



Full wwPDB EM Validation Report ⓘ

Oct 10, 2022 – 03:13 pm BST

PDB ID : 7PIB
EMDB ID : EMD-13435
Title : 70S ribosome with EF-G, A/P- and P/E-site tRNAs in spectinomycin-treated Mycoplasma pneumoniae cells
Authors : Xue, L.; Lenz, S.; Rappsilber, J.; Mahamid, J.
Deposited on : 2021-08-19
Resolution : 4.70 Å (reported)
Based on initial models : 7OOD, 7OOC, 4V7C, 4V7D

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:

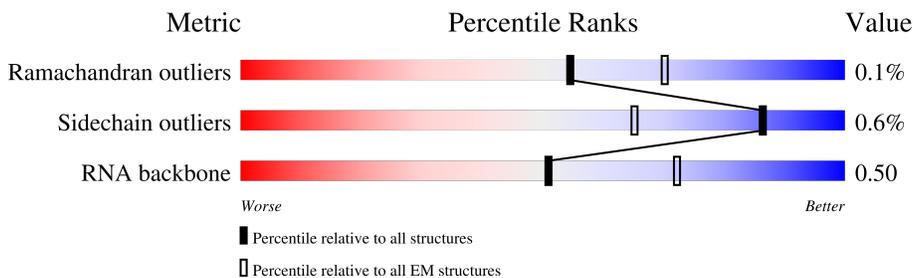
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 4.70 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.



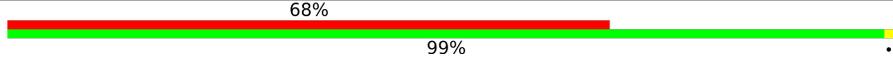
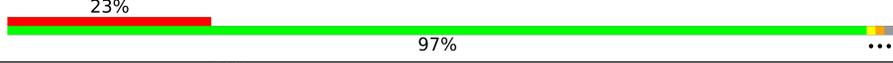
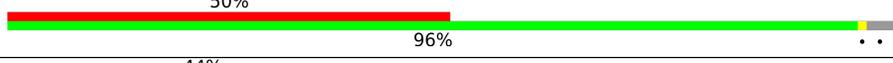
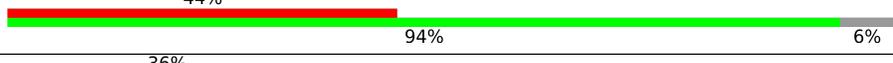
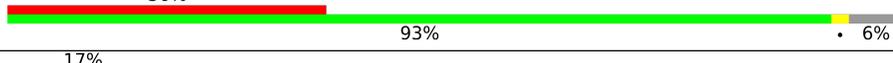
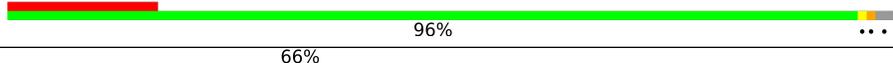
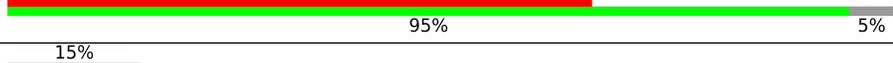
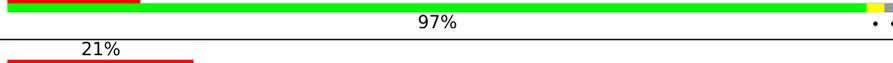
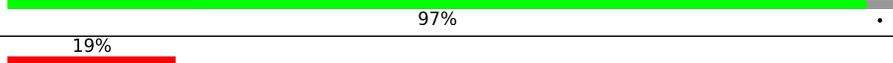
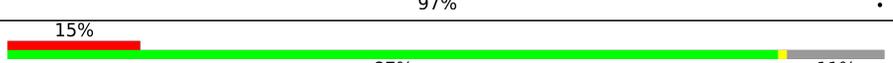
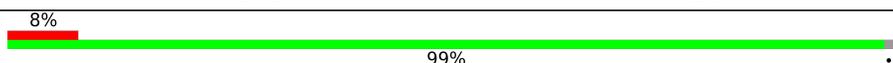
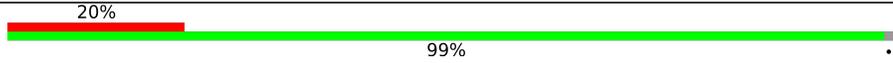
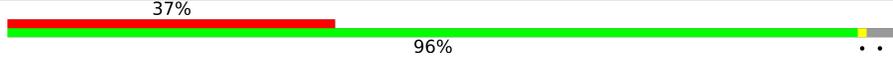
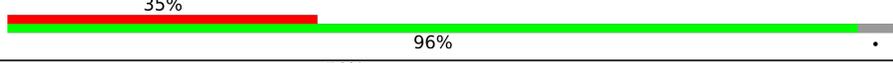
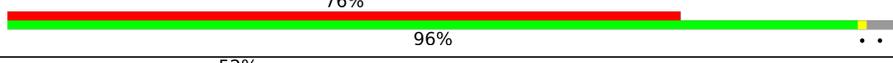
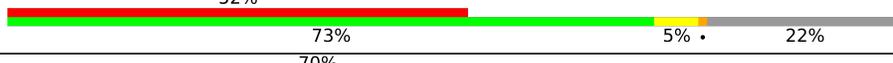
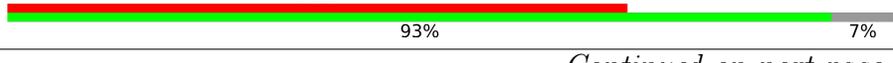
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	48	98%
2	1	59	10%
3	2	37	16%
4	9	688	66%
5	A	294	38%
6	B	273	81%
7	C	205	34%
8	D	219	79%
			39%
			99%
			18%
			21%
			16%
			69%
			30%

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Mol	Chain	Length	Quality of chain
9	E	215	
10	F	155	
11	G	142	
12	H	132	
13	I	108	
14	J	121	
15	K	139	
16	L	124	
17	M	61	
18	N	86	
19	O	94	
20	P	85	
21	Q	104	
22	R	87	
23	S	87	
24	T	60	
25	W	122	
26	a	287	
27	b	287	
28	c	212	
29	d	180	
30	e	184	
31	f	149	
32	g	161	
33	h	137	

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Mol	Chain	Length	Quality of chain
34	i	146	8% 99%
35	j	122	17% 100%
36	k	151	21% 97%
37	l	139	12% 98%
38	m	124	7% 96%
39	n	116	27% 97%
40	o	119	20% 95%
41	p	127	6% 90% 10%
42	q	100	17% 98%
43	r	159	9% 87% 13%
44	s	237	39% 61%
45	t	111	41% 100%
46	u	104	12% 82% 17%
47	v	65	20% 97%
48	w	111	25% 90% 10%
49	x	97	28% 45% 55%
50	y	57	18% 95%
51	z	53	11% 94% 6%
52	3	2907	73% 26%
53	4	108	66% 31%
54	5	1520	74% 24%
55	7	76	34% 61% 37%
55	8	76	13% 61% 37%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 152025 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 L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	47	380	236	81	61	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	59	477	300	99	77	1	0	0

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	37	304	189	65	46	4	0	0

- Molecule 4 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	9	682	5326	3369	911	1021	25	0	0

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	240	1921	1226	334	352	9	0	0

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	215	1698	1073	313	307	5	0	0

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	203	Total	C	N	O	S	0	0
			1660	1051	314	290	5		

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	153	Total	C	N	O	S	0	0
			1173	742	226	202	3		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	167	Total	C	N	O	S	0	0
			1362	857	240	263	2		

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	154	Total	C	N	O	S	0	0
			1246	785	239	216	6		

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	141	Total	C	N	O	S	0	0
			1110	723	193	192	2		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	128	Total	C	N	O	S	0	0
			1028	655	191	181	1		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	101	Total	C	N	O	S	0	0
			809	523	142	143	1		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	136	Total	C	N	O	S	0	0
			1076	680	213	181	2		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	118	Total	C	N	O	S	0	0
			951	594	191	166			

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	60	Total	C	N	O	S	0	0
			474	302	96	72	4		

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	83	Total	C	N	O	S	0	0
			673	428	125	120			

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	80	Total	C	N	O	S	0	0
			646	414	119	111	2		

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	83	Total	C	N	O	S	0	0
			675	425	135	115			

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	65	535	342	103	86	4	0	0

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	84	682	435	127	118	2	0	0

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	S	77	629	383	135	111	0	0

- Molecule 24 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	T	53	471	295	103	72	1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	W	69	534	342	87	103	2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	285	2225	1385	437	397	6	0	0

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	229	1762	1119	318	318	7	0	0

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	210	Total	C	N	O	S	0	0
			1644	1047	297	297	3		

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	175	Total	C	N	O	S	0	0
			1388	893	245	246	4		

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	e	176	Total	C	N	O	0	0
			1396	899	247	250		

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	145	Total	C	N	O	S	0	0
			1182	763	206	210	3		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	126	Total	C	N	O	S	0	0
			960	612	167	178	3		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	128	Total	C	N	O	S	0	0
			959	616	160	177	6		

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	144	Total	C	N	O	S	0	0
			1164	737	213	209	5		

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	122	944	595	178	167	4	0	0

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	148	1153	731	226	196		0	0

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	136	1079	694	196	182	7	0	0

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	m	119	958	609	175	171	3	0	0

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	112	889	557	175	155	2	0	0

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	115	938	592	180	165	1	0	0

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	114	947	603	188	154	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	q	99	811	525	148	134	4	0	0

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	139	1068	663	207	191	7	0	0

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	s	92	720	475	122	122	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	t	111	872	550	166	153	3	0	0

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	u	86	657	409	130	117	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	v	63	513	317	108	87	1	0	0

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	w	100	818	517	153	148	0	0

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	44	Total	C	N	O	S	0	0
			344	221	55	64	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

- Molecule 51 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 52 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3	2878	Total	C	N	O	P	0	0
			61664	27558	11236	19995	2875		

- Molecule 53 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	105	Total	C	N	O	P	0	0
			2239	1003	409	724	103		

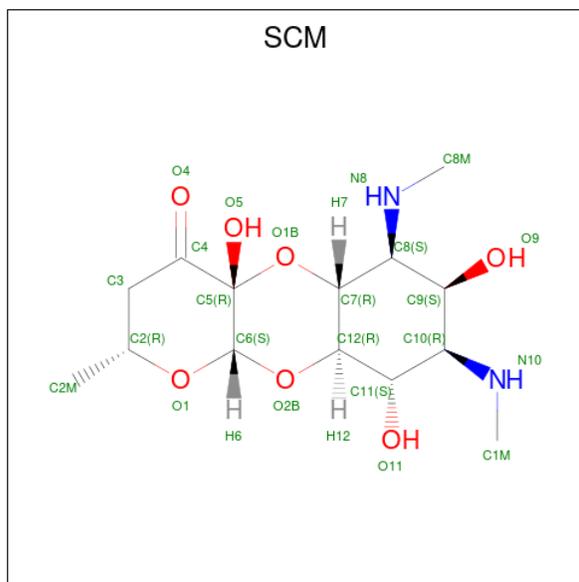
- Molecule 54 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	5	1493	Total	C	N	O	P	0	0
			31943	14279	5792	10382	1490		

- Molecule 55 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	76	Total	C	N	O	P	0	0
			1618	723	289	531	75		
55	8	76	Total	C	N	O	P	0	0
			1618	723	289	531	75		

- Molecule 56 is SPECTINOMYCIN (three-letter code: SCM) (formula: C₁₄H₂₄N₂O₇) (labeled as "Ligand of Interest" by depositor).

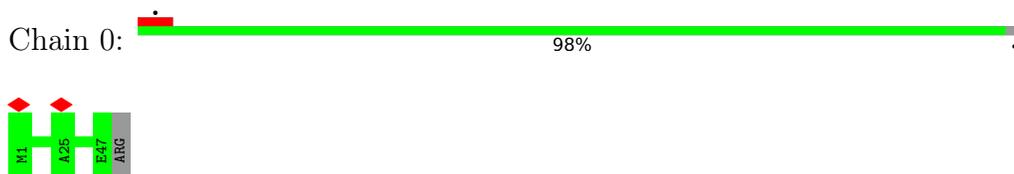


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
56	5	1	23	14	2	7	0

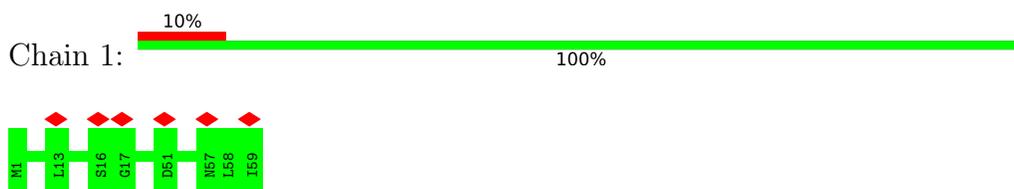
3 Residue-property plots [i](#)

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

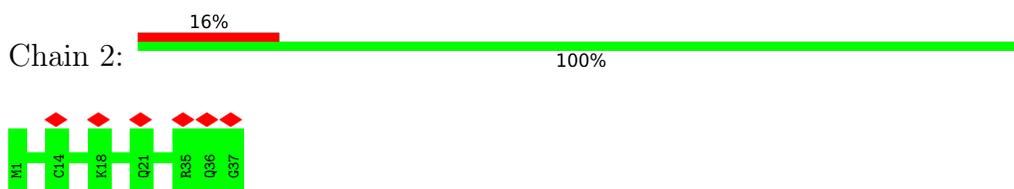
- Molecule 1: 50S ribosomal protein L34



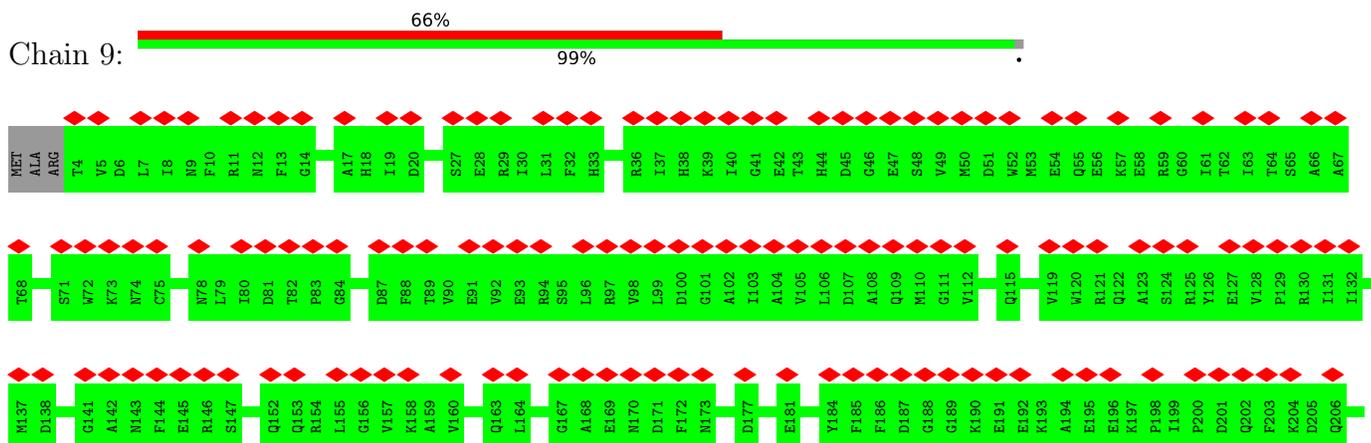
- Molecule 2: 50S ribosomal protein L35

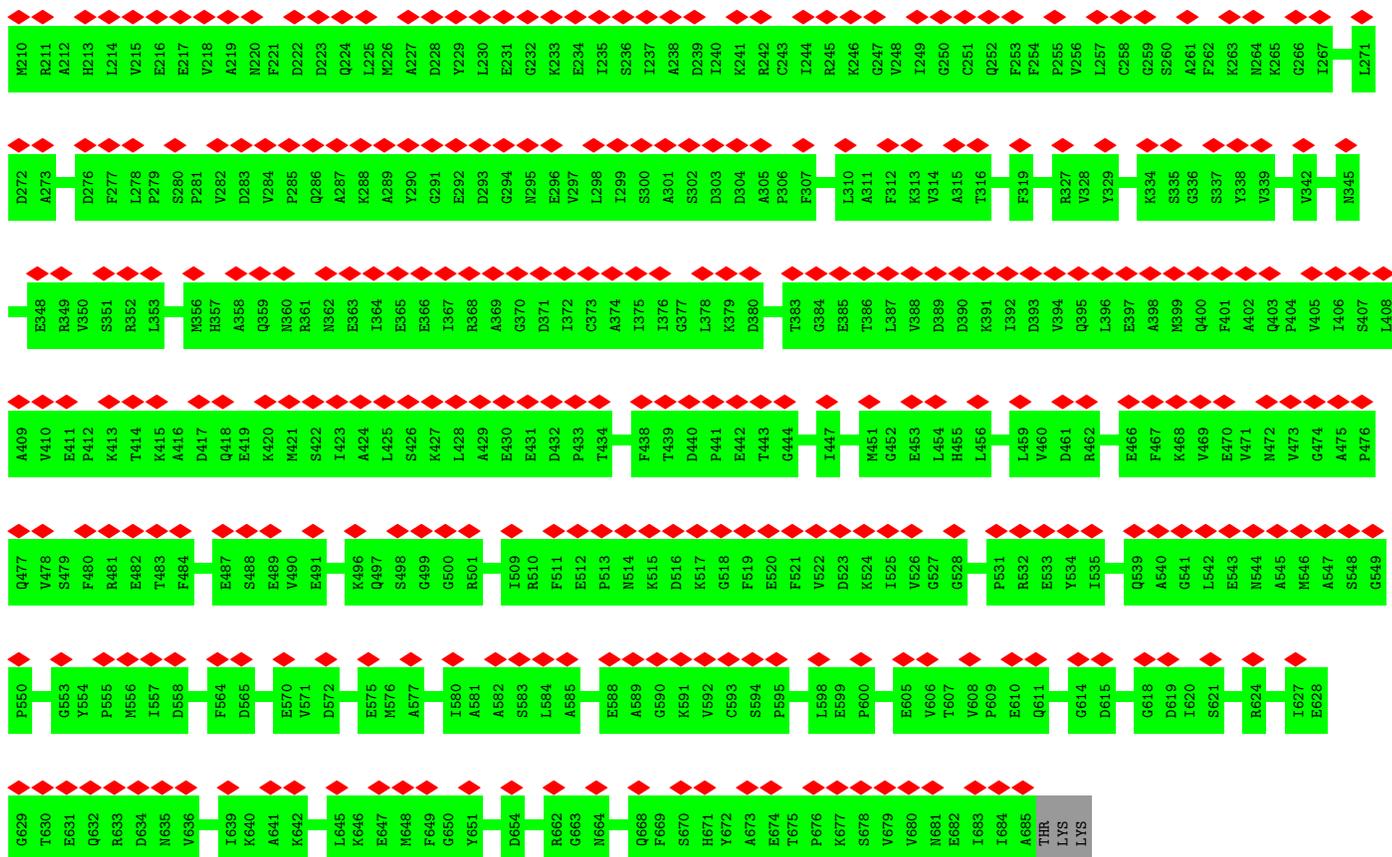


- Molecule 3: 50S ribosomal protein L36

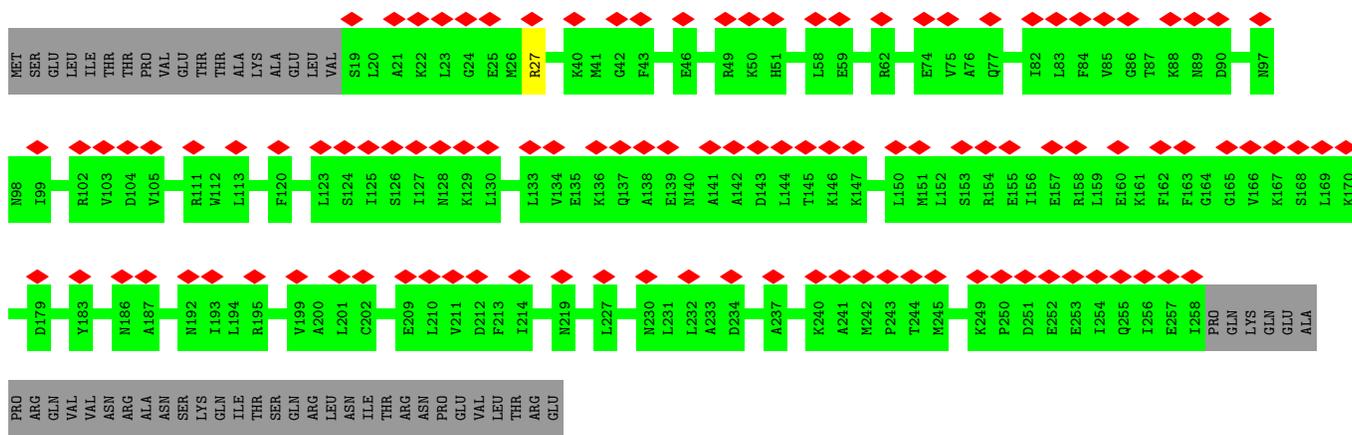
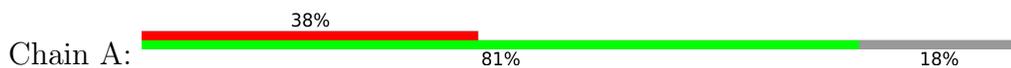


