



Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 03:52 pm BST

PDB ID : 8R55
EMDB ID : EMD-18901
Title : Bacillus subtilis MutS2-collided disome complex (collided 70S)
Authors : Park, E.; Mackens-Kiani, T.; Berhane, R.; Esser, H.; Erdenebat, C.; Burroughs, A.M.; Berninghausen, O.; Aravind, L.; Beckmann, R.; Green, R.; Buskirk, A.R.
Deposited on : 2023-11-16
Resolution : 3.57 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) : 2.39

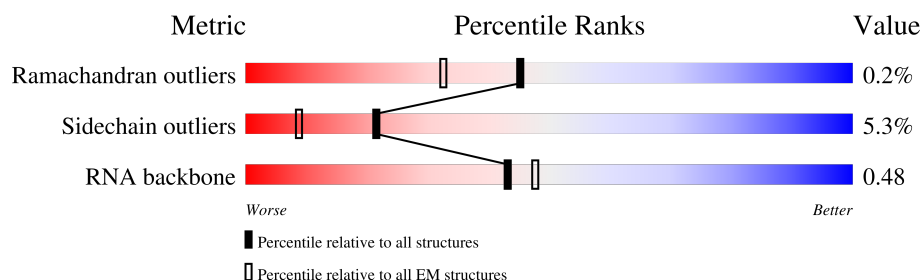
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.57 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	59	
2	1	48	
3	2	44	
4	3	66	
5	4	37	
6	6	64	
7	7	73	
8	A	1533	

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Mol	Chain	Length	Quality of chain
9	B	246	
10	C	218	
11	D	200	
12	E	166	
13	F	95	
14	G	156	
15	H	132	
16	I	130	
17	J	102	
18	K	131	
19	L	138	
20	M	121	
21	N	61	
22	O	89	
23	P	90	
24	Q	87	
25	R	79	
26	S	92	
27	T	88	
28	U	77	
29	V	33	
30	Y	112	
31	Z	275	
32	a	207	
33	b	205	

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Mol	Chain	Length	Quality of chain
34	c	178	
35	d	175	
36	e	142	
37	f	122	
38	i	146	
39	j	138	
40	k	119	
41	l	120	
42	m	115	
43	n	117	
44	o	101	
45	r	109	
46	s	93	
47	t	101	
48	u	82	
49	v	58	
50	w	65	
51	x	58	
52	X	2928	
53	z	785	

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 143867 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 2 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			402	244	80	74	4		

- Molecule 3 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	48	SER	ALA	conflict	UNP A0A063XFQ7

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 6 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	63	Total	C	N	O	S	0	0
			499	312	91	91	5		

- Molecule 7 is a RNA chain called tRNA (73-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	73	Total	C	N	O	P	0	0
			1560	695	279	513	73		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	3	G	C	conflict	GB 1851743410
7	70	C	G	conflict	GB 1851743410

- Molecule 8 is a RNA chain called 16S rRNA (1533-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	1533	Total	C	N	O	P	0	0
			32891	14667	6034	10657	1533		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	218	Total	C	N	O	S	0	0
			1757	1119	309	323	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	206	Total	C	N	O	S	0	0
			1619	1011	304	301	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	195	Total	C	N	O	S	0	0
			1569	991	291	285	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	164	Total	C	N	O	S	0	0
			1219	767	225	225	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	92	Total	C	N	O	S	0	0
			755	476	132	146	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	149	Total	C	N	O	S	0	0
			1181	740	220	215	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	131	Total	C	N	O	S	0	0
			1037	655	191	188	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	125	Total	C	N	O	S	0	0
			966	599	191	175	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	95	Total	C	N	O	S	0	0
			761	479	139	141	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	114	Total	C	N	O	S	0	0
			839	516	164	157	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	136	Total	C	N	O	S	0	0
			1052	653	211	186	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	108	Total	C	N	O	S	0	0
			868	534	176	158			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	60	Total	C	N	O	S	0	0
			498	317	98	78	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	85	Total	C	N	O	S	0	0
			710	436	144	129	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	88	Total	C	N	O	S	0	0
			695	441	128	124	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	84	Total	C	N	O	S	0	0
			691	435	128	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	64	Total	C	N	O	S	0	0
			518	332	96	88	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	78	Total	C	N	O	S	0	0
			633	409	112	110	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	83	Total	C	N	O	S	0	0
			637	390	130	116	1		

- Molecule 28 is a RNA chain called tRNA (77-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	77	Total	C	N	O	P	0	0
			1643	731	290	545	77		

- Molecule 29 is a RNA chain called mRNA (33-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	33	Total	C	N	O	P	0	0
			704	315	130	226	33		

- Molecule 30 is a RNA chain called 5S rRNA (112-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 31 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

- Molecule 32 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	205	Total	C	N	O	S	0	0
			1562	980	289	291	2		

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	176	Total	C	N	O	S	0	0
			1386	882	241	256	7		

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	175	Total	C	N	O	S	0	0
			1343	835	248	258	2		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	142	Total	C	N	O	S	0	0
			1124	710	206	203	5		

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	119	Total	C	N	O	S	0	0
			954	583	186	181	4		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	120	Total	C	N	O	S	0	0
			913	564	176	172	1		

- Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	115	Total	C	N	O	S	0	0
			945	600	185	159	1		

- Molecule 43 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	117	Total	C	N	O	S	0	0
			941	591	189	157	4		

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	101	Total	C	N	O	S	0	0
			787	501	139	147			

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	109	Total	C	N	O	S	0	0
			843	525	164	151	3		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	101	Total	C	N	O	S	0	0
			763	478	142	139	4		

- Molecule 48 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	82	Total	C	N	O		0	0
			631	390	123	118			

- Molecule 49 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	58	Total	C	N	O	S	0	0
			445	275	92	76	2		

- Molecule 50 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	65	Total	C	N	O	S	0	0
			531	328	102	99	2		

- Molecule 51 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	58	Total	C	N	O	S	0	0
			456	281	89	85	1		

- Molecule 52 is a RNA chain called 23S RNA (2887-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
52	X	2887	Total	C	N	O	P	0	0
			62005	27661	11460	19998	2886		

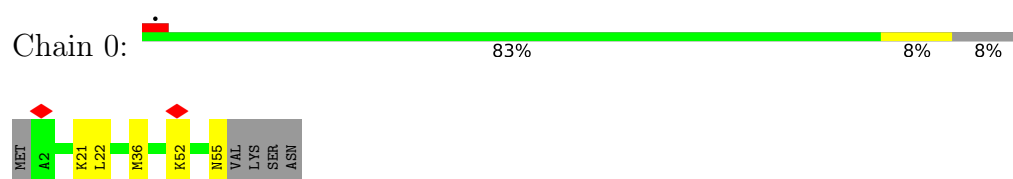
- Molecule 53 is a protein called Endonuclease MutS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	139	Total	C	N	O	S	0	0
			1083	683	195	204	1		

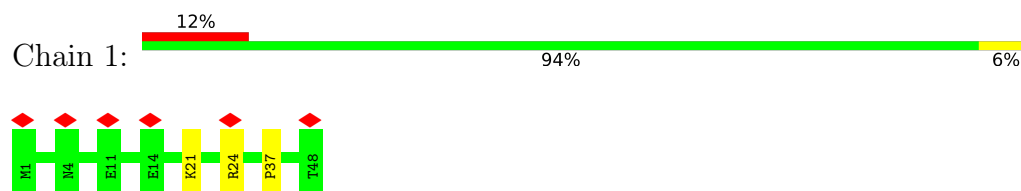
3 Residue-property plots [i](#)

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

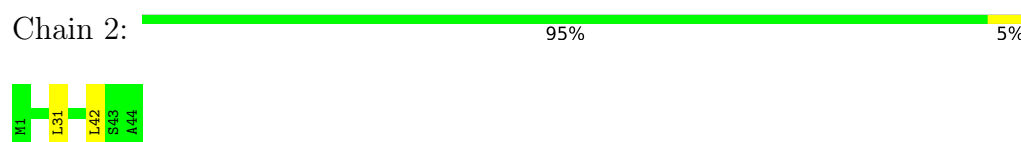
- Molecule 1: 50S ribosomal protein L32



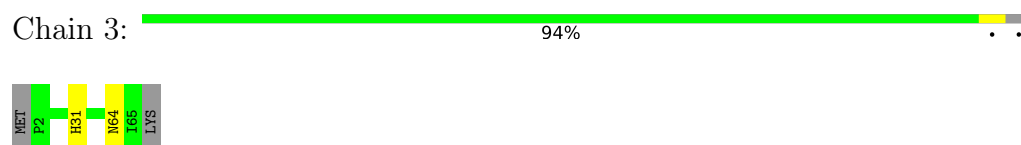
- Molecule 2: Large ribosomal subunit protein bL33



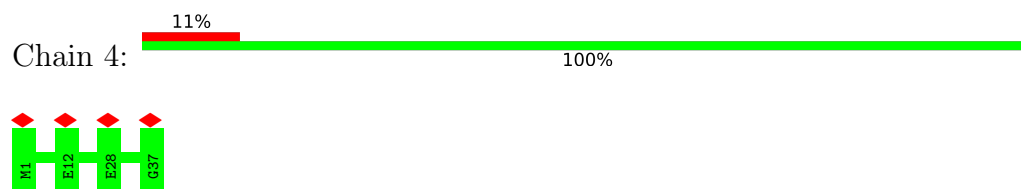
- Molecule 3: Large ribosomal subunit protein bL34



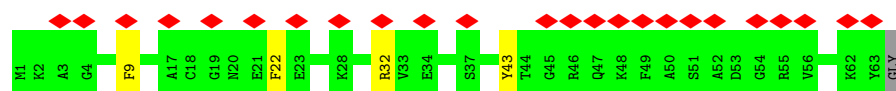
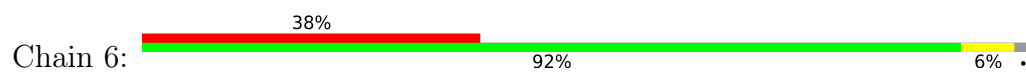
- Molecule 4: Large ribosomal subunit protein bL35



- Molecule 5: 50S ribosomal protein L36



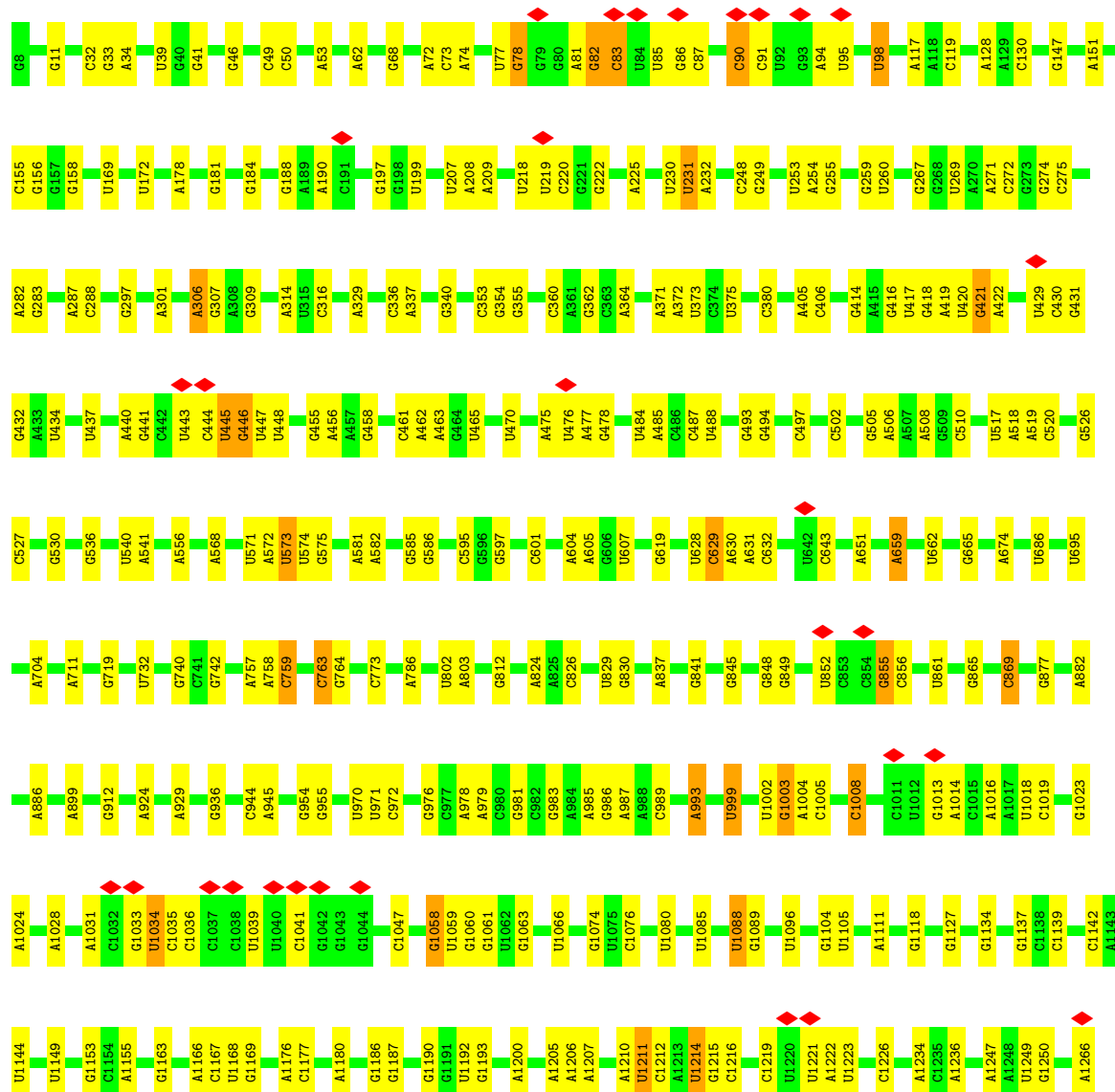
- Molecule 6: Large ribosomal subunit protein bL31



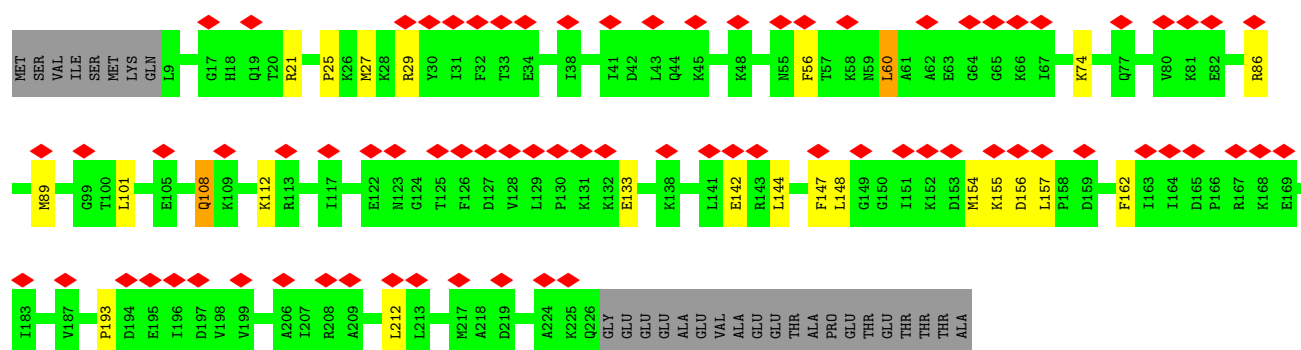
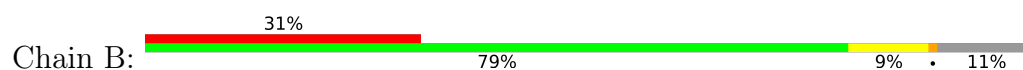
• Molecule 7: tRNA (73-MER)



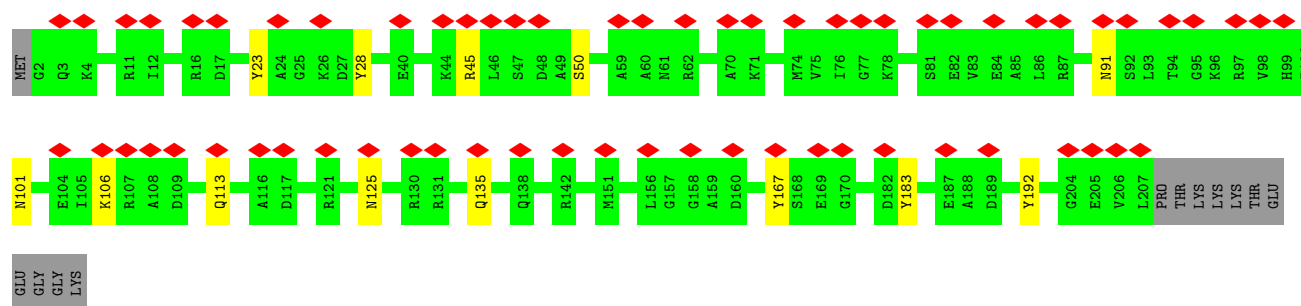
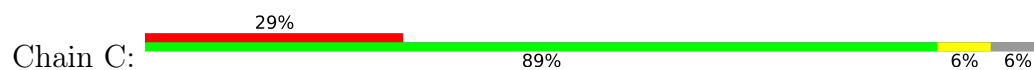
• Molecule 8: 16S rRNA (1533-MER)



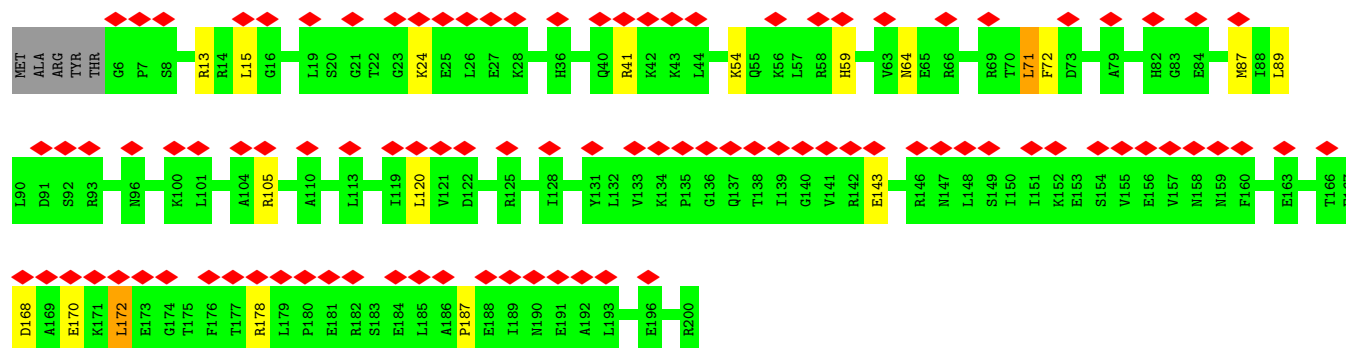
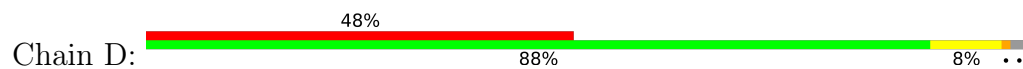
- Molecule 9: 30S ribosomal protein S2



- Molecule 10: 30S ribosomal protein S3

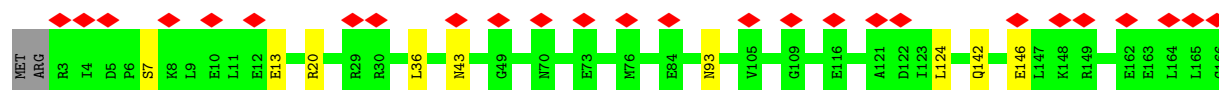


- Molecule 11: 30S ribosomal protein S4



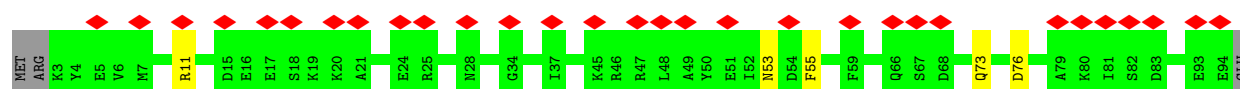
- Molecule 12: 30S ribosomal protein S5

Chain E: 




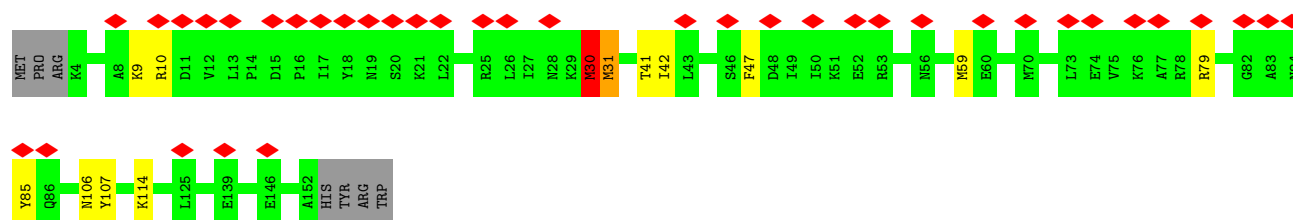
- Molecule 13: 30S ribosomal protein S6

Chain F: 



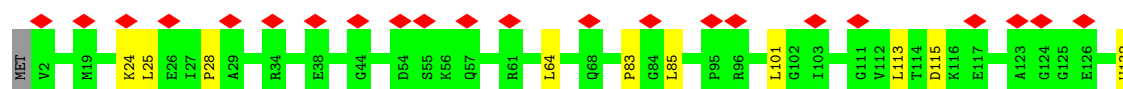
- Molecule 14: 30S ribosomal protein S7

Chain G: 




