



Full wwPDB EM Validation Report ⓘ

Dec 14, 2024 – 08:32 PM EST

PDB ID : 8UR0
EMDB ID : EMD-42479
Title : Escherichia coli transcription-translation coupled complex class B (TTC-B) containing RfaH bound to ops signal, NusA, mRNA with a 24 nt long spacer, and fMet-tRNAs in E-site and P-site of the ribosome
Authors : Molodtsov, V.; Wang, C.; Ebright, R.H.
Deposited on : 2023-10-25
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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.dev113
MolProbity : 4.02b-467
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) : 2.40

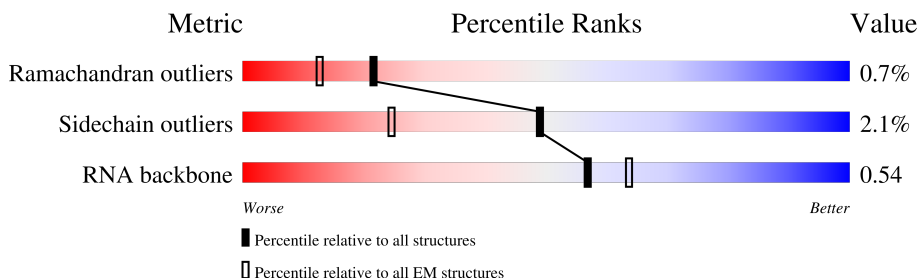
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	0	103	<div> <div>36%</div> <div>100%</div> </div>
2	1	110	<div> <div>20%</div> <div>100%</div> </div>
3	2	100	<div> <div>5%</div> <div>91%</div> <div>6%</div> </div>
4	3	104	<div> <div>32%</div> <div>99%</div> </div>
5	4	94	<div> <div>23%</div> <div>98%</div> </div>
6	5	38	<div> <div>37%</div> <div>58%</div> <div>34%</div> <div>8%</div> </div>
7	6	38	<div> <div>26%</div> <div>71%</div> <div>21%</div> <div>8%</div> </div>
8	7	41	<div> <div>12%</div> <div>17%</div> <div>68%</div> <div>5%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
9	9	165	
10	A	76	
10	B	76	
11	AA	1342	
12	AB	162	
13	AC	329	
13	AD	329	
14	AE	1407	
15	AF	91	
16	AG	495	
17	C	75	
18	D	1542	
19	E	87	
20	F	71	
21	G	241	
22	H	557	
23	I	233	
24	J	206	
25	K	167	
26	L	135	
27	M	179	
28	N	130	
29	O	130	
30	P	103	
31	Q	129	

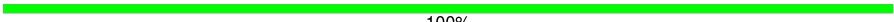


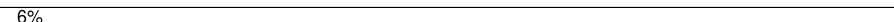
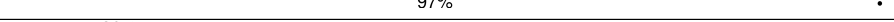
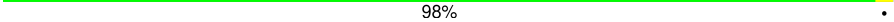
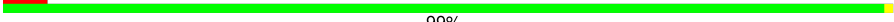


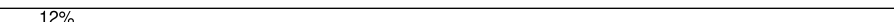
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Mol	Chain	Length	Quality of chain
32	R	124	
33	S	101	
34	T	89	
35	U	82	
36	V	84	
37	W	92	
38	X	118	
39	Y	142	
40	Z	121	
41	a	2904	
42	b	85	
43	c	78	
44	d	120	
45	e	63	
46	f	59	
47	g	70	
48	h	273	
49	i	57	
50	j	209	
51	k	55	
52	l	201	
53	m	46	
54	n	179	
55	o	65	
56	p	177	

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Mol	Chain	Length	Quality of chain
57	q	38	 100%
58	r	149	 37% 100%
59	s	142	 6% 97% ..
60	t	123	 6% 97% .
61	u	144	 26% 98% .
62	v	136	 5% 99% .
63	w	127	 9% 89% 5% 6%
64	x	117	 39% 99% .
65	y	115	 12% 97% ..
66	z	118	 12% 97% ..

2 Entry composition [i](#)

There are 68 unique types of molecules in this entry. The entry contains 280292 atoms, of which 98639 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 Ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	94	Total	C	H	N	O	S	0	0
			1557	470	811	140	134	2		

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	3	103	Total	C	H	N	O		0	0
			1632	498	844	148	142			

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 6 is a DNA chain called NT DNA ops.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	35	Total	C	N	O	P		0	0
			726	342	141	208	35			

- Molecule 7 is a DNA chain called T DNA ops.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	35	Total	C	N	O	P	0	0
			703	336	117	215	35		

- Molecule 8 is a RNA chain called mRNA with 24 nt long spacer.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	37	Total	C	N	O	P	0	0
			772	345	110	280	37		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 10 is a RNA chain called E-site and P-site fMet-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A	76	Total 2446	C 723	H 826	N 295	O 527	P 75	0	0
10	B	76	Total 2434	C 723	H 814	N 295	O 527	P 75	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	1316	Total	C	N	O	S	0	0
			10381	6514	1810	2014	43		

- Molecule 12 is a protein called Transcription antitermination protein RfaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AB	161	Total	C	N	O	S	0	0
			1286	828	222	232	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AC	221	Total	C	N	O	S	0	0
			1698	1060	299	333	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	AD	299	Total	C	N	O	S	0	0
			2078	1287	378	407	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AE	1337	Total	C	N	O	S	0	0
			10404	6535	1856	1963	50		

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AF	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 16 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AG	495	Total	C	N	O	S	0	0
			3852	2396	669	774	13		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	C	66	Total	C	H	N	O	S	0
			1103	344	559	102	97	1	0

- Molecule 18 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D	1524	Total	C	H	N	O	P	0
			49126	14585	16423	6003	10591	1524	0

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	86	Total	C	H	N	O	S	0
			1388	414	719	138	114	3	0

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	F	70	Total	C	H	N	O	S	0	0
			1218	366	629	125	97	1		

- Molecule 21 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 22 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 23 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 24 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 25 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 26 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 27 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	M	151	Total	C	H	N	O	S	0	0
			2416	735	1235	227	215	4		

- Molecule 28 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	N	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 29 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	O	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	P	99	Total	C	H	N	O	S	0	0
			1621	495	831	151	143	1		

- Molecule 31 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Q	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

- Molecule 32 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	R	121	Total	C	H	N	O	S	0	0
			1940	580	1001	194	161	4		

- Molecule 33 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	S	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 34 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 35 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 36 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 37 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 38 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 39 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Y	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 40 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Z	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 41 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	a	2880	Total	C	H	N	O	P	0	0
			92918	27587	31077	11398	19976	2880		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	b	76	Total	C	H	N	O	S	0	0
			1181	360	599	117	104	1		

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	c	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 44 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	d	120	Total	C	H	N	O	P	0	0
			3870	1144	1301	468	837	120		

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	e	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	f	58	Total	C	H	N	O	S	0	0
			936	281	488	87	78	2		

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	g	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

- Molecule 48 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	h	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	j	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	k	52	Total	C	H	N	O		0	0
			890	275	464	78	73			

- Molecule 52 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	l	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	m	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 54 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
55	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 58 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 59 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	s	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 60 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 61 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	u	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 62 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 63 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 64 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	x	116	Total	C	H	N	O	0	0
			1815	552	923	178	162		

- Molecule 65 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	y	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 66 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	z	117	Total	C	H	N	O	0	0
			1967	604	1020	192	151		

- Molecule 67 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
67	AE	1	Total	Mg	0
			1	1	

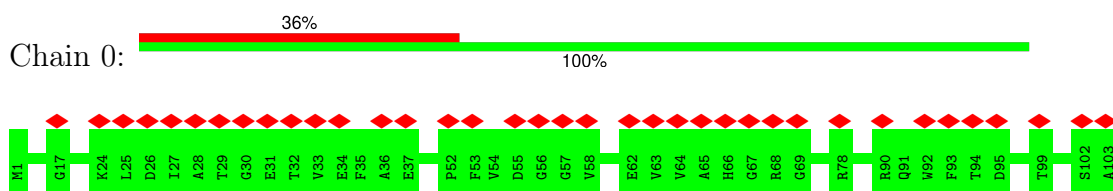
- Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
68	AE	2	Total	Zn	0
			2	2	

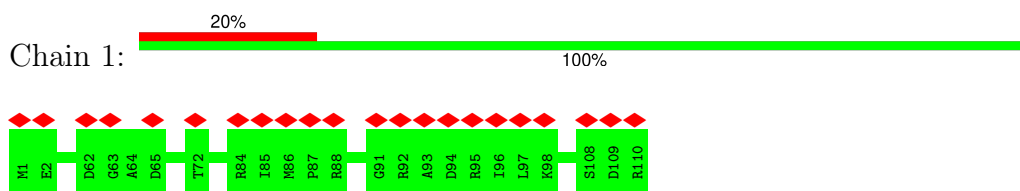
3 Residue-property plots [i](#)

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.

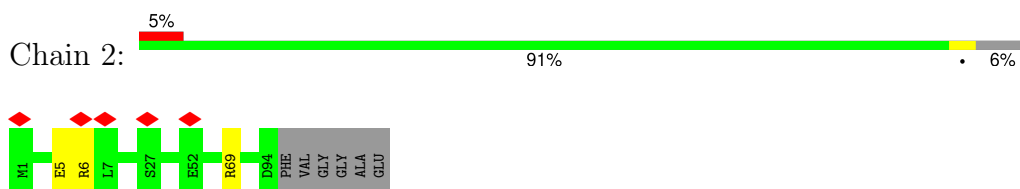
- Molecule 1: Ribosomal protein L21



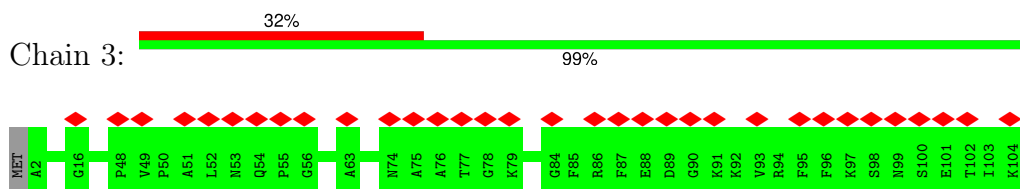
- Molecule 2: 50S ribosomal protein L22



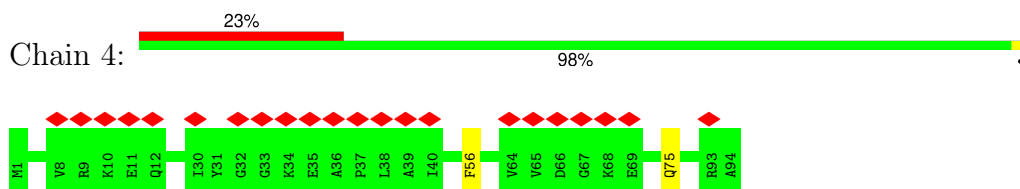
- Molecule 3: 50S ribosomal protein L23



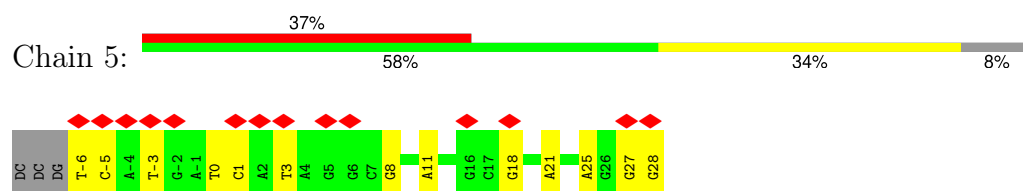
- Molecule 4: 50S ribosomal protein L24



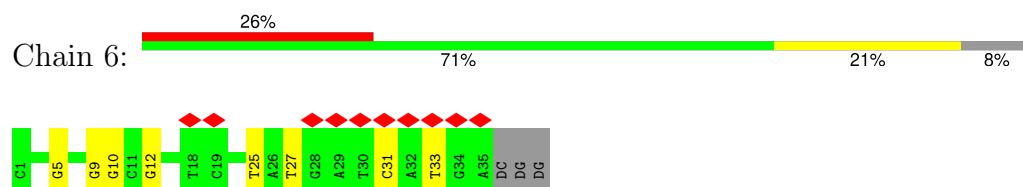
- Molecule 5: 50S ribosomal protein L25



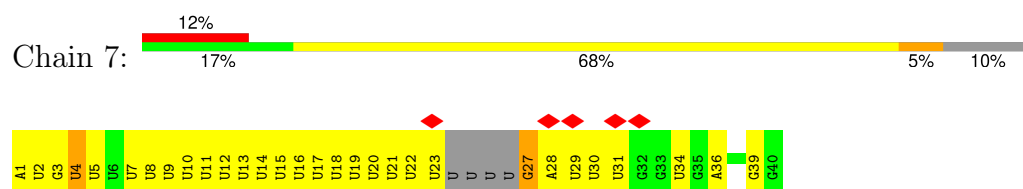
- Molecule 6: NT DNA ops



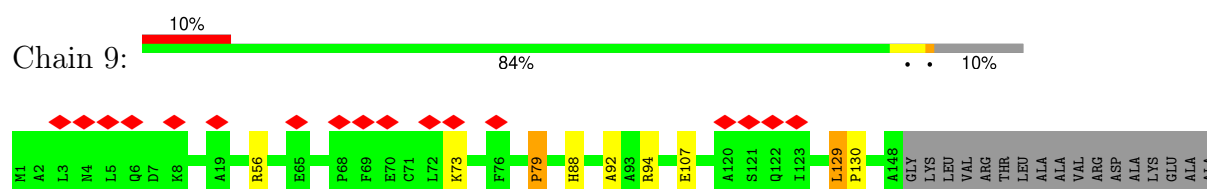
- Molecule 7: T DNA ops



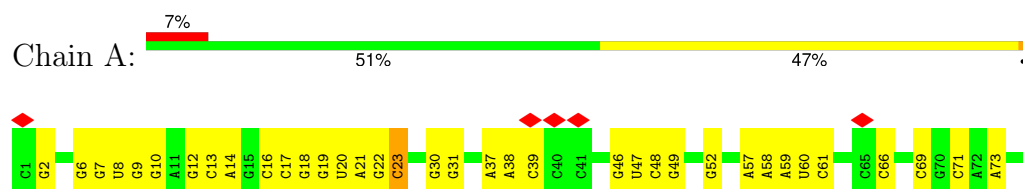
- Molecule 8: mRNA with 24 nt long spacer



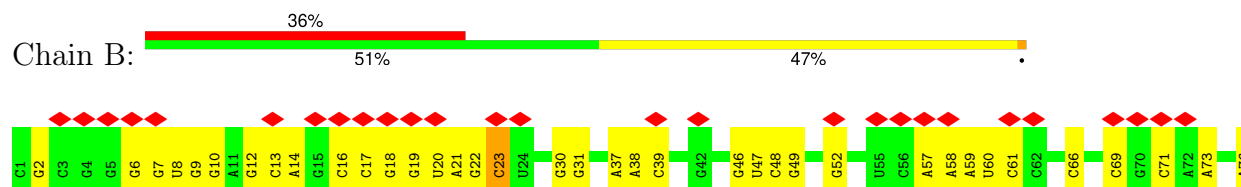
- Molecule 9: 50S ribosomal protein L10



- Molecule 10: E-site and P-site fMet-tRNA



- Molecule 10: E-site and P-site fMet-tRNA

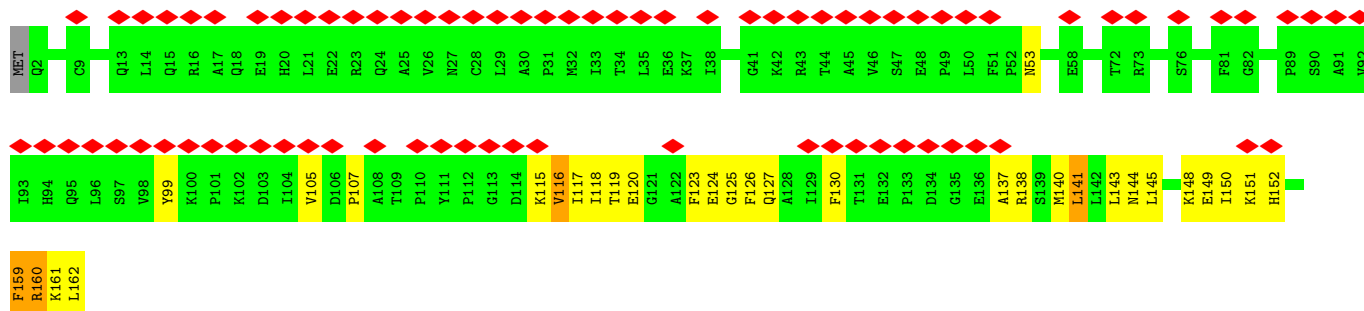
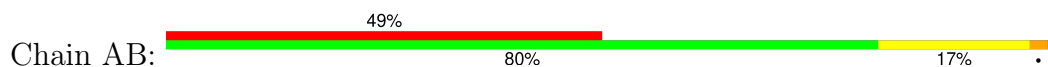


- Molecule 11: DNA-directed RNA polymerase subunit beta

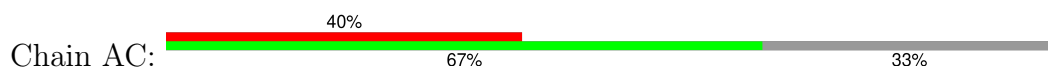


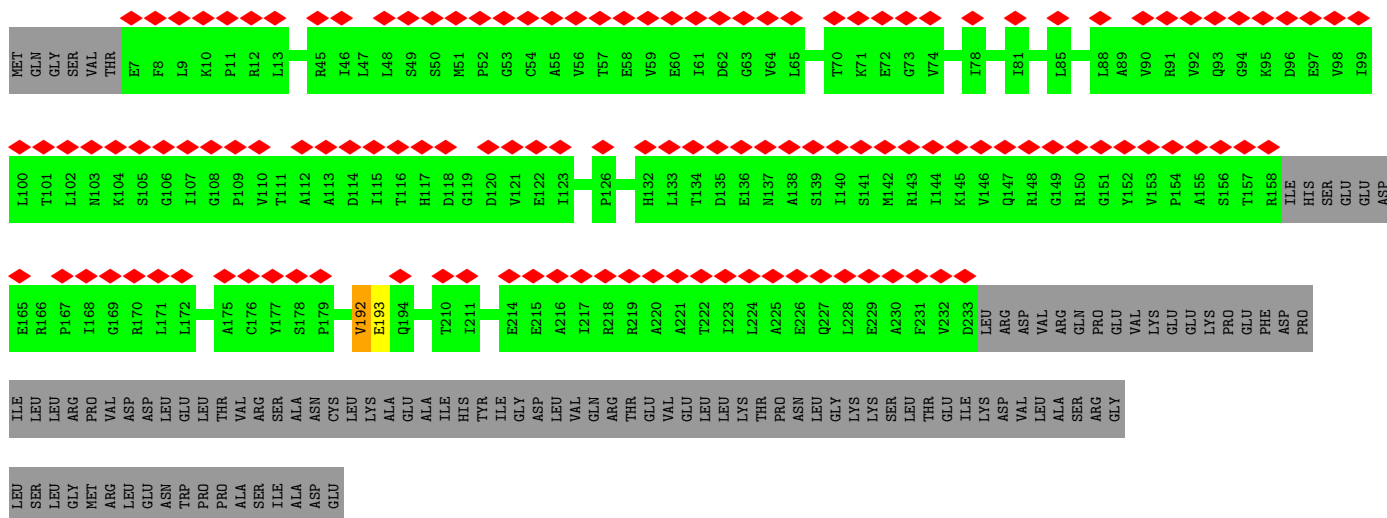


• Molecule 12: Transcription antitermination protein RfaH

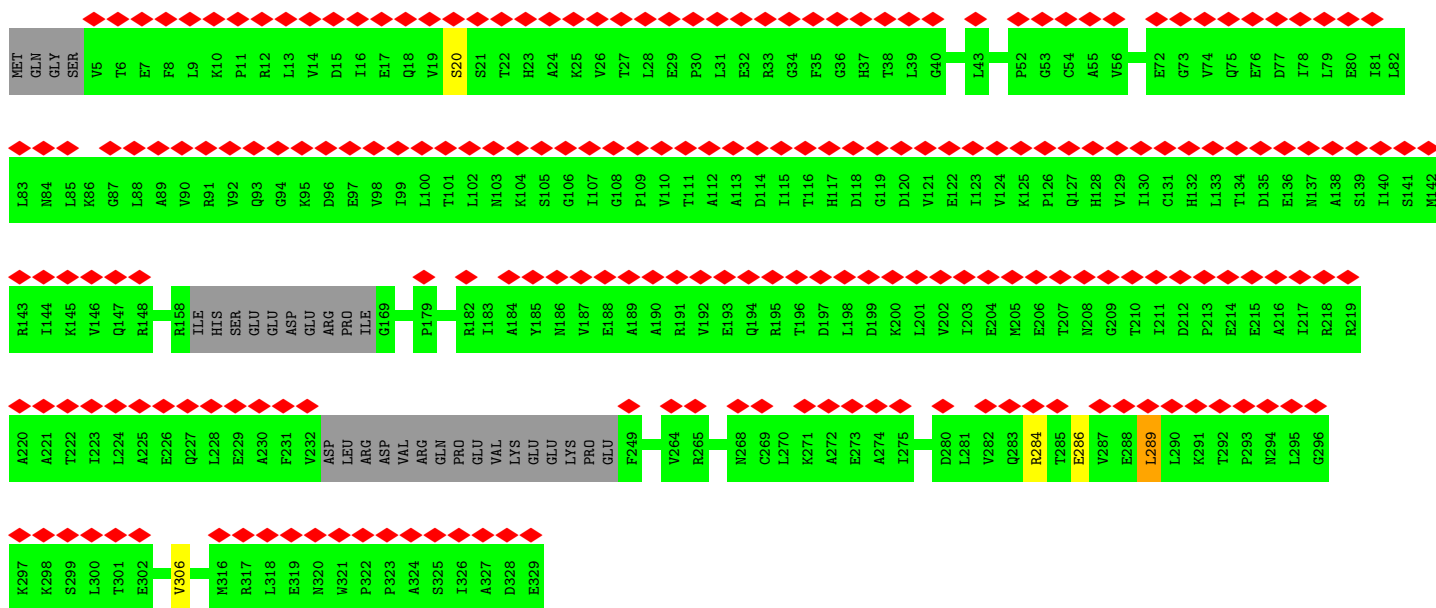
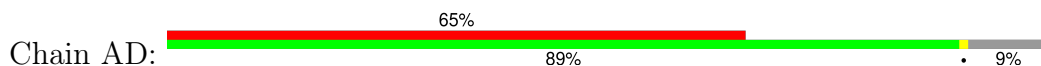