- Molecule 4: Elongation factor G

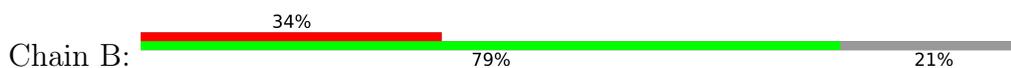


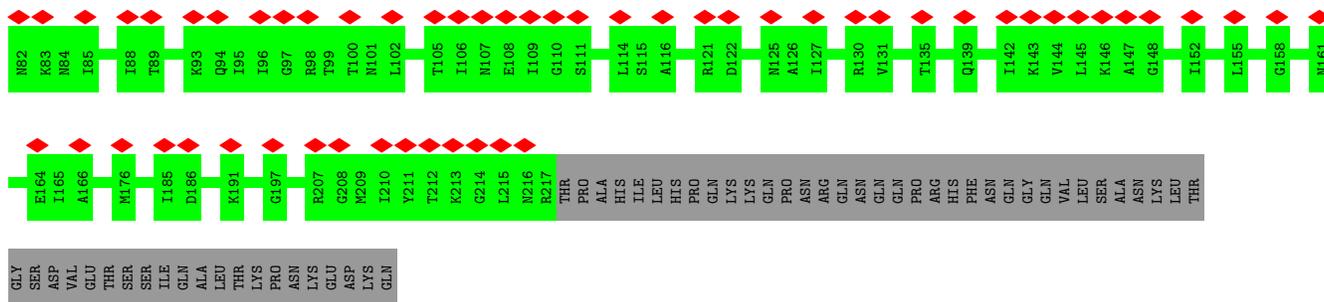


• Molecule 5: 30S ribosomal protein S2

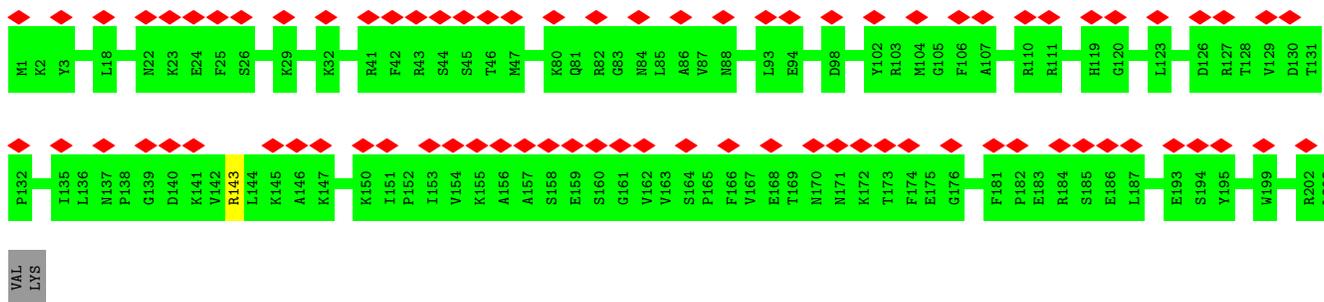
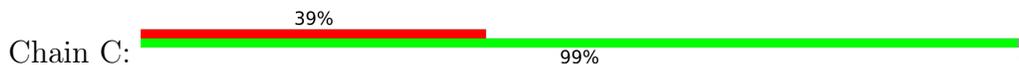


• Molecule 6: 30S ribosomal protein S3

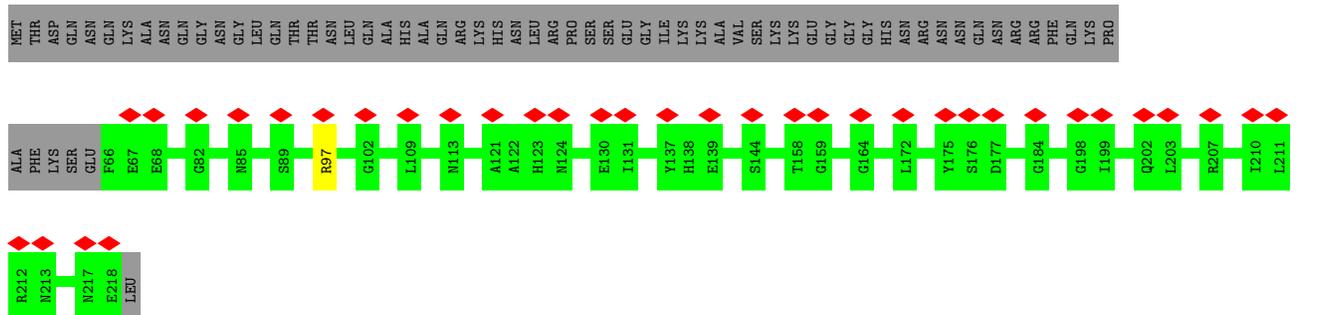




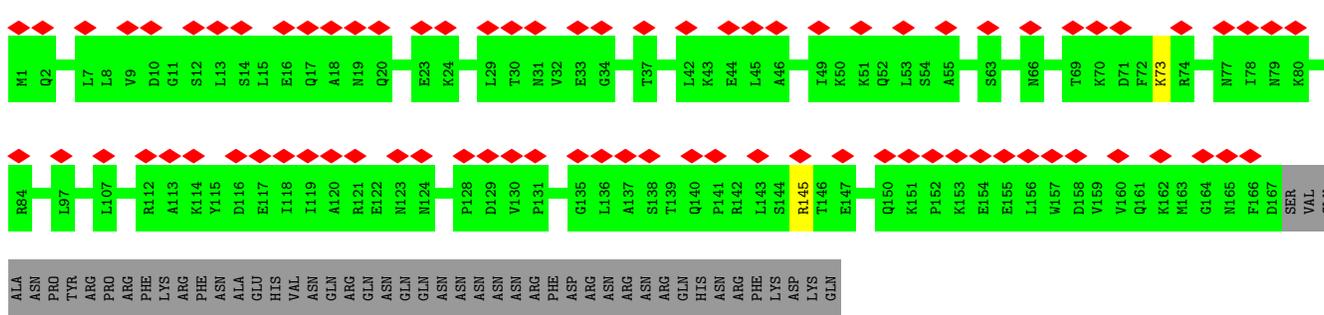
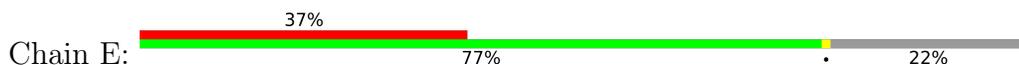
• Molecule 7: 30S ribosomal protein S4



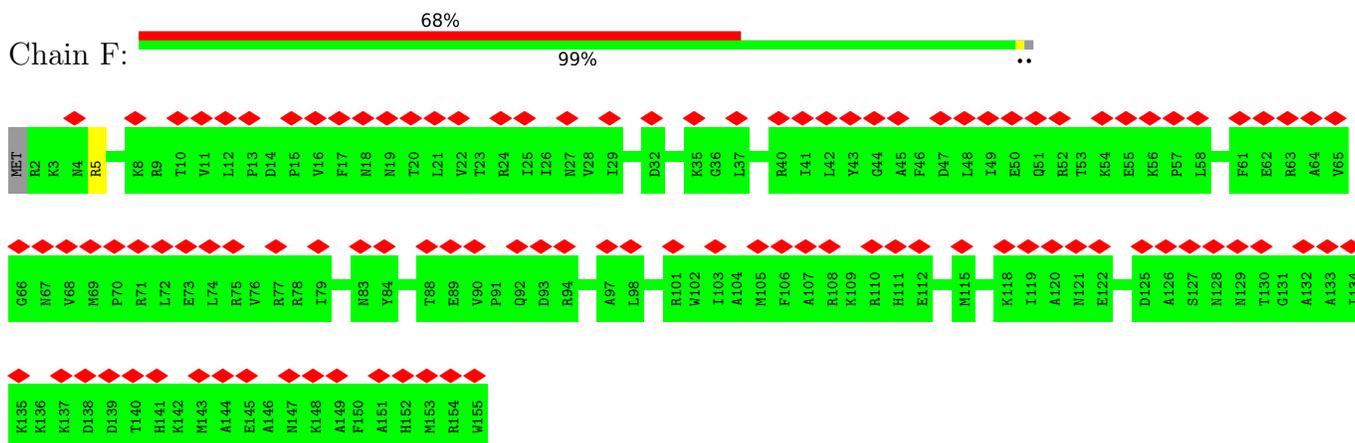
• Molecule 8: 30S ribosomal protein S5



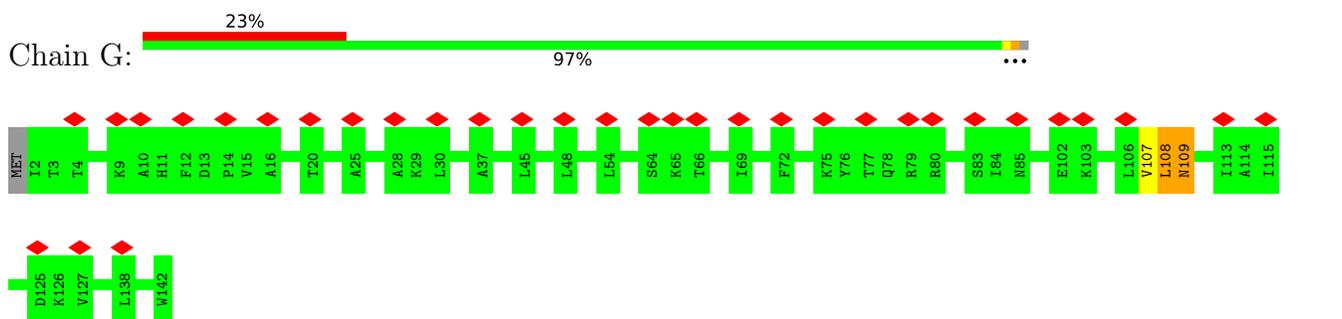
• Molecule 9: 30S ribosomal protein S6



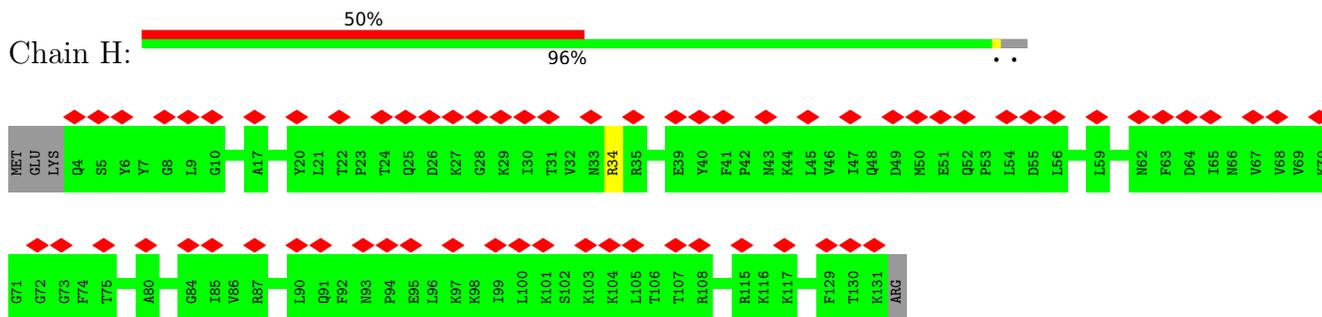
- Molecule 10: 30S ribosomal protein S7



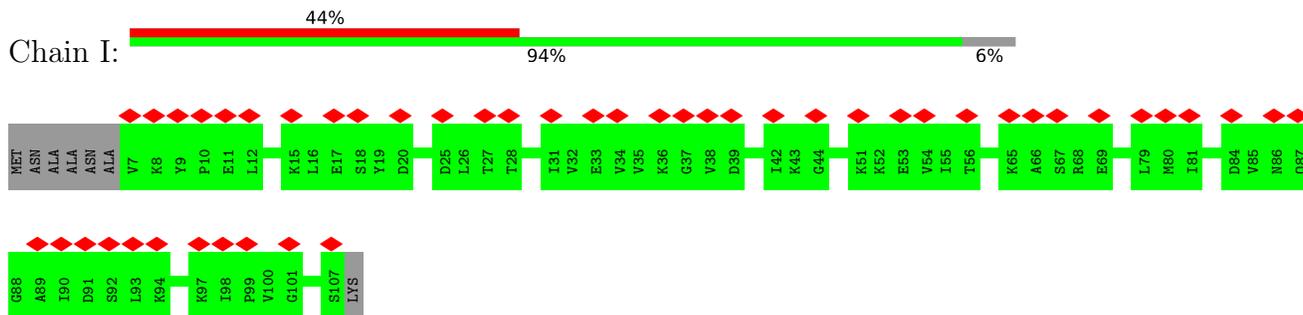
- Molecule 11: 30S ribosomal protein S8



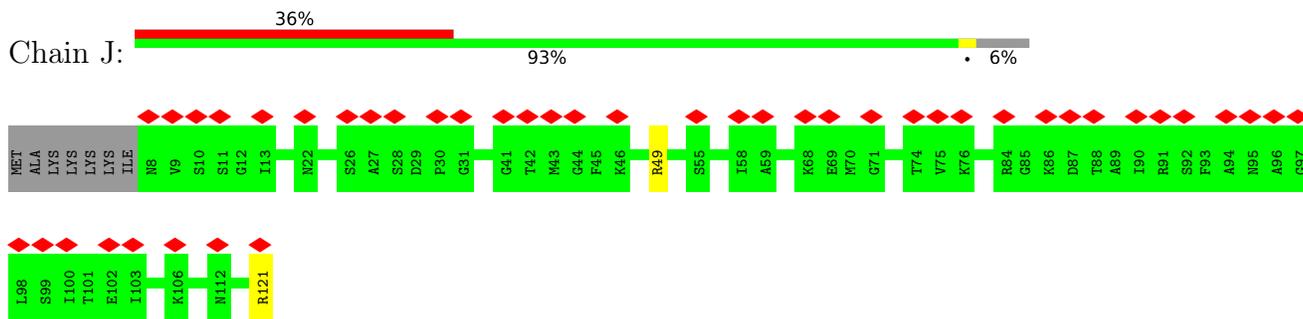
- Molecule 12: 30S ribosomal protein S9



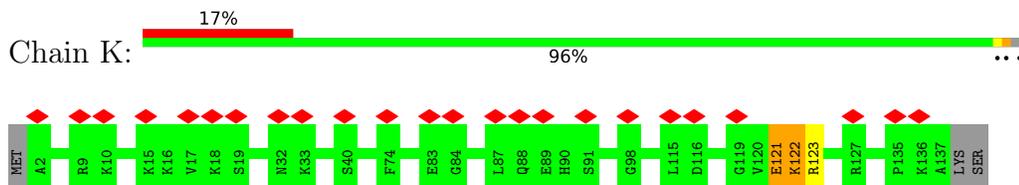
- Molecule 13: 30S ribosomal protein S10



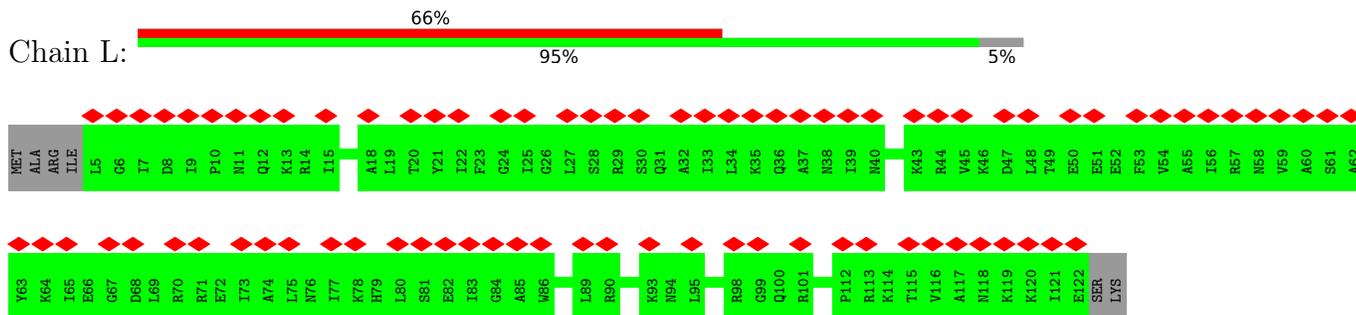
- Molecule 14: 30S ribosomal protein S11



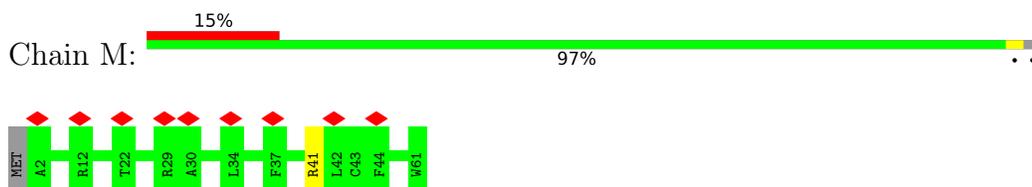
• Molecule 15: 30S ribosomal protein S12



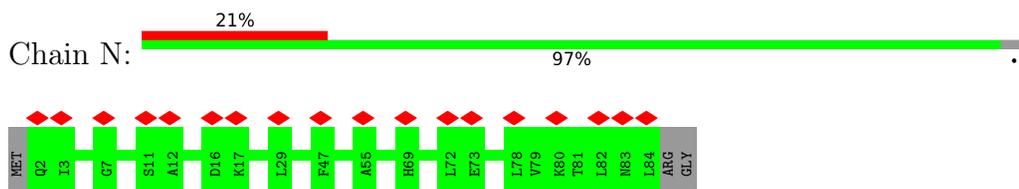
• Molecule 16: 30S ribosomal protein S13



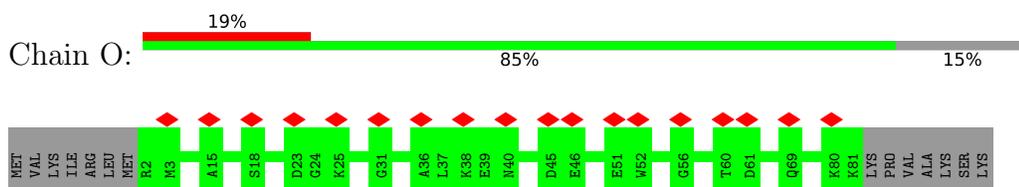
• Molecule 17: 30S ribosomal protein S14 type Z



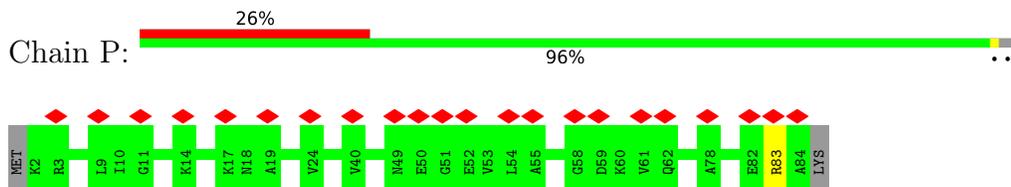
• Molecule 18: 30S ribosomal protein S15



