



Full wwPDB EM Validation Report ⓘ

Apr 24, 2023 – 05:45 pm BST

PDB ID : 8BIP
EMDB ID : EMD-16086
Title : Structure of a yeast 80S ribosome-bound N-Acetyltransferase B complex
Authors : Knorr, A.G.; Mackens-Kiani, T.; Musial, J.; Berninghausen, O.; Becker, T.;
Beatrix, B.; Beckmann, R.
Deposited on : 2022-11-02
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

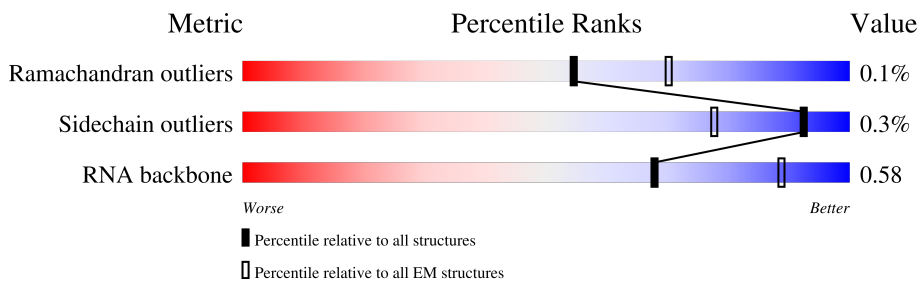
EMDB validation analysis : 0.0.1.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

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 3.10 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.



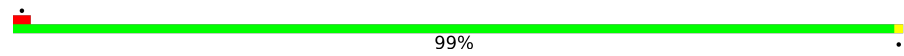
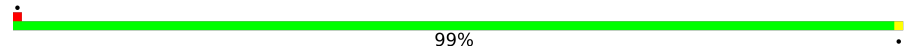
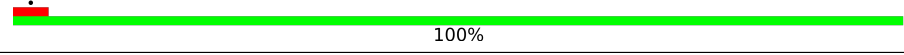
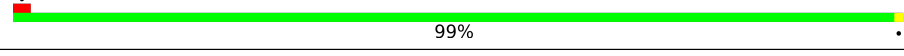
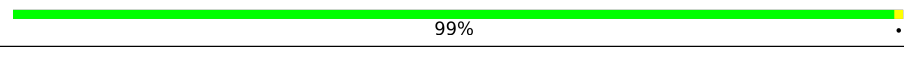
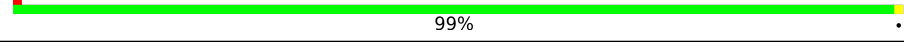
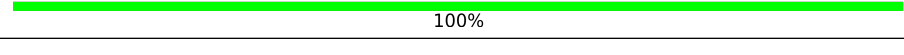
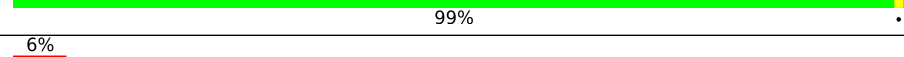
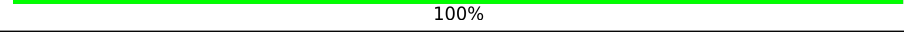
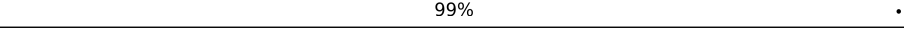
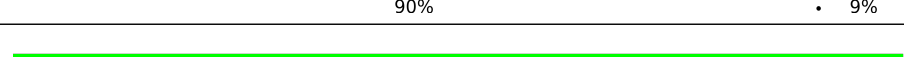
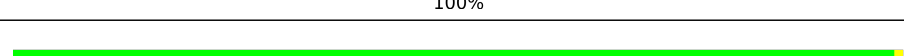
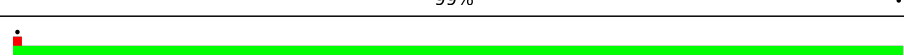
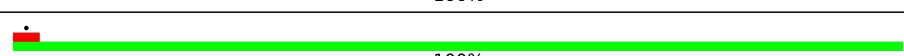
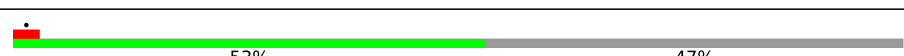
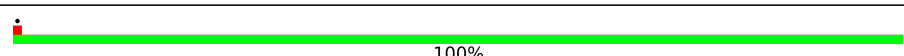
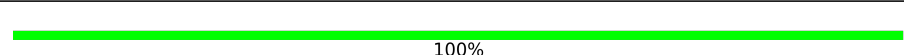
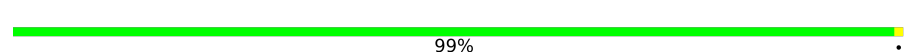

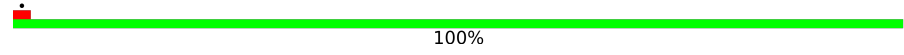
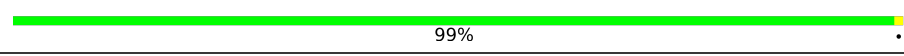
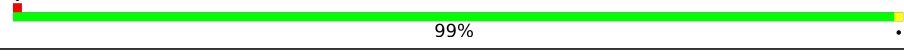
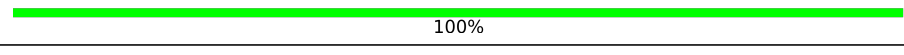
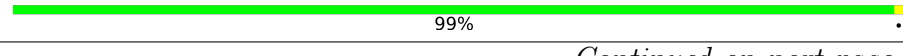

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	C4	121	
2	C3	158	
3	LA	251	
4	LB	386	
5	LC	361	
6	LD	294	
7	LE	175	
8	LF	222	

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Mol	Chain	Length	Quality of chain
9	LG	233	 99%
10	LH	191	 99%
11	LI	218	 100%
12	LJ	169	 99%
13	LL	193	 99%
14	LM	136	 99%
15	LN	203	 100%
16	LO	197	 99%
17	LP	183	 6% 100%
18	LQ	185	 99%
19	LR	188	 90% 9%
20	LS	171	 100%
21	LT	159	 99%
22	LU	100	 100%
23	LV	136	 100%
24	LW	126	 53% 47%
25	LX	121	 100%
26	LY	125	 100%
27	LZ	135	 99%
28	La	148	 100%
29	Lb	58	 100%
30	Lc	96	 99%
31	Ld	109	 99%
32	Le	127	 100%
33	Lf	106	 99%

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Mol	Chain	Length	Quality of chain
34	Lg	112	 99%
35	Lh	119	 99%
36	Li	99	 100%
37	Lj	85	 100%
38	Lk	77	 100%
39	Ll	50	 100%
40	Lm	52	 100%
41	Ln	25	 100%
42	Lo	103	 100%
43	Lp	91	 100%
44	1	3395	 80% 17%
45	A	195	 97%
46	B	796	 47% 100%
47	8	23	 22% 100%

2 Entry composition [i](#)

There are 49 unique types of molecules in this entry. The entry contains 134392 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 RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C4	121	2579	1152	461	845	121	0	0

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C3	158	3353	1500	586	1109	158	0	0

- Molecule 3 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	LA	251	1899	1182	385	331	1	0	0

- Molecule 4 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	LB	386	3075	1950	584	533	8	0	0

- Molecule 5 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LC	361	2748	1729	522	494	3	0	0

- Molecule 6 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LD	294	2351	1484	410	455	2	0	0

- Molecule 7 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	LE	167	1305	841	234	229	1	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LE	132	ALA	THR	conflict	UNP P05739
LE	146	ILE	LEU	conflict	UNP P05739
LE	173	MET	LEU	conflict	UNP P05739

- Molecule 8 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	LF	222	1784	1151	324	308	1	0	0

- Molecule 9 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LG	233	1804	1151	323	327	3	0	0

- Molecule 10 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LH	191	1508	957	274	273	4	0	0

- Molecule 11 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LI	218	1764	1117	334	306	7	0	0

- Molecule 12 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LJ	169	1350	846	253	247	4	0	0

- Molecule 13 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	LL	193	1543	962	315	266	0	0

- Molecule 14 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LM	136	1053	675	199	177	2	0	0

- Molecule 15 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LN	203	1720	1077	361	281	1	0	0

- Molecule 16 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	LO	197	1555	1003	289	262	1	197	0