• Molecule 13: DNA-directed RNA polymerase subunit alpha

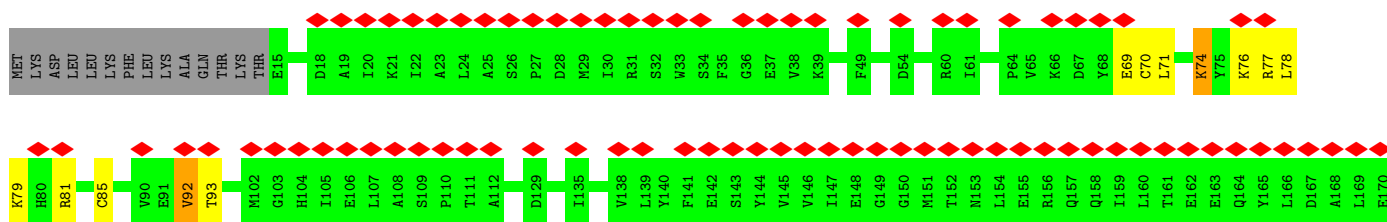


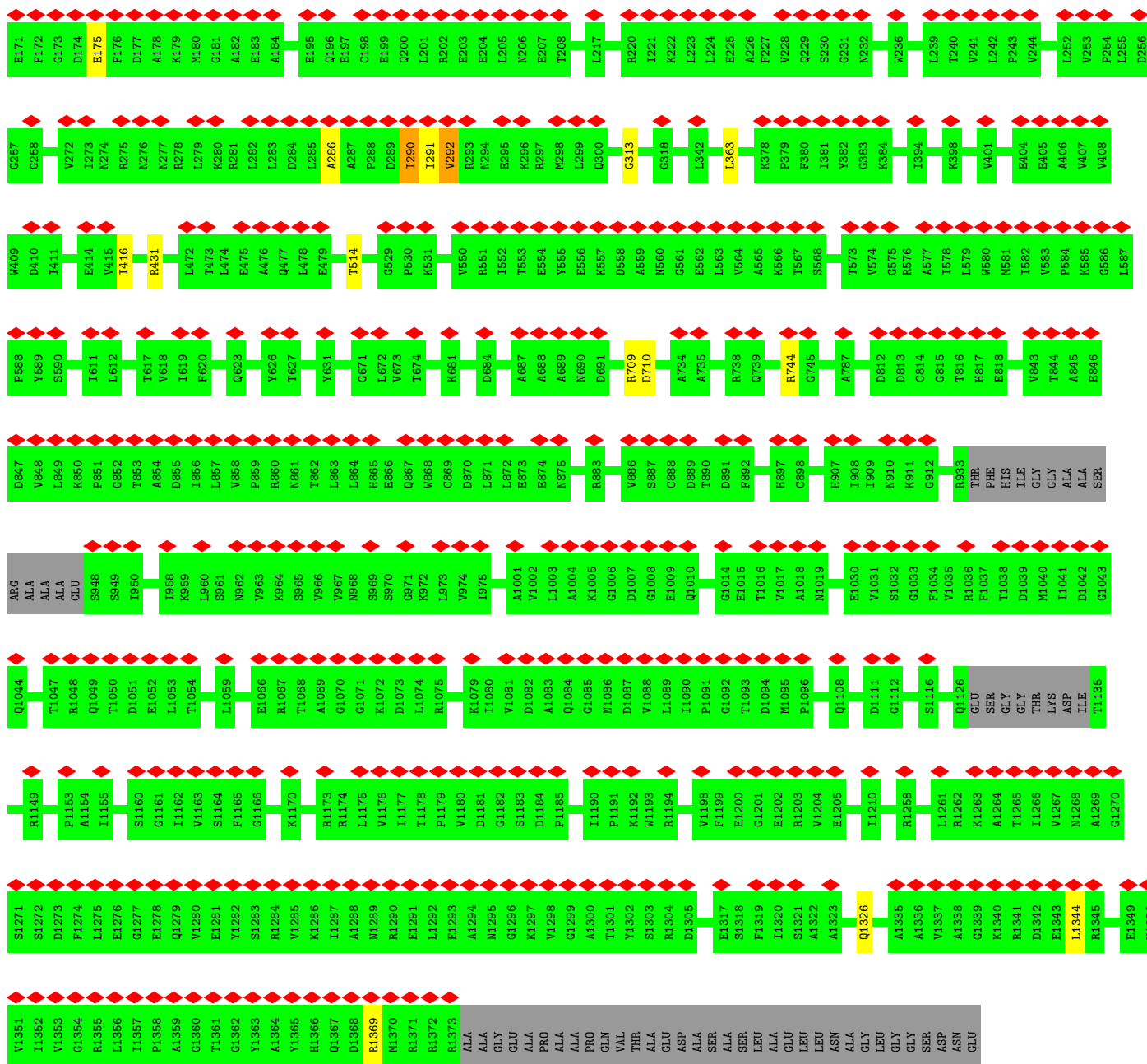


• Molecule 13: DNA-directed RNA polymerase subunit alpha

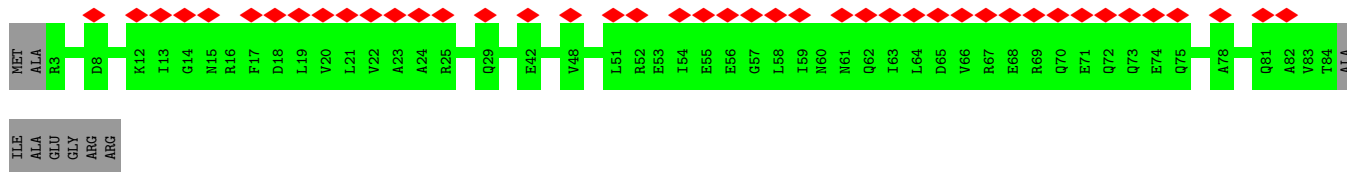
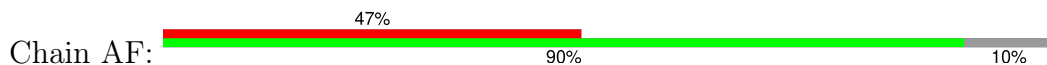


• Molecule 14: DNA-directed RNA polymerase subunit beta'

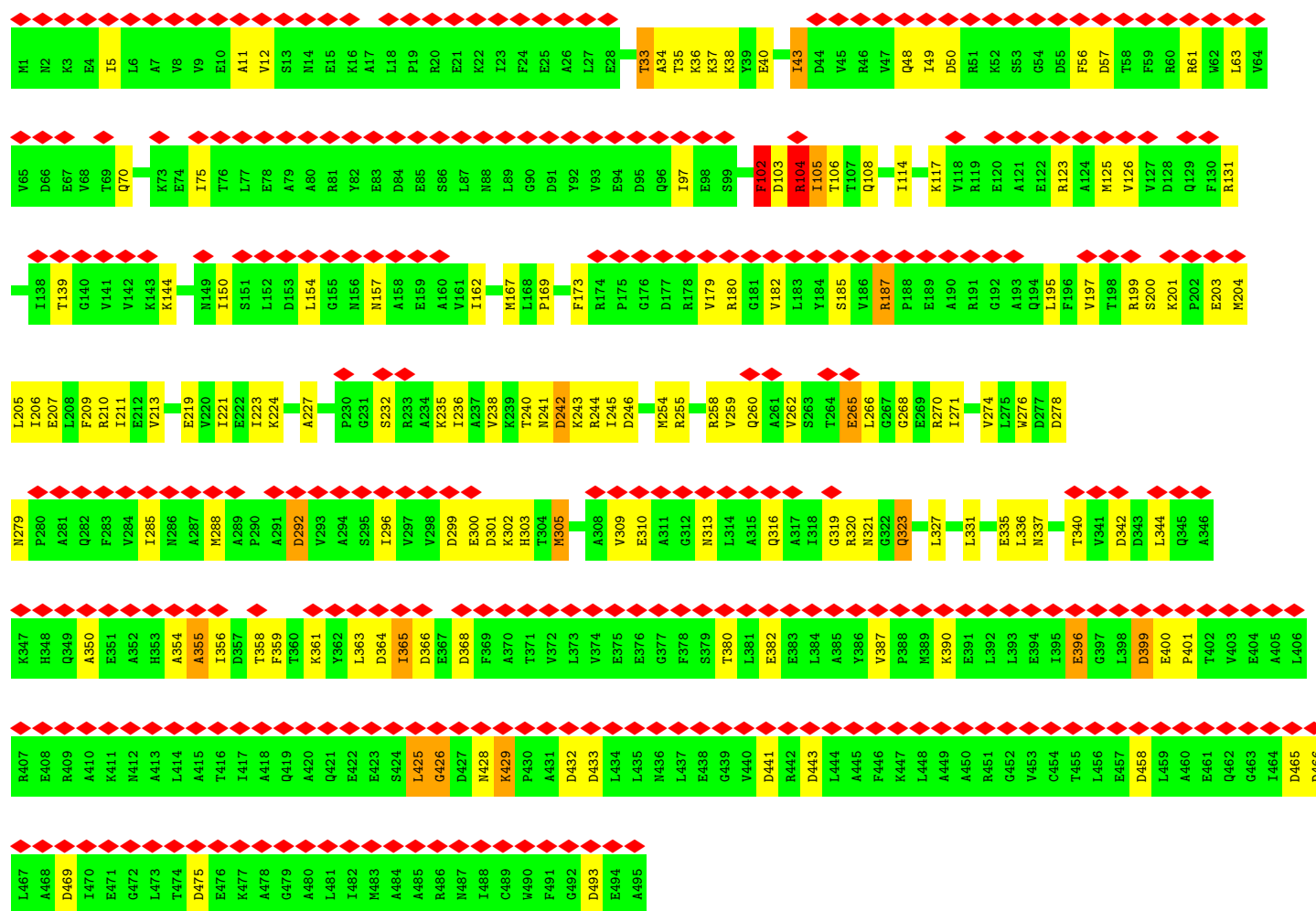
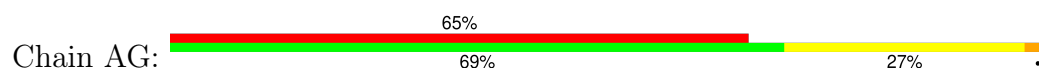




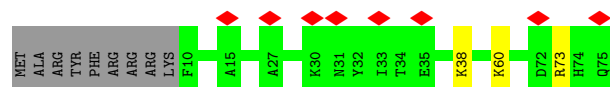
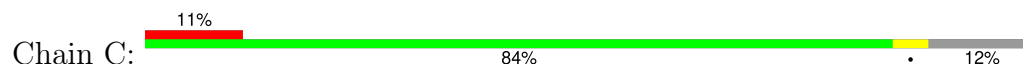
- Molecule 15: DNA-directed RNA polymerase subunit omega



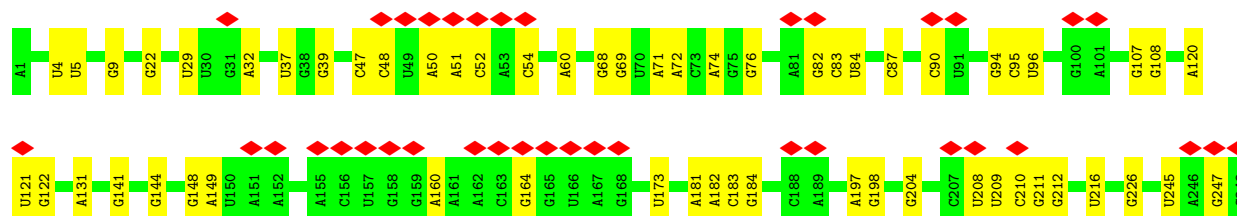
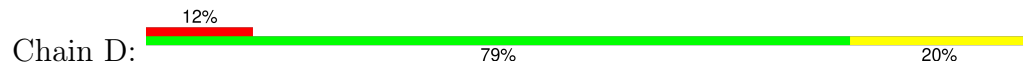
- Molecule 16: Transcription termination/antitermination protein NusA

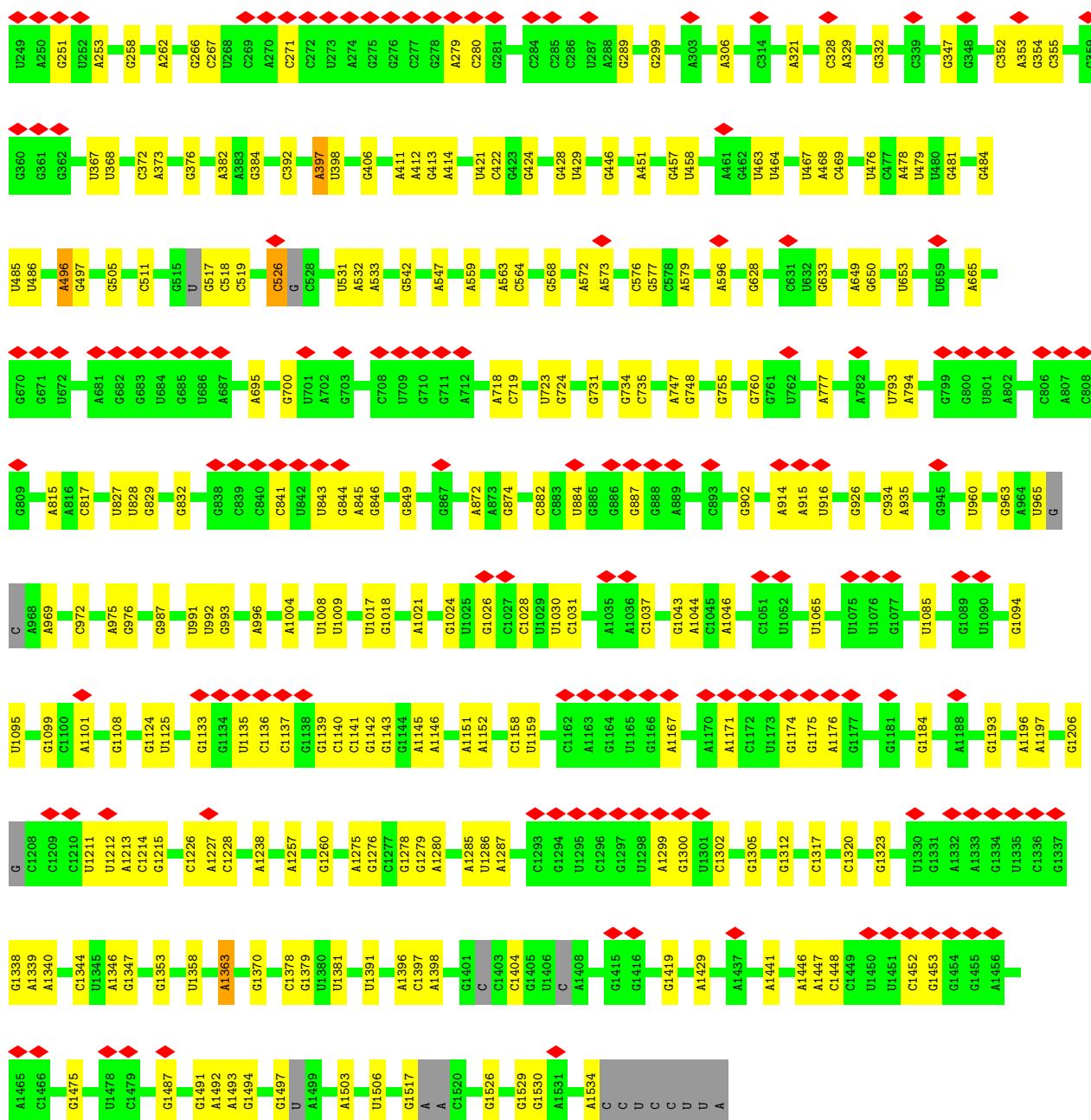


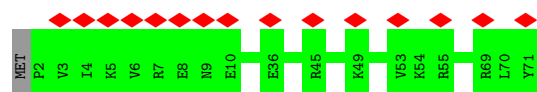
• Molecule 17: 30S ribosomal protein S18



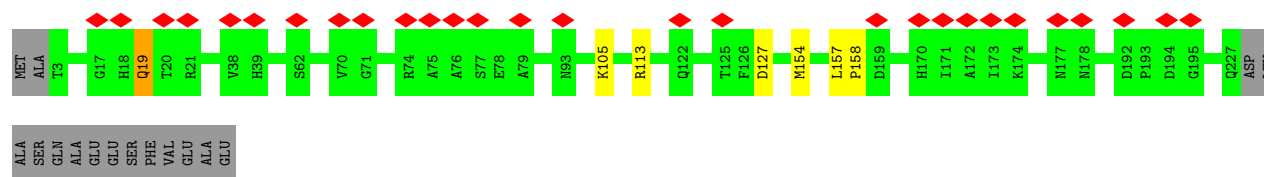
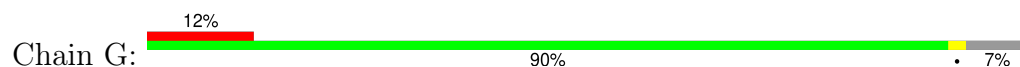
• Molecule 18: 16S rRNA



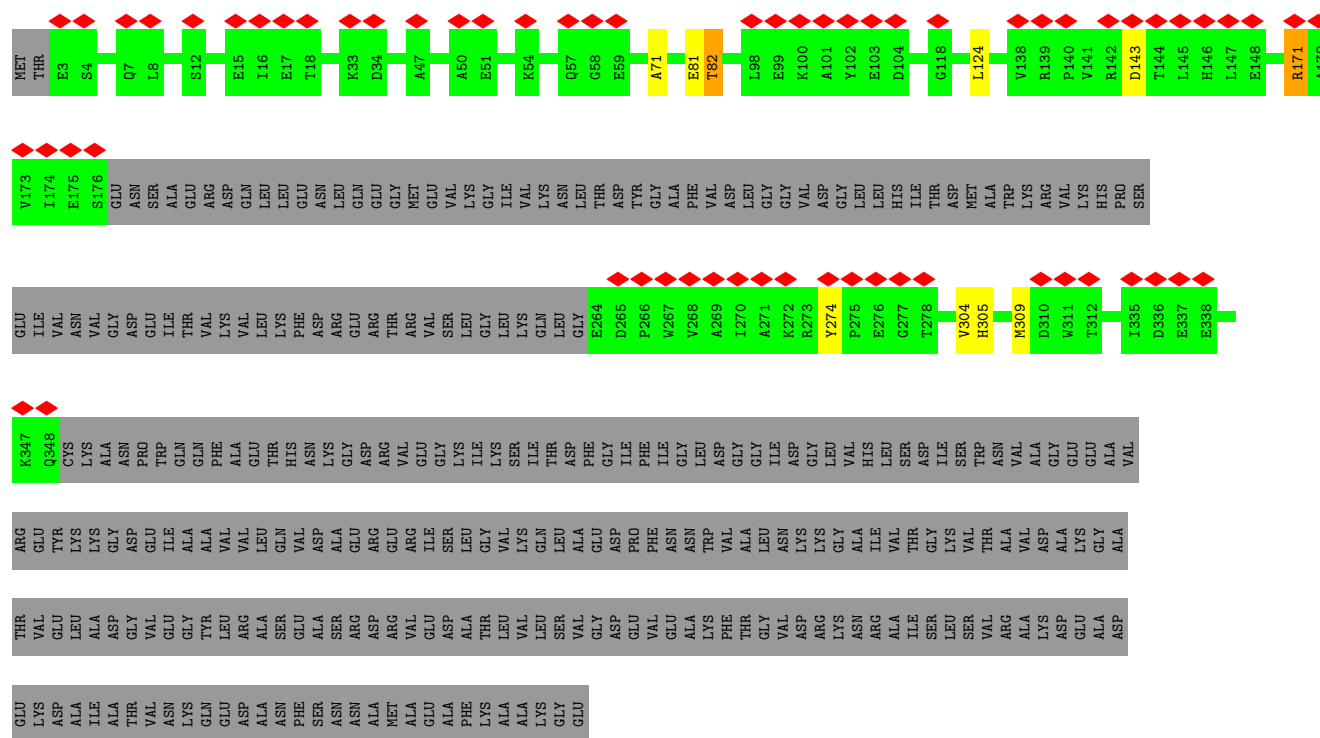




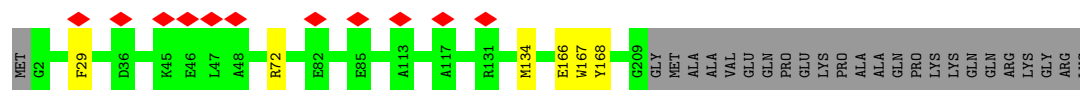
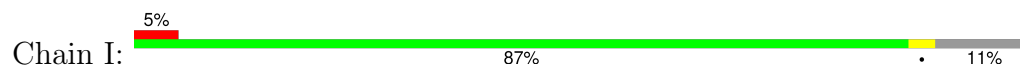
- Molecule 21: 30S ribosomal protein S2



- Molecule 22: 30S ribosomal protein S1



- Molecule 23: 30S ribosomal protein S3

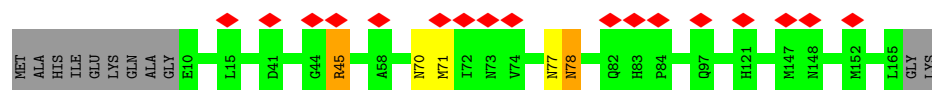
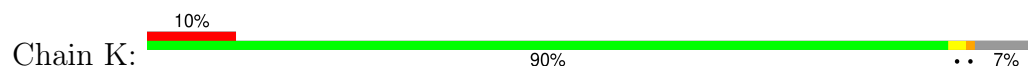


- Molecule 24: 30S ribosomal protein S4

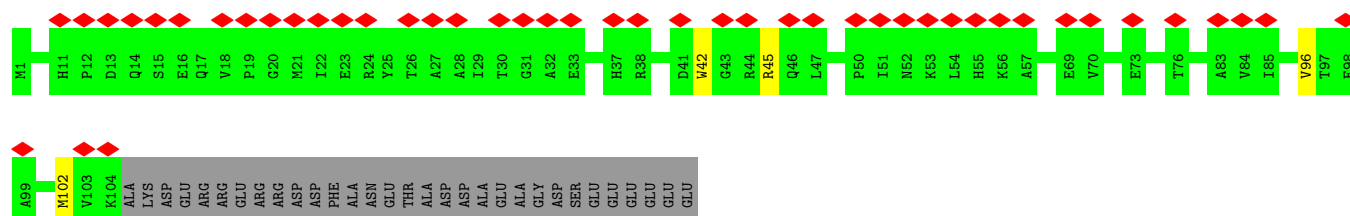
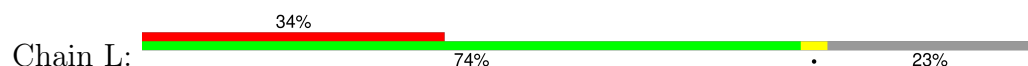




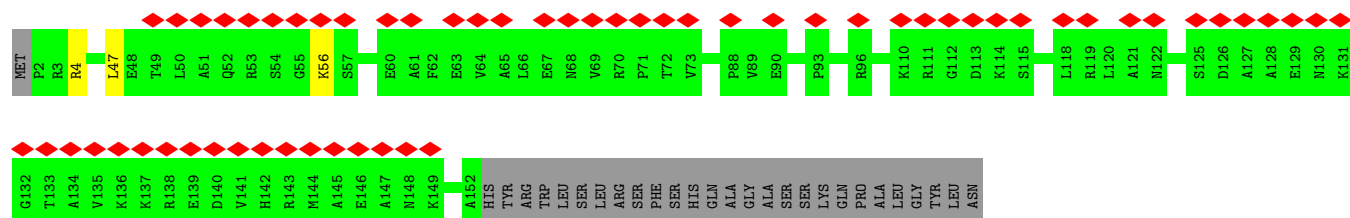
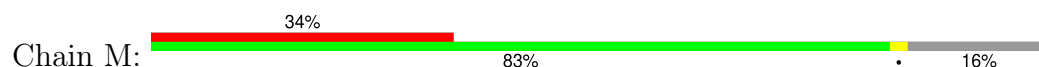
- Molecule 25: 30S ribosomal protein S5