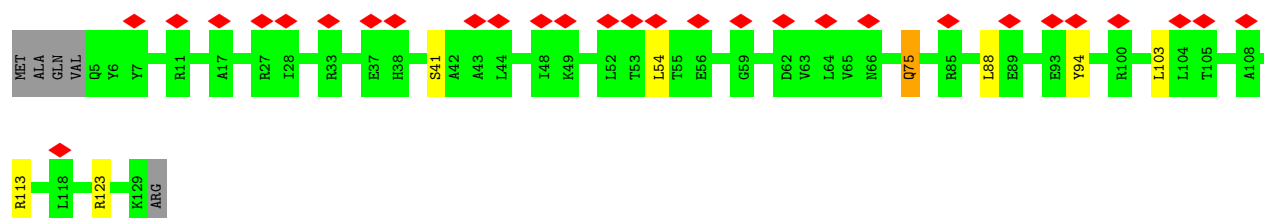
- Molecule 15: 30S ribosomal protein S8

Chain H: 




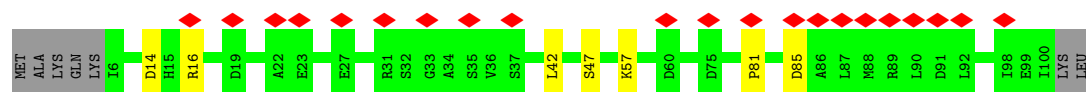
- Molecule 16: 30S ribosomal protein S9

Chain I: 

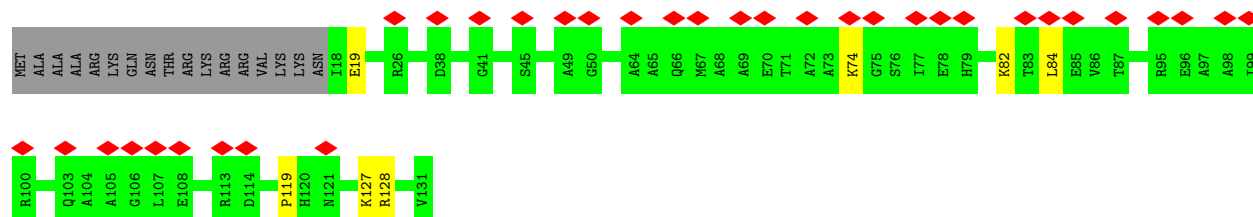
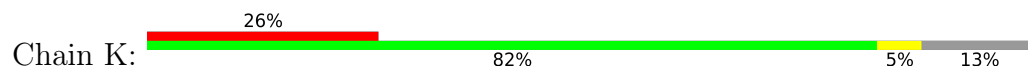


- Molecule 17: 30S ribosomal protein S10

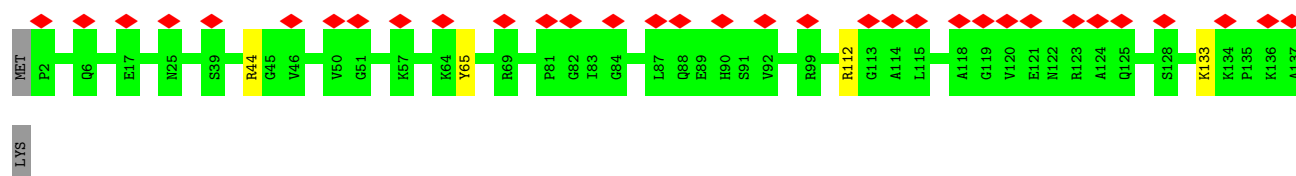
Chain J: 



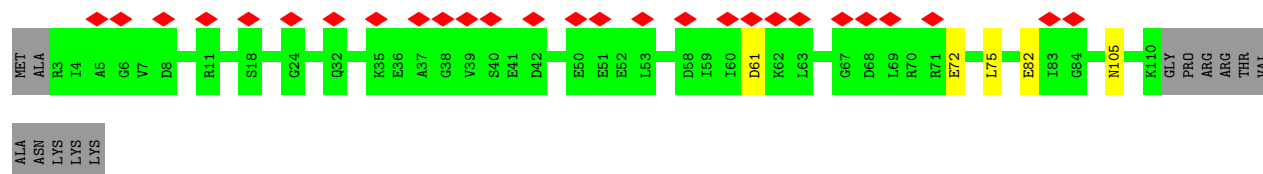
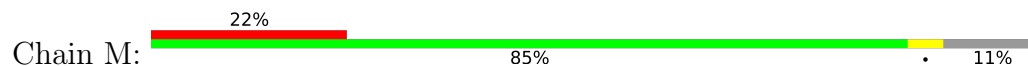
- Molecule 18: 30S ribosomal protein S11



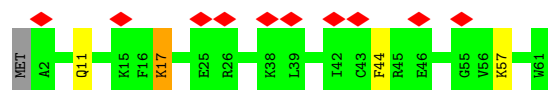
- Molecule 19: 30S ribosomal protein S12



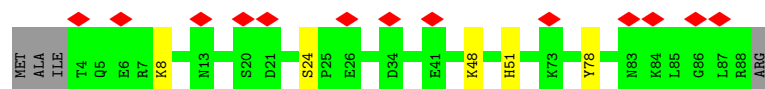
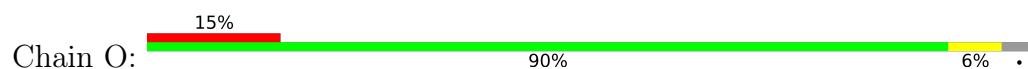
- Molecule 20: 30S ribosomal protein S13



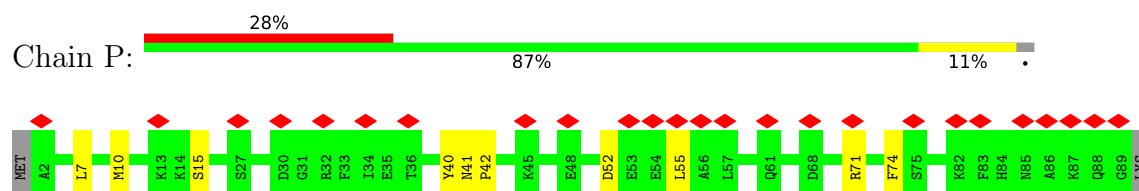
- Molecule 21: 30S ribosomal protein S14 type Z



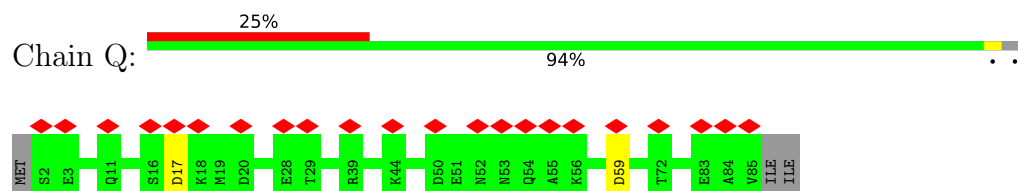
- Molecule 22: 30S ribosomal protein S15



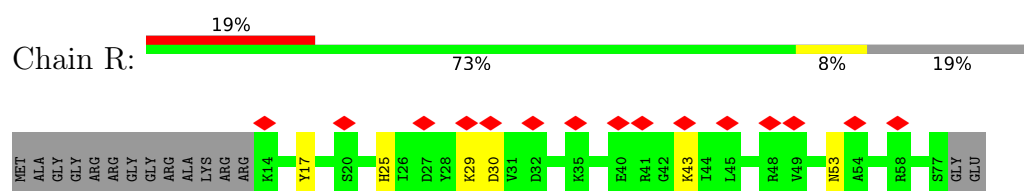
- Molecule 23: 30S ribosomal protein S16



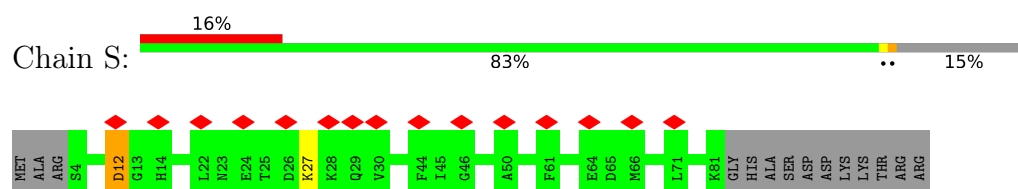
- Molecule 24: 30S ribosomal protein S17



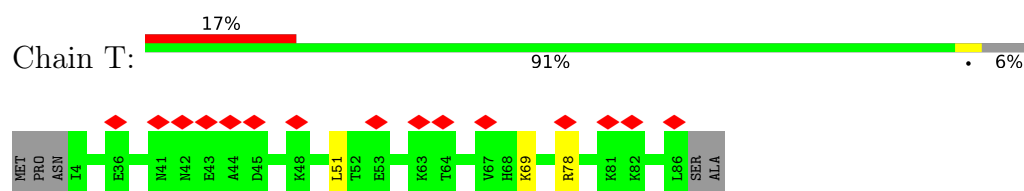
- Molecule 25: 30S ribosomal protein S18



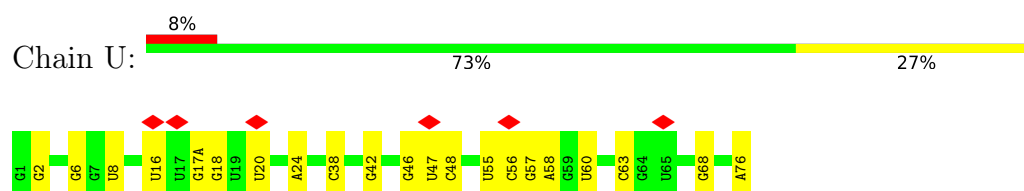
- Molecule 26: 30S ribosomal protein S19



- Molecule 27: 30S ribosomal protein S20



- Molecule 28: tRNA (77-MER)

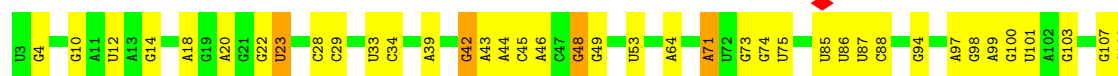


- Molecule 29: mRNA (33-MER)

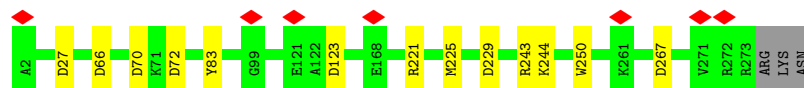




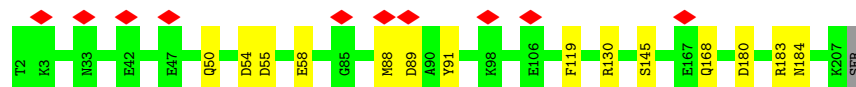
• Molecule 30: 5S rRNA (112-MER)



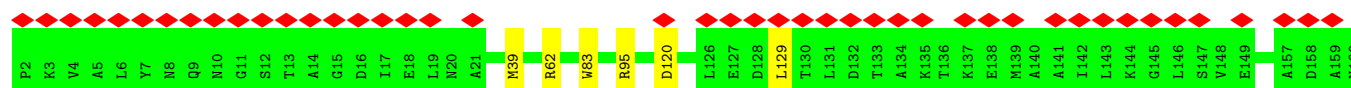
• Molecule 31: Large ribosomal subunit protein uL2



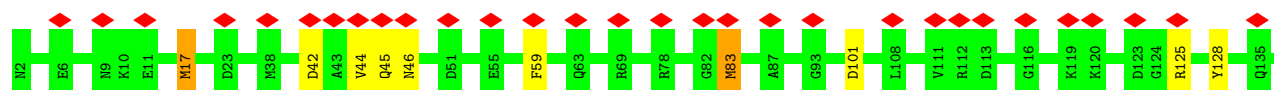
• Molecule 32: Large ribosomal subunit protein uL3

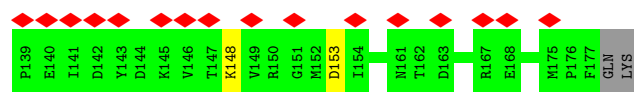


• Molecule 33: Large ribosomal subunit protein uL4

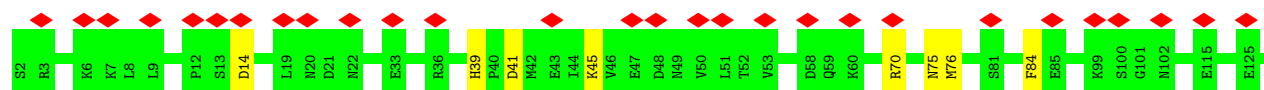


• Molecule 34: Large ribosomal subunit protein uL5

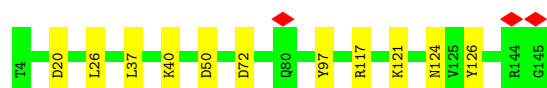
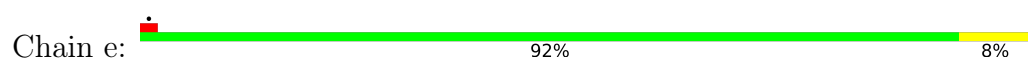




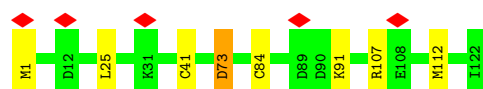
- Molecule 35: Large ribosomal subunit protein uL6



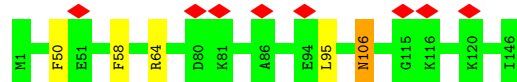
- Molecule 36: Large ribosomal subunit protein uL13



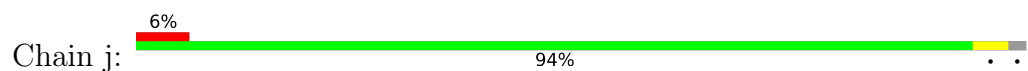
- Molecule 37: 50S ribosomal protein L14



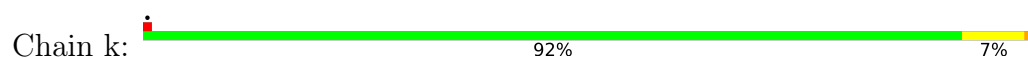
- Molecule 38: 50S ribosomal protein L15



- Molecule 39: Large ribosomal subunit protein uL16

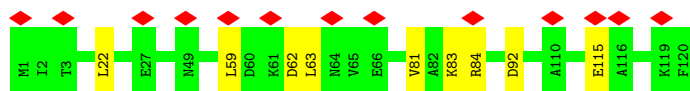
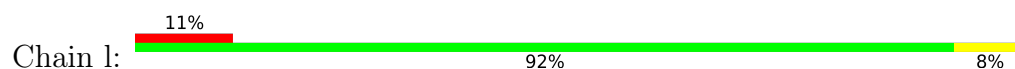


- Molecule 40: Large ribosomal subunit protein bL17

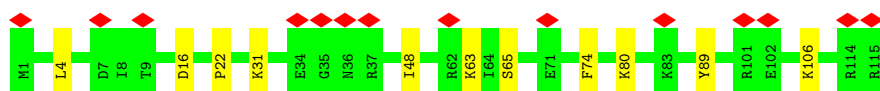




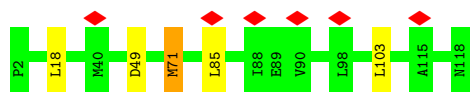
- Molecule 41: 50S ribosomal protein L18



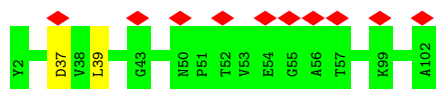
- Molecule 42: 50S ribosomal protein L19



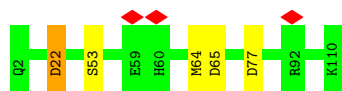
- Molecule 43: Large ribosomal subunit protein bL20



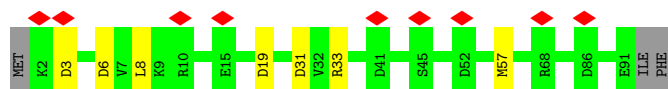
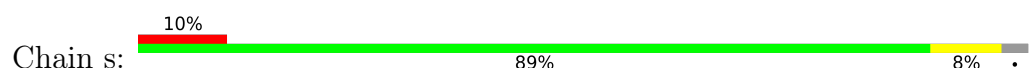
- Molecule 44: Large ribosomal subunit protein bL21



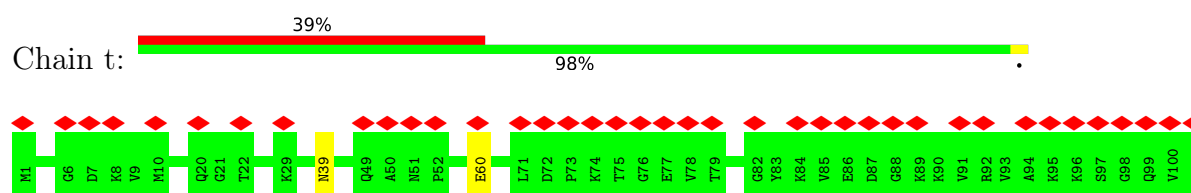
- Molecule 45: Large ribosomal subunit protein uL22



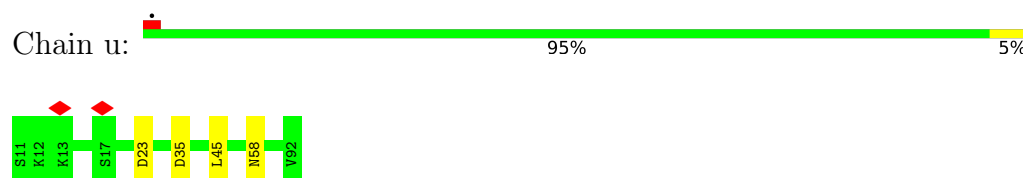
- Molecule 46: Large ribosomal subunit protein uL23



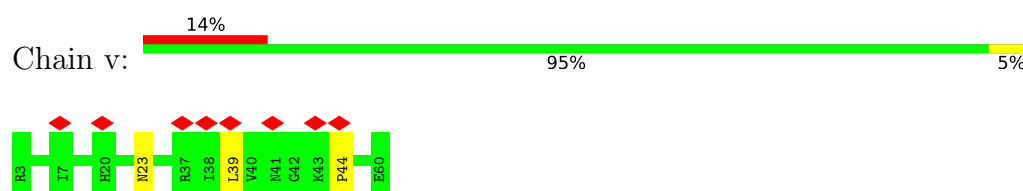
- Molecule 47: Large ribosomal subunit protein uL24



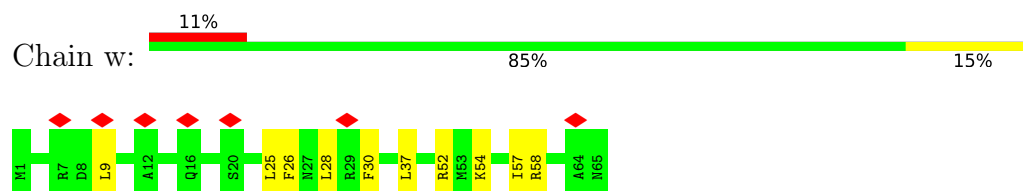
- Molecule 48: Large ribosomal subunit protein bL27



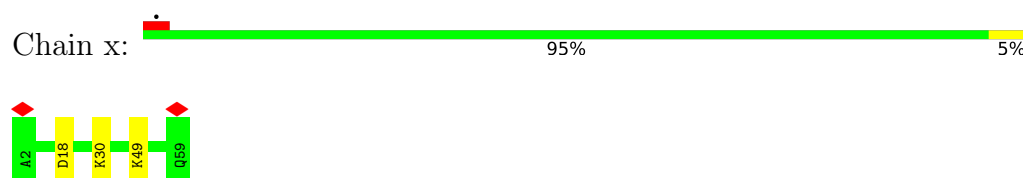
- Molecule 49: Large ribosomal subunit protein bL28



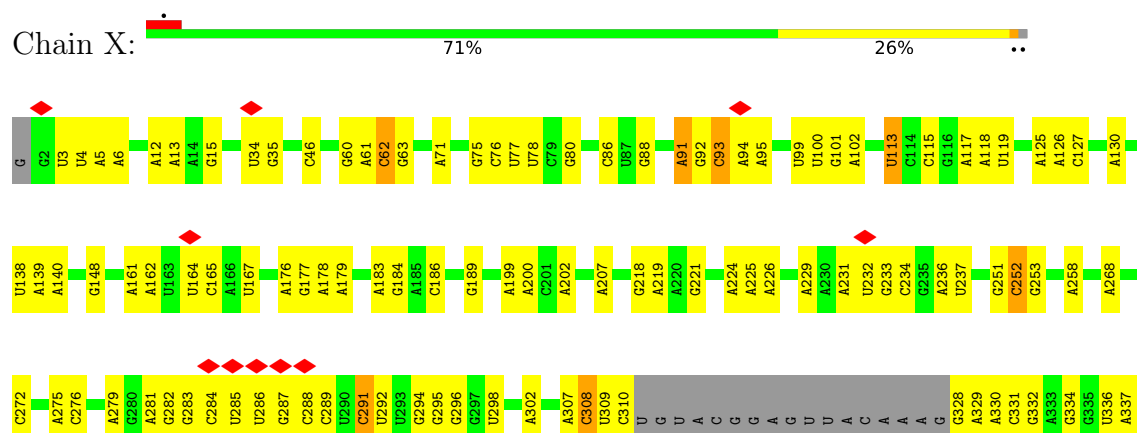
- Molecule 50: Large ribosomal subunit protein uL29

