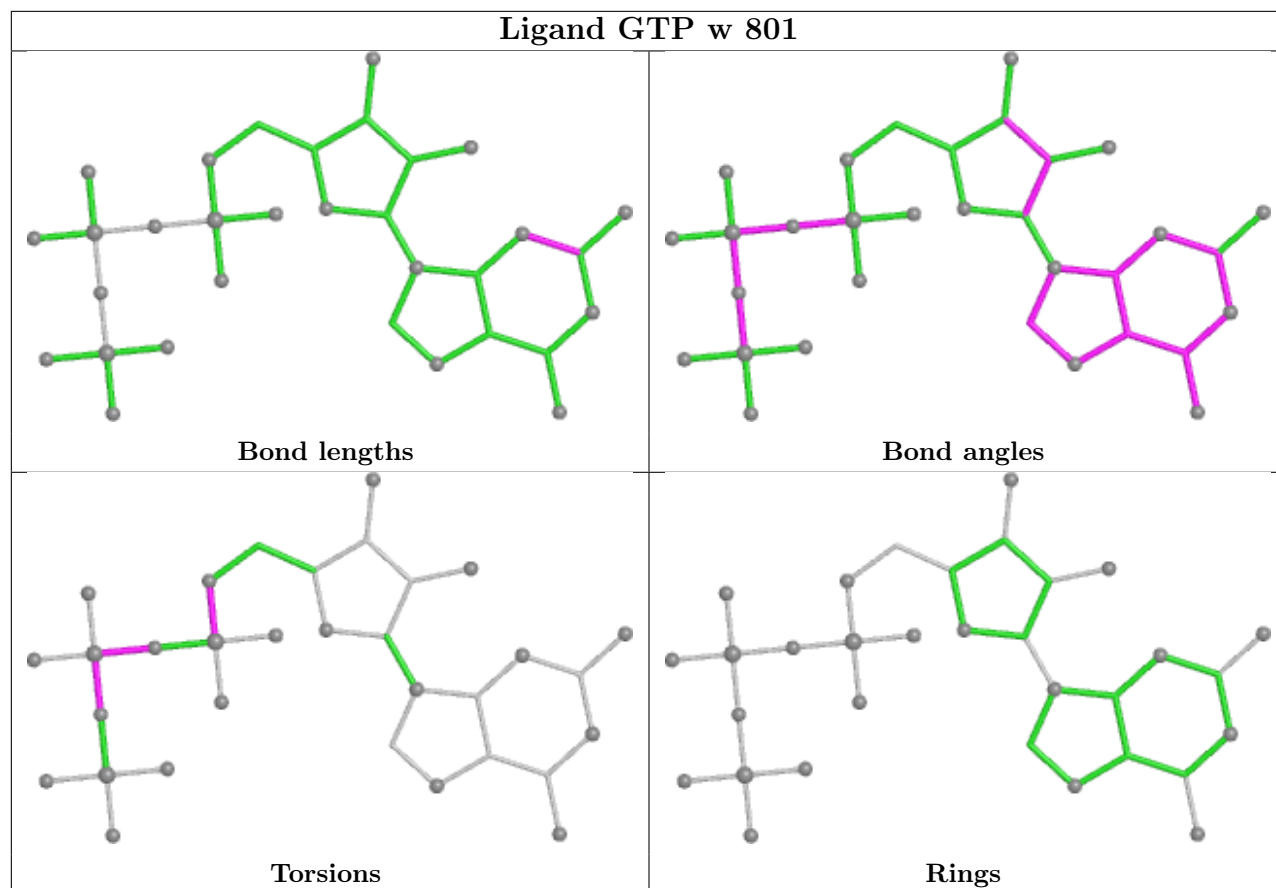
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	w	801	GTP	C5'-O5'-PA-O3A
59	w	801	GTP	PA-O3A-PB-O1B
59	w	801	GTP	C5'-O5'-PA-O2A
59	w	801	GTP	PG-O3B-PB-O3A
59	w	801	GTP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

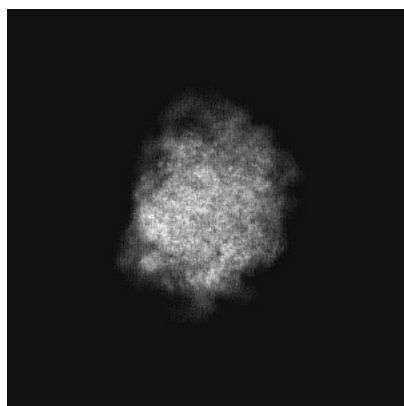
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35649. These allow visual inspection of the internal detail of the map and identification of artifacts.

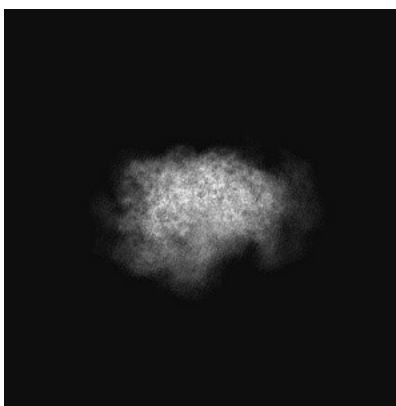
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