- Molecule 17 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	LP	183	1416	879	284	253	0	0

- Molecule 18 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	LQ	185	1441	908	290	241	2	0	0

- Molecule 19 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	LR	171	1378	850	294	234	0	0

- Molecule 20 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	LS	171	1437	925	266	243	3	0	0

- Molecule 21 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	LT	159	1276	805	246	221	4	0	0

- Molecule 22 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	LU	100	796	516	131	149	0	0

- Molecule 23 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LV	136	1003	628	189	179	7	0	0

- Molecule 24 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LW	67	538	345	106	86	1	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LW	104	GLN	ASN	conflict	UNP P04449
LW	109	GLN	LEU	conflict	UNP P04449
LW	112	ASP	ASN	conflict	UNP P04449
LW	119	ALA	GLU	conflict	UNP P04449

- Molecule 25 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LX	121	964	620	169	173	2	0	0

- Molecule 26 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	LY	125	984	620	191	173	0	0

- Molecule 27 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	LZ	135	1092	710	202	180	0	0

- Molecule 28 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	La	148	1173	749	231	190	3	0	0

- Molecule 29 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	Lb	58	462	289	100	73	0	0

- Molecule 30 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Lc	96	737	476	123	137	1	0	0

- Molecule 31 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Ld	109	880	559	168	152	1	0	0

- Molecule 32 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Le	127	1017	644	205	167	1	0	0

- Molecule 33 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Lf	106	850	540	165	144	1	0	0

- Molecule 34 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Lg	112	880	545	179	152	4	0	0

- Molecule 35 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Lh	119	969	615	186	167	1	0	0

- Molecule 36 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Li	99	766	478	154	132	2	0	0

- Molecule 37 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Lj	85	670	408	146	111	5	0	0

- Molecule 38 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	Lk	77	612	391	115	106	0	0

- Molecule 39 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Ll	50	436	272	97	65	2	0	0

- Molecule 40 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Lm	52	417	259	86	67	5	0	0

- Molecule 41 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Ln	25	229	139	62	27	1	0	0

- Molecule 42 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Lo	103	824	517	167	135	5	0	0

- Molecule 43 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Lp	91	694	429	138	121	6	0	0

- Molecule 44 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
44	1	3301	70586	31525	12690	23070	3301	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	G	deletion	GB 1262303
1	1962	A	G	conflict	GB 1262303

- Molecule 45 is a protein called N-terminal acetyltransferase B complex catalytic subunit NAT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	A	195	1612	1030	273	297	12	0	0

- Molecule 46 is a protein called N-terminal acetyltransferase B complex subunit MDM20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	B	796	6536	4195	1080	1231	30	0	0

- Molecule 47 is a protein called Nascent peptide chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	8	23	115	69	23	23	0	0

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	C4	1	Total	Mg	0
			1	1	
48	C3	1	Total	Mg	0
			1	1	
48	LA	2	Total	Mg	0
			2	2	
48	LB	1	Total	Mg	0
			1	1	
48	LN	1	Total	Mg	0
			1	1	
48	LP	1	Total	Mg	0
			1	1	
48	LR	1	Total	Mg	0
			1	1	
48	LV	1	Total	Mg	0
			1	1	
48	Le	1	Total	Mg	0
			1	1	
48	1	196	Total	Mg	0
			196	196	

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

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

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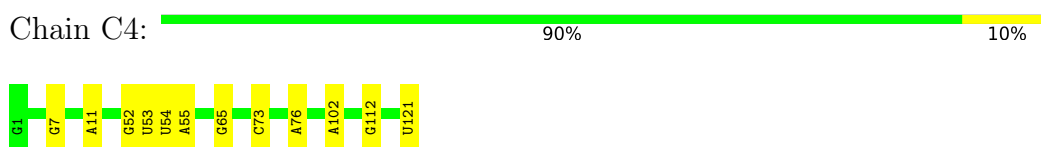
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Mol	Chain	Residues	Atoms		AltConf
49	Lo	1	Total 1	Zn 1	0
49	Lp	1	Total 1	Zn 1	0

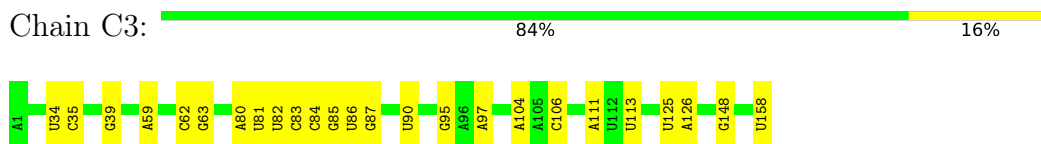
3 Residue-property plots [i](#)

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.

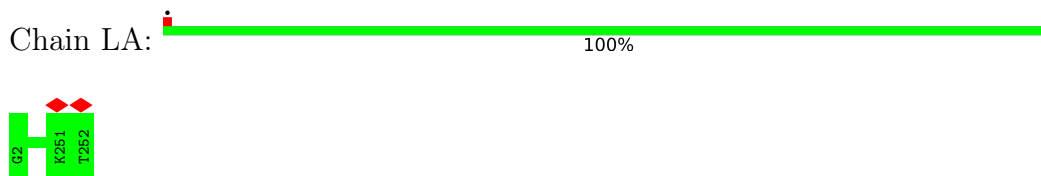
- Molecule 1: 5S rRNA



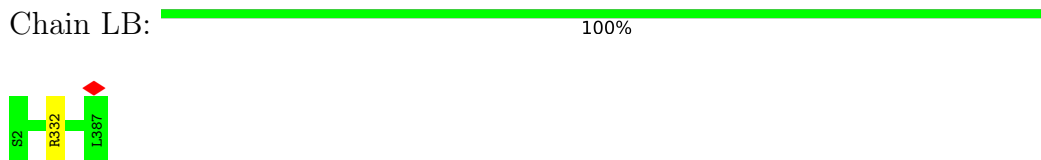
- Molecule 2: 5.8S rRNA



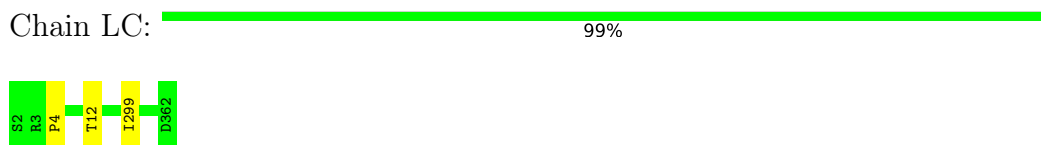
- Molecule 3: 60S ribosomal protein L2-A



- Molecule 4: 60S ribosomal protein L3

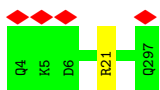


- Molecule 5: 60S ribosomal protein L4-A



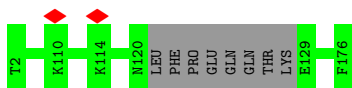
- Molecule 6: 60S ribosomal protein L5

Chain LD:  100%



- Molecule 7: 60S ribosomal protein L6-B

Chain LE:  95% 5%



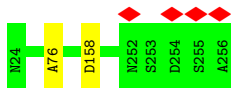
- Molecule 8: 60S ribosomal protein L7-A

Chain LF:  100%

There are no outlier residues recorded for this chain.

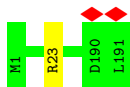
- Molecule 9: 60S ribosomal protein L8-A

Chain LG:  99%



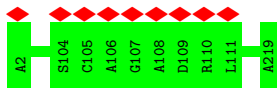
- Molecule 10: 60S ribosomal protein L9-A

Chain LH:  99%



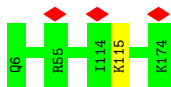
- Molecule 11: 60S ribosomal protein L10

Chain LI:  100%



- Molecule 12: 60S ribosomal protein L11-B

Chain LJ:  99%



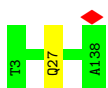
- Molecule 13: 60S ribosomal protein L13-A

Chain LL:  99%



- Molecule 14: 60S ribosomal protein L14-A

Chain LM:  99%



- Molecule 15: 60S ribosomal protein L15-A

Chain LN:  100%

There are no outlier residues recorded for this chain.

