



wwPDB EM Validation Summary Report ⓘ

Oct 31, 2023 – 04:30 pm GMT

PDB ID : 6Y6X
EMDB ID : EMD-10709
Title : Tetracenomycin X bound to the human ribosome
Authors : Buschauer, R.; Cheng, J.; Berninghausen, O.; Beckmann, R.; Wilson, D.N.
Deposited on : 2020-02-27
Resolution : 2.80 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70
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) : 2.36

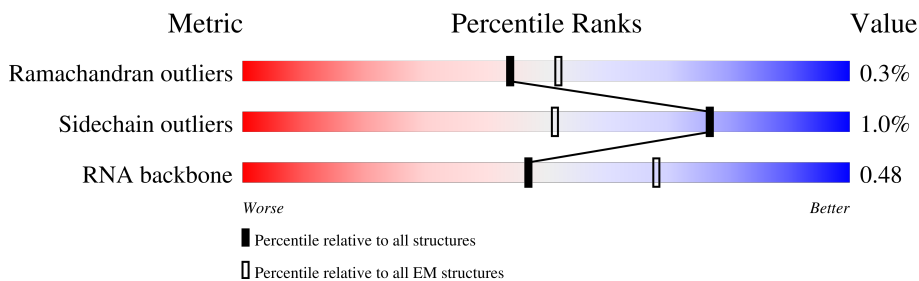
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	L5	5069	
2	L7	120	
3	L8	156	
4	LA	248	
5	LB	397	
6	LC	368	
7	LD	293	
8	LE	247	

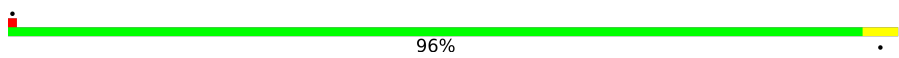
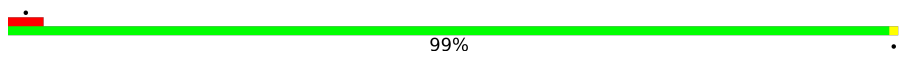
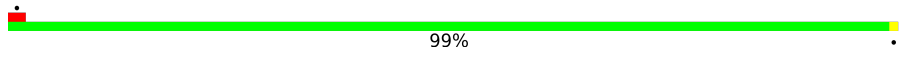
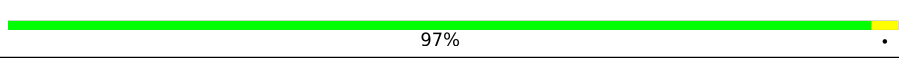
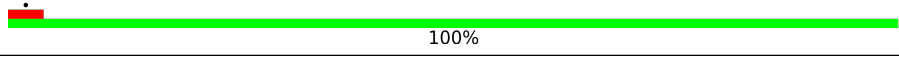
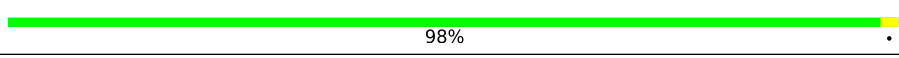
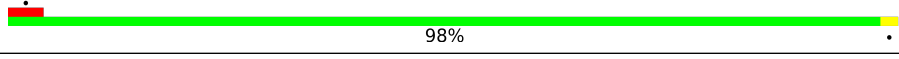
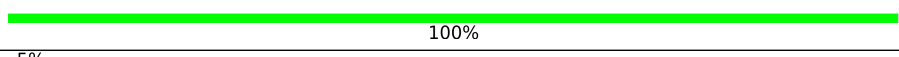
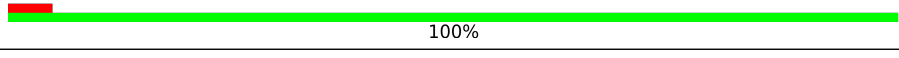
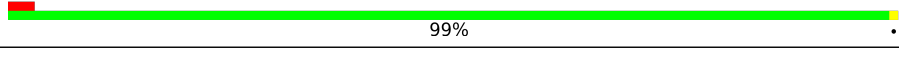
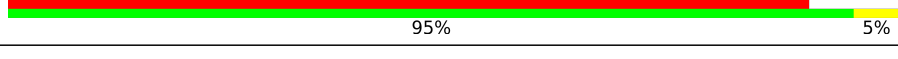
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	LF	225	100%
10	LG	241	11% 99%
11	LH	190	98%
12	LI	213	94% 5%
13	LJ	176	7% 96%
14	LL	210	100%
15	LM	139	98%
16	LN	203	98%
17	LO	201	99%
18	LP	153	99%
19	LQ	187	98%
20	LR	187	12% 100%
21	LS	175	98%
22	LT	159	97%
23	LU	99	96%
24	LV	131	99%
25	LW	124	43% 99%
26	LX	120	99%
27	LY	134	98%
28	LZ	135	100%
29	La	147	99%
30	Lb	121	8% 89% 10%
31	Lc	98	7% 97%
32	Ld	107	97%
33	Le	128	97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	Lf	109	 96%
35	Lg	114	 99%
36	Lh	122	 99%
37	Li	102	 99%
38	Lj	86	 97%
39	Lk	69	 100%
40	Ll	50	 98%
41	Lm	52	 98%
42	Ln	24	 100%
43	Lo	105	 100%
44	Lp	91	 99%
45	Lr	125	 99%
46	Lz	217	 95%

2 Entry composition [i](#)

There are 49 unique types of molecules in this entry. The entry contains 140991 atoms, of which 22 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L5	3773	80136	35654	14588	26122	3772	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L5	2113	C	G	conflict	GB NR_003287

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L7	120	2561	1141	456	844	120	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L8	156	3314	1480	585	1094	155	0	0

- Molecule 4 is a protein called 60S ribosomal protein L8.

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

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LB	397	3202	2039	602	547	14	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LC	368	2927	1840	583	489	15	0	0

- Molecule 7 is a protein called 60S ribosomal protein L5.

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

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	LE	236	1904	1222	361	317	4	0	0

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LF	225	1870	1202	358	301	9	0	0

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

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

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LI	202	1634	1037	314	269	14	0	0

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

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

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

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

- Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	LR	187	1434	889	305	231	9	0	0

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	LS	175	1453	925	283	235	10	0	0

- Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	LT	159	1298	823	252	217	6	0	0

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LU	99	809	519	141	147	2	0	0

- Molecule 24 is a protein called 60S ribosomal protein L23.

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

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LW	124	833	519	164	147	3	0	0

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LX	120	985	630	185	169	1	0	0

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Lg	114	906	566	187	147	6	0	0

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

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

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

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

- Molecule 46 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lz	217	Total	C	N	O	S	0	0
			1738	1110	312	307	9		

- Molecule 47 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

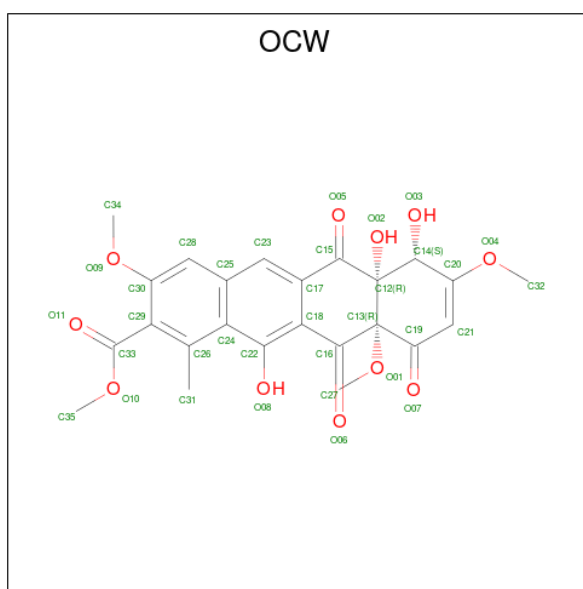
Mol	Chain	Residues	Atoms		AltConf
47	L5	214	Total	Mg	0
			214	214	
47	L7	3	Total	Mg	0
			3	3	
47	L8	4	Total	Mg	0
			4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
47	LA	1	1	1	0
47	LI	1	1	1	0
47	LP	1	1	1	0
47	LT	1	1	1	0
47	LV	1	1	1	0
47	Le	1	1	1	0
47	Lg	1	1	1	0
47	Lj	1	1	1	0

- Molecule 48 is Tetracenomycin X (three-letter code: OCW) (formula: C₂₄H₂₂O₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
48	L5	1	57	24	22	11	0