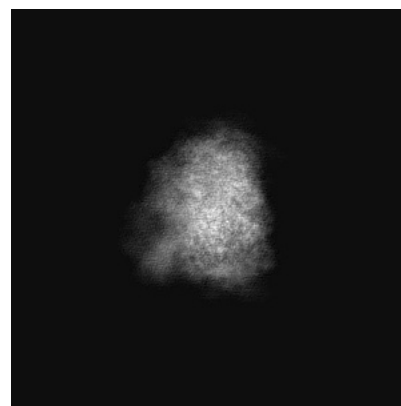
6.1.1 Primary map



X

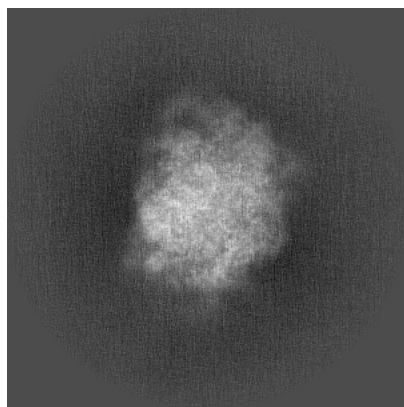


Y

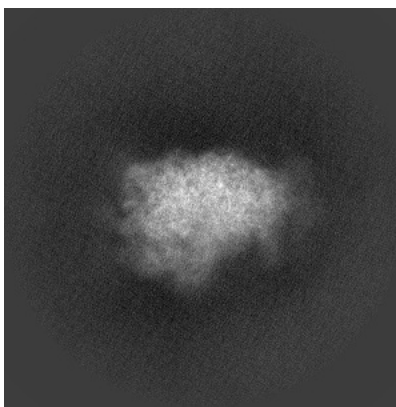


Z

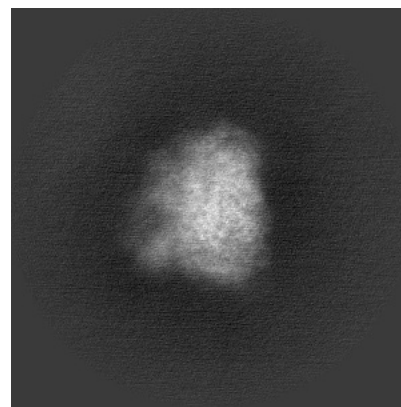
6.1.2 Raw map



X



Y

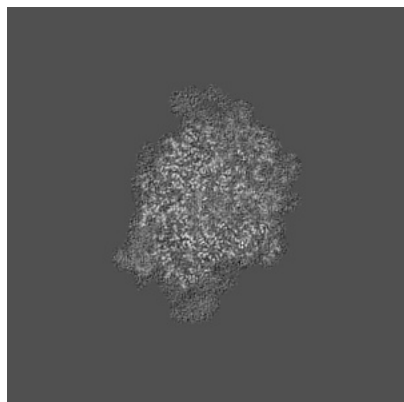


Z

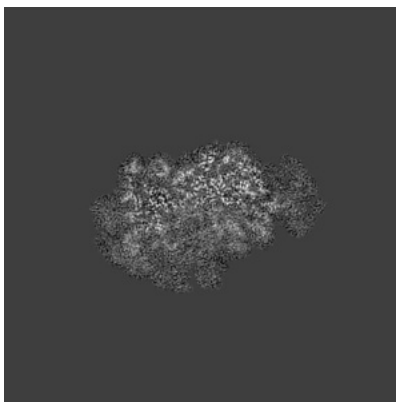
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

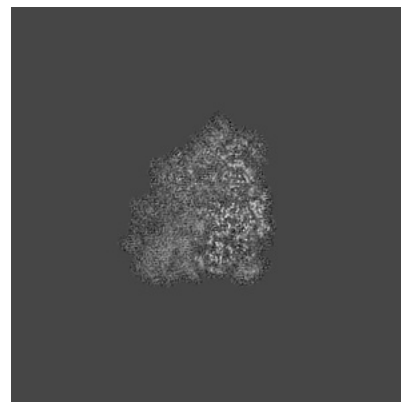
6.2.1 Primary map



X Index: 200

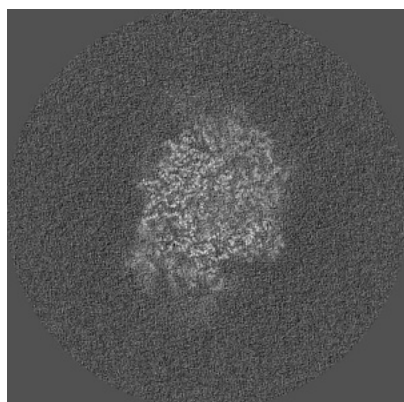


Y Index: 200

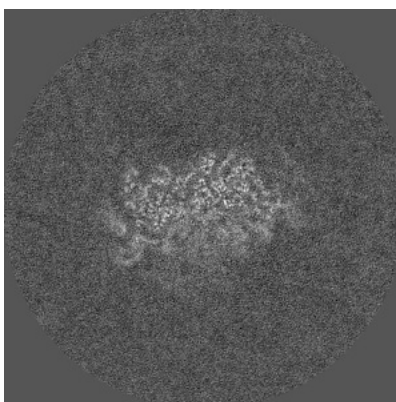


Z Index: 200

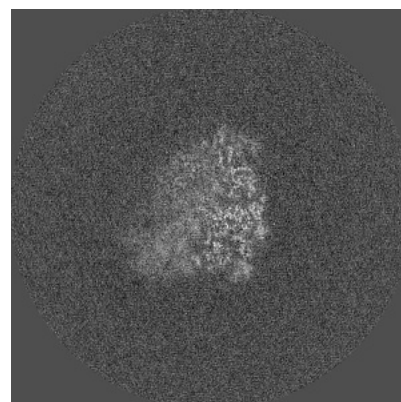
6.2.2 Raw map



X Index: 200



Y Index: 200

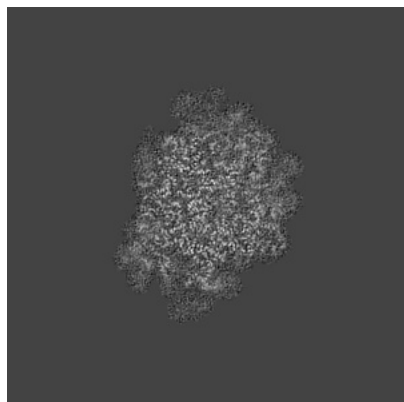


Z Index: 200

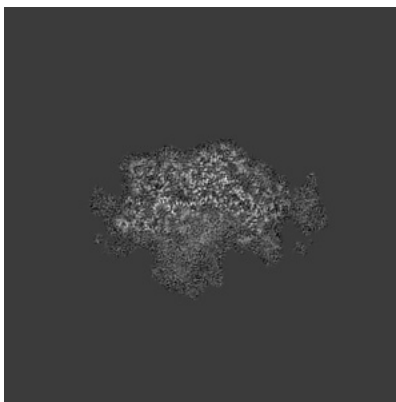
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