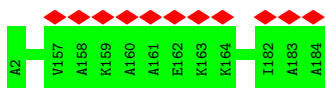
- Molecule 16: 60S ribosomal protein L16-A

Chain LO:  99%



- Molecule 17: 60S ribosomal protein L17-A

Chain LP:  100%



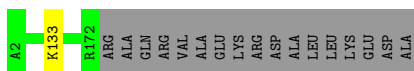
- Molecule 18: 60S ribosomal protein L18-A

Chain LQ:  99%



- Molecule 19: 60S ribosomal protein L19-A

Chain LR:  90% 9%



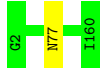
- Molecule 20: 60S ribosomal protein L20-A

Chain LS:  100%

There are no outlier residues recorded for this chain.

- Molecule 21: 60S ribosomal protein L21-A

Chain LT:  99%



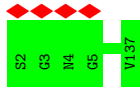
- Molecule 22: 60S ribosomal protein L22-A

Chain LU:  100%



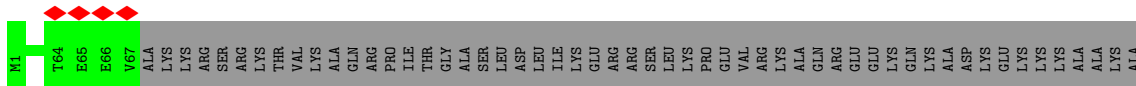
- Molecule 23: 60S ribosomal protein L23-A

Chain LV:  100%



- Molecule 24: 60S ribosomal protein L24-A

Chain LW:  53%



- Molecule 25: 60S ribosomal protein L25

Chain LX:  100%



- Molecule 26: 60S ribosomal protein L26-A

Chain LY:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 60S ribosomal protein L27-A

Chain LZ:  99%



- Molecule 28: 60S ribosomal protein L28

Chain La: 100%



- Molecule 29: 60S ribosomal protein L29

Chain Lb: 100%



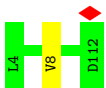
- Molecule 30: 60S ribosomal protein L30

Chain Lc: 99%



- Molecule 31: 60S ribosomal protein L31-A

Chain Ld: 99%



- Molecule 32: 60S ribosomal protein L32

Chain Le: 100%

There are no outlier residues recorded for this chain.

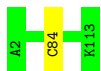
- Molecule 33: 60S ribosomal protein L33-A

Chain Lf: 99%



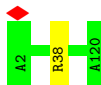
- Molecule 34: 60S ribosomal protein L34-A

Chain Lg: 99%



- Molecule 35: 60S ribosomal protein L35-A

Chain Lh:  99%



- Molecule 36: 60S ribosomal protein L36-A

Chain Li:  100%



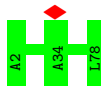
- Molecule 37: 60S ribosomal protein L37-A

Chain Lj:  100%

There are no outlier residues recorded for this chain.

- Molecule 38: 60S ribosomal protein L38

Chain Lk:  100%



- Molecule 39: 60S ribosomal protein L39

Chain Ll:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 60S ribosomal protein L40-A

Chain Lm:  100%



- Molecule 41: 60S ribosomal protein L41-A

Chain Ln:  100%



- Molecule 42: 60S ribosomal protein L42-A

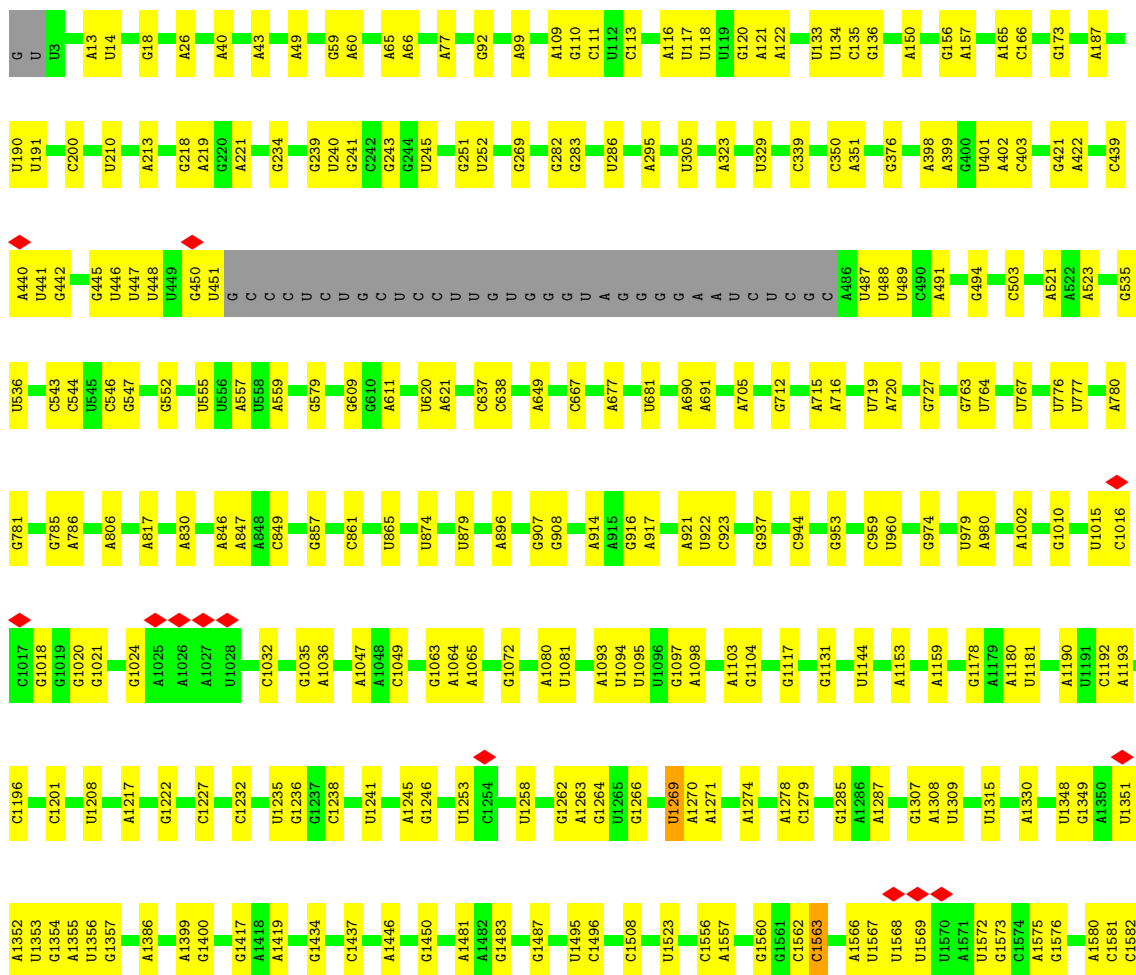
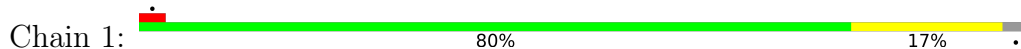


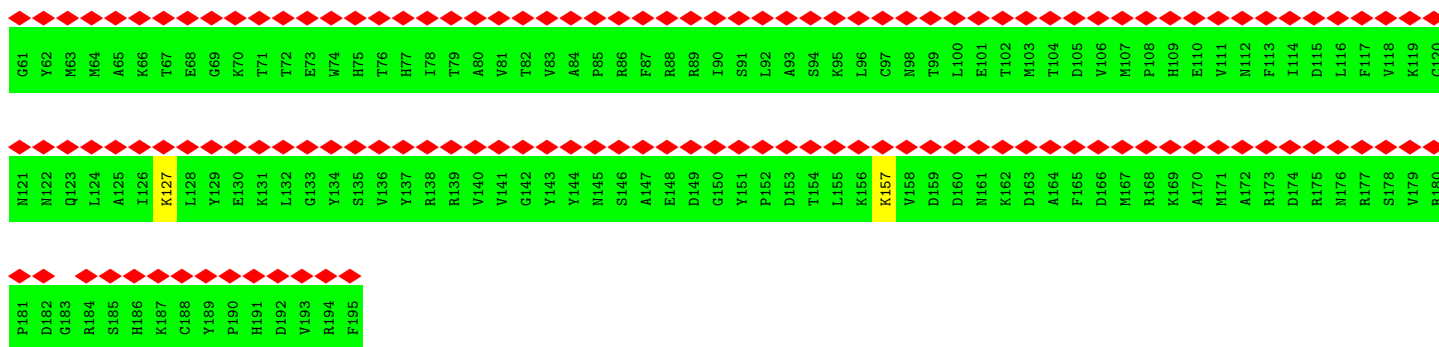
There are no outlier residues recorded for this chain.

