



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 09:16 PM JST

PDB ID : 5IMQ / pdb_00005imq
EMDB ID : EMD-6584
Title : Structure of ribosome bound to cofactor at 3.8 angstrom resolution
Authors : Kumar, V.; Ero, R.; Jian, G.K.; Ahmed, T.; Zhan, Y.; Bhushan, S.; Gao, Y.G.
Deposited on : 2016-03-06
Resolution : 3.80 Å(reported)
Based on initial models : 5AA0, 4W2E

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:

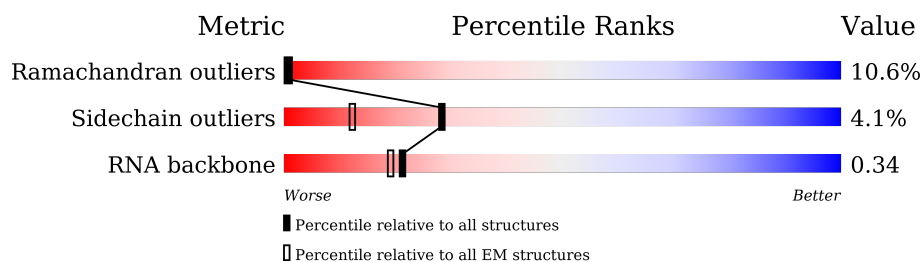
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	37	
2	2	173	
3	3	147	
4	4	77	
5	5	76	
6	A	1522	
7	D	2893	
8	E	123	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	256	
10	G	239	
11	H	209	
12	I	162	
13	J	101	
14	K	156	
15	L	138	
16	M	128	
17	N	105	
18	O	129	
19	P	132	
20	Q	126	
21	R	61	
22	S	89	
23	T	88	
24	U	105	
25	V	88	
26	W	93	
27	X	106	
28	Y	27	
29	Z	229	
30	a	276	
31	b	206	
32	c	210	
33	d	182	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	e	180	
35	f	140	
36	g	122	
37	h	150	
38	i	141	
39	j	118	
40	k	112	
41	l	146	
42	m	118	
43	n	101	
44	o	113	
45	p	96	
46	q	110	
47	r	206	
48	s	85	
49	t	67	
50	u	60	
51	v	71	
52	w	60	
53	x	54	
54	y	49	
55	z	65	
56	B	610	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 153046 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 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	37	Total	C	N	O	S	0	0
			307	188	68	47	4		

- Molecule 2 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	130	Total	C	N	O	0	0
			641	381	130	130		

- Molecule 3 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	134	Total	C	N	O	S	0	0
			993	632	175	181	5		

- Molecule 4 is a RNA chain called P- site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 5 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1515	Total	C	N	O	P	0	0
			32554	14490	6022	10527	1515		

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	2889	Total	C	N	O	P	0	0
			62218	27691	11629	20009	2889		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	123	Total	C	N	O	P	0	0
			2641	1175	488	855	123		

- Molecule 9 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 11 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 12 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 15 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	127	Total	C	N	O	S	0	0
			1010	639	197	174			

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	98	Total	C	N	O	S	0	0
			794	499	156	138	1		

- Molecule 18 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 19 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	114	Total	C	N	O	S	0	0
			914	565	189	158	2		

- Molecule 21 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 22 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 23 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 24 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	104	Total	C	N	O	S	0	0
			857	547	161	147	2		

- Molecule 25 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	V	73	Total	C	N	O	0	0
			597	380	118	99		

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	80	Total	C	N	O	S	0	0
			647	414	119	112	2		

- Molecule 27 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

- Molecule 28 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Y	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 29 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	228	Total	C	N	O	S	0	0
			1742	1102	318	319	3		

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	272	Total	C	N	O	S	0	0
			2124	1339	424	358	3		

- Molecule 31 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	206	Total	C	N	O	S	0	0
			1578	997	302	273	6		

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	208	Total	C	N	O	S	0	0
			1625	1034	303	286	2		

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	182	Total	C	N	O	S	0	0
			1482	947	269	261	5		

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	174	Total	C	N	O	S	0	0
			1328	844	248	235	1		

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	139	Total	C	N	O	S	0	0
			1113	717	207	186	3		

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	122	Total	C	N	O	S	0	0
			932	587	171	170	4		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	145	Total	C	N	O	S	0	0
			1106	688	226	190	2		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	136	Total	C	N	O	S	0	0
			1080	688	204	183	5		

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	j	117	Total	C	N	O	0	0
			960	599	202	159		

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	k	110	Total	C	N	O	0	0
			877	553	175	149		

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	117	Total	C	N	O	S	0	0
			976	614	197	164	1		

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	117	Total	C	N	O	S	0	0
			964	610	202	151	1		

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	110	Total	C	N	O	S	0	0
			876	552	171	151	2		

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	p	94	Total	C	N	O	0	0
			742	483	133	126		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	110	Total	C	N	O	S	0	0
			844	539	158	141	6		

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	180	Total	C	N	O	S	0	0
			1435	916	256	260	3		

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	79	Total	C	N	O	S	0	0
			625	387	131	106	1		

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	67	Total	C	N	O	S	0	0
			567	350	116	99	2		

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	59	Total	C	N	O		0	0
			469	298	90	81			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	71	Total	C	N	O	S	0	0
			581	364	108	104	5		

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	57	Total	C	N	O	S	0	0
			445	279	87	74	5		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	49	Total	C	N	O	S	0	0
			426	265	87	70	4		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	49	Total	C	N	O	S	0	0
			430	263	108	57	2		

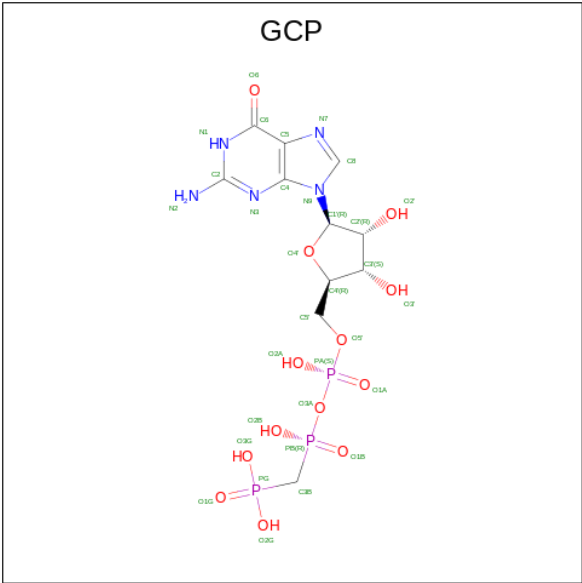
- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	64	Total	C	N	O	S	0	0
			515	331	102	79	3		

- Molecule 56 is a protein called Elongation factor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B	591	Total	C	N	O	S	0	0
			4628	2968	794	857	9		

- Molecule 57 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

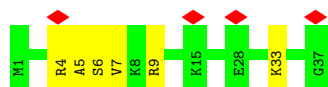
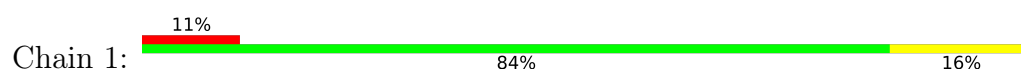