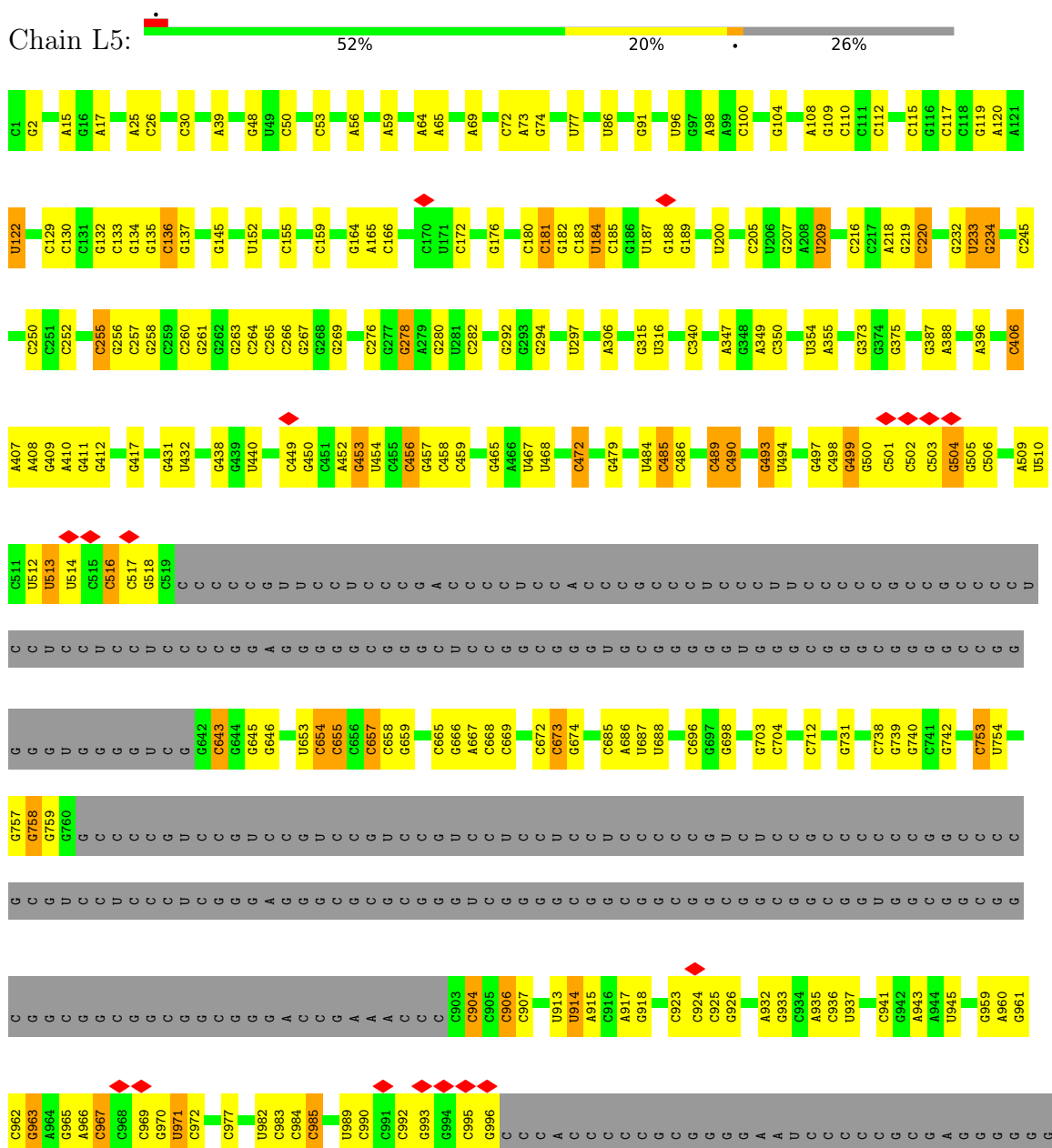
- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

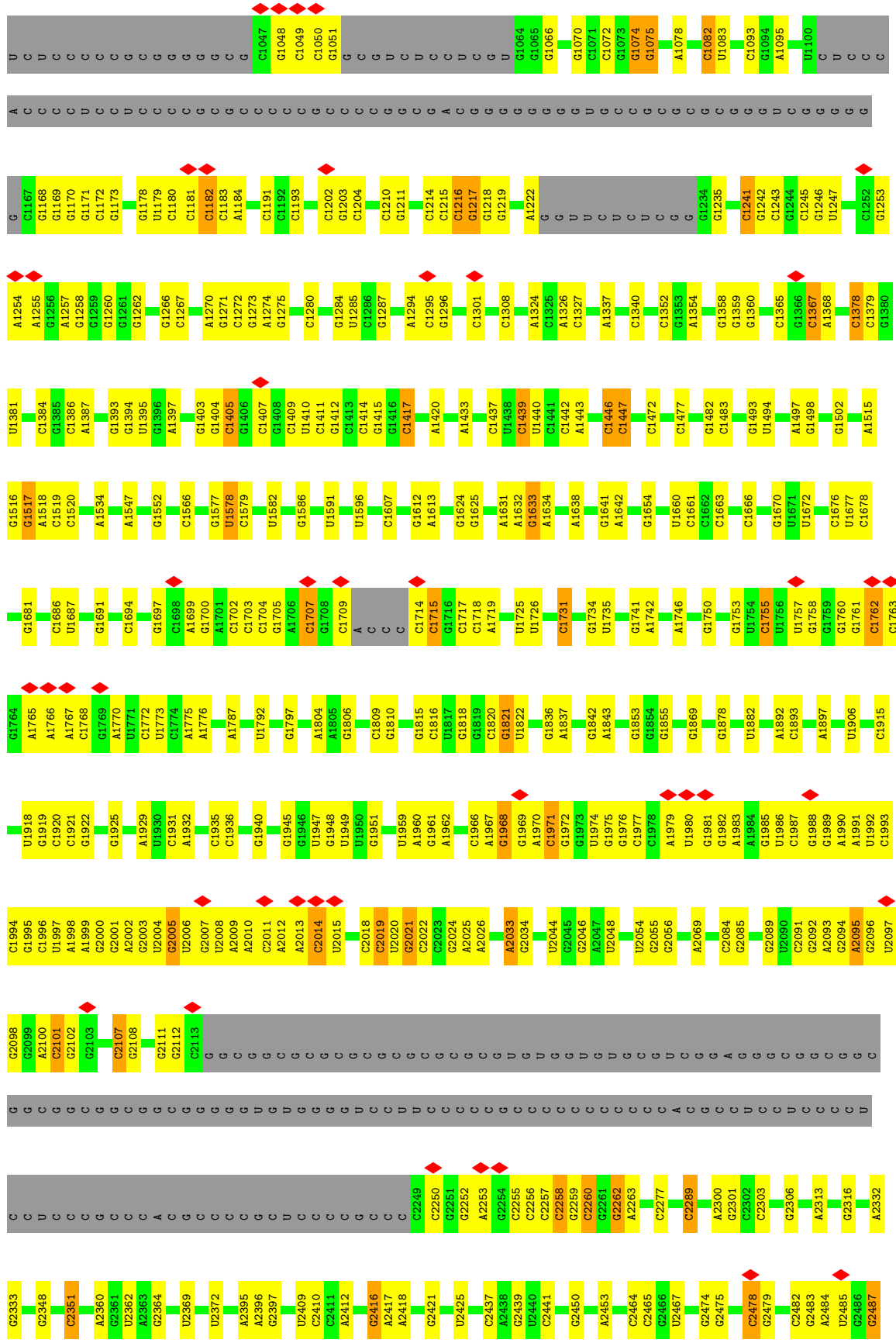
Mol	Chain	Residues	Atoms		AltConf
49	Lg	1	Total 1	Zn 1	0
49	Lj	1	Total 1	Zn 1	0
49	Lm	1	Total 1	Zn 1	0
49	Lo	1	Total 1	Zn 1	0
49	Lp	1	Total 1	Zn 1	0