- Molecule 43: 60S ribosomal protein L43-A

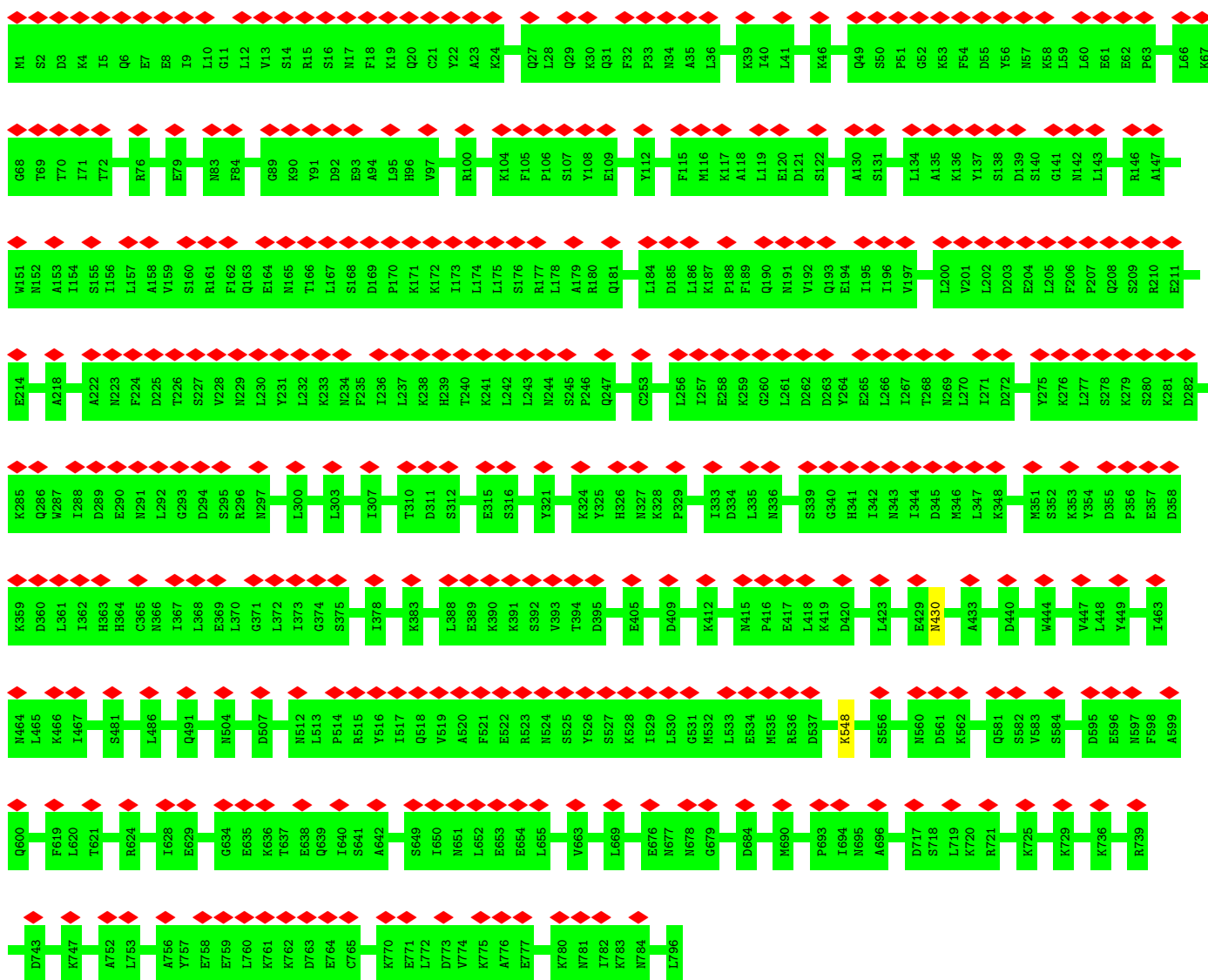


- Molecule 44: 25S rRNA

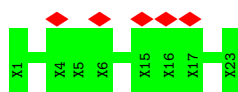




• Molecule 46: N-terminal acetyltransferase B complex subunit MDM20



• Molecule 47: Nascent peptide chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45530	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 ($e^-/\text{\AA}^2$)	45.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.563	Depositor
Minimum map value	-0.645	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.215	Depositor
Map size (Å)	417.99997, 417.99997, 417.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C4	0.33	0/2883	0.75	0/4491
2	C3	0.37	0/3746	0.77	0/5832
3	LA	0.29	0/1933	0.58	0/2598
4	LB	0.28	0/3146	0.53	0/4228
5	LC	0.28	0/2800	0.52	0/3790
6	LD	0.28	0/2400	0.51	0/3239
7	LE	0.28	0/1327	0.50	0/1790
8	LF	0.29	0/1821	0.48	0/2451
9	LG	0.27	0/1836	0.49	0/2481
10	LH	0.28	0/1529	0.54	0/2060
11	LI	0.28	0/1801	0.53	0/2416
12	LJ	0.27	0/1371	0.60	0/1838
13	LL	0.27	0/1568	0.58	0/2106
14	LM	0.27	0/1068	0.53	0/1438
15	LN	0.29	0/1757	0.58	0/2354
16	LO	0.29	0/1585	0.50	0/2128
17	LP	0.27	0/1439	0.55	0/1938
18	LQ	0.27	0/1465	0.55	0/1965
19	LR	0.27	0/1395	0.56	0/1861
20	LS	0.30	0/1473	0.56	0/1980
21	LT	0.30	0/1300	0.57	0/1743
22	LU	0.28	0/812	0.49	0/1099
23	LV	0.29	0/1018	0.57	0/1369
24	LW	0.29	0/550	0.55	0/731
25	LX	0.29	0/979	0.49	0/1321
26	LY	0.29	0/995	0.56	0/1329
27	LZ	0.30	0/1118	0.52	0/1497
28	La	0.28	0/1204	0.53	0/1612
29	Lb	0.27	0/473	0.55	0/629
30	Lc	0.28	0/745	0.47	0/1001
31	Ld	0.28	0/894	0.53	0/1200
32	Le	0.28	0/1038	0.51	0/1390