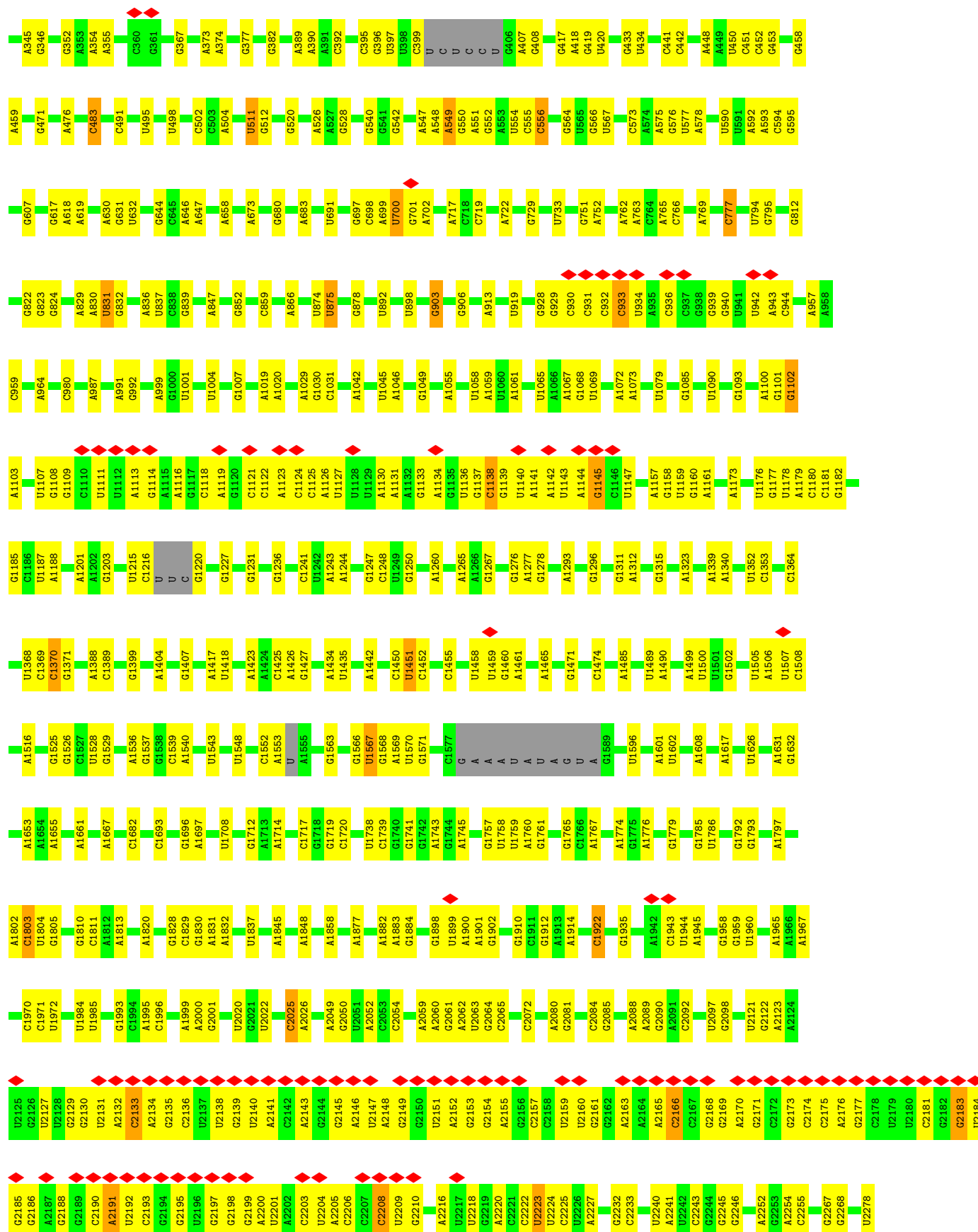


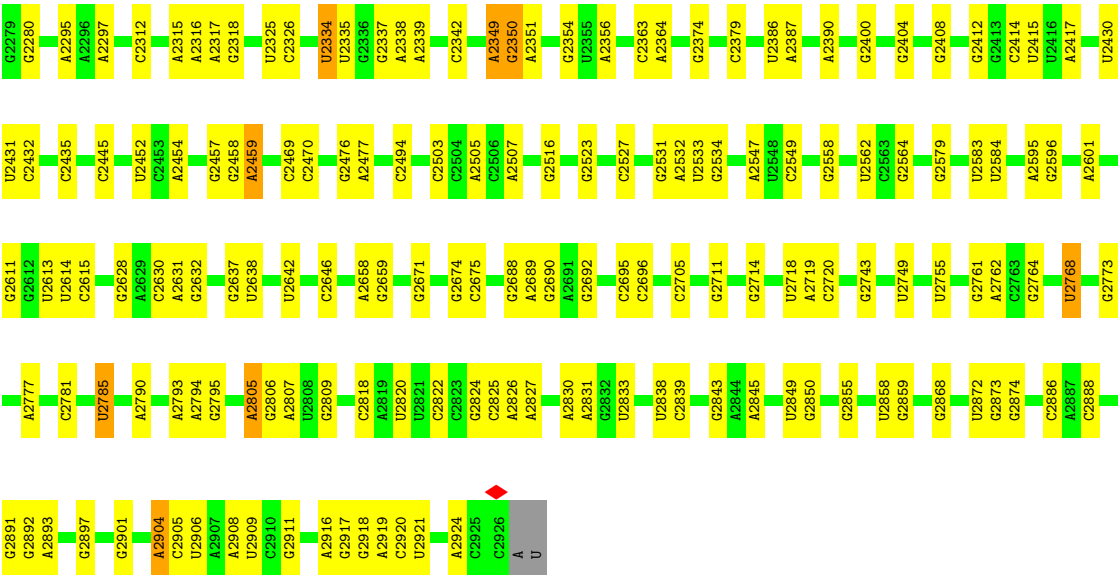
- Molecule 51: Large ribosomal subunit protein uL30



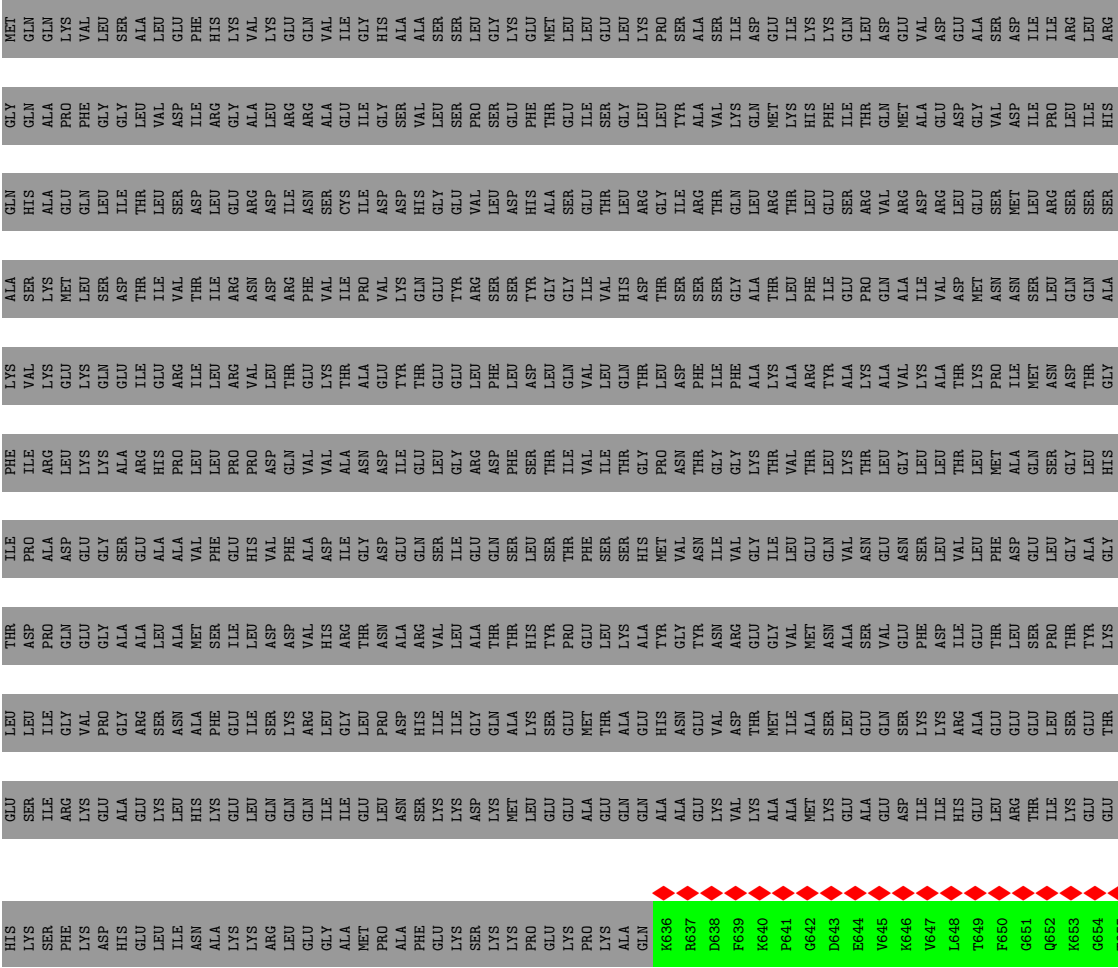
- Molecule 52: 23S RNA (2887-MER)







● Molecule 53: Endonuclease MutS2



	V781	V782	E783	L784	K785			G661	G662	N663	E664	W665	N666	V667	Q668	I669	G670	L671	L672	K673	M674	K675	V676	K677	E678	K679	D680	L681	E682	F683	I684	K685	S686	A687	P688	GLU	GLN	LYS	LYS	GLU	LYS	ILE	ILE	THR	ALA	VAL	K700	G701	K702	D703	Y704	H705	V706	S707	L708	E709	L710	D711	L712	R713	G714	E715	R716	Y717	E718	N719	A720
	L721	S722	R723	E725	K726	L727	L728	D729	D730	A731	V732	L733	A734	G735	Y736	P737	R738	V739	S740	I741	T742	H743	G744	K745	G746	T747	G748	A749	L750	R751	K752	G753	V754	Q755	D756	L757	L758	F759	N760	H761	R762	S763	V764	K765	S766	S767	R768	F769	G770	E771	A772	G773	E774	G775	S777	G778	V779	T780									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11794	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43.6	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.504	Depositor
Minimum map value	-1.281	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.41	0/433	0.84	1/574 (0.2%)
2	1	0.47	0/407	0.95	2/540 (0.4%)
3	2	0.36	0/371	0.87	2/483 (0.4%)
4	3	0.37	0/519	0.66	0/680
5	4	0.44	0/300	0.73	0/393
6	6	0.36	0/509	0.78	0/678
7	7	0.49	0/1743	1.14	12/2716 (0.4%)
8	A	0.60	1/36826 (0.0%)	1.03	112/57450 (0.2%)
9	B	0.39	0/1782	0.89	8/2392 (0.3%)
10	C	0.36	0/1641	0.79	1/2208 (0.0%)
11	D	0.37	0/1599	0.85	7/2147 (0.3%)
12	E	0.36	0/1231	0.75	0/1655
13	F	0.40	0/766	0.81	1/1031 (0.1%)
14	G	0.49	0/1196	0.80	1/1604 (0.1%)
15	H	0.40	0/1049	0.94	5/1407 (0.4%)
16	I	0.34	0/979	0.79	3/1315 (0.2%)
17	J	0.42	0/773	1.01	3/1044 (0.3%)
18	K	0.32	0/853	0.78	2/1153 (0.2%)
19	L	0.39	0/1069	0.77	0/1435
20	M	0.36	0/873	0.93	3/1166 (0.3%)
21	N	0.43	0/508	0.94	3/672 (0.4%)
22	O	0.41	0/718	0.82	0/960
23	P	0.43	0/708	1.00	4/950 (0.4%)
24	Q	0.41	0/699	0.78	1/933 (0.1%)
25	R	0.36	0/526	0.87	1/705 (0.1%)
26	S	0.38	0/649	0.88	2/872 (0.2%)
27	T	0.34	0/639	0.80	1/852 (0.1%)
28	U	0.47	0/1834	1.01	5/2858 (0.2%)
29	V	0.49	0/787	1.40	19/1224 (1.6%)
30	Y	0.58	0/2675	1.09	13/4170 (0.3%)
31	Z	0.41	0/2120	0.77	4/2845 (0.1%)
32	a	0.39	0/1591	0.73	2/2132 (0.1%)
33	b	0.35	0/1581	0.64	1/2132 (0.0%)
34	c	0.34	0/1405	0.77	4/1887 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	d	0.38	0/1361	0.72	1/1832 (0.1%)
36	e	0.39	0/1147	0.80	2/1542 (0.1%)
37	f	0.47	0/928	0.92	3/1245 (0.2%)
38	i	0.36	0/1094	0.74	2/1457 (0.1%)
39	j	0.40	0/1099	0.73	1/1468 (0.1%)
40	k	0.45	0/961	1.00	5/1284 (0.4%)
41	l	0.35	0/922	0.88	4/1236 (0.3%)
42	m	0.47	0/958	0.93	4/1279 (0.3%)
43	n	0.41	0/953	0.83	3/1266 (0.2%)
44	o	0.41	0/798	0.72	0/1070
45	r	0.39	0/852	0.89	3/1146 (0.3%)
46	s	0.43	0/731	1.00	4/974 (0.4%)
47	t	0.31	0/773	0.63	0/1032
48	u	0.39	0/639	0.80	1/847 (0.1%)
49	v	0.43	0/449	0.90	2/596 (0.3%)
50	w	0.67	0/532	1.20	4/707 (0.6%)
51	x	0.39	0/458	0.97	2/613 (0.3%)
52	X	0.71	0/69451	1.01	167/108344 (0.2%)
53	z	0.28	0/1097	0.61	0/1462
All	All	0.60	1/156562 (0.0%)	0.98	431/234663 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1503	A	N9-C4	-5.68	1.34	1.37