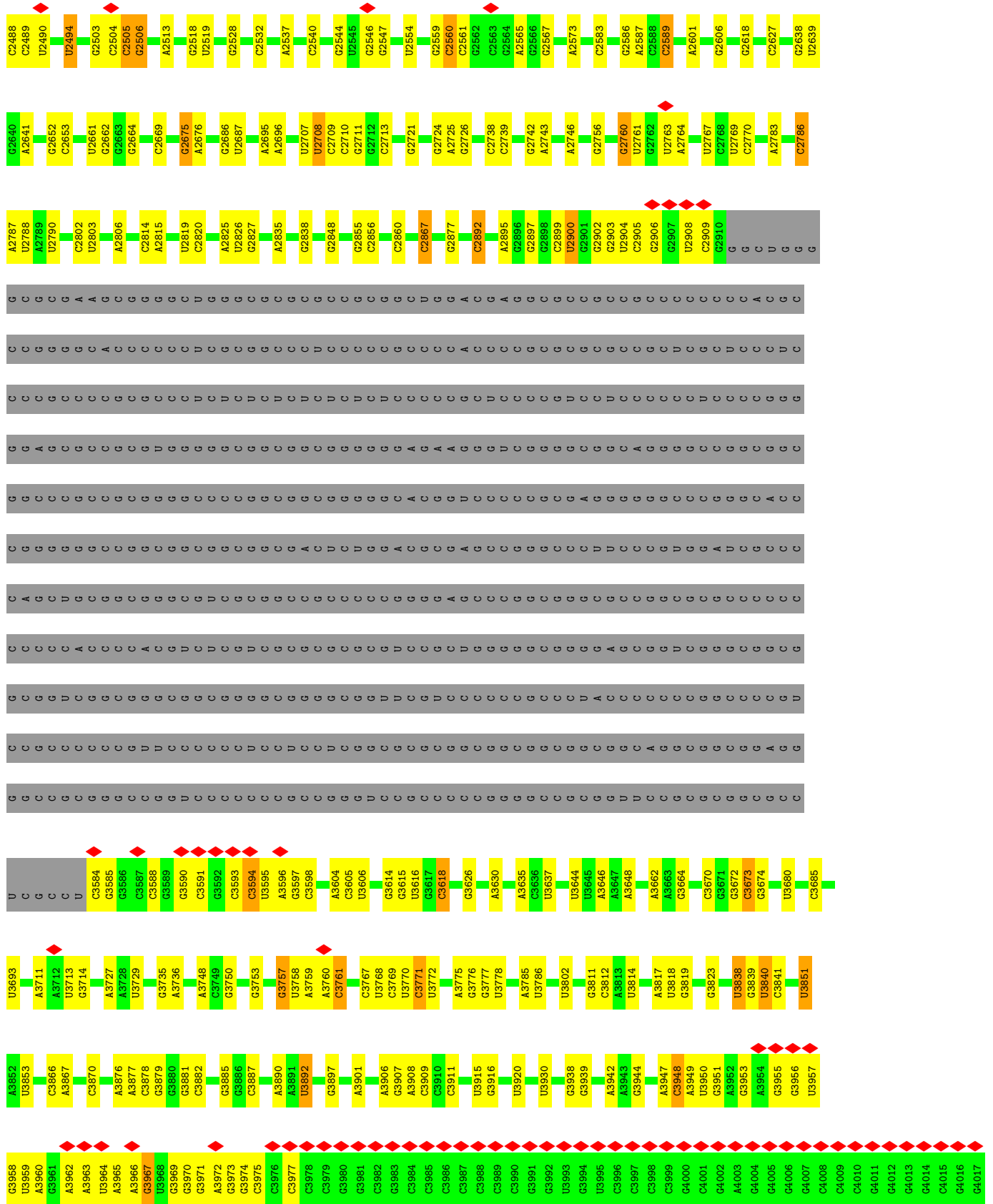
3 Residue-property plots i

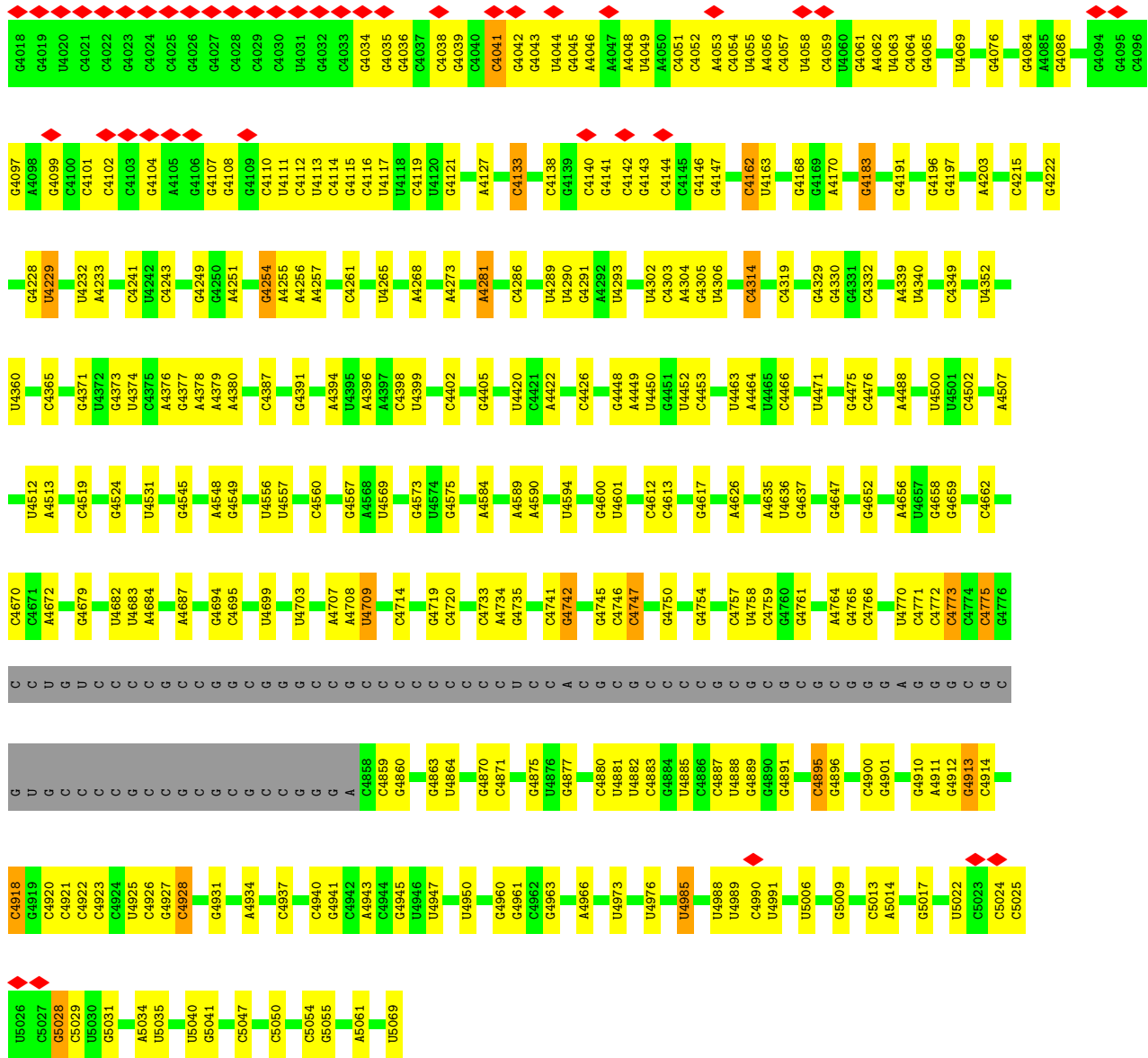
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 28S ribosomal RNA

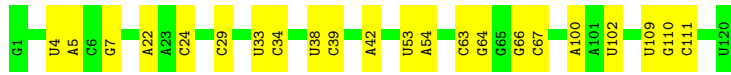
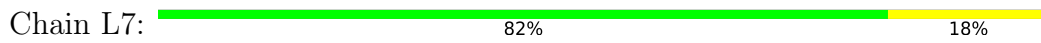




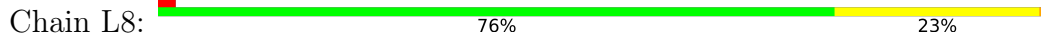




• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5.8S ribosomal RNA



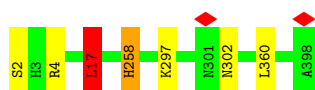
• Molecule 4: 60S ribosomal protein L8

Chain LA:  96%



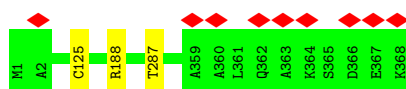
- Molecule 5: 60S ribosomal protein L3

Chain LB:  98%



- Molecule 6: 60S ribosomal protein L4

Chain LC:  99%



- Molecule 7: 60S ribosomal protein L5

Chain LD:  100%



- Molecule 8: 60S ribosomal protein L6

Chain LE:  93%



- Molecule 9: 60S ribosomal protein L7

Chain LF:  100%

There are no outlier residues recorded for this chain.

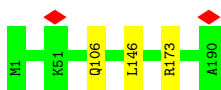
- Molecule 10: 60S ribosomal protein L7a

Chain LG:  99%



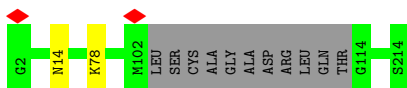
- Molecule 11: 60S ribosomal protein L9

Chain LH:  98%



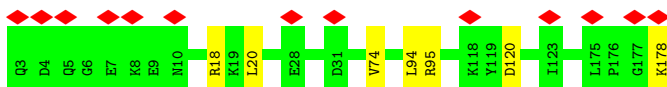
- Molecule 12: 60S ribosomal protein L10-like

Chain LI:  94% 5%



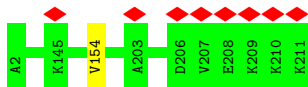
- Molecule 13: 60S ribosomal protein L11

Chain LJ:  7% 96%



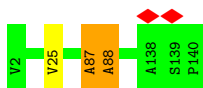
- Molecule 14: 60S ribosomal protein L13

Chain LL:  100%



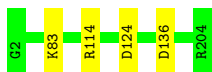
- Molecule 15: 60S ribosomal protein L14

Chain LM:  98%



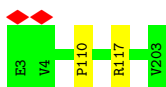
- Molecule 16: 60S ribosomal protein L15

Chain LN:  98%



- Molecule 17: 60S ribosomal protein L13a

Chain LO:  99%



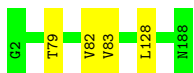
- Molecule 18: 60S ribosomal protein L17

Chain LP:  99%



- Molecule 19: 60S ribosomal protein L18

Chain LQ:  98%



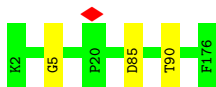
- Molecule 20: 60S ribosomal protein L19

Chain LR:  12% 100%



- Molecule 21: 60S ribosomal protein L18a

Chain LS:  98%



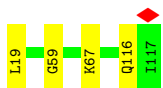
- Molecule 22: 60S ribosomal protein L21

Chain LT:  97%



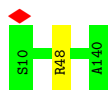
- Molecule 23: 60S ribosomal protein L22

Chain LU:  96%

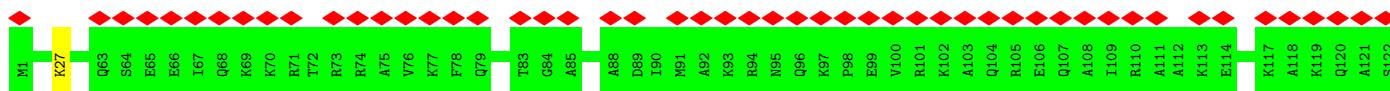
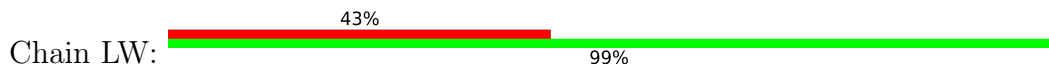


- Molecule 24: 60S ribosomal protein L23

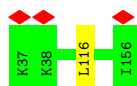
Chain LV:  99%



- Molecule 25: 60S ribosomal protein L24



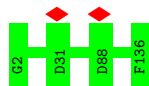
- Molecule 26: 60S ribosomal protein L23a



- Molecule 27: 60S ribosomal protein L26



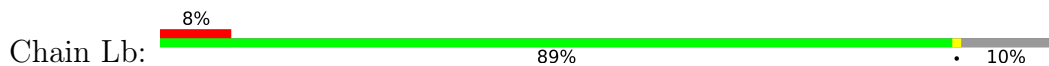
- Molecule 28: 60S ribosomal protein L27

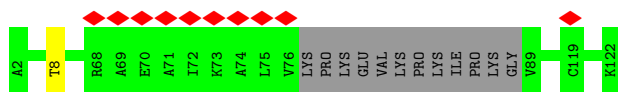


- Molecule 29: 60S ribosomal protein L27a



- Molecule 30: 60S ribosomal protein L29

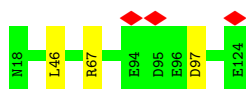




- Molecule 31: 60S ribosomal protein L30



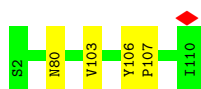
- Molecule 32: 60S ribosomal protein L31



- Molecule 33: 60S ribosomal protein L32



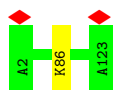
- Molecule 34: 60S ribosomal protein L35a



- Molecule 35: 60S ribosomal protein L34

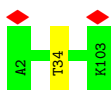


- Molecule 36: 60S ribosomal protein L35



- Molecule 37: 60S ribosomal protein L36

Chain Li:  99%



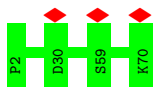
- Molecule 38: 60S ribosomal protein L37

Chain Lj:  97%



- Molecule 39: 60S ribosomal protein L38

Chain Lk:  100%



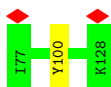
- Molecule 40: 60S ribosomal protein L39

Chain Ll:  98%



- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Lm:  98%



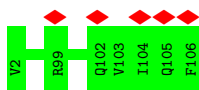
- Molecule 42: 60S ribosomal protein L41

Chain Ln:  100%

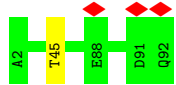
There are no outlier residues recorded for this chain.