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Lf	0.31	0/868	0.55	0/1168
34	Lg	0.28	0/890	0.57	0/1189
35	Lh	0.27	0/978	0.51	0/1301
36	Li	0.26	0/772	0.56	0/1026
37	Lj	0.28	0/685	0.58	0/908
38	Lk	0.29	0/618	0.57	0/826
39	Ll	0.28	0/443	0.62	0/588
40	Lm	0.28	0/423	0.60	0/562
41	Ln	0.24	0/230	0.72	0/296
42	Lo	0.28	0/836	0.56	0/1104
43	Lp	0.30	0/701	0.60	0/934
44	1	0.36	0/79000	0.78	16/123166 (0.0%)
45	A	0.24	0/1654	0.49	0/2237
46	B	0.24	0/6665	0.42	0/8979
All	All	0.33	0/144232	0.70	16/212189 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	LG	0	2
16	LO	0	1
All	All	0	3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1269	U	C2-N1-C1'	6.99	126.09	117.70
44	1	1269	U	N1-C2-O2	6.86	127.60	122.80
44	1	922	U	C2-N1-C1'	6.56	125.58	117.70
44	1	1269	U	N3-C2-O2	-6.44	117.69	122.20
44	1	1563	C	N3-C2-O2	-5.86	117.80	121.90
44	1	2080	C	N3-C2-O2	-5.76	117.87	121.90
44	1	922	U	N1-C2-O2	5.50	126.65	122.80
44	1	2867	C	N1-C2-O2	5.46	122.17	118.90
44	1	2080	C	N1-C2-O2	5.43	122.16	118.90
44	1	2836	C	C2-N1-C1'	5.40	124.74	118.80
44	1	2112	U	OP2-P-O3'	5.38	117.04	105.20
44	1	2237	C	N3-C2-O2	-5.23	118.24	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	1	1563	C	C6-N1-C2	-5.18	118.23	120.30
44	1	922	U	N3-C2-O2	-5.09	118.64	122.20
44	1	1496	C	C2-N1-C1'	5.06	124.37	118.80
44	1	2237	C	N1-C2-O2	5.01	121.90	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	LG	158	ASP	Peptide
9	LG	76	ALA	Peptide
16	LO	110[A]	PRO	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LA	249/251 (99%)	232 (93%)	17 (7%)	0	100	100
4	LB	384/386 (100%)	357 (93%)	27 (7%)	0	100	100
5	LC	359/361 (99%)	334 (93%)	24 (7%)	1 (0%)	41	73
6	LD	292/294 (99%)	279 (96%)	12 (4%)	1 (0%)	41	73
7	LE	163/175 (93%)	154 (94%)	9 (6%)	0	100	100
8	LF	220/222 (99%)	207 (94%)	13 (6%)	0	100	100
9	LG	231/233 (99%)	220 (95%)	11 (5%)	0	100	100
10	LH	189/191 (99%)	178 (94%)	11 (6%)	0	100	100
11	LI	216/218 (99%)	209 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	LJ	167/169 (99%)	152 (91%)	15 (9%)	0	100	100
13	LL	191/193 (99%)	175 (92%)	15 (8%)	1 (0%)	29	64
14	LM	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
15	LN	201/203 (99%)	188 (94%)	13 (6%)	0	100	100
16	LO	195/197 (99%)	188 (96%)	5 (3%)	2 (1%)	15	49
17	LP	181/183 (99%)	172 (95%)	9 (5%)	0	100	100
18	LQ	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
19	LR	169/188 (90%)	164 (97%)	5 (3%)	0	100	100
20	LS	169/171 (99%)	160 (95%)	9 (5%)	0	100	100
21	LT	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
22	LU	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
23	LV	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
24	LW	65/126 (52%)	63 (97%)	2 (3%)	0	100	100
25	LX	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
26	LY	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
27	LZ	133/135 (98%)	122 (92%)	11 (8%)	0	100	100
28	La	146/148 (99%)	130 (89%)	16 (11%)	0	100	100
29	Lb	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
30	Lc	94/96 (98%)	94 (100%)	0	0	100	100
31	Ld	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
32	Le	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
33	Lf	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
34	Lg	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
35	Lh	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
36	Li	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
37	Lj	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
38	Lk	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
39	Ll	48/50 (96%)	48 (100%)	0	0	100	100
40	Lm	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
41	Ln	23/25 (92%)	23 (100%)	0	0	100	100
42	Lo	101/103 (98%)	96 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
45	A	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
46	B	794/796 (100%)	784 (99%)	10 (1%)	0	100	100
All	All	7134/7306 (98%)	6797 (95%)	332 (5%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	LD	21	ARG
16	LO	111[A]	PRO
13	LL	63	VAL
16	LO	110[A]	PRO
5	LC	4	PRO

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	
3	LA	190/193 (98%)	190 (100%)	0	100	100
4	LB	319/322 (99%)	318 (100%)	1 (0%)	92	96
5	LC	288/288 (100%)	286 (99%)	2 (1%)	84	93
6	LD	241/243 (99%)	241 (100%)	0	100	100
7	LE	138/153 (90%)	138 (100%)	0	100	100
8	LF	186/186 (100%)	186 (100%)	0	100	100
9	LG	187/191 (98%)	187 (100%)	0	100	100
10	LH	168/171 (98%)	167 (99%)	1 (1%)	86	94
11	LI	185/185 (100%)	185 (100%)	0	100	100
12	LJ	146/147 (99%)	145 (99%)	1 (1%)	84	93
13	LL	154/154 (100%)	153 (99%)	1 (1%)	86	94
14	LM	107/107 (100%)	106 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	LN	175/175 (100%)	175 (100%)	0	100	100
16	LO	160/160 (100%)	160 (100%)	0	100	100
17	LP	138/145 (95%)	138 (100%)	0	100	100
18	LQ	150/150 (100%)	149 (99%)	1 (1%)	84	93
19	LR	139/153 (91%)	138 (99%)	1 (1%)	84	93
20	LS	155/155 (100%)	155 (100%)	0	100	100
21	LT	136/136 (100%)	135 (99%)	1 (1%)	84	93
22	LU	87/87 (100%)	87 (100%)	0	100	100
23	LV	104/104 (100%)	104 (100%)	0	100	100
24	LW	54/107 (50%)	54 (100%)	0	100	100
25	LX	104/105 (99%)	104 (100%)	0	100	100
26	LY	108/108 (100%)	108 (100%)	0	100	100
27	LZ	115/115 (100%)	114 (99%)	1 (1%)	78	91
28	La	118/118 (100%)	118 (100%)	0	100	100
29	Lb	46/46 (100%)	46 (100%)	0	100	100
30	Lc	81/81 (100%)	80 (99%)	1 (1%)	71	88
31	Ld	93/96 (97%)	92 (99%)	1 (1%)	73	89
32	Le	108/109 (99%)	108 (100%)	0	100	100
33	Lf	90/90 (100%)	89 (99%)	1 (1%)	73	89
34	Lg	95/95 (100%)	94 (99%)	1 (1%)	73	89
35	Lh	104/104 (100%)	103 (99%)	1 (1%)	76	90
36	Li	80/81 (99%)	80 (100%)	0	100	100
37	Lj	69/69 (100%)	69 (100%)	0	100	100
38	Lk	68/68 (100%)	68 (100%)	0	100	100
39	Ll	45/45 (100%)	45 (100%)	0	100	100
40	Lm	47/47 (100%)	47 (100%)	0	100	100
41	Ln	22/23 (96%)	22 (100%)	0	100	100
42	Lo	87/88 (99%)	87 (100%)	0	100	100
43	Lp	71/71 (100%)	71 (100%)	0	100	100
45	A	180/180 (100%)	178 (99%)	2 (1%)	73	89
46	B	743/743 (100%)	741 (100%)	2 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6081/6194 (98%)	6061 (100%)	20 (0%)	92 96

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LB	332	ARG
5	LC	12	THR
5	LC	299	ILE
10	LH	23	ARG
12	LJ	115	LYS
13	LL	104	ARG
14	LM	27	GLN
18	LQ	12	ARG
19	LR	133	LYS
21	LT	77	ASN
27	LZ	3	LYS
30	Lc	22	LYS
31	Ld	8	VAL
33	Lf	106	ASN
34	Lg	84	CYS
35	Lh	38	ARG
45	A	127	LYS
45	A	157	LYS
46	B	430	ASN
46	B	548	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	LA	83	HIS
5	LC	110	ASN
23	LV	98	ASN
27	LZ	128	GLN
34	Lg	34	HIS
39	Ll	11	GLN
42	Lo	47	GLN
42	Lo	53	GLN
46	B	126	GLN
46	B	699	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C4	120/121 (99%)	11 (9%)	1 (0%)
2	C3	157/158 (99%)	25 (15%)	1 (0%)
44	1	3297/3395 (97%)	579 (17%)	34 (1%)
All	All	3574/3674 (97%)	615 (17%)	36 (1%)

All (615) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C4	7	G
1	C4	11	A
1	C4	53	U
1	C4	54	U
1	C4	55	A
1	C4	65	G
1	C4	73	C
1	C4	76	A
1	C4	102	A
1	C4	112	G
1	C4	121	U
2	C3	34	U
2	C3	35	C
2	C3	39	G
2	C3	59	A
2	C3	62	C
2	C3	63	G
2	C3	80	A
2	C3	81	U
2	C3	82	U
2	C3	83	C
2	C3	84	C
2	C3	85	G
2	C3	86	U
2	C3	87	G
2	C3	90	U
2	C3	95	G
2	C3	97	A
2	C3	104	A
2	C3	106	C
2	C3	111	A
2	C3	113	U
2	C3	125	U

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Mol	Chain	Res	Type
2	C3	126	A
2	C3	148	G
2	C3	158	U
44	1	13	A
44	1	14	U
44	1	18	G
44	1	26	A
44	1	40	A
44	1	43	A
44	1	49	A
44	1	59	G
44	1	60	A
44	1	65	A
44	1	66	A
44	1	77	A
44	1	92	G
44	1	99	A
44	1	109	A
44	1	110	G
44	1	111	C
44	1	113	C
44	1	116	A
44	1	117	U
44	1	118	U
44	1	120	G
44	1	121	A
44	1	122	A
44	1	133	U
44	1	134	U
44	1	135	C
44	1	136	G
44	1	150	A
44	1	156	G
44	1	157	A
44	1	165	A
44	1	166	C
44	1	173	G
44	1	187	A
44	1	190	U
44	1	191	U
44	1	200	C
44	1	210	U