All (431) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	X	138	U	OP1-P-O3'	-30.62	37.83	105.20
52	X	139	A	OP1-P-OP2	-13.65	99.13	119.60
17	J	81	PRO	CA-N-CD	-11.77	95.02	111.50
29	V	448	U	C2-N1-C1'	11.64	131.66	117.70
52	X	1970	C	N1-C2-O2	11.16	125.59	118.90
52	X	1970	C	C2-N1-C1'	10.92	130.81	118.80
26	S	12	ASP	CB-CG-OD1	10.55	127.79	118.30
8	A	1472	C	N1-C2-O2	10.52	125.21	118.90
23	P	42	PRO	CA-N-CD	-10.45	96.87	111.50
8	A	1385	U	C2-N1-C1'	10.21	129.95	117.70
8	A	1472	C	C2-N1-C1'	10.20	130.03	118.80
29	V	448	U	N1-C2-O2	10.07	129.85	122.80
2	1	37	PRO	CA-N-CD	-9.55	98.13	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	11	GLN	CA-CB-CG	9.52	134.35	113.40
29	V	448	U	N3-C2-O2	-9.46	115.58	122.20
49	v	44	PRO	CA-N-CD	-9.44	98.29	111.50
52	X	875	U	C2-N1-C1'	9.35	128.92	117.70
7	7	49	C	N1-C2-O2	9.02	124.31	118.90
8	A	1385	U	N1-C2-O2	9.00	129.10	122.80
8	A	443	U	C2-N1-C1'	8.97	128.46	117.70
9	B	25	PRO	CA-N-CD	-8.88	99.06	111.50
40	k	20	LEU	CA-CB-CG	8.83	135.60	115.30
9	B	60	LEU	CA-CB-CG	8.78	135.50	115.30
52	X	1138	C	C5-C6-N1	8.77	125.39	121.00
52	X	1720	C	N1-C2-O2	8.65	124.09	118.90
8	A	629	C	C2-N1-C1'	8.57	128.23	118.80
52	X	1714	A	N7-C8-N9	8.57	118.08	113.80
8	A	1472	C	N3-C2-O2	-8.48	115.96	121.90
52	X	2223	U	C2-N1-C1'	8.48	127.88	117.70
15	H	83	PRO	CA-N-CD	-8.47	99.64	111.50
52	X	875	U	N1-C2-O2	8.45	128.71	122.80
52	X	138	U	OP2-P-O3'	8.42	123.72	105.20
42	m	16	ASP	CB-CG-OD1	8.38	125.84	118.30
17	J	85	ASP	CB-CG-OD1	8.37	125.83	118.30
52	X	2225	C	C6-N1-C2	-8.36	116.96	120.30
37	f	73	ASP	CB-CG-OD1	8.32	125.79	118.30
52	X	1720	C	C2-N1-C1'	8.25	127.88	118.80
8	A	1385	U	N3-C2-O2	-8.25	116.43	122.20
52	X	556	C	N1-C2-O2	8.16	123.80	118.90
52	X	1970	C	N3-C2-O2	-8.10	116.23	121.90
52	X	1970	C	C6-N1-C1'	-8.08	111.10	120.80
8	A	82	G	O4'-C1'-N9	8.02	114.61	108.20
23	P	41	ASN	C-N-CD	-8.01	102.98	120.60
8	A	83	C	C5-C6-N1	7.94	124.97	121.00
20	M	61	ASP	CB-CG-OD1	7.94	125.44	118.30
8	A	989	C	C2-N1-C1'	7.93	127.52	118.80
27	T	51	LEU	CA-CB-CG	7.92	133.51	115.30
28	U	38	C	N1-C2-O2	7.89	123.63	118.90
43	n	49	ASP	CB-CG-OD1	7.87	125.39	118.30
52	X	2243	C	N1-C2-O2	7.86	123.61	118.90
51	x	18	ASP	CB-CG-OD1	7.80	125.32	118.30
52	X	1138	C	C6-N1-C2	-7.79	117.19	120.30
8	A	1214	U	N1-C2-O2	7.72	128.21	122.80
46	s	31	ASP	CB-CG-OD1	7.72	125.25	118.30
7	7	59	U	N3-C2-O2	-7.71	116.80	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	e	50	ASP	CB-CG-OD1	7.71	125.23	118.30
52	X	1720	C	N3-C2-O2	-7.70	116.51	121.90
8	A	629	C	N1-C2-O2	7.68	123.51	118.90
40	k	28	GLU	CA-CB-CG	7.66	130.26	113.40
52	X	875	U	N3-C2-O2	-7.66	116.84	122.20
29	V	448	U	C6-N1-C1'	-7.59	110.57	121.20
52	X	272	C	C2-N1-C1'	7.55	127.10	118.80
3	2	42	LEU	CA-CB-CG	7.54	132.63	115.30
52	X	1352	U	C2-N1-C1'	7.54	126.74	117.70
52	X	2839	C	N1-C2-O2	7.51	123.41	118.90
8	A	90	C	N1-C2-O2	7.48	123.39	118.90
8	A	1474	G	N3-C4-N9	-7.41	121.55	126.00
8	A	78	G	N3-C4-N9	-7.37	121.58	126.00
46	s	6	ASP	CB-CG-OD1	7.37	124.93	118.30
30	Y	48	G	P-O3'-C3'	7.37	128.54	119.70
7	7	59	U	N1-C2-O2	7.36	127.95	122.80
52	X	2223	U	N3-C2-O2	-7.32	117.08	122.20
8	A	1034	U	C2-N1-C1'	7.32	126.48	117.70
45	r	22	ASP	CB-CG-OD1	7.31	124.88	118.30
45	r	77	ASP	CB-CG-OD1	7.27	124.84	118.30
8	A	83	C	N1-C2-O2	7.27	123.26	118.90
52	X	2225	C	N3-C2-O2	-7.25	116.82	121.90
52	X	1922	C	N1-C2-O2	7.25	123.25	118.90
37	f	112	MET	CA-CB-CG	7.24	125.61	113.30
42	m	22	PRO	CA-N-CD	-7.22	101.39	111.50
15	H	115	ASP	CB-CG-OD1	7.22	124.80	118.30
35	d	14	ASP	CB-CG-OD1	7.22	124.79	118.30
29	V	444	C	N1-C2-O2	7.17	123.20	118.90
8	A	1472	C	C6-N1-C1'	-7.15	112.22	120.80
8	A	421	G	N3-C4-N9	7.14	130.29	126.00
52	X	2166	C	C6-N1-C2	-7.14	117.44	120.30
8	A	1214	U	N3-C2-O2	-7.12	117.21	122.20
52	X	2243	C	N3-C2-O2	-7.11	116.93	121.90
8	A	421	G	N3-C4-C5	-7.10	125.05	128.60
8	A	989	C	N1-C2-O2	7.08	123.15	118.90
8	A	1008	C	N1-C2-O2	7.07	123.14	118.90
52	X	139	A	O5'-P-OP2	7.05	119.16	110.70
52	X	2342	C	C2-N1-C1'	7.04	126.54	118.80
7	7	1	G	OP1-P-OP2	-7.04	109.05	119.60
52	X	556	C	C2-N1-C1'	7.03	126.53	118.80
30	Y	23	U	N1-C2-O2	7.02	127.72	122.80
8	A	82	G	C4-N9-C1'	-7.02	117.37	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	X	931	C	N1-C2-O2	7.00	123.10	118.90
8	A	443	U	N1-C2-O2	6.99	127.69	122.80
50	w	28	LEU	CA-CB-CG	6.99	131.37	115.30
52	X	1922	C	N3-C2-O2	-6.98	117.01	121.90
31	Z	70	ASP	CB-CG-OD1	6.96	124.57	118.30
8	A	78	G	N3-C4-C5	6.95	132.07	128.60
8	A	763	C	C2-N1-C1'	6.94	126.43	118.80
46	s	8	LEU	CA-CB-CG	6.92	131.21	115.30
52	X	2785	U	C2-N1-C1'	6.91	125.99	117.70
8	A	443	U	N3-C2-O2	-6.89	117.38	122.20
46	s	3	ASP	CB-CG-OD1	6.89	124.50	118.30
52	X	328	G	OP1-P-OP2	-6.88	109.28	119.60
8	A	1385	U	C6-N1-C1'	-6.86	111.60	121.20
52	X	2646	C	C2-N1-C1'	6.82	126.30	118.80
52	X	2208	C	N1-C2-O2	6.81	122.98	118.90
52	X	2223	U	N1-C2-O2	6.78	127.55	122.80
52	X	167	U	N1-C2-O2	6.74	127.52	122.80
8	A	82	G	C8-N9-C1'	6.73	135.75	127.00
43	n	85	LEU	CA-CB-CG	6.70	130.71	115.30
52	X	1145	G	N3-C4-N9	6.67	130.00	126.00
32	a	54	ASP	CB-CG-OD1	6.62	124.26	118.30
52	X	1145	G	C8-N9-C1'	-6.61	118.40	127.00
52	X	167	U	C2-N1-C1'	6.61	125.63	117.70
52	X	93	C	N1-C2-O2	6.60	122.86	118.90
11	D	15	LEU	CB-CG-CD1	-6.59	99.80	111.00
52	X	1145	G	C4-N9-C1'	6.59	135.06	126.50
28	U	38	C	N3-C2-O2	-6.59	117.29	121.90
52	X	1220	G	OP1-P-OP2	-6.57	109.75	119.60
52	X	931	C	N3-C2-O2	-6.56	117.31	121.90
30	Y	29	C	C2-N1-C1'	6.56	126.01	118.80
8	A	1034	U	N1-C2-O2	6.54	127.38	122.80
52	X	1922	C	C2-N1-C1'	6.54	126.00	118.80
29	V	444	C	N3-C2-O2	-6.54	117.32	121.90
52	X	2183	G	C4-N9-C1'	6.54	135.00	126.50
8	A	231	U	C2-N1-C1'	6.54	125.54	117.70
7	7	49	C	N3-C2-O2	-6.53	117.33	121.90
52	X	1714	A	C4-N9-C1'	6.51	138.02	126.30
48	u	23	ASP	CB-CG-OD1	6.51	124.16	118.30
11	D	71	LEU	CA-CB-CG	6.50	130.25	115.30
29	V	435	G	C4-N9-C1'	6.49	134.94	126.50
40	k	55	ASP	CB-CG-OD1	6.47	124.12	118.30
52	X	875	U	C6-N1-C1'	-6.46	112.16	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Y	23	U	N3-C2-O2	-6.45	117.68	122.20
9	B	27	MET	CA-CB-CG	6.43	124.24	113.30
8	A	421	G	C4-N9-C1'	6.43	134.86	126.50
8	A	1008	C	N3-C2-O2	-6.42	117.41	121.90
52	X	1985	U	N3-C2-O2	-6.41	117.72	122.20
52	X	2191	A	C2-N3-C4	6.39	113.80	110.60
52	X	167	U	N3-C2-O2	-6.38	117.73	122.20
2	1	24	ARG	CG-CD-NE	6.38	125.20	111.80
29	V	443	C	N1-C2-O2	6.37	122.72	118.90
8	A	1472	C	C6-N1-C2	-6.37	117.75	120.30
52	X	1985	U	N1-C2-O2	6.37	127.26	122.80
8	A	231	U	N1-C2-O2	6.35	127.25	122.80
16	I	54	LEU	CA-CB-CG	6.35	129.91	115.30
9	B	154	MET	CG-SD-CE	6.34	110.35	100.20
52	X	1352	U	N1-C2-O2	6.34	127.24	122.80
11	D	168	ASP	CB-CG-OD1	6.34	124.00	118.30
52	X	2350	G	N3-C4-C5	-6.33	125.43	128.60
8	A	1474	G	C4-N9-C1'	-6.33	118.27	126.50
14	G	30	MET	CB-CG-SD	6.31	131.34	112.40
8	A	1167	C	C2-N1-C1'	6.31	125.74	118.80
52	X	2695	C	N1-C2-O2	6.30	122.68	118.90
39	j	80	GLU	CA-CB-CG	6.28	127.22	113.40
8	A	98	U	N1-C2-O2	6.26	127.19	122.80
29	V	444	C	C2-N1-C1'	6.26	125.69	118.80
40	k	119	LEU	CA-CB-CG	6.26	129.70	115.30
52	X	700	U	C2-N1-C1'	6.22	125.17	117.70
52	X	2223	U	C6-N1-C1'	-6.22	112.49	121.20
52	X	2183	G	N3-C4-C5	-6.22	125.49	128.60
8	A	1058	G	O5'-P-OP1	-6.20	100.12	105.70
52	X	1803	C	N1-C2-O2	6.20	122.62	118.90
51	x	49	LYS	CA-CB-CG	6.18	127.01	113.40
8	A	855	G	P-O3'-C3'	6.17	127.10	119.70
8	A	629	C	C6-N1-C1'	-6.17	113.40	120.80
52	X	308	C	N1-C2-O2	6.15	122.59	118.90
50	w	37	LEU	CA-CB-CG	6.15	129.45	115.30
18	K	119	PRO	CA-N-CD	-6.14	102.90	111.50
8	A	1474	G	C8-N9-C1'	6.13	134.97	127.00
49	v	39	LEU	CA-CB-CG	6.12	129.39	115.30
52	X	2025	C	N1-C2-O2	6.12	122.57	118.90
52	X	1352	U	N3-C2-O2	-6.10	117.93	122.20
8	A	1299	U	C2-N1-C1'	6.09	125.01	117.70
52	X	1102	G	O4'-C1'-N9	6.08	113.06	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	65	G	N3-C4-N9	6.05	129.63	126.00
17	J	81	PRO	N-CD-CG	-6.05	94.13	103.20
41	l	63	LEU	CA-CB-CG	6.05	129.21	115.30
8	A	607	U	C2-N1-C1'	6.04	124.95	117.70
8	A	90	C	N3-C2-O2	-6.03	117.68	121.90
8	A	510	C	C5-C6-N1	6.03	124.02	121.00
52	X	831	U	N3-C2-O2	-6.01	117.99	122.20
8	A	989	C	N3-C2-O2	-6.00	117.70	121.90
11	D	87	MET	CA-CB-CG	6.00	123.50	113.30
41	l	92	ASP	CB-CG-OD1	6.00	123.70	118.30
8	A	629	C	N3-C2-O2	-6.00	117.70	121.90
8	A	607	U	N1-C2-O2	5.99	127.00	122.80
28	U	38	C	C2-N1-C1'	5.99	125.39	118.80
52	X	2785	U	C6-N1-C1'	-5.98	112.83	121.20
15	H	25	LEU	CA-CB-CG	5.96	129.02	115.30
25	R	30	ASP	CB-CG-OD1	5.96	123.67	118.30
52	X	1720	C	C6-N1-C1'	-5.96	113.64	120.80
8	A	607	U	N3-C2-O2	-5.94	118.04	122.20
52	X	308	C	N3-C2-O2	-5.92	117.75	121.90
52	X	1353	C	C2-N1-C1'	5.92	125.31	118.80
52	X	556	C	N3-C2-O2	-5.92	117.76	121.90
52	X	2906	U	C2-N1-C1'	5.91	124.80	117.70
41	l	62	ASP	CB-CG-OD1	5.91	123.62	118.30
8	A	1060	G	N1-C6-O6	-5.91	116.36	119.90
8	A	629	C	C6-N1-C2	-5.90	117.94	120.30
8	A	1390	U	N1-C2-O2	5.89	126.92	122.80
52	X	2459	A	C2-N3-C4	5.88	113.54	110.60
52	X	62	C	N1-C2-O2	5.88	122.43	118.90
52	X	2334	U	P-O3'-C3'	5.88	126.75	119.70
8	A	98	U	N3-C2-O2	-5.87	118.09	122.20
42	m	4	LEU	CA-CB-CG	5.87	128.81	115.30
34	c	101	ASP	CB-CG-OD1	5.87	123.58	118.30
52	X	700	U	N1-C2-O2	5.85	126.90	122.80
15	H	64	LEU	CA-CB-CG	5.84	128.74	115.30
52	X	1247	G	O4'-C1'-N9	5.83	112.86	108.20
34	c	17	MET	CA-CB-CG	5.82	123.19	113.30
29	V	443	C	C2-N1-C1'	5.81	125.19	118.80
8	A	78	G	C4-N9-C1'	-5.80	118.96	126.50
8	A	972	C	C2-N1-C1'	5.79	125.17	118.80
9	B	108	GLN	CA-CB-CG	5.79	126.13	113.40
7	7	21	A	P-O3'-C3'	5.78	126.64	119.70
52	X	237	U	N1-C2-O2	5.78	126.84	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	X	1145	G	N9-C4-C5	-5.77	103.09	105.40
52	X	1803	C	N3-C2-O2	-5.77	117.86	121.90
8	A	83	C	C2-N1-C1'	5.76	125.14	118.80
50	w	25	LEU	CA-CB-CG	5.75	128.52	115.30
24	Q	59	ASP	CB-CG-OD1	5.75	123.47	118.30
11	D	172	LEU	CA-CB-CG	5.73	128.48	115.30
29	V	435	G	N3-C4-C5	-5.73	125.73	128.60
52	X	1596	U	N3-C2-O2	-5.72	118.20	122.20
8	A	1390	U	N3-C2-O2	-5.71	118.20	122.20
52	X	2054	C	C2-N1-C1'	5.71	125.09	118.80
42	m	48	ILE	CG1-CB-CG2	-5.71	98.85	111.40
52	X	331	C	N1-C2-O2	5.70	122.32	118.90
15	H	85	LEU	CA-CB-CG	5.70	128.41	115.30
8	A	443	U	C5-C6-N1	5.70	125.55	122.70
8	A	421	G	C6-C5-N7	-5.69	126.98	130.40
52	X	2138	U	C2-N1-C1'	5.69	124.53	117.70
10	C	135	GLN	CA-CB-CG	5.69	125.91	113.40
52	X	2243	C	C2-N1-C1'	5.68	125.05	118.80
52	X	186	C	N3-C2-O2	-5.68	117.93	121.90
18	K	84	LEU	CA-CB-CG	5.67	128.34	115.30
52	X	1970	C	C6-N1-C2	-5.67	118.03	120.30
8	A	989	C	C6-N1-C1'	-5.67	114.00	120.80
37	f	91	LYS	C-N-CA	5.67	135.87	121.70
52	X	700	U	N3-C2-O2	-5.67	118.23	122.20
34	c	83	MET	CB-CG-SD	5.67	129.40	112.40
52	X	2092	C	N1-C2-O2	5.66	122.30	118.90
8	A	855	G	OP1-P-O3'	5.66	117.66	105.20
29	V	448	U	C5-C6-N1	5.65	125.53	122.70
52	X	2342	C	N1-C2-O2	5.65	122.29	118.90
8	A	231	U	N3-C2-O2	-5.65	118.25	122.20
52	X	1970	C	C5-C6-N1	5.64	123.82	121.00
16	I	75	GLN	CA-CB-CG	5.64	125.80	113.40
36	e	20	ASP	CB-CG-OD1	5.63	123.37	118.30
52	X	2133	C	OP1-P-O3'	5.62	117.57	105.20
52	X	1370	C	N1-C2-O2	5.62	122.27	118.90
8	A	445	U	P-O3'-C3'	5.61	126.43	119.70
52	X	483	C	N1-C2-O2	5.61	122.27	118.90
30	Y	99	A	C2-N3-C4	5.61	113.41	110.60
52	X	2839	C	C2-N1-C1'	5.60	124.96	118.80
8	A	1219	C	C6-N1-C1'	5.60	127.52	120.80
52	X	2177	G	N3-C4-N9	-5.58	122.65	126.00
52	X	2138	U	N1-C2-O2	5.57	126.70	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	X	113	U	C2-N1-C1'	5.54	124.35	117.70
52	X	2906	U	N3-C2-O2	-5.54	118.32	122.20
52	X	2904	A	P-O3'-C3'	5.54	126.34	119.70
52	X	631	G	N3-C4-C5	5.53	131.36	128.60
52	X	2349	A	C2-N3-C4	5.52	113.36	110.60
8	A	1385	U	C5-C6-N1	5.52	125.46	122.70
52	X	2785	U	N1-C2-O2	5.51	126.66	122.80
52	X	2839	C	N3-C2-O2	-5.51	118.04	121.90
28	U	63	C	C2-N1-C1'	5.51	124.86	118.80
52	X	1804	U	C5-C4-O4	-5.51	122.59	125.90
30	Y	23	U	C2-N1-C1'	5.50	124.30	117.70
8	A	572	A	C4-N9-C1'	5.50	136.20	126.30
52	X	2805	A	P-O3'-C3'	5.49	126.29	119.70
31	Z	66	ASP	CB-CG-OD1	5.46	123.21	118.30
30	Y	29	C	N1-C2-O2	5.46	122.17	118.90
9	B	157	LEU	CA-CB-CG	5.45	127.84	115.30
29	V	435	G	N3-C4-N9	5.45	129.27	126.00
52	X	2924	A	C8-N9-C4	-5.44	103.62	105.80
8	A	443	U	C6-N1-C1'	-5.43	113.59	121.20
52	X	2768	U	N1-C2-O2	5.43	126.60	122.80
8	A	629	C	C5-C6-N1	5.42	123.71	121.00
52	X	1714	A	C8-N9-C4	-5.42	103.63	105.80
52	X	252	C	P-O3'-C3'	5.41	126.20	119.70
52	X	483	C	N3-C2-O2	-5.41	118.11	121.90
8	A	1088	U	P-O3'-C3'	5.41	126.19	119.70
8	A	1317	C	C2-N1-C1'	5.41	124.75	118.80
52	X	2025	C	N3-C2-O2	-5.41	118.11	121.90
29	V	448	U	C6-N1-C2	-5.40	117.76	121.00
52	X	2838	U	N3-C2-O2	-5.39	118.42	122.20
11	D	87	MET	CB-CG-SD	5.39	128.57	112.40
52	X	932	C	N3-C2-O2	-5.39	118.12	121.90
52	X	2705	C	C2-N1-C1'	5.39	124.73	118.80
8	A	1034	U	N3-C2-O2	-5.39	118.43	122.20
8	A	1211	U	C5-C6-N1	5.39	125.39	122.70
13	F	76	ASP	CB-CG-OD1	5.38	123.15	118.30
34	c	83	MET	CA-CB-CG	5.37	122.43	113.30
29	V	444	C	C6-N1-C2	-5.37	118.15	120.30
52	X	1352	U	C6-N1-C1'	-5.37	113.69	121.20
8	A	1474	G	N3-C4-C5	5.36	131.28	128.60
52	X	272	C	C6-N1-C1'	-5.36	114.36	120.80
52	X	1714	A	C5-N7-C8	-5.36	101.22	103.90
52	X	2749	U	N3-C2-O2	-5.36	118.45	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	443	U	C6-N1-C2	-5.34	117.79	121.00
45	r	77	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	0	22	LEU	CA-CB-CG	5.34	127.58	115.30
8	A	1167	C	N3-C2-O2	-5.34	118.17	121.90
52	X	2092	C	C2-N1-C1'	5.33	124.66	118.80
8	A	993	A	C2-N3-C4	5.33	113.27	110.60
20	M	75	LEU	CA-CB-CG	5.33	127.55	115.30
8	A	595	C	C2-N1-C1'	5.33	124.66	118.80
8	A	1034	U	C6-N1-C1'	-5.33	113.75	121.20
52	X	2092	C	N3-C2-O2	-5.32	118.17	121.90
8	A	773	C	C2-N1-C1'	5.31	124.65	118.80
8	A	659	A	N1-C6-N6	-5.31	115.41	118.60
11	D	89	LEU	CA-CB-CG	5.31	127.52	115.30
8	A	869	C	N1-C2-O2	5.31	122.08	118.90
52	X	511	U	P-O3'-C3'	5.30	126.06	119.70
41	l	59	LEU	CA-CB-CG	5.30	127.50	115.30
31	Z	27	ASP	CB-CG-OD1	5.30	123.07	118.30
52	X	2820	U	C2-N1-C1'	5.29	124.05	117.70
43	n	71	MET	CA-CB-CG	5.29	122.30	113.30
52	X	2350	G	N3-C4-N9	5.29	129.18	126.00
7	7	19	G	P-O3'-C3'	5.29	126.05	119.70
8	A	1503	A	C8-N9-C4	5.28	107.91	105.80
31	Z	123	ASP	CB-CG-OD1	5.28	123.05	118.30
52	X	1451	U	N3-C2-O2	-5.28	118.51	122.20
8	A	1276	C	P-O3'-C3'	5.28	126.03	119.70
52	X	2888	C	N1-C2-O2	5.27	122.06	118.90
52	X	939	G	N1-C2-N2	-5.27	111.46	116.20
8	A	572	A	C8-N9-C1'	-5.26	118.23	127.70
8	A	1472	C	C5-C6-N1	5.25	123.63	121.00
8	A	1167	C	N1-C2-O2	5.25	122.05	118.90
30	Y	28	C	C2-N1-C1'	5.25	124.57	118.80
8	A	601	C	C2-N1-C1'	5.25	124.57	118.80
8	A	78	G	C8-N9-C1'	5.24	133.82	127.00
52	X	831	U	N1-C2-O2	5.24	126.47	122.80
52	X	2255	C	N1-C2-O2	5.24	122.04	118.90
32	a	180	ASP	CB-CG-OD1	5.23	123.01	118.30
52	X	1101	G	N1-C6-O6	-5.23	116.76	119.90
7	7	4	C	C2-N1-C1'	5.23	124.55	118.80
52	X	1145	G	C6-C5-N7	-5.23	127.26	130.40
52	X	777	C	N1-C2-O2	5.22	122.03	118.90
52	X	2166	C	N3-C2-O2	-5.22	118.25	121.90
52	X	331	C	N3-C2-O2	-5.22	118.25	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1474	G	C6-C5-N7	5.20	133.52	130.40
52	X	1714	A	C8-N9-C1'	-5.20	118.34	127.70
3	2	31	LEU	CA-CB-CG	5.20	127.25	115.30
33	b	129	LEU	CA-CB-CG	5.20	127.25	115.30
8	A	39	U	N1-C2-O2	5.19	126.44	122.80
9	B	144	LEU	CA-CB-CG	5.19	127.24	115.30
52	X	2191	A	N3-C4-N9	5.19	131.55	127.40
8	A	573	U	P-O3'-C3'	5.19	125.92	119.70
52	X	1567	U	P-O3'-C3'	5.18	125.92	119.70
7	7	6	G	N3-C4-N9	5.17	129.10	126.00
52	X	1203	G	C4-N9-C1'	5.17	133.22	126.50
8	A	1219	C	C2-N1-C1'	-5.16	113.13	118.80
52	X	91	A	C2-N3-C4	5.15	113.18	110.60
52	X	1353	C	C6-N1-C2	-5.15	118.24	120.30
30	Y	42	G	N3-C4-N9	5.15	129.09	126.00
52	X	115	C	C2-N1-C1'	5.15	124.46	118.80
30	Y	98	G	N3-C4-N9	5.14	129.09	126.00
28	U	38	C	C6-N1-C2	-5.14	118.25	120.30
38	i	95	LEU	CA-CB-CG	5.14	127.12	115.30
8	A	421	G	C8-N9-C1'	-5.14	120.32	127.00
38	i	106	ASN	CB-CA-C	5.14	120.67	110.40
29	V	435	G	C8-N9-C1'	-5.13	120.33	127.00
29	V	454	G	N3-C4-N9	5.13	129.08	126.00
52	X	308	C	C6-N1-C2	-5.13	118.25	120.30
52	X	1922	C	C6-N1-C2	-5.13	118.25	120.30
52	X	237	U	N3-C2-O2	-5.12	118.61	122.20
8	A	1085	U	C2-N1-C1'	5.12	123.85	117.70
52	X	291	C	C2-N1-C1'	-5.12	113.17	118.80
8	A	446	G	O4'-C1'-N9	5.12	112.30	108.20
40	k	46	LYS	CA-CB-CG	5.12	124.66	113.40
52	X	1145	G	C4-C5-N7	5.11	112.85	110.80
52	X	898	U	N3-C2-O2	-5.11	118.62	122.20
8	A	763	C	C6-N1-C1'	-5.11	114.67	120.80
8	A	1003	G	C4-N9-C1'	5.11	133.14	126.50
8	A	82	G	C6-C5-N7	5.11	133.47	130.40
8	A	999	U	N3-C2-O2	-5.11	118.63	122.20
8	A	1003	G	N3-C4-N9	5.11	129.06	126.00
8	A	1391	C	N1-C2-O2	5.10	121.96	118.90
52	X	186	C	N1-C2-O2	5.10	121.96	118.90
52	X	93	C	N3-C2-O2	-5.10	118.33	121.90
52	X	3	U	C2-N1-C1'	5.10	123.82	117.70
8	A	306	A	P-O3'-C3'	5.10	125.82	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	X	2696	C	N1-C2-O2	5.10	121.96	118.90
29	V	443	C	N3-C2-O2	-5.09	118.33	121.90
8	A	98	U	C2-N1-C1'	5.09	123.80	117.70
52	X	777	C	N3-C2-O2	-5.08	118.34	121.90
52	X	766	C	N1-C2-O2	5.08	121.95	118.90
52	X	2904	A	OP2-P-O3'	5.08	116.37	105.20
8	A	1503	A	C4-C5-C6	-5.08	114.46	117.00
52	X	933	C	N1-C2-O2	5.07	121.94	118.90
21	N	11	GLN	N-CA-CB	5.07	119.72	110.60
52	X	2208	C	N3-C2-O2	-5.07	118.35	121.90
52	X	2768	U	N3-C2-O2	-5.07	118.65	122.20
23	P	7	LEU	CA-CB-CG	5.07	126.95	115.30
29	V	454	G	N3-C4-C5	-5.07	126.07	128.60
8	A	773	C	C6-N1-C2	-5.06	118.27	120.30
8	A	972	C	N1-C2-O2	5.06	121.94	118.90
9	B	212	LEU	CA-CB-CG	5.06	126.94	115.30
52	X	1682	C	N1-C2-O2	5.06	121.94	118.90
52	X	2138	U	C5-C6-N1	5.06	125.23	122.70
52	X	2183	G	C8-N9-C4	-5.05	104.38	106.40
7	7	19	G	OP2-P-O3'	5.04	116.29	105.20
7	7	21	A	OP1-P-O3'	5.04	116.29	105.20
21	N	17	LYS	CA-CB-CG	5.04	124.49	113.40
30	Y	29	C	C6-N1-C1'	-5.04	114.75	120.80
52	X	556	C	C5-C6-N1	5.04	123.52	121.00
52	X	291	C	C6-N1-C1'	5.04	126.84	120.80
8	A	1369	A	P-O3'-C3'	5.03	125.74	119.70
30	Y	99	A	N3-C4-N9	5.03	131.43	127.40
26	S	12	ASP	CB-CG-OD2	-5.03	113.77	118.30
52	X	2695	C	N3-C2-O2	-5.03	118.38	121.90
8	A	1005	C	O4'-C1'-N1	5.03	112.22	108.20
20	M	72	GLU	CA-CB-CG	5.03	124.46	113.40
16	I	88	LEU	CB-CG-CD1	-5.02	102.46	111.00
52	X	903	G	N3-C4-N9	5.02	129.01	126.00
50	w	9	LEU	CA-CB-CG	5.02	126.84	115.30
52	X	1241	C	C2-N1-C1'	5.02	124.32	118.80
8	A	759	C	C6-N1-C2	-5.01	118.30	120.30
30	Y	71	A	C6-N1-C2	5.01	121.61	118.60
23	P	55	LEU	CA-CB-CG	5.01	126.82	115.30
52	X	549	A	P-O3'-C3'	5.00	125.70	119.70
52	X	1215	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	52/59 (88%)	52 (100%)	0	0	100	100
2	1	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
3	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
4	3	62/66 (94%)	58 (94%)	4 (6%)	0	100	100
5	4	35/37 (95%)	35 (100%)	0	0	100	100
6	6	61/64 (95%)	53 (87%)	8 (13%)	0	100	100
9	B	216/246 (88%)	192 (89%)	23 (11%)	1 (0%)	25	59
10	C	204/218 (94%)	184 (90%)	19 (9%)	1 (0%)	25	59
11	D	193/200 (96%)	172 (89%)	19 (10%)	2 (1%)	13	46
12	E	162/166 (98%)	153 (94%)	9 (6%)	0	100	100
13	F	90/95 (95%)	84 (93%)	6 (7%)	0	100	100
14	G	147/156 (94%)	134 (91%)	11 (8%)	2 (1%)	9	40
15	H	129/132 (98%)	118 (92%)	11 (8%)	0	100	100
16	I	123/130 (95%)	112 (91%)	11 (9%)	0	100	100
17	J	93/102 (91%)	87 (94%)	6 (6%)	0	100	100
18	K	112/131 (86%)	108 (96%)	4 (4%)	0	100	100
19	L	134/138 (97%)	122 (91%)	12 (9%)	0	100	100
20	M	106/121 (88%)	97 (92%)	9 (8%)	0	100	100
21	N	58/61 (95%)	51 (88%)	7 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	O	83/89 (93%)	77 (93%)	6 (7%)	0	100	100
23	P	86/90 (96%)	80 (93%)	6 (7%)	0	100	100
24	Q	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
25	R	62/79 (78%)	58 (94%)	4 (6%)	0	100	100
26	S	76/92 (83%)	73 (96%)	3 (4%)	0	100	100
27	T	81/88 (92%)	76 (94%)	4 (5%)	1 (1%)	11	43
31	Z	270/275 (98%)	252 (93%)	17 (6%)	1 (0%)	30	62
32	a	204/207 (99%)	194 (95%)	10 (5%)	0	100	100
33	b	203/205 (99%)	189 (93%)	14 (7%)	0	100	100
34	c	174/178 (98%)	166 (95%)	7 (4%)	1 (1%)	22	55
35	d	173/175 (99%)	159 (92%)	14 (8%)	0	100	100
36	e	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
37	f	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
38	i	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
39	j	133/138 (96%)	124 (93%)	9 (7%)	0	100	100
40	k	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	14	48
41	l	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
42	m	113/115 (98%)	102 (90%)	10 (9%)	1 (1%)	14	48
43	n	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
44	o	99/101 (98%)	85 (86%)	14 (14%)	0	100	100
45	r	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
46	s	88/93 (95%)	85 (97%)	3 (3%)	0	100	100
47	t	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
48	u	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
49	v	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
50	w	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
51	x	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
53	z	135/785 (17%)	130 (96%)	5 (4%)	0	100	100
All	All	5342/6250 (86%)	4963 (93%)	368 (7%)	11 (0%)	45	74