- Molecule 43: 60S ribosomal protein L36a

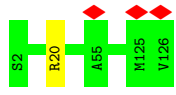
Chain Lo:  5% 100%



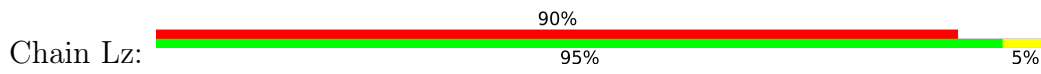
- Molecule 44: 60S ribosomal protein L37a



• Molecule 45: 60S ribosomal protein L28



• Molecule 46: 60S ribosomal protein L10a



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	302737	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.604	Depositor
Minimum map value	-0.200	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	487.8, 487.8, 487.8	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	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: MG, ZN, OCW

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	L5	0.65	1/89592 (0.0%)	1.16	641/139681 (0.5%)
2	L7	0.62	0/2861	1.08	11/4459 (0.2%)
3	L8	0.64	0/3701	1.09	10/5766 (0.2%)
4	LA	0.43	0/1936	0.67	2/2596 (0.1%)
5	LB	0.41	0/3270	0.66	2/4377 (0.0%)
6	LC	0.40	0/2981	0.65	0/4002
7	LD	0.38	0/2428	0.58	0/3252
8	LE	0.36	0/1942	0.66	0/2606
9	LF	0.41	0/1905	0.60	0/2539
10	LG	0.38	0/1960	0.62	0/2637
11	LH	0.41	0/1537	0.65	1/2066 (0.0%)
12	LI	0.39	0/1673	0.58	0/2233
13	LJ	0.39	0/1433	0.77	2/1915 (0.1%)
14	LL	0.38	0/1732	0.62	0/2315
15	LM	0.38	0/1161	0.61	1/1554 (0.1%)
16	LN	0.42	0/1746	0.64	1/2338 (0.0%)
17	LO	0.40	0/1682	0.54	0/2250
18	LP	0.44	0/1268	0.61	0/1701
19	LQ	0.39	0/1537	0.64	1/2052 (0.0%)
20	LR	0.38	0/1450	0.59	0/1935
21	LS	0.39	0/1493	0.58	0/2003
22	LT	0.41	0/1326	0.64	0/1770
23	LU	0.37	0/823	0.65	0/1104
24	LV	0.40	0/993	0.64	0/1332
25	LW	0.37	0/846	0.55	0/1146
26	LX	0.38	0/1002	0.61	1/1345 (0.1%)
27	LY	0.39	0/1132	0.63	0/1504
28	LZ	0.40	0/1130	0.66	0/1507
29	La	0.39	0/1191	0.58	0/1591
30	Lb	0.33	0/889	0.62	0/1175
31	Lc	0.38	0/774	0.64	0/1038
32	Ld	0.41	0/903	0.65	2/1216 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Le	0.40	0/1071	0.64	0/1429
34	Lf	0.42	0/895	0.64	0/1198
35	Lg	0.37	0/916	0.64	0/1220
36	Lh	0.34	0/1023	0.58	0/1351
37	Li	0.36	0/843	0.59	0/1115
38	Lj	0.42	0/720	0.63	0/952
39	Lk	0.35	0/575	0.61	0/761
40	Ll	0.36	0/454	0.63	0/599
41	Lm	0.37	0/435	0.65	0/575
42	Ln	0.32	0/231	0.62	0/294
43	Lo	0.37	0/876	0.58	0/1156
44	Lp	0.41	0/718	0.55	0/953
45	Lr	0.38	0/1017	0.61	0/1364
46	Lz	0.38	0/1766	0.75	3/2367 (0.1%)
All	All	0.57	1/151837 (0.0%)	1.01	678/224339 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	LA	0	2
5	LB	0	3
8	LE	0	1
11	LH	0	2
12	LI	0	1
13	LJ	0	1
14	LL	0	1
15	LM	0	2
17	LO	0	1
21	LS	0	1
22	LT	0	1
34	Lf	0	2
36	Lh	0	1
38	Lj	0	1
45	Lr	0	1
46	Lz	0	1
All	All	0	22

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4764	A	N9-C4	-5.18	1.34	1.37

The worst 5 of 678 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	969	C	N1-C2-O2	14.79	127.78	118.90
1	L5	2710	C	N1-C2-O2	14.29	127.48	118.90
1	L5	485	C	C2-N1-C1'	14.12	134.33	118.80
1	L5	969	C	C2-N1-C1'	13.05	133.15	118.80
1	L5	2019	C	N3-C2-O2	-12.21	113.35	121.90

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	LA	110	GLY	Peptide
4	LA	54	ARG	Peptide
5	LB	17	LEU	Peptide
5	LB	2	SER	Peptide
5	LB	258	HIS	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/248 (99%)	221 (90%)	24 (10%)	1 (0%)	34	66
5	LB	395/397 (100%)	366 (93%)	27 (7%)	2 (0%)	29	61
6	LC	366/368 (100%)	336 (92%)	30 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	LD	291/293 (99%)	275 (94%)	16 (6%)	0	100	100
8	LE	232/247 (94%)	208 (90%)	23 (10%)	1 (0%)	34	66
9	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
10	LG	239/241 (99%)	218 (91%)	21 (9%)	0	100	100
11	LH	188/190 (99%)	168 (89%)	20 (11%)	0	100	100
12	LI	198/213 (93%)	184 (93%)	14 (7%)	0	100	100
13	LJ	174/176 (99%)	155 (89%)	18 (10%)	1 (1%)	25	56
14	LL	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
15	LM	137/139 (99%)	127 (93%)	9 (7%)	1 (1%)	22	53
16	LN	201/203 (99%)	189 (94%)	10 (5%)	2 (1%)	15	44
17	LO	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
18	LP	151/153 (99%)	140 (93%)	10 (7%)	1 (1%)	22	53
19	LQ	185/187 (99%)	174 (94%)	11 (6%)	0	100	100
20	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
21	LS	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
22	LT	157/159 (99%)	146 (93%)	10 (6%)	1 (1%)	25	56
23	LU	97/99 (98%)	82 (84%)	13 (13%)	2 (2%)	7	23
24	LV	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
25	LW	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
26	LX	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
27	LY	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
28	LZ	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
29	La	145/147 (99%)	135 (93%)	9 (6%)	1 (1%)	22	53
30	Lb	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
31	Lc	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
32	Ld	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
33	Le	126/128 (98%)	118 (94%)	6 (5%)	2 (2%)	9	31
34	Lf	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	8	26
35	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
36	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
37	Li	100/102 (98%)	96 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	Lj	84/86 (98%)	77 (92%)	6 (7%)	1 (1%)	13	39
39	Lk	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
40	Ll	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
41	Lm	50/52 (96%)	49 (98%)	0	1 (2%)	7	24
42	Ln	22/24 (92%)	22 (100%)	0	0	100	100
43	Lo	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
44	Lp	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
45	Lr	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
46	Lz	215/217 (99%)	171 (80%)	43 (20%)	1 (0%)	29	61
All	All	6696/6822 (98%)	6206 (93%)	470 (7%)	20 (0%)	44	72

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	LN	124	ASP
23	LU	116	GLN
33	Le	73	GLY
33	Le	92	ASN
34	Lf	80	ASN

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	
4	LA	190/190 (100%)	185 (97%)	5 (3%)	46	79
5	LB	345/345 (100%)	342 (99%)	3 (1%)	78	94
6	LC	306/306 (100%)	303 (99%)	3 (1%)	76	93
7	LD	246/247 (100%)	245 (100%)	1 (0%)	91	97
8	LE	209/220 (95%)	205 (98%)	4 (2%)	57	85
9	LF	194/194 (100%)	194 (100%)	0	100	100
10	LG	203/205 (99%)	201 (99%)	2 (1%)	76	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	LH	169/169 (100%)	169 (100%)	0	100	100
12	LI	172/180 (96%)	171 (99%)	1 (1%)	86	96
13	LJ	148/148 (100%)	145 (98%)	3 (2%)	55	84
14	LL	176/176 (100%)	176 (100%)	0	100	100
15	LM	118/118 (100%)	117 (99%)	1 (1%)	81	94
16	LN	171/171 (100%)	170 (99%)	1 (1%)	86	96
17	LO	173/173 (100%)	172 (99%)	1 (1%)	86	96
18	LP	134/134 (100%)	133 (99%)	1 (1%)	84	95
19	LQ	164/164 (100%)	161 (98%)	3 (2%)	59	86
20	LR	133/166 (80%)	133 (100%)	0	100	100
21	LS	156/156 (100%)	154 (99%)	2 (1%)	69	91
22	LT	139/139 (100%)	136 (98%)	3 (2%)	52	83
23	LU	89/89 (100%)	87 (98%)	2 (2%)	52	83
24	LV	101/101 (100%)	100 (99%)	1 (1%)	76	93
25	LW	56/103 (54%)	55 (98%)	1 (2%)	59	86
26	LX	108/108 (100%)	108 (100%)	0	100	100
27	LY	124/124 (100%)	121 (98%)	3 (2%)	49	81
28	LZ	117/117 (100%)	117 (100%)	0	100	100
29	La	120/120 (100%)	120 (100%)	0	100	100
30	Lb	88/101 (87%)	87 (99%)	1 (1%)	73	92
31	Lc	83/83 (100%)	80 (96%)	3 (4%)	35	69
32	Ld	98/98 (100%)	97 (99%)	1 (1%)	76	93
33	Le	114/114 (100%)	111 (97%)	3 (3%)	46	79
34	Lf	88/88 (100%)	88 (100%)	0	100	100
35	Lg	98/98 (100%)	97 (99%)	1 (1%)	76	93
36	Lh	109/109 (100%)	109 (100%)	0	100	100
37	Li	86/86 (100%)	85 (99%)	1 (1%)	71	92
38	Lj	73/73 (100%)	72 (99%)	1 (1%)	67	90
39	Lk	64/64 (100%)	64 (100%)	0	100	100
40	Ll	47/47 (100%)	46 (98%)	1 (2%)	53	84
41	Lm	48/48 (100%)	48 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	Ln	23/23 (100%)	23 (100%)	0	100	100
43	Lo	93/93 (100%)	93 (100%)	0	100	100
44	Lp	74/74 (100%)	73 (99%)	1 (1%)	67	90
45	Lr	109/109 (100%)	109 (100%)	0	100	100
46	Lz	194/196 (99%)	189 (97%)	5 (3%)	46	79
All	All	5750/5867 (98%)	5691 (99%)	59 (1%)	77	93