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Mol	Chain	Res	Type
44	1	213	A
44	1	218	G
44	1	219	A
44	1	221	A
44	1	234	G
44	1	240	U
44	1	241	G
44	1	243	G
44	1	245	U
44	1	251	G
44	1	252	U
44	1	269	G
44	1	283	G
44	1	286	U
44	1	295	A
44	1	305	U
44	1	323	A
44	1	329	U
44	1	339	C
44	1	350	C
44	1	351	A
44	1	376	G
44	1	398	A
44	1	399	A
44	1	401	U
44	1	402	A
44	1	403	C
44	1	421	G
44	1	422	A
44	1	439	C
44	1	440	A
44	1	441	U
44	1	442	G
44	1	445	G
44	1	446	U
44	1	447	U
44	1	448	U
44	1	450	G
44	1	451	U
44	1	487	U
44	1	488	U
44	1	489	U

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Mol	Chain	Res	Type
44	1	491	A
44	1	494	G
44	1	503	C
44	1	521	A
44	1	523	A
44	1	535	G
44	1	536	U
44	1	543	C
44	1	544	C
44	1	546	C
44	1	547	G
44	1	552	G
44	1	555	U
44	1	557	A
44	1	559	A
44	1	579	G
44	1	609	G
44	1	611	A
44	1	620	U
44	1	621	A
44	1	637	C
44	1	638	C
44	1	649	A
44	1	667	C
44	1	677	A
44	1	681	U
44	1	690	A
44	1	691	A
44	1	705	A
44	1	712	G
44	1	716	A
44	1	719	U
44	1	720	A
44	1	727	G
44	1	764	U
44	1	767	U
44	1	776	U
44	1	777	U
44	1	780	A
44	1	781	G
44	1	785	G
44	1	786	A

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Mol	Chain	Res	Type
44	1	806	A
44	1	817	A
44	1	830	A
44	1	846	A
44	1	847	A
44	1	849	C
44	1	857	G
44	1	861	C
44	1	865	U
44	1	874	U
44	1	879	U
44	1	896	A
44	1	907	G
44	1	908	G
44	1	914	A
44	1	916	G
44	1	917	A
44	1	921	A
44	1	923	C
44	1	937	G
44	1	944	C
44	1	953	G
44	1	959	C
44	1	960	U
44	1	974	G
44	1	979	U
44	1	980	A
44	1	1002	A
44	1	1010	G
44	1	1015	U
44	1	1016	C
44	1	1018	G
44	1	1020	G
44	1	1021	G
44	1	1024	G
44	1	1032	C
44	1	1035	G
44	1	1036	A
44	1	1047	A
44	1	1049	C
44	1	1063	G
44	1	1064	A

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Mol	Chain	Res	Type
44	1	1065	A
44	1	1072	G
44	1	1080	A
44	1	1081	U
44	1	1093	A
44	1	1094	U
44	1	1095	U
44	1	1097	G
44	1	1098	A
44	1	1103	A
44	1	1104	G
44	1	1117	G
44	1	1131	G
44	1	1144	U
44	1	1153	A
44	1	1159	A
44	1	1178	G
44	1	1180	A
44	1	1181	U
44	1	1190	A
44	1	1192	C
44	1	1193	A
44	1	1196	C
44	1	1201	C
44	1	1208	U
44	1	1217	A
44	1	1222	G
44	1	1227	C
44	1	1232	C
44	1	1235	U
44	1	1236	G
44	1	1238	C
44	1	1241	U
44	1	1245	A
44	1	1246	G
44	1	1253	U
44	1	1258	U
44	1	1262	G
44	1	1263	A
44	1	1264	G
44	1	1266	G
44	1	1269	U

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Mol	Chain	Res	Type
44	1	1270	A
44	1	1271	A
44	1	1274	A
44	1	1278	A
44	1	1279	C
44	1	1285	G
44	1	1287	A
44	1	1307	G
44	1	1308	A
44	1	1309	U
44	1	1315	U
44	1	1330	A
44	1	1348	U
44	1	1349	G
44	1	1351	U
44	1	1352	A
44	1	1353	U
44	1	1354	G
44	1	1355	A
44	1	1356	U
44	1	1357	G
44	1	1386	A
44	1	1399	A
44	1	1400	G
44	1	1417	G
44	1	1419	A
44	1	1434	G
44	1	1437	C
44	1	1446	A
44	1	1450	G
44	1	1481	A
44	1	1483	G
44	1	1487	G
44	1	1495	U
44	1	1508	C
44	1	1523	U
44	1	1556	C
44	1	1557	A
44	1	1560	G
44	1	1562	C
44	1	1563	C
44	1	1566	A

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Mol	Chain	Res	Type
44	1	1567	U
44	1	1568	U
44	1	1569	U
44	1	1572	U
44	1	1573	G
44	1	1575	A
44	1	1576	G
44	1	1580	A
44	1	1581	C
44	1	1582	C
44	1	1583	A
44	1	1587	A
44	1	1588	A
44	1	1589	A
44	1	1605	A
44	1	1607	U
44	1	1619	A
44	1	1620	U
44	1	1621	A
44	1	1629	U
44	1	1639	C
44	1	1642	A
44	1	1643	A
44	1	1645	U
44	1	1657	C
44	1	1683	A
44	1	1688	U
44	1	1717	U
44	1	1724	U
44	1	1725	C
44	1	1736	G
44	1	1741	A
44	1	1750	A
44	1	1751	G
44	1	1761	C
44	1	1765	U
44	1	1766	G
44	1	1770	G
44	1	1775	G
44	1	1780	G
44	1	1788	C
44	1	1797	A

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Mol	Chain	Res	Type
44	1	1808	G
44	1	1814	A
44	1	1816	A
44	1	1817	G
44	1	1819	U
44	1	1820	U
44	1	1821	U
44	1	1835	A
44	1	1839	A
44	1	1840	U
44	1	1841	A
44	1	1842	A
44	1	1846	C
44	1	1849	C
44	1	1850	A
44	1	1866	C
44	1	1867	A
44	1	1878	G
44	1	1880	U
44	1	1893	A
44	1	1906	G
44	1	1952	G
44	1	1953	G
44	1	1954	G
44	1	1955	U
44	1	1958	U
44	1	1960	A
44	1	1961	G
44	1	1962	A
44	1	1963	G
44	1	1964	C
44	1	1972	A
44	1	1973	G
44	1	1976	G
44	1	1981	G
44	1	1984	C
44	1	1985	G
44	1	1988	C
44	1	1994	G
44	1	2001	U
44	1	2006	G
44	1	2010	U

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Mol	Chain	Res	Type
44	1	2013	C
44	1	2017	G
44	1	2020	A
44	1	2022	G
44	1	2025	G
44	1	2035	G
44	1	2039	C
44	1	2044	U
44	1	2045	G
44	1	2047	A
44	1	2048	G
44	1	2049	A
44	1	2050	C
44	1	2059	U
44	1	2081	U
44	1	2082	U
44	1	2087	C
44	1	2088	A
44	1	2093	A
44	1	2101	C
44	1	2102	U
44	1	2107	A
44	1	2111	G
44	1	2112	U
44	1	2113	A
44	1	2114	C
44	1	2121	G
44	1	2122	G
44	1	2131	A
44	1	2144	A
44	1	2158	A
44	1	2169	G
44	1	2170	U
44	1	2171	G
44	1	2188	A
44	1	2192	C
44	1	2193	U
44	1	2194	G
44	1	2206	G
44	1	2209	U
44	1	2210	G
44	1	2222	A

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Mol	Chain	Res	Type
44	1	2223	A
44	1	2244	A
44	1	2249	G
44	1	2250	G
44	1	2255	A
44	1	2256	A
44	1	2270	A
44	1	2272	G
44	1	2273	G
44	1	2281	A
44	1	2282	U
44	1	2288	G
44	1	2307	G
44	1	2310	U
44	1	2313	A
44	1	2314	U
44	1	2315	G
44	1	2336	U
44	1	2373	A
44	1	2374	C
44	1	2375	G
44	1	2385	G
44	1	2388	U
44	1	2393	G
44	1	2394	G
44	1	2397	A
44	1	2402	A
44	1	2403	G
44	1	2404	A
44	1	2411	U
44	1	2435	G
44	1	2437	G
44	1	2438	A
44	1	2439	A
44	1	2445	A
44	1	2446	U
44	1	2447	A
44	1	2452	G
44	1	2496	C
44	1	2498	U
44	1	2501	U
44	1	2502	A