Mol	Chain	Residues	Atoms					AltConf
57	B	1	Total	C	N	O	P	0
			32	11	5	13	3	

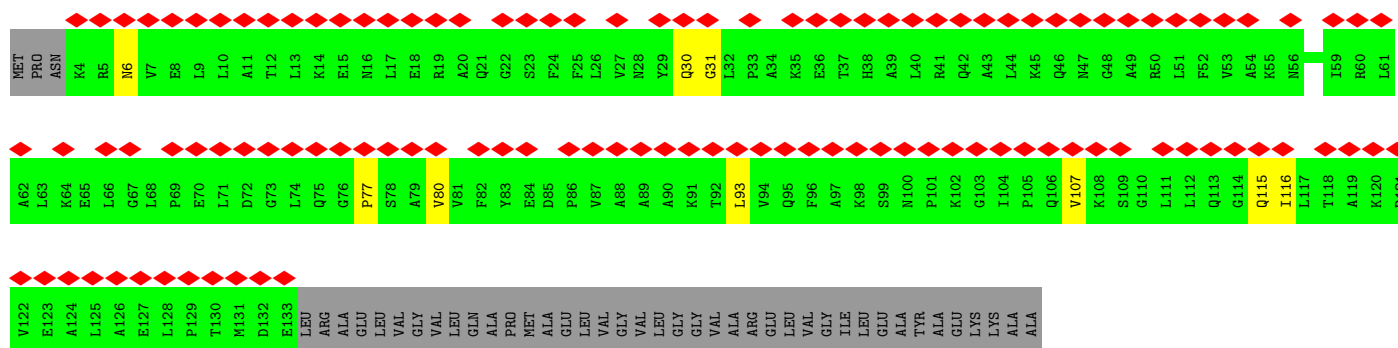
3 Residue-property plots

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

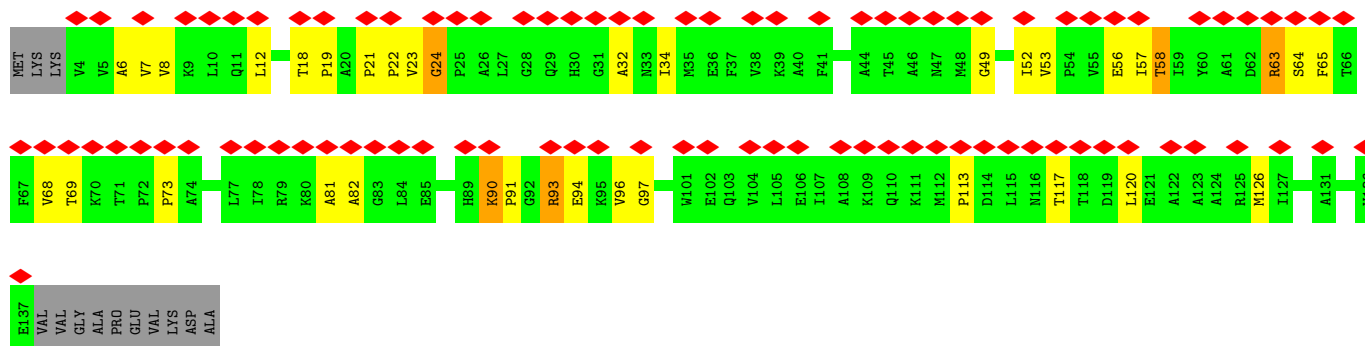
- Molecule 1: 50S ribosomal protein L36



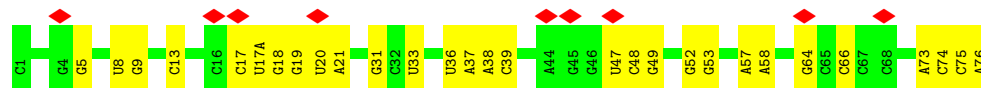
- Molecule 2: 50S ribosomal protein L10



- Molecule 3: 50S ribosomal protein L11



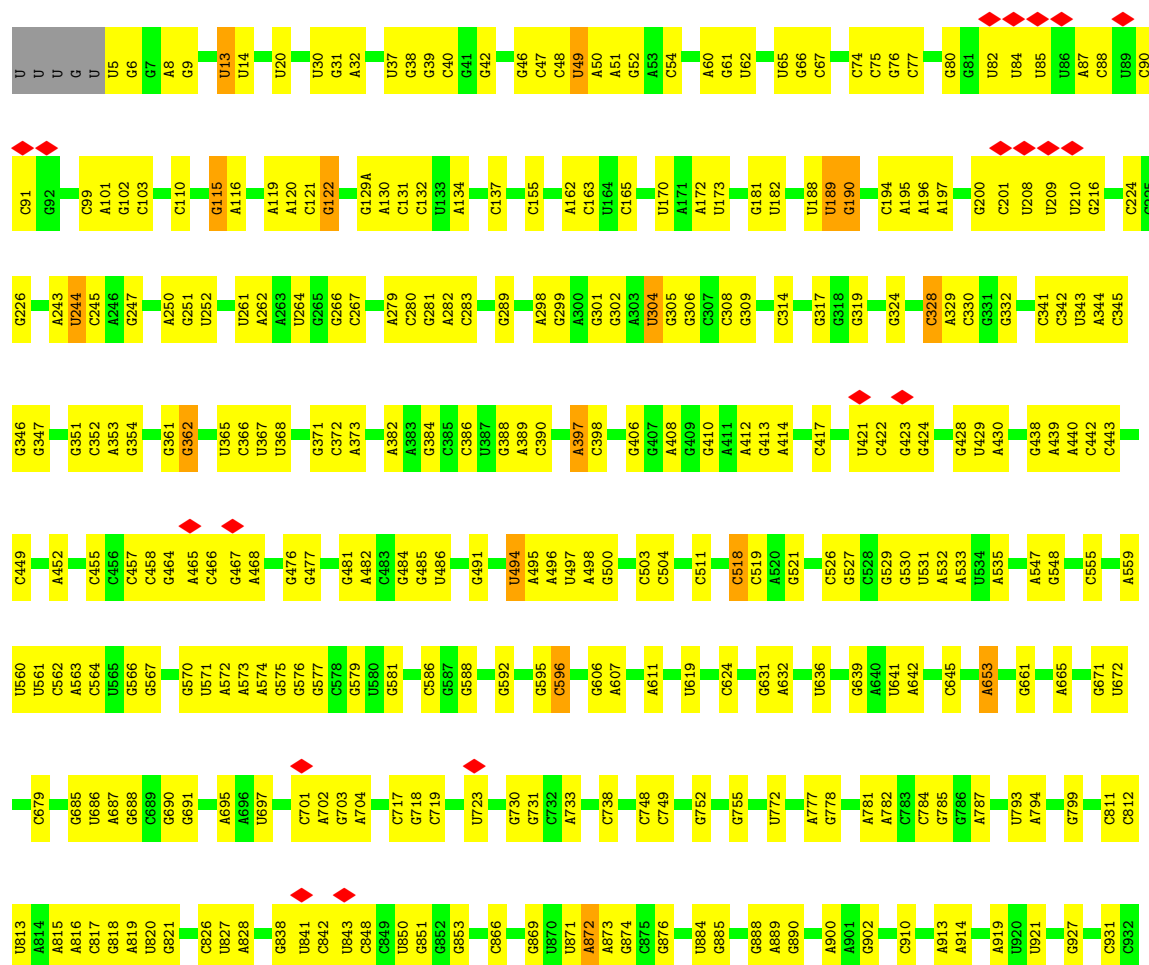
- Molecule 4: P- site tRNA

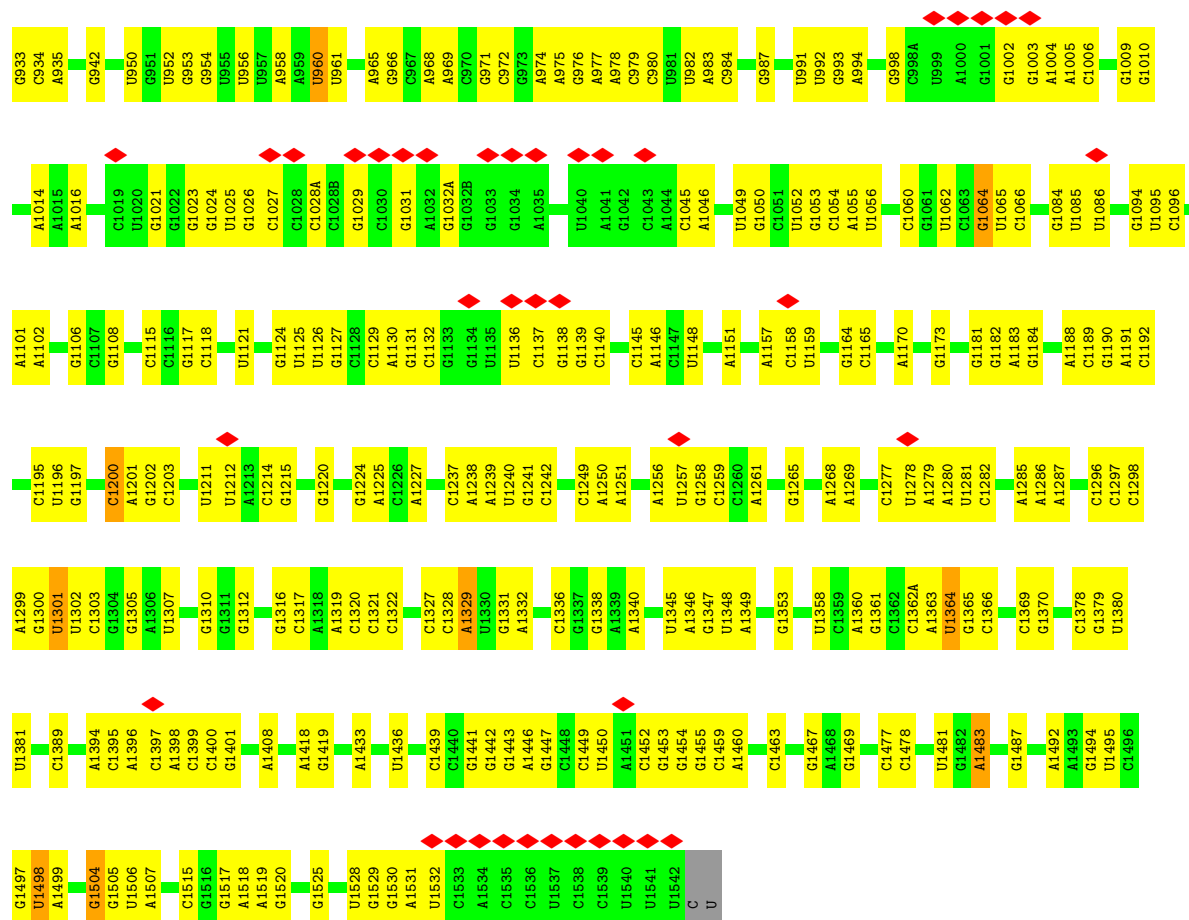


- Molecule 5: E site tRNA



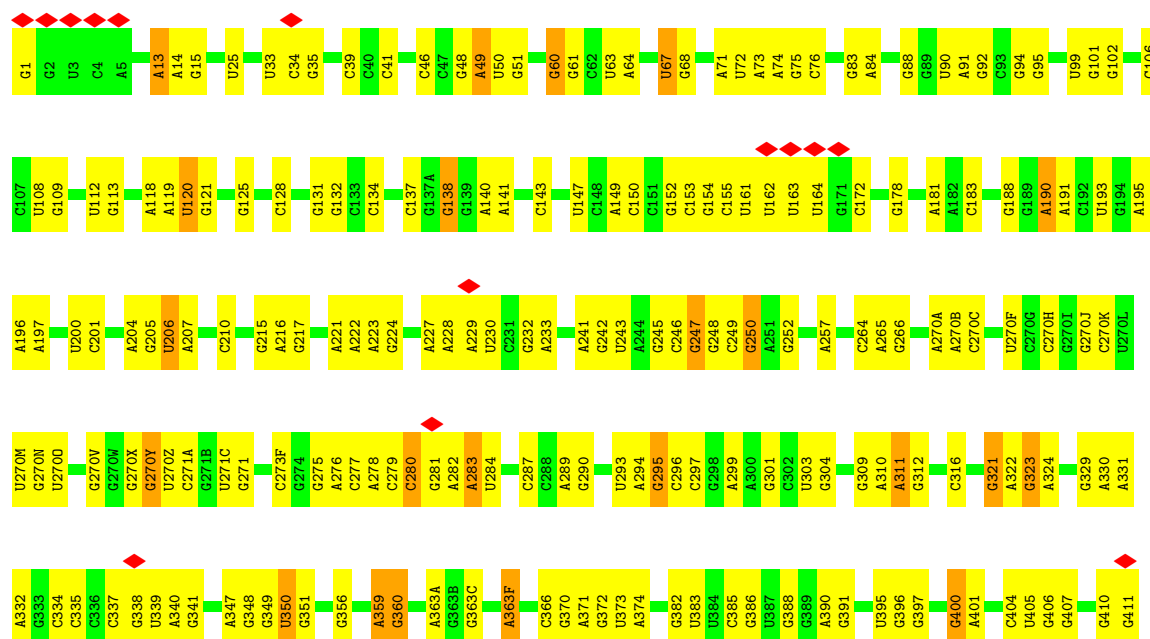
- Molecule 6: 16S ribosomal RNA

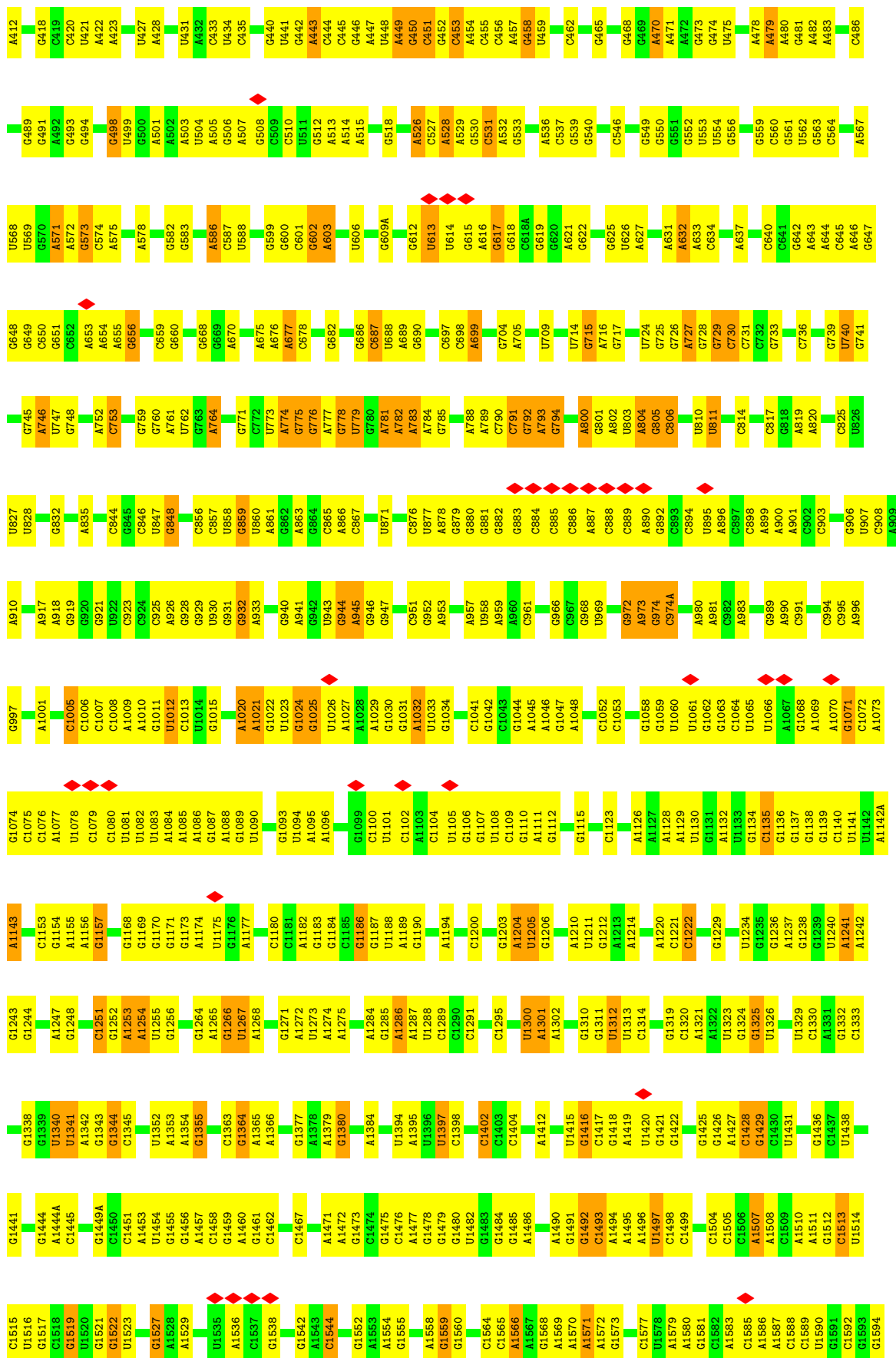




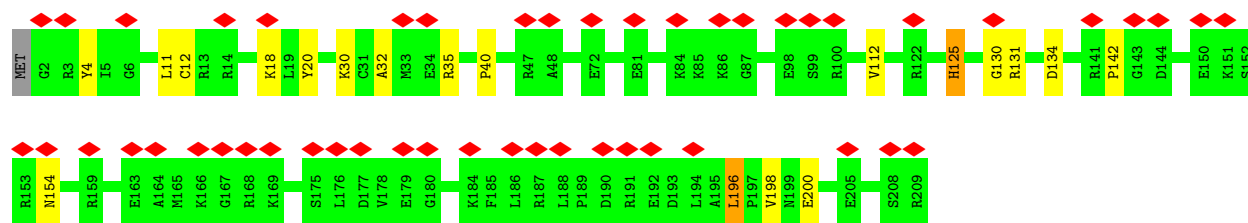
• Molecule 7: 23S ribosomal RNA

Chain D:









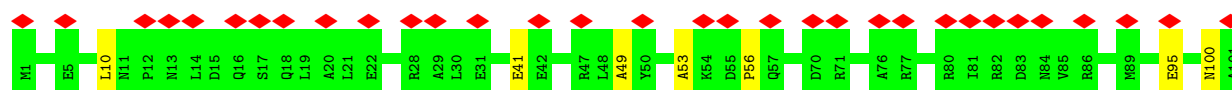
- Molecule 12: 30S ribosomal protein S5

Chain I: 87% 6% 7%



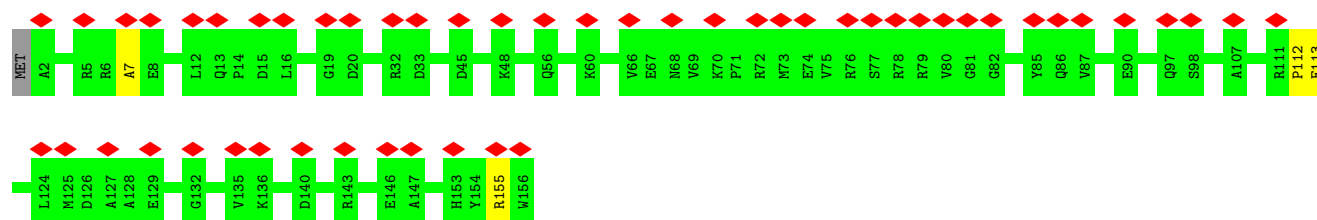
- Molecule 13: 30S ribosomal protein S6

Chain J: 32% 93% 7%



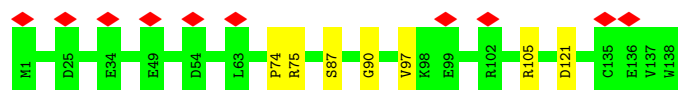
- Molecule 14: 30S ribosomal protein S7

Chain K: 33% 97% . .