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	D	143	GLU
42	m	106	LYS
14	G	31	MET
10	C	50	SER
34	c	42	ASP
14	G	30	MET
27	T	69	LYS
40	k	28	GLU
31	Z	244	LYS
9	B	193	PRO
11	D	187	PRO

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	48/53 (91%)	44 (92%)	4 (8%)	9 34
2	1	46/46 (100%)	45 (98%)	1 (2%)	47 70
3	2	39/39 (100%)	39 (100%)	0	100 100
4	3	54/57 (95%)	52 (96%)	2 (4%)	29 58
5	4	35/35 (100%)	35 (100%)	0	100 100
6	6	53/53 (100%)	49 (92%)	4 (8%)	11 37
9	B	189/212 (89%)	172 (91%)	17 (9%)	8 32
10	C	168/178 (94%)	157 (94%)	11 (6%)	14 42
11	D	169/173 (98%)	156 (92%)	13 (8%)	10 36
12	E	128/130 (98%)	119 (93%)	9 (7%)	12 39
13	F	81/84 (96%)	77 (95%)	4 (5%)	21 50
14	G	125/132 (95%)	112 (90%)	13 (10%)	5 27
15	H	111/112 (99%)	106 (96%)	5 (4%)	23 53
16	I	98/102 (96%)	92 (94%)	6 (6%)	15 44
17	J	86/92 (94%)	81 (94%)	5 (6%)	17 45
18	K	86/100 (86%)	81 (94%)	5 (6%)	17 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	L	114/116 (98%)	110 (96%)	4 (4%)	31	60
20	M	94/104 (90%)	92 (98%)	2 (2%)	48	71
21	N	53/54 (98%)	50 (94%)	3 (6%)	17	46
22	O	80/83 (96%)	75 (94%)	5 (6%)	15	43
23	P	74/76 (97%)	68 (92%)	6 (8%)	9	34
24	Q	77/80 (96%)	76 (99%)	1 (1%)	65	82
25	R	56/64 (88%)	51 (91%)	5 (9%)	8	32
26	S	70/81 (86%)	68 (97%)	2 (3%)	37	63
27	T	66/70 (94%)	65 (98%)	1 (2%)	60	79
31	Z	220/223 (99%)	212 (96%)	8 (4%)	30	59
32	a	167/168 (99%)	155 (93%)	12 (7%)	12	38
33	b	169/169 (100%)	163 (96%)	6 (4%)	30	59
34	c	151/153 (99%)	141 (93%)	10 (7%)	14	42
35	d	148/148 (100%)	140 (95%)	8 (5%)	18	47
36	e	120/120 (100%)	111 (92%)	9 (8%)	11	37
37	f	101/101 (100%)	95 (94%)	6 (6%)	16	45
38	i	110/110 (100%)	106 (96%)	4 (4%)	30	59
39	j	109/111 (98%)	105 (96%)	4 (4%)	29	58
40	k	99/99 (100%)	93 (94%)	6 (6%)	15	44
41	l	93/93 (100%)	88 (95%)	5 (5%)	18	47
42	m	100/100 (100%)	94 (94%)	6 (6%)	16	44
43	n	96/96 (100%)	93 (97%)	3 (3%)	35	62
44	o	83/83 (100%)	81 (98%)	2 (2%)	44	68
45	r	90/90 (100%)	86 (96%)	4 (4%)	24	53
46	s	81/84 (96%)	78 (96%)	3 (4%)	29	58
47	t	85/85 (100%)	83 (98%)	2 (2%)	44	68
48	u	64/64 (100%)	61 (95%)	3 (5%)	22	51
49	v	47/47 (100%)	46 (98%)	1 (2%)	48	71
50	w	56/56 (100%)	50 (89%)	6 (11%)	5	26
51	x	52/52 (100%)	51 (98%)	1 (2%)	52	73
53	z	115/673 (17%)	111 (96%)	4 (4%)	31	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4556/5251 (87%)	4315 (95%)	241 (5%)	21	48

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	21	LYS
1	0	36	MET
1	0	52	LYS
1	0	55	ASN
2	1	21	LYS
4	3	31	HIS
4	3	64	ASN
6	6	9	PHE
6	6	22	PHE
6	6	32	ARG
6	6	43	TYR
9	B	21	ARG
9	B	29	ARG
9	B	56	PHE
9	B	60	LEU
9	B	74	LYS
9	B	86	ARG
9	B	89	MET
9	B	101	LEU
9	B	108	GLN
9	B	112	LYS
9	B	133	GLU
9	B	142	GLU
9	B	147	PHE
9	B	148	LEU
9	B	155	LYS
9	B	156	ASP
9	B	162	PHE
10	C	23	TYR
10	C	28	TYR
10	C	45	ARG
10	C	91	ASN
10	C	101	ASN
10	C	106	LYS
10	C	113	GLN
10	C	125	ASN
10	C	167	TYR

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Mol	Chain	Res	Type
10	C	183	TYR
10	C	192	TYR
11	D	13	ARG
11	D	24	LYS
11	D	41	ARG
11	D	54	LYS
11	D	59	HIS
11	D	64	ASN
11	D	71	LEU
11	D	72	PHE
11	D	105	ARG
11	D	120	LEU
11	D	170	GLU
11	D	172	LEU
11	D	178	ARG
12	E	7	SER
12	E	13	GLU
12	E	20	ARG
12	E	36	LEU
12	E	43	ASN
12	E	93	ASN
12	E	124	LEU
12	E	142	GLN
12	E	146	GLU
13	F	11	ARG
13	F	53	ASN
13	F	55	PHE
13	F	73	GLN
14	G	9	LYS
14	G	10	ARG
14	G	30	MET
14	G	31	MET
14	G	41	THR
14	G	42	ILE
14	G	47	PHE
14	G	59	MET
14	G	79	ARG
14	G	85	TYR
14	G	106	ASN
14	G	107	TYR
14	G	114	LYS
15	H	24	LYS

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Mol	Chain	Res	Type
15	H	28	PRO
15	H	101	LEU
15	H	113	LEU
15	H	132	TRP
16	I	41	SER
16	I	75	GLN
16	I	94	TYR
16	I	103	LEU
16	I	113	ARG
16	I	123	ARG
17	J	14	ASP
17	J	16	ARG
17	J	42	LEU
17	J	47	SER
17	J	57	LYS
18	K	19	GLU
18	K	74	LYS
18	K	82	LYS
18	K	127	LYS
18	K	128	ARG
19	L	44	ARG
19	L	65	TYR
19	L	112	ARG
19	L	133	LYS
20	M	82	GLU
20	M	105	ASN
21	N	17	LYS
21	N	44	PHE
21	N	57	LYS
22	O	8	LYS
22	O	24	SER
22	O	48	LYS
22	O	51	HIS
22	O	78	TYR
23	P	10	MET
23	P	15	SER
23	P	40	TYR
23	P	52	ASP
23	P	71	ARG
23	P	74	PHE
24	Q	17	ASP
25	R	17	TYR

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Mol	Chain	Res	Type
25	R	25	HIS
25	R	29	LYS
25	R	43	LYS
25	R	53	ASN
26	S	12	ASP
26	S	27	LYS
27	T	78	ARG
31	Z	72	ASP
31	Z	83	TYR
31	Z	221	ARG
31	Z	225	MET
31	Z	229	ASP
31	Z	243	ARG
31	Z	250	TRP
31	Z	267	ASP
32	a	50	GLN
32	a	55	ASP
32	a	58	GLU
32	a	88	MET
32	a	89	ASP
32	a	91	TYR
32	a	119	PHE
32	a	130	ARG
32	a	145	SER
32	a	168	GLN
32	a	183	ARG
32	a	184	ASN
33	b	39	MET
33	b	62	ARG
33	b	83	TRP
33	b	95	ARG
33	b	120	ASP
33	b	190	GLU
34	c	17	MET
34	c	44	VAL
34	c	45	GLN
34	c	46	ASN
34	c	59	PHE
34	c	83	MET
34	c	125	ARG
34	c	128	TYR
34	c	148	LYS

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Mol	Chain	Res	Type
34	c	153	ASP
35	d	39	HIS
35	d	41	ASP
35	d	45	LYS
35	d	70	ARG
35	d	75	ASN
35	d	76	MET
35	d	84	PHE
35	d	154	SER
36	e	26	LEU
36	e	37	LEU
36	e	40	LYS
36	e	72	ASP
36	e	97	TYR
36	e	117	ARG
36	e	121	LYS
36	e	124	ASN
36	e	126	TYR
37	f	1	MET
37	f	25	LEU
37	f	41	CYS
37	f	73	ASP
37	f	84	CYS
37	f	107	ARG
38	i	50	PHE
38	i	58	PHE
38	i	64	ARG
38	i	106	ASN
39	j	40	SER
39	j	43	THR
39	j	122	SER
39	j	131	PHE
40	k	40	LEU
40	k	42	SER
40	k	46	LYS
40	k	78	ASP
40	k	84	PHE
40	k	92	GLU
41	l	22	LEU
41	l	81	VAL
41	l	83	LYS
41	l	84	ARG

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Mol	Chain	Res	Type
41	l	115	GLU
42	m	31	LYS
42	m	63	LYS
42	m	65	SER
42	m	74	PHE
42	m	80	LYS
42	m	89	TYR
43	n	18	LEU
43	n	71	MET
43	n	103	LEU
44	o	37	ASP
44	o	39	LEU
45	r	22	ASP
45	r	53	SER
45	r	64	MET
45	r	65	ASP
46	s	19	ASP
46	s	33	ARG
46	s	57	MET
47	t	39	ASN
47	t	60	GLU
48	u	35	ASP
48	u	45	LEU
48	u	58	ASN
49	v	23	ASN
50	w	26	PHE
50	w	30	PHE
50	w	52	ARG
50	w	54	LYS
50	w	57	ILE
50	w	58	ARG
51	x	30	LYS
53	z	679	LYS
53	z	752	LYS
53	z	765	LYS
53	z	771	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	35	ASN
11	D	52	GLN

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Mol	Chain	Res	Type
11	D	55	GLN
11	D	118	HIS
13	F	73	GLN
19	L	125	GLN
22	O	10	GLN
22	O	13	ASN
23	P	88	GLN
26	S	23	ASN
49	v	23	ASN
49	v	34	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	U	76/77 (98%)	19 (25%)	0
29	V	32/33 (96%)	21 (65%)	0
30	Y	111/112 (99%)	35 (31%)	2 (1%)
52	X	2881/2928 (98%)	737 (25%)	23 (0%)
7	7	72/73 (98%)	25 (34%)	2 (2%)
8	A	1532/1533 (99%)	369 (24%)	14 (0%)
All	All	4704/4756 (98%)	1206 (25%)	41 (0%)

All (1206) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	7	4	C
7	7	6	G
7	7	7	A
7	7	8	U
7	7	9	A
7	7	13	C
7	7	14	A
7	7	16	U
7	7	17	C
7	7	18	G
7	7	19	G
7	7	20	U
7	7	22	G
7	7	45	U
7	7	46	G
7	7	47	U

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Mol	Chain	Res	Type
7	7	48	C
7	7	49	C
7	7	50	U
7	7	56	C
7	7	59	U
7	7	60	U
7	7	61	C
7	7	63	G
7	7	73	A
8	A	11	G
8	A	32	C
8	A	33	G
8	A	34	A
8	A	41	G
8	A	46	G
8	A	49	C
8	A	50	C
8	A	53	A
8	A	62	A
8	A	68	G
8	A	72	A
8	A	73	C
8	A	74	A
8	A	77	U
8	A	78	G
8	A	81	A
8	A	82	G
8	A	83	C
8	A	85	U
8	A	86	G
8	A	87	C
8	A	90	C
8	A	91	C
8	A	94	A
8	A	95	U
8	A	98	U
8	A	117	A
8	A	119	C
8	A	128	A
8	A	130	C
8	A	147	G
8	A	151	A

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Mol	Chain	Res	Type
8	A	155	C
8	A	156	G
8	A	158	G
8	A	169	U
8	A	172	U
8	A	178	A
8	A	181	G
8	A	184	G
8	A	188	G
8	A	190	A
8	A	197	G
8	A	199	U
8	A	207	U
8	A	208	A
8	A	209	A
8	A	218	U
8	A	219	U
8	A	220	C
8	A	222	G
8	A	225	A
8	A	230	U
8	A	231	U
8	A	232	A
8	A	248	C
8	A	249	G
8	A	253	U
8	A	254	A
8	A	255	G
8	A	259	G
8	A	260	U
8	A	267	G
8	A	269	U
8	A	271	A
8	A	272	C
8	A	274	G
8	A	275	C
8	A	282	A
8	A	283	G
8	A	287	A
8	A	288	C
8	A	297	G
8	A	301	A

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Mol	Chain	Res	Type
8	A	306	A
8	A	307	G
8	A	309	G
8	A	314	A
8	A	316	C
8	A	329	A
8	A	336	C
8	A	337	A
8	A	340	G
8	A	353	C
8	A	354	G
8	A	355	G
8	A	360	C
8	A	362	G
8	A	364	A
8	A	371	A
8	A	373	U
8	A	375	U
8	A	380	C
8	A	405	A
8	A	406	C
8	A	414	G
8	A	416	G
8	A	417	U
8	A	418	G
8	A	419	A
8	A	420	U
8	A	421	G
8	A	422	A
8	A	429	U
8	A	430	C
8	A	431	G
8	A	432	G
8	A	434	U
8	A	437	U
8	A	440	A
8	A	441	G
8	A	444	C
8	A	446	G
8	A	447	U
8	A	448	U
8	A	456	A

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Mol	Chain	Res	Type
8	A	458	G
8	A	461	C
8	A	462	A
8	A	463	A
8	A	465	U
8	A	470	U
8	A	475	A
8	A	476	U
8	A	477	A
8	A	478	G
8	A	484	U
8	A	485	A
8	A	487	C
8	A	488	U
8	A	493	G
8	A	494	G
8	A	497	C
8	A	502	C
8	A	505	G
8	A	506	A
8	A	508	A
8	A	517	U
8	A	518	A
8	A	519	A
8	A	520	C
8	A	526	G
8	A	527	C
8	A	530	G
8	A	536	G
8	A	540	U
8	A	541	A
8	A	556	A
8	A	568	A
8	A	571	U
8	A	573	U
8	A	574	U
8	A	575	G
8	A	581	A
8	A	582	A
8	A	585	G
8	A	586	G
8	A	597	G

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Mol	Chain	Res	Type
8	A	604	A
8	A	605	A
8	A	619	G
8	A	628	U
8	A	629	C
8	A	630	A
8	A	631	A
8	A	632	C
8	A	643	C
8	A	651	A
8	A	659	A
8	A	662	U
8	A	665	G
8	A	674	A
8	A	686	U
8	A	695	U
8	A	704	A
8	A	711	A
8	A	719	G
8	A	732	U
8	A	740	G
8	A	742	G
8	A	757	A
8	A	758	A
8	A	759	C
8	A	763	C
8	A	764	G
8	A	786	A
8	A	802	U
8	A	803	A
8	A	812	G
8	A	824	A
8	A	826	C
8	A	829	U
8	A	830	G
8	A	837	A
8	A	841	G
8	A	845	G
8	A	849	G
8	A	852	U
8	A	856	C
8	A	861	U

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Mol	Chain	Res	Type
8	A	865	G
8	A	869	C
8	A	877	G
8	A	882	A
8	A	886	A
8	A	899	A
8	A	912	G
8	A	924	A
8	A	929	A
8	A	936	G
8	A	944	C
8	A	945	A
8	A	954	G
8	A	955	G
8	A	970	U
8	A	971	U
8	A	976	G
8	A	978	A
8	A	979	A
8	A	981	G
8	A	983	G
8	A	985	A
8	A	986	G
8	A	987	A
8	A	993	A
8	A	999	U
8	A	1002	U
8	A	1003	G
8	A	1004	A
8	A	1008	C
8	A	1013	G
8	A	1014	A
8	A	1016	A
8	A	1018	U
8	A	1019	C
8	A	1023	G
8	A	1024	A
8	A	1028	A
8	A	1031	A
8	A	1033	G
8	A	1034	U
8	A	1035	C