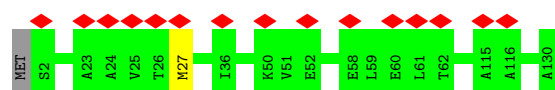
- Molecule 26: 30S ribosomal protein S6



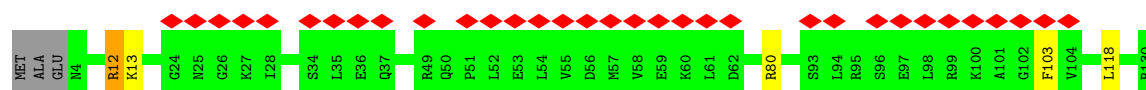
- Molecule 27: 30S ribosomal protein S7



- Molecule 28: 30S ribosomal protein S8



- Molecule 29: 30S ribosomal protein S9




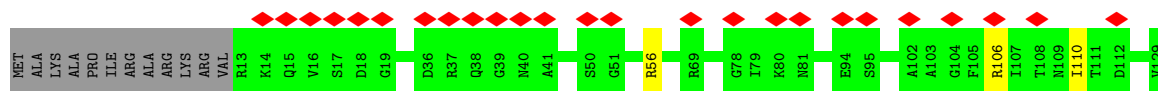
- Molecule 30: 30S ribosomal protein S10

Chain P:  92%



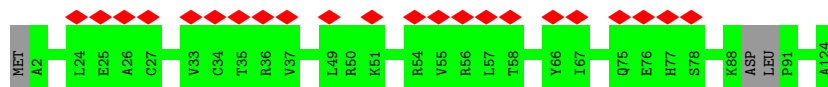
- Molecule 31: 30S ribosomal protein S11

Chain Q:  19% 88% 9%



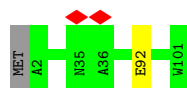
- Molecule 32: 30S ribosomal protein S12

Chain R:  18% 98%

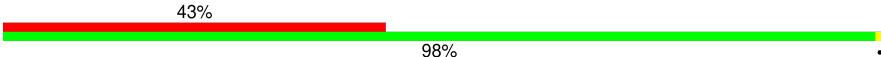


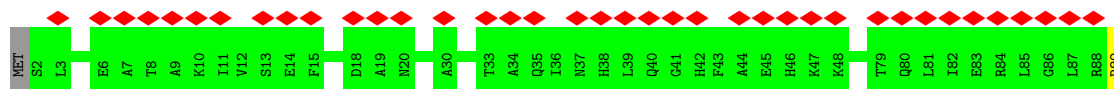
- Molecule 33: 30S ribosomal protein S14

Chain S:  98%



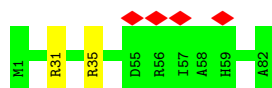
- Molecule 34: 30S ribosomal protein S15

Chain T:  43% 98%




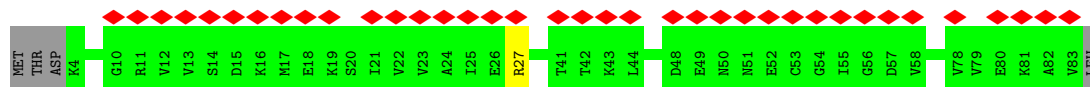
- Molecule 35: 30S ribosomal protein S16

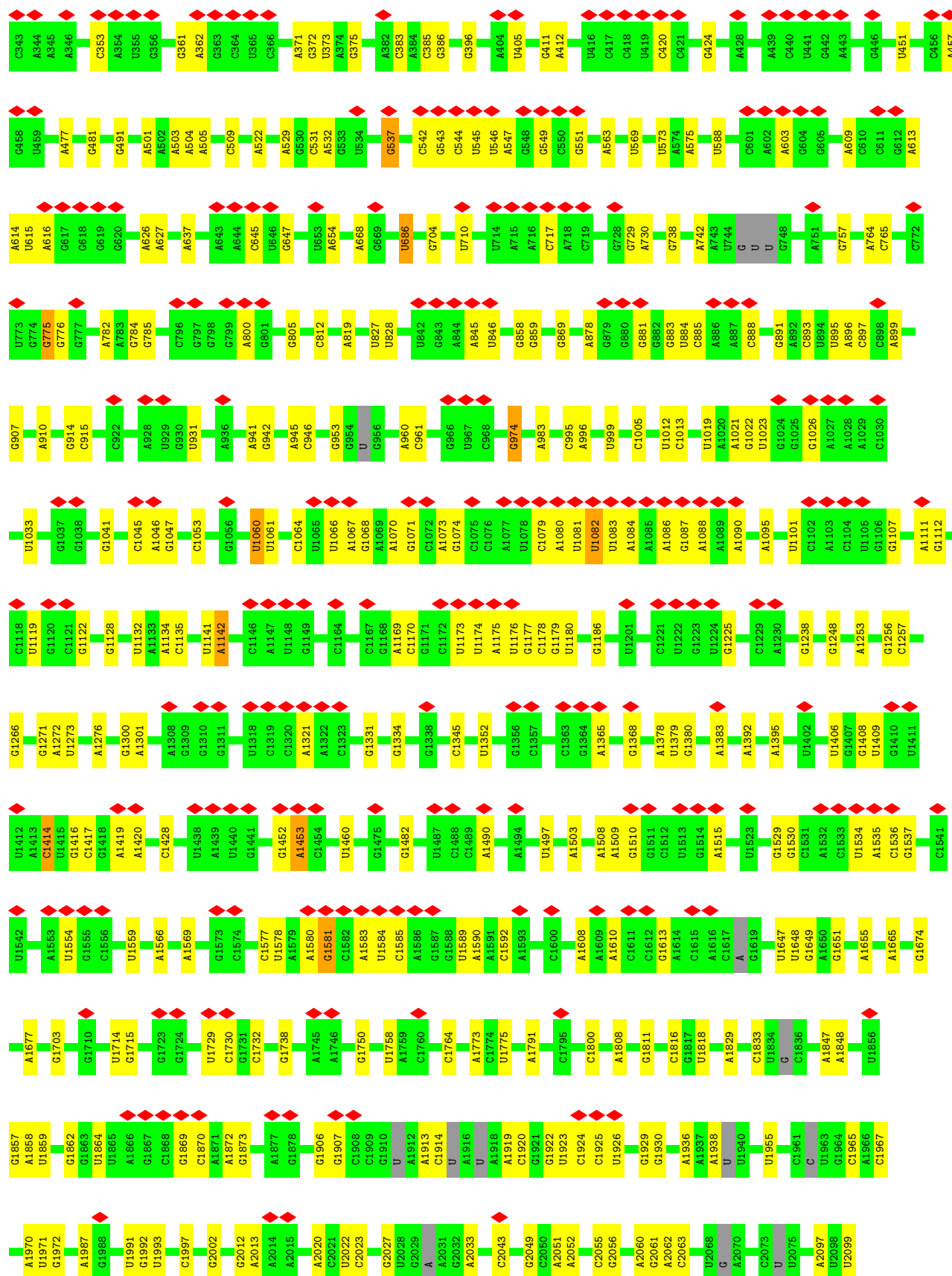
Chain U:  5% 98%

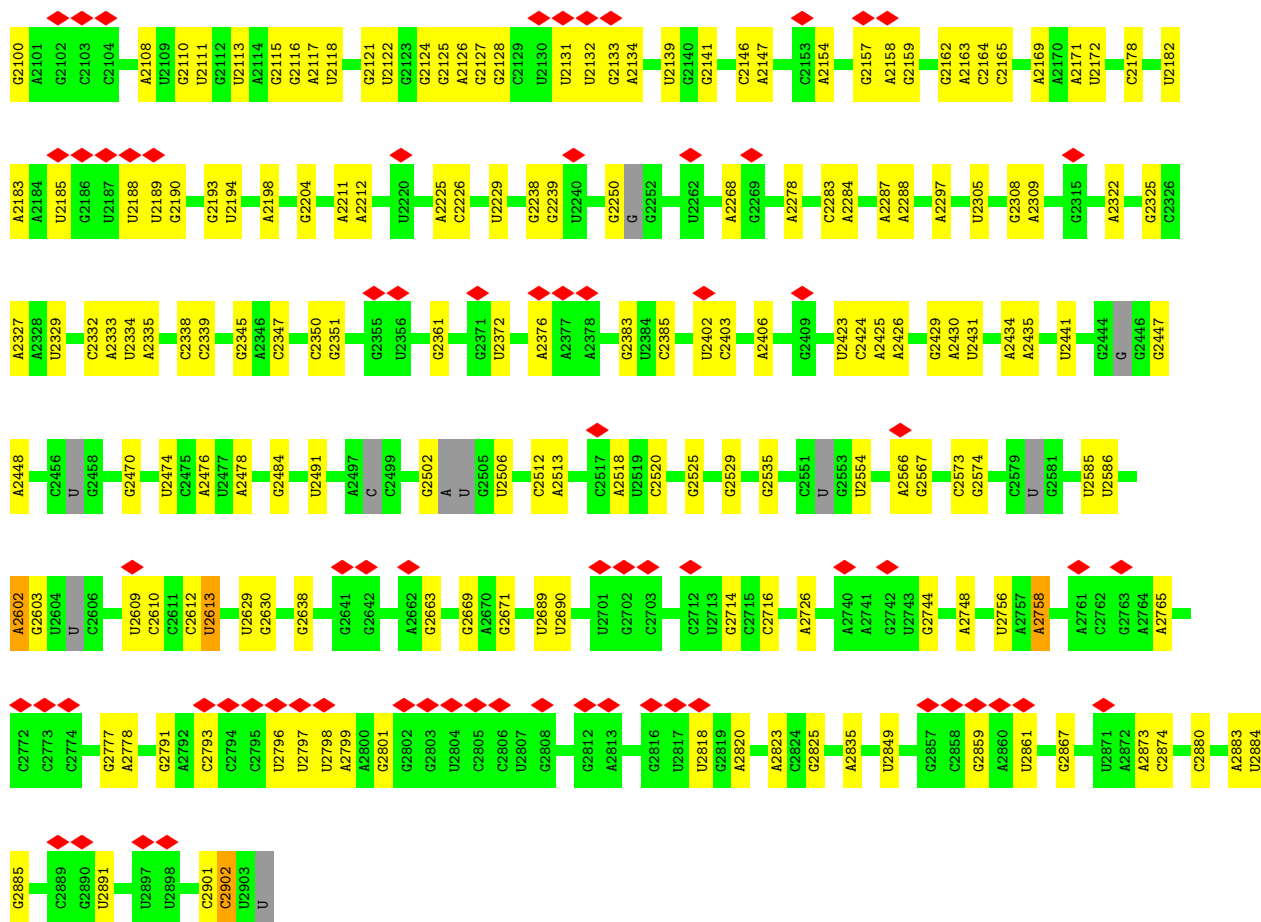


- Molecule 36: 30S ribosomal protein S17

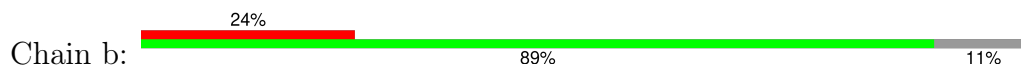
Chain V:  44% 94% 5%



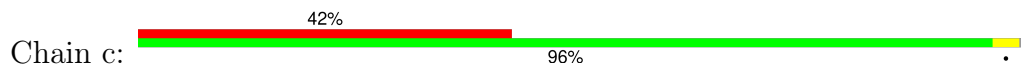




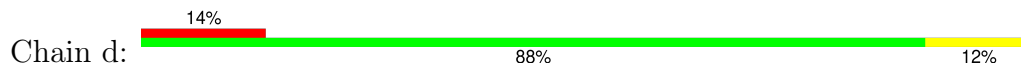
- Molecule 42: 50S ribosomal protein L27



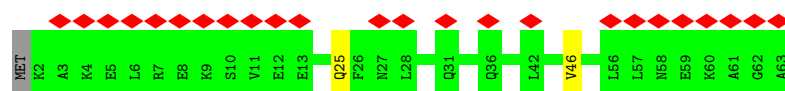
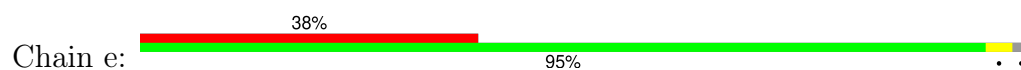
- Molecule 43: 50S ribosomal protein L28



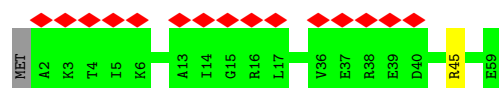
- Molecule 44: 5S rRNA



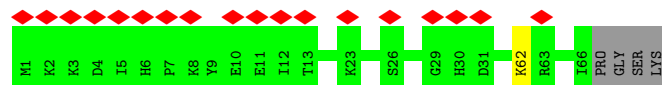
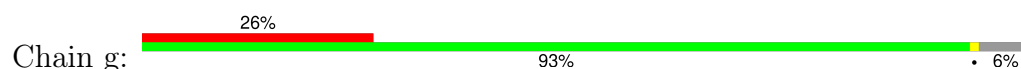
- Molecule 45: 50S ribosomal protein L29



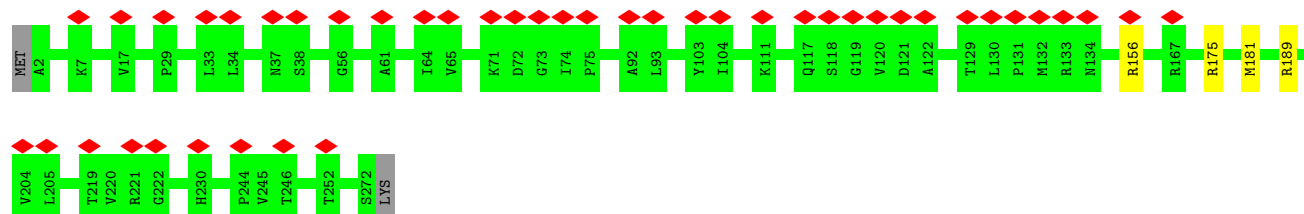
- Molecule 46: 50S ribosomal protein L30



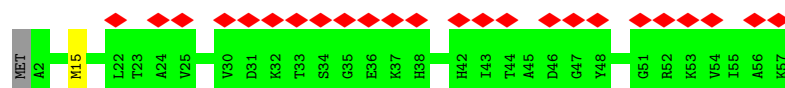
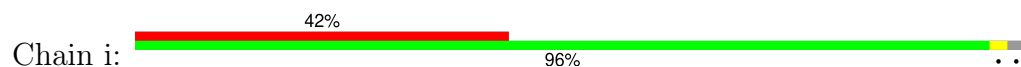
- Molecule 47: 50S ribosomal protein L31



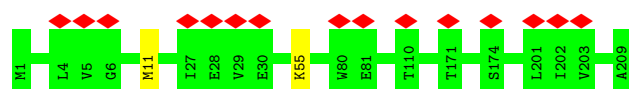
- Molecule 48: 50S ribosomal protein L2



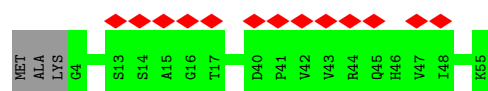
- Molecule 49: 50S ribosomal protein L32



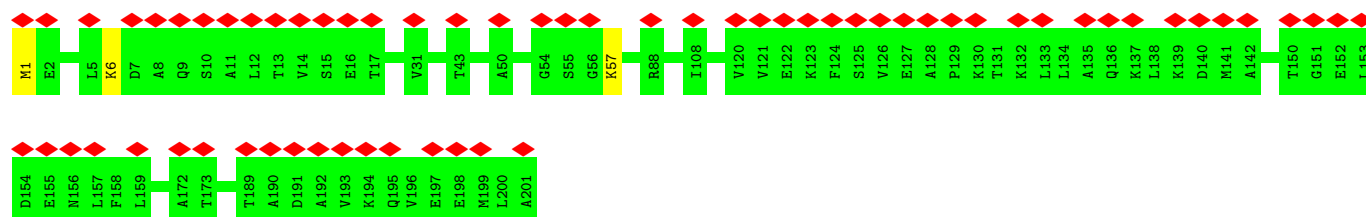
- Molecule 50: 50S ribosomal protein L3



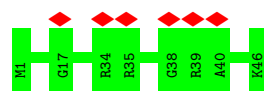
- Molecule 51: 50S ribosomal protein L33



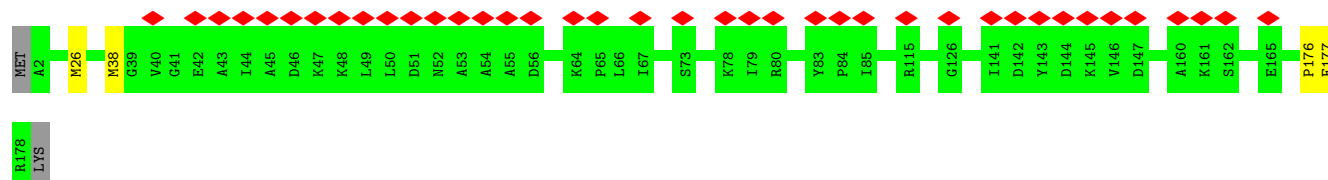
• Molecule 52: 50S ribosomal protein L4



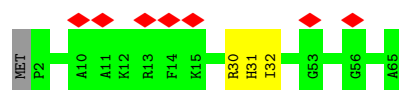
• Molecule 53: 50S ribosomal protein L34



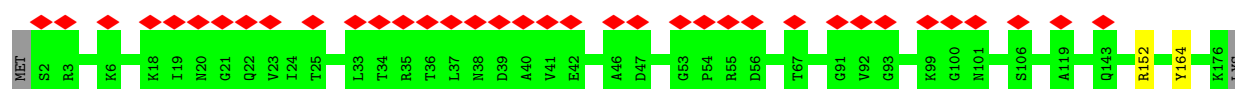
• Molecule 54: 50S ribosomal protein L5



• Molecule 55: 50S ribosomal protein L35



• Molecule 56: 50S ribosomal protein L6



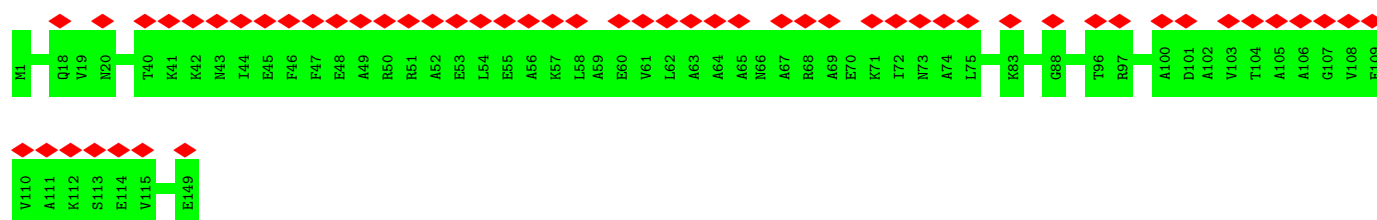
- Molecule 57: 50S ribosomal protein L36

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L9

Chain r:  37%
100%



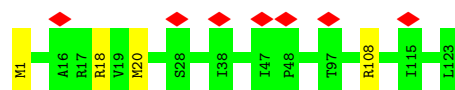
- Molecule 59: 50S ribosomal protein L13

Chain s:  6%
97%



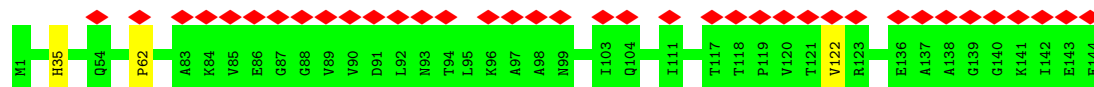
- Molecule 60: 50S ribosomal protein L14

Chain t:  6%
97%



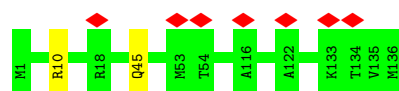
- Molecule 61: 50S ribosomal protein L15

Chain u:  26%
98%




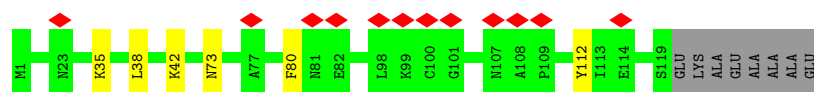
- Molecule 62: 50S ribosomal protein L16

Chain v:  5%
99%

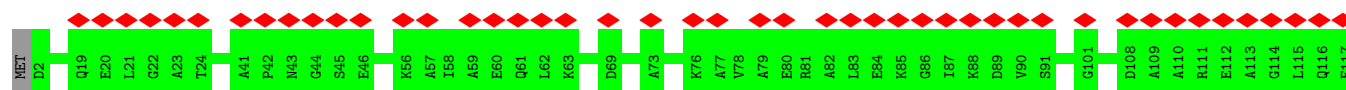
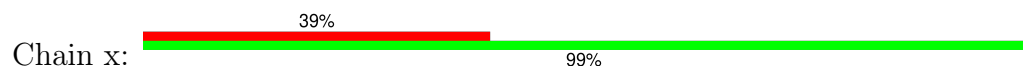


- Molecule 63: 50S ribosomal protein L17

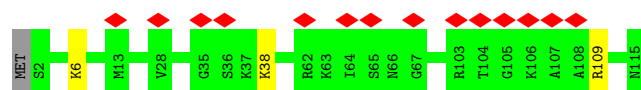
Chain w:  9%
89% 5% 6%



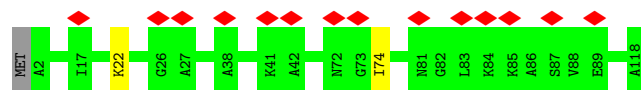
- Molecule 64: 50S ribosomal protein L18