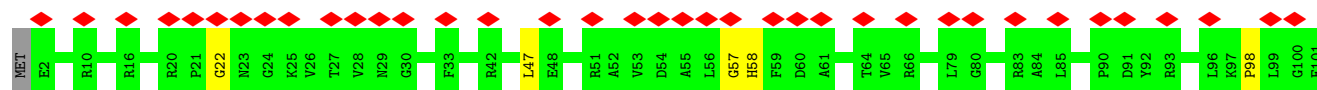
- Molecule 15: 30S ribosomal protein S8

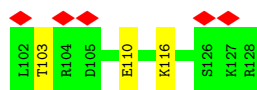
Chain L: 7% 95% 5%



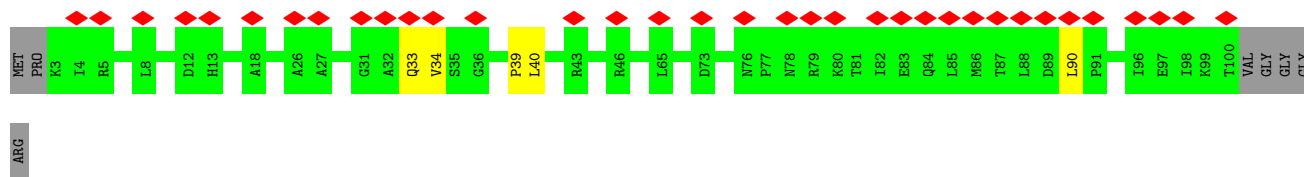
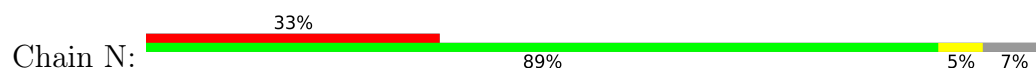
- Molecule 16: 30S ribosomal protein S9

Chain M: 33% 93% 6% .

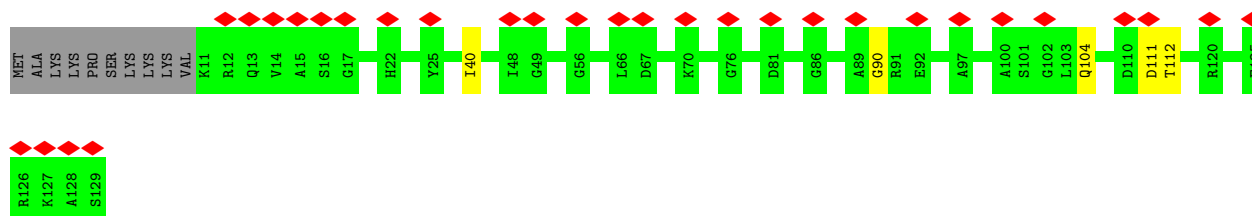
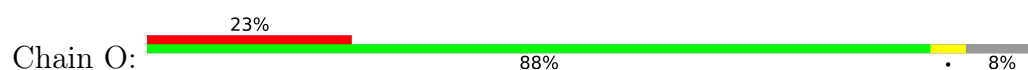




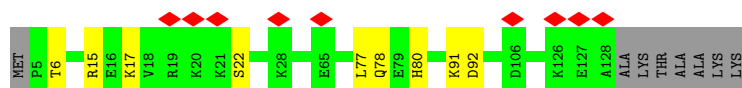
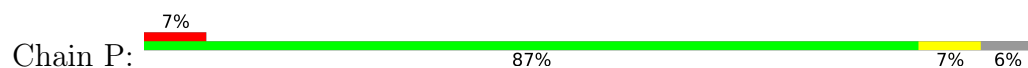
- Molecule 17: 30S ribosomal protein S10



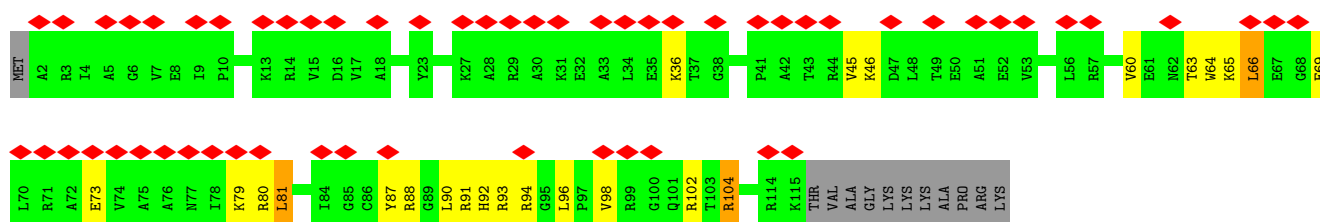
- Molecule 18: 30S ribosomal protein S11



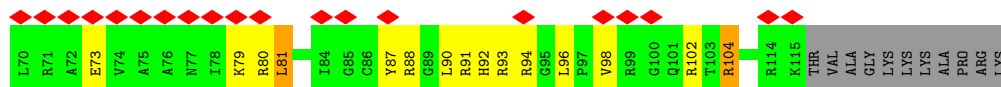
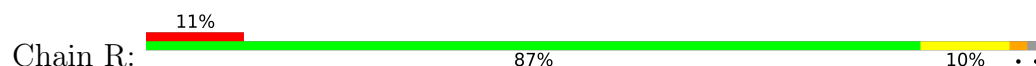
- Molecule 19: 30S ribosomal protein S12

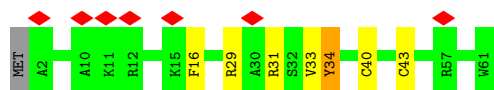


- Molecule 20: 30S ribosomal protein S13

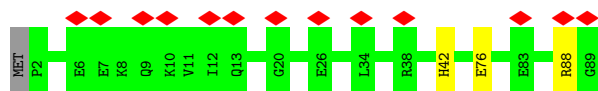


- Molecule 21: 30S ribosomal protein S14 type Z

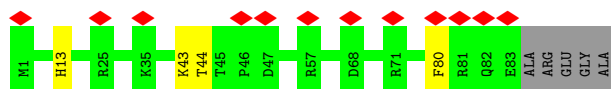




- Molecule 22: 30S ribosomal protein S15



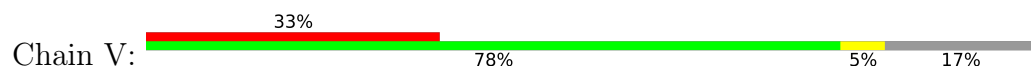
- Molecule 23: 30S ribosomal protein S16



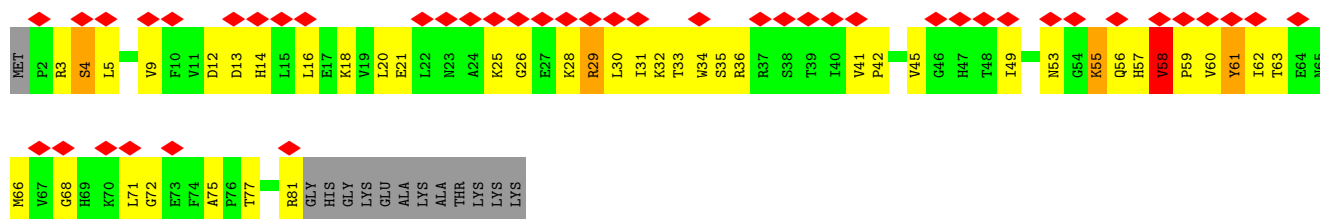
- Molecule 24: 30S ribosomal protein S17



- Molecule 25: 30S ribosomal protein S18

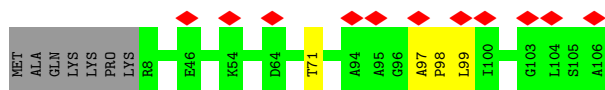


- Molecule 26: 30S ribosomal protein S19

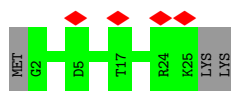
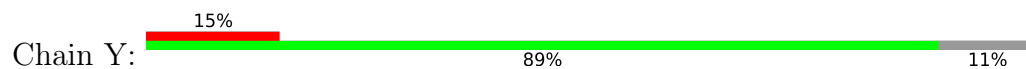


- Molecule 27: 30S ribosomal protein S20

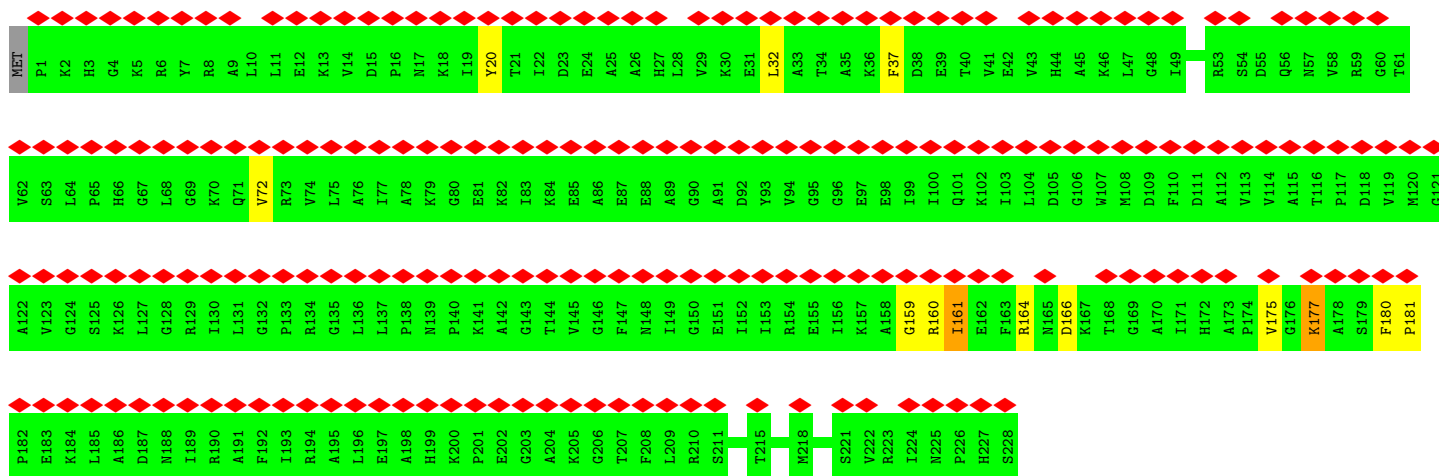




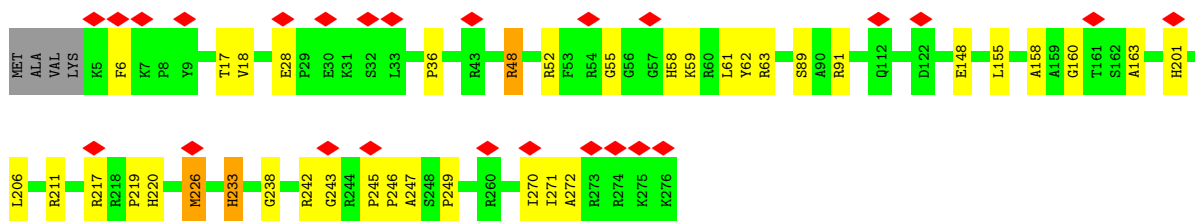
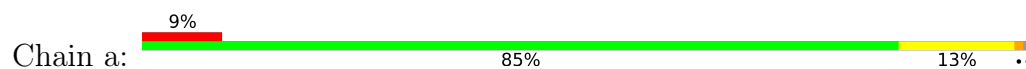
- Molecule 28: 30S ribosomal protein Thx