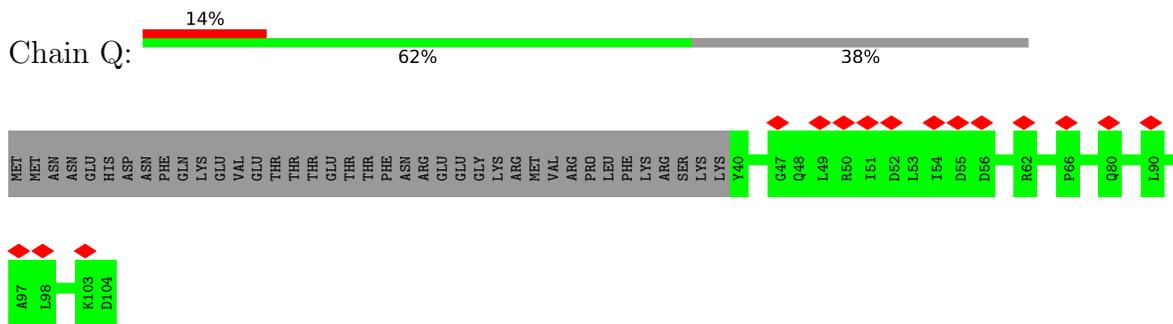
• Molecule 19: 30S ribosomal protein S16



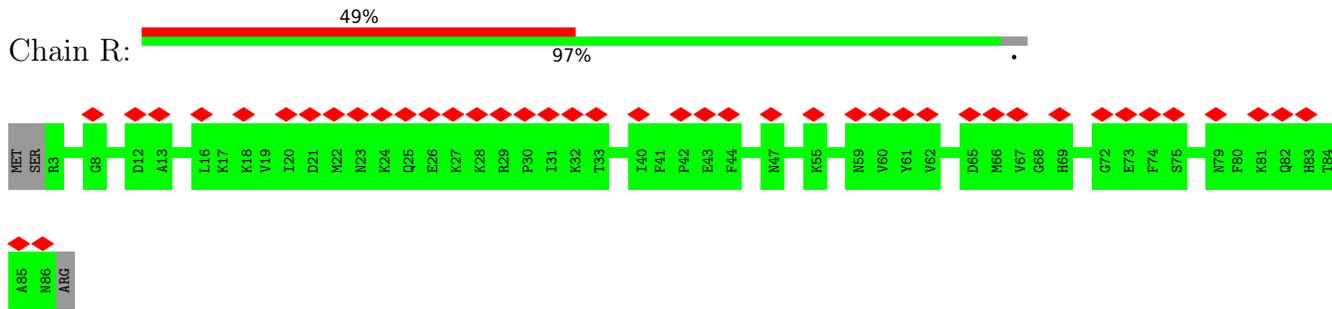
• Molecule 20: 30S ribosomal protein S17



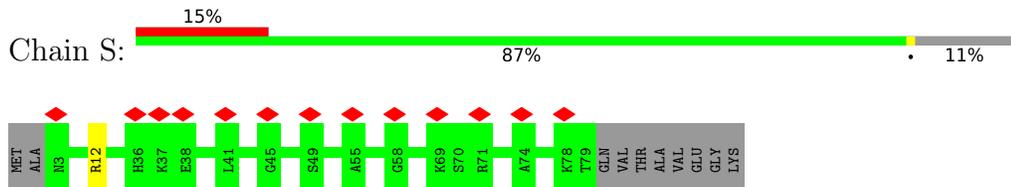
• Molecule 21: 30S ribosomal protein S18



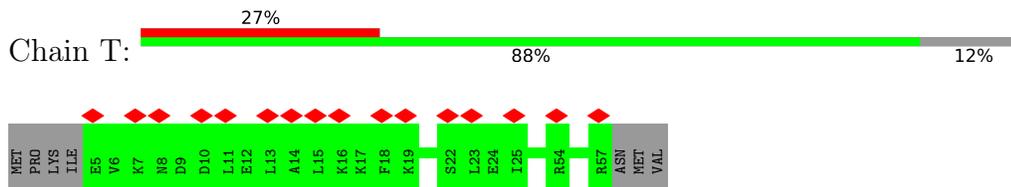
• Molecule 22: 30S ribosomal protein S19



• Molecule 23: 30S ribosomal protein S20

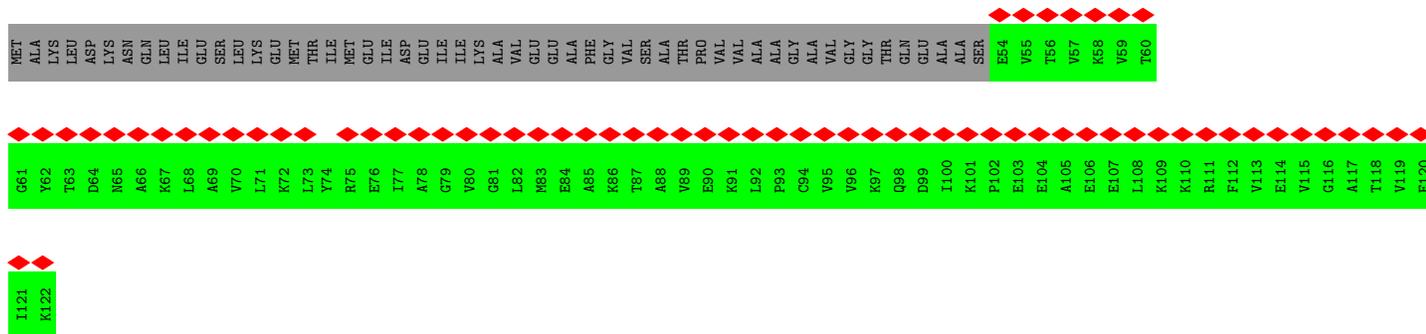


• Molecule 24: 30S ribosomal protein S21



• Molecule 25: 50S ribosomal protein L7/L12

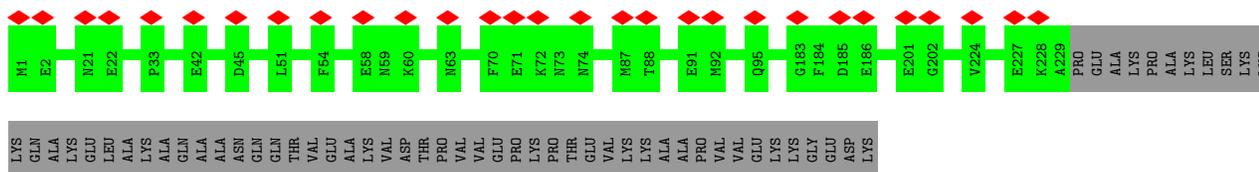
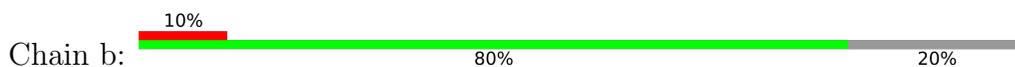




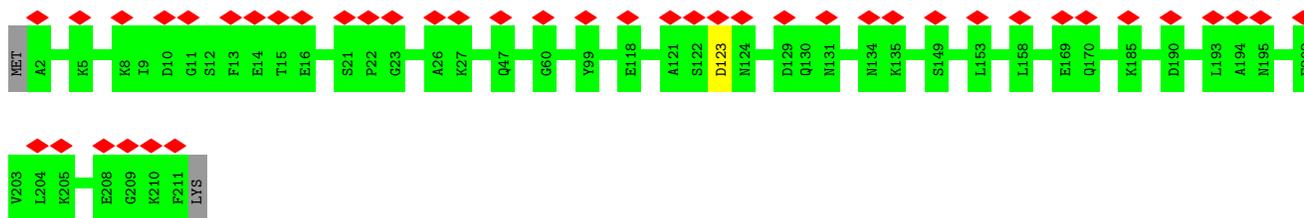
• Molecule 26: 50S ribosomal protein L2



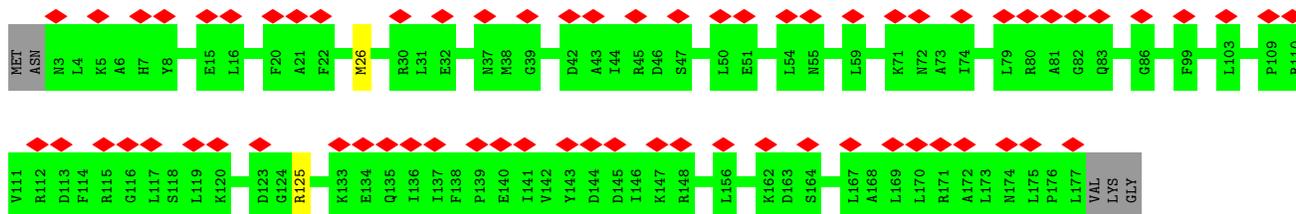
• Molecule 27: 50S ribosomal protein L3



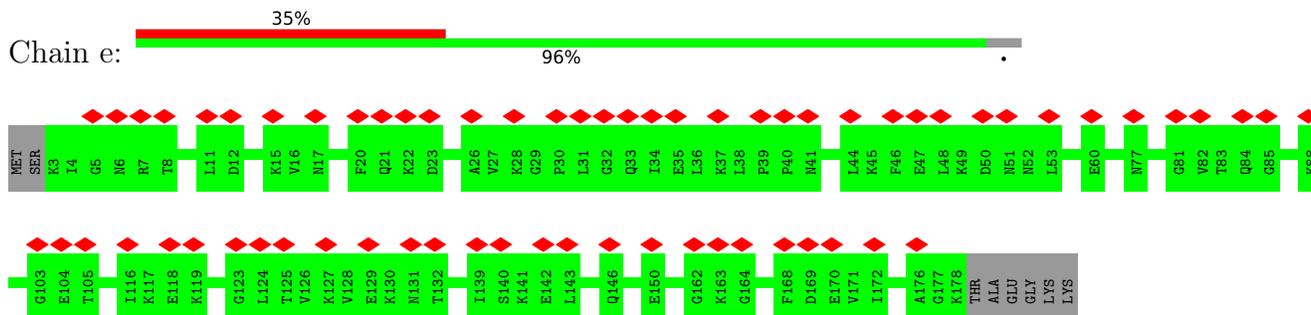
• Molecule 28: 50S ribosomal protein L4



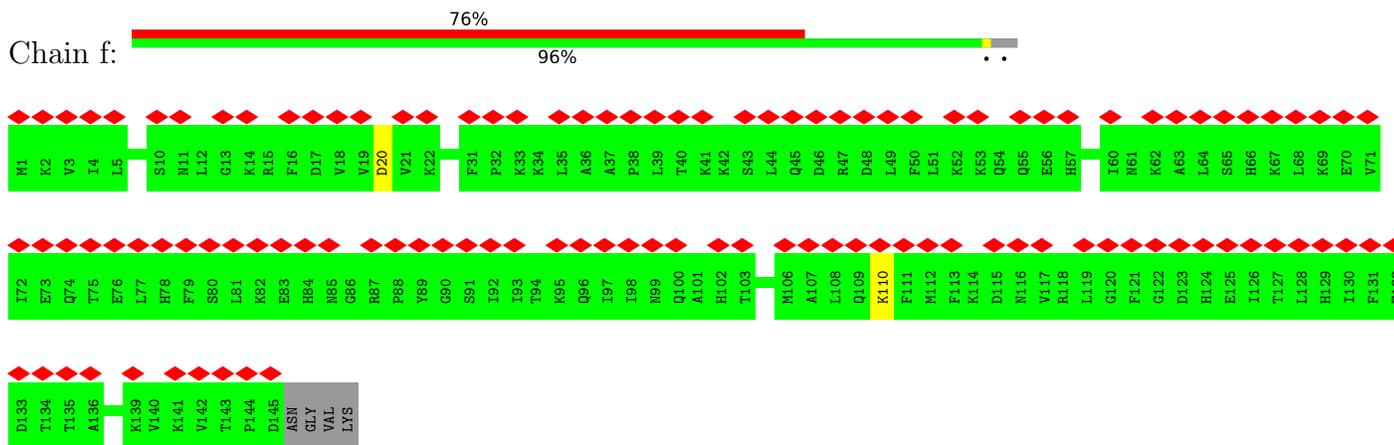
• Molecule 29: 50S ribosomal protein L5



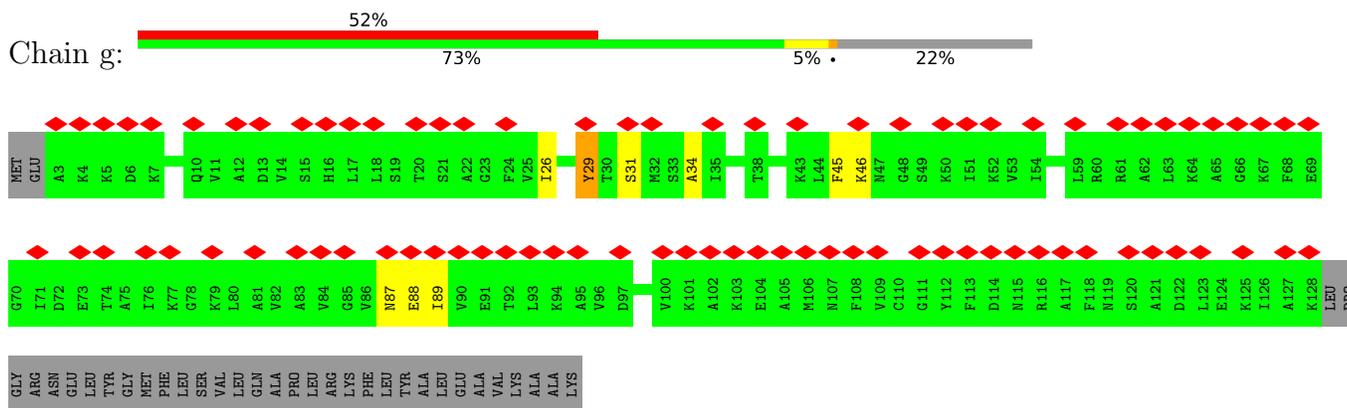
- Molecule 30: 50S ribosomal protein L6



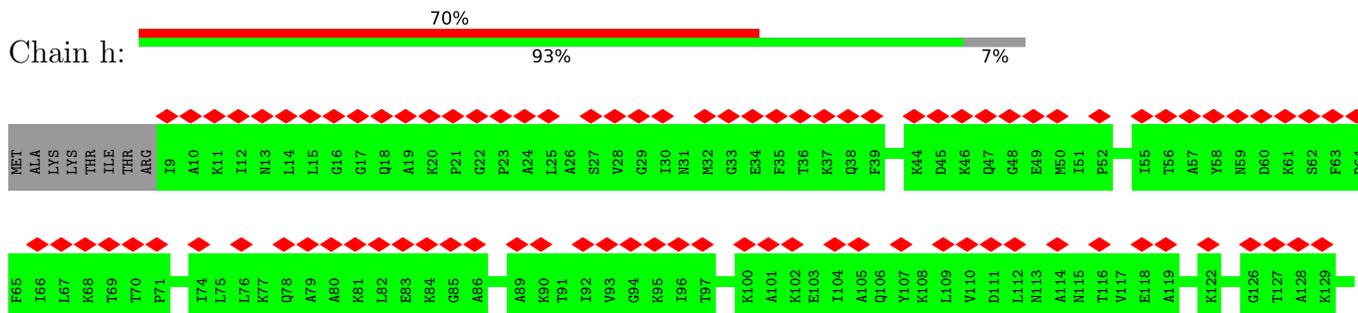
- Molecule 31: 50S ribosomal protein L9



- Molecule 32: 50S ribosomal protein L10

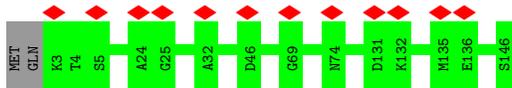


- Molecule 33: 50S ribosomal protein L11

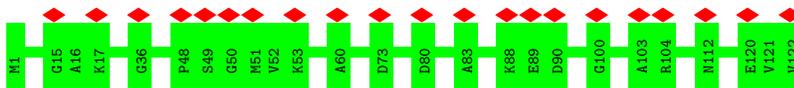




- Molecule 34: 50S ribosomal protein L13



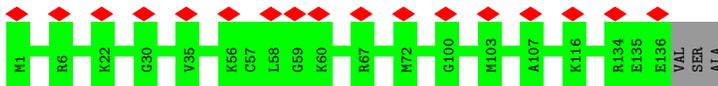
- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15



- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17



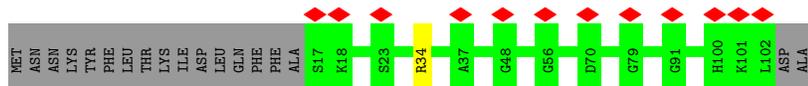
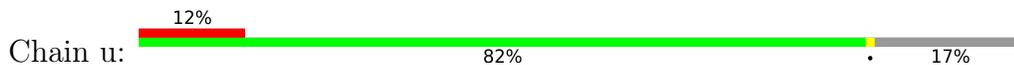
- Molecule 39: 50S ribosomal protein L18



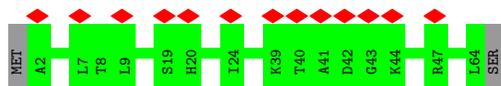
- Molecule 40: 50S ribosomal protein L19



• Molecule 46: 50S ribosomal protein L27



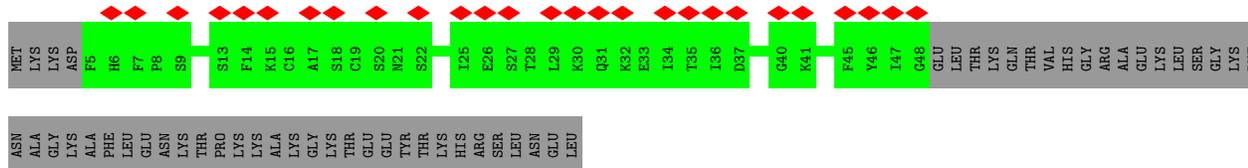
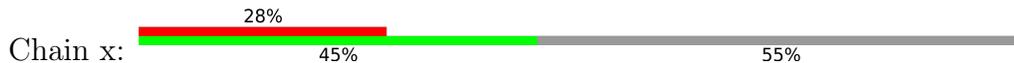
• Molecule 47: 50S ribosomal protein L28



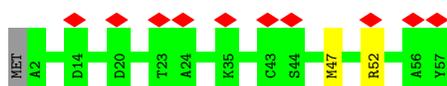
• Molecule 48: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L31



• Molecule 50: 50S ribosomal protein L32



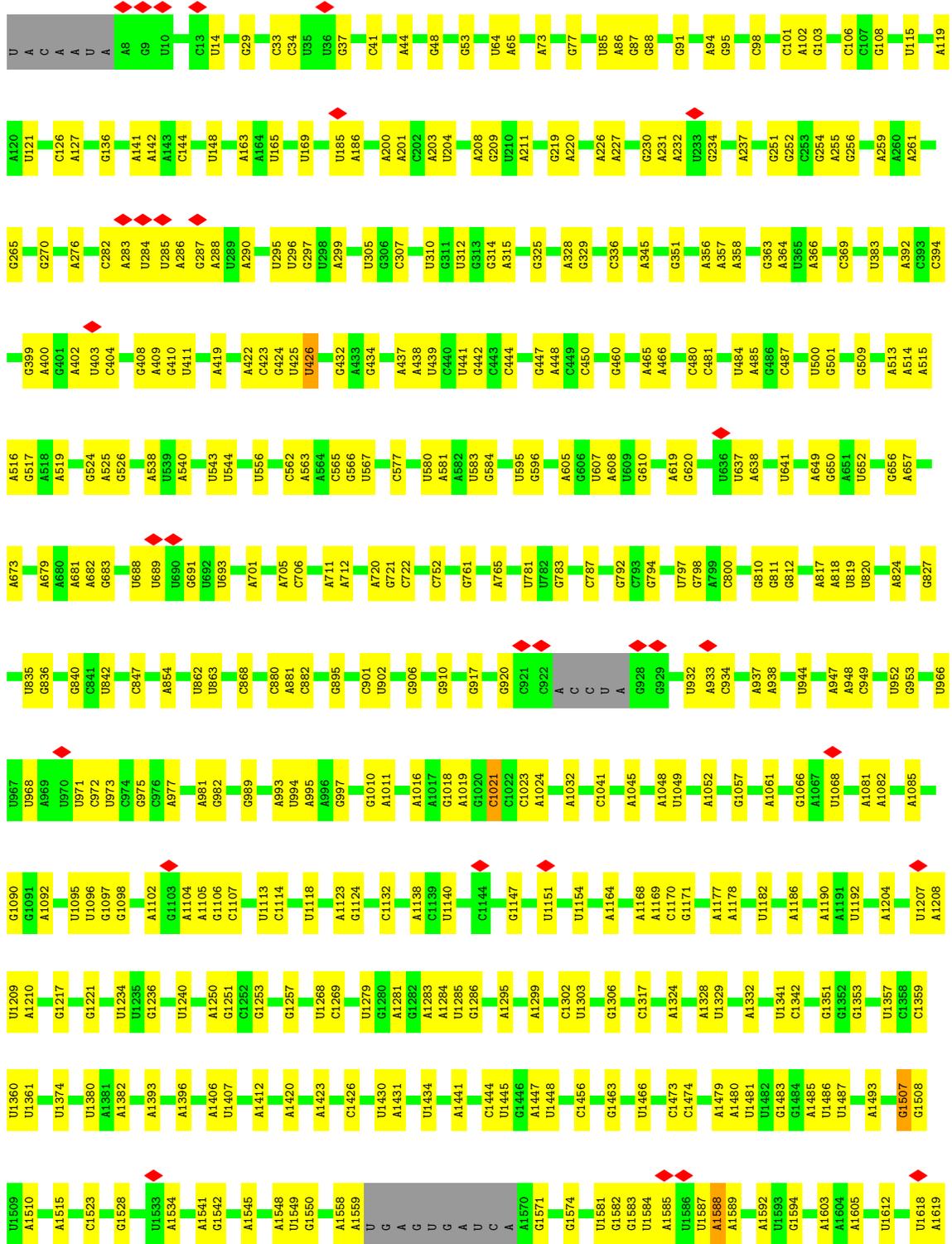
• Molecule 51: 50S ribosomal protein L33 1