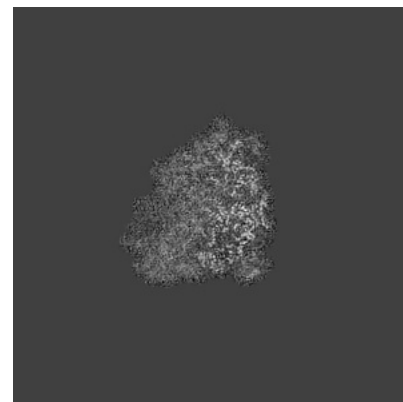
6.3.1 Primary map



X Index: 207

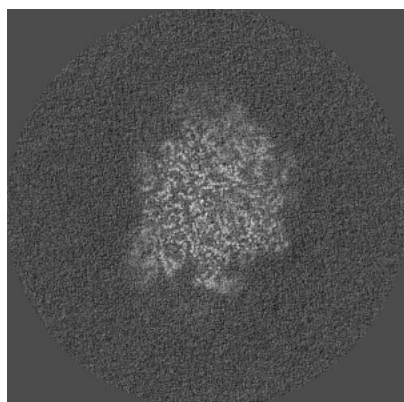


Y Index: 181

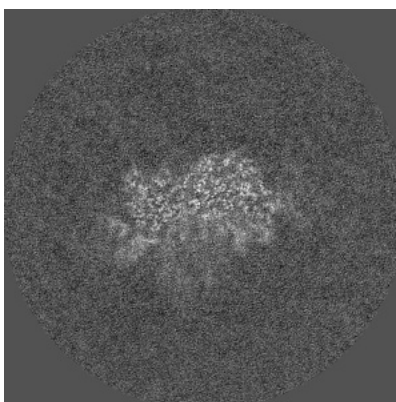


Z Index: 198

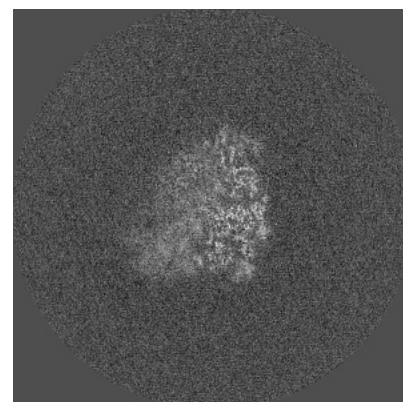
6.3.2 Raw map



X Index: 205



Y Index: 199

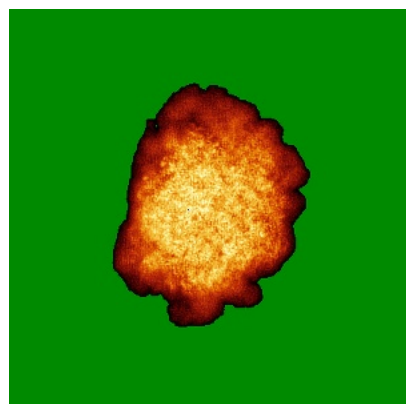


Z Index: 200

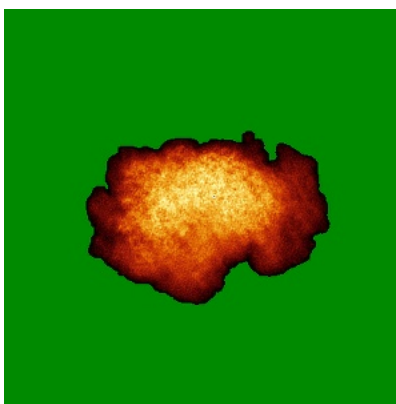
The images above show the largest variance slices of the map in three orthogonal directions.