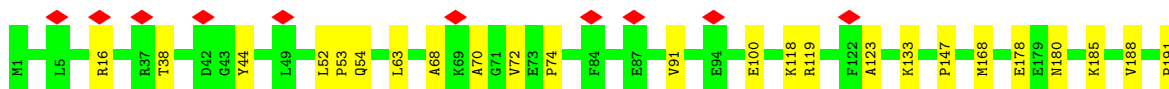
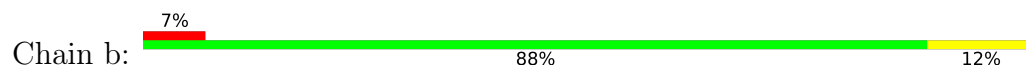
- Molecule 29: 50S ribosomal protein L1

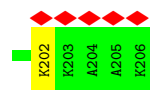


- Molecule 30: 50S ribosomal protein L2

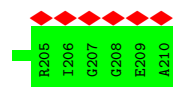


- Molecule 31: 50S ribosomal protein L3

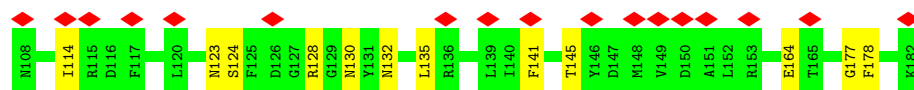
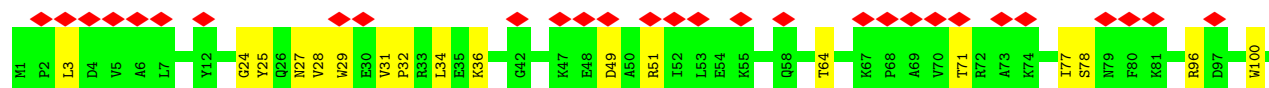
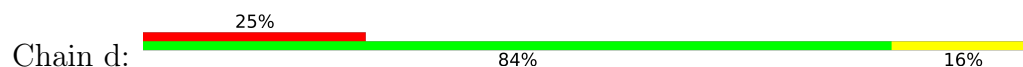




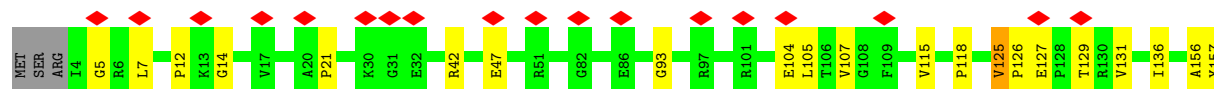
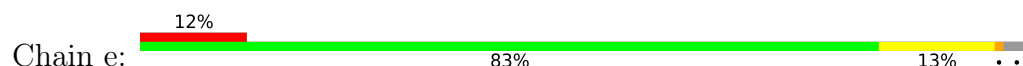
- Molecule 32: 50S ribosomal protein L4



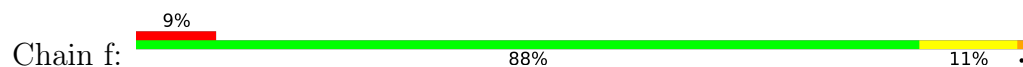
- Molecule 33: 50S ribosomal protein L5



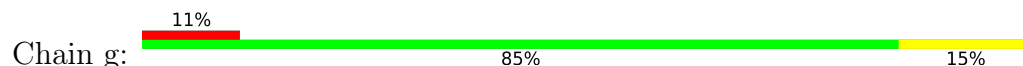
- Molecule 34: 50S ribosomal protein L6

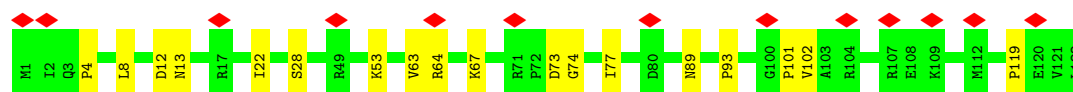


- Molecule 35: 50S ribosomal protein L13

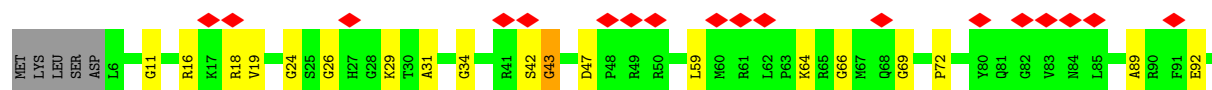
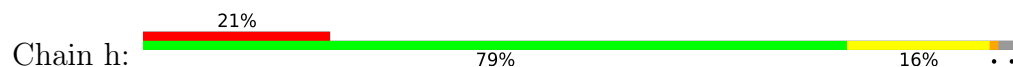


- Molecule 36: 50S ribosomal protein L14

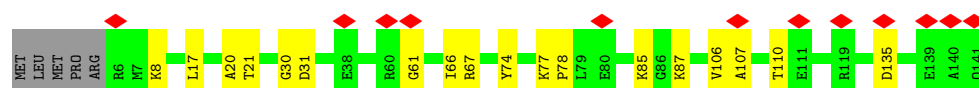
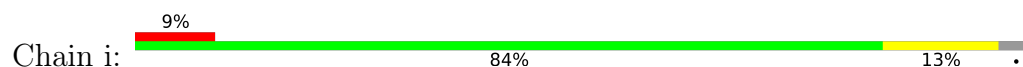




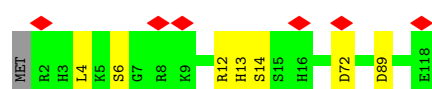
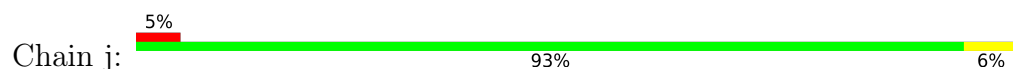
- Molecule 37: 50S ribosomal protein L15



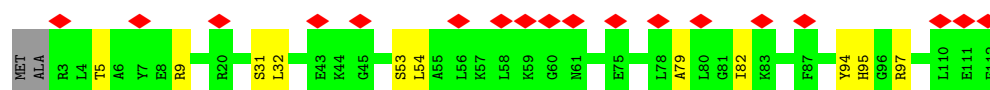
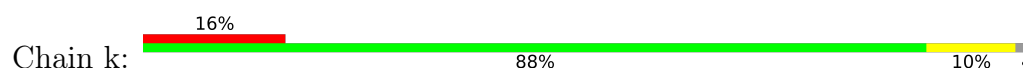
- Molecule 38: 50S ribosomal protein L16



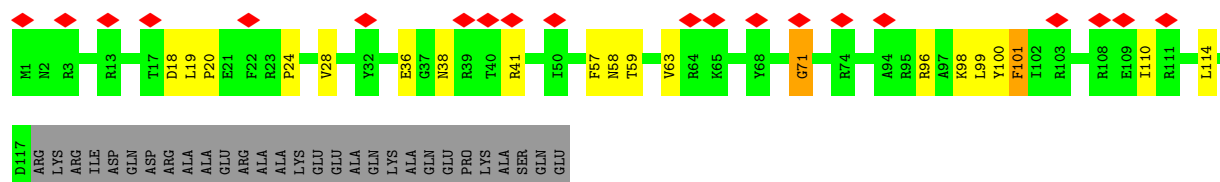
- Molecule 39: 50S ribosomal protein L17



- Molecule 40: 50S ribosomal protein L18

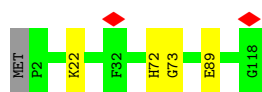


- Molecule 41: 50S ribosomal protein L19




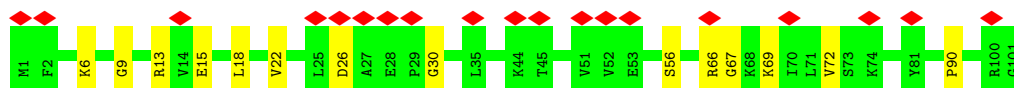
- Molecule 42: 50S ribosomal protein L20

Chain m:  96%




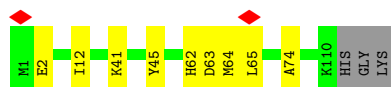
- Molecule 43: 50S ribosomal protein L21

Chain n:  19% 86% 14%

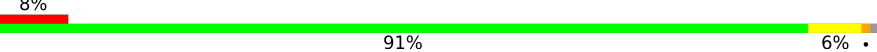


- Molecule 44: 50S ribosomal protein L22

Chain o:  89% 8%




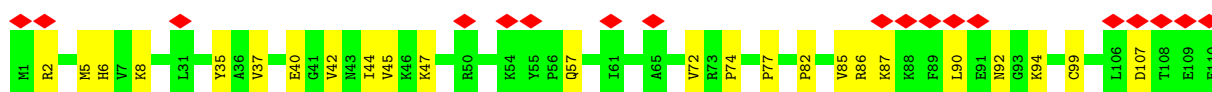
- Molecule 45: 50S ribosomal protein L23

Chain p:  8% 91% 6%




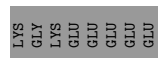
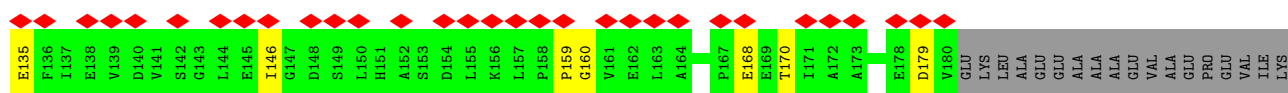
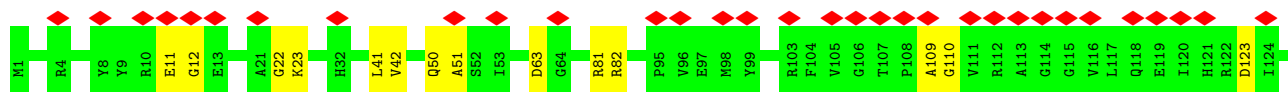
- Molecule 46: 50S ribosomal protein L24

Chain q:  16% 78% 22%

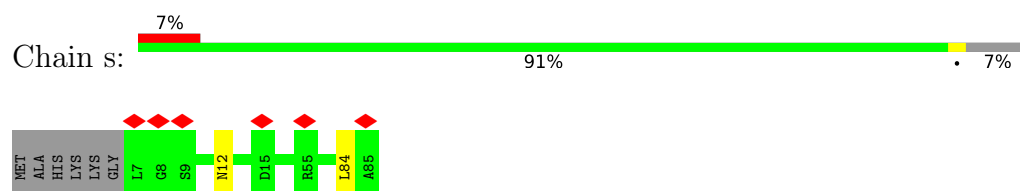


- Molecule 47: 50S ribosomal protein L25

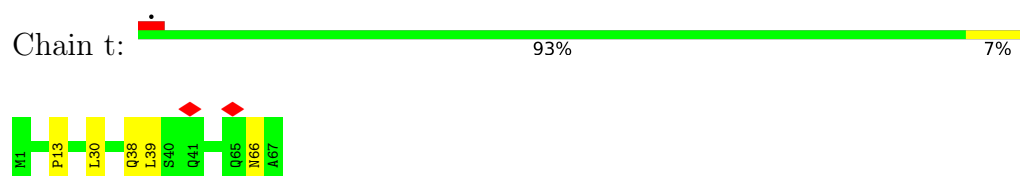
Chain r:  31% 77% 10% 13%



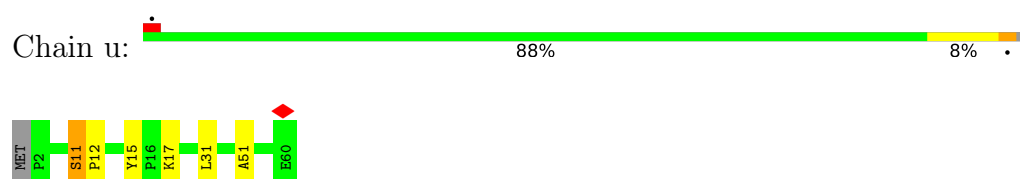
- Molecule 48: 50S ribosomal protein L27



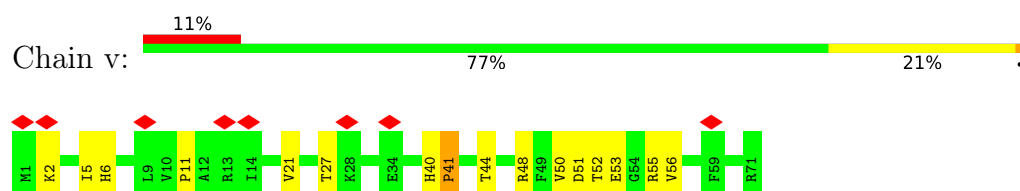
- Molecule 49: 50S ribosomal protein L29