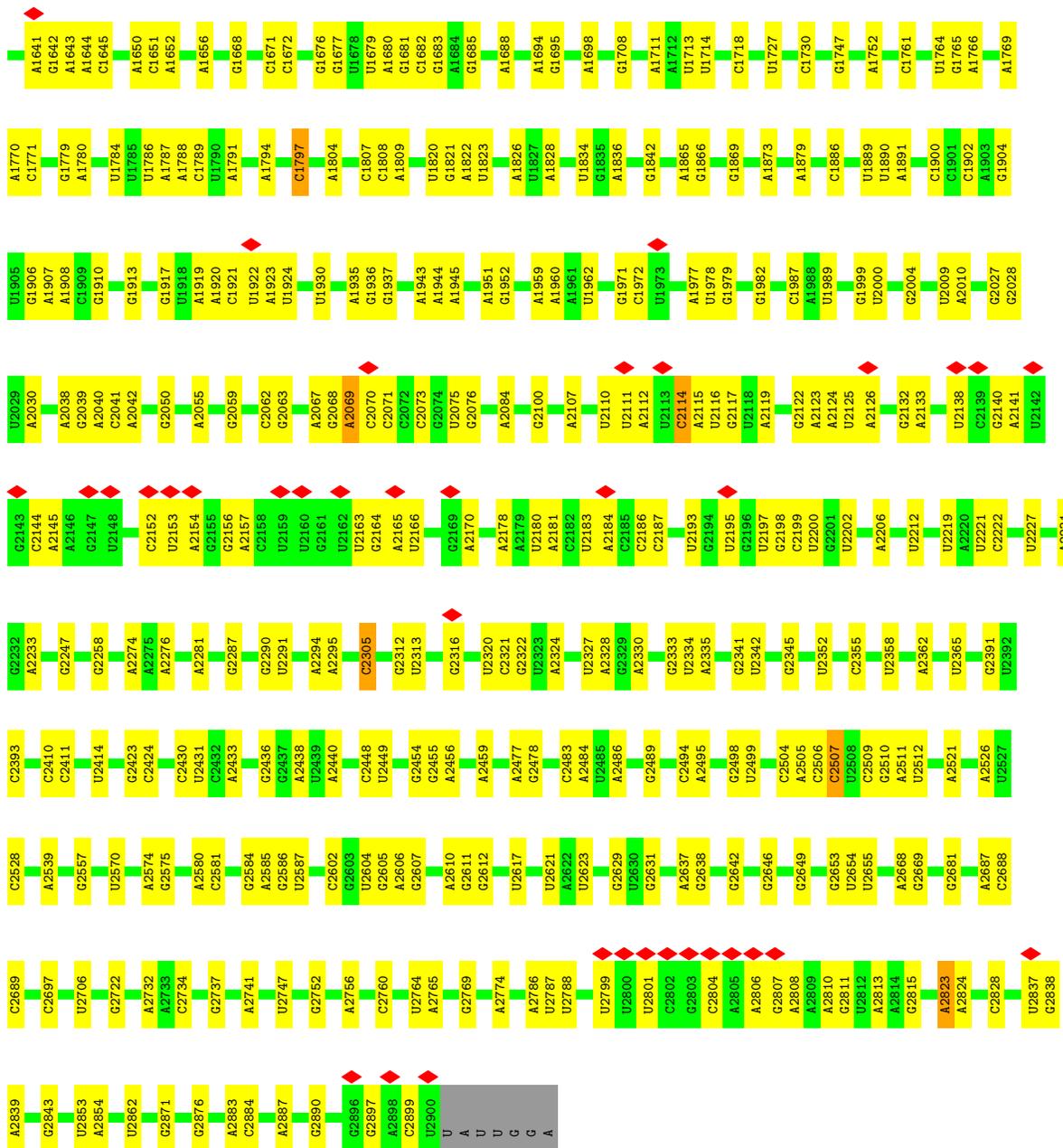




• Molecule 52: 23S ribosomal RNA

Chain 3: 73% 26%

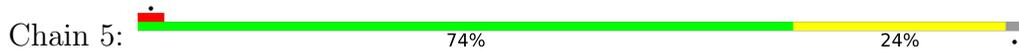


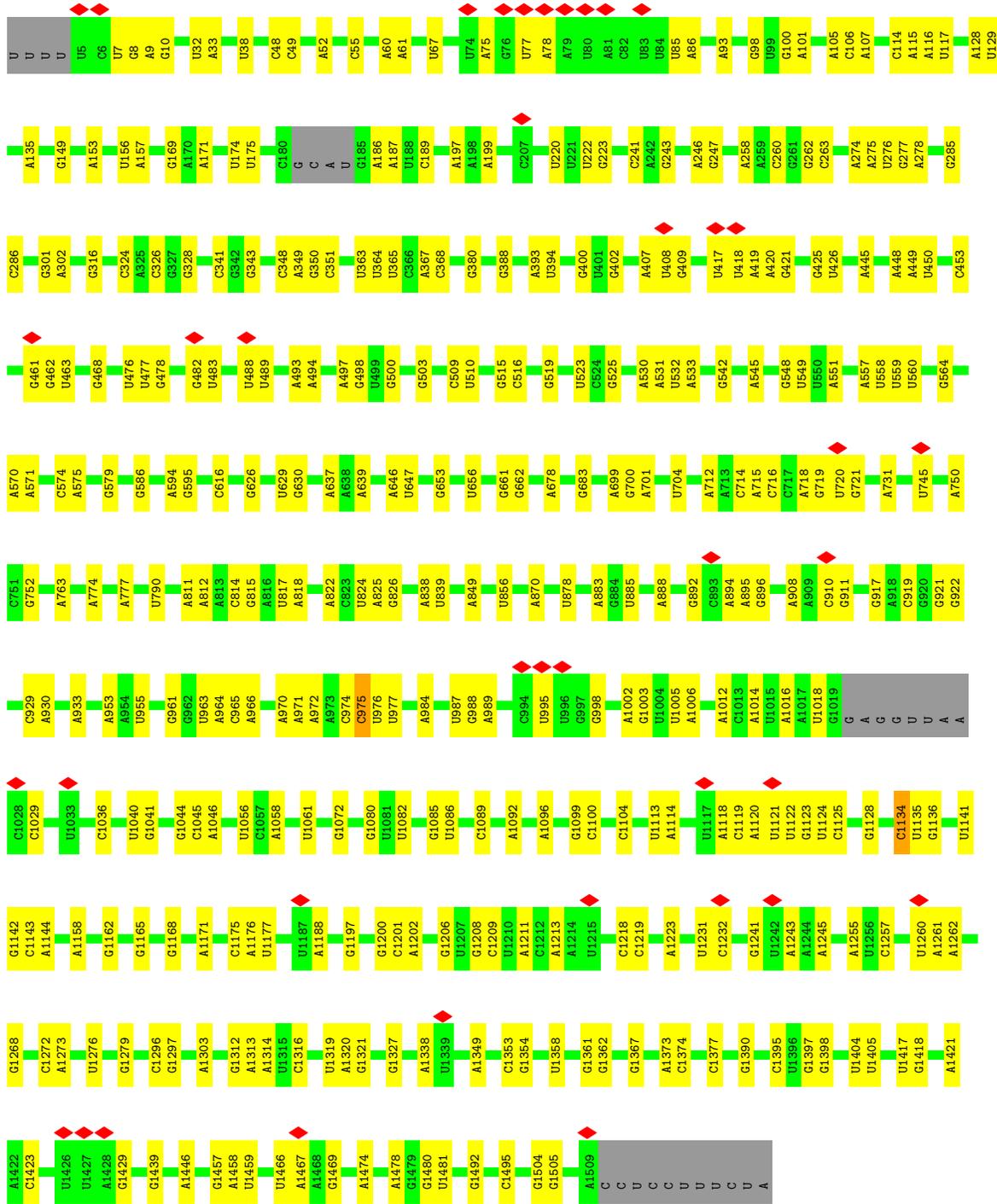


• Molecule 53: 5S ribosomal RNA



• Molecule 54: 16S ribosomal RNA

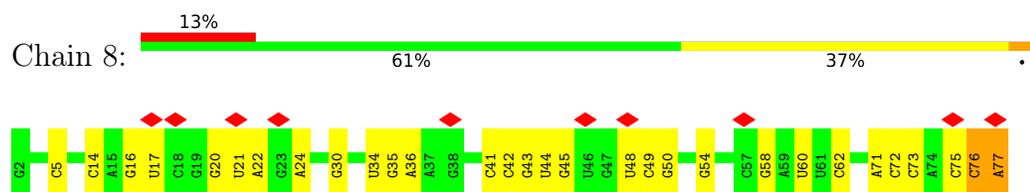




• Molecule 55: tRNA-Phe



• Molecule 55: tRNA-Phe



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	8371	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 ($e^-/\text{\AA}^2$)	3.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.055	Depositor
Minimum map value	-1.778	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.164	Depositor
Recommended contour level	0.66	Depositor
Map size (Å)	435.328, 435.328, 435.328	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7005, 1.7005, 1.7005	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.23	0/383	0.44	0/504
2	1	0.24	0/484	0.46	0/637
3	2	0.22	0/306	0.43	0/401
4	9	0.25	0/5419	0.44	0/7307
5	A	0.25	0/1954	0.44	0/2642
6	B	0.24	0/1721	0.48	0/2323
7	C	0.24	0/1691	0.42	0/2267
8	D	0.24	0/1188	0.47	0/1593
9	E	0.24	0/1384	0.47	0/1867
10	F	0.23	0/1266	0.42	0/1700
11	G	0.26	0/1126	0.50	0/1517
12	H	0.24	0/1044	0.45	0/1395
13	I	0.23	0/820	0.48	0/1103
14	J	0.24	0/844	0.43	0/1136
15	K	0.27	0/1094	0.56	0/1468
16	L	0.23	0/962	0.44	0/1289
17	M	0.24	0/483	0.42	0/643
18	N	0.23	0/679	0.44	0/907
19	O	0.23	0/659	0.42	0/885
20	P	0.23	0/684	0.46	0/913
21	Q	0.24	0/545	0.41	0/730
22	R	0.25	0/698	0.44	0/936
23	S	0.23	0/631	0.40	0/838
24	T	0.23	0/475	0.43	0/621
25	W	0.24	0/538	0.45	0/722
26	a	0.24	0/2267	0.47	0/3044
27	b	0.25	0/1795	0.47	0/2412
28	c	0.24	0/1671	0.46	1/2246 (0.0%)
29	d	0.24	0/1409	0.48	0/1894
30	e	0.25	0/1420	0.46	0/1912
31	f	0.25	0/1205	0.47	1/1616 (0.1%)
32	g	0.34	0/969	0.61	1/1295 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.24	0/968	0.44	0/1298
34	i	0.23	0/1186	0.43	0/1592
35	j	0.24	0/953	0.48	0/1275
36	k	0.24	0/1170	0.44	0/1559
37	l	0.26	0/1104	0.47	0/1481
38	m	0.23	0/973	0.44	0/1309
39	n	0.23	0/897	0.47	0/1198
40	o	0.24	0/948	0.44	0/1262
41	p	0.24	0/961	0.38	0/1278
42	q	0.24	0/828	0.47	0/1111
43	r	0.24	0/1077	0.43	0/1441
44	s	0.25	0/732	0.48	0/988
45	t	0.24	0/879	0.47	0/1165
46	u	0.28	0/665	0.48	0/884
47	v	0.26	0/519	0.56	0/695
48	w	0.23	0/826	0.43	0/1104
49	x	0.25	0/353	0.43	0/474
50	y	0.28	0/457	0.56	0/601
51	z	0.23	0/412	0.45	0/547
52	3	0.20	0/69073	0.80	66/107710 (0.1%)
53	4	0.19	0/2505	0.78	3/3902 (0.1%)
54	5	0.18	0/35768	0.76	14/55764 (0.0%)
55	7	0.33	0/1808	1.05	8/2817 (0.3%)
55	8	0.34	0/1808	1.05	9/2817 (0.3%)
All	All	0.22	0/164684	0.71	103/245035 (0.0%)

There are no bond length outliers.

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	3	2454	G	N3-C4-N9	11.62	132.97	126.00
52	3	1900	C	N3-C2-O2	-9.85	115.00	121.90
52	3	1987	C	N3-C2-O2	-9.18	115.47	121.90
52	3	2454	G	N3-C4-C5	-8.87	124.17	128.60
52	3	426	U	C2-N1-C1'	8.37	127.74	117.70
52	3	1900	C	N1-C2-O2	8.12	123.77	118.90
52	3	1341	U	C2-N1-C1'	7.87	127.14	117.70
52	3	1718	C	N3-C2-O2	-7.81	116.43	121.90
52	3	1303	U	C2-N1-C1'	7.63	126.86	117.70
54	5	974	C	C2-N1-C1'	7.52	127.08	118.80
52	3	394	C	N3-C2-O2	-7.49	116.66	121.90
52	3	1303	U	N1-C2-O2	7.34	127.94	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	5	714	C	N3-C2-O2	-7.34	116.76	121.90
52	3	2454	G	C6-C5-N7	-7.33	126.00	130.40
52	3	1902	C	N3-C2-O2	-7.25	116.82	121.90
52	3	1672	C	N3-C2-O2	-7.19	116.87	121.90
52	3	1021	C	N3-C2-O2	-7.17	116.88	121.90
52	3	1341	U	N1-C2-O2	7.15	127.80	122.80
54	5	974	C	N1-C2-O2	7.05	123.13	118.90
52	3	426	U	C6-N1-C1'	-6.90	111.53	121.20
55	8	76	C	N1-C1'-C2'	-6.84	104.48	112.00
55	7	76	C	N1-C1'-C2'	-6.81	104.51	112.00
52	3	34	C	N3-C2-O2	-6.73	117.19	121.90
52	3	1341	U	N3-C2-O2	-6.69	117.52	122.20
55	8	77	A	O5'-P-OP1	6.69	118.73	110.70
55	7	77	A	O5'-P-OP1	6.64	118.67	110.70
55	7	73	C	N3-C2-O2	-6.60	117.28	121.90
55	8	73	C	N3-C2-O2	-6.59	117.29	121.90
52	3	2321	C	N3-C2-O2	-6.52	117.34	121.90
52	3	1303	U	N3-C2-O2	-6.51	117.65	122.20
52	3	2114	C	N3-C2-O2	-6.46	117.38	121.90
52	3	2454	G	C6-N1-C2	-6.45	121.23	125.10
52	3	2804	C	C2-N1-C1'	6.39	125.83	118.80
54	5	463	U	C2-N1-C1'	6.37	125.34	117.70
52	3	2454	G	C8-N9-C1'	-6.34	118.75	127.00
52	3	2454	G	N9-C4-C5	-6.34	102.86	105.40
52	3	2454	G	C4-N9-C1'	6.29	134.68	126.50
55	8	42	C	N3-C2-O2	-6.26	117.52	121.90
55	7	42	C	N3-C2-O2	-6.23	117.54	121.90
52	3	444	C	N3-C2-O2	-6.18	117.57	121.90
52	3	1507	G	O4'-C1'-N9	6.18	113.14	108.20
52	3	2454	G	C5-C6-N1	6.16	114.58	111.50
52	3	2507	C	C2-N1-C1'	6.15	125.56	118.80
52	3	144	C	N3-C2-O2	-6.04	117.67	121.90
52	3	1474	C	C6-N1-C2	-5.98	117.91	120.30
52	3	394	C	C6-N1-C2	-5.95	117.92	120.30
52	3	1474	C	N3-C2-O2	-5.93	117.75	121.90
52	3	1588	A	P-O3'-C3'	5.83	126.70	119.70
53	4	58	C	N3-C2-O2	-5.81	117.83	121.90
54	5	974	C	N3-C2-O2	-5.79	117.85	121.90
55	7	76	C	O4'-C1'-N1	5.79	112.83	108.20
55	7	76	C	C3'-C2'-C1'	5.78	106.13	101.50
52	3	1021	C	N1-C2-O2	5.78	122.37	118.90
54	5	463	U	N1-C2-O2	5.77	126.84	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	3	2804	C	N1-C2-O2	5.71	122.33	118.90
55	8	76	C	O4'-C1'-N1	5.70	112.76	108.20
52	3	2507	C	N1-C2-O2	5.70	122.32	118.90
55	8	76	C	C3'-C2'-C1'	5.70	106.06	101.50
53	4	78	C	C2-N1-C1'	5.68	125.05	118.80
52	3	481	C	N1-C2-O2	5.62	122.27	118.90
52	3	1797	C	N1-C2-O2	5.62	122.27	118.90
52	3	2454	G	C4-C5-N7	5.61	113.05	110.80
54	5	974	C	C6-N1-C2	-5.61	118.06	120.30
54	5	1134	C	C6-N1-C2	-5.60	118.06	120.30
52	3	1473	C	N1-C2-O2	5.57	122.24	118.90
55	7	30	G	N3-C4-N9	5.57	129.34	126.00
52	3	1987	C	N1-C2-O2	5.57	122.24	118.90
52	3	1797	C	C2-N1-C1'	5.56	124.92	118.80
52	3	2069	A	C4'-C3'-O3'	5.54	124.09	113.00
54	5	975	C	C6-N1-C2	-5.54	118.08	120.30
52	3	1779	G	N1-C6-O6	-5.49	116.60	119.90
54	5	714	C	N1-C2-O2	5.48	122.19	118.90
52	3	480	C	N3-C2-O2	-5.48	118.07	121.90
55	8	30	G	N3-C4-N9	5.48	129.29	126.00
54	5	463	U	N3-C2-O2	-5.47	118.37	122.20
52	3	1886	C	N3-C2-O2	-5.46	118.08	121.90
52	3	972	C	N1-C2-O2	5.44	122.16	118.90
54	5	1080	G	N1-C6-O6	-5.43	116.64	119.90
52	3	34	C	C6-N1-C2	-5.41	118.14	120.30
52	3	2199	C	C2-N1-C1'	5.40	124.74	118.80
52	3	1672	C	C6-N1-C2	-5.37	118.15	120.30
52	3	2305	C	C2-N1-C1'	5.33	124.67	118.80
52	3	2823	A	OP1-P-O3'	5.28	116.82	105.20
52	3	2612	G	N1-C6-O6	-5.26	116.74	119.90
52	3	1987	C	C6-N1-C2	-5.24	118.20	120.30
54	5	1134	C	C2-N1-C1'	5.24	124.56	118.80
52	3	33	C	N1-C2-O2	5.24	122.04	118.90
52	3	1779	G	C5-C6-O6	5.21	131.73	128.60
31	f	20	ASP	CB-CG-OD2	5.21	122.99	118.30
55	8	77	A	C5-C6-N1	5.19	120.29	117.70
32	g	29	TYR	CB-CA-C	5.15	120.69	110.40
52	3	1779	G	N1-C2-N2	-5.15	111.57	116.20
52	3	1588	A	OP1-P-O3'	5.14	116.52	105.20
28	c	123	ASP	CB-CG-OD1	5.13	122.92	118.30
53	4	78	C	N1-C2-O2	5.13	121.98	118.90
52	3	426	U	N1-C2-O2	5.12	126.39	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	3	2688	C	N1-C2-O2	5.11	121.97	118.90
54	5	975	C	C2-N1-C1'	5.07	124.38	118.80
55	7	73	C	N1-C2-O2	5.06	121.94	118.90
52	3	1303	U	C6-N1-C1'	-5.05	114.13	121.20
52	3	480	C	N1-C2-O2	5.02	121.91	118.90
52	3	1341	U	C6-N1-C1'	-5.00	114.20	121.20
55	8	73	C	N1-C2-O2	5.00	121.90	118.90