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

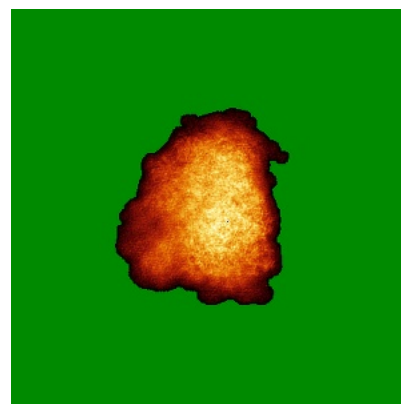
6.4.1 Primary map



X

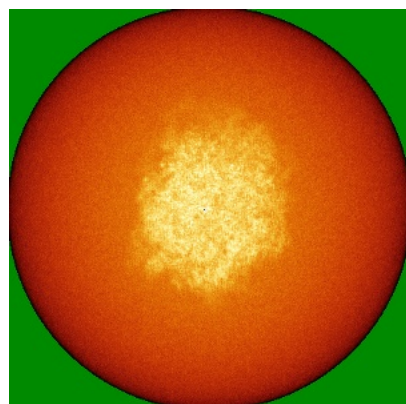


Y

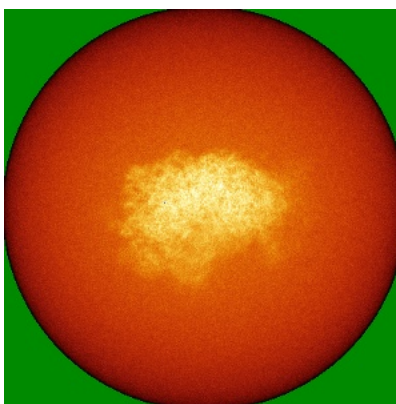


Z

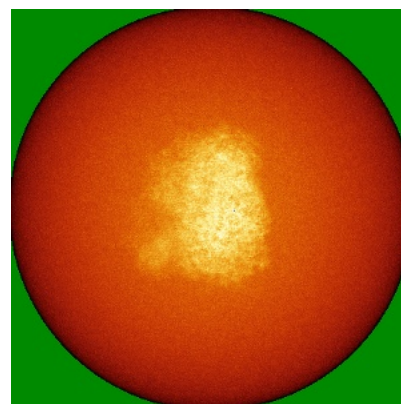
6.4.2 Raw map



X



Y

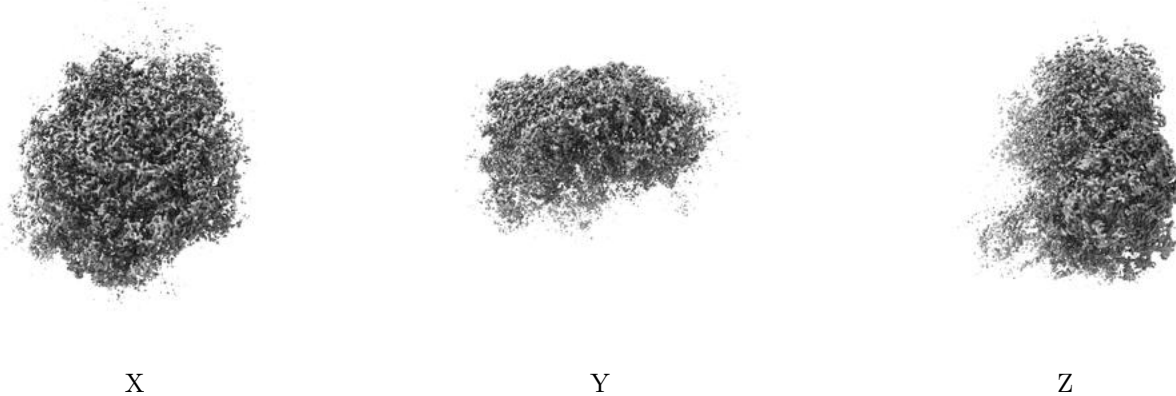


Z

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

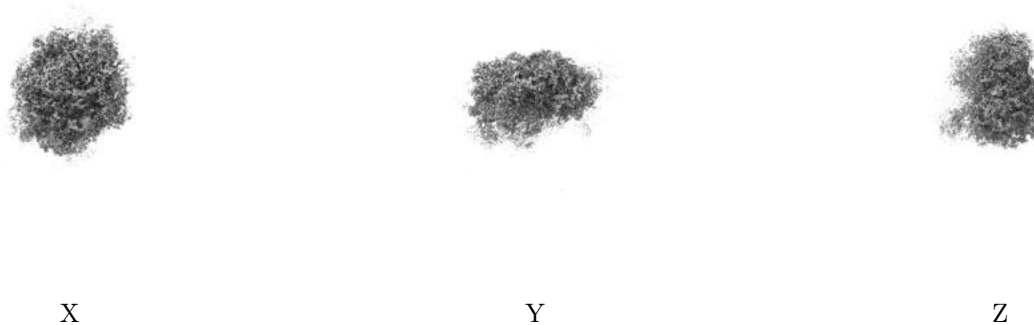
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

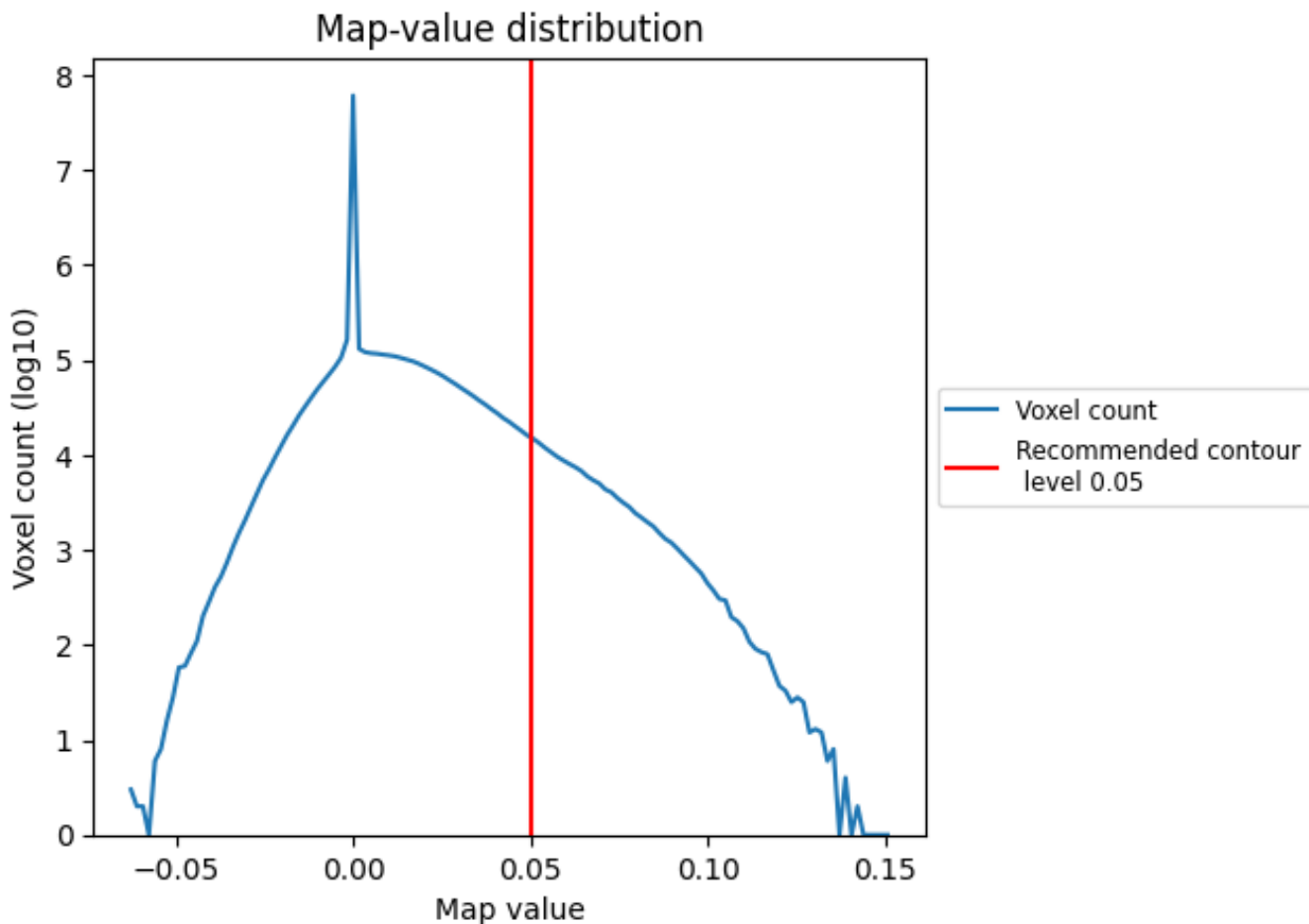
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