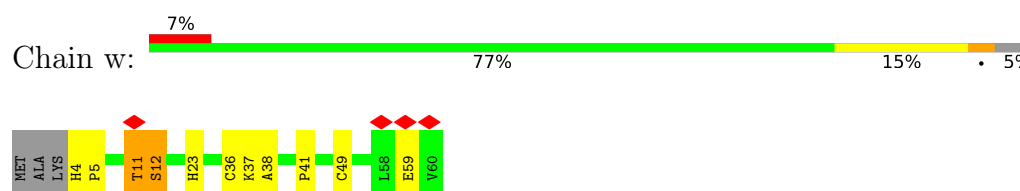
- Molecule 50: 50S ribosomal protein L30



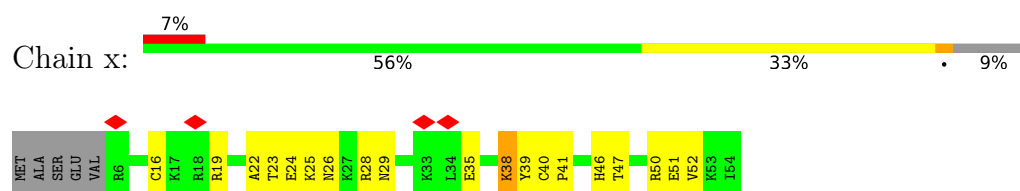
- Molecule 51: 50S ribosomal protein L31



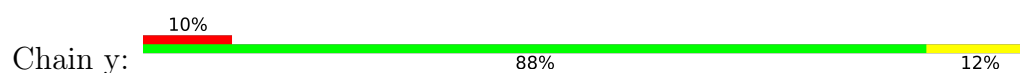
- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L34



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110981	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)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.616	Depositor
Minimum map value	-0.387	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.095	Depositor
Map size (\AA)	414.72, 414.72, 414.72	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.28, 1.28, 1.28	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.77	0/310	0.90	0/407
2	2	0.26	0/640	0.50	0/889
3	3	0.54	0/1012	0.82	6/1373 (0.4%)
4	4	0.85	0/1832	1.03	0/2855
5	5	0.62	2/1813 (0.1%)	1.14	7/2823 (0.2%)
6	A	1.00	4/36438 (0.0%)	1.10	59/56869 (0.1%)
7	D	1.40	164/69685 (0.2%)	1.34	623/108786 (0.6%)
8	E	1.10	1/2954 (0.0%)	1.15	6/4606 (0.1%)
9	F	0.50	0/1935	0.74	0/2609
10	G	0.54	0/1636	0.67	0/2205
11	H	0.53	0/1733	0.76	3/2318 (0.1%)
12	I	0.69	0/1162	0.80	0/1564
13	J	0.48	0/856	0.70	1/1154 (0.1%)
14	K	0.47	0/1276	0.66	0/1709
15	L	0.59	0/1136	0.73	0/1527
16	M	0.46	0/1029	0.68	0/1379
17	N	0.49	0/807	0.69	0/1085
18	O	0.51	0/900	0.64	0/1213
19	P	0.67	0/986	0.79	0/1320
20	Q	0.39	0/924	0.66	1/1238 (0.1%)
21	R	0.64	0/501	0.76	1/664 (0.2%)
22	S	0.54	0/745	0.77	0/992
23	T	0.60	0/716	0.73	0/963
24	U	0.54	0/870	0.74	0/1159
25	V	0.44	0/603	0.71	0/799
26	W	0.39	0/661	0.50	2/890 (0.2%)
27	X	0.52	0/765	0.77	0/1007
28	Y	0.51	0/212	0.67	0/277
29	Z	0.37	0/1775	0.63	1/2393 (0.0%)
30	a	0.81	0/2174	0.93	3/2927 (0.1%)
31	b	0.77	0/1611	0.94	1/2171 (0.0%)
32	c	0.77	0/1660	0.90	0/2247

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.55	0/1507	0.81	1/2027 (0.0%)
34	e	0.58	0/1354	0.78	1/1831 (0.1%)
35	f	0.75	0/1140	0.95	2/1537 (0.1%)
36	g	0.79	0/942	0.93	2/1268 (0.2%)
37	h	0.64	0/1123	1.03	3/1493 (0.2%)
38	i	0.75	0/1100	0.90	0/1470
39	j	0.74	0/974	0.91	0/1302
40	k	0.61	0/887	0.95	0/1180
41	l	0.70	0/990	0.93	2/1325 (0.2%)
42	m	0.91	0/982	0.96	0/1306
43	n	0.65	0/790	0.94	1/1057 (0.1%)
44	o	0.78	0/886	0.83	0/1189
45	p	0.71	0/756	0.85	1/1015 (0.1%)
46	q	0.51	0/857	0.84	0/1142
47	r	0.56	0/1467	0.75	0/1992
48	s	0.81	0/633	0.84	0/843
49	t	0.59	0/569	0.82	1/751 (0.1%)
50	u	0.69	0/474	0.93	1/635 (0.2%)
51	v	0.82	0/594	1.11	2/795 (0.3%)
52	w	0.80	0/459	0.99	1/621 (0.2%)
53	x	0.67	0/433	1.00	2/576 (0.3%)
54	y	0.83	0/438	0.98	1/575 (0.2%)
55	z	0.79	0/523	0.96	1/690 (0.1%)
56	B	0.41	0/4718	0.52	25/6392 (0.4%)
All	All	1.09	171/165953 (0.1%)	1.14	761/247430 (0.3%)

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
9	F	0	1
17	N	0	1
19	P	0	1
21	R	0	1
30	a	0	4
32	c	0	2
33	d	0	2
35	f	0	3
37	h	0	1
40	k	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
41	l	0	3
47	r	0	1
51	v	0	1
52	w	0	5
53	x	0	3
55	z	0	3
All	All	0	34

The worst 5 of 171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1786	A	N9-C4	12.42	1.45	1.37
5	5	1	G	OP3-P	-10.94	1.48	1.61
7	D	1	G	OP3-P	-10.91	1.48	1.61
8	E	-1	A	OP3-P	-10.79	1.48	1.61
7	D	363(F)	A	O3'-P	9.72	1.72	1.61

The worst 5 of 761 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	775	G	N3-C4-C5	-15.67	120.77	128.60
7	D	2491	U	C6-N1-C2	-13.29	113.03	121.00
7	D	1664	A	C8-N9-C4	-13.09	100.56	105.80
7	D	1779	U	C5-C4-O4	-12.85	118.19	125.90
7	D	775	G	C8-N9-C4	-12.80	101.28	106.40

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	F	95	GLN	Peptide
17	N	33	GLN	Peptide
19	P	15	ARG	Peptide
21	R	34	TYR	Peptide
30	a	226	MET	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	35/37 (95%)	23 (66%)	6 (17%)	6 (17%)	0	2
2	2	128/173 (74%)	96 (75%)	23 (18%)	9 (7%)	1	12
3	3	132/147 (90%)	68 (52%)	37 (28%)	27 (20%)	0	1
9	F	232/256 (91%)	179 (77%)	32 (14%)	21 (9%)	0	9
10	G	204/239 (85%)	170 (83%)	21 (10%)	13 (6%)	1	14
11	H	206/209 (99%)	172 (84%)	17 (8%)	17 (8%)	0	10
12	I	148/162 (91%)	125 (84%)	15 (10%)	8 (5%)	1	17
13	J	99/101 (98%)	85 (86%)	8 (8%)	6 (6%)	1	15
14	K	153/156 (98%)	138 (90%)	11 (7%)	4 (3%)	4	28
15	L	136/138 (99%)	112 (82%)	17 (12%)	7 (5%)	1	17
16	M	125/128 (98%)	90 (72%)	27 (22%)	8 (6%)	1	14
17	N	96/105 (91%)	80 (83%)	12 (12%)	4 (4%)	2	20
18	O	117/129 (91%)	104 (89%)	8 (7%)	5 (4%)	2	20
19	P	122/132 (92%)	91 (75%)	24 (20%)	7 (6%)	1	16
20	Q	112/126 (89%)	77 (69%)	23 (20%)	12 (11%)	0	6
21	R	58/61 (95%)	43 (74%)	9 (16%)	6 (10%)	0	7
22	S	86/89 (97%)	74 (86%)	10 (12%)	2 (2%)	5	30
23	T	81/88 (92%)	69 (85%)	8 (10%)	4 (5%)	2	18
24	U	102/105 (97%)	80 (78%)	16 (16%)	6 (6%)	1	15
25	V	71/88 (81%)	57 (80%)	10 (14%)	4 (6%)	1	16
26	W	78/93 (84%)	30 (38%)	25 (32%)	23 (30%)	0	0
27	X	97/106 (92%)	85 (88%)	8 (8%)	4 (4%)	2	20
28	Y	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
29	Z	226/229 (99%)	187 (83%)	28 (12%)	11 (5%)	2	18
30	a	270/276 (98%)	201 (74%)	38 (14%)	31 (12%)	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	b	204/206 (99%)	150 (74%)	31 (15%)	23 (11%)	0	5
32	c	206/210 (98%)	165 (80%)	25 (12%)	16 (8%)	1	11
33	d	180/182 (99%)	115 (64%)	42 (23%)	23 (13%)	0	4
34	e	172/180 (96%)	125 (73%)	24 (14%)	23 (13%)	0	3
35	f	137/140 (98%)	107 (78%)	19 (14%)	11 (8%)	1	11
36	g	120/122 (98%)	81 (68%)	24 (20%)	15 (12%)	0	4
37	h	143/150 (95%)	93 (65%)	28 (20%)	22 (15%)	0	3
38	i	134/141 (95%)	92 (69%)	25 (19%)	17 (13%)	0	4
39	j	115/118 (98%)	104 (90%)	6 (5%)	5 (4%)	2	20
40	k	108/112 (96%)	77 (71%)	22 (20%)	9 (8%)	0	10
41	l	115/146 (79%)	80 (70%)	19 (16%)	16 (14%)	0	3
42	m	115/118 (98%)	100 (87%)	11 (10%)	4 (4%)	3	23
43	n	99/101 (98%)	66 (67%)	20 (20%)	13 (13%)	0	3
44	o	108/113 (96%)	86 (80%)	14 (13%)	8 (7%)	1	12
45	p	92/96 (96%)	71 (77%)	14 (15%)	7 (8%)	1	11
46	q	108/110 (98%)	63 (58%)	21 (19%)	24 (22%)	0	1
47	r	178/206 (86%)	130 (73%)	28 (16%)	20 (11%)	0	5
48	s	77/85 (91%)	65 (84%)	10 (13%)	2 (3%)	4	28
49	t	65/67 (97%)	54 (83%)	7 (11%)	4 (6%)	1	15
50	u	57/60 (95%)	44 (77%)	8 (14%)	5 (9%)	0	9
51	v	69/71 (97%)	35 (51%)	21 (30%)	13 (19%)	0	2
52	w	55/60 (92%)	37 (67%)	11 (20%)	7 (13%)	0	4
53	x	47/54 (87%)	16 (34%)	16 (34%)	15 (32%)	0	0
54	y	47/49 (96%)	33 (70%)	9 (19%)	5 (11%)	0	6
55	z	62/65 (95%)	45 (73%)	8 (13%)	9 (14%)	0	3
56	B	587/610 (96%)	267 (46%)	188 (32%)	132 (22%)	0	0
All	All	6536/6972 (94%)	4756 (73%)	1087 (17%)	693 (11%)	1	6