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	LQ	83	VAL
46	Lz	9	THR
23	LU	67	LYS
46	Lz	7	ARG
35	Lg	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
17	LO	173	GLN
45	Lr	30	ASN
19	LQ	45	GLN
44	Lp	56	HIS
46	Lz	143	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3706/5069 (73%)	965 (26%)	19 (0%)
2	L7	119/120 (99%)	15 (12%)	0
3	L8	155/156 (99%)	33 (21%)	0
All	All	3980/5345 (74%)	1013 (25%)	19 (0%)

5 of 1013 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	2	G
1	L5	15	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L5	17	A
1	L5	25	A
1	L5	26	C

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	3614	G
1	L5	4378	A
1	L5	4913	G
1	L5	4045	G
1	L5	2019	C

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](#)

Of 235 ligands modelled in this entry, 234 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	OCW	L5	5315	47	34,38,38	1.86	12 (35%)	41,61,61	2.65	10 (24%)

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
48	OCW	L5	5315	47	-	5/13/62/62	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	L5	5315	OCW	C17-C18	-4.28	1.34	1.41
48	L5	5315	OCW	O10-C33	2.87	1.39	1.33
48	L5	5315	OCW	C21-C19	2.86	1.51	1.45
48	L5	5315	OCW	O04-C20	2.63	1.40	1.35
48	L5	5315	OCW	O05-C15	-2.46	1.17	1.21

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	L5	5315	OCW	O04-C20-C14	10.27	118.75	110.06
48	L5	5315	OCW	O04-C20-C21	-8.25	118.55	126.00
48	L5	5315	OCW	C19-C21-C20	-5.43	116.20	121.12
48	L5	5315	OCW	C31-C26-C29	-3.17	117.05	121.52
48	L5	5315	OCW	O09-C30-C28	-3.03	121.32	125.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

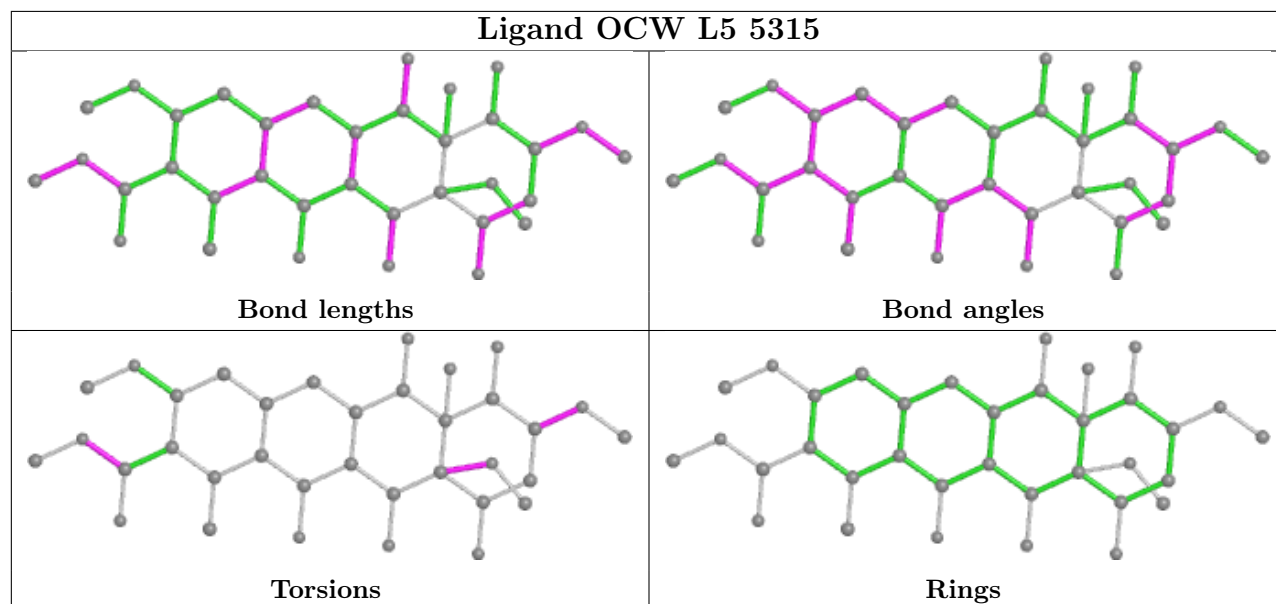
Mol	Chain	Res	Type	Atoms
48	L5	5315	OCW	C14-C20-O04-C32
48	L5	5315	OCW	C29-C33-O10-C35
48	L5	5315	OCW	O11-C33-O10-C35
48	L5	5315	OCW	C19-C13-O01-C27
48	L5	5315	OCW	C12-C13-O01-C27

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.

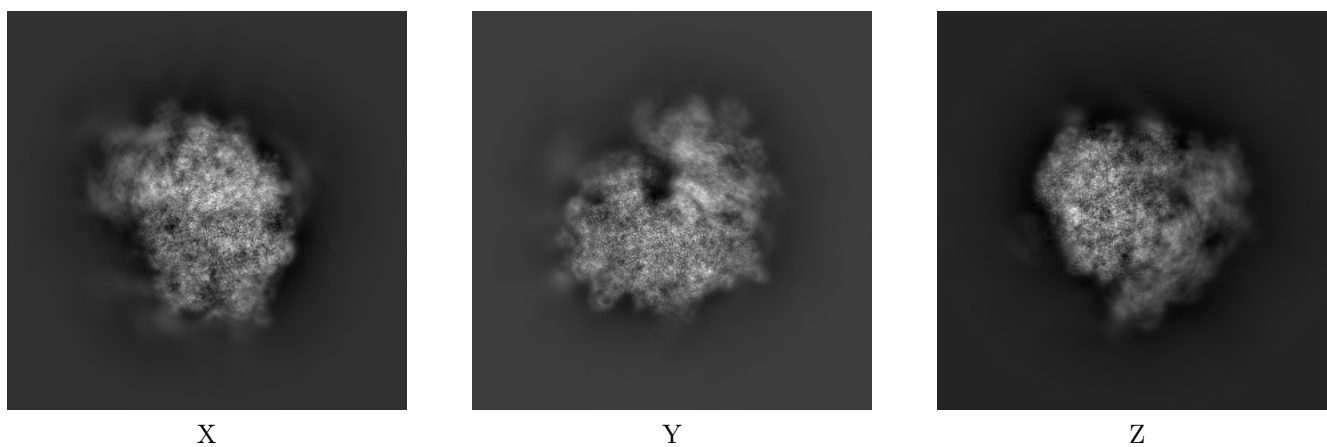
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10709. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

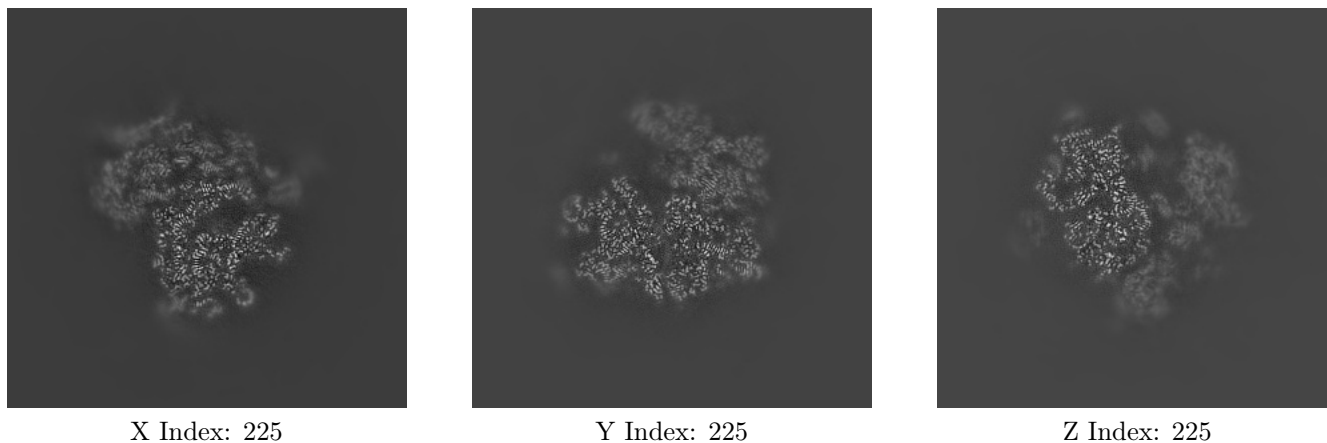
6.1.1 Primary map



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

6.2 Central slices [i](#)

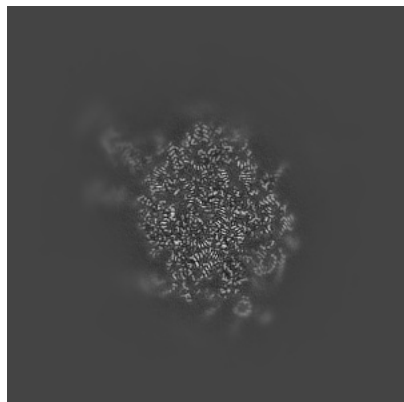
6.2.1 Primary map



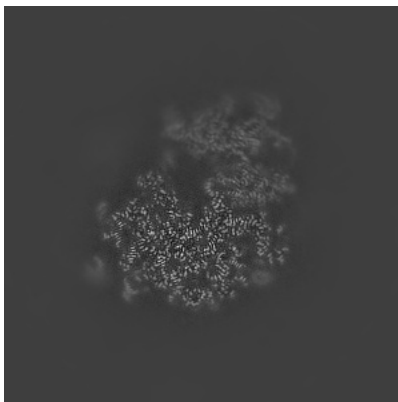
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