- Molecule 65: 50S ribosomal protein L19



- Molecule 66: 50S ribosomal protein L20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14614	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0017	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.46	0/829	0.61	0/1107
2	1	0.58	0/864	0.69	0/1156
3	2	0.67	1/752 (0.1%)	0.72	1/1005 (0.1%)
4	3	0.41	0/796	0.55	0/1062
5	4	0.65	2/766 (0.3%)	0.69	0/1025
6	5	1.14	11/816 (1.3%)	1.13	2/1259 (0.2%)
7	6	1.12	8/783 (1.0%)	1.10	0/1203
8	7	0.53	2/856 (0.2%)	0.89	4/1326 (0.3%)
9	9	0.36	0/1131	0.66	2/1524 (0.1%)
10	A	0.55	1/1810 (0.1%)	1.26	12/2821 (0.4%)
10	B	0.55	1/1810 (0.1%)	1.26	12/2821 (0.4%)
11	AA	0.43	0/10547	0.61	1/14232 (0.0%)
12	AB	0.47	0/1317	0.86	5/1786 (0.3%)
13	AC	0.41	0/1718	0.62	0/2328
13	AD	0.36	0/2096	0.62	1/2854 (0.0%)
14	AE	0.42	0/10561	0.63	3/14258 (0.0%)
15	AF	0.34	0/652	0.57	0/879
16	AG	0.65	2/3897 (0.1%)	0.89	31/5273 (0.6%)
17	C	0.70	0/553	0.92	4/743 (0.5%)
18	D	0.59	13/36610 (0.0%)	1.03	65/57091 (0.1%)
19	E	0.57	0/675	0.71	0/895
20	F	0.62	0/597	0.60	0/792
21	G	0.66	2/1791 (0.1%)	0.83	8/2413 (0.3%)
22	H	0.43	0/1746	0.70	0/2382
23	I	0.62	2/1663 (0.1%)	0.71	4/2241 (0.2%)
24	J	0.54	2/1665 (0.1%)	0.59	0/2227
25	K	0.68	1/1165 (0.1%)	0.75	2/1568 (0.1%)
26	L	0.79	3/867 (0.3%)	0.82	3/1171 (0.3%)
27	M	0.54	0/1195	0.70	2/1602 (0.1%)
28	N	0.52	0/989	0.63	1/1326 (0.1%)
29	O	0.68	4/1034 (0.4%)	0.82	4/1375 (0.3%)
30	P	0.52	0/800	0.70	2/1082 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Q	0.71	1/893 (0.1%)	0.82	4/1205 (0.3%)
32	R	0.56	0/952	0.65	0/1274
33	S	0.63	1/817 (0.1%)	0.64	0/1088
34	T	0.56	0/722	0.72	1/964 (0.1%)
35	U	0.45	0/659	0.65	1/884 (0.1%)
36	V	0.56	0/657	0.70	0/881
37	W	0.56	1/680 (0.1%)	0.69	3/915 (0.3%)
38	X	0.48	0/909	0.72	1/1215 (0.1%)
39	Y	0.42	1/1046 (0.1%)	0.57	2/1410 (0.1%)
40	Z	0.23	0/227	0.37	0/304
41	a	0.61	15/69247 (0.0%)	1.03	129/107985 (0.1%)
42	b	0.47	0/589	0.57	0/779
43	c	0.56	1/635 (0.2%)	0.66	1/848 (0.1%)
44	d	0.50	0/2872	0.95	0/4478
45	e	0.81	2/502 (0.4%)	0.66	0/667
46	f	0.53	0/452	0.72	2/605 (0.3%)
47	g	0.50	1/531 (0.2%)	0.67	1/709 (0.1%)
48	h	0.53	2/2121 (0.1%)	0.67	6/2852 (0.2%)
49	i	0.42	0/450	0.64	1/599 (0.2%)
50	j	0.53	0/1586	0.64	2/2134 (0.1%)
51	k	0.50	0/433	0.68	0/576
52	l	0.54	1/1571 (0.1%)	0.64	1/2113 (0.0%)
53	m	0.43	0/380	0.60	0/498
54	n	0.51	0/1434	0.68	2/1926 (0.1%)
55	o	0.51	0/513	0.85	1/676 (0.1%)
56	p	0.50	0/1333	0.68	3/1805 (0.2%)
57	q	0.46	0/303	0.61	0/397
58	r	0.34	0/1122	0.52	0/1515
59	s	0.83	5/1152 (0.4%)	0.81	4/1551 (0.3%)
60	t	0.55	1/955 (0.1%)	0.89	5/1279 (0.4%)
61	u	0.47	1/1062 (0.1%)	0.63	0/1413
62	v	0.62	1/1093 (0.1%)	0.75	1/1460 (0.1%)
63	w	0.90	5/964 (0.5%)	0.95	9/1289 (0.7%)
64	x	0.42	0/902	0.57	0/1209
65	y	0.46	0/929	0.58	1/1242 (0.1%)
66	z	0.63	1/960 (0.1%)	0.60	0/1278
All	All	0.58	95/195004 (0.0%)	0.92	350/286850 (0.1%)

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	9	0	3
12	AB	0	2
13	AC	0	1
13	AD	0	2
14	AE	0	4
16	AG	0	6
21	G	0	1
22	H	0	5
23	I	0	1
25	K	0	2
29	O	0	1
38	X	0	1
39	Y	0	1
54	n	0	1
55	o	0	1
59	s	0	1
61	u	0	2
All	All	0	35

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	w	35	LYS	CE-NZ	-15.20	1.11	1.49
26	L	42	TRP	CB-CG	-12.36	1.28	1.50
3	2	5	GLU	CG-CD	-11.60	1.34	1.51
45	e	46	VAL	CB-CG1	-11.26	1.29	1.52
63	w	42	LYS	CD-CE	-10.82	1.24	1.51
25	K	45	ARG	CG-CD	9.49	1.75	1.51
18	D	718	A	N9-C4	-8.83	1.32	1.37
16	AG	429	LYS	C-N	8.82	1.51	1.34
29	O	80	ARG	CD-NE	-8.78	1.31	1.46
59	s	74	TYR	CZ-OH	-8.67	1.23	1.37
59	s	74	TYR	CE2-CZ	-8.46	1.27	1.38
16	AG	246	ASP	C-N	8.43	1.50	1.34
21	G	19	GLN	CB-CG	-8.42	1.29	1.52
41	a	1141	U	N3-C4	-7.87	1.31	1.38
59	s	74	TYR	CD1-CE1	-7.80	1.27	1.39
6	5	25	DA	C1'-N9	-7.57	1.36	1.47
41	a	1453	A	N9-C4	-7.50	1.33	1.37
63	w	112	TYR	CG-CD1	-7.49	1.29	1.39
8	7	39	G	C1'-N9	-7.33	1.36	1.46
6	5	18	DG	C1'-N9	-7.28	1.37	1.47
24	J	182	PHE	CE2-CZ	-7.13	1.23	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	563	A	C6-N1	-7.12	1.30	1.35
37	W	66	MET	CG-SD	-7.09	1.62	1.81
18	D	1339	A	N9-C4	-7.08	1.33	1.37
18	D	397	A	C6-N1	-6.96	1.30	1.35
7	6	9	DG	C1'-N9	-6.91	1.37	1.47
8	7	2	U	C1'-N1	6.85	1.59	1.48
52	l	6	LYS	CE-NZ	-6.85	1.31	1.49
6	5	21	DA	C1'-N9	-6.83	1.37	1.47
41	a	1019	U	N3-C4	-6.78	1.32	1.38
39	Y	5	GLN	CB-CG	-6.71	1.34	1.52
18	D	872	A	C6-N1	-6.69	1.30	1.35
29	O	80	ARG	CZ-NH2	6.61	1.41	1.33
18	D	1363	A	C6-N1	-6.57	1.30	1.35
7	6	12	DG	C1'-N9	-6.52	1.38	1.47
47	g	62	LYS	CE-NZ	-6.48	1.32	1.49
66	z	74	ILE	CB-CG2	-6.48	1.32	1.52
26	L	42	TRP	CZ3-CH2	-6.47	1.29	1.40
41	a	1021	A	C6-N1	-6.45	1.31	1.35
23	I	29	PHE	CD2-CE2	-6.36	1.26	1.39
29	O	118	LEU	CG-CD2	-6.35	1.28	1.51
41	a	1142	A	C6-N1	-6.29	1.31	1.35
6	5	-5	DC	C1'-N1	6.28	1.57	1.49
23	I	166	GLU	CG-CD	-6.28	1.42	1.51
26	L	42	TRP	CE3-CZ3	-6.27	1.27	1.38
21	G	158	PRO	CG-CD	6.25	1.71	1.50
6	5	1	DC	C1'-N1	6.24	1.57	1.49
18	D	1358	U	N3-C4	-6.23	1.32	1.38
10	A	37	A	N9-C4	-6.23	1.34	1.37
41	a	2013	A	C6-N6	-6.21	1.28	1.33
18	D	827	U	N3-C4	-6.19	1.32	1.38
7	6	5	DG	C1'-N9	-6.17	1.38	1.47
6	5	28	DG	C1'-N9	-6.17	1.38	1.47
18	D	37	U	N3-C4	-6.13	1.32	1.38
41	a	67	U	C4-O4	-6.12	1.18	1.23
6	5	27	DG	C1'-N9	-6.11	1.38	1.47
10	B	37	A	N9-C4	-6.08	1.34	1.37
33	S	92	GLU	CD-OE1	-6.03	1.19	1.25
45	e	25	GLN	CB-CG	-5.94	1.36	1.52
48	h	181	MET	CG-SD	-5.94	1.65	1.81
41	a	2613	U	N3-C4	-5.91	1.33	1.38
59	s	92	MET	CG-SD	-5.89	1.65	1.81
18	D	872	A	C6-N6	-5.88	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	w	35	LYS	CD-CE	5.82	1.65	1.51
41	a	1257	C	N1-C2	-5.81	1.34	1.40
41	a	2756	U	C4-O4	-5.81	1.19	1.23
62	v	45	GLN	CB-CG	-5.71	1.37	1.52
18	D	884	U	N3-C4	-5.63	1.33	1.38
29	O	103	PHE	CE2-CZ	-5.63	1.26	1.37
5	4	56	PHE	CB-CG	-5.63	1.41	1.51
41	a	2013	A	C6-N1	-5.56	1.31	1.35
43	c	70	GLU	CG-CD	-5.54	1.43	1.51
61	u	122	VAL	CB-CG1	-5.54	1.41	1.52
41	a	1082	U	C4-O4	-5.52	1.19	1.23
24	J	72	PHE	CB-CG	-5.52	1.42	1.51
59	s	74	TYR	CD2-CE2	-5.50	1.31	1.39
48	h	175	ARG	CB-CG	5.49	1.67	1.52
31	Q	106	ARG	CD-NE	-5.42	1.37	1.46
5	4	75	GLN	CB-CG	-5.41	1.38	1.52
18	D	563	A	C6-N6	-5.34	1.29	1.33
6	5	-3	DT	C1'-N1	5.31	1.56	1.49
60	t	18	ARG	CZ-NH1	-5.24	1.26	1.33
6	5	0	DT	C1'-N1	5.23	1.56	1.49
63	w	80	PHE	CB-CG	-5.21	1.42	1.51
6	5	-6	DT	C1'-N1	5.19	1.55	1.49
7	6	31	DC	C1'-N1	5.18	1.55	1.49
7	6	27	DT	C1'-N1	5.18	1.55	1.49
41	a	1021	A	C6-N6	-5.17	1.29	1.33
6	5	3	DT	C1'-N1	5.15	1.55	1.49
41	a	2613	U	C4-O4	-5.13	1.19	1.23
7	6	10	DG	C1'-N9	-5.10	1.40	1.47
7	6	25	DT	C1'-N1	5.09	1.55	1.49
18	D	397	A	C6-N6	-5.08	1.29	1.33
7	6	33	DT	C1'-N1	5.03	1.55	1.49
41	a	1655	A	N9-C4	-5.02	1.34	1.37