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Mol	Chain	Res	Type
44	1	2506	U
44	1	2507	C
44	1	2508	U
44	1	2514	U
44	1	2515	A
44	1	2522	G
44	1	2524	A
44	1	2525	G
44	1	2531	C
44	1	2537	U
44	1	2538	U
44	1	2539	C
44	1	2540	A
44	1	2541	U
44	1	2542	U
44	1	2544	U
44	1	2547	A
44	1	2548	C
44	1	2549	G
44	1	2552	C
44	1	2561	A
44	1	2569	A
44	1	2570	U
44	1	2571	U
44	1	2572	C
44	1	2573	G
44	1	2585	G
44	1	2593	A
44	1	2606	G
44	1	2607	G
44	1	2614	G
44	1	2635	A
44	1	2638	C
44	1	2652	U
44	1	2656	A
44	1	2672	G
44	1	2674	A
44	1	2677	G
44	1	2689	A
44	1	2691	A
44	1	2694	A
44	1	2696	A

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Mol	Chain	Res	Type
44	1	2704	A
44	1	2719	U
44	1	2728	G
44	1	2729	U
44	1	2737	C
44	1	2752	U
44	1	2753	G
44	1	2755	C
44	1	2772	C
44	1	2773	C
44	1	2777	G
44	1	2778	G
44	1	2788	C
44	1	2796	G
44	1	2800	G
44	1	2801	A
44	1	2803	A
44	1	2810	C
44	1	2816	G
44	1	2817	A
44	1	2821	C
44	1	2842	U
44	1	2844	C
44	1	2845	A
44	1	2867	C
44	1	2871	G
44	1	2872	A
44	1	2873	U
44	1	2875	U
44	1	2887	A
44	1	2889	C
44	1	2911	A
44	1	2915	U
44	1	2923	U
44	1	2935	U
44	1	2936	A
44	1	2947	G
44	1	2971	A
44	1	2983	C
44	1	2992	U
44	1	2996	U
44	1	2997	G

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Mol	Chain	Res	Type
44	1	3012	A
44	1	3030	G
44	1	3059	G
44	1	3074	G
44	1	3078	U
44	1	3086	A
44	1	3092	C
44	1	3093	C
44	1	3101	G
44	1	3104	U
44	1	3113	A
44	1	3119	U
44	1	3122	A
44	1	3129	A
44	1	3130	A
44	1	3131	U
44	1	3142	A
44	1	3143	C
44	1	3153	U
44	1	3154	C
44	1	3155	U
44	1	3156	U
44	1	3157	U
44	1	3165	A
44	1	3170	A
44	1	3173	G
44	1	3174	A
44	1	3176	G
44	1	3179	U
44	1	3181	C
44	1	3187	A
44	1	3196	U
44	1	3198	U
44	1	3207	U
44	1	3210	A
44	1	3217	C
44	1	3218	A
44	1	3219	G
44	1	3227	A
44	1	3229	G
44	1	3242	G
44	1	3243	A

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Mol	Chain	Res	Type
44	1	3245	A
44	1	3247	G
44	1	3259	U
44	1	3263	G
44	1	3269	U
44	1	3270	U
44	1	3273	A
44	1	3276	G
44	1	3281	U
44	1	3287	U
44	1	3288	G
44	1	3289	G
44	1	3292	A
44	1	3294	A
44	1	3304	U
44	1	3313	U
44	1	3316	A
44	1	3318	G
44	1	3319	U
44	1	3320	A
44	1	3334	U
44	1	3341	U
44	1	3345	G
44	1	3347	A
44	1	3351	U
44	1	3352	U
44	1	3353	G
44	1	3354	U
44	1	3355	U
44	1	3369	G
44	1	3375	A
44	1	3378	C
44	1	3383	G
44	1	3386	G
44	1	3389	U
44	1	3390	G

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C4	52	G
2	C3	85	G

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Mol	Chain	Res	Type
44	1	13	A
44	1	239	G
44	1	282	G
44	1	637	C
44	1	715	A
44	1	763	G
44	1	916	G
44	1	1064	A
44	1	1097	G
44	1	1307	G
44	1	1355	A
44	1	1562	C
44	1	1568	U
44	1	1815	U
44	1	1820	U
44	1	1959	G
44	1	1983	G
44	1	2086	A
44	1	2101	C
44	1	2112	U
44	1	2249	G
44	1	2446	U
44	1	2495	C
44	1	2537	U
44	1	2541	U
44	1	2547	A
44	1	3121	U
44	1	3218	A
44	1	3228	C
44	1	3269	U
44	1	3275	U
44	1	3319	U
44	1	3350	C
44	1	3351	U

5.4 Non-standard residues in protein, DNA, RNA chains

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 211 ligands modelled in this entry, 211 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

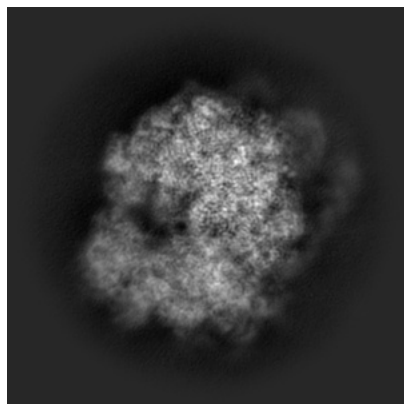
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16086. These allow visual inspection of the internal detail of the map and identification of artifacts.

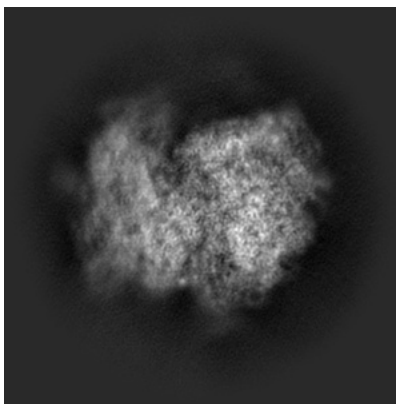
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

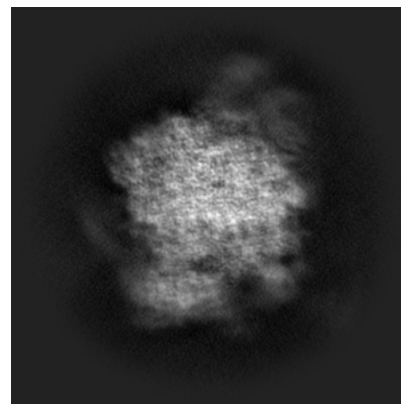
6.1.1 Primary map



X

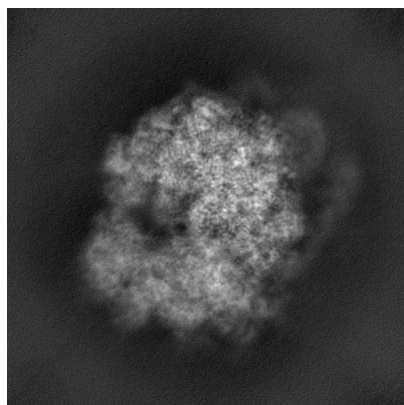


Y

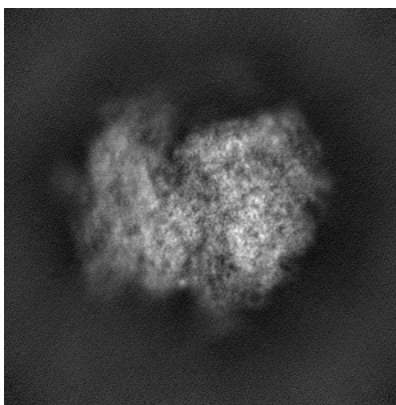


Z

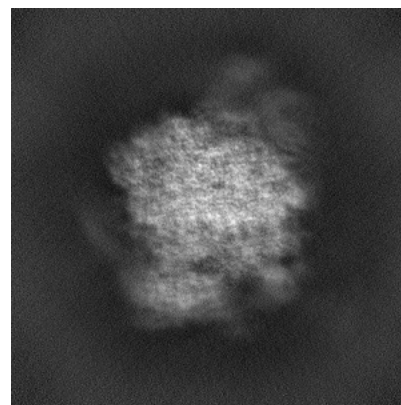
6.1.2 Raw map



X



Y

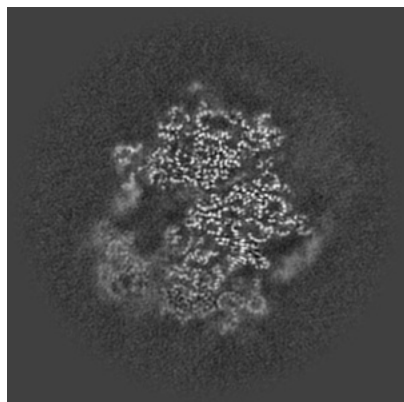


Z

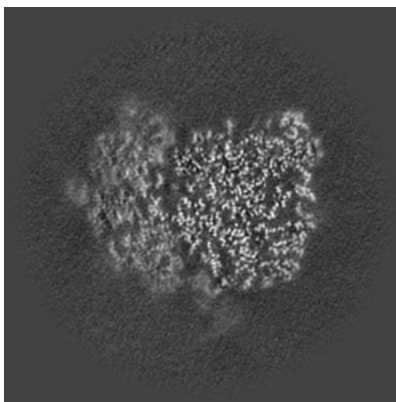
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