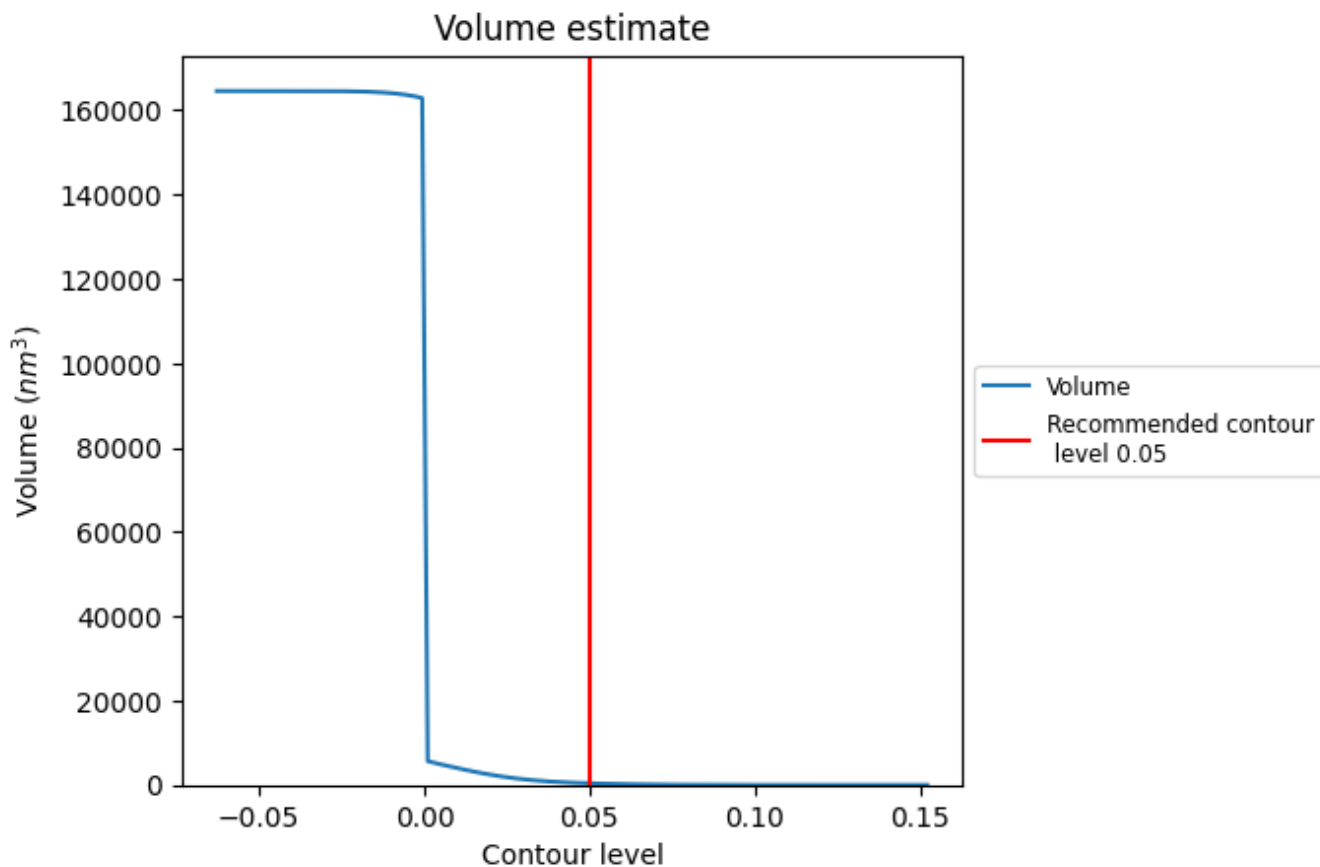
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