5 of 693 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	ARG
1	1	33	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	77	PRO
2	2	93	LEU
2	2	107	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	34/34 (100%)	34 (100%)	0	100	100
3	3	101/111 (91%)	93 (92%)	8 (8%)	10	34
9	F	202/220 (92%)	201 (100%)	1 (0%)	86	90
10	G	160/188 (85%)	159 (99%)	1 (1%)	84	88
11	H	180/181 (99%)	179 (99%)	1 (1%)	84	88
12	I	115/123 (94%)	114 (99%)	1 (1%)	75	82
13	J	90/90 (100%)	90 (100%)	0	100	100
14	K	126/127 (99%)	126 (100%)	0	100	100
15	L	119/119 (100%)	119 (100%)	0	100	100
16	M	98/99 (99%)	98 (100%)	0	100	100
17	N	88/92 (96%)	88 (100%)	0	100	100
18	O	90/99 (91%)	90 (100%)	0	100	100
19	P	104/109 (95%)	103 (99%)	1 (1%)	73	80
20	Q	92/101 (91%)	78 (85%)	14 (15%)	2	14
21	R	49/50 (98%)	49 (100%)	0	100	100
22	S	79/80 (99%)	78 (99%)	1 (1%)	65	76
23	T	72/74 (97%)	72 (100%)	0	100	100
24	U	96/97 (99%)	96 (100%)	0	100	100
25	V	64/77 (83%)	64 (100%)	0	100	100
26	W	71/80 (89%)	47 (66%)	24 (34%)	0	1
27	X	76/82 (93%)	76 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	Y	19/22 (86%)	19 (100%)	0	100	100
29	Z	180/181 (99%)	177 (98%)	3 (2%)	56	72
30	a	215/218 (99%)	212 (99%)	3 (1%)	62	75
31	b	166/166 (100%)	165 (99%)	1 (1%)	84	88
32	c	164/166 (99%)	161 (98%)	3 (2%)	54	71
33	d	156/156 (100%)	152 (97%)	4 (3%)	41	61
34	e	143/148 (97%)	142 (99%)	1 (1%)	81	86
35	f	118/119 (99%)	117 (99%)	1 (1%)	79	84
36	g	100/100 (100%)	99 (99%)	1 (1%)	73	80
37	h	111/116 (96%)	109 (98%)	2 (2%)	54	71
38	i	106/111 (96%)	105 (99%)	1 (1%)	75	82
39	j	100/101 (99%)	98 (98%)	2 (2%)	50	68
40	k	87/88 (99%)	87 (100%)	0	100	100
41	l	105/127 (83%)	104 (99%)	1 (1%)	73	80
42	m	93/94 (99%)	93 (100%)	0	100	100
43	n	82/82 (100%)	82 (100%)	0	100	100
44	o	90/92 (98%)	89 (99%)	1 (1%)	70	79
45	p	76/78 (97%)	76 (100%)	0	100	100
46	q	91/91 (100%)	91 (100%)	0	100	100
47	r	159/179 (89%)	159 (100%)	0	100	100
48	s	63/67 (94%)	63 (100%)	0	100	100
49	t	62/62 (100%)	62 (100%)	0	100	100
50	u	51/52 (98%)	50 (98%)	1 (2%)	50	68
51	v	63/63 (100%)	62 (98%)	1 (2%)	58	73
52	w	50/52 (96%)	50 (100%)	0	100	100
53	x	48/52 (92%)	48 (100%)	0	100	100
54	y	42/42 (100%)	42 (100%)	0	100	100
55	z	54/55 (98%)	52 (96%)	2 (4%)	29	53
56	B	490/505 (97%)	347 (71%)	143 (29%)	0	1
All	All	5390/5618 (96%)	5167 (96%)	223 (4%)	28	50

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	B	164	ILE
56	B	591	GLU
56	B	294	PHE
56	B	582	LYS
56	B	495	LEU

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

Mol	Chain	Res	Type
39	j	13	HIS
49	t	4	GLN
40	k	38	GLN
44	o	34	ASN
51	v	47	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	4	76/77 (98%)	29 (38%)	0
5	5	75/76 (98%)	32 (42%)	3 (4%)
6	A	1515/1522 (99%)	529 (34%)	102 (6%)
7	D	2888/2893 (99%)	1316 (45%)	205 (7%)
8	E	122/123 (99%)	48 (39%)	4 (3%)
All	All	4676/4691 (99%)	1954 (41%)	314 (6%)

5 of 1954 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	4	5	G
4	4	8	U
4	4	9	G
4	4	13	C
4	4	17	C

5 of 314 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	D	1784	A
7	D	2449	U
7	D	1913	A
7	D	2115	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	D	2732	G

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](#)

1 ligand is 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	$\# Z > 2$
57	GCP	B	701	-	27,34,34	1.53	6 (22%)	34,54,54	1.98	8 (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
57	GCP	B	701	-	-	4/15/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	B	701	GCP	C5-C6	4.19	1.48	1.41
57	B	701	GCP	PG-O3G	2.86	1.61	1.54
57	B	701	GCP	PB-O3A	2.84	1.61	1.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	B	701	GCP	PG-O2G	2.84	1.61	1.54
57	B	701	GCP	C5-C4	2.46	1.47	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	B	701	GCP	C2-N3-C4	4.94	121.00	115.36
57	B	701	GCP	C2-N1-C6	4.02	122.32	115.93
57	B	701	GCP	C5-C6-N1	-3.96	118.01	123.43
57	B	701	GCP	PB-O3A-PA	-3.82	120.45	132.56
57	B	701	GCP	C4-C5-C6	-3.71	117.26	120.80

There are no chirality outliers.

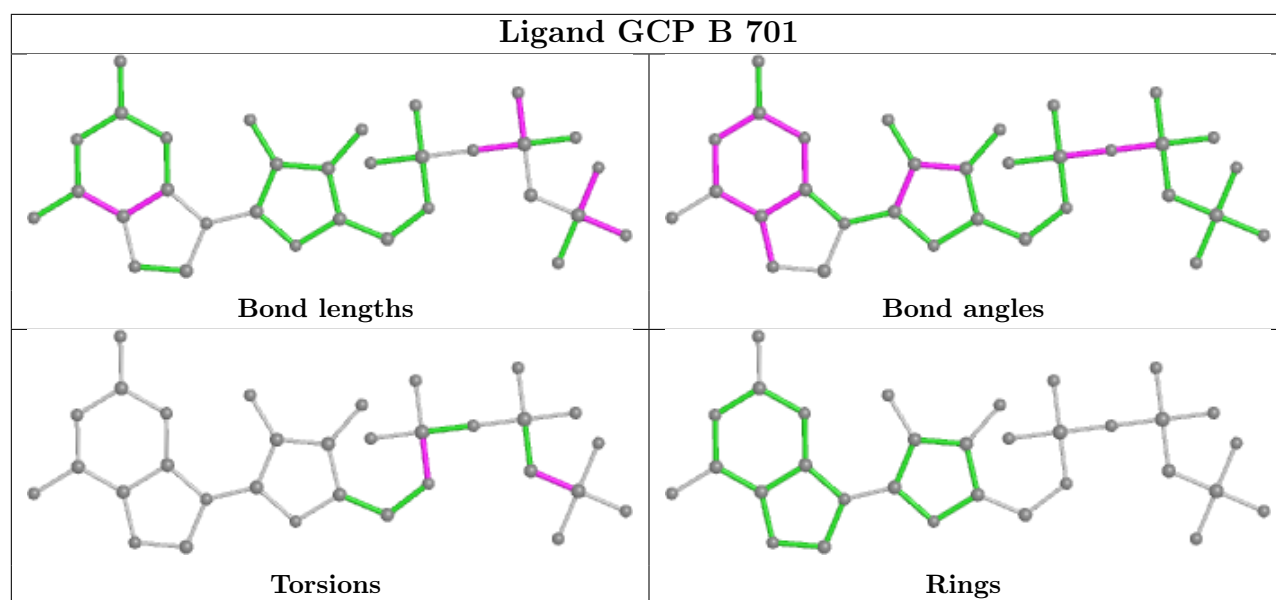
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	B	701	GCP	C5'-O5'-PA-O3A
57	B	701	GCP	C5'-O5'-PA-O1A
57	B	701	GCP	C5'-O5'-PA-O2A
57	B	701	GCP	PB-C3B-PG-O1G

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.

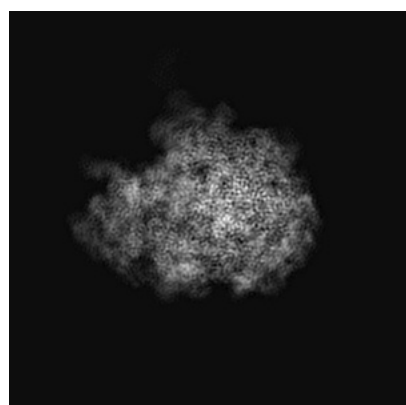
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6584. These allow visual inspection of the internal detail of the map and identification of artifacts.

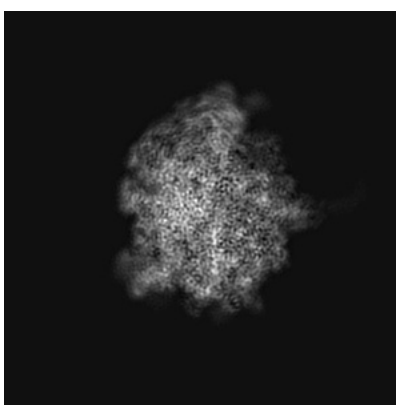
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

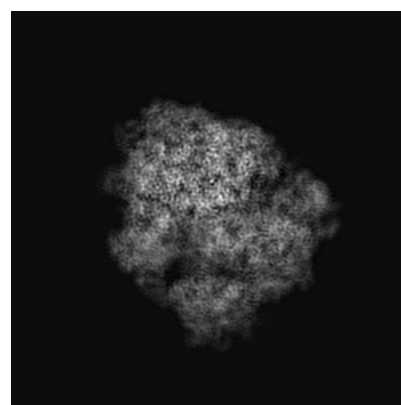
6.1.1 Primary map



X



Y

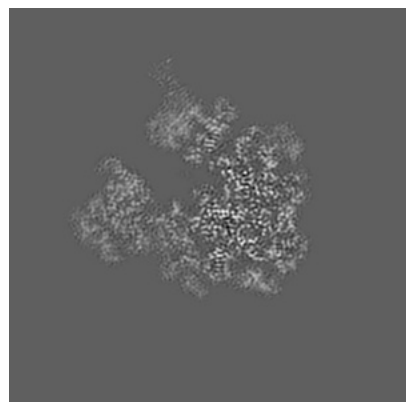


Z

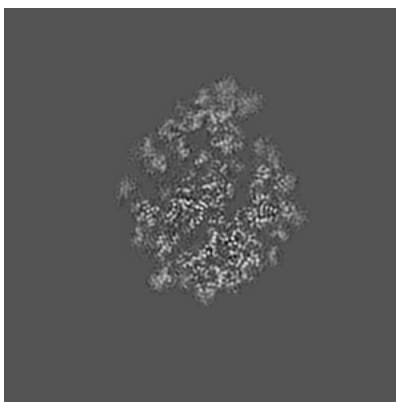
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

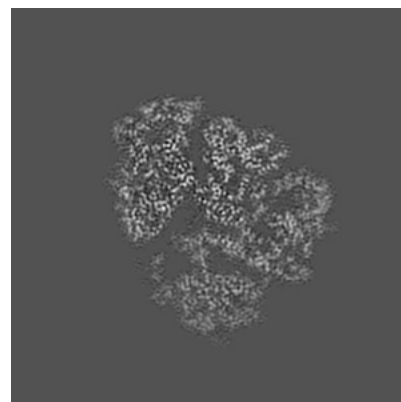
6.2.1 Primary map



X Index: 162



Y Index: 162

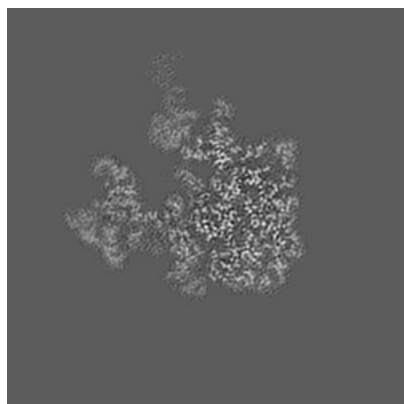


Z Index: 162

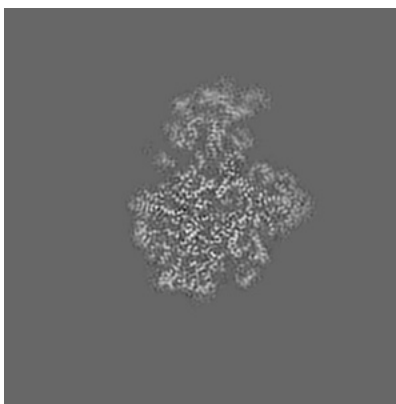
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

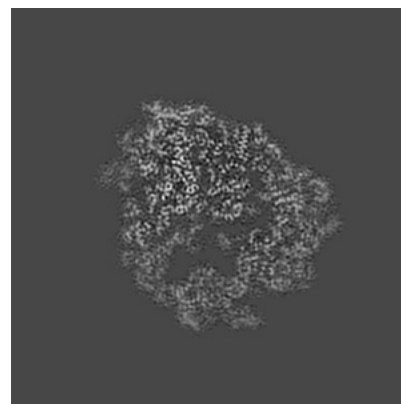
6.3.1 Primary map



X Index: 168



Y Index: 169

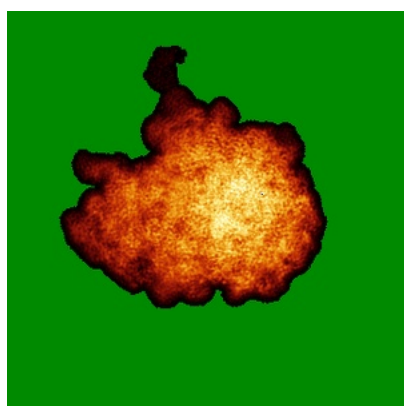


Z Index: 170

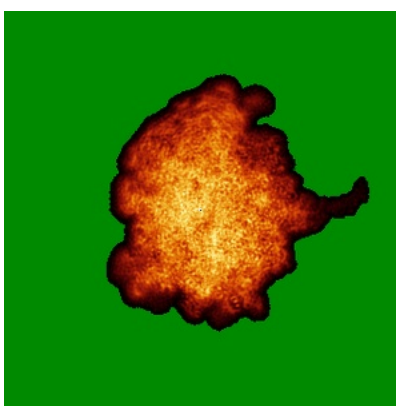
The images above show the largest variance slices of the map in three orthogonal directions.