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Mol	Chain	Res	Type
8	A	1036	C
8	A	1039	U
8	A	1041	C
8	A	1047	C
8	A	1058	G
8	A	1059	U
8	A	1061	G
8	A	1063	G
8	A	1066	U
8	A	1074	G
8	A	1076	C
8	A	1080	U
8	A	1088	U
8	A	1089	G
8	A	1096	U
8	A	1104	G
8	A	1105	U
8	A	1111	A
8	A	1118	G
8	A	1127	G
8	A	1134	G
8	A	1137	G
8	A	1139	C
8	A	1142	C
8	A	1144	U
8	A	1149	U
8	A	1153	G
8	A	1155	A
8	A	1163	G
8	A	1166	A
8	A	1168	U
8	A	1169	G
8	A	1176	A
8	A	1177	C
8	A	1180	A
8	A	1186	G
8	A	1187	G
8	A	1190	G
8	A	1192	U
8	A	1193	G
8	A	1200	A
8	A	1205	A

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Mol	Chain	Res	Type
8	A	1206	A
8	A	1207	A
8	A	1210	A
8	A	1211	U
8	A	1212	C
8	A	1214	U
8	A	1215	G
8	A	1216	C
8	A	1221	U
8	A	1222	A
8	A	1223	U
8	A	1226	C
8	A	1234	A
8	A	1236	A
8	A	1247	A
8	A	1249	U
8	A	1250	G
8	A	1266	A
8	A	1269	G
8	A	1277	G
8	A	1279	G
8	A	1283	A
8	A	1289	A
8	A	1290	U
8	A	1294	A
8	A	1295	C
8	A	1296	A
8	A	1306	U
8	A	1308	A
8	A	1311	U
8	A	1314	G
8	A	1317	C
8	A	1329	C
8	A	1337	C
8	A	1340	G
8	A	1345	U
8	A	1349	A
8	A	1355	A
8	A	1356	G
8	A	1362	G
8	A	1369	A
8	A	1370	G

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Mol	Chain	Res	Type
8	A	1373	U
8	A	1381	U
8	A	1383	A
8	A	1384	A
8	A	1385	U
8	A	1386	A
8	A	1387	C
8	A	1388	G
8	A	1396	G
8	A	1406	C
8	A	1410	G
8	A	1414	G
8	A	1428	G
8	A	1435	A
8	A	1443	A
8	A	1445	U
8	A	1446	C
8	A	1447	G
8	A	1448	G
8	A	1451	A
8	A	1453	G
8	A	1454	U
8	A	1455	A
8	A	1459	U
8	A	1462	U
8	A	1463	A
8	A	1464	G
8	A	1465	G
8	A	1466	A
8	A	1467	G
8	A	1468	C
8	A	1471	G
8	A	1473	C
8	A	1474	G
8	A	1500	U
8	A	1503	A
8	A	1504	G
8	A	1510	A
8	A	1513	A
8	A	1516	U
8	A	1539	G
8	A	1540	G

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Mol	Chain	Res	Type
28	U	2	G
28	U	6	G
28	U	8	U
28	U	16	U
28	U	17(A)	G
28	U	18	G
28	U	20	U
28	U	24	A
28	U	42	G
28	U	46	G
28	U	47	U
28	U	48	C
28	U	55	U
28	U	56	C
28	U	57	G
28	U	58	A
28	U	60	U
28	U	68	G
28	U	76	A
29	V	436	A
29	V	438	C
29	V	439	A
29	V	442	G
29	V	443	C
29	V	444	C
29	V	446	U
29	V	447	G
29	V	448	U
29	V	449	A
29	V	450	C
29	V	451	G
29	V	452	U
29	V	453	C
29	V	454	G
29	V	455	C
29	V	458	U
29	V	459	C
29	V	460	G
29	V	461	G
29	V	462	A
30	Y	4	G
30	Y	10	G

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Mol	Chain	Res	Type
30	Y	12	U
30	Y	14	G
30	Y	18	A
30	Y	20	A
30	Y	22	G
30	Y	23	U
30	Y	33	U
30	Y	34	C
30	Y	39	A
30	Y	42	G
30	Y	43	A
30	Y	44	A
30	Y	45	C
30	Y	46	A
30	Y	49	G
30	Y	53	U
30	Y	64	A
30	Y	71	A
30	Y	73	G
30	Y	74	G
30	Y	75	U
30	Y	85	U
30	Y	86	U
30	Y	87	U
30	Y	88	C
30	Y	94	G
30	Y	97	A
30	Y	100	G
30	Y	101	U
30	Y	103	G
30	Y	107	G
30	Y	108	C
30	Y	109	C
52	X	4	U
52	X	5	A
52	X	6	A
52	X	12	A
52	X	13	A
52	X	15	G
52	X	34	U
52	X	35	G
52	X	46	C

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Mol	Chain	Res	Type
52	X	60	G
52	X	61	A
52	X	62	C
52	X	63	G
52	X	71	A
52	X	75	G
52	X	76	C
52	X	77	U
52	X	78	U
52	X	80	G
52	X	86	C
52	X	88	G
52	X	91	A
52	X	92	G
52	X	93	C
52	X	94	A
52	X	95	A
52	X	99	U
52	X	100	U
52	X	101	G
52	X	102	A
52	X	113	U
52	X	117	A
52	X	118	A
52	X	119	U
52	X	125	A
52	X	126	A
52	X	127	C
52	X	130	A
52	X	140	A
52	X	148	G
52	X	161	A
52	X	162	A
52	X	164	U
52	X	165	C
52	X	176	A
52	X	177	G
52	X	178	A
52	X	179	A
52	X	183	A
52	X	184	G
52	X	189	G

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Mol	Chain	Res	Type
52	X	199	A
52	X	200	A
52	X	202	A
52	X	207	A
52	X	218	G
52	X	219	A
52	X	221	G
52	X	224	A
52	X	225	A
52	X	226	A
52	X	229	A
52	X	231	A
52	X	232	U
52	X	233	G
52	X	234	C
52	X	236	A
52	X	251	G
52	X	252	C
52	X	253	G
52	X	258	A
52	X	268	A
52	X	275	A
52	X	276	C
52	X	279	A
52	X	281	A
52	X	282	G
52	X	283	G
52	X	284	C
52	X	285	U
52	X	286	U
52	X	287	G
52	X	288	C
52	X	289	C
52	X	291	C
52	X	292	U
52	X	294	G
52	X	295	G
52	X	296	G
52	X	298	U
52	X	302	A
52	X	307	A
52	X	308	C

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Mol	Chain	Res	Type
52	X	309	U
52	X	310	C
52	X	329	A
52	X	330	A
52	X	332	G
52	X	334	G
52	X	336	U
52	X	337	A
52	X	338	G
52	X	345	A
52	X	346	G
52	X	352	G
52	X	354	A
52	X	355	A
52	X	367	G
52	X	373	A
52	X	374	A
52	X	377	G
52	X	382	G
52	X	389	A
52	X	390	A
52	X	392	C
52	X	395	C
52	X	396	G
52	X	397	U
52	X	399	C
52	X	407	A
52	X	408	G
52	X	417	G
52	X	418	A
52	X	419	G
52	X	420	U
52	X	433	G
52	X	434	U
52	X	442	C
52	X	448	A
52	X	451	C
52	X	452	C
52	X	453	G
52	X	458	G
52	X	459	A
52	X	471	G

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Mol	Chain	Res	Type
52	X	476	A
52	X	483	C
52	X	491	C
52	X	495	U
52	X	498	U
52	X	502	C
52	X	504	A
52	X	512	G
52	X	520	G
52	X	526	A
52	X	528	G
52	X	540	G
52	X	542	G
52	X	547	A
52	X	548	A
52	X	550	G
52	X	551	A
52	X	552	G
52	X	554	U
52	X	555	C
52	X	556	C
52	X	564	G
52	X	566	G
52	X	567	U
52	X	573	C
52	X	575	A
52	X	576	G
52	X	577	U
52	X	578	A
52	X	590	U
52	X	592	A
52	X	593	A
52	X	594	C
52	X	595	G
52	X	607	G
52	X	617	G
52	X	618	A
52	X	619	A
52	X	630	A
52	X	632	U
52	X	644	G
52	X	646	A

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Mol	Chain	Res	Type
52	X	647	A
52	X	658	A
52	X	673	A
52	X	680	G
52	X	683	A
52	X	691	U
52	X	697	G
52	X	698	C
52	X	699	A
52	X	700	U
52	X	701	G
52	X	702	A
52	X	717	A
52	X	719	C
52	X	722	A
52	X	729	G
52	X	733	U
52	X	752	A
52	X	762	A
52	X	763	A
52	X	765	A
52	X	769	A
52	X	777	C
52	X	794	U
52	X	795	G
52	X	812	G
52	X	822	G
52	X	823	G
52	X	824	G
52	X	829	A
52	X	830	A
52	X	831	U
52	X	832	G
52	X	836	A
52	X	837	U
52	X	839	G
52	X	847	A
52	X	852	G
52	X	859	C
52	X	866	A
52	X	874	U
52	X	875	U

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Mol	Chain	Res	Type
52	X	878	G
52	X	892	U
52	X	903	G
52	X	906	G
52	X	913	A
52	X	919	U
52	X	928	G
52	X	929	G
52	X	930	C
52	X	933	C
52	X	934	U
52	X	936	C
52	X	940	G
52	X	942	U
52	X	943	A
52	X	944	C
52	X	957	A
52	X	959	C
52	X	964	A
52	X	980	C
52	X	987	A
52	X	991	A
52	X	992	G
52	X	999	A
52	X	1001	U
52	X	1004	U
52	X	1007	G
52	X	1019	A
52	X	1020	A
52	X	1029	A
52	X	1030	G
52	X	1031	C
52	X	1042	A
52	X	1046	A
52	X	1049	G
52	X	1055	A
52	X	1058	U
52	X	1059	A
52	X	1061	A
52	X	1065	U
52	X	1067	A
52	X	1068	G

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Mol	Chain	Res	Type
52	X	1069	U
52	X	1072	A
52	X	1073	A
52	X	1079	U
52	X	1085	G
52	X	1090	U
52	X	1093	G
52	X	1100	A
52	X	1102	G
52	X	1103	A
52	X	1107	U
52	X	1108	G
52	X	1109	G
52	X	1111	U
52	X	1113	A
52	X	1114	G
52	X	1116	A
52	X	1118	C
52	X	1119	A
52	X	1121	C
52	X	1122	C
52	X	1123	A
52	X	1124	C
52	X	1125	C
52	X	1126	A
52	X	1127	U
52	X	1130	A
52	X	1131	A
52	X	1133	G
52	X	1134	A
52	X	1136	U
52	X	1137	G
52	X	1138	C
52	X	1139	G
52	X	1140	U
52	X	1141	A
52	X	1142	A
52	X	1143	U
52	X	1144	A
52	X	1145	G
52	X	1147	U
52	X	1157	A

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Mol	Chain	Res	Type
52	X	1158	G
52	X	1159	U
52	X	1160	G
52	X	1161	A
52	X	1173	A
52	X	1177	G
52	X	1178	U
52	X	1179	A
52	X	1180	C
52	X	1181	C
52	X	1182	G
52	X	1185	G
52	X	1187	U
52	X	1188	A
52	X	1201	A
52	X	1216	C
52	X	1227	G
52	X	1231	G
52	X	1236	G
52	X	1243	A
52	X	1244	A
52	X	1248	C
52	X	1250	G
52	X	1260	A
52	X	1265	A
52	X	1267	G
52	X	1276	G
52	X	1277	A
52	X	1278	G
52	X	1293	A
52	X	1296	G
52	X	1311	G
52	X	1312	A
52	X	1315	G
52	X	1323	A
52	X	1339	A
52	X	1340	A
52	X	1364	C
52	X	1368	U
52	X	1369	C
52	X	1370	C
52	X	1371	G

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Mol	Chain	Res	Type
52	X	1388	A
52	X	1389	C
52	X	1399	G
52	X	1404	A
52	X	1407	G
52	X	1417	A
52	X	1418	U
52	X	1423	A
52	X	1425	C
52	X	1426	A
52	X	1427	G
52	X	1434	A
52	X	1435	U
52	X	1442	A
52	X	1450	C
52	X	1452	C
52	X	1455	C
52	X	1458	U
52	X	1459	U
52	X	1460	G
52	X	1461	A
52	X	1465	A
52	X	1471	G
52	X	1474	C
52	X	1485	A
52	X	1489	U
52	X	1490	A
52	X	1499	A
52	X	1500	U
52	X	1502	G
52	X	1505	U
52	X	1506	A
52	X	1507	U
52	X	1508	C
52	X	1516	A
52	X	1525	G
52	X	1526	G
52	X	1528	U
52	X	1529	G
52	X	1536	A
52	X	1537	G
52	X	1539	C

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Mol	Chain	Res	Type
52	X	1540	A
52	X	1543	U
52	X	1548	U
52	X	1552	C
52	X	1553	A
52	X	1563	G
52	X	1566	G
52	X	1567	U
52	X	1568	G
52	X	1569	A
52	X	1570	U
52	X	1571	G
52	X	1601	A
52	X	1602	U
52	X	1608	A
52	X	1617	A
52	X	1626	U
52	X	1631	A
52	X	1632	G
52	X	1653	A
52	X	1655	A
52	X	1661	A
52	X	1667	A
52	X	1693	C
52	X	1696	G
52	X	1697	A
52	X	1708	U
52	X	1712	G
52	X	1717	C
52	X	1719	G
52	X	1738	U
52	X	1739	C
52	X	1741	G
52	X	1743	A
52	X	1745	A
52	X	1757	G
52	X	1758	U
52	X	1759	U
52	X	1760	A
52	X	1761	G
52	X	1765	G
52	X	1767	A

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Mol	Chain	Res	Type
52	X	1774	A
52	X	1776	A
52	X	1779	G
52	X	1785	G
52	X	1786	U
52	X	1792	G
52	X	1793	G
52	X	1797	A
52	X	1802	A
52	X	1803	C
52	X	1805	G
52	X	1810	G
52	X	1811	C
52	X	1813	A
52	X	1820	A
52	X	1828	G
52	X	1829	C
52	X	1830	G
52	X	1831	A
52	X	1832	A
52	X	1837	U
52	X	1845	A
52	X	1848	A
52	X	1858	A
52	X	1877	A
52	X	1882	A
52	X	1883	A
52	X	1884	G
52	X	1898	G
52	X	1899	U
52	X	1900	A
52	X	1901	A
52	X	1902	G
52	X	1910	G
52	X	1912	G
52	X	1914	A
52	X	1922	C
52	X	1935	G
52	X	1943	C
52	X	1944	U
52	X	1945	A
52	X	1958	G

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Mol	Chain	Res	Type
52	X	1959	G
52	X	1960	U
52	X	1965	A
52	X	1967	A
52	X	1971	C
52	X	1972	U
52	X	1984	U
52	X	1993	G
52	X	1995	A
52	X	1996	C
52	X	1999	A
52	X	2000	A
52	X	2001	G
52	X	2020	U
52	X	2022	U
52	X	2025	C
52	X	2026	A
52	X	2049	A
52	X	2050	G
52	X	2052	A
52	X	2059	A
52	X	2060	A
52	X	2061	G
52	X	2062	A
52	X	2063	U
52	X	2064	G
52	X	2065	C
52	X	2072	C
52	X	2080	A
52	X	2081	G
52	X	2084	C
52	X	2085	G
52	X	2088	A
52	X	2089	A
52	X	2090	G
52	X	2097	U
52	X	2098	G
52	X	2121	U
52	X	2122	G
52	X	2123	A
52	X	2127	U
52	X	2129	G

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Mol	Chain	Res	Type
52	X	2130	G
52	X	2131	U
52	X	2132	A
52	X	2133	C
52	X	2134	A
52	X	2135	G
52	X	2136	C
52	X	2139	G
52	X	2140	U
52	X	2141	A
52	X	2143	A
52	X	2145	G
52	X	2146	A
52	X	2147	U
52	X	2148	A
52	X	2149	G
52	X	2151	U
52	X	2152	A
52	X	2153	G
52	X	2154	G
52	X	2155	A
52	X	2157	C
52	X	2159	U
52	X	2160	U
52	X	2161	G
52	X	2163	A
52	X	2165	A
52	X	2166	C
52	X	2168	G
52	X	2169	G
52	X	2170	A
52	X	2171	G
52	X	2173	G
52	X	2174	C
52	X	2175	C
52	X	2176	A
52	X	2181	C
52	X	2183	G
52	X	2184	U
52	X	2185	G
52	X	2186	G
52	X	2188	G

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Mol	Chain	Res	Type
52	X	2190	C
52	X	2191	A
52	X	2193	C
52	X	2195	G
52	X	2197	G
52	X	2198	G
52	X	2199	G
52	X	2200	A
52	X	2201	U
52	X	2203	C
52	X	2204	U
52	X	2205	A
52	X	2206	C
52	X	2208	C
52	X	2209	U
52	X	2210	G
52	X	2216	A
52	X	2218	U
52	X	2220	A
52	X	2222	C
52	X	2223	U
52	X	2224	U
52	X	2227	A
52	X	2232	G
52	X	2233	C
52	X	2240	U
52	X	2241	A
52	X	2245	G
52	X	2246	G
52	X	2252	A
52	X	2254	A
52	X	2267	G
52	X	2268	G
52	X	2278	U
52	X	2280	G
52	X	2295	A
52	X	2297	A
52	X	2312	C
52	X	2315	A
52	X	2316	A
52	X	2317	A
52	X	2318	G

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Mol	Chain	Res	Type
52	X	2325	U
52	X	2326	C
52	X	2334	U
52	X	2335	U
52	X	2337	G
52	X	2338	A
52	X	2339	A
52	X	2349	A
52	X	2350	G
52	X	2351	A
52	X	2354	G
52	X	2356	A
52	X	2363	C
52	X	2364	A
52	X	2374	G
52	X	2379	C
52	X	2386	U
52	X	2387	A
52	X	2390	A
52	X	2400	G
52	X	2404	G
52	X	2408	G
52	X	2412	G
52	X	2414	C
52	X	2415	U
52	X	2417	A
52	X	2430	U
52	X	2431	U
52	X	2432	C
52	X	2435	C
52	X	2445	C
52	X	2452	U
52	X	2454	A
52	X	2457	G
52	X	2458	G
52	X	2459	A
52	X	2469	C
52	X	2470	C
52	X	2476	G
52	X	2477	A
52	X	2494	C
52	X	2503	C

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Mol	Chain	Res	Type
52	X	2505	A
52	X	2507	A
52	X	2516	G
52	X	2523	G
52	X	2527	C
52	X	2531	G
52	X	2532	A
52	X	2533	U
52	X	2534	G
52	X	2547	A
52	X	2549	C
52	X	2558	G
52	X	2562	U
52	X	2564	G
52	X	2579	G
52	X	2583	U
52	X	2584	U
52	X	2595	A
52	X	2596	G
52	X	2601	A
52	X	2611	G
52	X	2613	U
52	X	2614	U
52	X	2615	C
52	X	2628	G
52	X	2630	C
52	X	2631	A
52	X	2632	G
52	X	2637	G
52	X	2638	U
52	X	2642	U
52	X	2658	A
52	X	2659	G
52	X	2671	G
52	X	2674	G
52	X	2675	C
52	X	2688	G
52	X	2689	A
52	X	2690	G
52	X	2692	G
52	X	2711	G
52	X	2714	G

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Mol	Chain	Res	Type
52	X	2718	U
52	X	2719	A
52	X	2720	C
52	X	2743	G
52	X	2755	U
52	X	2761	G
52	X	2762	A
52	X	2764	G
52	X	2768	U
52	X	2773	G
52	X	2777	A
52	X	2781	C
52	X	2785	U
52	X	2790	A
52	X	2793	A
52	X	2794	A
52	X	2795	G
52	X	2806	G
52	X	2807	A
52	X	2809	G
52	X	2818	C
52	X	2822	C
52	X	2824	G
52	X	2825	C
52	X	2826	A
52	X	2827	A
52	X	2830	A
52	X	2831	A
52	X	2833	U
52	X	2843	G
52	X	2845	A
52	X	2849	U
52	X	2850	G
52	X	2855	G
52	X	2858	U
52	X	2859	G
52	X	2868	G
52	X	2872	U
52	X	2873	G
52	X	2874	G
52	X	2886	C
52	X	2891	G

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Mol	Chain	Res	Type
52	X	2892	G
52	X	2893	A
52	X	2897	G
52	X	2901	G
52	X	2905	C
52	X	2908	A
52	X	2909	U
52	X	2911	G
52	X	2916	A
52	X	2917	G
52	X	2918	G
52	X	2919	A
52	X	2920	C
52	X	2921	U

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	7	19	G
7	7	21	A
8	A	81	A
8	A	306	A
8	A	372	A
8	A	445	U
8	A	455	G
8	A	487	C
8	A	573	U
8	A	848	G
8	A	855	G
8	A	1088	U
8	A	1211	U
8	A	1276	C
8	A	1369	A
8	A	1463	A
30	Y	33	U
30	Y	48	G
52	X	101	G
52	X	164	U
52	X	252	C
52	X	441	C
52	X	450	U
52	X	511	U

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Mol	Chain	Res	Type
52	X	549	A
52	X	751	G
52	X	762	A
52	X	1045	U
52	X	1176	U
52	X	1451	U
52	X	1507	U
52	X	1525	G
52	X	1567	U
52	X	1882	A
52	X	1900	A
52	X	2133	C
52	X	2192	U
52	X	2334	U
52	X	2337	G
52	X	2805	A
52	X	2904	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](#)

There are no ligands in this entry.

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.

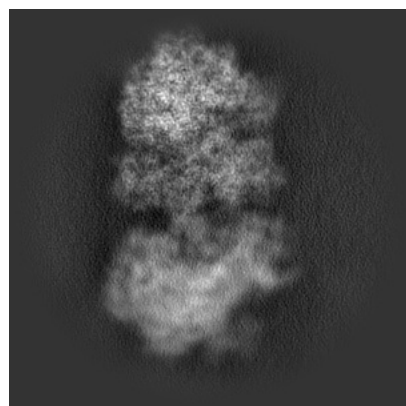
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18901. These allow visual inspection of the internal detail of the map and identification of artifacts.