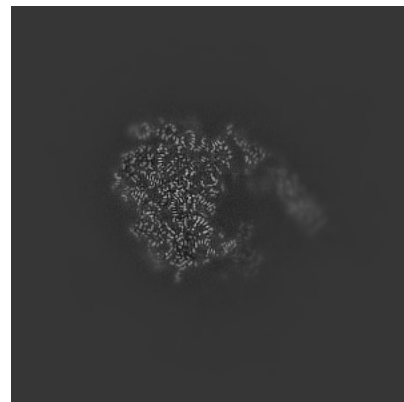
6.3.1 Primary map



X Index: 198



Y Index: 240

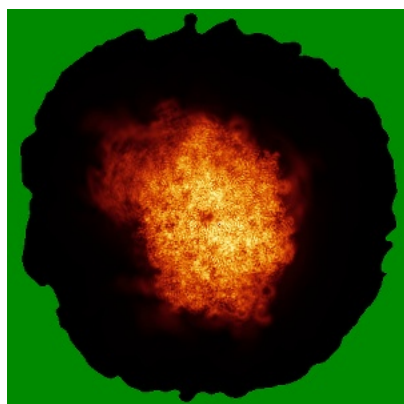


Z Index: 193

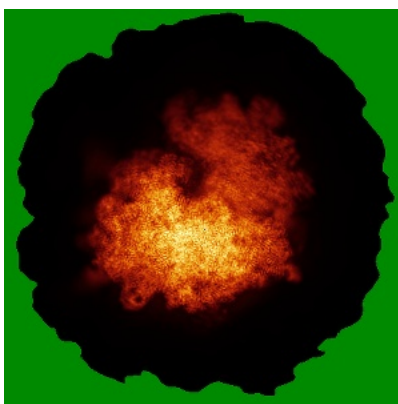
The images above show the largest variance slices of the map in three orthogonal directions.

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

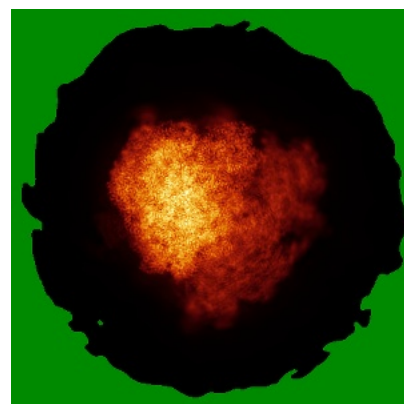
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

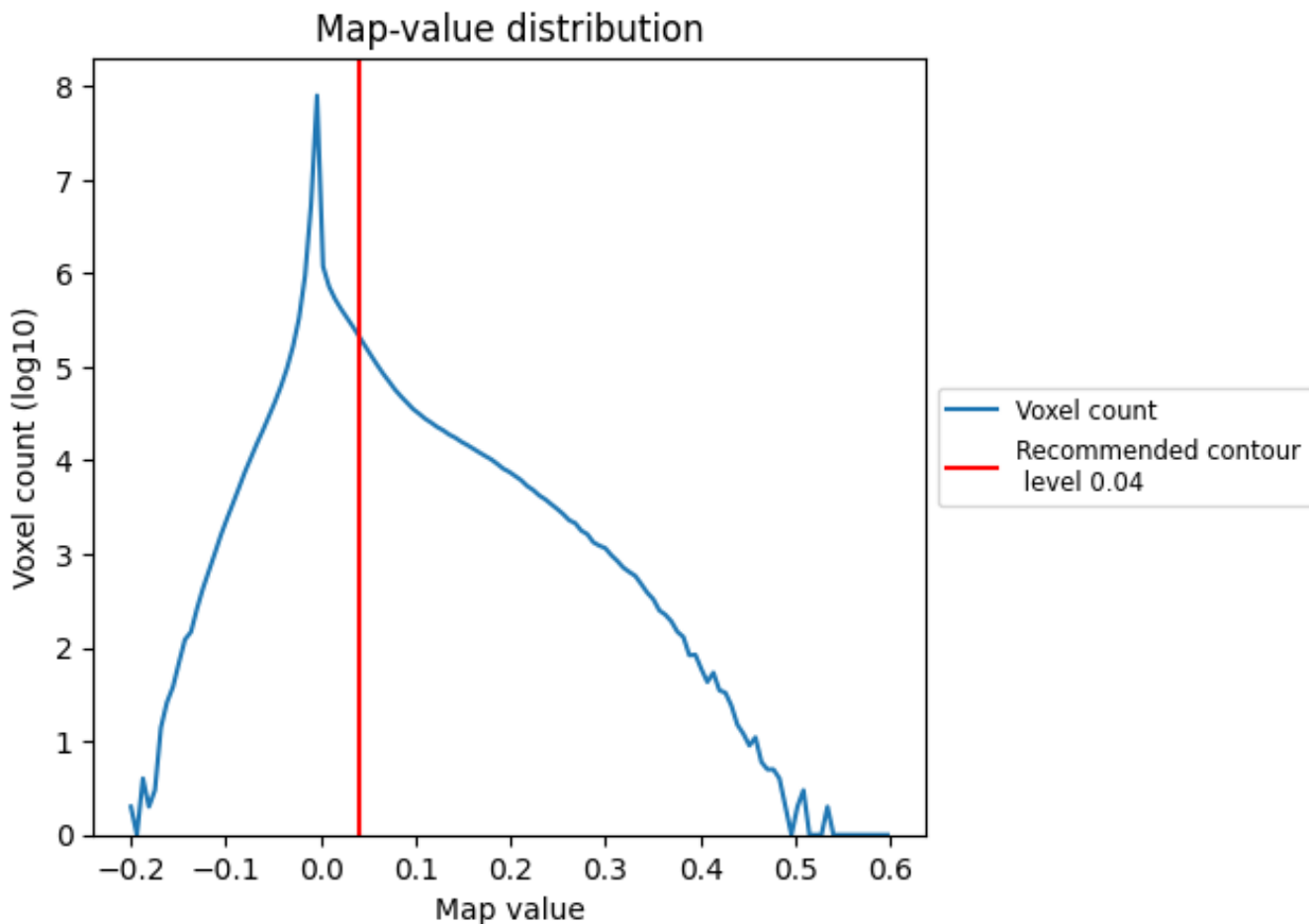
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

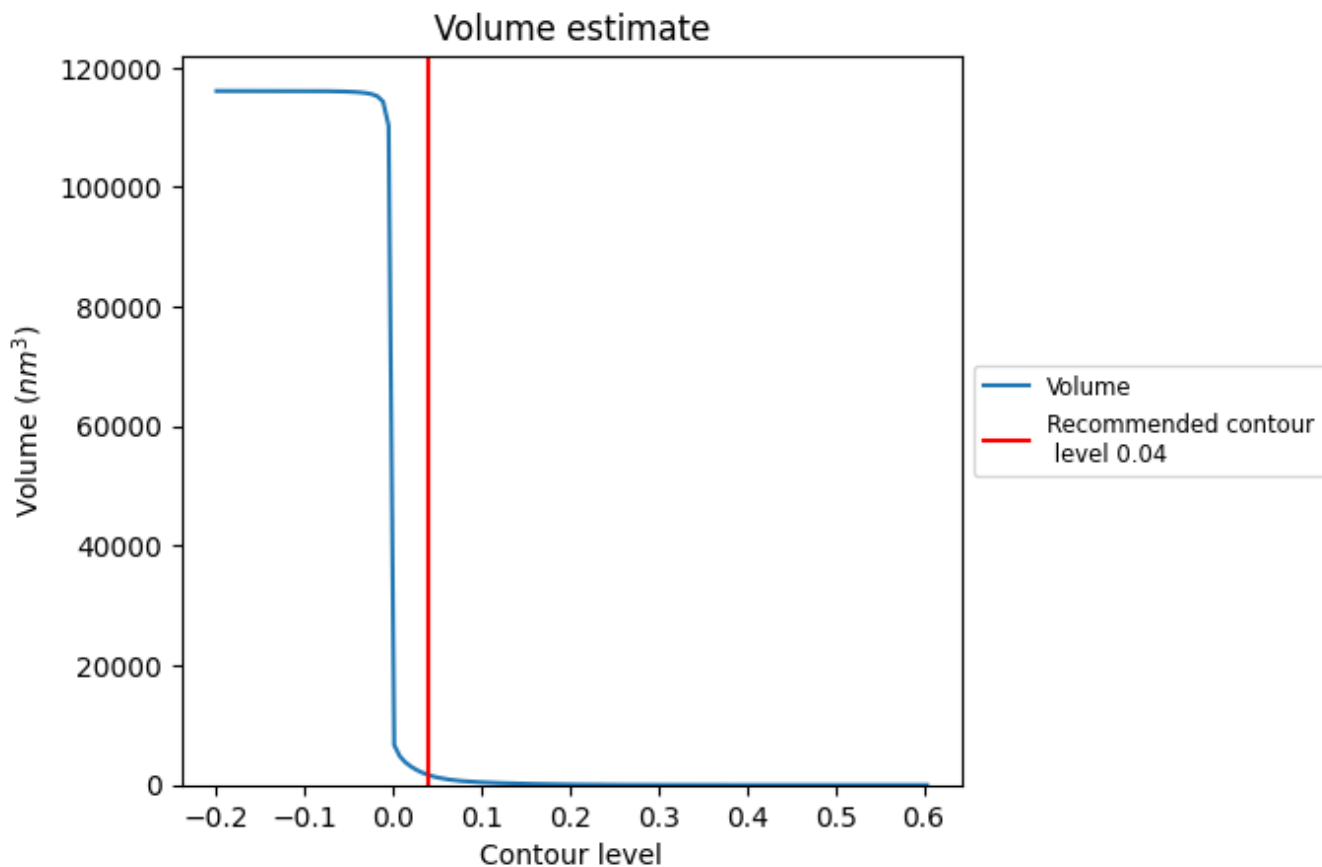
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