All (350) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	a	1019	U	C5-C4-O4	30.71	144.33	125.90
41	a	1141	U	C5-C4-O4	29.53	143.62	125.90
18	D	37	U	C5-C4-O4	29.39	143.53	125.90
18	D	1358	U	C5-C4-O4	29.16	143.40	125.90
18	D	827	U	C5-C4-O4	28.71	143.13	125.90
18	D	37	U	N3-C4-O4	-28.37	99.54	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	827	U	N3-C4-O4	-27.57	100.10	119.40
41	a	1019	U	N3-C4-O4	-27.35	100.25	119.40
18	D	1358	U	N3-C4-O4	-27.11	100.42	119.40
41	a	2613	U	C5-C4-O4	26.10	141.56	125.90
18	D	884	U	C5-C4-O4	25.38	141.13	125.90
41	a	2613	U	N3-C4-O4	-25.38	101.63	119.40
41	a	1082	U	N3-C4-O4	-25.36	101.65	119.40
18	D	884	U	N3-C4-O4	-24.71	102.10	119.40
41	a	1082	U	C5-C4-O4	23.83	140.20	125.90
41	a	1141	U	N3-C4-O4	-23.74	102.78	119.40
41	a	1257	C	C6-N1-C2	19.96	128.28	120.30
18	D	872	A	N1-C6-N6	-17.66	108.00	118.60
41	a	1021	A	N1-C6-N6	-17.29	108.23	118.60
18	D	563	A	N1-C6-N6	-17.01	108.39	118.60
18	D	397	A	N1-C6-N6	-16.63	108.62	118.60
41	a	1141	U	C2-N3-C4	16.47	136.88	127.00
41	a	1142	A	N1-C6-N6	-16.26	108.84	118.60
41	a	2756	U	N3-C4-O4	-16.12	108.12	119.40
18	D	1363	A	N1-C6-N6	-15.86	109.08	118.60
41	a	67	U	N3-C4-O4	-15.18	108.77	119.40
63	w	112	TYR	CZ-CE2-CD2	-14.97	106.33	119.80
41	a	2013	A	N1-C6-N6	-14.90	109.66	118.60
10	B	39	C	C4-C5-C6	14.79	124.80	117.40
10	A	39	C	C4-C5-C6	14.77	124.78	117.40
41	a	1019	U	C2-N3-C4	14.61	135.77	127.00
41	a	1086	A	N1-C6-N6	-14.42	109.95	118.60
21	G	113	ARG	NE-CZ-NH2	14.29	127.44	120.30
16	AG	104	ARG	C-N-CA	13.00	154.21	121.70
55	o	30	ARG	NE-CZ-NH1	-12.84	113.88	120.30
41	a	1019	U	N1-C2-N3	-12.76	107.24	114.90
59	s	92	MET	CG-SD-CE	-12.43	80.32	100.20
10	A	39	C	N3-C4-C5	-12.21	117.02	121.90
60	t	18	ARG	NE-CZ-NH2	12.20	126.40	120.30
41	a	1141	U	N1-C2-N3	-12.19	107.59	114.90
10	B	39	C	N3-C4-C5	-12.17	117.03	121.90
60	t	18	ARG	NE-CZ-NH1	-11.59	114.50	120.30
17	C	73	ARG	NE-CZ-NH2	11.27	125.93	120.30
41	a	2756	U	C5-C4-O4	11.13	132.58	125.90
18	D	1358	U	C2-N3-C4	11.11	133.66	127.00
18	D	718	A	N3-C4-C5	11.09	134.56	126.80
21	G	158	PRO	N-CD-CG	-10.96	86.75	103.20
41	a	960	A	N1-C6-N6	10.95	125.17	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	102	MET	CA-CB-CG	-10.84	94.87	113.30
41	a	1021	A	C5-C6-N6	10.67	132.24	123.70
18	D	1358	U	N1-C2-N3	-10.64	108.52	114.90
41	a	1142	A	C5-C6-N6	10.55	132.14	123.70
18	D	397	A	C5-C6-N6	10.31	131.95	123.70
41	a	960	A	C5-C6-N6	-10.12	115.61	123.70
18	D	872	A	C5-C6-N6	9.93	131.65	123.70
18	D	1363	A	C5-C6-N6	9.92	131.63	123.70
18	D	827	U	N1-C2-N3	-9.67	109.10	114.90
16	AG	354	ALA	O-C-N	-9.61	107.32	122.70
63	w	112	TYR	CB-CG-CD2	-9.60	115.24	121.00
16	AG	292	ASP	O-C-N	-9.56	107.40	122.70
18	D	563	A	C5-C6-N6	9.53	131.32	123.70
41	a	67	U	C5-C4-O4	9.51	131.61	125.90
18	D	718	A	C4-C5-C6	-9.35	112.33	117.00
29	O	103	PHE	CD1-CE1-CZ	-9.11	109.17	120.10
21	G	157	LEU	C-N-CD	-8.96	100.89	120.60
18	D	827	U	C2-N3-C4	8.95	132.37	127.00
41	a	1257	C	O4'-C1'-N1	-8.73	101.22	108.20
16	AG	355	ALA	CB-CA-C	8.71	123.17	110.10
41	a	1060	U	N3-C4-O4	8.66	125.47	119.40
41	a	1021	A	N1-C2-N3	-8.63	124.98	129.30
41	a	1019	U	C4-C5-C6	-8.50	114.60	119.70
62	v	10	ARG	NE-CZ-NH1	-8.44	116.08	120.30
41	a	1060	U	C5-C4-O4	-8.42	120.85	125.90
34	T	89	ARG	NE-CZ-NH2	-8.41	116.09	120.30
31	Q	106	ARG	NE-CZ-NH1	-8.41	116.10	120.30
41	a	1257	C	C5-C6-N1	-8.38	116.81	121.00
41	a	1775	U	C5-C4-O4	-8.33	120.90	125.90
18	D	718	A	N3-C4-N9	-8.23	120.81	127.40
41	a	2334	U	OP2-P-O3'	-8.19	87.19	105.20
14	AE	710	ASP	CB-CG-OD1	8.18	125.66	118.30
18	D	1125	U	C5-C4-O4	-8.11	121.03	125.90
41	a	2012	G	O5'-P-OP1	-8.11	98.41	105.70
18	D	718	A	N1-C2-N3	-8.09	125.25	129.30
9	9	129	LEU	C-N-CD	-8.08	102.82	120.60
31	Q	56	ARG	NE-CZ-NH1	8.08	124.34	120.30
25	K	78	ASN	N-CA-CB	-8.05	96.11	110.60
46	f	45	ARG	NE-CZ-NH1	8.04	124.32	120.30
10	B	76	A	N1-C6-N6	-8.04	113.78	118.60
18	D	884	U	N1-C2-N3	-8.02	110.09	114.90
10	A	76	A	N1-C6-N6	-7.98	113.81	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	U	31	ARG	NE-CZ-NH2	-7.92	116.34	120.30
18	D	37	U	N1-C2-N3	-7.92	110.15	114.90
29	O	80	ARG	CG-CD-NE	7.84	128.27	111.80
18	D	884	U	C2-N3-C4	7.78	131.66	127.00
41	a	1530	G	C5-C6-O6	-7.75	123.95	128.60
41	a	1257	C	N3-C4-C5	7.71	124.98	121.90
18	D	397	A	N1-C2-N3	-7.69	125.45	129.30
38	X	81	MET	CG-SD-CE	-7.55	88.13	100.20
10	A	37	A	C2-N3-C4	-7.54	106.83	110.60
18	D	718	A	C6-N1-C2	7.53	123.12	118.60
10	B	37	A	C2-N3-C4	-7.52	106.84	110.60
41	a	626	A	N1-C6-N6	-7.47	114.12	118.60
41	a	626	A	N1-C2-N3	7.39	133.00	129.30
23	I	166	GLU	OE1-CD-OE2	7.39	132.17	123.30
18	D	827	U	C4-C5-C6	-7.39	115.27	119.70
63	w	112	TYR	OH-CZ-CE2	-7.38	100.17	120.10
41	a	1655	A	C8-N9-C4	7.38	108.75	105.80
63	w	38	LEU	CB-CG-CD1	-7.37	98.48	111.00
23	I	134	MET	CG-SD-CE	-7.35	88.44	100.20
29	O	103	PHE	CG-CD1-CE1	7.32	128.85	120.80
21	G	154	MET	CG-SD-CE	-7.28	88.55	100.20
10	A	39	C	C5-C6-N1	-7.28	117.36	121.00
18	D	1358	U	C4-C5-C6	-7.28	115.33	119.70
41	a	1086	A	C5-C6-N6	7.28	129.52	123.70
10	B	39	C	C5-C6-N1	-7.23	117.38	121.00
41	a	1530	G	N1-C6-O6	7.23	124.24	119.90
10	A	37	A	C5-N7-C8	-7.21	100.29	103.90
41	a	1276	A	C8-N9-C4	7.20	108.68	105.80
8	7	1	A	OP2-P-O3'	7.17	120.96	105.20
16	AG	108	GLN	N-CA-CB	7.13	123.44	110.60
41	a	1775	U	N3-C4-O4	7.12	124.38	119.40
41	a	2013	A	C5-C6-N6	7.12	129.40	123.70
41	a	1453	A	C2-N3-C4	-7.10	107.05	110.60
18	D	37	U	C2-N3-C4	7.09	131.25	127.00
23	I	134	MET	CB-CG-SD	-7.08	91.17	112.40
18	D	1125	U	N3-C4-O4	7.06	124.34	119.40
41	a	1581	G	N9-C4-C5	-7.05	102.58	105.40
41	a	2902	C	C2-N1-C1'	-7.03	111.06	118.80
10	B	37	A	N1-C2-N3	7.02	132.81	129.30
41	a	960	A	N9-C4-C5	-6.98	103.01	105.80
41	a	2612	C	C6-N1-C2	6.96	123.08	120.30
10	A	37	A	N1-C2-N3	6.92	132.76	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	a	1453	A	N3-C4-C5	6.88	131.62	126.80
10	B	37	A	C5-N7-C8	-6.86	100.47	103.90
47	g	62	LYS	CD-CE-NZ	-6.85	95.94	111.70
12	AB	159	PHE	CB-CA-C	6.83	124.06	110.40
8	7	1	A	O3'-P-O5'	-6.81	91.06	104.00
18	D	37	U	C4-C5-C6	-6.79	115.62	119.70
16	AG	355	ALA	N-CA-CB	6.78	119.58	110.10
41	a	2758	A	N1-C6-N6	-6.77	114.54	118.60
30	P	88	MET	CG-SD-CE	-6.76	89.38	100.20
41	a	542	C	C6-N1-C2	6.76	123.00	120.30
18	D	1526	G	N3-C2-N2	-6.76	115.17	119.90
17	C	38	LYS	CD-CE-NZ	-6.75	96.19	111.70
21	G	19	GLN	CA-CB-CG	6.71	128.16	113.40
41	a	196	A	O4'-C1'-N9	6.69	113.56	108.20
21	G	158	PRO	CA-N-CD	-6.69	102.14	111.50
63	w	42	LYS	CD-CE-NZ	6.68	127.07	111.70
41	a	960	A	C4-C5-N7	6.68	114.04	110.70
18	D	280	C	C2-N3-C4	6.66	123.23	119.90
41	a	1818	U	C5-C6-N1	6.59	126.00	122.70
16	AG	108	GLN	CB-CA-C	-6.59	97.23	110.40
16	AG	354	ALA	CA-C-N	6.56	131.63	117.20
41	a	1453	A	C6-N1-C2	6.53	122.52	118.60
41	a	2013	A	C5-C6-N1	6.49	120.94	117.70
18	D	476	U	C5-C4-O4	-6.49	122.01	125.90
41	a	2351	G	C5-C6-O6	-6.46	124.73	128.60
48	h	181	MET	CG-SD-CE	-6.45	89.89	100.20
41	a	1581	G	C4-C5-N7	6.43	113.37	110.80
41	a	1082	U	C4-C5-C6	-6.39	115.87	119.70
52	l	1	MET	CG-SD-CE	-6.37	90.00	100.20
18	D	718	A	C8-N9-C4	6.37	108.35	105.80
41	a	2188	U	C5-C4-O4	-6.37	122.08	125.90
18	D	1339	A	N3-C4-N9	-6.37	122.31	127.40
41	a	2756	U	N1-C2-N3	-6.36	111.08	114.90
18	D	280	C	C5-C6-N1	6.32	124.16	121.00
18	D	884	U	C4-C5-C6	-6.29	115.93	119.70
21	G	154	MET	CA-CB-CG	-6.27	102.64	113.30
59	s	120	ARG	NE-CZ-NH1	-6.24	117.18	120.30
29	O	80	ARG	CB-CG-CD	-6.24	95.38	111.60
37	W	40	ILE	CG1-CB-CG2	6.24	125.12	111.40
41	a	1276	A	N9-C4-C5	-6.22	103.31	105.80
18	D	60	A	O4'-C1'-N9	6.21	113.17	108.20
59	s	92	MET	CB-CG-SD	-6.20	93.81	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	476	U	N3-C4-O4	6.19	123.74	119.40
12	AB	99	TYR	C-N-CA	6.19	137.16	121.70
41	a	942	G	N1-C6-O6	-6.18	116.19	119.90
10	B	31	G	O4'-C1'-N9	6.18	113.14	108.20
41	a	1257	C	N3-C2-O2	6.15	126.21	121.90
46	f	45	ARG	NE-CZ-NH2	-6.14	117.23	120.30
10	A	31	G	O4'-C1'-N9	6.14	113.11	108.20
12	AB	141	LEU	C-N-CA	-6.13	106.37	121.70
18	D	718	A	P-O5'-C5'	-6.13	111.09	120.90
49	i	15	MET	CG-SD-CE	-6.12	90.41	100.20
56	p	152	ARG	NE-CZ-NH1	-6.12	117.24	120.30
16	AG	105	ILE	C-N-CA	6.10	136.95	121.70
41	a	2902	C	C6-N1-C2	6.09	122.74	120.30
41	a	893	C	C2-N3-C4	-6.09	116.86	119.90
48	h	175	ARG	NE-CZ-NH2	-6.06	117.27	120.30
41	a	2613	U	C4-C5-C6	-6.06	116.06	119.70
18	D	1363	A	N9-C4-C5	-6.06	103.38	105.80
12	AB	162	LEU	CA-CB-CG	6.03	129.17	115.30
41	a	2638	G	O4'-C1'-N9	6.03	113.02	108.20
63	w	112	TYR	CG-CD1-CE1	-6.01	116.49	121.30
48	h	156	ARG	NE-CZ-NH1	6.00	123.30	120.30
14	AE	363	LEU	CA-CB-CG	5.98	129.05	115.30
63	w	38	LEU	CB-CG-CD2	5.98	121.16	111.00
41	a	2901	C	C6-N1-C2	5.96	122.69	120.30
37	W	40	ILE	CA-CB-CG1	-5.96	99.67	111.00
16	AG	106	THR	OG1-CB-CG2	-5.94	96.33	110.00
41	a	729	G	O4'-C1'-N9	5.94	112.95	108.20
16	AG	33	THR	CA-CB-CG2	5.94	120.71	112.40
41	a	2602	A	C3'-C2'-C1'	5.90	106.22	101.50
16	AG	426	GLY	O-C-N	-5.87	113.30	122.70
41	a	1257	C	N1-C2-N3	-5.86	115.10	119.20
41	a	2334	U	OP1-P-O3'	5.83	118.02	105.20
41	a	1581	G	N1-C6-O6	5.82	123.39	119.90
41	a	686	U	N3-C4-C5	5.82	118.09	114.60
50	j	55	LYS	CD-CE-NZ	-5.82	98.32	111.70
41	a	136	G	N9-C4-C5	-5.81	103.08	105.40
18	D	1344	C	O5'-P-OP1	-5.79	100.49	105.70
27	M	47	LEU	CB-CG-CD2	-5.79	101.16	111.00
18	D	280	C	N1-C2-O2	5.79	122.37	118.90
41	a	2351	G	C4-C5-N7	5.79	113.12	110.80
41	a	2049	G	N3-C2-N2	-5.77	115.86	119.90
48	h	175	ARG	NE-CZ-NH1	5.77	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	915	A	N9-C4-C5	-5.77	103.49	105.80
41	a	1577	C	C6-N1-C2	5.77	122.61	120.30
41	a	1019	U	N3-C2-O2	5.76	126.23	122.20
27	M	4	ARG	NE-CZ-NH1	-5.75	117.43	120.30
17	C	73	ARG	NE-CZ-NH1	-5.74	117.43	120.30
41	a	2756	U	C4-C5-C6	-5.74	116.26	119.70
56	p	164	TYR	CB-CG-CD2	5.73	124.44	121.00
41	a	942	G	C5-C6-O6	5.72	132.03	128.60
18	D	526	C	C6-N1-C2	5.72	122.59	120.30
60	t	18	ARG	CG-CD-NE	-5.72	99.80	111.80
41	a	1142	A	N1-C2-N3	-5.71	126.45	129.30
41	a	686	U	N3-C4-O4	-5.71	115.41	119.40
48	h	189	ARG	NE-CZ-NH2	5.68	123.14	120.30
30	P	85	ASP	CB-CG-OD2	-5.66	113.21	118.30
26	L	45	ARG	NE-CZ-NH2	-5.66	117.47	120.30
41	a	1334	G	N3-C4-C5	5.64	131.42	128.60
16	AG	33	THR	C-N-CA	5.64	135.80	121.70
16	AG	102	PHE	C-N-CA	5.64	135.80	121.70
12	AB	159	PHE	C-N-CA	5.63	135.77	121.70
41	a	1857	G	O4'-C1'-N9	5.62	112.69	108.20
41	a	1086	A	C5-C6-N1	5.60	120.50	117.70
16	AG	35	THR	CA-CB-OG1	-5.60	97.24	109.00
41	a	1082	U	N1-C2-N3	-5.60	111.54	114.90
41	a	2188	U	N3-C4-O4	5.60	123.32	119.40
31	Q	110	ILE	CG1-CB-CG2	-5.59	99.10	111.40
41	a	1225	G	N3-C4-C5	5.59	131.40	128.60
41	a	542	C	N3-C4-C5	5.59	124.14	121.90
48	h	156	ARG	NE-CZ-NH2	-5.58	117.51	120.30
18	D	563	A	N9-C4-C5	-5.57	103.57	105.80
17	C	60	LYS	CD-CE-NZ	-5.56	98.90	111.70
10	B	23	C	N1-C2-O2	5.55	122.23	118.90
41	a	1141	U	C4-C5-C6	-5.54	116.38	119.70
41	a	1414	C	C2-N1-C1'	-5.53	112.72	118.80
41	a	2329	U	C5-C6-N1	5.53	125.47	122.70
18	D	1339	A	C2-N3-C4	-5.53	107.84	110.60
41	a	974	G	O4'-C1'-N9	5.52	112.61	108.20
60	t	1	MET	CG-SD-CE	-5.52	91.37	100.20
41	a	1021	A	C4-C5-C6	-5.50	114.25	117.00
41	a	253	C	C6-N1-C2	5.50	122.50	120.30
43	c	71	LEU	CA-CB-CG	5.49	127.93	115.30
41	a	2332	C	C6-N1-C2	5.49	122.50	120.30
10	A	38	A	C5'-C4'-O4'	5.49	115.68	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AE	709	ARG	C-N-CA	5.48	135.41	121.70
41	a	544	C	C6-N1-C2	5.48	122.49	120.30
18	D	719	C	C6-N1-C2	5.47	122.49	120.30
26	L	45	ARG	NE-CZ-NH1	5.47	123.04	120.30
10	A	23	C	N1-C2-O2	5.47	122.18	118.90
10	B	38	A	C5'-C4'-O4'	5.45	115.64	109.10
41	a	742	A	C6-N1-C2	-5.45	115.33	118.60
18	D	280	C	C5-C4-N4	5.45	124.01	120.20
16	AG	104	ARG	O-C-N	5.43	131.39	122.70
41	a	1141	U	N1-C2-O2	5.43	126.60	122.80
8	7	27	G	C2'-C3'-O3'	5.43	122.39	113.70
18	D	1158	C	O4'-C1'-N1	5.42	112.54	108.20
50	j	11	MET	CB-CG-SD	-5.42	96.14	112.40
41	a	221	A	O4'-C1'-N9	5.41	112.53	108.20
41	a	775	G	O4'-C1'-N9	5.41	112.53	108.20
41	a	1257	C	C6-N1-C1'	-5.41	114.31	120.80
10	A	37	A	N7-C8-N9	5.41	116.50	113.80
3	2	69	ARG	NE-CZ-NH1	5.40	123.00	120.30
41	a	2338	C	C6-N1-C2	5.39	122.46	120.30
16	AG	104	ARG	CA-C-N	-5.37	105.38	117.20
41	a	883	G	N3-C2-N2	-5.36	116.15	119.90
65	y	109	ARG	NE-CZ-NH1	5.36	122.98	120.30
41	a	1142	A	C4-C5-C6	-5.36	114.32	117.00
41	a	1581	G	C6-C5-N7	-5.35	127.19	130.40
59	s	92	MET	CA-CB-CG	-5.35	104.20	113.30
23	I	168	TYR	N-CA-CB	5.34	120.22	110.60
41	a	2613	U	C2-N3-C4	5.34	130.20	127.00
6	5	8	DG	P-O3'-C3'	5.33	126.10	119.70
31	Q	56	ARG	NE-CZ-NH2	-5.32	117.64	120.30
9	9	130	PRO	CA-N-CD	-5.32	104.06	111.50
16	AG	458	ASP	CB-CG-OD2	5.30	123.07	118.30
63	w	112	TYR	CE1-CZ-CE2	5.30	128.28	119.80
16	AG	469	ASP	CB-CG-OD2	5.30	123.07	118.30
16	AG	465	ASP	CB-CG-OD2	5.30	123.07	118.30
16	AG	466	ASP	CB-CG-OD2	5.29	123.06	118.30
18	D	872	A	C5-C6-N1	5.29	120.35	117.70
18	D	476	U	C2-N1-C1'	5.29	124.05	117.70
41	a	1021	A	C6-N1-C2	5.29	121.77	118.60
18	D	397	A	C4-C5-N7	5.29	113.34	110.70
41	a	542	C	C2-N1-C1'	-5.28	112.99	118.80
16	AG	432	ASP	CB-CG-OD2	5.26	123.04	118.30
6	5	11	DA	P-O3'-C3'	5.26	126.02	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AG	102	PHE	N-CA-C	5.26	125.20	111.00
41	a	1257	C	O5'-P-OP2	-5.26	100.97	105.70
41	a	67	U	N1-C2-N3	-5.25	111.75	114.90
41	a	1019	U	N1-C2-O2	5.25	126.47	122.80
16	AG	475	ASP	CB-CG-OD2	5.25	123.02	118.30
41	a	1053	C	C6-N1-C2	5.24	122.40	120.30
16	AG	433	ASP	CB-CG-OD2	5.23	123.01	118.30
16	AG	368	ASP	CB-CG-OD2	5.23	123.00	118.30
60	t	20	MET	CA-CB-CG	5.23	122.19	113.30
39	Y	5	GLN	CB-CA-C	-5.21	99.98	110.40
41	a	27	G	O4'-C1'-N9	5.21	112.37	108.20
16	AG	443	ASP	CB-CG-OD2	5.21	122.98	118.30
56	p	152	ARG	NE-CZ-NH2	5.20	122.90	120.30
37	W	62	VAL	CG1-CB-CG2	5.20	119.21	110.90
54	n	26	MET	CG-SD-CE	-5.19	91.89	100.20
41	a	2602	A	P-O3'-C3'	5.19	125.93	119.70
41	a	385	C	C6-N1-C2	5.19	122.38	120.30
41	a	1414	C	C6-N1-C2	5.19	122.38	120.30
41	a	2284	A	C8-N9-C4	5.19	107.88	105.80
16	AG	366	ASP	CB-CG-OD2	5.17	122.95	118.30
41	a	704	G	O4'-C1'-N9	5.16	112.33	108.20
41	a	2013	A	N9-C4-C5	-5.16	103.73	105.80
41	a	2901	C	C2-N1-C1'	-5.15	113.14	118.80
18	D	107	G	N9-C1'-C2'	-5.15	106.34	112.00
18	D	563	A	C5-C6-N1	5.14	120.27	117.70
16	AG	493	ASP	CB-CG-OD2	5.14	122.92	118.30
16	AG	441	ASP	CB-CG-OD2	5.13	122.92	118.30
10	B	37	A	N7-C8-N9	5.12	116.36	113.80
8	7	4	U	C2'-C3'-O3'	5.12	121.89	113.70
41	a	2756	U	N3-C4-C5	5.11	117.67	114.60
63	w	112	TYR	CG-CD2-CE2	5.11	125.39	121.30
28	N	27	MET	CG-SD-CE	-5.11	92.03	100.20
16	AG	246	ASP	C-N-CD	-5.10	109.38	120.60
54	n	38	MET	CG-SD-CE	5.10	108.36	100.20
25	K	45	ARG	CB-CG-CD	-5.10	98.35	111.60
41	a	1331	G	N1-C6-O6	-5.09	116.84	119.90
13	AD	289	LEU	C-N-CA	-5.09	108.97	121.70
18	D	397	A	N9-C4-C5	-5.09	103.76	105.80
18	D	496	A	C2-N3-C4	5.09	113.14	110.60
41	a	2613	U	N1-C2-N3	-5.05	111.87	114.90
18	D	368	U	C2-N1-C1'	5.04	123.75	117.70
11	AA	516	ASP	CB-CG-OD2	5.04	122.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	882	C	C6-N1-C2	5.04	122.31	120.30
18	D	1358	U	N3-C2-O2	5.03	125.72	122.20
10	A	39	C	C2-N3-C4	5.03	122.42	119.90
21	G	113	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
10	B	76	A	N9-C4-C5	5.02	107.81	105.80
41	a	537	G	OP1-P-OP2	5.02	127.13	119.60
41	a	1592	C	C2-N1-C1'	-5.02	113.27	118.80
39	Y	5	GLN	CA-CB-CG	5.01	124.43	113.40

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	107	GLU	Peptide
9	9	79	PRO	Peptide
9	9	92	ALA	Peptide
12	AB	140	MET	Peptide
12	AB	151	LYS	Peptide
13	AC	192	VAL	Peptide
13	AD	20	SER	Peptide
13	AD	284	ARG	Mainchain
14	AE	1326	GLN	Peptide
14	AE	1344	LEU	Peptide
14	AE	313	GLY	Peptide
14	AE	416	ILE	Peptide
16	AG	102	PHE	Peptide
16	AG	104	ARG	Peptide,Mainchain
16	AG	11	ALA	Peptide
16	AG	292	ASP	Mainchain
16	AG	426	GLY	Mainchain
21	G	19	GLN	Sidechain
22	H	124	LEU	Peptide
22	H	171	ARG	Peptide
22	H	274	TYR	Peptide
22	H	81	GLU	Peptide
22	H	82	THR	Peptide
23	I	167	TRP	Mainchain
25	K	45	ARG	Mainchain
25	K	77	ASN	Peptide
29	O	12	ARG	Peptide
38	X	65	VAL	Peptide
39	Y	5	GLN	Peptide

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Mol	Chain	Res	Type	Group
54	n	176	PRO	Peptide
55	o	31	HIS	Peptide
59	s	74	TYR	Sidechain
61	u	35	HIS	Peptide
61	u	62	PRO	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
2	1	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
3	2	92/100 (92%)	87 (95%)	5 (5%)	0	100	100
4	3	101/104 (97%)	98 (97%)	3 (3%)	0	100	100
5	4	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
9	9	146/165 (88%)	101 (69%)	42 (29%)	3 (2%)	5	24
11	AA	1312/1342 (98%)	1197 (91%)	114 (9%)	1 (0%)	48	78
12	AB	159/162 (98%)	106 (67%)	42 (26%)	11 (7%)	1	6
13	AC	217/329 (66%)	204 (94%)	11 (5%)	2 (1%)	14	41
13	AD	293/329 (89%)	263 (90%)	27 (9%)	3 (1%)	13	39
14	AE	1331/1407 (95%)	1212 (91%)	113 (8%)	6 (0%)	25	54
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
16	AG	493/495 (100%)	376 (76%)	86 (17%)	31 (6%)	1	7
17	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
20	F	68/71 (96%)	68 (100%)	0	0	100	100
21	G	223/241 (92%)	212 (95%)	10 (4%)	1 (0%)	30	60
22	H	255/557 (46%)	182 (71%)	66 (26%)	7 (3%)	4	21
23	I	206/233 (88%)	193 (94%)	13 (6%)	0	100	100
24	J	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
25	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	22	50
26	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	13	39
27	M	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	19	47
28	N	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
29	O	125/130 (96%)	116 (93%)	8 (6%)	1 (1%)	16	44
30	P	97/103 (94%)	89 (92%)	8 (8%)	0	100	100
31	Q	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
32	R	117/124 (94%)	112 (96%)	5 (4%)	0	100	100
33	S	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
34	T	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
35	U	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
36	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
37	W	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
38	X	114/118 (97%)	103 (90%)	9 (8%)	2 (2%)	7	27
39	Y	139/142 (98%)	102 (73%)	37 (27%)	0	100	100
40	Z	28/121 (23%)	22 (79%)	6 (21%)	0	100	100
42	b	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
43	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
45	e	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
46	f	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
47	g	64/70 (91%)	62 (97%)	2 (3%)	0	100	100
48	h	269/273 (98%)	255 (95%)	14 (5%)	0	100	100
49	i	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
50	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
51	k	50/55 (91%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	l	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
53	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	n	175/179 (98%)	160 (91%)	14 (8%)	1 (1%)	22	50
55	o	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	8	29
56	p	173/177 (98%)	162 (94%)	11 (6%)	0	100	100
57	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
58	r	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
59	s	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
60	t	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
61	u	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
62	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
63	w	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
64	x	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
65	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
66	z	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
All	All	10058/11053 (91%)	9180 (91%)	805 (8%)	73 (1%)	21	47

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AB	107	PRO
12	AB	125	GLY
12	AB	130	PHE
12	AB	137	ALA
12	AB	141	LEU
12	AB	152	HIS
12	AB	160	ARG
13	AD	286	GLU
16	AG	34	ALA
16	AG	105	ILE
16	AG	187	ARG
16	AG	227	ALA
21	G	127	ASP
22	H	304	VAL
27	M	56	LYS
55	o	32	ILE
12	AB	105	VAL

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Mol	Chain	Res	Type
14	AE	92	VAL
14	AE	175	GLU
16	AG	63	LEU
16	AG	104	ARG
16	AG	242	ASP
16	AG	268	GLY
16	AG	279	ASN
16	AG	350	ALA
16	AG	365	ILE
22	H	171	ARG
22	H	305	HIS
22	H	309	MET
12	AB	127	GLN
16	AG	33	THR
16	AG	102	PHE
16	AG	200	SER
16	AG	305	MET
16	AG	319	GLY
16	AG	355	ALA
16	AG	396	GLU
16	AG	425	LEU
25	K	78	ASN
26	L	96	VAL
29	O	13	LYS
54	n	177	PHE
13	AC	193	GLU
16	AG	48	GLN
16	AG	265	GLU
16	AG	363	LEU
16	AG	401	PRO
22	H	82	THR
12	AB	53	ASN
13	AD	289	LEU
14	AE	74	LYS
14	AE	286	ALA
16	AG	224	LYS
16	AG	399	ASP
22	H	143	ASP
38	X	6	GLY
38	X	66	GLU
9	9	79	PRO
9	9	88	HIS

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Mol	Chain	Res	Type
13	AC	192	VAL
13	AD	306	VAL
14	AE	290	ILE
16	AG	43	ILE
16	AG	70	GLN
16	AG	169	PRO
16	AG	323	GLN
16	AG	364	ASP
16	AG	382	GLU
22	H	71	ALA
14	AE	292	VAL
9	9	129	LEU
11	AA	1317	PRO
12	AB	116	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	0	84/84 (100%)	84 (100%)	0	100	100
2	1	93/93 (100%)	93 (100%)	0	100	100
3	2	81/84 (96%)	80 (99%)	1 (1%)	67	80
4	3	84/85 (99%)	84 (100%)	0	100	100
5	4	78/78 (100%)	78 (100%)	0	100	100
9	9	112/123 (91%)	109 (97%)	3 (3%)	40	63
11	AA	1135/1157 (98%)	1134 (100%)	1 (0%)	92	97
12	AB	141/142 (99%)	122 (86%)	19 (14%)	3	12
13	AC	186/286 (65%)	186 (100%)	0	100	100
13	AD	185/286 (65%)	185 (100%)	0	100	100
14	AE	1122/1168 (96%)	1103 (98%)	19 (2%)	56	74
15	AF	70/75 (93%)	70 (100%)	0	100	100
16	AG	409/409 (100%)	297 (73%)	112 (27%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	C	57/65 (88%)	57 (100%)	0	100	100
19	E	65/66 (98%)	65 (100%)	0	100	100
20	F	60/61 (98%)	60 (100%)	0	100	100
21	G	187/199 (94%)	186 (100%)	1 (0%)	86	91
22	H	137/461 (30%)	137 (100%)	0	100	100
23	I	171/190 (90%)	170 (99%)	1 (1%)	84	90
24	J	172/173 (99%)	171 (99%)	1 (1%)	84	90
25	K	119/126 (94%)	117 (98%)	2 (2%)	56	74
26	L	91/116 (78%)	91 (100%)	0	100	100
27	M	124/147 (84%)	124 (100%)	0	100	100
28	N	104/105 (99%)	104 (100%)	0	100	100
29	O	105/107 (98%)	104 (99%)	1 (1%)	73	83
30	P	86/90 (96%)	84 (98%)	2 (2%)	45	67
31	Q	90/99 (91%)	90 (100%)	0	100	100
32	R	101/104 (97%)	101 (100%)	0	100	100
33	S	83/84 (99%)	83 (100%)	0	100	100
34	T	76/77 (99%)	76 (100%)	0	100	100
35	U	65/65 (100%)	64 (98%)	1 (2%)	60	76
36	V	74/78 (95%)	73 (99%)	1 (1%)	62	77
37	W	72/79 (91%)	72 (100%)	0	100	100
38	X	94/96 (98%)	94 (100%)	0	100	100
39	Y	109/110 (99%)	108 (99%)	1 (1%)	75	86
40	Z	26/85 (31%)	26 (100%)	0	100	100
42	b	58/63 (92%)	58 (100%)	0	100	100
43	c	67/68 (98%)	67 (100%)	0	100	100
45	e	54/55 (98%)	54 (100%)	0	100	100
46	f	48/49 (98%)	48 (100%)	0	100	100
47	g	59/62 (95%)	59 (100%)	0	100	100
48	h	216/218 (99%)	216 (100%)	0	100	100
49	i	47/48 (98%)	47 (100%)	0	100	100
50	j	164/164 (100%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	k	47/49 (96%)	47 (100%)	0	100	100
52	l	165/165 (100%)	164 (99%)	1 (1%)	84	90
53	m	38/38 (100%)	38 (100%)	0	100	100
54	n	148/150 (99%)	148 (100%)	0	100	100
55	o	51/52 (98%)	51 (100%)	0	100	100
56	p	136/138 (99%)	136 (100%)	0	100	100
57	q	34/34 (100%)	34 (100%)	0	100	100
58	r	114/114 (100%)	114 (100%)	0	100	100
59	s	116/116 (100%)	115 (99%)	1 (1%)	75	86
60	t	104/104 (100%)	103 (99%)	1 (1%)	73	83
61	u	103/103 (100%)	103 (100%)	0	100	100
62	v	109/109 (100%)	109 (100%)	0	100	100
63	w	99/103 (96%)	98 (99%)	1 (1%)	73	83
64	x	86/87 (99%)	86 (100%)	0	100	100
65	y	99/100 (99%)	97 (98%)	2 (2%)	50	70
66	z	89/90 (99%)	88 (99%)	1 (1%)	70	81
All	All	8299/9132 (91%)	8126 (98%)	173 (2%)	49	69