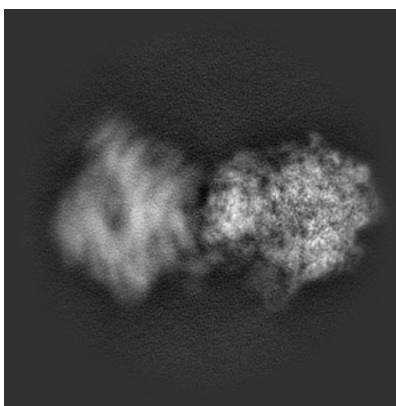
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

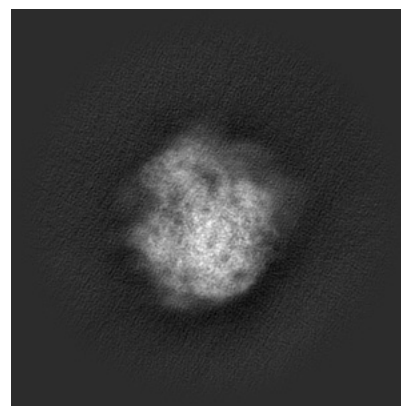
6.1.1 Primary map



X

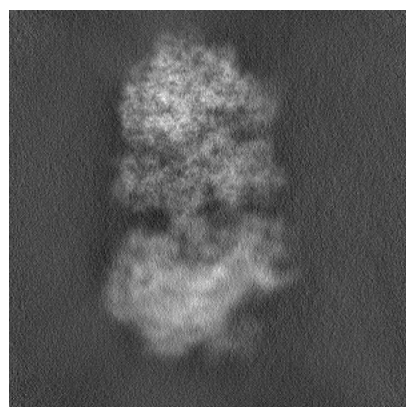


Y

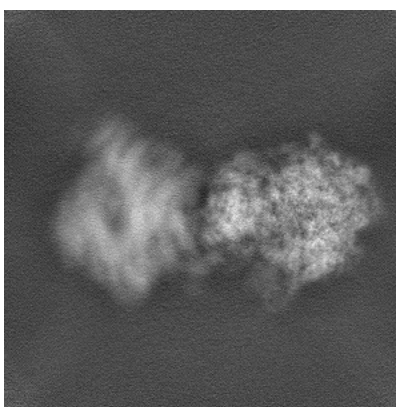


Z

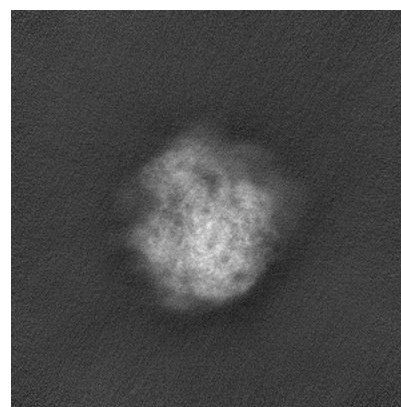
6.1.2 Raw map



X



Y

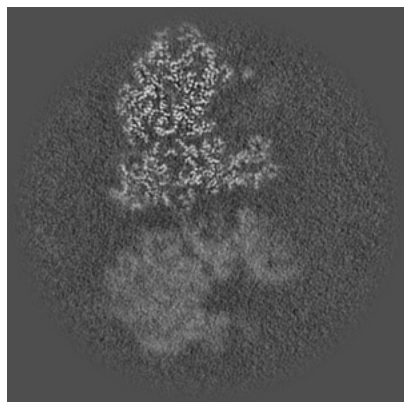


Z

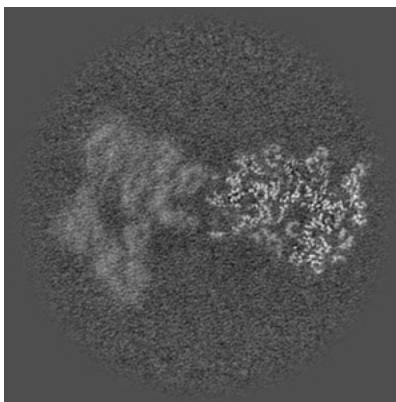
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

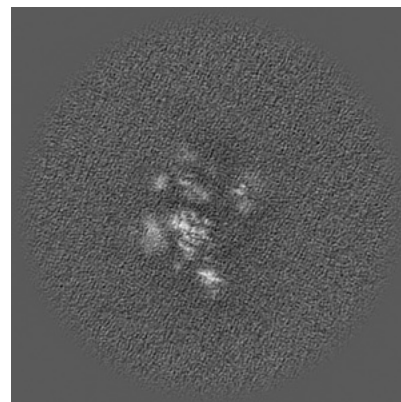
6.2.1 Primary map



X Index: 250

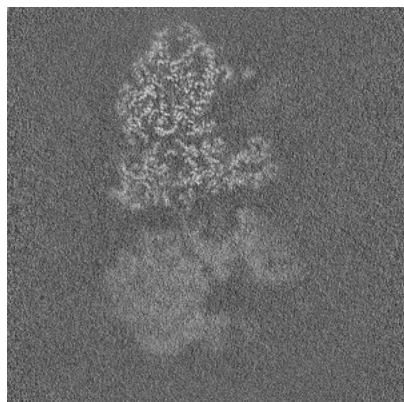


Y Index: 250

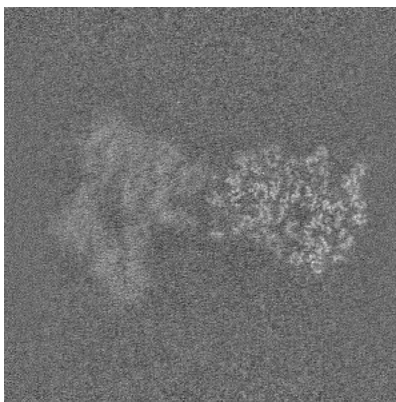


Z Index: 250

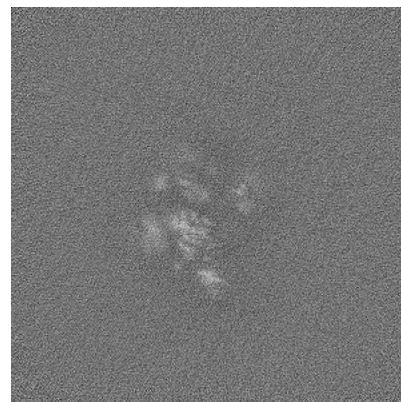
6.2.2 Raw map



X Index: 250



Y Index: 250

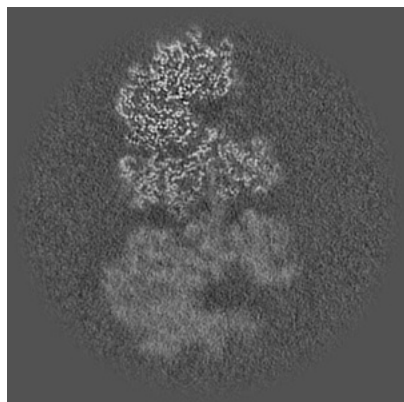


Z Index: 250

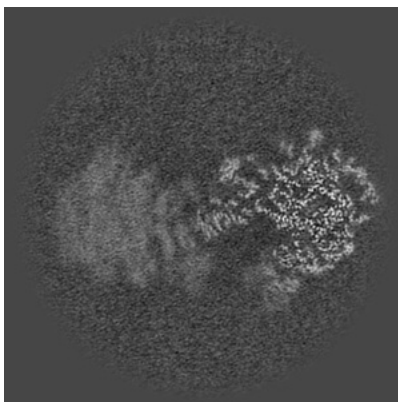
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

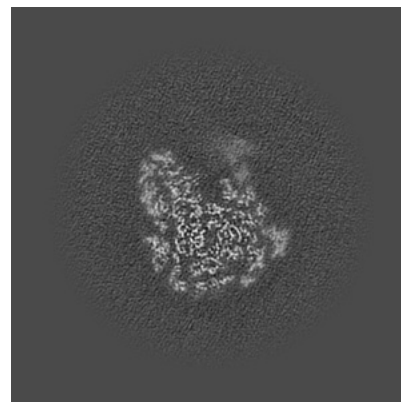
6.3.1 Primary map



X Index: 238

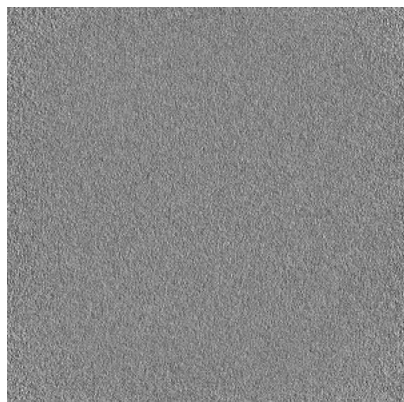


Y Index: 209

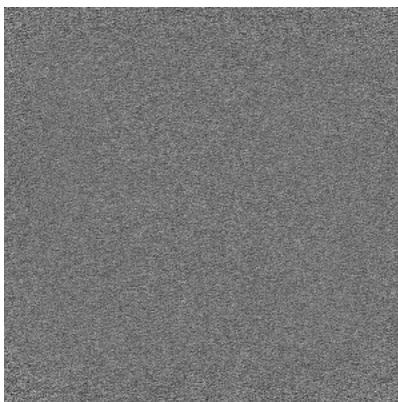


Z Index: 387

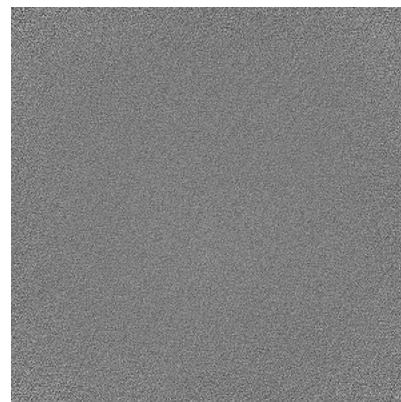
6.3.2 Raw map



X Index: 0



Y Index: 0

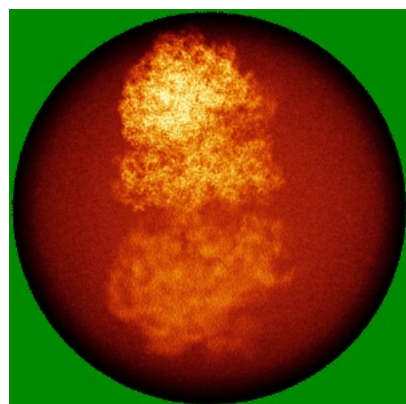


Z Index: 0

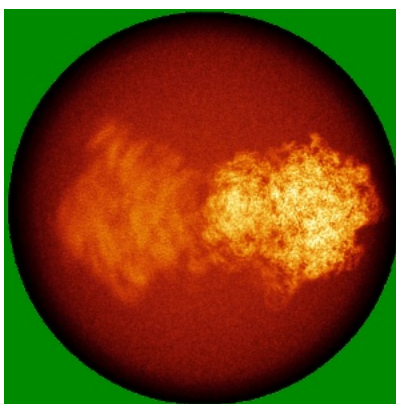
The images above show the largest variance slices of the map in three orthogonal directions.

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

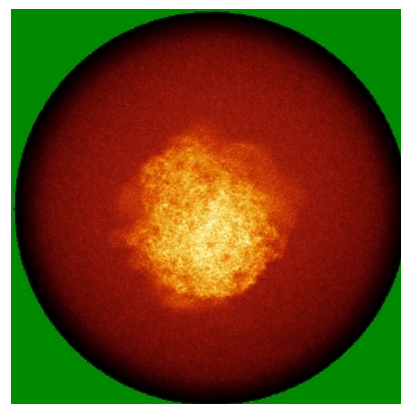
6.4.1 Primary map



X

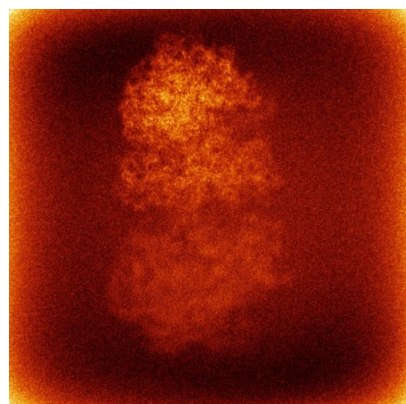


Y

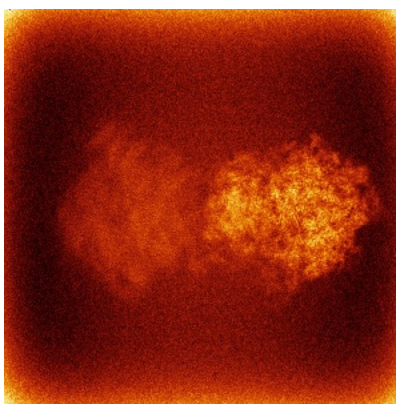


Z

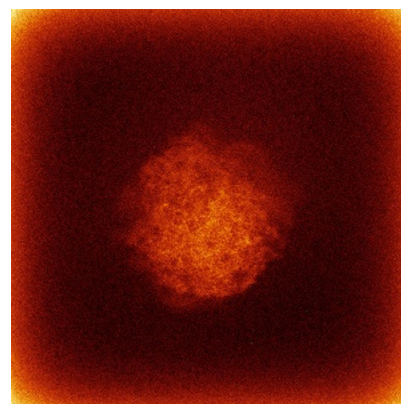
6.4.2 Raw map



X



Y

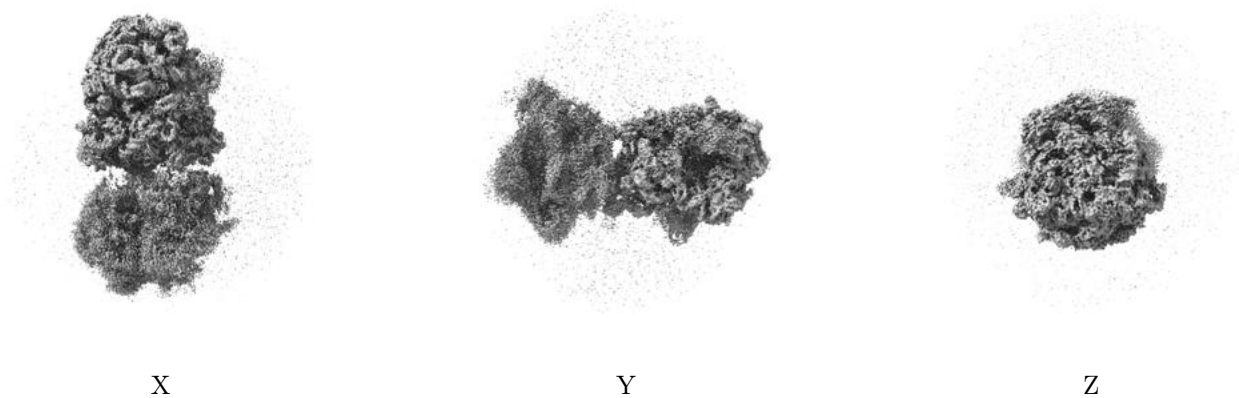


Z

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.

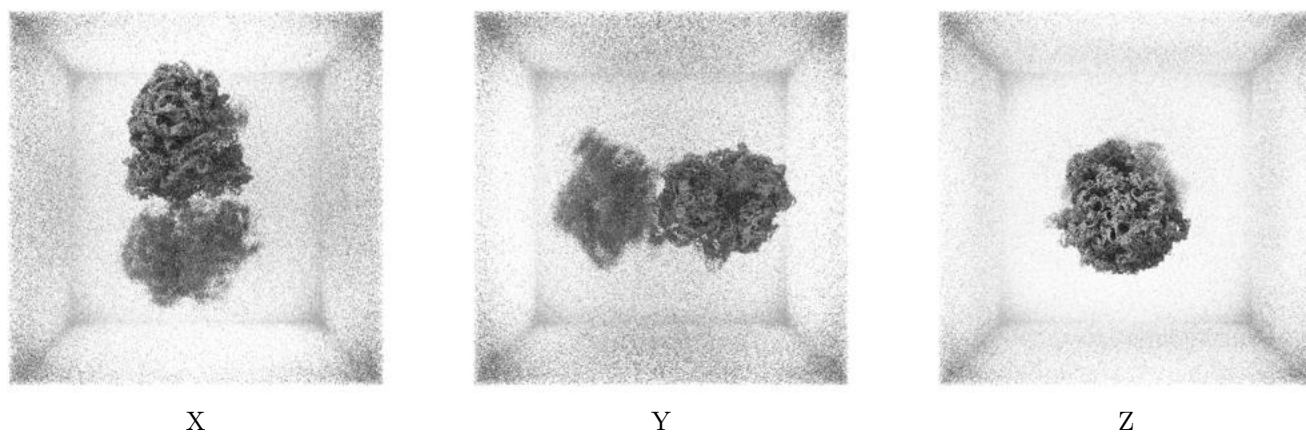
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

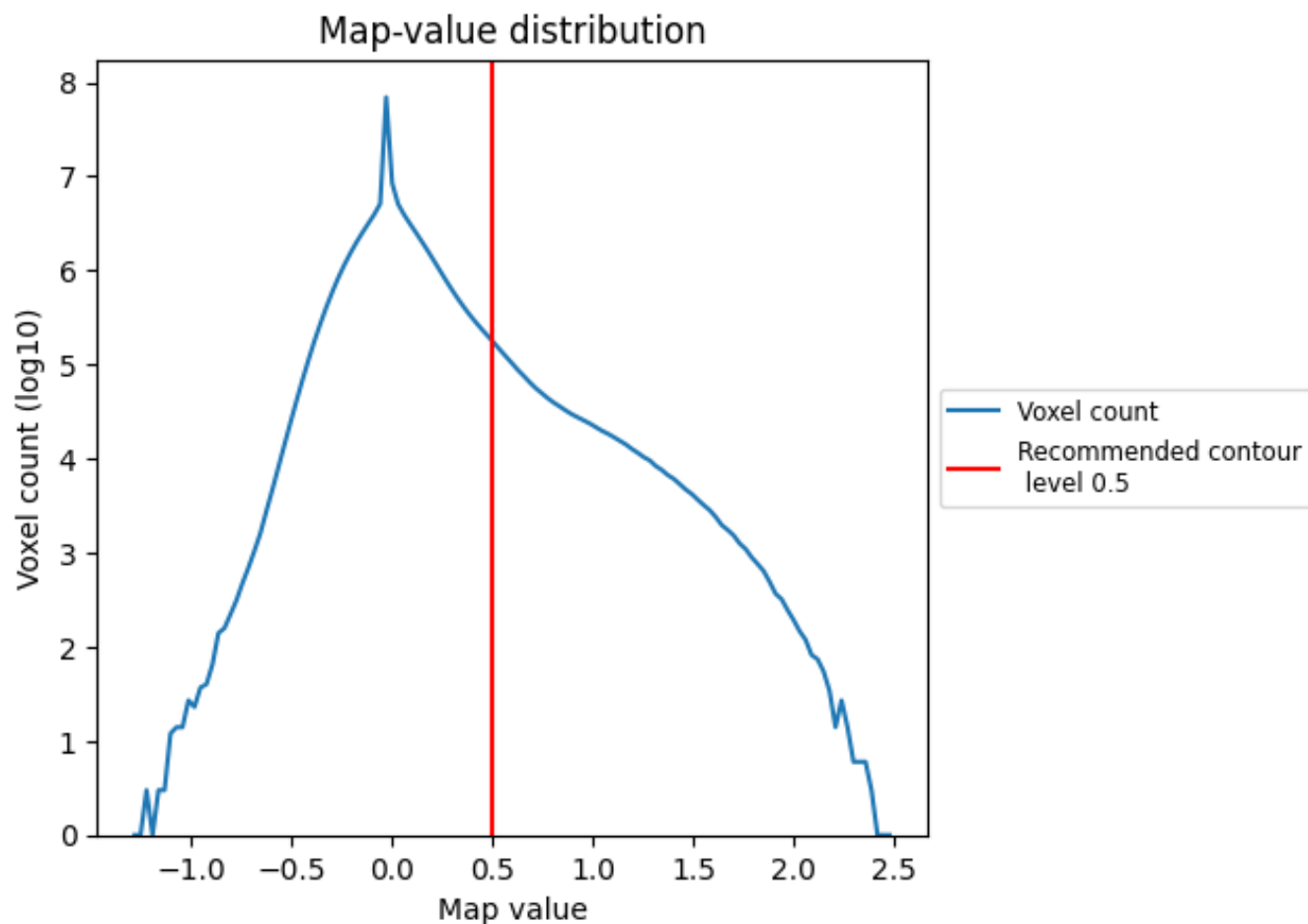
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

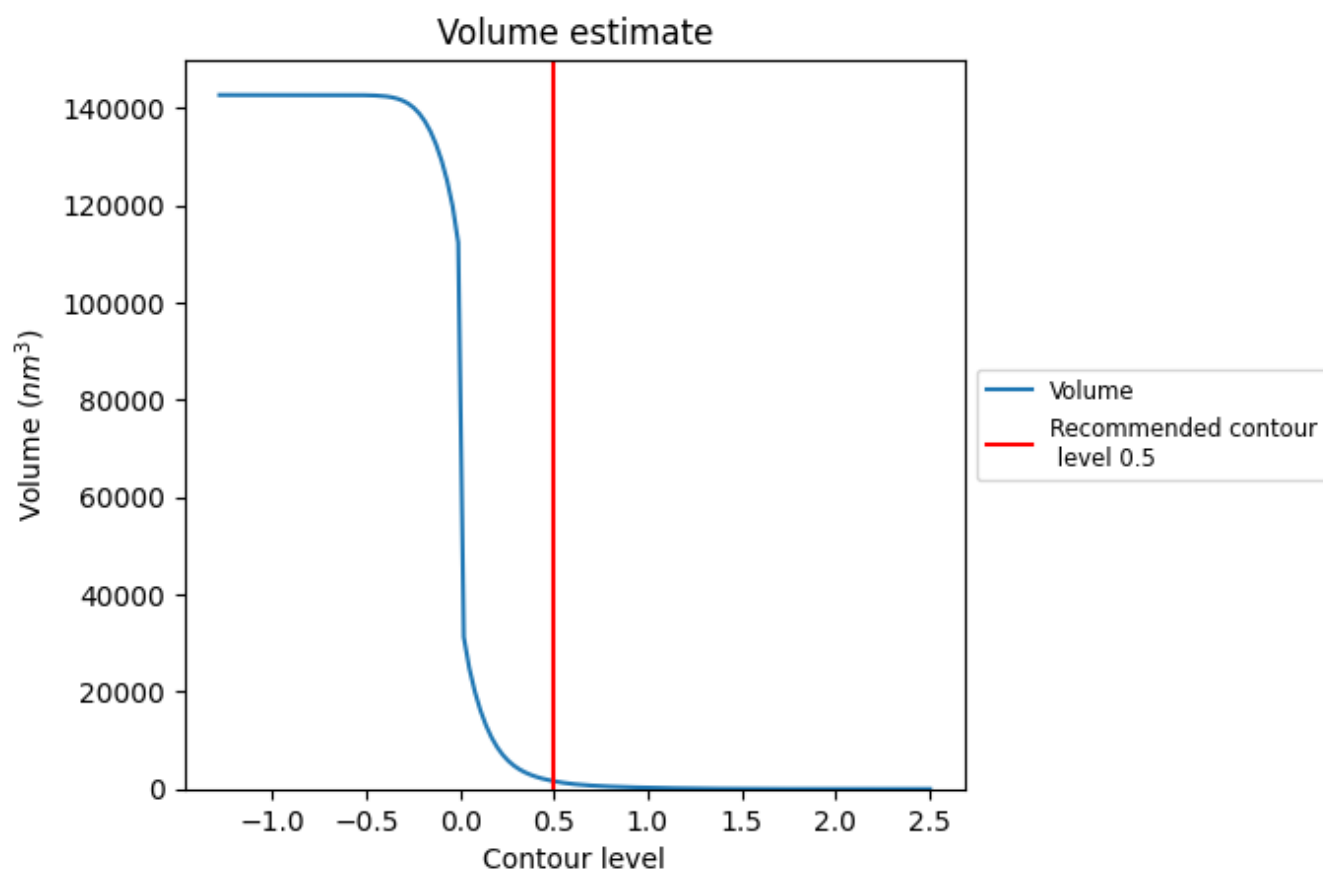
This section contains the results of statistical analysis of the map.