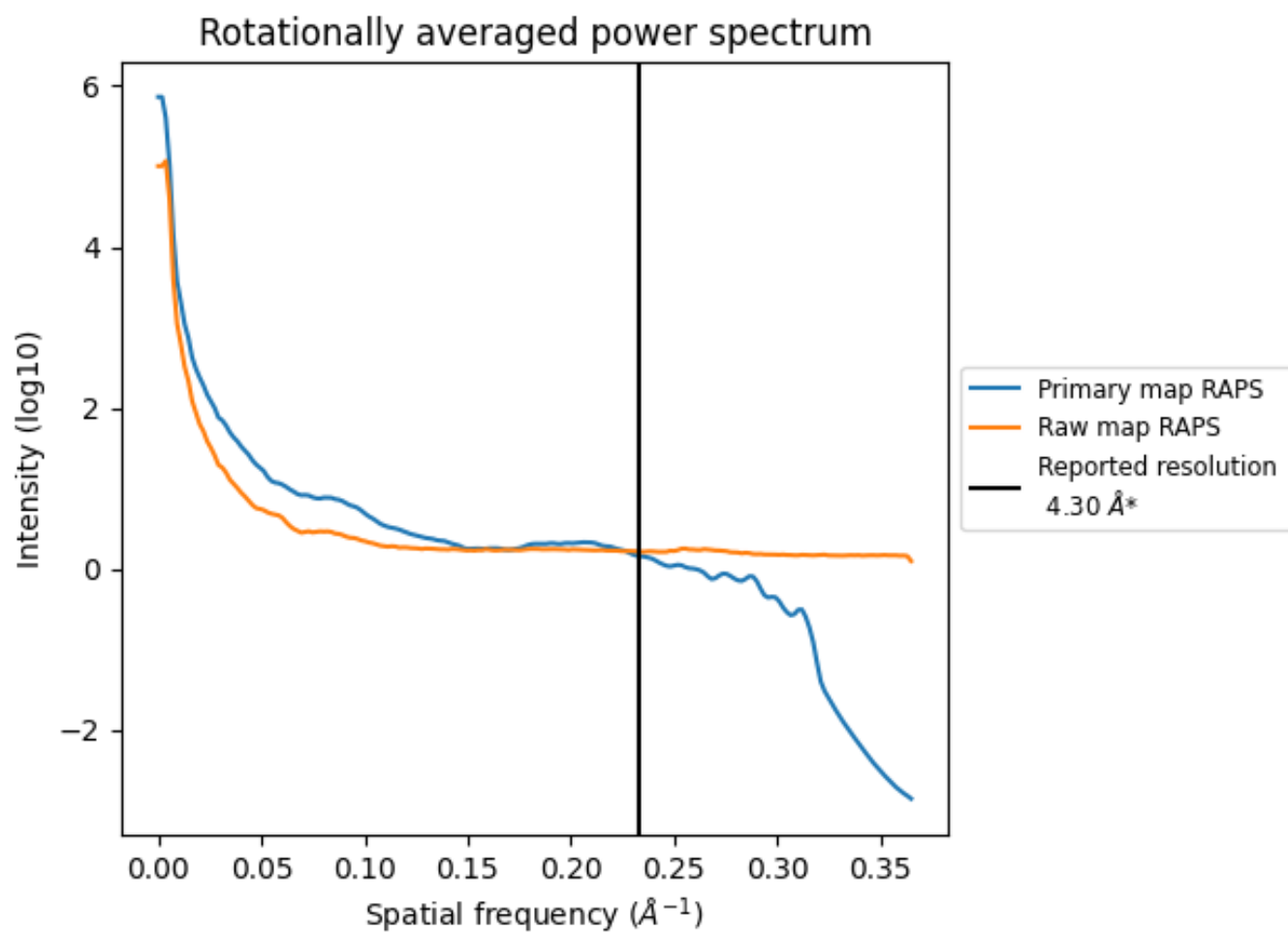
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 388 nm³; this corresponds to an approximate mass of 351 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