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	6	ARG
9	9	56	ARG
9	9	73	LYS
9	9	94	ARG
11	AA	914	LYS
12	AB	115	LYS
12	AB	116	VAL
12	AB	117	ILE
12	AB	118	ILE
12	AB	119	THR
12	AB	120	GLU
12	AB	123	PHE
12	AB	124	GLU
12	AB	126	PHE
12	AB	138	ARG

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Mol	Chain	Res	Type
12	AB	143	LEU
12	AB	144	ASN
12	AB	145	LEU
12	AB	148	LYS
12	AB	149	GLU
12	AB	150	ILE
12	AB	159	PHE
12	AB	160	ARG
12	AB	161	LYS
14	AE	69	GLU
14	AE	70	CYS
14	AE	71	LEU
14	AE	74	LYS
14	AE	76	LYS
14	AE	77	ARG
14	AE	78	LEU
14	AE	79	LYS
14	AE	81	ARG
14	AE	85	CYS
14	AE	92	VAL
14	AE	93	THR
14	AE	290	ILE
14	AE	291	ILE
14	AE	292	VAL
14	AE	431	ARG
14	AE	514	THR
14	AE	744	ARG
14	AE	1369	ARG
16	AG	5	ILE
16	AG	12	VAL
16	AG	36	LYS
16	AG	37	LYS
16	AG	38	LYS
16	AG	40	GLU
16	AG	43	ILE
16	AG	49	ILE
16	AG	50	ASP
16	AG	56	PHE
16	AG	57	ASP
16	AG	61	ARG
16	AG	75	ILE
16	AG	97	ILE

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Mol	Chain	Res	Type
16	AG	103	ASP
16	AG	104	ARG
16	AG	114	ILE
16	AG	117	LYS
16	AG	123	ARG
16	AG	125	MET
16	AG	126	VAL
16	AG	131	ARG
16	AG	139	THR
16	AG	144	LYS
16	AG	150	ILE
16	AG	154	LEU
16	AG	157	ASN
16	AG	162	ILE
16	AG	167	MET
16	AG	173	PHE
16	AG	179	VAL
16	AG	180	ARG
16	AG	182	VAL
16	AG	185	SER
16	AG	187	ARG
16	AG	195	LEU
16	AG	197	VAL
16	AG	199	ARG
16	AG	201	LYS
16	AG	203	GLU
16	AG	204	MET
16	AG	205	LEU
16	AG	206	ILE
16	AG	207	GLU
16	AG	209	PHE
16	AG	210	ARG
16	AG	211	ILE
16	AG	213	VAL
16	AG	219	GLU
16	AG	221	ILE
16	AG	223	ILE
16	AG	232	SER
16	AG	235	LYS
16	AG	236	ILE
16	AG	238	VAL
16	AG	240	THR

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Mol	Chain	Res	Type
16	AG	241	ASN
16	AG	242	ASP
16	AG	243	LYS
16	AG	244	ARG
16	AG	245	ILE
16	AG	254	MET
16	AG	255	ARG
16	AG	258	ARG
16	AG	259	VAL
16	AG	260	GLN
16	AG	262	VAL
16	AG	265	GLU
16	AG	266	LEU
16	AG	270	ARG
16	AG	271	ILE
16	AG	274	VAL
16	AG	276	TRP
16	AG	278	ASP
16	AG	285	ILE
16	AG	288	MET
16	AG	296	ILE
16	AG	299	ASP
16	AG	300	GLU
16	AG	301	ASP
16	AG	302	LYS
16	AG	303	HIS
16	AG	305	MET
16	AG	309	VAL
16	AG	310	GLU
16	AG	313	ASN
16	AG	316	GLN
16	AG	320	ARG
16	AG	321	ASN
16	AG	323	GLN
16	AG	327	LEU
16	AG	331	LEU
16	AG	335	GLU
16	AG	336	LEU
16	AG	337	ASN
16	AG	340	THR
16	AG	342	ASP
16	AG	344	LEU

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Mol	Chain	Res	Type
16	AG	356	ILE
16	AG	358	THR
16	AG	359	PHE
16	AG	361	LYS
16	AG	365	ILE
16	AG	380	THR
16	AG	387	VAL
16	AG	390	LYS
16	AG	396	GLU
16	AG	399	ASP
16	AG	400	GLU
16	AG	425	LEU
16	AG	428	ASN
16	AG	429	LYS
21	G	105	LYS
23	I	72	ARG
24	J	47	ARG
25	K	70	ASN
25	K	71	MET
29	O	12	ARG
30	P	5	ARG
30	P	89	ARG
35	U	35	ARG
36	V	27	ARG
39	Y	44	LYS
52	l	57	LYS
59	s	86	GLN
60	t	108	ARG
63	w	73	ASN
65	y	6	LYS
65	y	38	LYS
66	z	22	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	6	GLN
2	1	7	HIS
3	2	15	HIS
9	9	9	GLN
11	AA	69	GLN
11	AA	150	HIS

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Mol	Chain	Res	Type
11	AA	314	ASN
11	AA	387	ASN
11	AA	513	GLN
11	AA	554	HIS
11	AA	580	GLN
11	AA	604	HIS
11	AA	688	GLN
11	AA	1268	GLN
11	AA	1313	HIS
12	AB	65	HIS
13	AC	147	GLN
13	AD	66	HIS
13	AD	117	HIS
14	AE	157	GLN
14	AE	450	HIS
14	AE	777	HIS
14	AE	805	GLN
14	AE	910	ASN
14	AE	1108	GLN
14	AE	1326	GLN
14	AE	1367	GLN
15	AF	31	GLN
16	AG	194	GLN
16	AG	241	ASN
16	AG	260	GLN
16	AG	282	GLN
16	AG	316	GLN
16	AG	323	GLN
16	AG	337	ASN
17	C	54	GLN
19	E	13	GLN
19	E	61	GLN
20	F	9	ASN
21	G	18	HIS
21	G	39	HIS
21	G	58	ASN
21	G	109	GLN
23	I	3	GLN
23	I	6	HIS
23	I	32	ASN
23	I	190	HIS
24	J	131	ASN

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Mol	Chain	Res	Type
24	J	198	HIS
26	L	3	HIS
26	L	68	GLN
27	M	68	ASN
29	O	5	GLN
34	T	80	GLN
35	U	26	ASN
39	Y	5	GLN
45	e	25	GLN
45	e	31	GLN
46	f	20	HIS
48	h	53	HIS
50	j	173	GLN
52	l	92	HIS
53	m	29	GLN
54	n	5	HIS
55	o	24	HIS
57	q	13	ASN
59	s	132	HIS
62	v	45	GLN
62	v	97	GLN
63	w	18	GLN
64	x	19	GLN
64	x	38	GLN
65	y	10	GLN
65	y	77	HIS
66	z	37	GLN
66	z	72	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	8 (10%)
10	B	75/76 (98%)	29 (38%)	8 (10%)
18	D	1514/1542 (98%)	290 (19%)	20 (1%)
41	a	2859/2904 (98%)	507 (17%)	0
44	d	119/120 (99%)	15 (12%)	0
8	7	36/41 (87%)	26 (72%)	5 (13%)
All	All	4678/4759 (98%)	896 (19%)	41 (0%)

All (896) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	3	G
8	7	4	U
8	7	5	U
8	7	7	U
8	7	8	U
8	7	9	U
8	7	10	U
8	7	11	U
8	7	12	U
8	7	13	U
8	7	14	U
8	7	15	U
8	7	16	U
8	7	17	U
8	7	18	U
8	7	19	U
8	7	20	U
8	7	21	U
8	7	22	U
8	7	23	U
8	7	28	A
8	7	29	U
8	7	30	U
8	7	31	U
8	7	34	U
8	7	36	A
10	A	2	G
10	A	6	G
10	A	7	G
10	A	8	U
10	A	10	G
10	A	13	C
10	A	14	A
10	A	16	C
10	A	17	C
10	A	18	G
10	A	19	G
10	A	20	U
10	A	21	A
10	A	22	G
10	A	23	C
10	A	30	G
10	A	46	G

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Mol	Chain	Res	Type
10	A	47	U
10	A	48	C
10	A	49	G
10	A	52	G
10	A	57	A
10	A	58	A
10	A	59	A
10	A	61	C
10	A	66	C
10	A	69	C
10	A	71	C
10	A	73	A
10	B	2	G
10	B	6	G
10	B	7	G
10	B	8	U
10	B	10	G
10	B	13	C
10	B	14	A
10	B	16	C
10	B	17	C
10	B	18	G
10	B	19	G
10	B	20	U
10	B	21	A
10	B	22	G
10	B	23	C
10	B	30	G
10	B	46	G
10	B	47	U
10	B	48	C
10	B	49	G
10	B	52	G
10	B	57	A
10	B	58	A
10	B	59	A
10	B	61	C
10	B	66	C
10	B	69	C
10	B	71	C
10	B	73	A
18	D	4	U

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Mol	Chain	Res	Type
18	D	5	U
18	D	9	G
18	D	22	G
18	D	29	U
18	D	32	A
18	D	39	G
18	D	47	C
18	D	48	C
18	D	50	A
18	D	51	A
18	D	52	C
18	D	54	C
18	D	68	G
18	D	69	G
18	D	71	A
18	D	72	A
18	D	74	A
18	D	76	G
18	D	82	G
18	D	83	C
18	D	84	U
18	D	87	C
18	D	90	C
18	D	94	G
18	D	95	C
18	D	96	U
18	D	108	G
18	D	120	A
18	D	121	U
18	D	122	G
18	D	131	A
18	D	141	G
18	D	144	G
18	D	148	G
18	D	149	A
18	D	160	A
18	D	164	G
18	D	173	U
18	D	181	A
18	D	182	A
18	D	183	C
18	D	184	G

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Mol	Chain	Res	Type
18	D	197	A
18	D	198	G
18	D	204	G
18	D	208	U
18	D	209	U
18	D	210	C
18	D	211	G
18	D	212	G
18	D	216	U
18	D	226	G
18	D	245	U
18	D	247	G
18	D	251	G
18	D	253	A
18	D	258	G
18	D	262	A
18	D	266	G
18	D	267	C
18	D	271	C
18	D	279	A
18	D	289	G
18	D	299	G
18	D	306	A
18	D	321	A
18	D	328	C
18	D	329	A
18	D	332	G
18	D	347	G
18	D	352	C
18	D	353	A
18	D	354	G
18	D	355	C
18	D	367	U
18	D	372	C
18	D	373	A
18	D	376	G
18	D	382	A
18	D	384	G
18	D	392	C
18	D	397	A
18	D	398	U
18	D	406	G

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Mol	Chain	Res	Type
18	D	411	A
18	D	412	A
18	D	413	G
18	D	414	A
18	D	421	U
18	D	422	C
18	D	424	G
18	D	429	U
18	D	446	G
18	D	451	A
18	D	457	G
18	D	458	U
18	D	463	U
18	D	464	U
18	D	467	U
18	D	468	A
18	D	469	C
18	D	478	A
18	D	479	U
18	D	481	G
18	D	484	G
18	D	485	U
18	D	486	U
18	D	496	A
18	D	497	G
18	D	505	G
18	D	511	C
18	D	518	C
18	D	519	C
18	D	526	C
18	D	531	U
18	D	532	A
18	D	533	A
18	D	542	G
18	D	547	A
18	D	559	A
18	D	564	C
18	D	568	G
18	D	572	A
18	D	573	A
18	D	576	C
18	D	577	G

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Mol	Chain	Res	Type
18	D	579	A
18	D	596	A
18	D	628	G
18	D	633	G
18	D	649	A
18	D	650	G
18	D	653	U
18	D	665	A
18	D	695	A
18	D	700	G
18	D	723	U
18	D	724	G
18	D	731	G
18	D	734	G
18	D	735	C
18	D	747	A
18	D	748	G
18	D	755	G
18	D	760	G
18	D	777	A
18	D	793	U
18	D	794	A
18	D	815	A
18	D	817	C
18	D	828	U
18	D	829	G
18	D	832	G
18	D	841	C
18	D	843	U
18	D	844	G
18	D	845	A
18	D	846	G
18	D	849	G
18	D	874	G
18	D	887	G
18	D	902	G
18	D	914	A
18	D	916	U
18	D	926	G
18	D	934	C
18	D	935	A
18	D	960	U

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Mol	Chain	Res	Type
18	D	963	G
18	D	965	U
18	D	969	A
18	D	972	C
18	D	975	A
18	D	976	G
18	D	987	G
18	D	991	U
18	D	992	U
18	D	993	G
18	D	996	A
18	D	1004	A
18	D	1008	U
18	D	1009	U
18	D	1017	U
18	D	1018	G
18	D	1021	A
18	D	1024	G
18	D	1026	G
18	D	1028	C
18	D	1030	U
18	D	1031	C
18	D	1037	C
18	D	1043	G
18	D	1044	A
18	D	1046	A
18	D	1065	U
18	D	1085	U
18	D	1094	G
18	D	1095	U
18	D	1099	G
18	D	1101	A
18	D	1108	G
18	D	1124	G
18	D	1133	G
18	D	1135	U
18	D	1136	C
18	D	1137	C
18	D	1139	G
18	D	1140	C
18	D	1141	C
18	D	1142	G

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Mol	Chain	Res	Type
18	D	1143	G
18	D	1145	A
18	D	1146	A
18	D	1151	A
18	D	1152	A
18	D	1159	U
18	D	1167	A
18	D	1171	A
18	D	1174	G
18	D	1175	G
18	D	1176	A
18	D	1184	G
18	D	1193	G
18	D	1196	A
18	D	1197	A
18	D	1206	G
18	D	1211	U
18	D	1212	U
18	D	1213	A
18	D	1214	C
18	D	1215	G
18	D	1226	C
18	D	1227	A
18	D	1228	C
18	D	1238	A
18	D	1257	A
18	D	1260	G
18	D	1275	A
18	D	1276	G
18	D	1278	G
18	D	1279	G
18	D	1280	A
18	D	1285	A
18	D	1286	U
18	D	1287	A
18	D	1299	A
18	D	1300	G
18	D	1302	C
18	D	1305	G
18	D	1312	G
18	D	1317	C
18	D	1320	C

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Mol	Chain	Res	Type
18	D	1323	G
18	D	1338	G
18	D	1340	A
18	D	1346	A
18	D	1347	G
18	D	1353	G
18	D	1363	A
18	D	1370	G
18	D	1378	C
18	D	1379	G
18	D	1381	U
18	D	1391	U
18	D	1396	A
18	D	1397	C
18	D	1398	A
18	D	1404	C
18	D	1419	G
18	D	1429	A
18	D	1441	A
18	D	1446	A
18	D	1447	A
18	D	1448	C
18	D	1452	C
18	D	1453	G
18	D	1475	G
18	D	1487	G
18	D	1491	G
18	D	1492	A
18	D	1493	A
18	D	1494	G
18	D	1497	G
18	D	1503	A
18	D	1506	U
18	D	1517	G
18	D	1529	G
18	D	1530	G
18	D	1534	A
41	a	4	U
41	a	10	A
41	a	15	G
41	a	23	G
41	a	34	U

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Mol	Chain	Res	Type
41	a	35	G
41	a	46	G
41	a	58	G
41	a	60	G
41	a	62	U
41	a	63	A
41	a	71	A
41	a	74	A
41	a	75	G
41	a	83	A
41	a	84	A
41	a	85	G
41	a	96	C
41	a	101	A
41	a	102	U
41	a	103	A
41	a	110	G
41	a	118	A
41	a	119	A
41	a	120	U
41	a	131	A
41	a	136	G
41	a	139	U
41	a	140	C
41	a	141	G
41	a	163	C
41	a	165	A
41	a	181	A
41	a	196	A
41	a	215	G
41	a	216	A
41	a	222	A
41	a	225	C
41	a	248	G
41	a	249	C
41	a	261	G
41	a	264	C
41	a	265	A
41	a	266	G
41	a	267	C
41	a	271	G
41	a	272	A

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Mol	Chain	Res	Type
41	a	275	C
41	a	276	U
41	a	278	A
41	a	285	G
41	a	291	G
41	a	311	A
41	a	329	G
41	a	330	A
41	a	353	C
41	a	361	G
41	a	362	A
41	a	371	A
41	a	372	G
41	a	373	U
41	a	375	G
41	a	383	C
41	a	386	G
41	a	396	G
41	a	405	U
41	a	411	G
41	a	412	A
41	a	420	C
41	a	424	G
41	a	451	U
41	a	457	A
41	a	477	A
41	a	481	G
41	a	491	G
41	a	501	A
41	a	503	A
41	a	504	A
41	a	505	A
41	a	509	C
41	a	522	A
41	a	529	A
41	a	531	C
41	a	532	A
41	a	537	G
41	a	543	G
41	a	545	U
41	a	546	U
41	a	547	A

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Mol	Chain	Res	Type
41	a	549	G
41	a	551	G
41	a	563	A
41	a	569	U
41	a	573	U
41	a	575	A
41	a	588	U
41	a	603	A
41	a	609	A
41	a	613	A
41	a	614	A
41	a	615	U
41	a	616	A
41	a	627	A
41	a	637	A
41	a	645	C
41	a	647	G
41	a	654	A
41	a	668	A
41	a	686	U
41	a	710	U
41	a	717	C
41	a	730	A
41	a	738	G
41	a	757	G
41	a	764	A
41	a	765	C
41	a	775	G
41	a	776	G
41	a	782	A
41	a	784	G
41	a	785	G
41	a	800	A
41	a	805	G
41	a	812	C
41	a	819	A
41	a	827	U
41	a	828	U
41	a	845	A
41	a	846	U
41	a	858	G
41	a	859	G

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Mol	Chain	Res	Type
41	a	869	G
41	a	878	A
41	a	881	G
41	a	884	U
41	a	885	C
41	a	888	C
41	a	891	G
41	a	895	U
41	a	896	A
41	a	897	C
41	a	899	A
41	a	907	G
41	a	910	A
41	a	914	G
41	a	915	C
41	a	931	U
41	a	941	A
41	a	945	A
41	a	946	C
41	a	953	G
41	a	961	C
41	a	974	G
41	a	983	A
41	a	995	C
41	a	996	A
41	a	999	U
41	a	1005	C
41	a	1012	U
41	a	1013	C
41	a	1022	G
41	a	1023	U
41	a	1026	G
41	a	1033	U
41	a	1041	G
41	a	1045	C
41	a	1046	A
41	a	1047	G
41	a	1060	U
41	a	1061	U
41	a	1064	C
41	a	1066	U
41	a	1067	A

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Mol	Chain	Res	Type
41	a	1068	G
41	a	1070	A
41	a	1071	G
41	a	1073	A
41	a	1074	G
41	a	1079	C
41	a	1080	A
41	a	1081	U
41	a	1082	U
41	a	1083	U
41	a	1084	A
41	a	1087	G
41	a	1088	A
41	a	1090	A
41	a	1095	A
41	a	1101	U
41	a	1107	G
41	a	1111	A
41	a	1112	G
41	a	1119	U
41	a	1122	G
41	a	1128	G
41	a	1132	U
41	a	1134	A
41	a	1135	C
41	a	1142	A
41	a	1169	A
41	a	1170	C
41	a	1173	U
41	a	1174	U
41	a	1175	A
41	a	1176	U
41	a	1177	G
41	a	1178	C
41	a	1179	G
41	a	1180	U
41	a	1186	G
41	a	1238	G
41	a	1248	G
41	a	1253	A
41	a	1256	G
41	a	1266	G

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Mol	Chain	Res	Type
41	a	1271	G
41	a	1272	A
41	a	1273	U
41	a	1300	G
41	a	1301	A
41	a	1321	A
41	a	1345	C
41	a	1352	U
41	a	1365	A
41	a	1368	G
41	a	1378	A
41	a	1379	U
41	a	1380	G
41	a	1383	A
41	a	1392	A
41	a	1395	A
41	a	1406	U
41	a	1408	G
41	a	1409	U
41	a	1414	C
41	a	1416	G
41	a	1417	C
41	a	1419	A
41	a	1420	A
41	a	1428	C
41	a	1452	G
41	a	1453	A
41	a	1460	U
41	a	1482	G
41	a	1490	A
41	a	1497	U
41	a	1503	A
41	a	1508	A
41	a	1509	A
41	a	1510	G
41	a	1515	A
41	a	1529	G
41	a	1534	U
41	a	1535	A
41	a	1536	C
41	a	1537	G
41	a	1554	U

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Mol	Chain	Res	Type
41	a	1559	U
41	a	1566	A
41	a	1569	A
41	a	1578	U
41	a	1580	A
41	a	1581	G
41	a	1583	A
41	a	1584	U
41	a	1585	C
41	a	1589	U
41	a	1590	A
41	a	1608	A
41	a	1610	A
41	a	1613	G
41	a	1647	U
41	a	1648	U
41	a	1649	G
41	a	1651	G
41	a	1665	A
41	a	1674	G
41	a	1677	A
41	a	1703	G
41	a	1714	U
41	a	1715	G
41	a	1729	U
41	a	1730	C
41	a	1732	C
41	a	1738	G
41	a	1750	G
41	a	1758	U
41	a	1764	C
41	a	1773	A
41	a	1791	A
41	a	1800	C
41	a	1808	A
41	a	1811	G
41	a	1816	C
41	a	1829	A
41	a	1833	C
41	a	1847	A
41	a	1848	A
41	a	1858	A

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Mol	Chain	Res	Type
41	a	1859	U
41	a	1862	G
41	a	1864	U
41	a	1869	G
41	a	1870	C
41	a	1872	A
41	a	1873	G
41	a	1906	G
41	a	1907	G
41	a	1913	A
41	a	1914	C
41	a	1919	A
41	a	1920	C
41	a	1922	G
41	a	1923	U
41	a	1924	C
41	a	1925	C
41	a	1926	U
41	a	1929	G
41	a	1930	G
41	a	1936	A
41	a	1938	A
41	a	1955	U
41	a	1965	C
41	a	1967	C
41	a	1970	A
41	a	1971	U
41	a	1972	G
41	a	1987	A
41	a	1991	U
41	a	1992	G
41	a	1993	U
41	a	1997	C
41	a	2002	G
41	a	2020	A
41	a	2022	U
41	a	2023	C
41	a	2027	G
41	a	2033	A
41	a	2043	C
41	a	2051	A
41	a	2052	A

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Mol	Chain	Res	Type
41	a	2055	C
41	a	2056	G
41	a	2060	A
41	a	2061	G
41	a	2062	A
41	a	2063	C
41	a	2097	A
41	a	2099	U
41	a	2100	G
41	a	2108	A
41	a	2110	G
41	a	2111	U
41	a	2113	U
41	a	2115	G
41	a	2116	G
41	a	2117	A
41	a	2118	U
41	a	2121	G
41	a	2122	U
41	a	2124	G
41	a	2125	G
41	a	2126	A
41	a	2127	G
41	a	2128	G
41	a	2131	U
41	a	2132	U
41	a	2133	G
41	a	2134	A
41	a	2139	U
41	a	2141	G
41	a	2146	C
41	a	2147	A
41	a	2154	A
41	a	2157	G
41	a	2158	A
41	a	2159	G
41	a	2162	G
41	a	2163	A
41	a	2164	C
41	a	2165	C
41	a	2169	A
41	a	2171	A