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

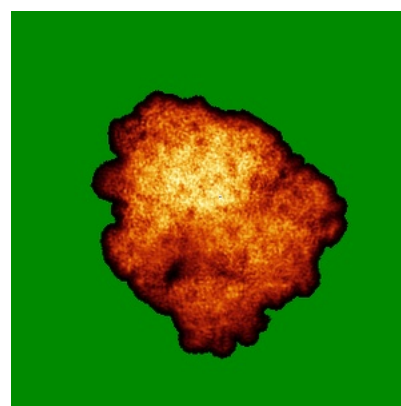
6.4.1 Primary map



X



Y

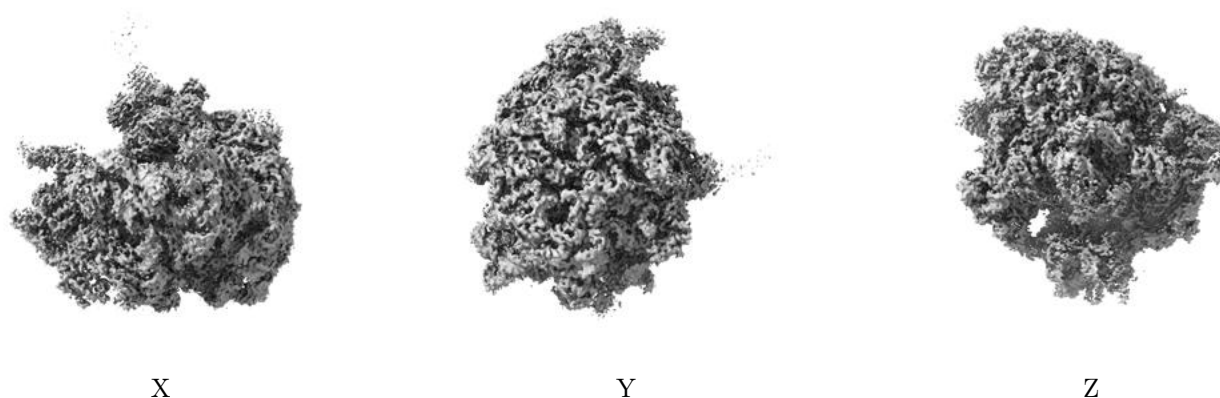


Z

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 0.095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

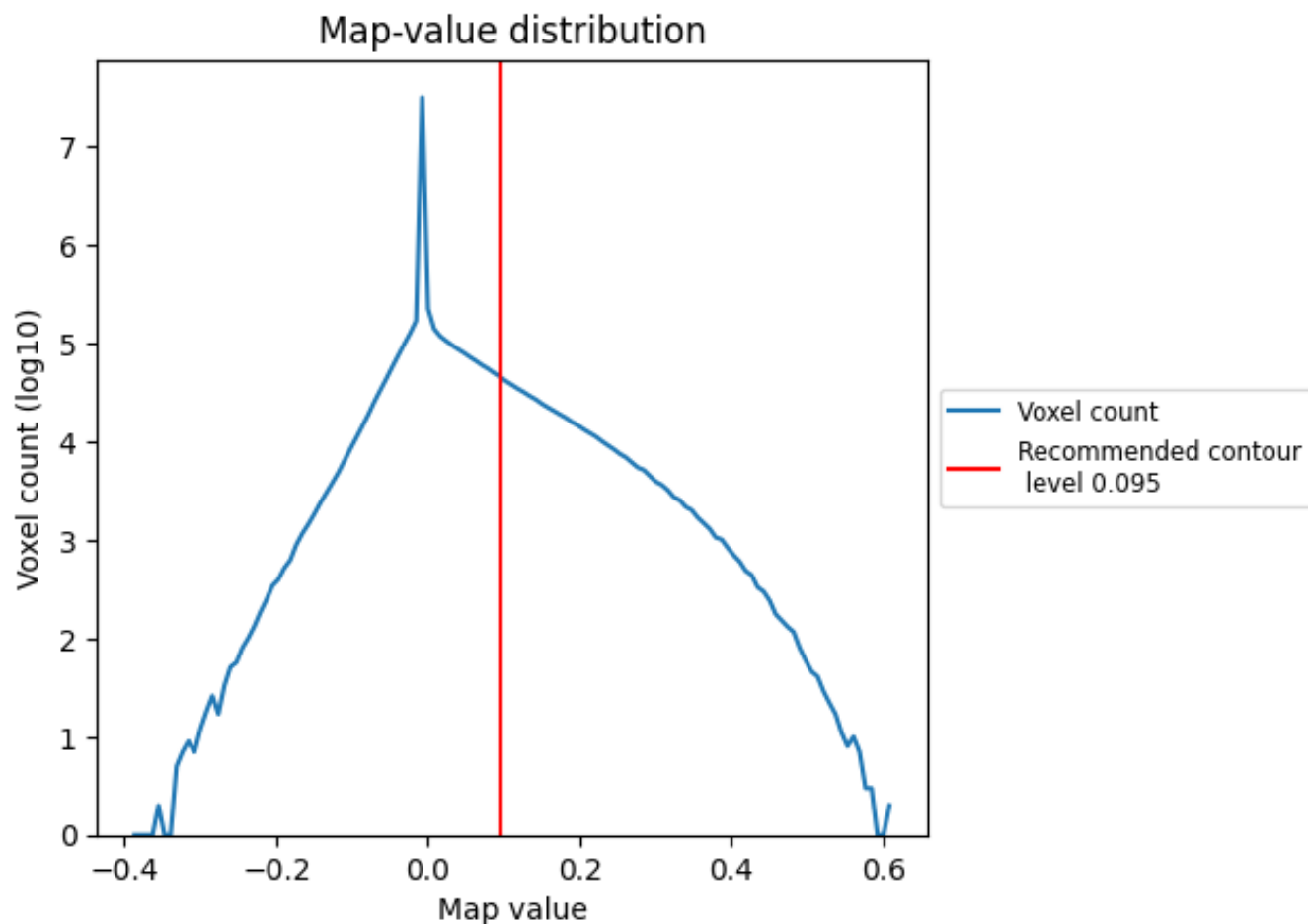
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

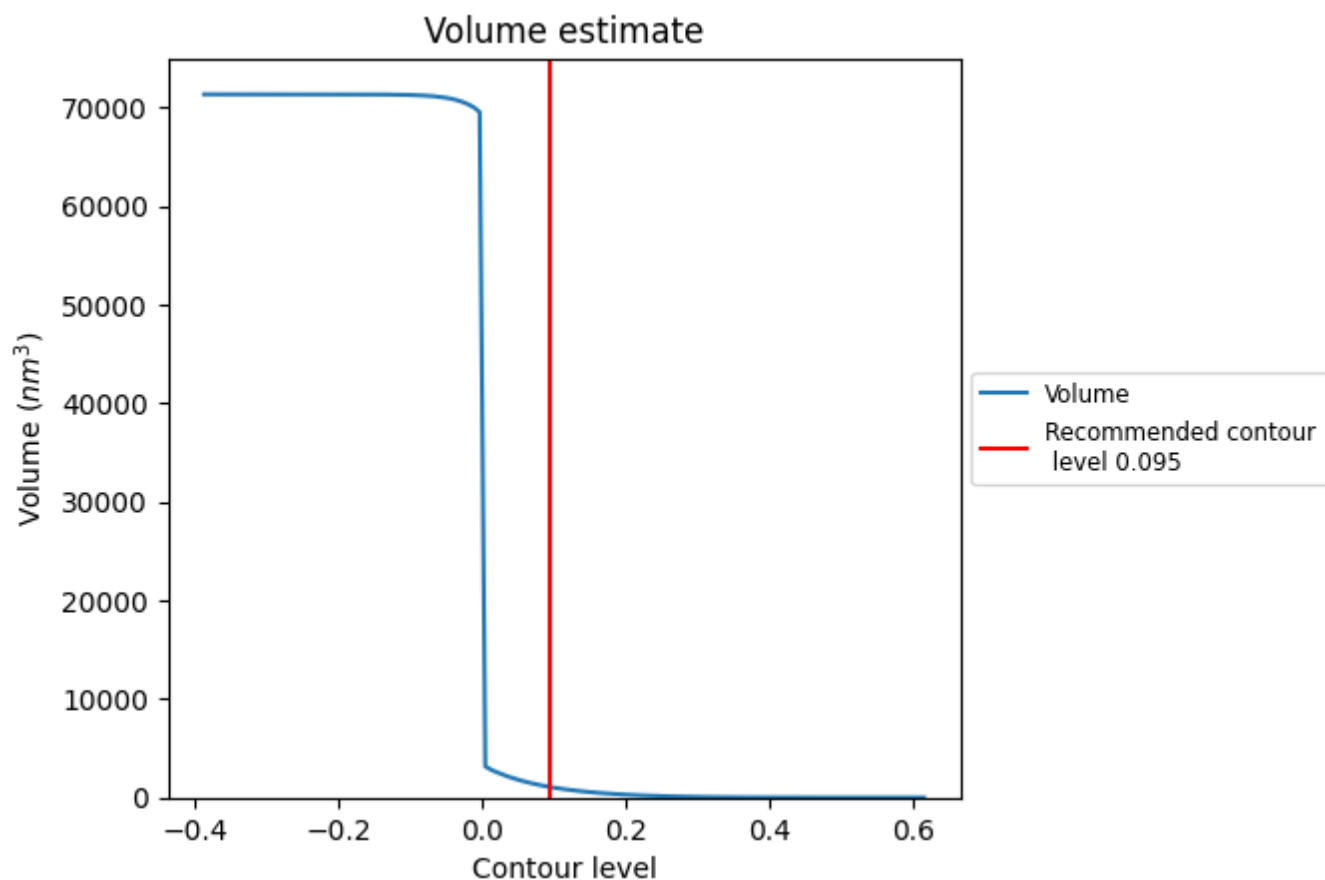
This section contains the results of statistical analysis of the map.

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.

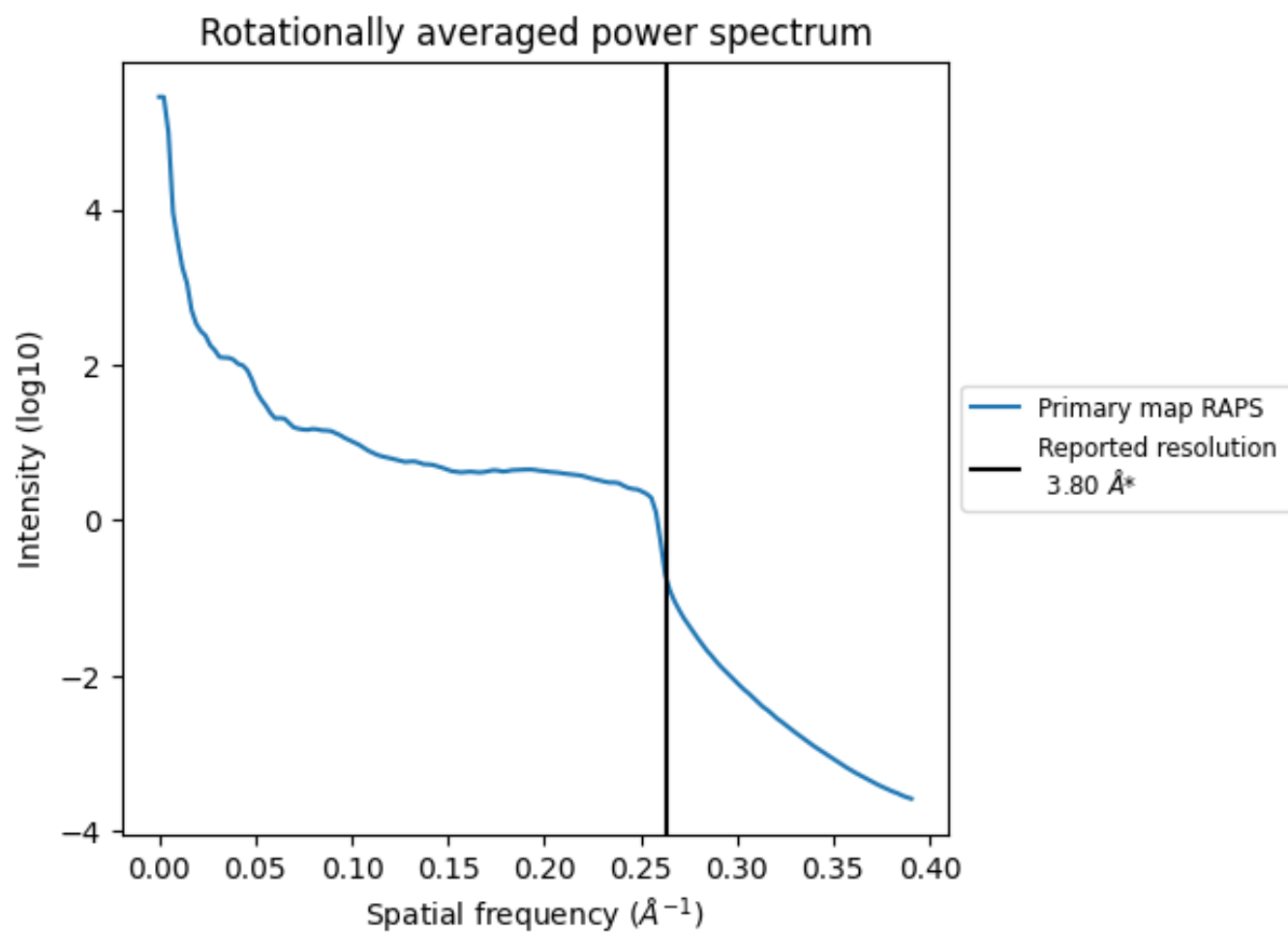
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1072 nm³; this corresponds to an approximate mass of 968 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