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	45/48 (94%)	44 (98%)	1 (2%)	0	100	100
2	1	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
3	2	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
4	9	680/688 (99%)	622 (92%)	58 (8%)	0	100	100
5	A	238/294 (81%)	219 (92%)	19 (8%)	0	100	100
6	B	213/273 (78%)	201 (94%)	12 (6%)	0	100	100
7	C	201/205 (98%)	196 (98%)	5 (2%)	0	100	100
8	D	151/219 (69%)	147 (97%)	4 (3%)	0	100	100
9	E	165/215 (77%)	140 (85%)	25 (15%)	0	100	100
10	F	152/155 (98%)	146 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	G	139/142 (98%)	123 (88%)	14 (10%)	2 (1%)	11	47
12	H	126/132 (96%)	111 (88%)	15 (12%)	0	100	100
13	I	99/108 (92%)	94 (95%)	5 (5%)	0	100	100
14	J	112/121 (93%)	109 (97%)	3 (3%)	0	100	100
15	K	134/139 (96%)	121 (90%)	10 (8%)	3 (2%)	6	37
16	L	116/124 (94%)	109 (94%)	7 (6%)	0	100	100
17	M	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
18	N	81/86 (94%)	78 (96%)	3 (4%)	0	100	100
19	O	78/94 (83%)	71 (91%)	7 (9%)	0	100	100
20	P	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
21	Q	63/104 (61%)	57 (90%)	6 (10%)	0	100	100
22	R	82/87 (94%)	75 (92%)	7 (8%)	0	100	100
23	S	75/87 (86%)	75 (100%)	0	0	100	100
24	T	51/60 (85%)	50 (98%)	1 (2%)	0	100	100
25	W	67/122 (55%)	63 (94%)	4 (6%)	0	100	100
26	a	283/287 (99%)	260 (92%)	23 (8%)	0	100	100
27	b	227/287 (79%)	213 (94%)	14 (6%)	0	100	100
28	c	208/212 (98%)	202 (97%)	6 (3%)	0	100	100
29	d	173/180 (96%)	160 (92%)	13 (8%)	0	100	100
30	e	174/184 (95%)	162 (93%)	12 (7%)	0	100	100
31	f	143/149 (96%)	132 (92%)	11 (8%)	0	100	100
32	g	124/161 (77%)	111 (90%)	11 (9%)	2 (2%)	9	45
33	h	126/137 (92%)	120 (95%)	6 (5%)	0	100	100
34	i	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
35	j	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
36	k	146/151 (97%)	136 (93%)	10 (7%)	0	100	100
37	l	134/139 (96%)	126 (94%)	8 (6%)	0	100	100
38	m	117/124 (94%)	114 (97%)	3 (3%)	0	100	100
39	n	108/116 (93%)	101 (94%)	7 (6%)	0	100	100
40	o	113/119 (95%)	108 (96%)	5 (4%)	0	100	100
41	p	112/127 (88%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	q	97/100 (97%)	85 (88%)	12 (12%)	0	100	100
43	r	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
44	s	90/237 (38%)	86 (96%)	4 (4%)	0	100	100
45	t	109/111 (98%)	101 (93%)	8 (7%)	0	100	100
46	u	84/104 (81%)	78 (93%)	6 (7%)	0	100	100
47	v	61/65 (94%)	58 (95%)	3 (5%)	0	100	100
48	w	96/111 (86%)	88 (92%)	8 (8%)	0	100	100
49	x	42/97 (43%)	38 (90%)	4 (10%)	0	100	100
50	y	54/57 (95%)	47 (87%)	7 (13%)	0	100	100
51	z	48/53 (91%)	45 (94%)	3 (6%)	0	100	100
All	All	6567/7480 (88%)	6123 (93%)	437 (7%)	7 (0%)	54	85

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	K	122	LYS
15	K	123	ARG
11	G	108	LEU
15	K	121	GLU
32	g	45	PHE
11	G	109	ASN
32	g	34	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	40/41 (98%)	40 (100%)	0	100	100
2	1	51/51 (100%)	51 (100%)	0	100	100
3	2	35/35 (100%)	35 (100%)	0	100	100
4	9	579/584 (99%)	579 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	212/262 (81%)	211 (100%)	1 (0%)	88	93
6	B	180/232 (78%)	180 (100%)	0	100	100
7	C	181/183 (99%)	180 (99%)	1 (1%)	86	92
8	D	123/178 (69%)	122 (99%)	1 (1%)	81	89
9	E	150/196 (76%)	148 (99%)	2 (1%)	69	82
10	F	131/132 (99%)	130 (99%)	1 (1%)	81	89
11	G	123/124 (99%)	120 (98%)	3 (2%)	49	69
12	H	111/115 (96%)	110 (99%)	1 (1%)	78	88
13	I	95/99 (96%)	95 (100%)	0	100	100
14	J	91/97 (94%)	89 (98%)	2 (2%)	52	71
15	K	117/120 (98%)	115 (98%)	2 (2%)	60	78
16	L	100/105 (95%)	100 (100%)	0	100	100
17	M	47/48 (98%)	46 (98%)	1 (2%)	53	72
18	N	76/78 (97%)	76 (100%)	0	100	100
19	O	69/82 (84%)	69 (100%)	0	100	100
20	P	73/75 (97%)	72 (99%)	1 (1%)	67	81
21	Q	56/94 (60%)	56 (100%)	0	100	100
22	R	74/77 (96%)	74 (100%)	0	100	100
23	S	70/77 (91%)	69 (99%)	1 (1%)	67	81
24	T	49/56 (88%)	49 (100%)	0	100	100
25	W	58/98 (59%)	58 (100%)	0	100	100
26	a	241/243 (99%)	240 (100%)	1 (0%)	91	94
27	b	186/233 (80%)	186 (100%)	0	100	100
28	c	182/184 (99%)	182 (100%)	0	100	100
29	d	150/154 (97%)	148 (99%)	2 (1%)	69	82
30	e	153/159 (96%)	153 (100%)	0	100	100
31	f	131/134 (98%)	130 (99%)	1 (1%)	81	89
32	g	101/129 (78%)	94 (93%)	7 (7%)	15	42
33	h	102/110 (93%)	102 (100%)	0	100	100
34	i	126/128 (98%)	126 (100%)	0	100	100
35	j	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	123/126 (98%)	122 (99%)	1 (1%)	81	89
37	l	113/115 (98%)	113 (100%)	0	100	100
38	m	105/109 (96%)	105 (100%)	0	100	100
39	n	96/99 (97%)	96 (100%)	0	100	100
40	o	101/105 (96%)	99 (98%)	2 (2%)	55	73
41	p	100/108 (93%)	100 (100%)	0	100	100
42	q	90/91 (99%)	89 (99%)	1 (1%)	73	85
43	r	116/132 (88%)	115 (99%)	1 (1%)	78	88
44	s	82/208 (39%)	82 (100%)	0	100	100
45	t	96/96 (100%)	96 (100%)	0	100	100
46	u	69/85 (81%)	68 (99%)	1 (1%)	67	81
47	v	58/60 (97%)	58 (100%)	0	100	100
48	w	87/98 (89%)	87 (100%)	0	100	100
49	x	41/86 (48%)	41 (100%)	0	100	100
50	y	48/49 (98%)	46 (96%)	2 (4%)	30	55
51	z	47/50 (94%)	47 (100%)	0	100	100
All	All	5738/6433 (89%)	5702 (99%)	36 (1%)	86	92

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	27	ARG
7	C	143	ARG
8	D	97	ARG
9	E	73	LYS
9	E	145	ARG
10	F	5	ARG
11	G	107	VAL
11	G	108	LEU
11	G	109	ASN
12	H	34	ARG
14	J	49	ARG
14	J	121	ARG
15	K	121	GLU
15	K	122	LYS
17	M	41	ARG

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Mol	Chain	Res	Type
20	P	83	ARG
23	S	12	ARG
26	a	4	LYS
29	d	26	MET
29	d	125	ARG
31	f	110	LYS
32	g	26	ILE
32	g	29	TYR
32	g	31	SER
32	g	46	LYS
32	g	87	ASN
32	g	88	GLU
32	g	89	ILE
36	k	30	LYS
40	o	40	LYS
40	o	58	LYS
42	q	24	LYS
43	r	114	ARG
46	u	34	ARG
50	y	47	MET
50	y	52	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
4	9	12	ASN
4	9	264	ASN
4	9	357	HIS
4	9	506	HIS
6	B	8	ASN
7	C	119	HIS
8	D	138	HIS
8	D	202	GLN
9	E	79	ASN
11	G	109	ASN
26	a	208	HIS
28	c	113	HIS
31	f	28	HIS
32	g	47	ASN
32	g	87	ASN
35	j	9	ASN
35	j	18	GLN

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Mol	Chain	Res	Type
41	p	36	GLN
46	u	84	GLN
47	v	34	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	3	2875/2907 (98%)	724 (25%)	27 (0%)
53	4	103/108 (95%)	31 (30%)	2 (1%)
54	5	1490/1520 (98%)	358 (24%)	6 (0%)
55	7	75/76 (98%)	26 (34%)	2 (2%)
55	8	75/76 (98%)	26 (34%)	2 (2%)
All	All	4618/4687 (98%)	1165 (25%)	39 (0%)

All (1165) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	3	14	U
52	3	29	G
52	3	37	G
52	3	41	C
52	3	44	A
52	3	48	G
52	3	53	G
52	3	64	U
52	3	65	A
52	3	73	A
52	3	77	G
52	3	86	A
52	3	87	G
52	3	88	G
52	3	91	G
52	3	94	A
52	3	95	G
52	3	98	C
52	3	101	C
52	3	102	A
52	3	103	G
52	3	106	C
52	3	108	G
52	3	115	U

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Mol	Chain	Res	Type
52	3	119	A
52	3	121	U
52	3	126	C
52	3	127	A
52	3	136	G
52	3	141	A
52	3	142	A
52	3	148	U
52	3	163	A
52	3	165	U
52	3	169	U
52	3	185	U
52	3	186	A
52	3	200	A
52	3	201	A
52	3	203	A
52	3	204	U
52	3	208	A
52	3	209	G
52	3	211	A
52	3	219	G
52	3	220	A
52	3	226	A
52	3	227	A
52	3	230	G
52	3	231	A
52	3	232	A
52	3	234	G
52	3	237	A
52	3	251	G
52	3	252	G
52	3	254	G
52	3	255	A
52	3	256	G
52	3	259	A
52	3	261	A
52	3	265	G
52	3	270	G
52	3	276	A
52	3	282	C
52	3	283	A
52	3	284	U

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Mol	Chain	Res	Type
52	3	285	U
52	3	286	A
52	3	287	G
52	3	288	A
52	3	290	A
52	3	295	U
52	3	296	U
52	3	297	G
52	3	299	A
52	3	305	U
52	3	307	C
52	3	310	U
52	3	312	U
52	3	314	G
52	3	315	A
52	3	325	G
52	3	328	A
52	3	329	G
52	3	336	C
52	3	345	A
52	3	351	G
52	3	356	A
52	3	357	A
52	3	358	A
52	3	363	G
52	3	364	A
52	3	366	A
52	3	369	C
52	3	383	U
52	3	392	A
52	3	399	G
52	3	400	A
52	3	402	A
52	3	403	U
52	3	404	C
52	3	408	G
52	3	409	A
52	3	410	G
52	3	411	U
52	3	419	A
52	3	422	A
52	3	423	C

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Mol	Chain	Res	Type
52	3	424	G
52	3	425	U
52	3	426	U
52	3	432	G
52	3	434	G
52	3	437	A
52	3	438	A
52	3	439	U
52	3	441	U
52	3	442	G
52	3	447	G
52	3	448	A
52	3	450	C
52	3	460	G
52	3	465	A
52	3	466	A
52	3	484	U
52	3	485	A
52	3	487	C
52	3	501	G
52	3	509	G
52	3	514	A
52	3	515	A
52	3	516	A
52	3	517	G
52	3	519	A
52	3	525	A
52	3	526	G
52	3	538	A
52	3	540	A
52	3	543	U
52	3	544	U
52	3	556	U
52	3	562	C
52	3	563	A
52	3	565	C
52	3	566	G
52	3	567	U
52	3	577	C
52	3	580	U
52	3	581	A
52	3	583	U

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Mol	Chain	Res	Type
52	3	584	G
52	3	595	U
52	3	596	G
52	3	605	A
52	3	607	U
52	3	608	A
52	3	610	G
52	3	619	A
52	3	620	G
52	3	637	U
52	3	638	A
52	3	641	U
52	3	649	A
52	3	650	G
52	3	652	U
52	3	656	G
52	3	657	A
52	3	673	A
52	3	679	A
52	3	681	A
52	3	682	A
52	3	683	G
52	3	688	U
52	3	689	U
52	3	691	G
52	3	693	U
52	3	701	A
52	3	705	A
52	3	706	C
52	3	711	A
52	3	712	A
52	3	720	A
52	3	721	G
52	3	722	C
52	3	752	C
52	3	761	G
52	3	765	A
52	3	781	U
52	3	783	G
52	3	787	C
52	3	792	G
52	3	794	G

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Mol	Chain	Res	Type
52	3	797	U
52	3	798	G
52	3	800	C
52	3	810	G
52	3	811	G
52	3	812	G
52	3	817	A
52	3	818	A
52	3	819	U
52	3	820	U
52	3	824	A
52	3	827	G
52	3	835	U
52	3	836	G
52	3	840	G
52	3	842	U
52	3	847	C
52	3	854	A
52	3	862	U
52	3	863	U
52	3	868	C
52	3	880	C
52	3	882	C
52	3	895	G
52	3	902	U
52	3	906	G
52	3	910	G
52	3	917	G
52	3	920	G
52	3	932	U
52	3	933	A
52	3	934	C
52	3	937	A
52	3	938	A
52	3	944	U
52	3	947	A
52	3	948	A
52	3	949	C
52	3	952	U
52	3	953	G
52	3	966	U
52	3	968	U

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Mol	Chain	Res	Type
52	3	971	U
52	3	973	U
52	3	975	G
52	3	977	A
52	3	981	A
52	3	982	G
52	3	989	G
52	3	993	A
52	3	994	U
52	3	995	A
52	3	997	G
52	3	1010	G
52	3	1011	A
52	3	1016	A
52	3	1018	G
52	3	1019	A
52	3	1021	C
52	3	1023	C
52	3	1024	A
52	3	1032	A
52	3	1041	C
52	3	1045	A
52	3	1048	A
52	3	1049	U
52	3	1052	A
52	3	1057	G
52	3	1061	A
52	3	1066	G
52	3	1068	U
52	3	1081	A
52	3	1082	A
52	3	1085	A
52	3	1090	G
52	3	1092	A
52	3	1095	U
52	3	1096	U
52	3	1097	G
52	3	1098	G
52	3	1102	A
52	3	1104	A
52	3	1105	A
52	3	1106	G

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Mol	Chain	Res	Type
52	3	1107	C
52	3	1113	U
52	3	1114	C
52	3	1118	U
52	3	1123	A
52	3	1124	G
52	3	1132	C
52	3	1138	A
52	3	1140	U
52	3	1147	G
52	3	1151	U
52	3	1154	U
52	3	1164	A
52	3	1168	A
52	3	1169	A
52	3	1170	C
52	3	1171	G
52	3	1177	A
52	3	1178	A
52	3	1182	U
52	3	1186	A
52	3	1190	A
52	3	1192	U
52	3	1204	A
52	3	1207	U
52	3	1208	A
52	3	1209	U
52	3	1210	A
52	3	1217	G
52	3	1221	G
52	3	1234	U
52	3	1236	G
52	3	1240	U
52	3	1250	A
52	3	1251	G
52	3	1253	G
52	3	1257	G
52	3	1268	U
52	3	1269	C
52	3	1279	U
52	3	1281	A
52	3	1283	A

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Mol	Chain	Res	Type
52	3	1284	A
52	3	1285	U
52	3	1286	G
52	3	1295	A
52	3	1299	A
52	3	1302	C
52	3	1306	G
52	3	1317	C
52	3	1324	A
52	3	1328	A
52	3	1329	U
52	3	1332	A
52	3	1342	C
52	3	1351	G
52	3	1353	G
52	3	1357	U
52	3	1359	C
52	3	1360	U
52	3	1361	U
52	3	1374	U
52	3	1380	U
52	3	1382	A
52	3	1393	A
52	3	1396	A
52	3	1406	A
52	3	1407	U
52	3	1412	A
52	3	1420	A
52	3	1423	A
52	3	1426	C
52	3	1430	U
52	3	1431	A
52	3	1434	U
52	3	1441	A
52	3	1444	C
52	3	1445	U
52	3	1447	A
52	3	1448	U
52	3	1456	C
52	3	1463	G
52	3	1466	U
52	3	1479	A

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Mol	Chain	Res	Type
52	3	1480	A
52	3	1481	U
52	3	1483	G
52	3	1485	A
52	3	1486	U
52	3	1487	U
52	3	1493	A
52	3	1507	G
52	3	1508	G
52	3	1510	A
52	3	1515	A
52	3	1523	C
52	3	1528	G
52	3	1534	A
52	3	1541	A
52	3	1542	G
52	3	1545	A
52	3	1548	A
52	3	1549	U
52	3	1550	G
52	3	1558	A
52	3	1559	A
52	3	1571	G
52	3	1574	G
52	3	1581	U
52	3	1582	G
52	3	1584	U
52	3	1585	A
52	3	1587	U
52	3	1588	A
52	3	1589	A
52	3	1592	A
52	3	1594	G
52	3	1603	A
52	3	1605	A
52	3	1612	U
52	3	1618	U
52	3	1619	A
52	3	1641	A
52	3	1642	G
52	3	1643	A
52	3	1644	A

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Mol	Chain	Res	Type
52	3	1645	C
52	3	1650	A
52	3	1651	C
52	3	1652	A
52	3	1656	A
52	3	1668	G
52	3	1671	C
52	3	1676	G
52	3	1677	G
52	3	1679	U
52	3	1680	A
52	3	1681	G
52	3	1682	C
52	3	1683	G
52	3	1685	G
52	3	1688	A
52	3	1694	A
52	3	1695	G
52	3	1698	A
52	3	1708	G
52	3	1711	A
52	3	1713	U
52	3	1714	U
52	3	1727	U
52	3	1730	C
52	3	1747	G
52	3	1752	A
52	3	1761	C
52	3	1764	U
52	3	1765	G
52	3	1766	A
52	3	1769	A
52	3	1770	A
52	3	1771	C
52	3	1780	A
52	3	1784	U
52	3	1786	U
52	3	1787	A
52	3	1788	A
52	3	1789	C
52	3	1791	A
52	3	1794	A

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Mol	Chain	Res	Type
52	3	1797	C
52	3	1804	A
52	3	1807	C
52	3	1808	C
52	3	1809	A
52	3	1821	G
52	3	1822	A
52	3	1823	U
52	3	1826	A
52	3	1828	A
52	3	1834	U
52	3	1836	A
52	3	1842	G
52	3	1865	A
52	3	1866	G
52	3	1869	G
52	3	1873	A
52	3	1879	A
52	3	1889	U
52	3	1890	U
52	3	1891	A
52	3	1904	G
52	3	1906	G
52	3	1907	A
52	3	1908	A
52	3	1910	G
52	3	1913	G
52	3	1917	G
52	3	1919	A
52	3	1920	A
52	3	1921	C
52	3	1922	U
52	3	1923	A
52	3	1924	U
52	3	1930	U
52	3	1935	A
52	3	1936	G
52	3	1937	G
52	3	1943	A
52	3	1944	A
52	3	1945	A
52	3	1951	A

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Mol	Chain	Res	Type
52	3	1952	G
52	3	1959	A
52	3	1960	A
52	3	1962	U
52	3	1971	G
52	3	1972	C
52	3	1977	A
52	3	1978	U
52	3	1979	G
52	3	1982	G
52	3	1989	U
52	3	1999	G
52	3	2000	U
52	3	2004	G
52	3	2009	U
52	3	2010	A
52	3	2027	G
52	3	2028	G
52	3	2030	A
52	3	2038	A
52	3	2039	G
52	3	2040	A
52	3	2041	C
52	3	2042	A
52	3	2050	G
52	3	2055	A
52	3	2059	G
52	3	2062	C
52	3	2063	G
52	3	2067	A
52	3	2068	G
52	3	2069	A
52	3	2070	C
52	3	2071	C
52	3	2073	C
52	3	2075	U
52	3	2076	G
52	3	2084	A
52	3	2100	G
52	3	2107	A
52	3	2110	U
52	3	2111	U