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Mol	Chain	Res	Type
41	a	2172	U
41	a	2178	C
41	a	2182	U
41	a	2183	A
41	a	2185	U
41	a	2189	U
41	a	2190	G
41	a	2193	G
41	a	2194	U
41	a	2198	A
41	a	2204	G
41	a	2211	A
41	a	2212	A
41	a	2225	A
41	a	2226	C
41	a	2229	U
41	a	2238	G
41	a	2239	G
41	a	2250	G
41	a	2268	A
41	a	2278	A
41	a	2283	C
41	a	2287	A
41	a	2288	A
41	a	2297	A
41	a	2305	U
41	a	2308	G
41	a	2309	A
41	a	2322	A
41	a	2325	G
41	a	2327	A
41	a	2333	A
41	a	2335	A
41	a	2339	C
41	a	2345	G
41	a	2347	C
41	a	2350	C
41	a	2361	G
41	a	2372	U
41	a	2376	A
41	a	2383	G
41	a	2385	C

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Mol	Chain	Res	Type
41	a	2402	U
41	a	2403	C
41	a	2406	A
41	a	2423	U
41	a	2424	C
41	a	2425	A
41	a	2426	A
41	a	2429	G
41	a	2430	A
41	a	2431	U
41	a	2434	A
41	a	2435	A
41	a	2441	U
41	a	2447	G
41	a	2448	A
41	a	2470	G
41	a	2474	U
41	a	2476	A
41	a	2478	A
41	a	2484	G
41	a	2491	U
41	a	2502	G
41	a	2506	U
41	a	2512	C
41	a	2513	A
41	a	2518	A
41	a	2520	C
41	a	2525	G
41	a	2529	G
41	a	2535	G
41	a	2554	U
41	a	2566	A
41	a	2567	G
41	a	2573	C
41	a	2574	G
41	a	2585	U
41	a	2586	U
41	a	2602	A
41	a	2603	G
41	a	2609	U
41	a	2610	C
41	a	2613	U

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Mol	Chain	Res	Type
41	a	2629	U
41	a	2630	G
41	a	2663	G
41	a	2669	G
41	a	2671	G
41	a	2689	U
41	a	2690	U
41	a	2714	G
41	a	2716	C
41	a	2726	A
41	a	2744	G
41	a	2748	A
41	a	2758	A
41	a	2765	A
41	a	2777	G
41	a	2778	A
41	a	2791	G
41	a	2793	C
41	a	2796	U
41	a	2797	U
41	a	2798	U
41	a	2799	A
41	a	2801	G
41	a	2818	U
41	a	2820	A
41	a	2823	A
41	a	2825	G
41	a	2835	A
41	a	2849	U
41	a	2859	G
41	a	2861	U
41	a	2867	G
41	a	2873	A
41	a	2874	C
41	a	2880	C
41	a	2883	A
41	a	2884	U
41	a	2885	G
41	a	2891	U
41	a	2902	C
44	d	2	G
44	d	13	G

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Mol	Chain	Res	Type
44	d	16	G
44	d	17	C
44	d	35	C
44	d	45	A
44	d	51	G
44	d	56	G
44	d	57	A
44	d	66	A
44	d	88	C
44	d	89	U
44	d	90	C
44	d	99	A
44	d	109	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	4	U
8	7	7	U
8	7	10	U
8	7	18	U
8	7	27	G
10	A	6	G
10	A	7	G
10	A	9	G
10	A	12	G
10	A	21	A
10	A	22	G
10	A	57	A
10	A	60	U
10	B	6	G
10	B	7	G
10	B	9	G
10	B	12	G
10	B	21	A
10	B	22	G
10	B	57	A
10	B	60	U
18	D	121	U
18	D	181	A
18	D	183	C
18	D	197	A

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Mol	Chain	Res	Type
18	D	209	U
18	D	428	G
18	D	496	A
18	D	517	G
18	D	991	U
18	D	992	U
18	D	1145	A
18	D	1196	A
18	D	1211	U
18	D	1212	U
18	D	1213	A
18	D	1214	C
18	D	1447	A
18	D	1491	G
18	D	1492	A
18	D	1493	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

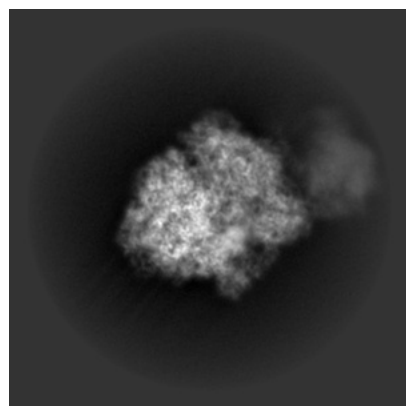
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42479. These allow visual inspection of the internal detail of the map and identification of artifacts.

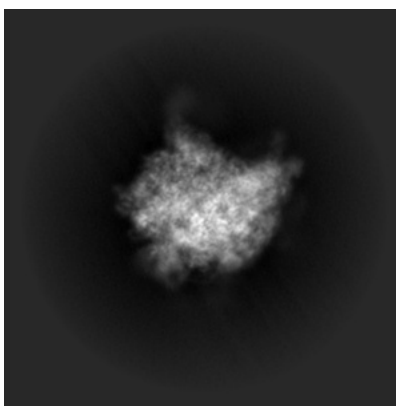
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

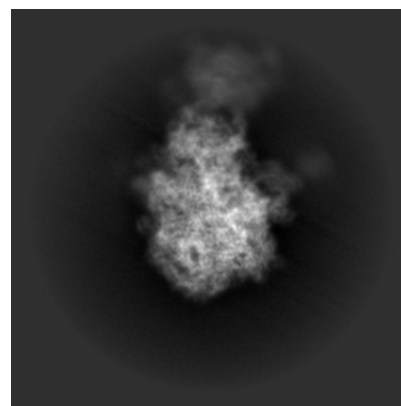
6.1.1 Primary map



X



Y

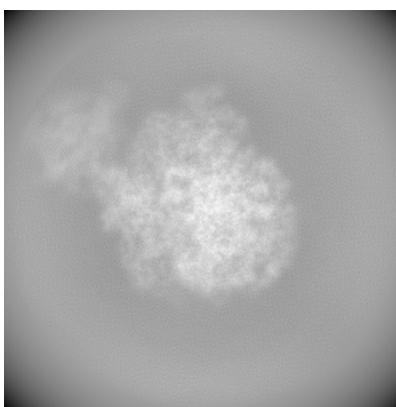


Z

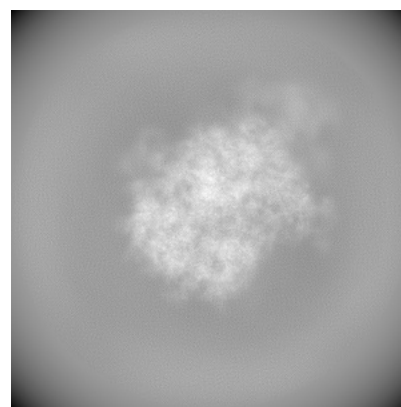
6.1.2 Raw map



X



Y

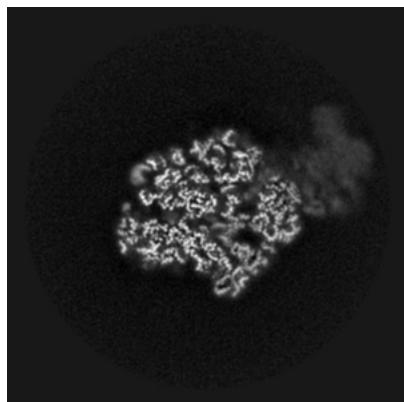


Z

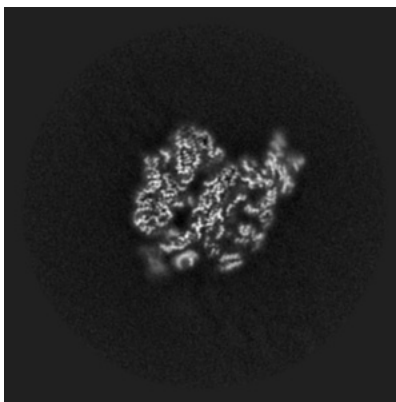
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

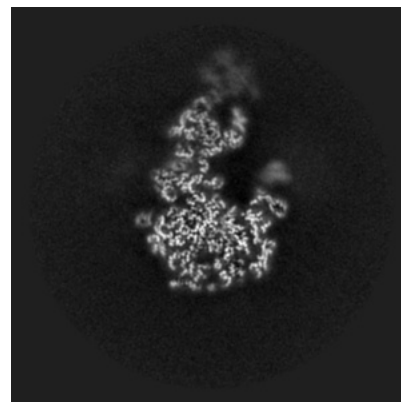
6.2.1 Primary map



X Index: 256

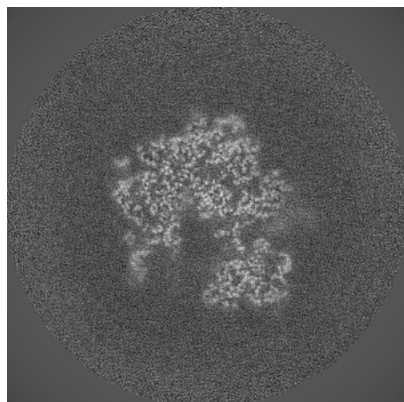


Y Index: 256

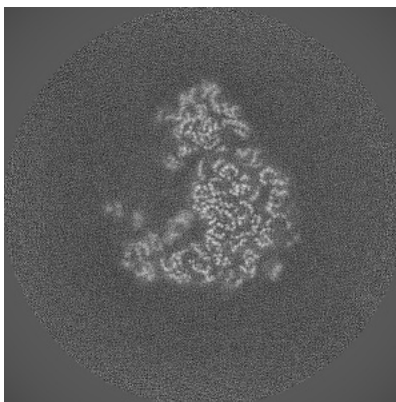


Z Index: 256

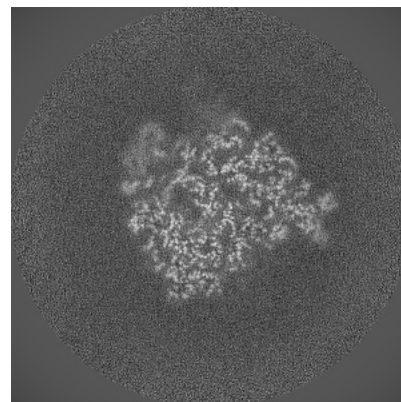
6.2.2 Raw map



X Index: 288



Y Index: 288

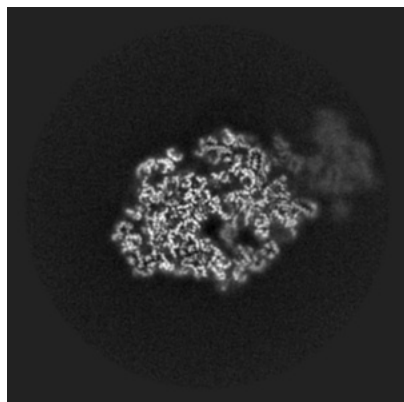


Z Index: 288

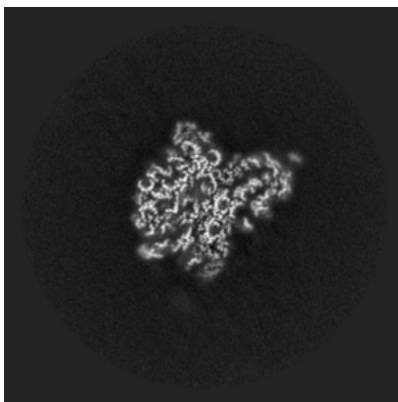
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

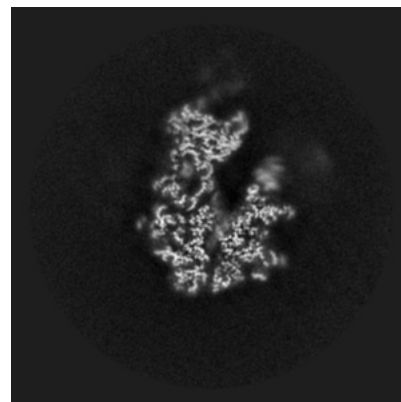
6.3.1 Primary map



X Index: 245

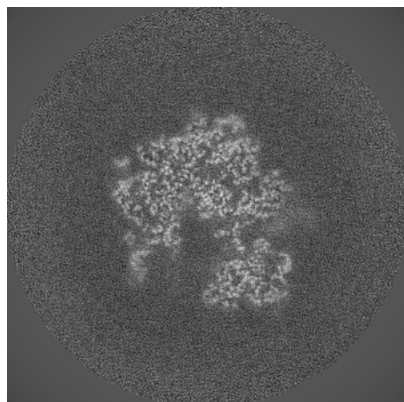


Y Index: 246

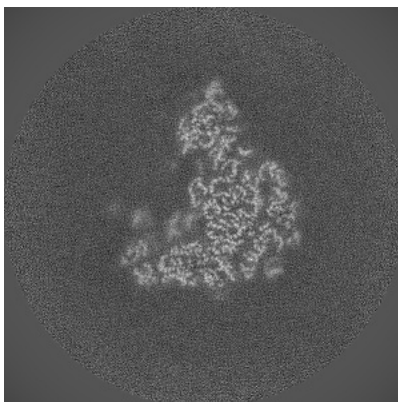


Z Index: 243

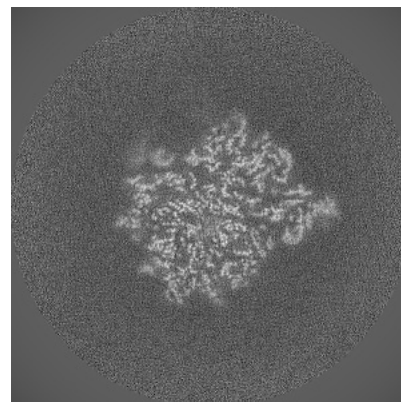
6.3.2 Raw map



X Index: 288



Y Index: 281

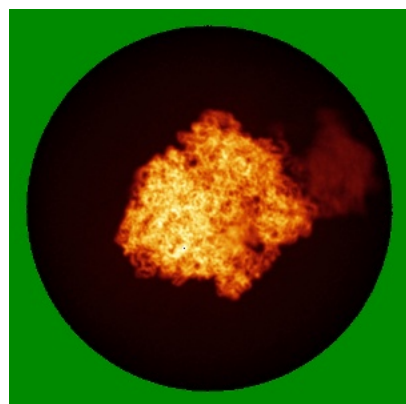


Z Index: 300

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

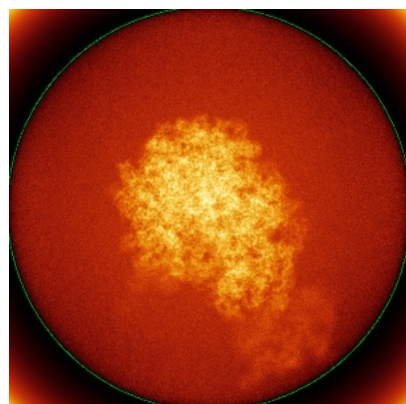


Y

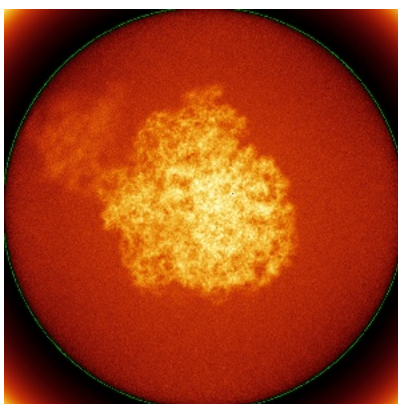


Z

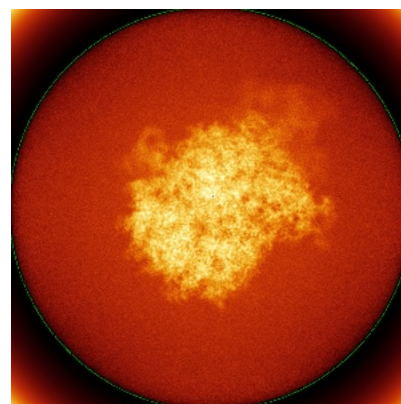
6.4.2 Raw map



X



Y

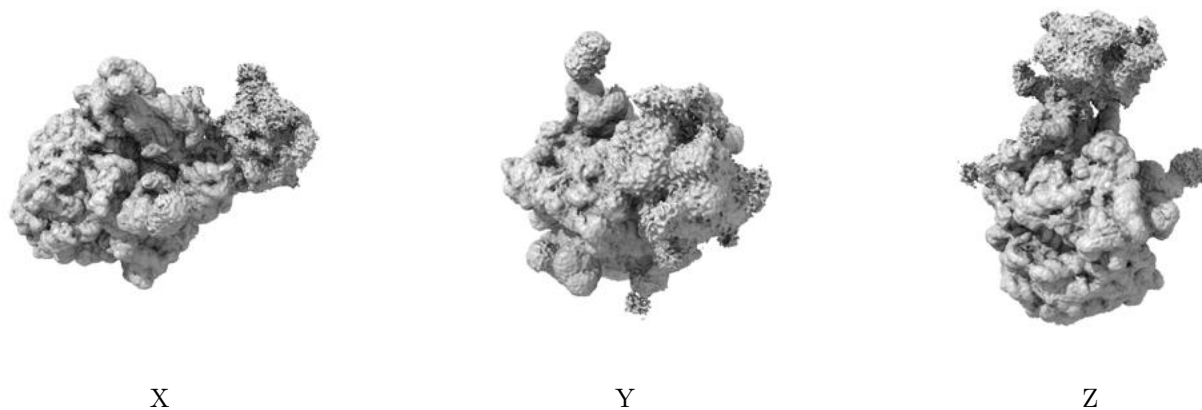


Z

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.

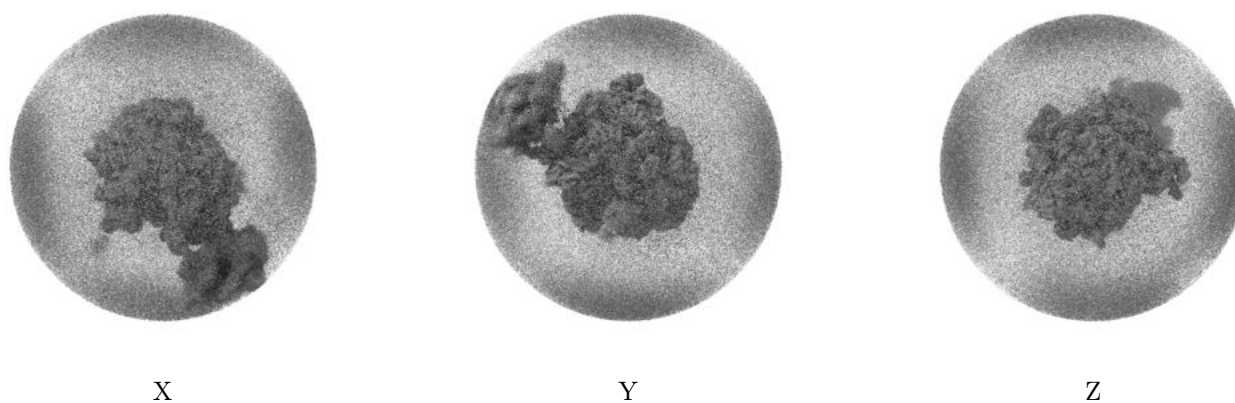
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0017. 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.

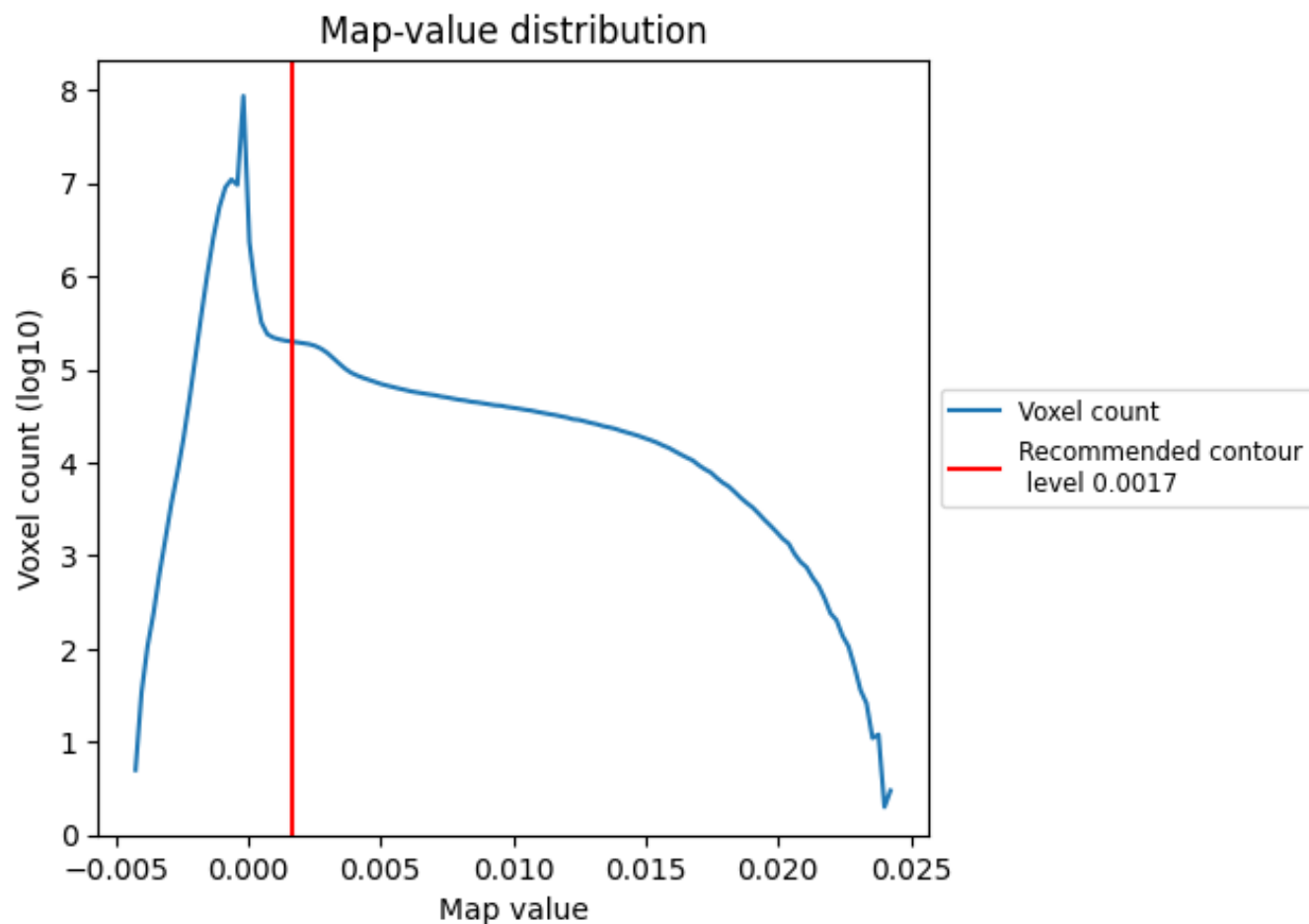
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