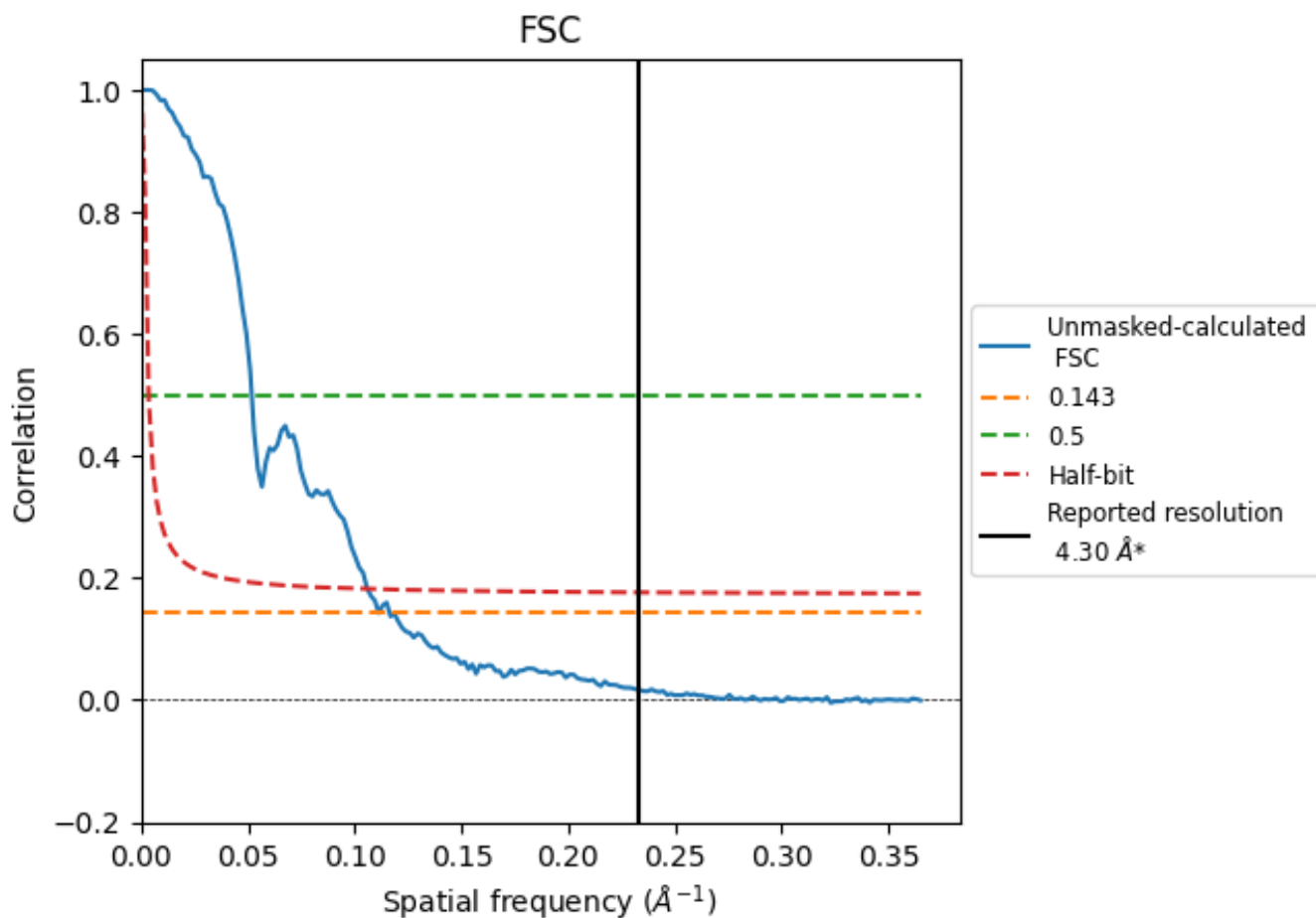


*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

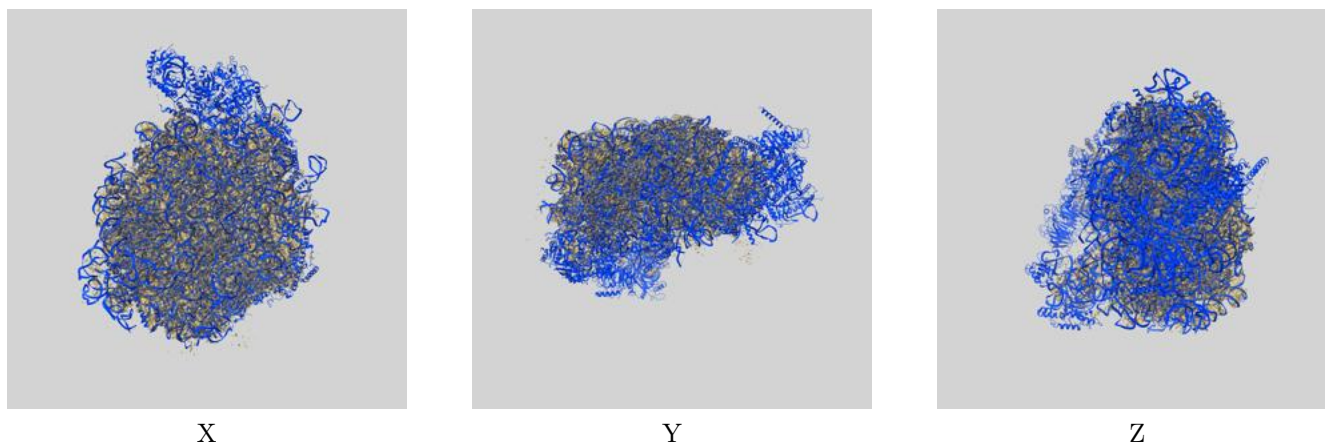
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.98	19.31	9.43

*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 8.98 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

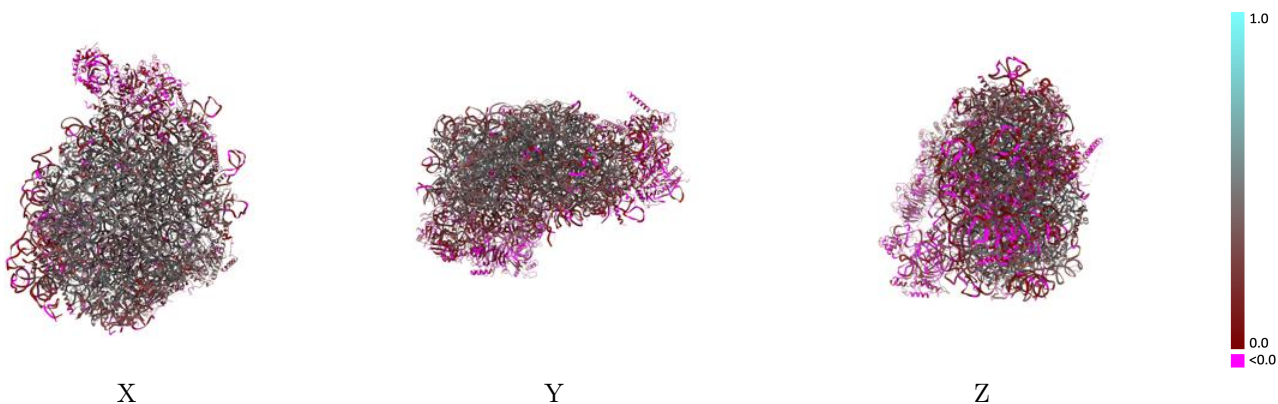
This section contains information regarding the fit between EMDB map EMD-35649 and PDB model 8IPX. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



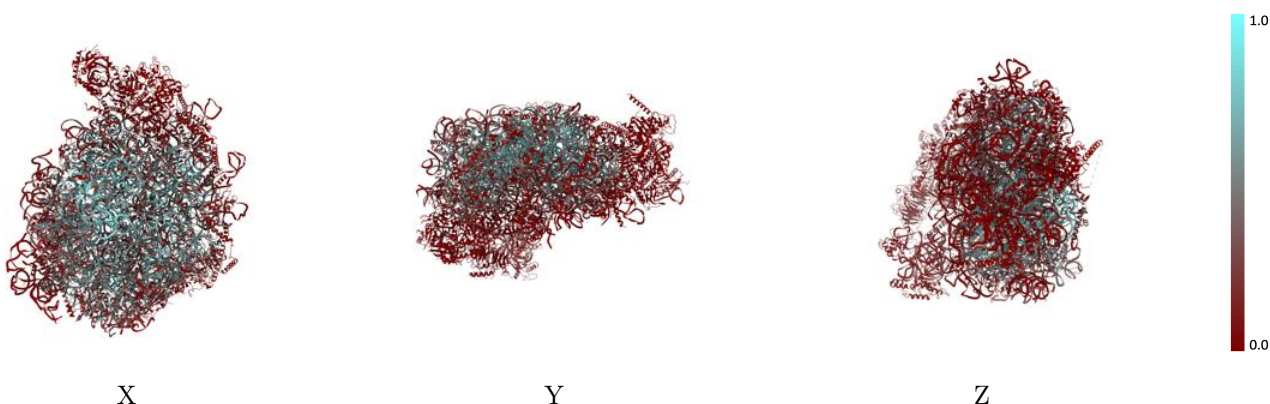
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