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Mol	Chain	Res	Type
52	3	2112	A
52	3	2114	C
52	3	2115	A
52	3	2116	U
52	3	2117	G
52	3	2119	A
52	3	2122	G
52	3	2123	A
52	3	2124	A
52	3	2125	U
52	3	2126	A
52	3	2132	G
52	3	2133	A
52	3	2138	U
52	3	2140	G
52	3	2141	A
52	3	2144	C
52	3	2145	A
52	3	2152	C
52	3	2153	U
52	3	2154	A
52	3	2156	G
52	3	2157	A
52	3	2163	U
52	3	2164	G
52	3	2165	A
52	3	2166	U
52	3	2170	A
52	3	2178	A
52	3	2180	U
52	3	2181	A
52	3	2183	U
52	3	2184	A
52	3	2186	C
52	3	2187	C
52	3	2193	U
52	3	2195	U
52	3	2197	U
52	3	2198	G
52	3	2200	U
52	3	2202	U
52	3	2206	A

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Mol	Chain	Res	Type
52	3	2212	U
52	3	2219	U
52	3	2221	U
52	3	2222	C
52	3	2227	U
52	3	2231	A
52	3	2233	A
52	3	2247	G
52	3	2258	G
52	3	2274	A
52	3	2276	A
52	3	2281	A
52	3	2287	G
52	3	2290	G
52	3	2291	U
52	3	2294	A
52	3	2295	A
52	3	2305	C
52	3	2312	G
52	3	2313	U
52	3	2316	G
52	3	2320	U
52	3	2322	G
52	3	2324	A
52	3	2327	U
52	3	2328	A
52	3	2330	A
52	3	2333	G
52	3	2334	U
52	3	2335	A
52	3	2341	G
52	3	2342	U
52	3	2345	G
52	3	2352	U
52	3	2355	C
52	3	2358	U
52	3	2362	A
52	3	2365	U
52	3	2391	G
52	3	2393	C
52	3	2410	C
52	3	2411	C

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Mol	Chain	Res	Type
52	3	2414	U
52	3	2423	G
52	3	2424	C
52	3	2430	C
52	3	2431	U
52	3	2433	A
52	3	2436	G
52	3	2438	A
52	3	2440	A
52	3	2448	C
52	3	2449	U
52	3	2455	G
52	3	2456	A
52	3	2459	A
52	3	2477	A
52	3	2478	G
52	3	2483	C
52	3	2484	A
52	3	2486	A
52	3	2489	G
52	3	2494	C
52	3	2495	A
52	3	2498	G
52	3	2499	U
52	3	2505	A
52	3	2506	C
52	3	2507	C
52	3	2509	C
52	3	2510	G
52	3	2511	A
52	3	2512	U
52	3	2521	A
52	3	2526	A
52	3	2528	C
52	3	2539	A
52	3	2557	G
52	3	2570	U
52	3	2574	A
52	3	2575	G
52	3	2580	A
52	3	2581	C
52	3	2584	G

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Mol	Chain	Res	Type
52	3	2585	A
52	3	2586	G
52	3	2587	U
52	3	2602	C
52	3	2605	G
52	3	2606	A
52	3	2607	G
52	3	2610	A
52	3	2611	G
52	3	2617	U
52	3	2621	U
52	3	2623	U
52	3	2629	G
52	3	2631	G
52	3	2637	A
52	3	2638	G
52	3	2642	G
52	3	2646	G
52	3	2649	G
52	3	2653	G
52	3	2654	U
52	3	2655	U
52	3	2668	A
52	3	2669	G
52	3	2681	G
52	3	2687	A
52	3	2689	C
52	3	2697	C
52	3	2706	U
52	3	2722	G
52	3	2732	A
52	3	2734	C
52	3	2737	G
52	3	2741	A
52	3	2747	U
52	3	2752	G
52	3	2756	A
52	3	2760	C
52	3	2765	A
52	3	2769	G
52	3	2774	A
52	3	2786	A

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Mol	Chain	Res	Type
52	3	2787	U
52	3	2788	U
52	3	2799	U
52	3	2801	U
52	3	2806	A
52	3	2807	G
52	3	2808	A
52	3	2810	A
52	3	2811	G
52	3	2813	A
52	3	2815	G
52	3	2824	A
52	3	2828	C
52	3	2837	U
52	3	2838	G
52	3	2839	A
52	3	2843	G
52	3	2853	U
52	3	2854	A
52	3	2862	U
52	3	2871	G
52	3	2876	G
52	3	2883	A
52	3	2884	C
52	3	2887	A
52	3	2890	G
52	3	2897	G
52	3	2899	C
53	4	10	C
53	4	11	A
53	4	12	U
53	4	13	G
53	4	14	U
53	4	22	G
53	4	23	A
53	4	28	C
53	4	34	U
53	4	38	U
53	4	39	U
53	4	40	U
53	4	41	C
53	4	42	G

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Mol	Chain	Res	Type
53	4	47	C
53	4	49	G
53	4	54	U
53	4	55	A
53	4	60	C
53	4	64	G
53	4	65	G
53	4	66	A
53	4	76	A
53	4	77	G
53	4	80	G
53	4	85	A
53	4	88	G
53	4	89	A
53	4	99	A
53	4	100	G
53	4	108	C
54	5	7	U
54	5	8	G
54	5	9	A
54	5	10	G
54	5	32	U
54	5	33	A
54	5	38	U
54	5	48	C
54	5	49	C
54	5	52	A
54	5	55	C
54	5	61	A
54	5	67	U
54	5	75	A
54	5	77	U
54	5	78	A
54	5	85	U
54	5	86	A
54	5	93	A
54	5	98	G
54	5	100	G
54	5	101	A
54	5	105	A
54	5	106	C
54	5	107	A

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Mol	Chain	Res	Type
54	5	114	C
54	5	115	A
54	5	116	A
54	5	117	U
54	5	128	A
54	5	129	U
54	5	135	A
54	5	149	G
54	5	153	A
54	5	156	U
54	5	157	A
54	5	169	G
54	5	171	A
54	5	174	U
54	5	175	U
54	5	186	A
54	5	187	A
54	5	189	C
54	5	197	A
54	5	199	A
54	5	220	U
54	5	222	U
54	5	223	G
54	5	241	C
54	5	243	G
54	5	246	A
54	5	247	G
54	5	258	A
54	5	260	C
54	5	262	G
54	5	263	C
54	5	274	A
54	5	275	A
54	5	276	U
54	5	277	G
54	5	278	A
54	5	285	G
54	5	286	C
54	5	301	G
54	5	302	A
54	5	316	G
54	5	324	C

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Mol	Chain	Res	Type
54	5	326	C
54	5	328	G
54	5	341	C
54	5	343	G
54	5	348	C
54	5	349	A
54	5	350	G
54	5	351	C
54	5	363	U
54	5	364	U
54	5	365	U
54	5	367	A
54	5	368	C
54	5	380	G
54	5	388	G
54	5	393	A
54	5	394	U
54	5	400	G
54	5	402	G
54	5	407	A
54	5	408	U
54	5	409	G
54	5	417	U
54	5	418	U
54	5	419	A
54	5	420	A
54	5	421	G
54	5	425	G
54	5	426	U
54	5	445	A
54	5	448	A
54	5	449	A
54	5	450	U
54	5	453	C
54	5	461	G
54	5	462	G
54	5	468	G
54	5	476	U
54	5	477	U
54	5	478	G
54	5	482	G
54	5	483	U

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Mol	Chain	Res	Type
54	5	488	U
54	5	489	U
54	5	493	A
54	5	494	A
54	5	497	A
54	5	498	G
54	5	500	G
54	5	503	G
54	5	509	C
54	5	510	U
54	5	515	G
54	5	516	C
54	5	519	G
54	5	523	U
54	5	525	G
54	5	530	A
54	5	531	A
54	5	533	A
54	5	542	G
54	5	545	A
54	5	548	G
54	5	549	U
54	5	551	A
54	5	557	A
54	5	558	U
54	5	559	U
54	5	560	U
54	5	564	G
54	5	570	A
54	5	571	A
54	5	574	C
54	5	575	A
54	5	579	G
54	5	586	G
54	5	594	A
54	5	595	G
54	5	616	C
54	5	626	G
54	5	629	U
54	5	630	G
54	5	637	A
54	5	639	A

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Mol	Chain	Res	Type
54	5	646	A
54	5	647	U
54	5	653	G
54	5	656	U
54	5	661	G
54	5	662	G
54	5	678	A
54	5	683	G
54	5	699	A
54	5	700	G
54	5	701	A
54	5	704	U
54	5	712	A
54	5	715	A
54	5	716	C
54	5	718	A
54	5	719	G
54	5	720	U
54	5	721	G
54	5	731	A
54	5	745	U
54	5	750	A
54	5	752	G
54	5	763	A
54	5	774	A
54	5	777	A
54	5	790	U
54	5	811	A
54	5	812	A
54	5	814	C
54	5	815	G
54	5	817	U
54	5	818	A
54	5	822	A
54	5	824	U
54	5	825	A
54	5	826	G
54	5	838	A
54	5	839	U
54	5	849	A
54	5	856	U
54	5	870	A

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Mol	Chain	Res	Type
54	5	878	U
54	5	883	A
54	5	885	U
54	5	888	A
54	5	892	G
54	5	895	A
54	5	896	G
54	5	908	A
54	5	910	C
54	5	911	G
54	5	917	G
54	5	919	C
54	5	921	G
54	5	922	G
54	5	929	C
54	5	930	A
54	5	933	A
54	5	953	A
54	5	955	U
54	5	961	G
54	5	963	U
54	5	964	A
54	5	965	C
54	5	966	A
54	5	970	A
54	5	971	A
54	5	972	A
54	5	975	C
54	5	976	U
54	5	977	U
54	5	984	A
54	5	987	U
54	5	988	G
54	5	989	A
54	5	995	U
54	5	998	G
54	5	1002	A
54	5	1003	G
54	5	1005	U
54	5	1006	A
54	5	1012	A
54	5	1014	A

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Mol	Chain	Res	Type
54	5	1016	A
54	5	1018	U
54	5	1029	C
54	5	1036	C
54	5	1040	U
54	5	1041	G
54	5	1044	G
54	5	1045	C
54	5	1046	A
54	5	1056	U
54	5	1058	A
54	5	1061	U
54	5	1072	G
54	5	1082	U
54	5	1085	G
54	5	1086	U
54	5	1089	C
54	5	1092	A
54	5	1096	A
54	5	1100	C
54	5	1104	C
54	5	1113	U
54	5	1114	A
54	5	1118	A
54	5	1119	C
54	5	1120	A
54	5	1121	U
54	5	1122	U
54	5	1123	G
54	5	1124	U
54	5	1125	C
54	5	1128	G
54	5	1134	C
54	5	1135	U
54	5	1136	G
54	5	1141	U
54	5	1142	G
54	5	1144	A
54	5	1158	A
54	5	1162	G
54	5	1165	G
54	5	1168	G

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Mol	Chain	Res	Type
54	5	1171	A
54	5	1175	C
54	5	1176	A
54	5	1177	U
54	5	1188	A
54	5	1197	G
54	5	1200	G
54	5	1201	C
54	5	1202	A
54	5	1206	G
54	5	1208	G
54	5	1209	C
54	5	1211	A
54	5	1213	A
54	5	1218	C
54	5	1219	C
54	5	1223	A
54	5	1231	U
54	5	1232	C
54	5	1241	G
54	5	1243	A
54	5	1245	A
54	5	1255	A
54	5	1257	C
54	5	1260	U
54	5	1261	A
54	5	1262	A
54	5	1268	G
54	5	1272	C
54	5	1273	A
54	5	1276	U
54	5	1279	G
54	5	1296	C
54	5	1297	G
54	5	1303	A
54	5	1312	G
54	5	1313	A
54	5	1314	A
54	5	1316	C
54	5	1319	U
54	5	1320	A
54	5	1321	G

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Mol	Chain	Res	Type
54	5	1327	G
54	5	1338	A
54	5	1349	A
54	5	1353	C
54	5	1354	G
54	5	1358	U
54	5	1361	G
54	5	1362	G
54	5	1367	G
54	5	1373	A
54	5	1374	C
54	5	1377	C
54	5	1390	G
54	5	1395	C
54	5	1397	G
54	5	1398	G
54	5	1404	U
54	5	1405	U
54	5	1417	U
54	5	1418	G
54	5	1421	A
54	5	1423	C
54	5	1429	G
54	5	1439	G
54	5	1446	A
54	5	1457	G
54	5	1458	A
54	5	1459	U
54	5	1466	U
54	5	1467	A
54	5	1469	G
54	5	1474	A
54	5	1478	A
54	5	1480	G
54	5	1481	U
54	5	1492	G
54	5	1495	C
54	5	1504	G
54	5	1505	G
55	7	5	C
55	7	14	C
55	7	17	U

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Mol	Chain	Res	Type
55	7	20	G
55	7	21	U
55	7	22	A
55	7	24	A
55	7	34	U
55	7	35	G
55	7	36	A
55	7	41	C
55	7	43	G
55	7	44	U
55	7	45	G
55	7	48	U
55	7	49	C
55	7	50	G
55	7	54	G
55	7	58	G
55	7	60	U
55	7	62	C
55	7	71	A
55	7	72	C
55	7	75	C
55	7	76	C
55	7	77	A
55	8	5	C
55	8	14	C
55	8	17	U
55	8	20	G
55	8	21	U
55	8	22	A
55	8	24	A
55	8	34	U
55	8	35	G
55	8	36	A
55	8	41	C
55	8	43	G
55	8	44	U
55	8	45	G
55	8	48	U
55	8	49	C
55	8	50	G
55	8	54	G
55	8	58	G

Continued on next page...

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Mol	Chain	Res	Type
55	8	60	U
55	8	62	C
55	8	71	A
55	8	72	C
55	8	75	C
55	8	76	C
55	8	77	A

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	3	85	U
52	3	410	G
52	3	500	U
52	3	513	A
52	3	514	A
52	3	524	G
52	3	688	U
52	3	881	A
52	3	901	C
52	3	952	U
52	3	1048	A
52	3	1104	A
52	3	1209	U
52	3	1507	G
52	3	1583	G
52	3	1587	U
52	3	1588	A
52	3	1820	U
52	3	2070	C
52	3	2165	A
52	3	2333	G
52	3	2504	C
52	3	2506	C
52	3	2604	U
52	3	2668	A
52	3	2764	U
52	3	2823	A
53	4	54	U
53	4	59	A
54	5	60	A
54	5	532	U

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Mol	Chain	Res	Type
54	5	894	A
54	5	988	G
54	5	1099	G
54	5	1143	C
55	7	16	G
55	7	71	A
55	8	16	G
55	8	71	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	SCM	5	1601	-	23,25,25	1.66	7 (30%)	26,39,39	1.32	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SCM	5	1601	-	-	2/4/57/57	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	5	1601	SCM	C3-C2	3.03	1.58	1.51
56	5	1601	SCM	C9-C8	2.89	1.58	1.53
56	5	1601	SCM	C3-C4	2.53	1.54	1.50
56	5	1601	SCM	C12-C7	2.40	1.57	1.52
56	5	1601	SCM	O2B-C12	2.24	1.47	1.44
56	5	1601	SCM	O5-C5	2.19	1.43	1.39
56	5	1601	SCM	C8-N8	2.06	1.51	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	5	1601	SCM	C1M-N10-C10	-4.87	107.29	114.38
56	5	1601	SCM	C2M-C2-C3	-2.40	108.54	113.22

There are no chirality outliers.

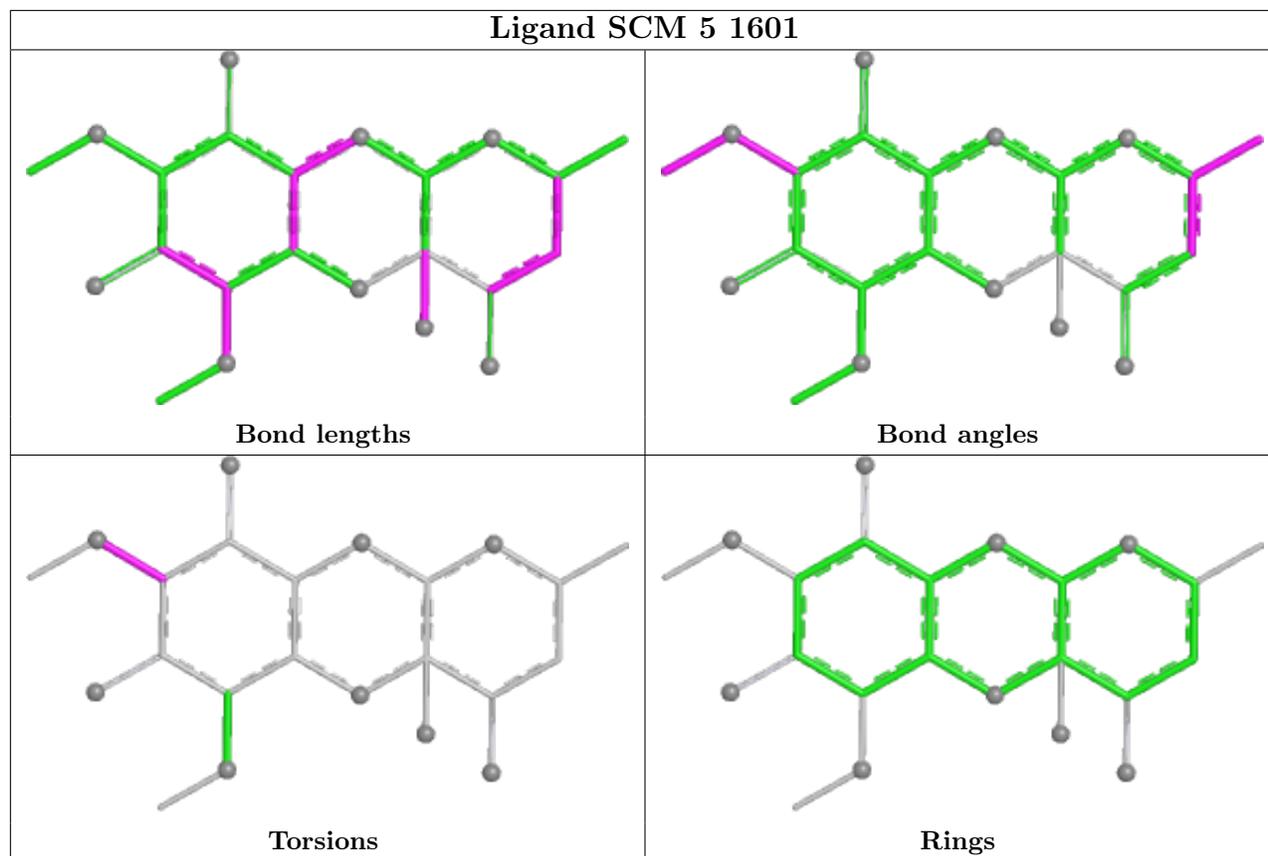
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	5	1601	SCM	C9-C10-N10-C1M
56	5	1601	SCM	C11-C10-N10-C1M

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

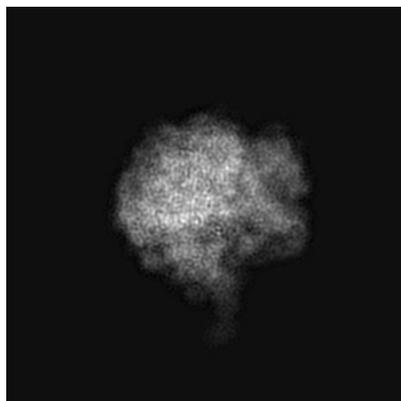
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13435. These allow visual inspection of the internal detail of the map and identification of artifacts.