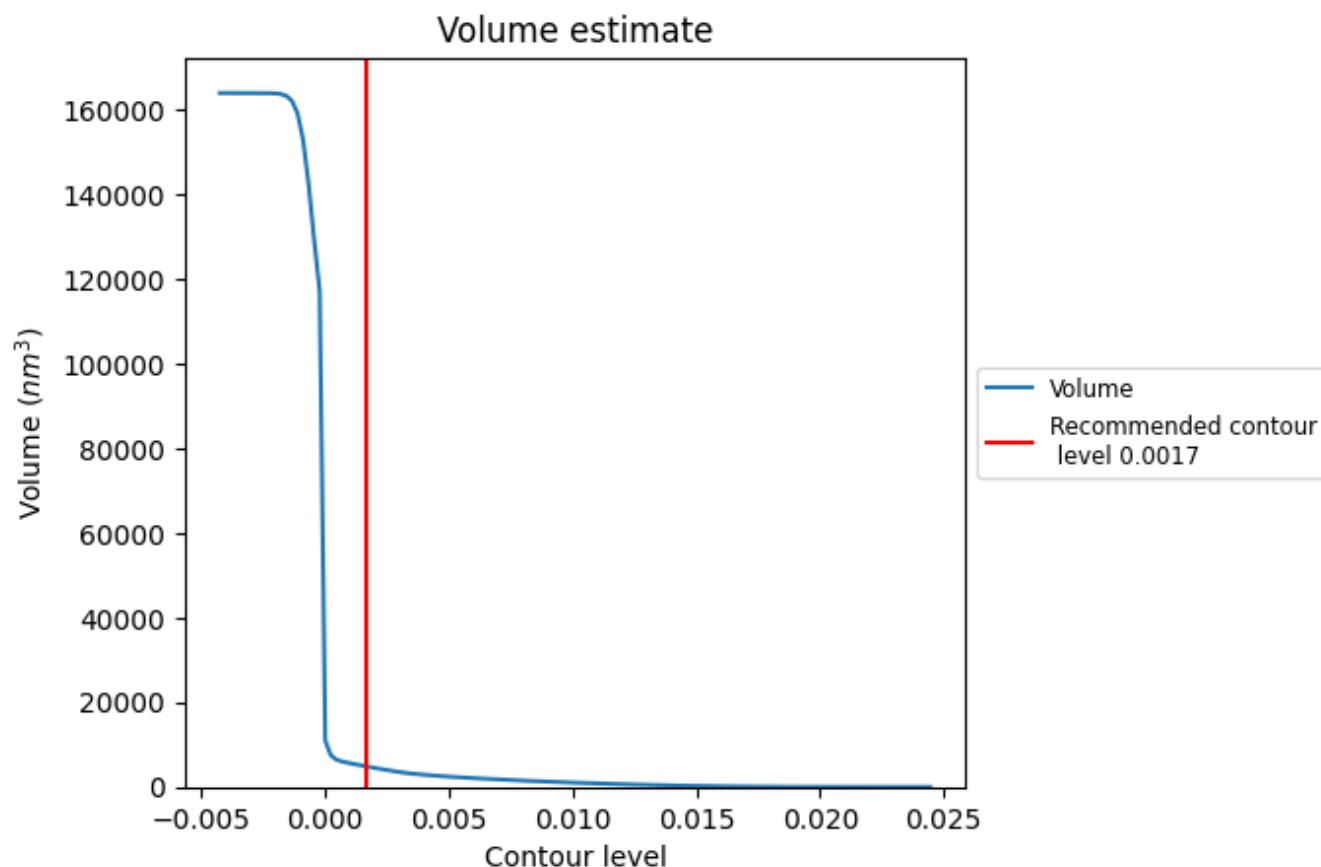
This section contains the results of statistical analysis of the map.

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.

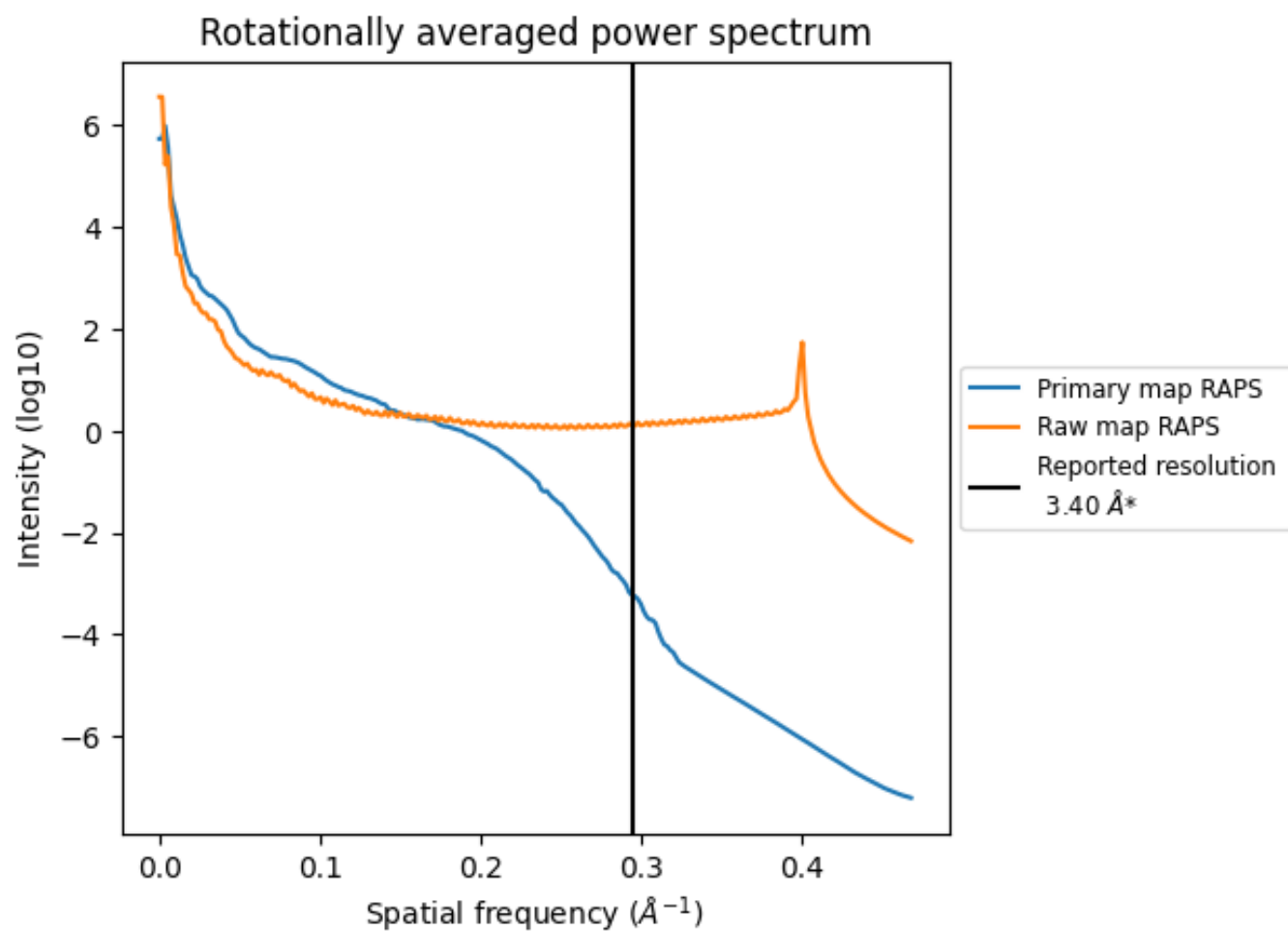
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4832 nm³; this corresponds to an approximate mass of 4365 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 ⓘ

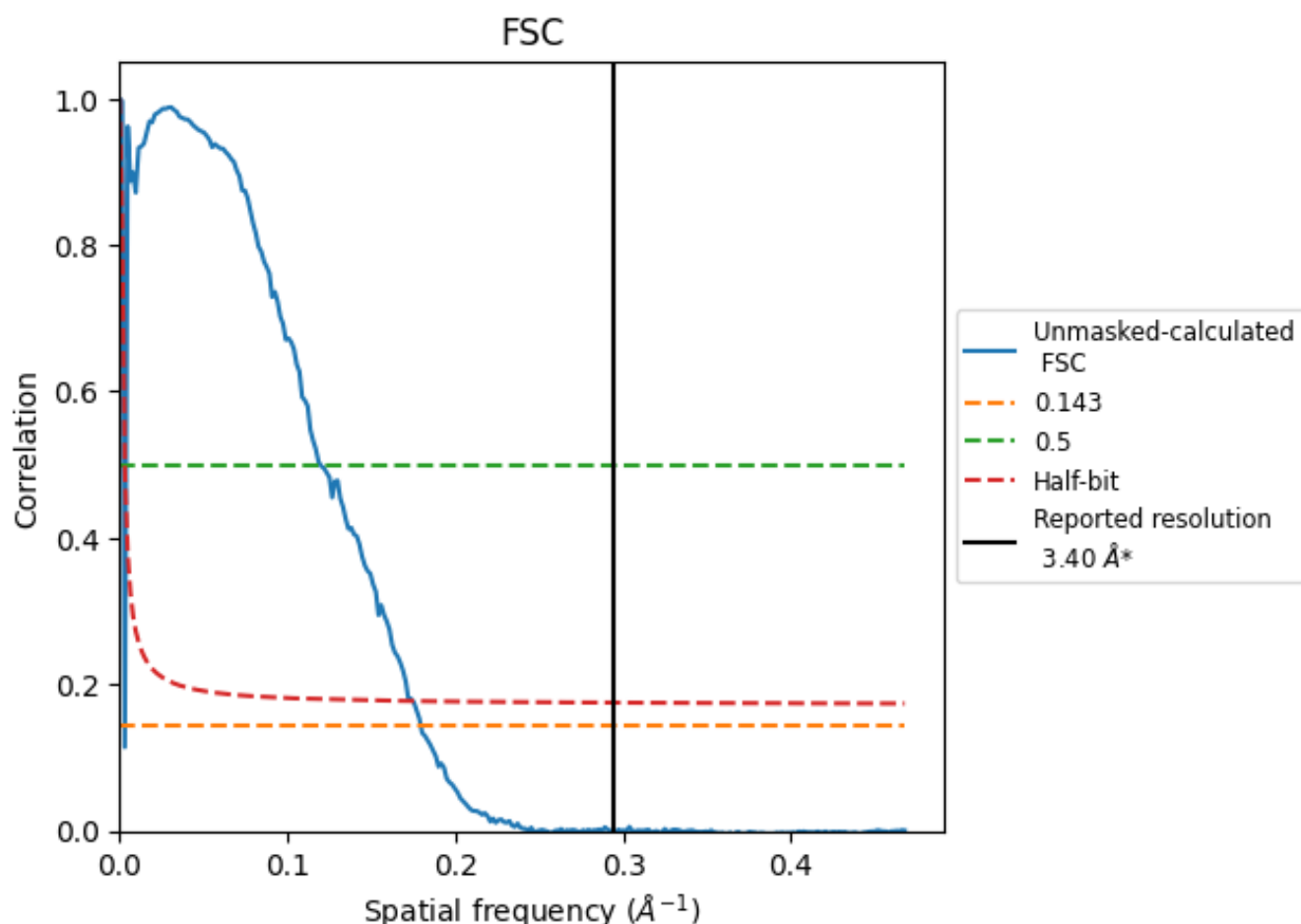


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

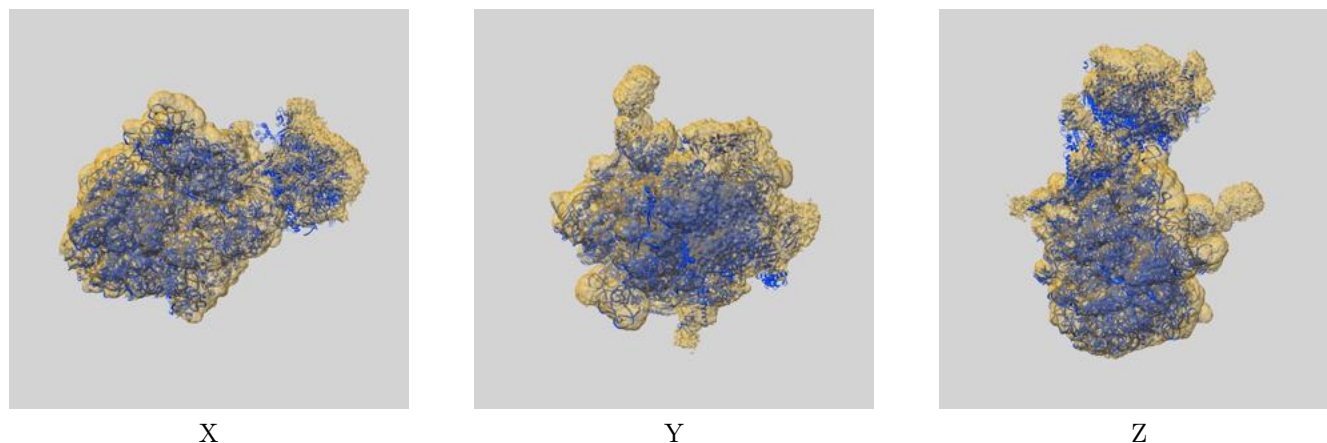
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	312.50	400.00	476.19

*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 312.50 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

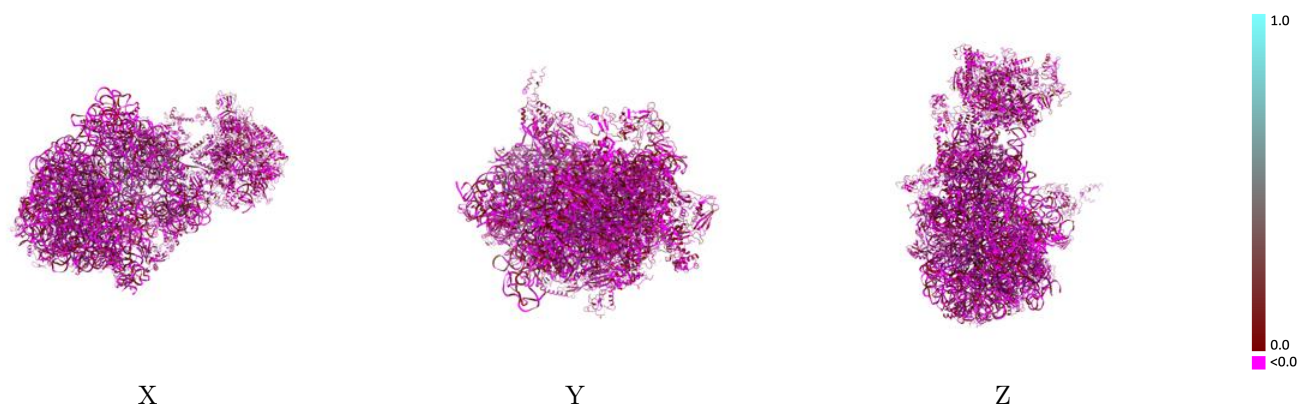
This section contains information regarding the fit between EMDB map EMD-42479 and PDB model 8UR0. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



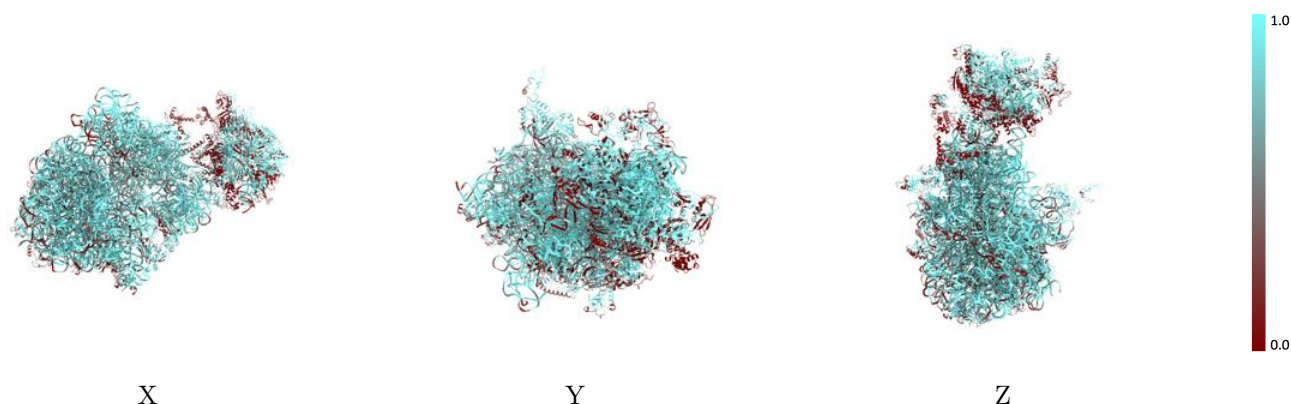
The images above show the 3D surface view of the map at the recommended contour level 0.0017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



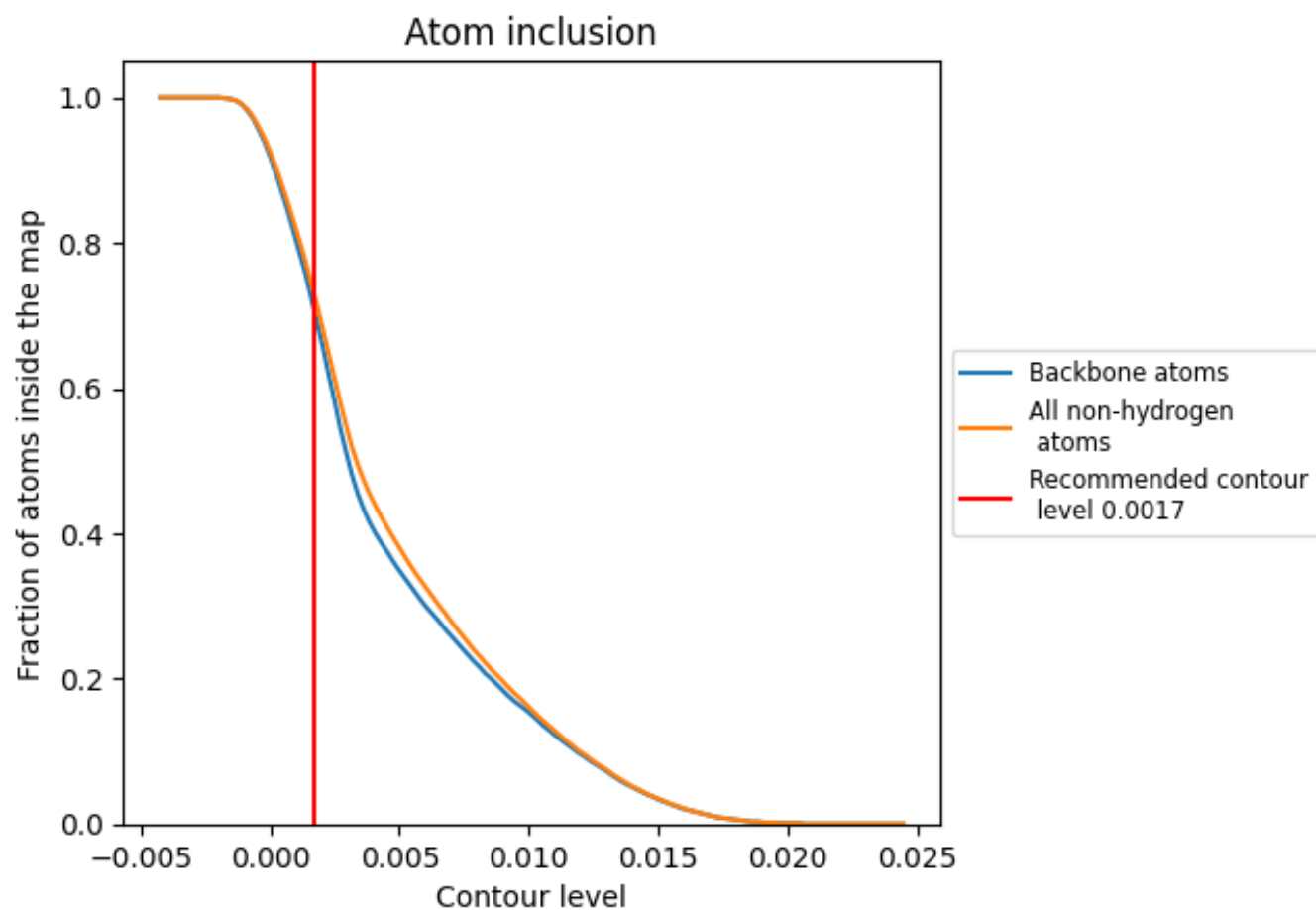
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0017).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



































































The table lists the average atom inclusion at the recommended contour level (0.0017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7300	 -0.0190
0	 0.5720	 0.0060
1	 0.7340	 -0.0160
2	 0.8780	 -0.0080
3	 0.6240	 -0.0180
4	 0.7520	 -0.0120
5	 0.5790	 0.0040
6	 0.6440	 -0.0190
7	 0.7970	 -0.0060
9	 0.8550	 0.0110
A	 0.8820	 0.0170
AA	 0.6580	 -0.0020
AB	 0.4930	 -0.0040
AC	 0.3820	 0.0060
AD	 0.2530	 0.0050
AE	 0.5830	 0.0040
AF	 0.3960	 0.0070
AG	 0.3200	 -0.0070
B	 0.5800	 -0.0370
C	 0.8030	 -0.0220
D	 0.8270	 -0.0270
E	 0.6650	 -0.0280
F	 0.7530	 -0.0110
G	 0.8500	 -0.0090
H	 0.7140	 -0.0020
I	 0.9130	 -0.0060
J	 0.9270	 -0.0050
K	 0.8540	 -0.0240
L	 0.5150	 -0.0420
M	 0.5780	 -0.0190
N	 0.8520	 -0.0460
O	 0.6890	 -0.0110
P	 0.9690	 -0.0120
Q	 0.7580	 -0.0340
R	 0.7520	 0.0040



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Chain	Atom inclusion	Q-score
S	 0.9690	 -0.0360
T	 0.5220	 -0.0290
U	 0.9070	 -0.0210
V	 0.5650	 -0.0180
W	 0.6630	 -0.0130
X	 0.5350	 -0.0430
Y	 0.8710	 0.0130
Z	 0.5680	 -0.0100
a	 0.7970	 -0.0270
b	 0.7170	 -0.0100
c	 0.5320	 -0.0370
d	 0.8140	 -0.0140
e	 0.5670	 -0.0580
f	 0.6950	 0.0120
g	 0.6670	 -0.0170
h	 0.7890	 -0.0330
i	 0.5790	 -0.0310
j	 0.8850	 -0.0290
k	 0.7110	 -0.0250
l	 0.6330	 -0.0120
m	 0.8540	 -0.0420
n	 0.7420	 -0.0340
o	 0.8660	 -0.0390
p	 0.7650	 -0.0170
q	 0.9900	 0.0020
r	 0.6030	 0.0110
s	 0.8790	 -0.0200
t	 0.8830	 -0.0030
u	 0.6950	 -0.0270
v	 0.9090	 -0.0390
w	 0.8580	 -0.0180
x	 0.5550	 -0.0090
y	 0.8480	 -0.0460
z	 0.8470	 -0.0100