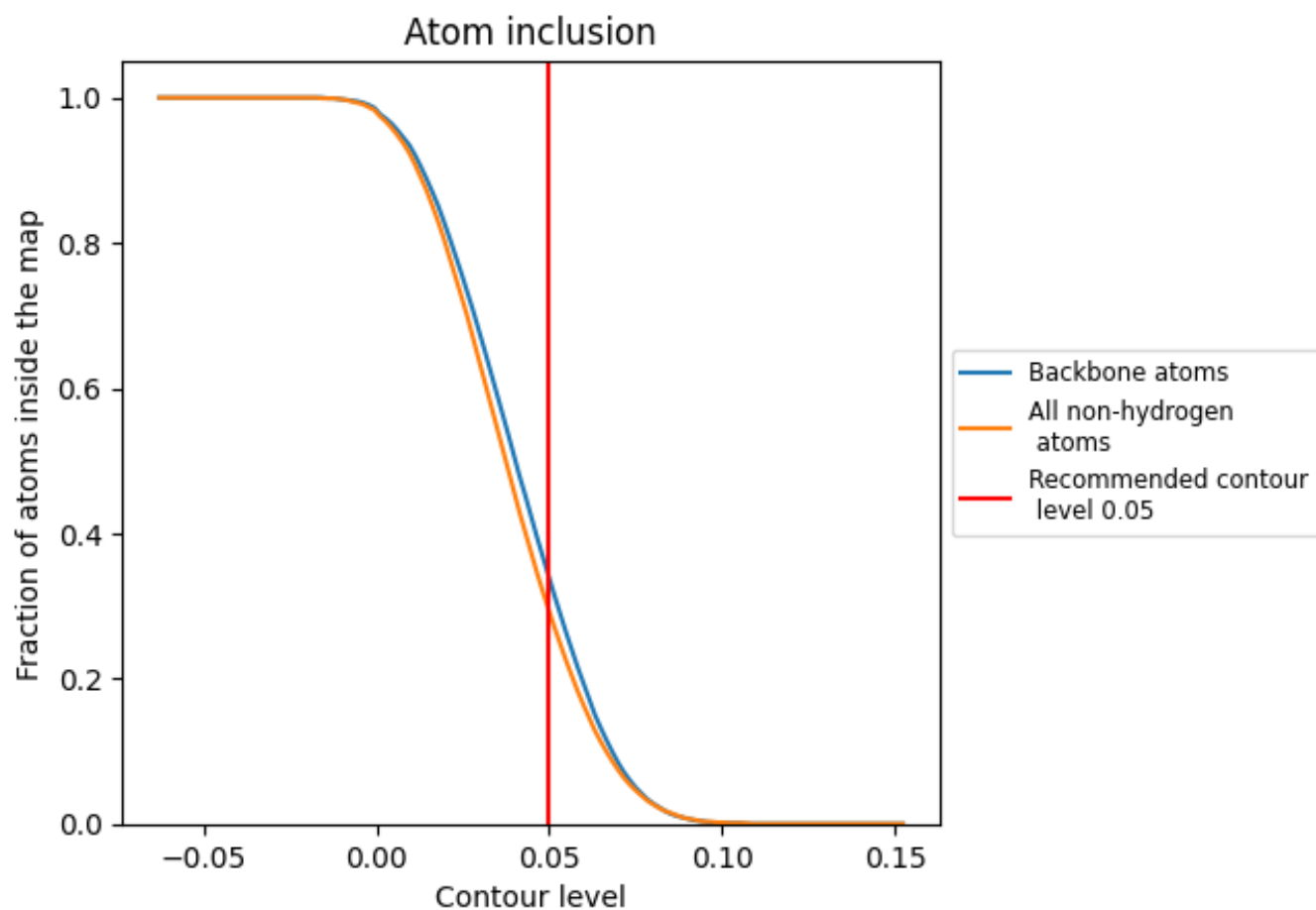
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 29% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2920	 0.2920
1	 0.0010	 0.1020
2	 0.3950	 0.3190
3	 0.0950	 0.1160
4	 0.1000	 0.2600
6	 0.1430	 0.2940
7	 0.2360	 0.3640
8	 0.5910	 0.4070
9	 0.0220	 0.1700
A	 0.0470	 0.2120
B	 0.3730	 0.4160
C	 0.0010	 0.0130
D	 0.4580	 0.4280
E	 0.0670	 0.2370
F	 0.2420	 0.3550
G	 0.1610	 0.2710
H	 0.3360	 0.3750
I	 0.2290	 0.3480
J	 0.0340	 0.2070
K	 0.2470	 0.3340
L	 0.3710	 0.4000
M	 0.5040	 0.4210
N	 0.0000	 0.0090
O	 0.1290	 0.2870
P	 0.4820	 0.4440
Q	 0.3040	 0.3510
R	 0.0030	 0.0200
S	 0.3320	 0.3800
T	 0.0700	 0.1290
U	 0.4170	 0.4160
V	 0.4510	 0.4200
W	 0.0000	 0.0380
X	 0.1380	 0.2790
Y	 0.4360	 0.4010
Z	 0.4340	 0.4410



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Chain	Atom inclusion	Q-score
a	 0.2390	 0.3490
b	 0.3490	 0.4060
d	 0.1830	 0.3170
e	 0.2930	 0.3910
f	 0.0020	 0.1560
g	 0.2730	 0.3340
h	 0.4110	 0.3970
i	 0.0780	 0.2720
j	 0.3390	 0.3860
k	 0.4790	 0.4390
l	 0.4290	 0.4270
m	 0.0950	 0.2830
n	 0.4890	 0.4640
o	 0.2200	 0.3260
p	 0.4030	 0.4040
q	 0.0140	 0.1640
r	 0.0000	 0.0710
t	 0.0010	 0.0740
u	 0.0220	 0.1340
v	 0.0090	 0.1390
w	 0.0350	 0.2120
x	 0.0000	 0.0240
y	 0.0060	 0.0830
z	 0.0650	 0.2300