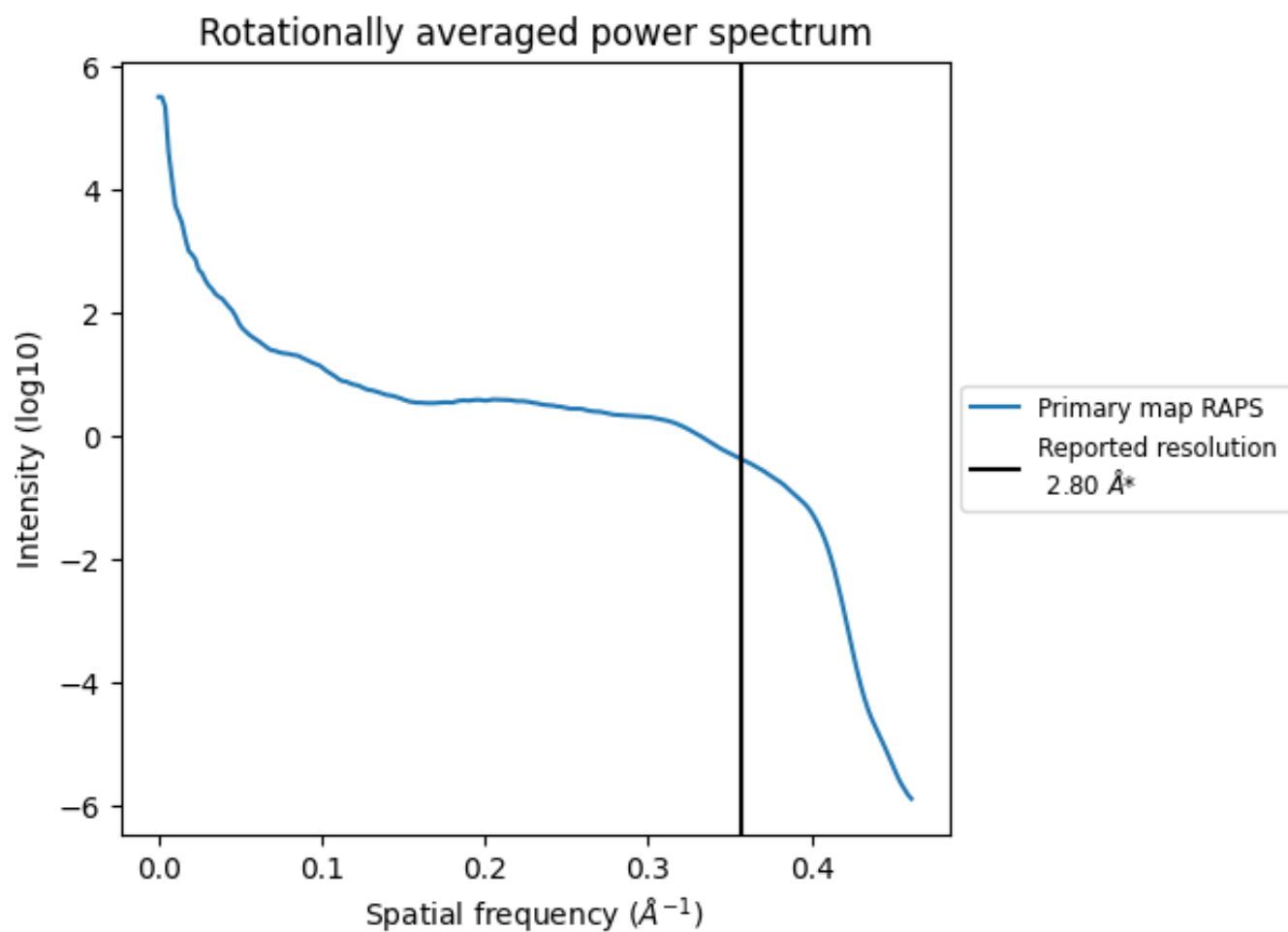
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1664 nm^3 ; this corresponds to an approximate mass of 1503 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

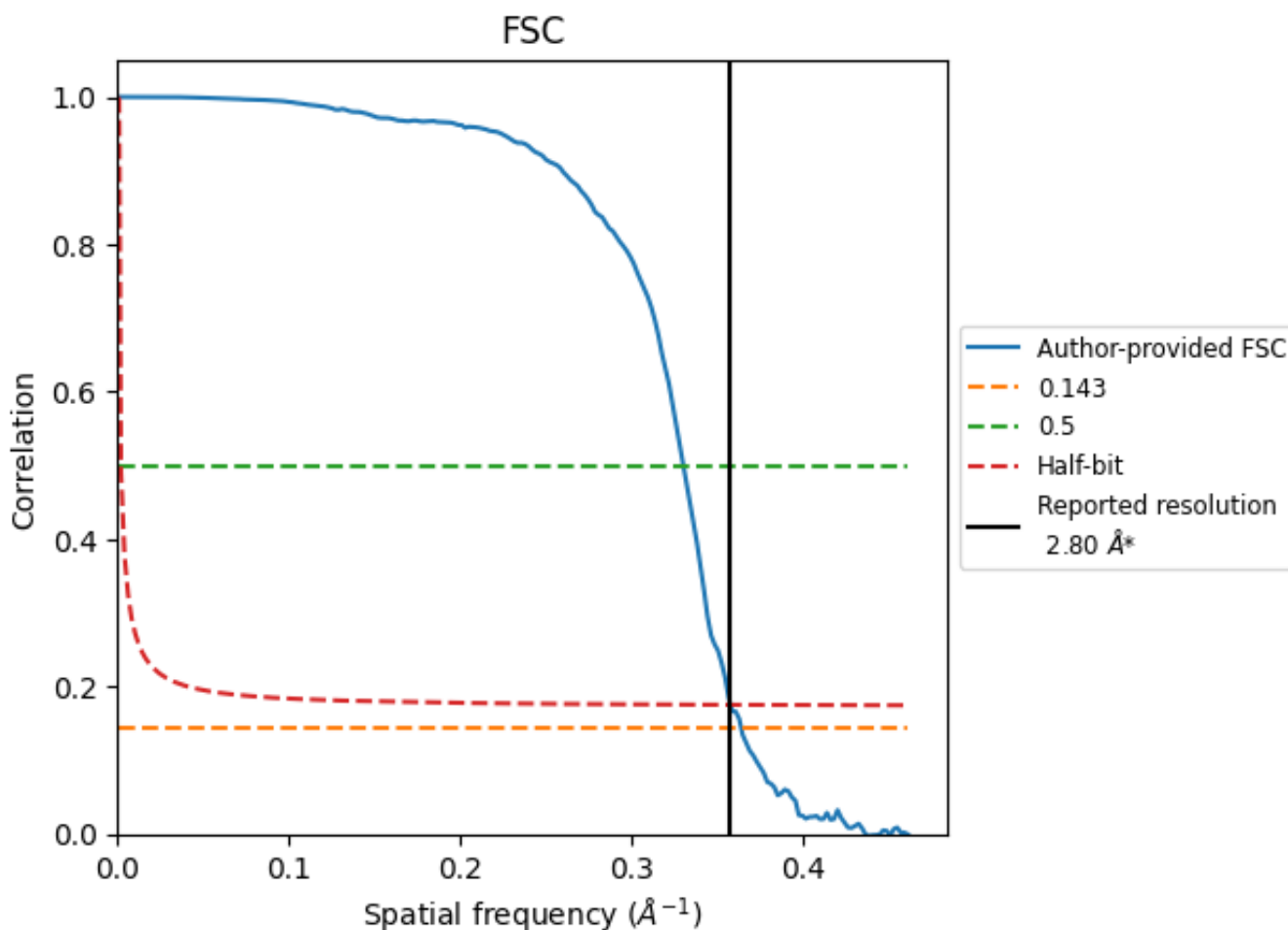


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

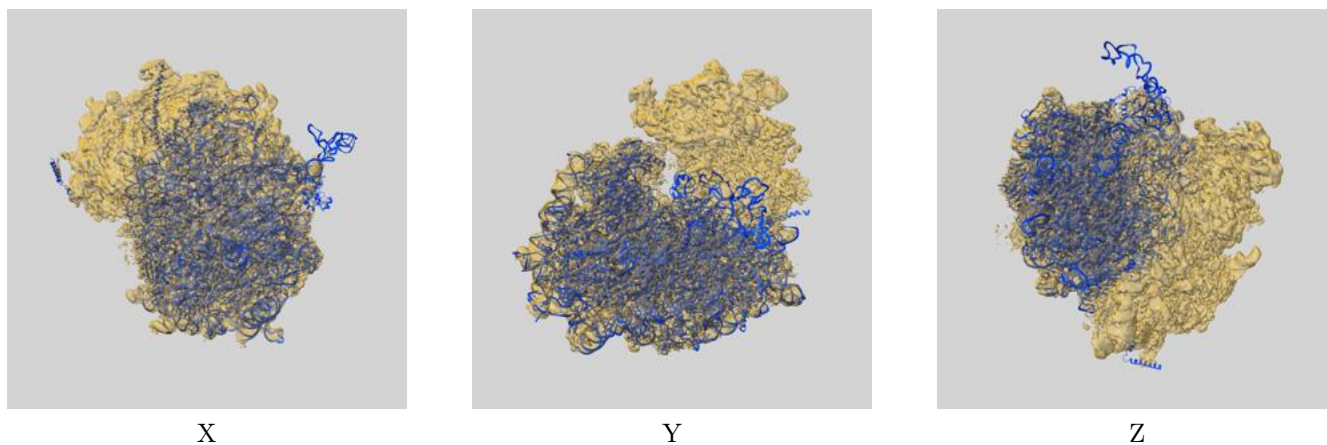
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.75	3.03	2.79
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