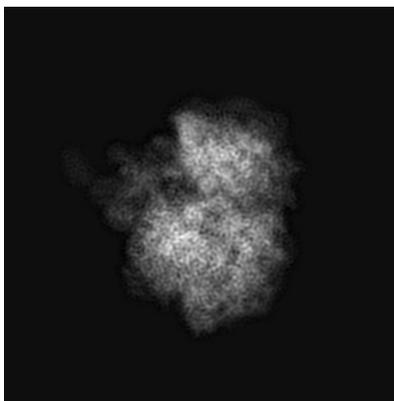
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

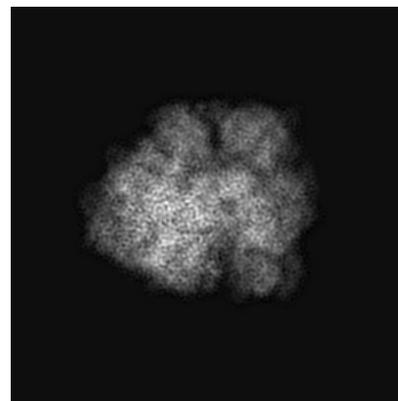
6.1.1 Primary map



X

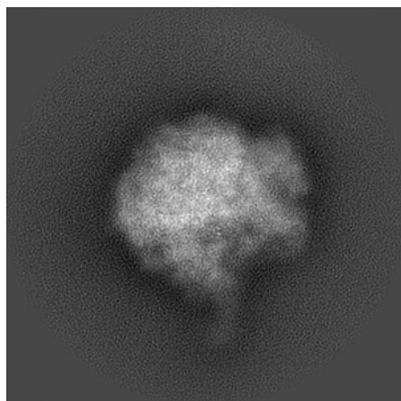


Y

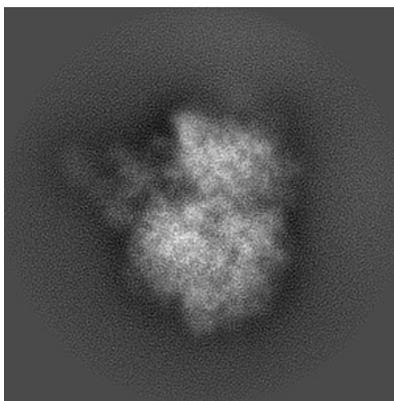


Z

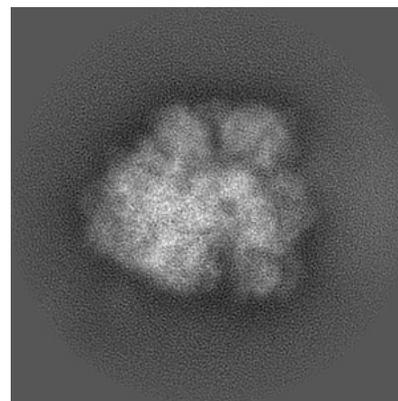
6.1.2 Raw map



X



Y

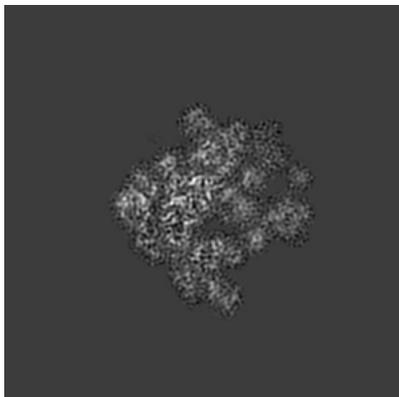


Z

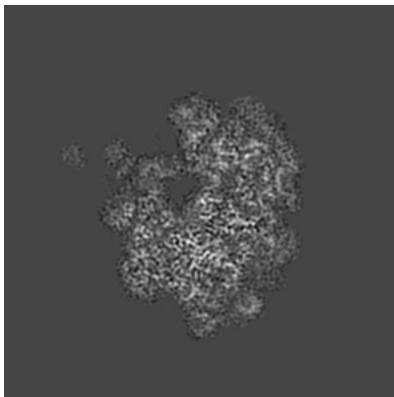
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

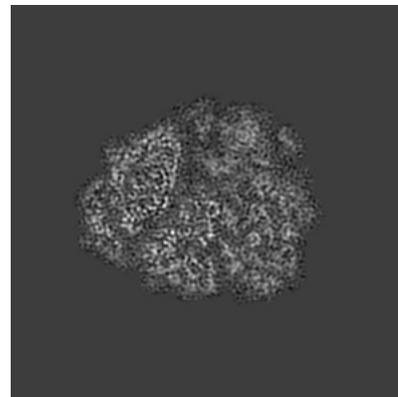
6.2.1 Primary map



X Index: 128

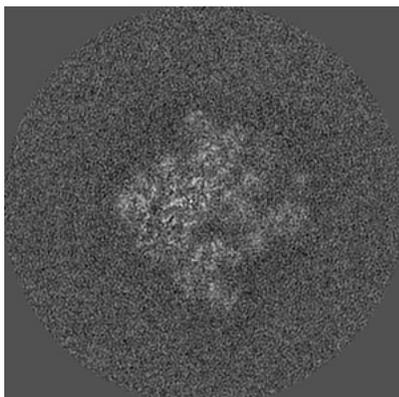


Y Index: 128

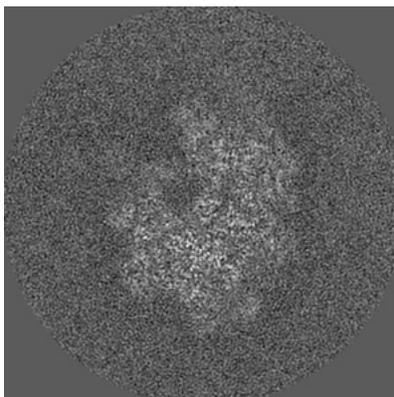


Z Index: 128

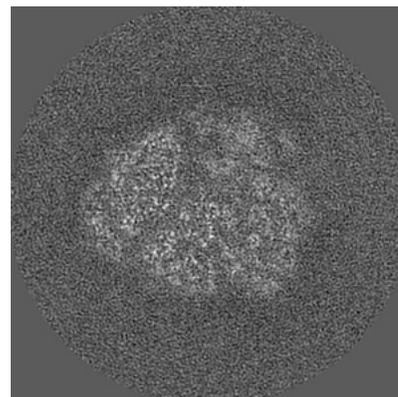
6.2.2 Raw map



X Index: 128



Y Index: 128

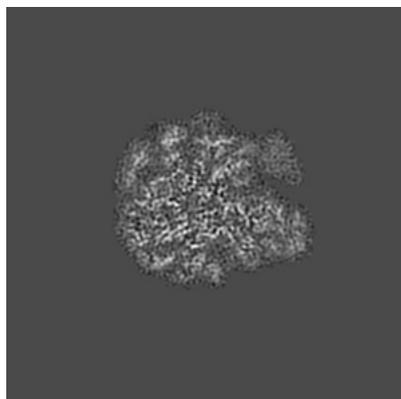


Z Index: 128

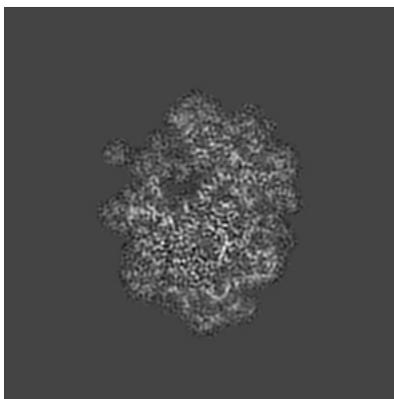
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

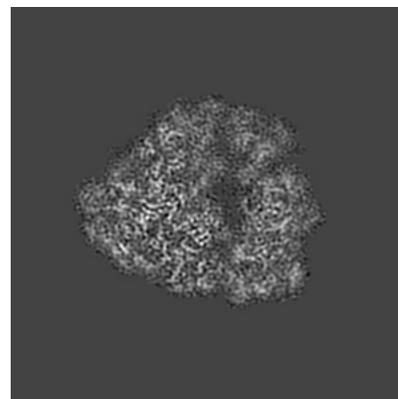
6.3.1 Primary map



X Index: 104

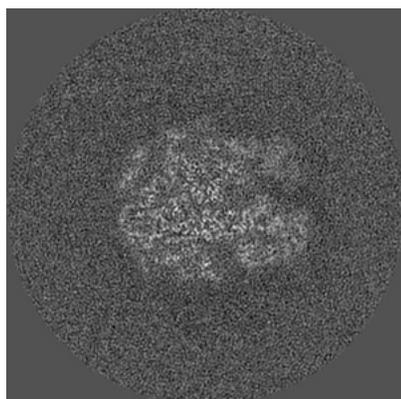


Y Index: 121

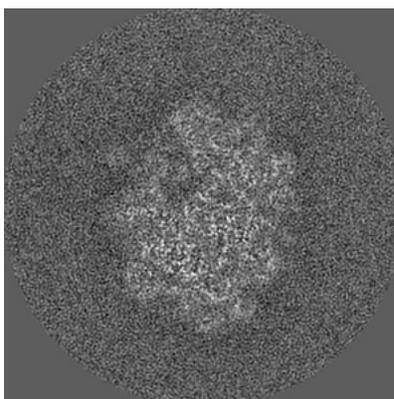


Z Index: 122

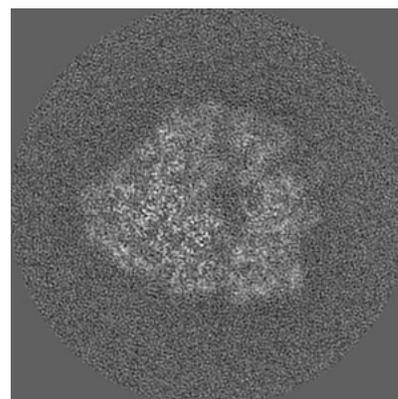
6.3.2 Raw map



X Index: 107



Y Index: 122

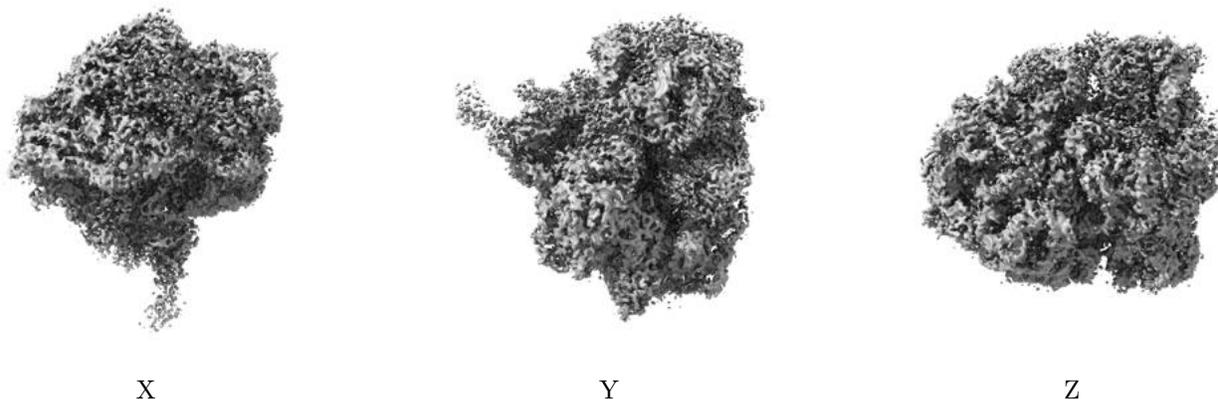


Z Index: 122

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

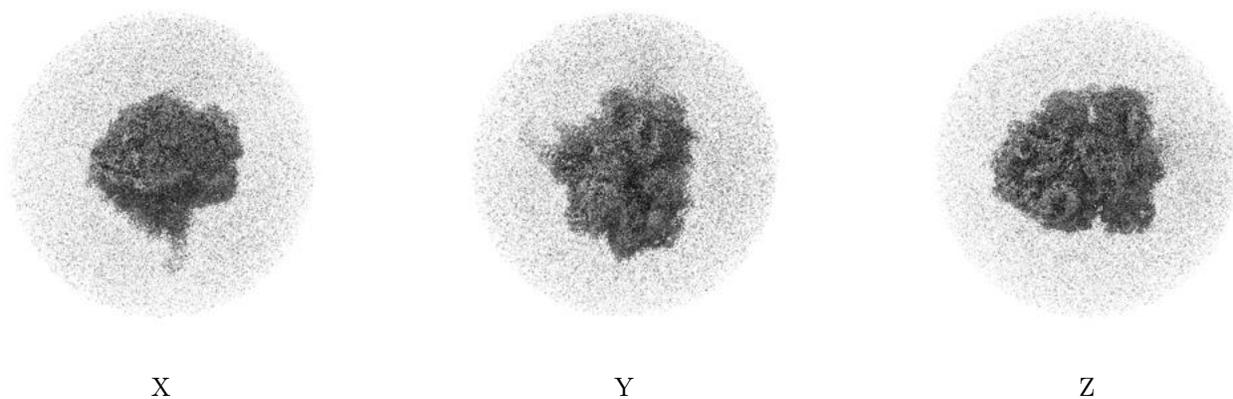
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.66. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

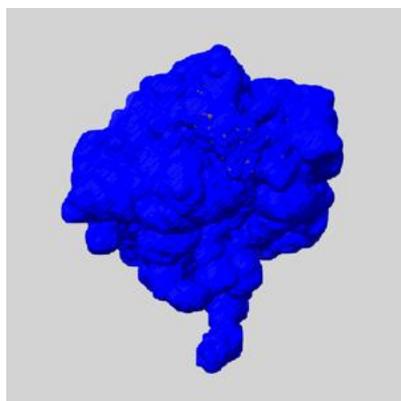
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

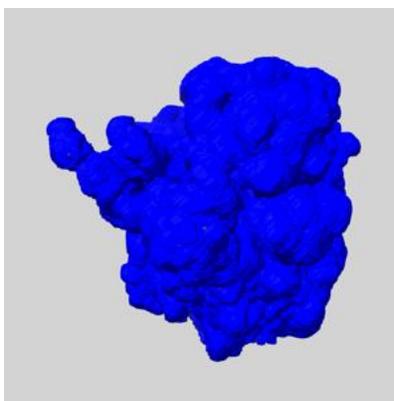
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

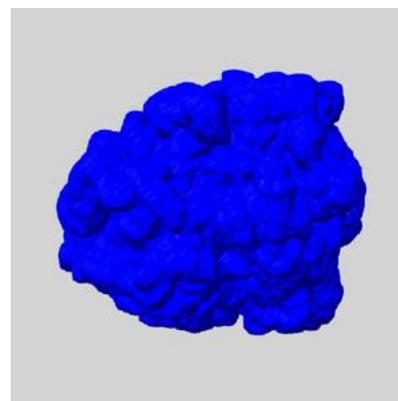
6.5.1 emd_13435_msk_1.map [i](#)



X



Y

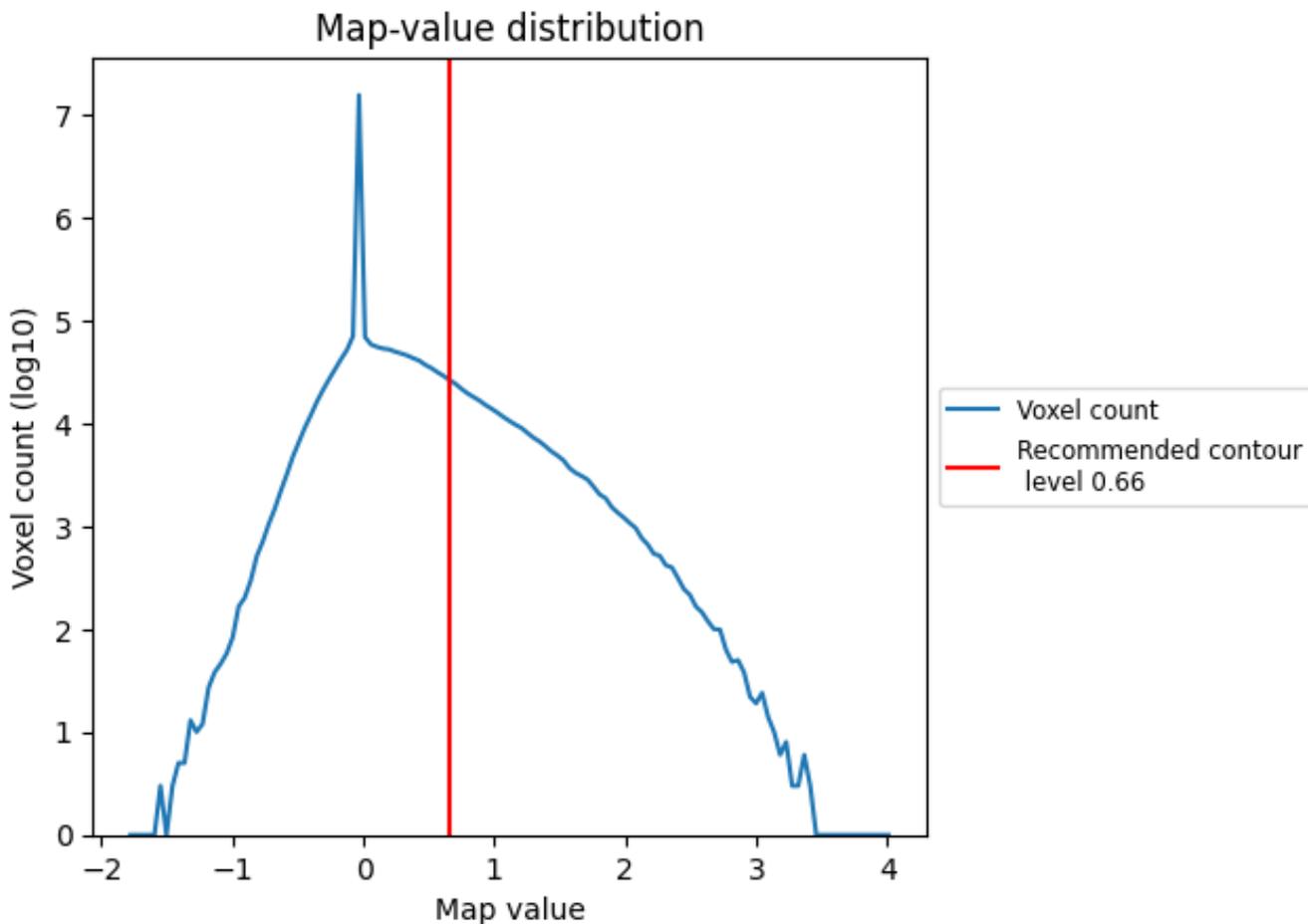


Z

7 Map analysis [i](#)

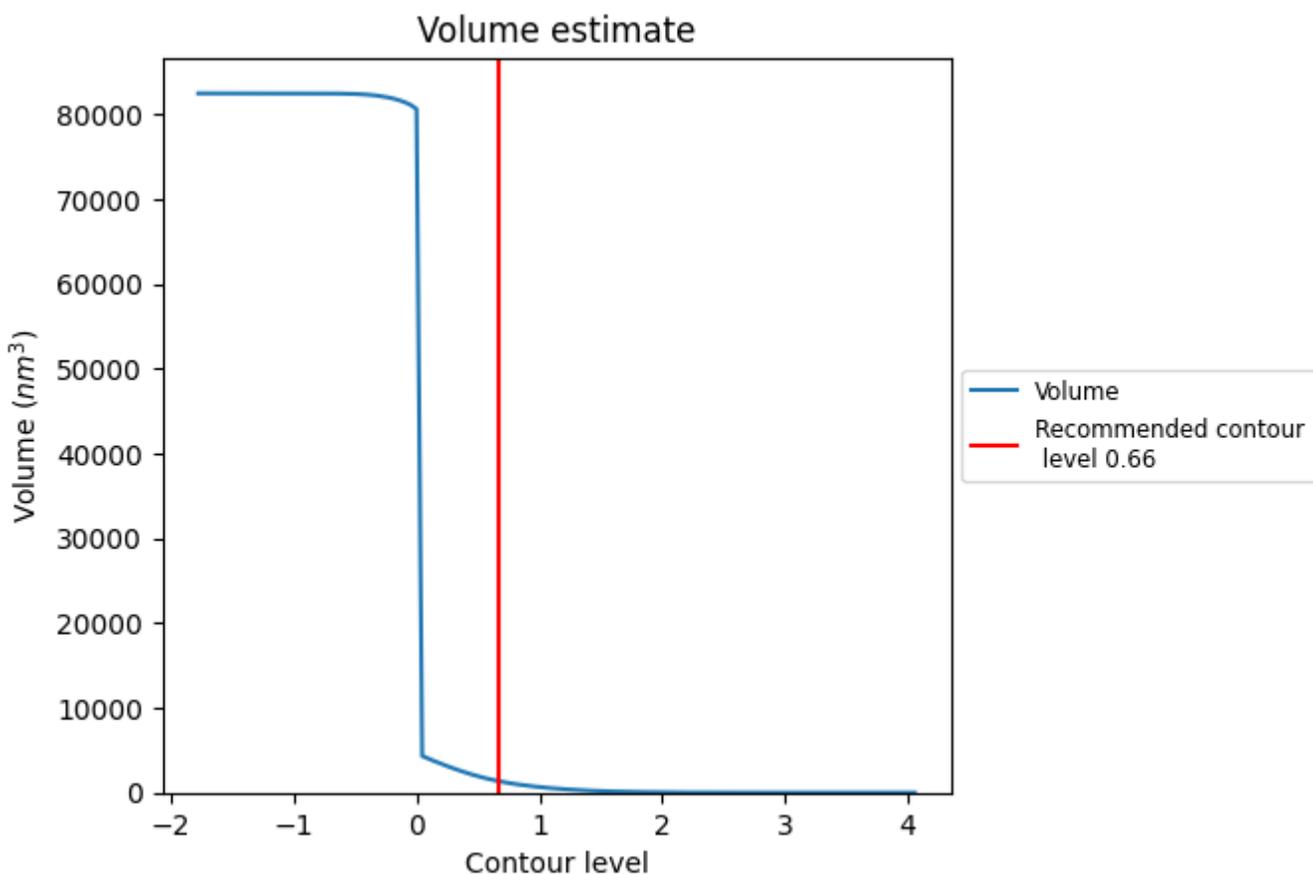
This section contains the results of statistical analysis of the map.