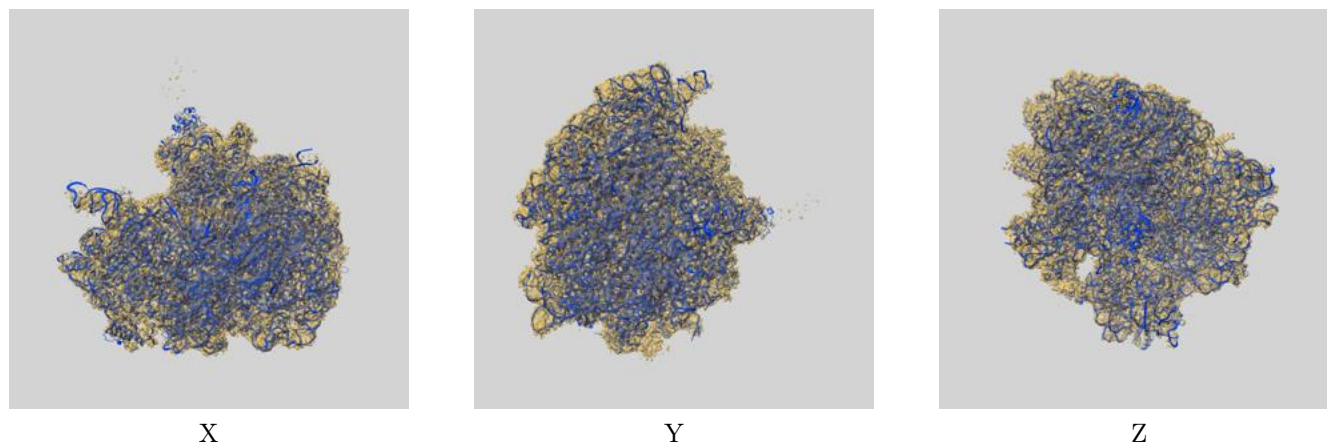
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

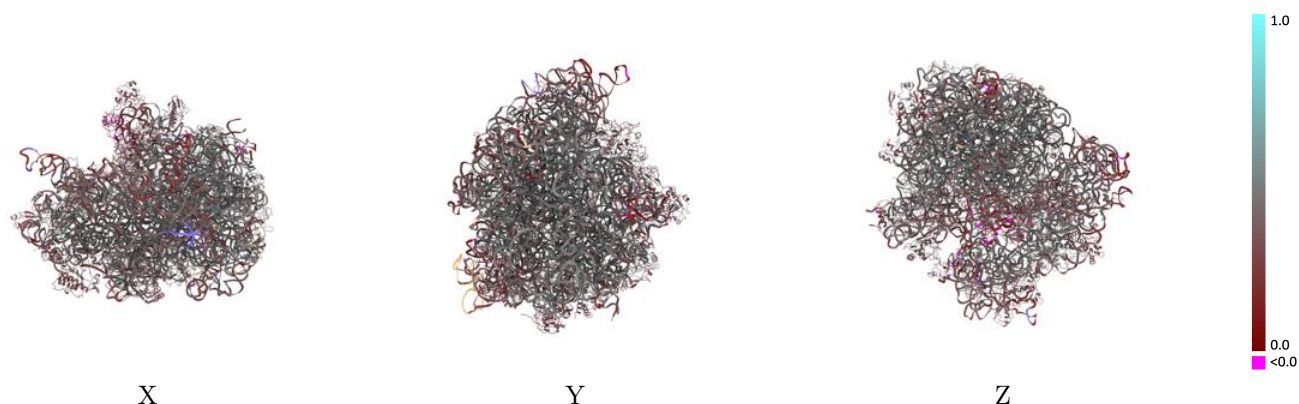
This section contains information regarding the fit between EMDB map EMD-6584 and PDB model 5IMQ. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



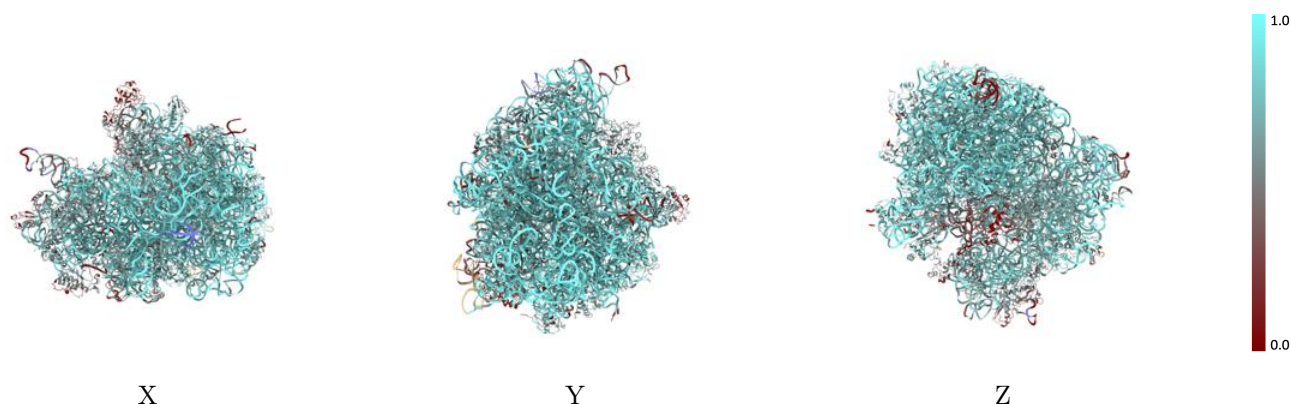
The images above show the 3D surface view of the map at the recommended contour level 0.095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



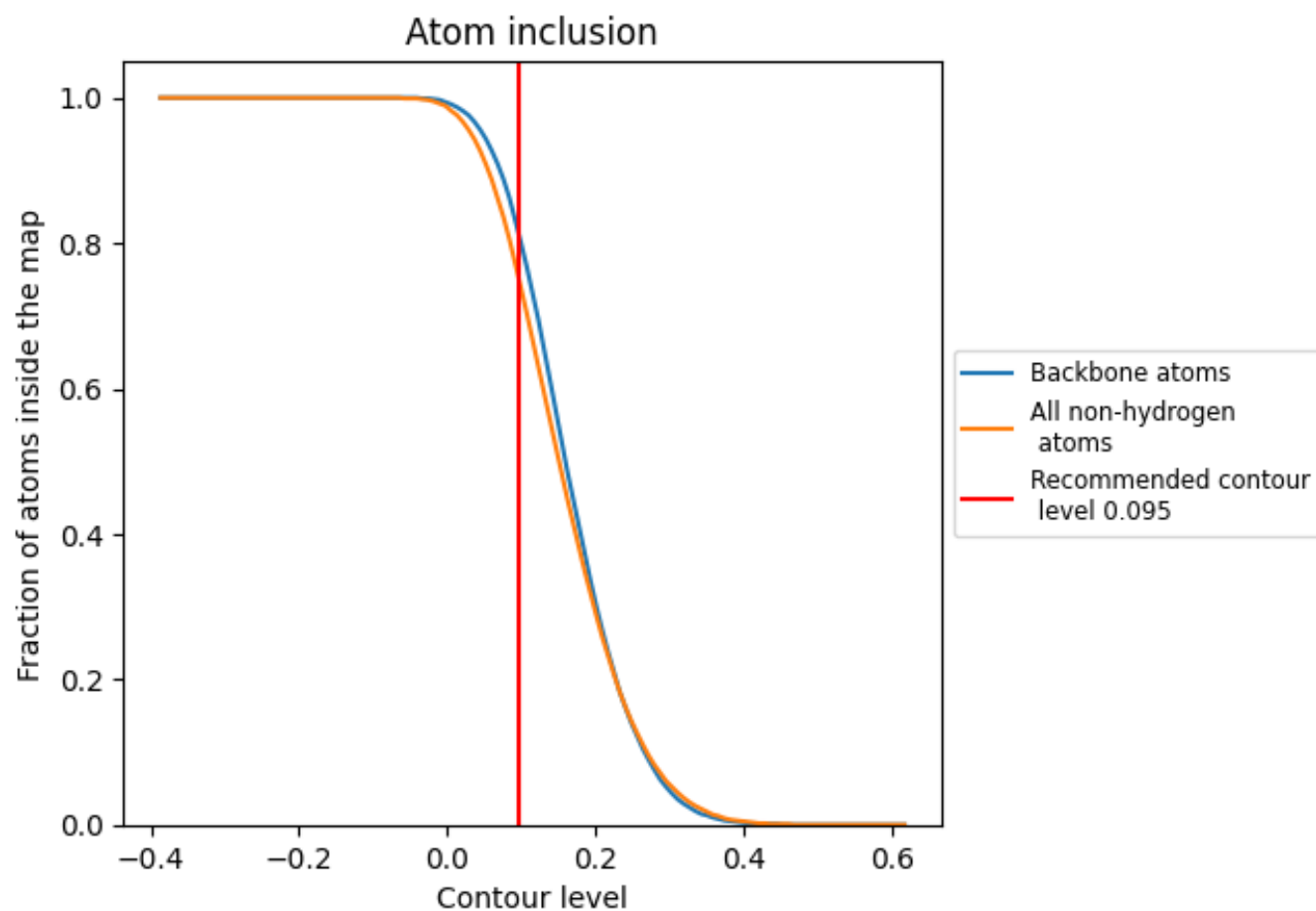
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.095).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ













































The table lists the average atom inclusion at the recommended contour level (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7560	 0.4020
1	 0.7650	 0.4810
2	 0.1920	 0.3240
3	 0.3170	 0.1780
4	 0.6350	 0.4010
5	 0.2730	 0.2430
A	 0.8310	 0.4030
B	 0.5040	 0.3030
D	 0.8640	 0.4290
E	 0.8960	 0.4250
F	 0.5090	 0.3650
G	 0.5850	 0.4070
H	 0.6020	 0.3710
I	 0.6800	 0.4430
J	 0.5040	 0.3330
K	 0.4890	 0.3660
L	 0.6710	 0.4270
M	 0.5060	 0.3610
N	 0.4770	 0.3540
O	 0.5790	 0.3990
P	 0.6790	 0.4600
Q	 0.4300	 0.2670
R	 0.6250	 0.4330
S	 0.6170	 0.3790
T	 0.6630	 0.3900
U	 0.5980	 0.3900
V	 0.5020	 0.3570
W	 0.3710	 0.1910
X	 0.6200	 0.3910
Y	 0.6810	 0.4310
Z	 0.1310	 0.2160
a	 0.6970	 0.4310
b	 0.7160	 0.4330
c	 0.6850	 0.4010
d	 0.5710	 0.3180



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.6480	 0.3860
f	 0.6850	 0.4130
g	 0.6710	 0.4210
h	 0.6020	 0.3350
i	 0.6850	 0.4220
j	 0.7430	 0.4460
k	 0.6350	 0.3260
l	 0.6290	 0.3950
m	 0.7700	 0.4360
n	 0.6500	 0.3650
o	 0.7490	 0.4560
p	 0.6840	 0.4190
q	 0.6080	 0.3660
r	 0.5290	 0.3770
s	 0.7300	 0.4570
t	 0.7000	 0.4210
u	 0.7110	 0.4390
v	 0.6480	 0.3690
w	 0.7760	 0.4230
x	 0.6800	 0.3610
y	 0.7210	 0.4510
z	 0.6640	 0.4210