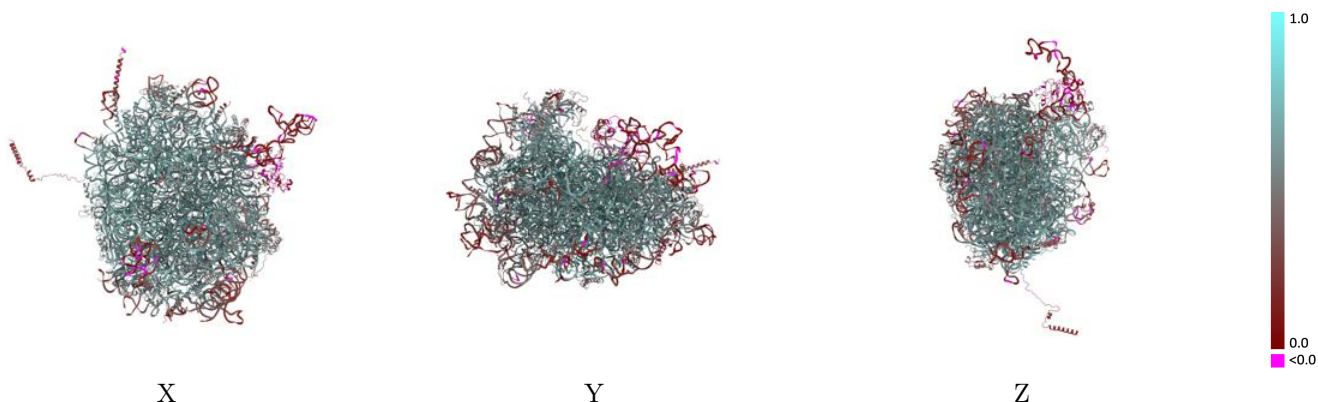
This section contains information regarding the fit between EMDB map EMD-10709 and PDB model 6Y6X. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



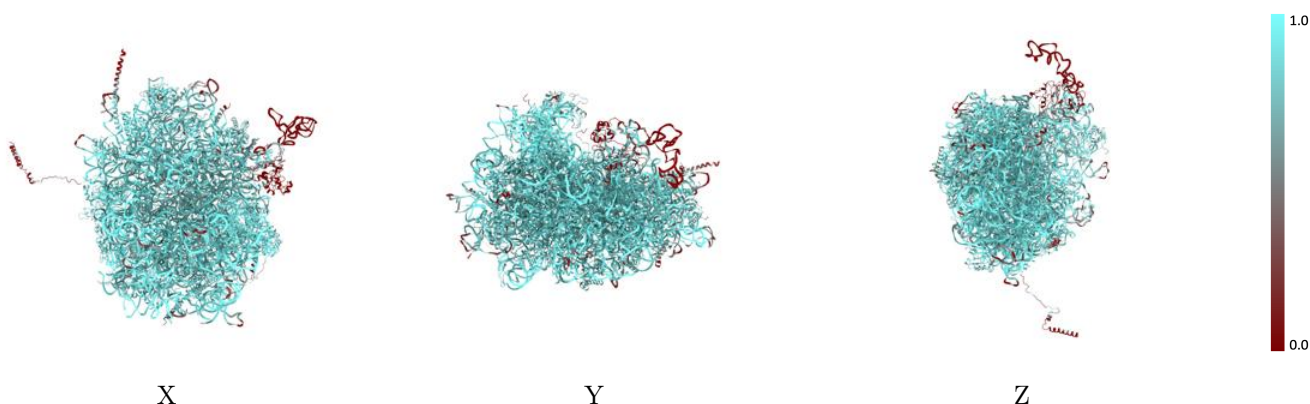
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



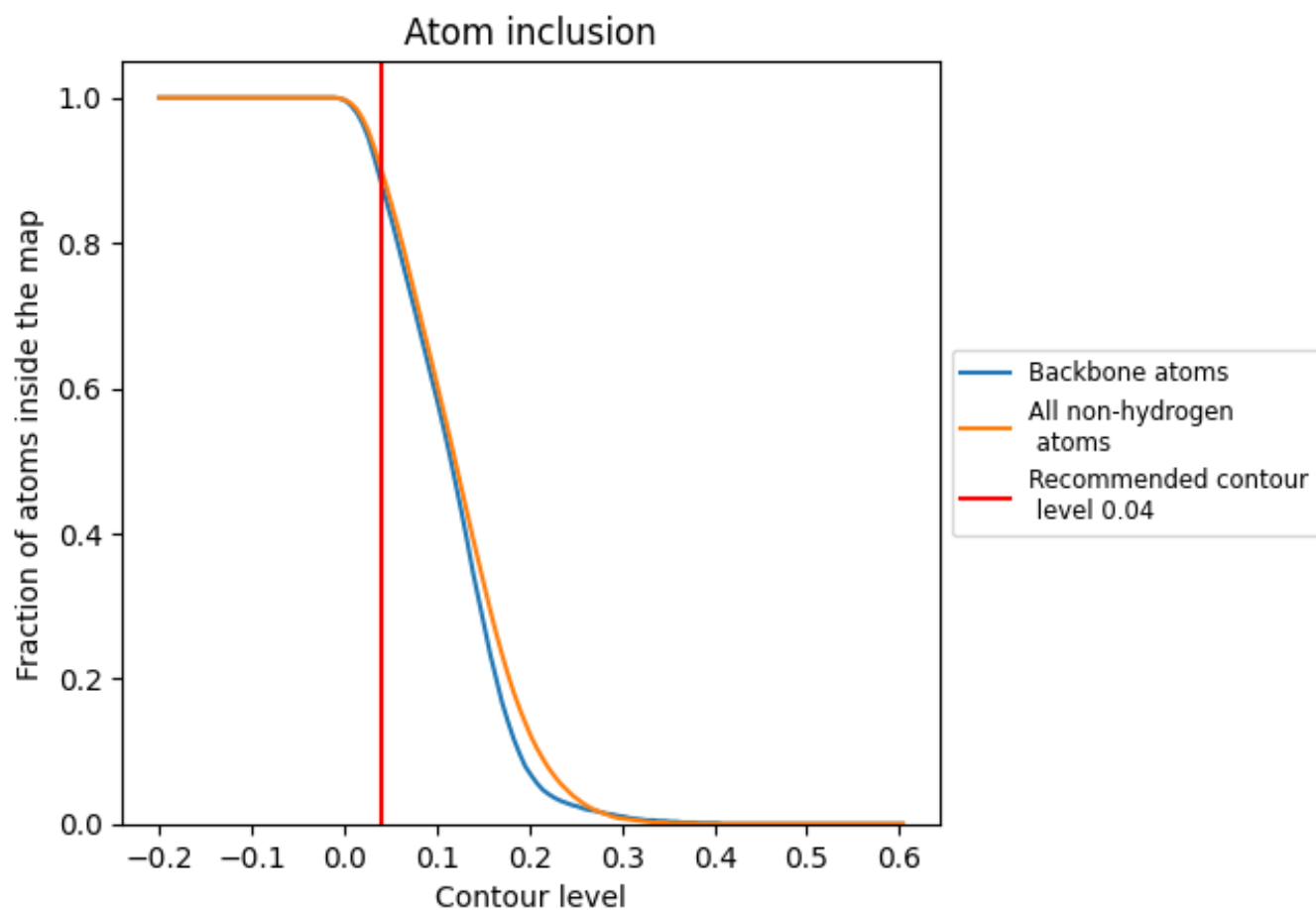
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 90% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.5460
L5	 0.9290	 0.5420
L7	 0.9950	 0.6130
L8	 0.9590	 0.5830
LA	 0.9370	 0.6240
LB	 0.9150	 0.5970
LC	 0.9010	 0.5750
LD	 0.8980	 0.5270
LE	 0.8070	 0.4820
LF	 0.9190	 0.6020
LG	 0.7920	 0.4790
LH	 0.8980	 0.5650
LI	 0.9030	 0.5830
LJ	 0.7800	 0.4410
LL	 0.8610	 0.5380
LM	 0.9080	 0.5560
LN	 0.9540	 0.6290
LO	 0.9250	 0.6100
LP	 0.9240	 0.6070
LQ	 0.9320	 0.6100
LR	 0.8440	 0.5400
LS	 0.9470	 0.6150
LT	 0.8960	 0.5650
LU	 0.8240	 0.4590
LV	 0.9110	 0.6080
LW	 0.6220	 0.4360
LX	 0.8690	 0.5510
LY	 0.8780	 0.5440
LZ	 0.8540	 0.4840
La	 0.9440	 0.6160
Lb	 0.7900	 0.4940
Lc	 0.8390	 0.5160
Ld	 0.8890	 0.5720
Le	 0.9240	 0.6110
Lf	 0.9360	 0.6290



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lg	 0.8840	 0.5830
Lh	 0.8560	 0.5260
Li	 0.8580	 0.5420
Lj	 0.9480	 0.6220
Lk	 0.7770	 0.4580
Ll	 0.9170	 0.5900
Lm	 0.8990	 0.5780
Ln	 0.8520	 0.5420
Lo	 0.8580	 0.5800
Lp	 0.8550	 0.5980
Lr	 0.9180	 0.5710
Lz	 0.0890	 0.0730