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.

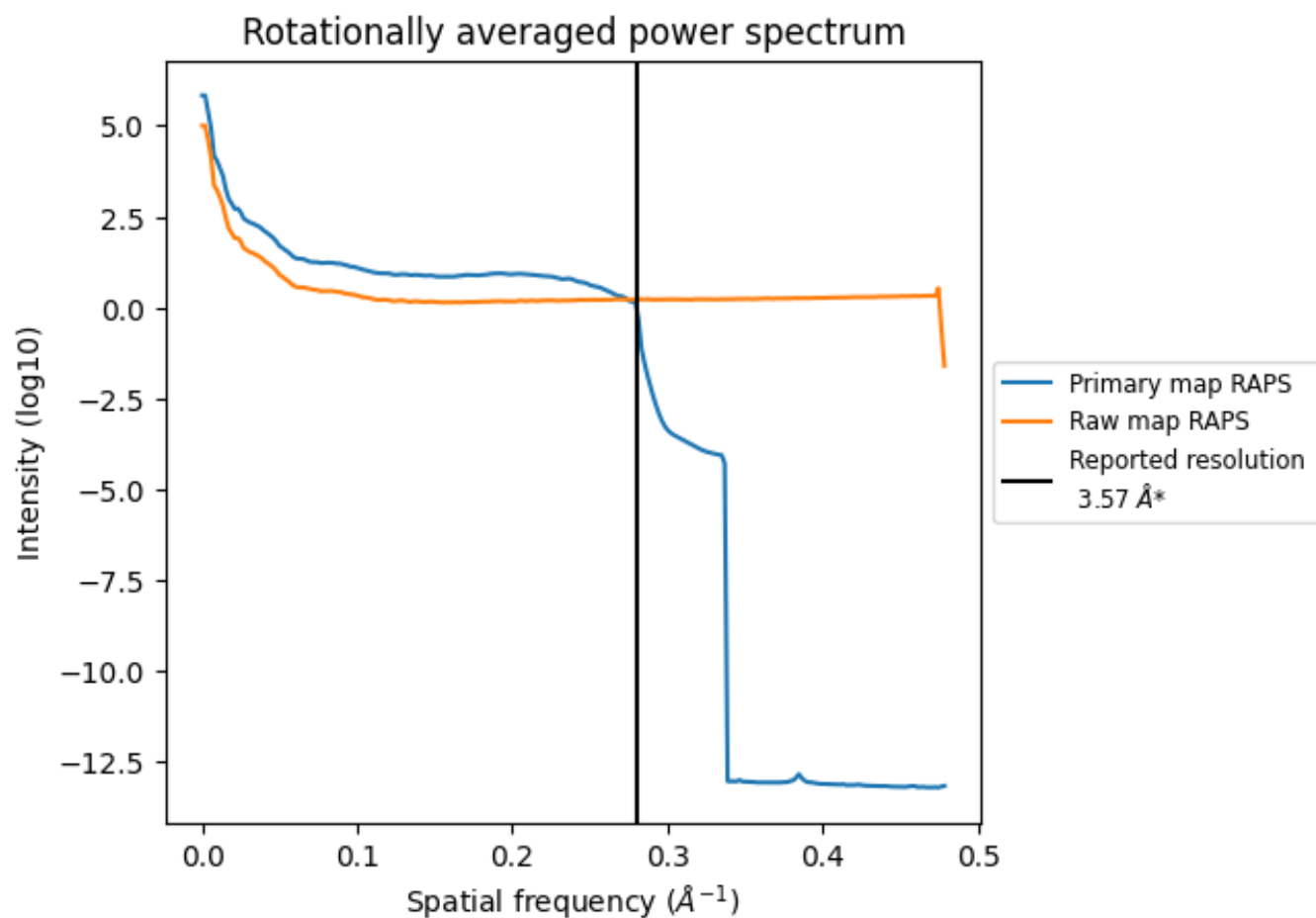
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1594 nm³; this corresponds to an approximate mass of 1440 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 ⓘ

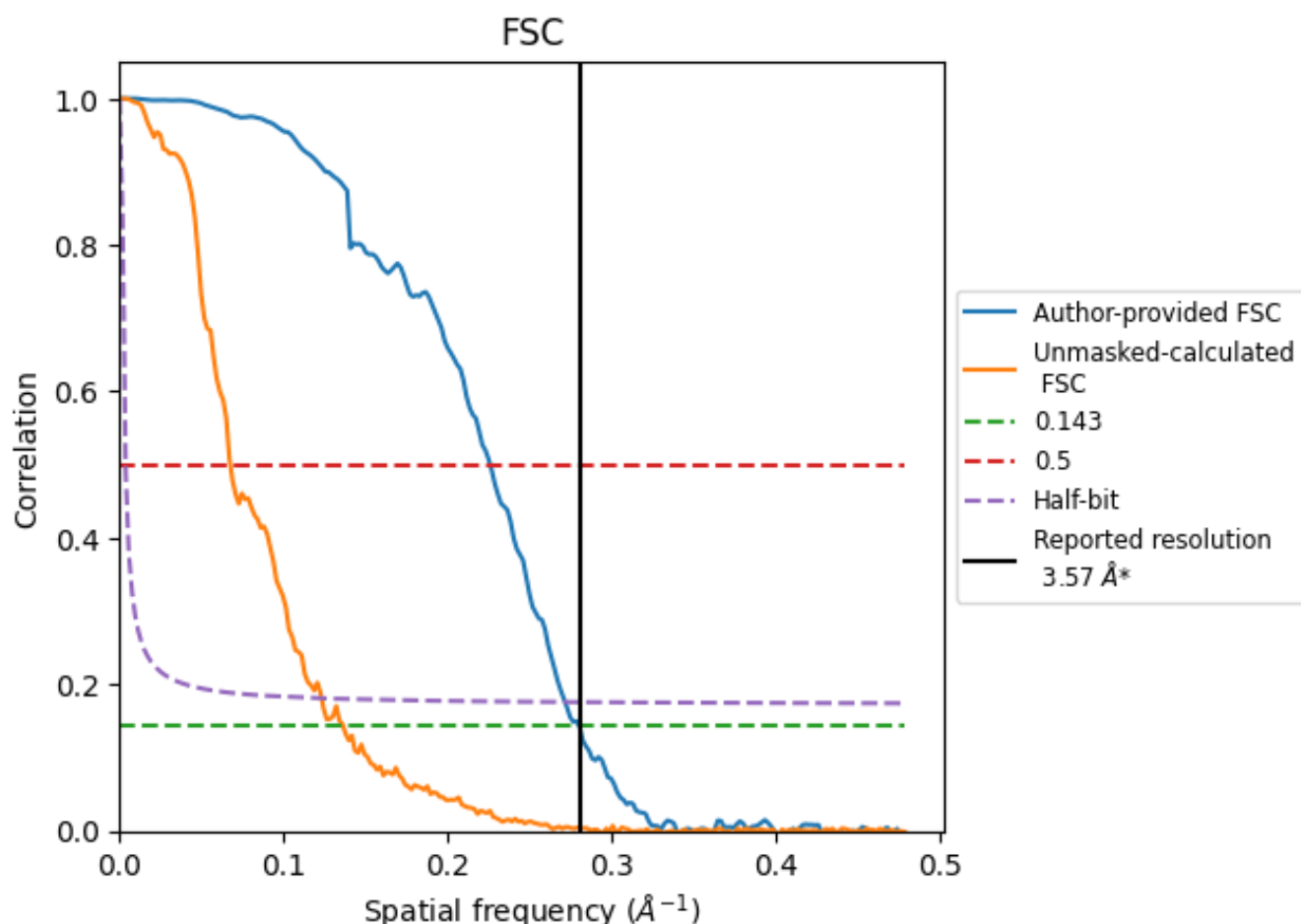


*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

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 0.280 Å⁻¹

8.2 Resolution estimates [i](#)

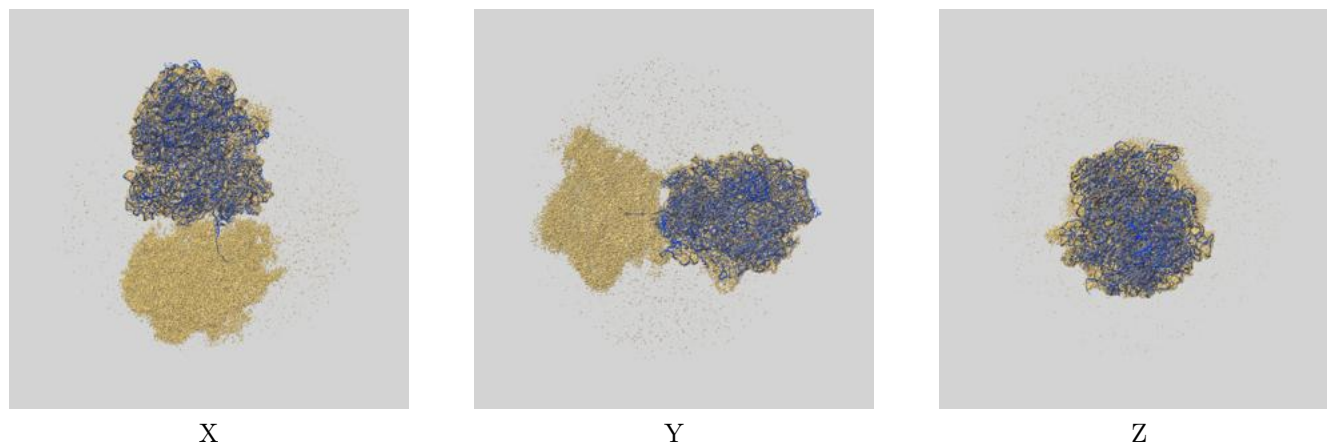
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	4.43	3.68
Unmasked-calculated*	7.34	14.81	8.12

*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 7.34 differs from the reported value 3.57 by more than 10 %

9 Map-model fit [i](#)

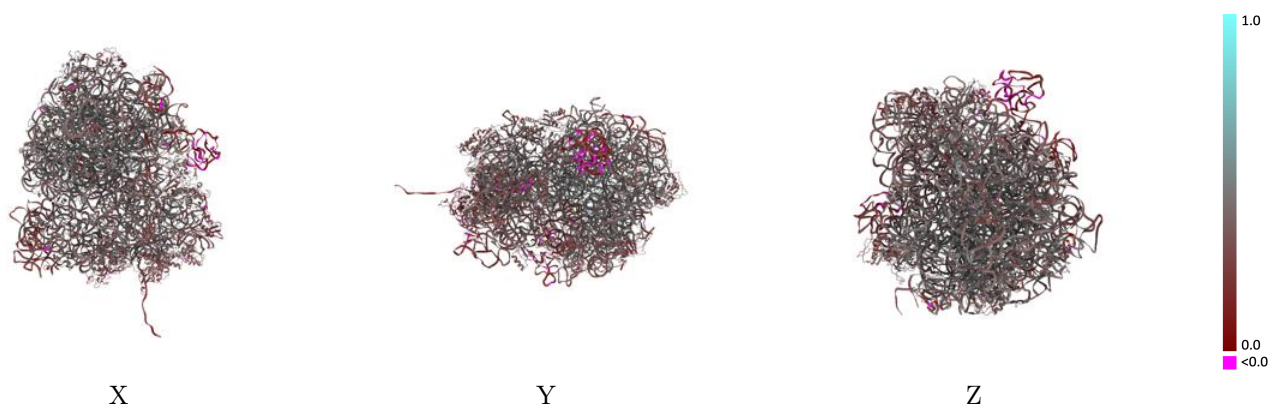
This section contains information regarding the fit between EMDB map EMD-18901 and PDB model 8R55. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



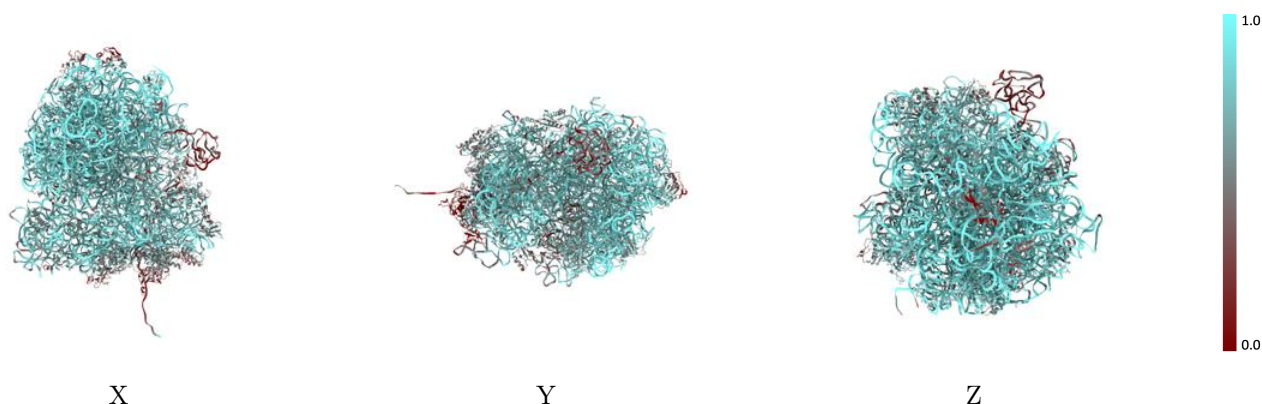
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



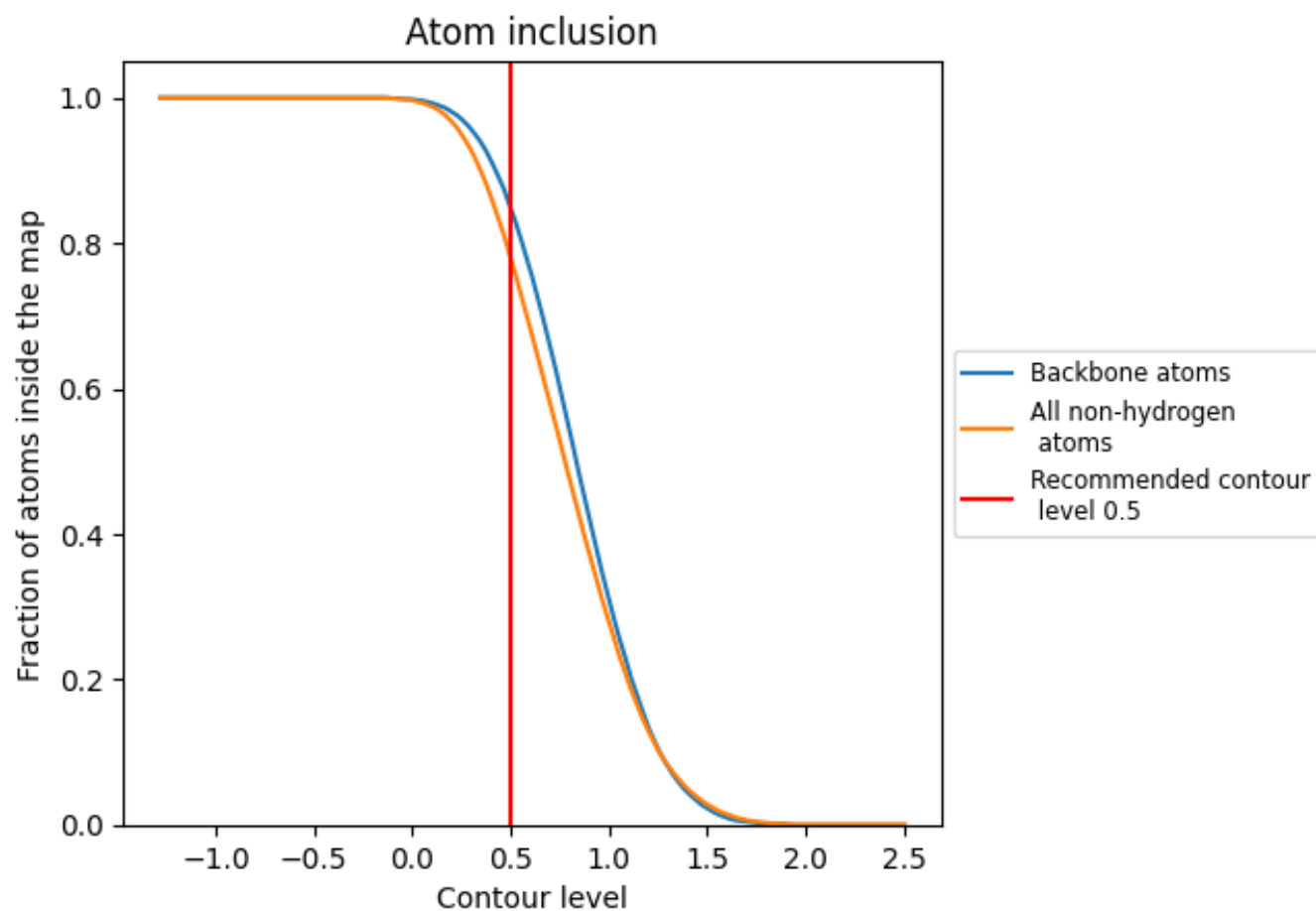
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.3860
0	 0.7630	 0.4470
1	 0.6210	 0.3610
2	 0.8440	 0.4770
3	 0.7340	 0.4550
4	 0.7150	 0.4440
6	 0.4830	 0.2930
7	 0.5310	 0.2370
A	 0.8400	 0.3740
B	 0.4810	 0.3300
C	 0.5300	 0.3800
D	 0.3950	 0.2890
E	 0.5860	 0.4140
F	 0.5430	 0.3600
G	 0.5550	 0.3350
H	 0.6080	 0.3720
I	 0.6070	 0.3310
J	 0.5510	 0.3630
K	 0.5290	 0.3630
L	 0.5660	 0.3120
M	 0.5950	 0.3510
N	 0.6110	 0.3900
O	 0.6730	 0.3860
P	 0.5500	 0.3600
Q	 0.5330	 0.3590
R	 0.5900	 0.3860
S	 0.6030	 0.3610
T	 0.5950	 0.3280
U	 0.6660	 0.3450
V	 0.4060	 0.2580
X	 0.8740	 0.4040
Y	 0.9060	 0.3570
Z	 0.7300	 0.4600
a	 0.7200	 0.4480
b	 0.5750	 0.3930



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Chain	Atom inclusion	Q-score
c	 0.5550	 0.3110
d	 0.5580	 0.3380
e	 0.7250	 0.4280
f	 0.6950	 0.4530
i	 0.7250	 0.4150
j	 0.7110	 0.4360
k	 0.7360	 0.4200
l	 0.6700	 0.3460
m	 0.6720	 0.4190
n	 0.7650	 0.4150
o	 0.7070	 0.3990
r	 0.7460	 0.4350
s	 0.7100	 0.4230
t	 0.4380	 0.3690
u	 0.7510	 0.4340
v	 0.6280	 0.4350
w	 0.6620	 0.3590
x	 0.7330	 0.4250
z	 0.0480	 0.2260