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.

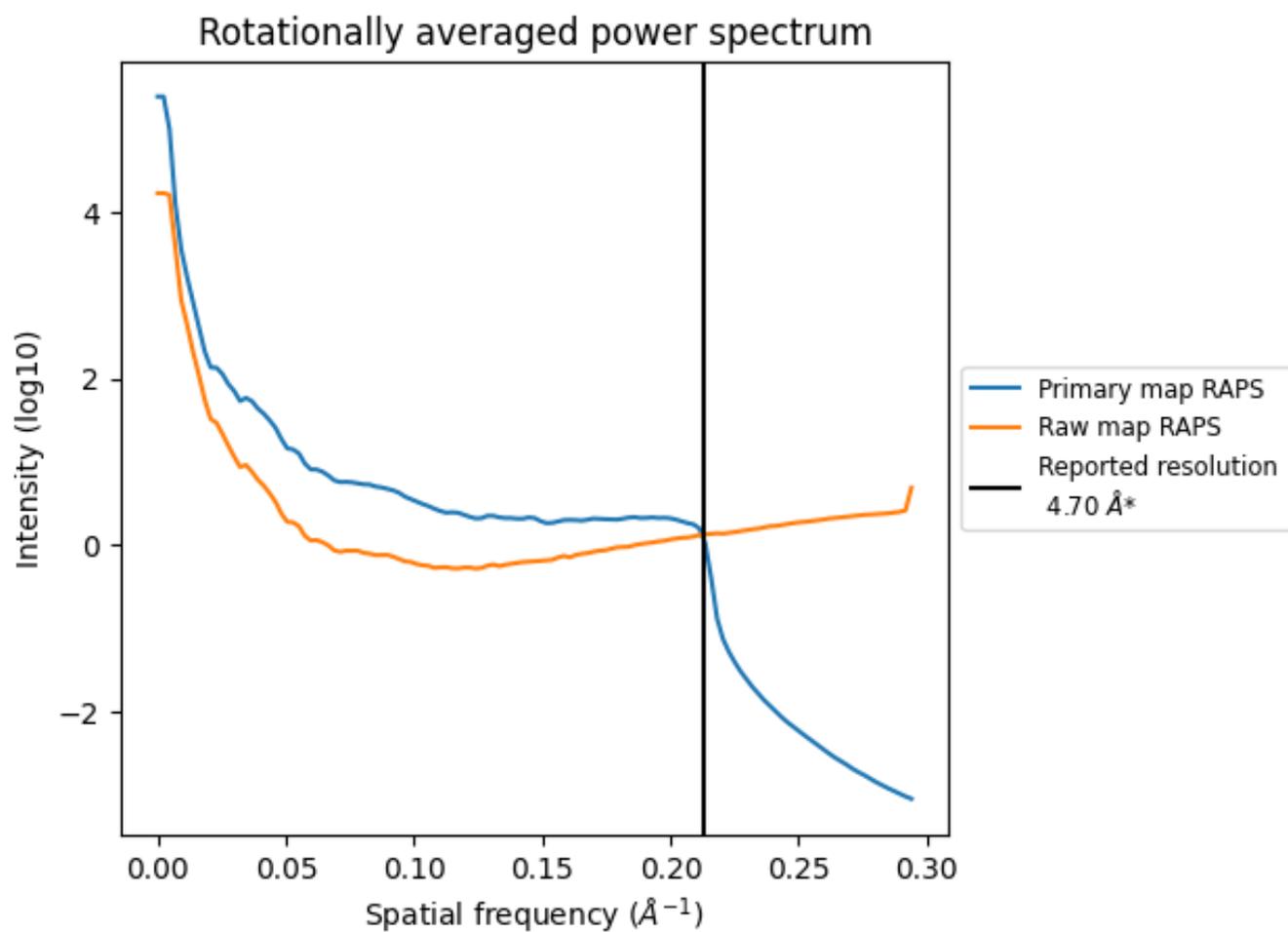
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1378 nm³; this corresponds to an approximate mass of 1245 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

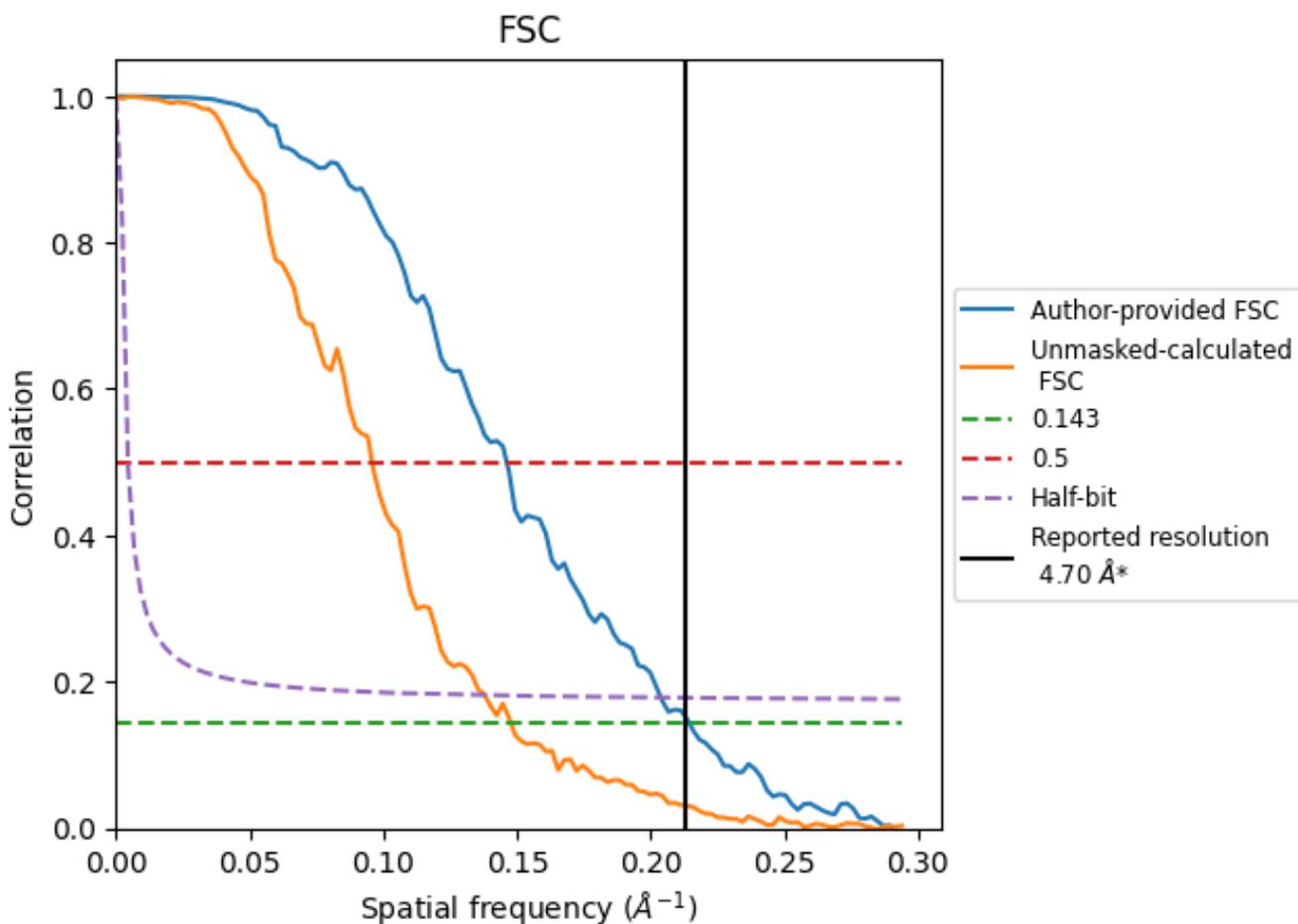


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

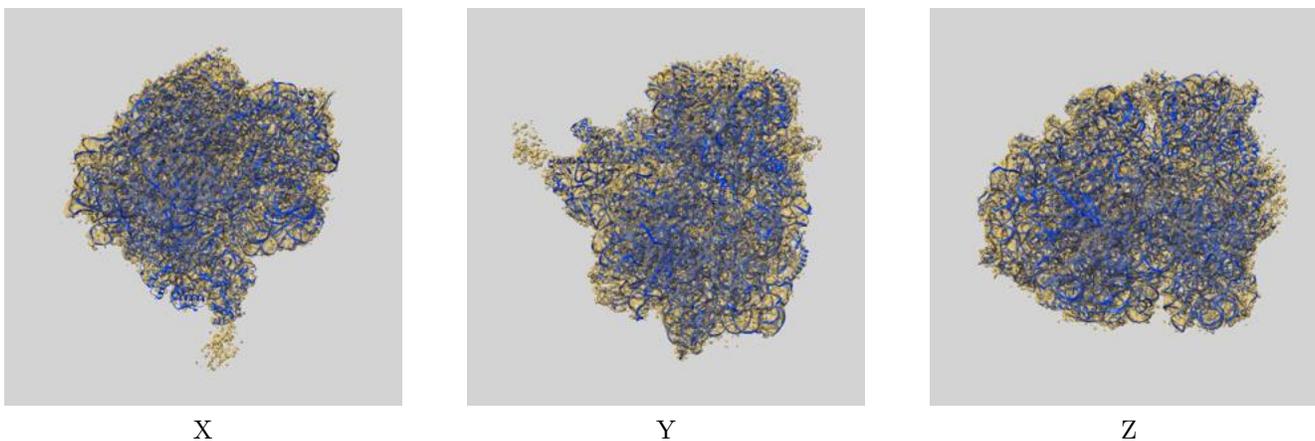
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.66	6.84	4.90
Unmasked-calculated*	6.77	10.44	7.25

*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 6.77 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

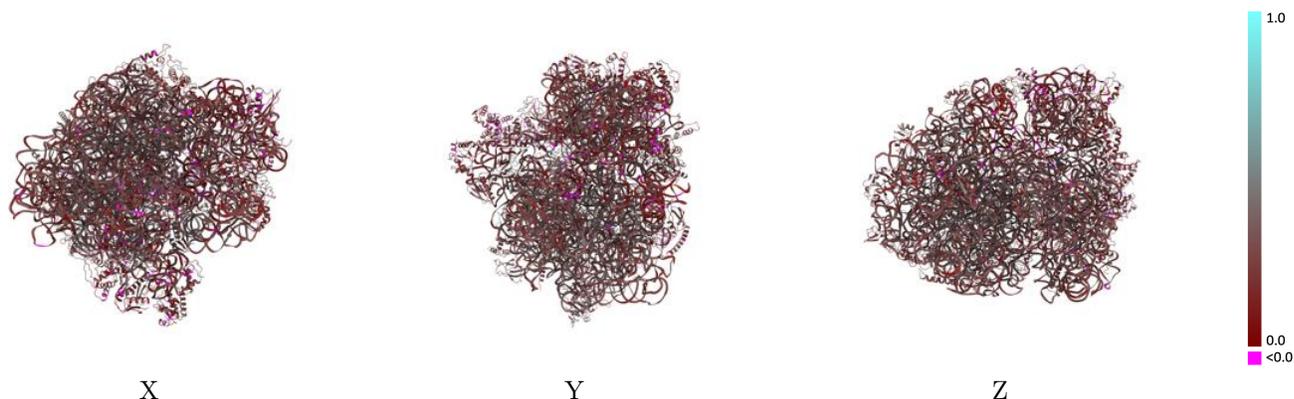
This section contains information regarding the fit between EMDB map EMD-13435 and PDB model 7PIB. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



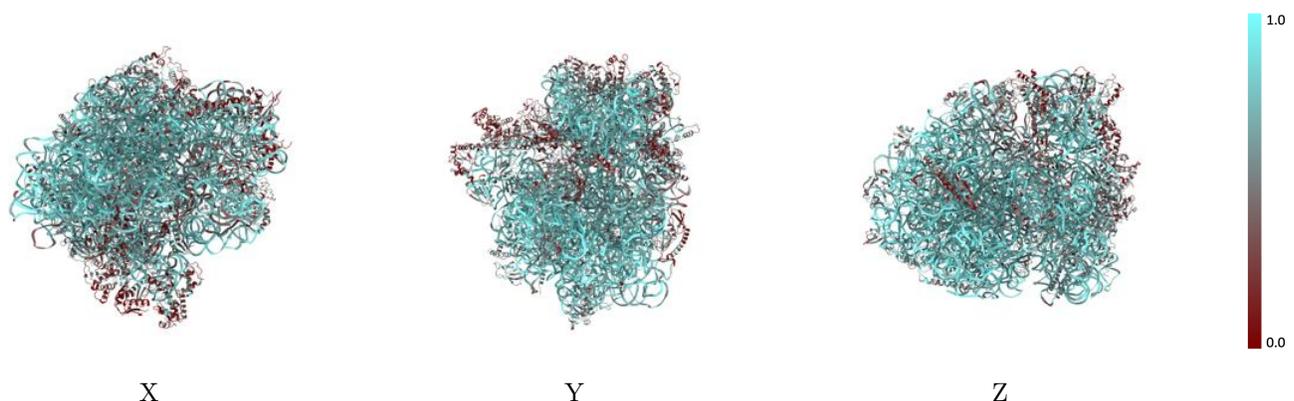
The images above show the 3D surface view of the map at the recommended contour level 0.66 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



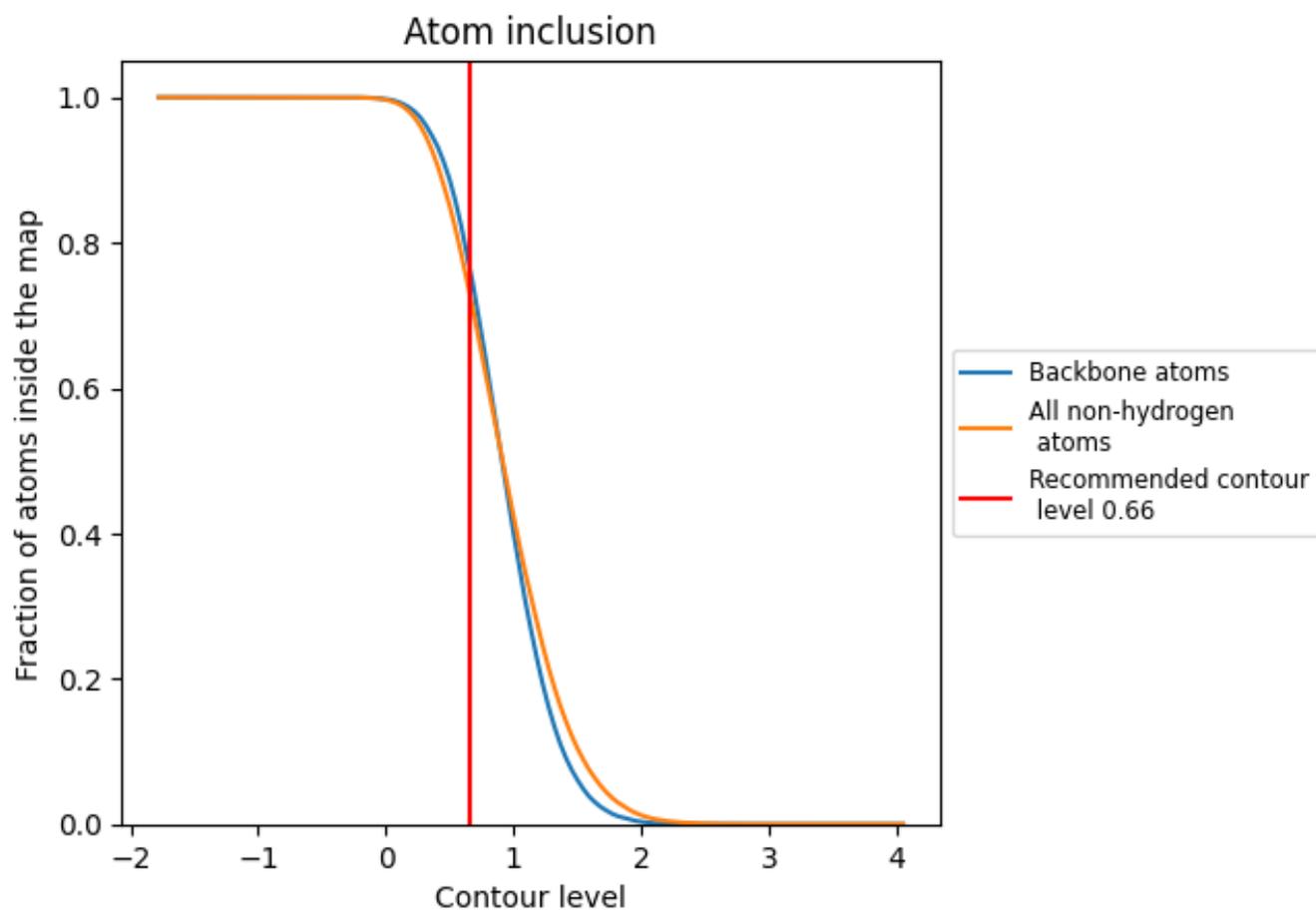
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.66).

9.4 Atom inclusion [i](#)

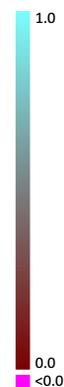


At the recommended contour level, 76% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.66) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7286	 0.2990
0	 0.7589	 0.3750
1	 0.6845	 0.3500
2	 0.6757	 0.3730
3	 0.8632	 0.3180
4	 0.8191	 0.2810
5	 0.8354	 0.2890
7	 0.5130	 0.0850
8	 0.6514	 0.1860
9	 0.3112	 0.2380
A	 0.4400	 0.2790
B	 0.4517	 0.2740
C	 0.4748	 0.2560
D	 0.5459	 0.3130
E	 0.4394	 0.2850
F	 0.2950	 0.2140
G	 0.5637	 0.3120
H	 0.3916	 0.2290
I	 0.4164	 0.2810
J	 0.5435	 0.3040
K	 0.5996	 0.3420
L	 0.3279	 0.2360
M	 0.6308	 0.3220
N	 0.5650	 0.2920
O	 0.6137	 0.3080
P	 0.5616	 0.3200
Q	 0.5581	 0.2790
R	 0.4343	 0.2350
S	 0.6066	 0.2650
T	 0.5223	 0.2980
W	 0.0890	 0.1830
a	 0.6822	 0.3520
b	 0.6411	 0.3530
c	 0.5995	 0.3380
d	 0.4750	 0.2760



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Chain	Atom inclusion	Q-score
e	 0.5182	 0.3160
f	 0.2331	 0.2220
g	 0.3074	 0.2330
h	 0.2706	 0.2180
i	 0.6713	 0.3440
j	 0.6130	 0.3560
k	 0.6125	 0.3390
l	 0.6521	 0.3370
m	 0.6741	 0.3290
n	 0.5571	 0.2990
o	 0.5818	 0.3270
p	 0.6896	 0.3270
q	 0.6270	 0.3590
r	 0.6511	 0.3320
s	 0.6601	 0.3580
t	 0.4530	 0.2900
u	 0.6547	 0.3440
v	 0.5980	 0.2990
w	 0.5743	 0.2760
x	 0.3440	 0.2400
y	 0.6313	 0.3190
z	 0.6474	 0.3470