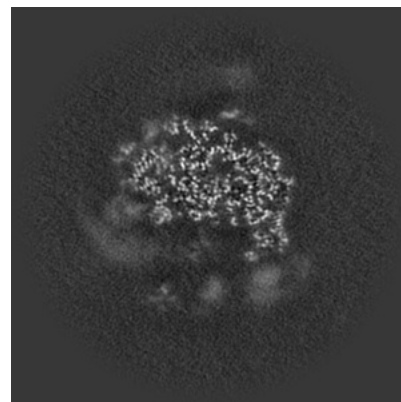
6.2.1 Primary map



X Index: 200

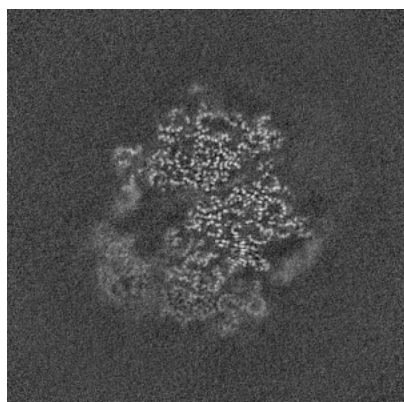


Y Index: 200

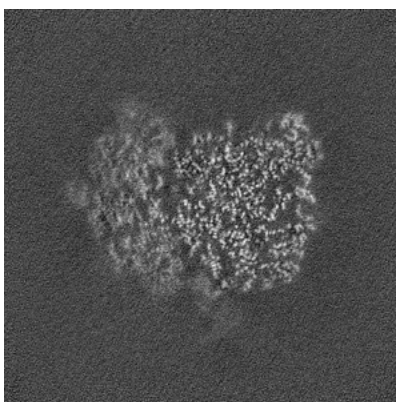


Z Index: 200

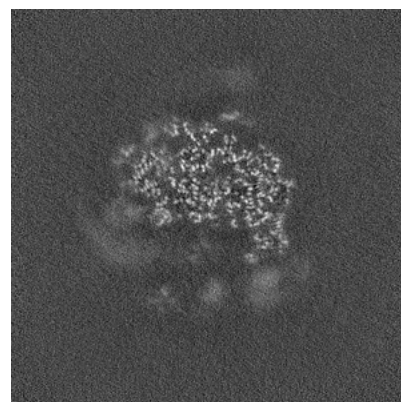
6.2.2 Raw map



X Index: 200



Y Index: 200

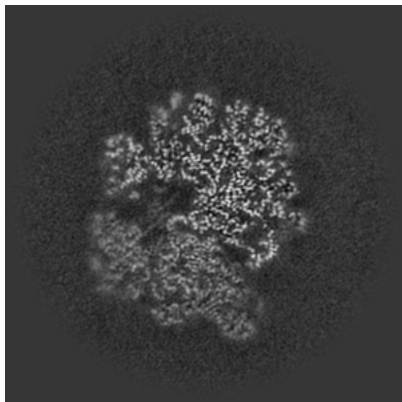


Z Index: 200

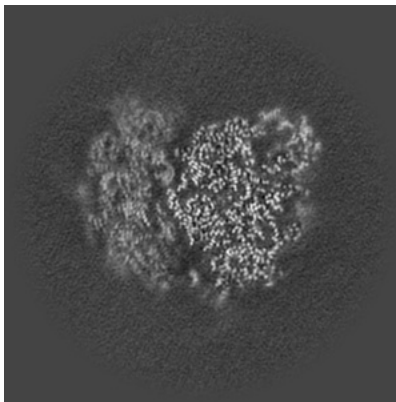
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

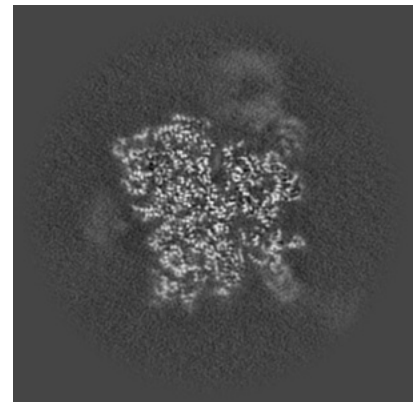
6.3.1 Primary map



X Index: 182

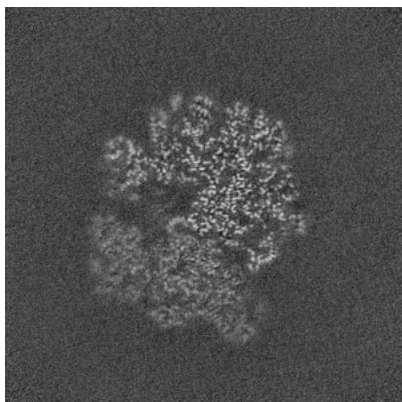


Y Index: 210

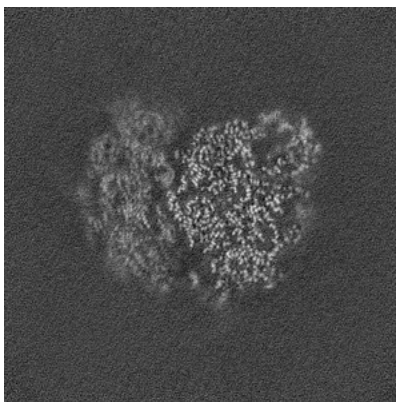


Z Index: 235

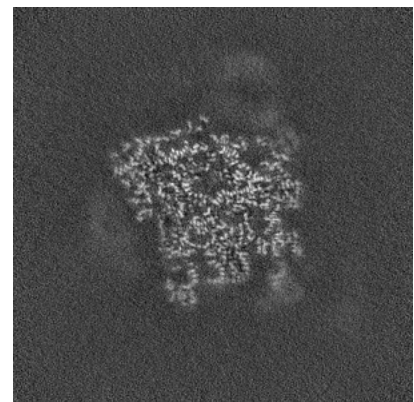
6.3.2 Raw map



X Index: 183



Y Index: 210

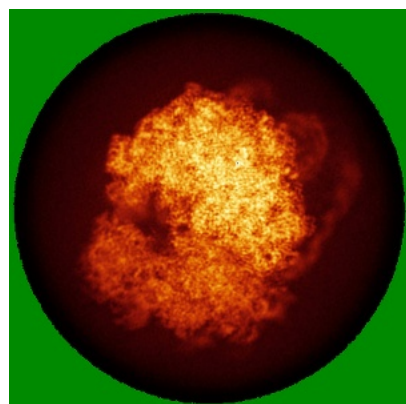


Z Index: 226

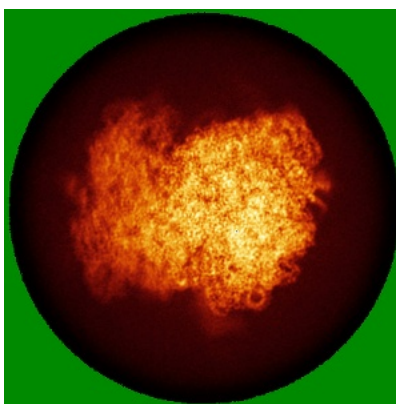
The images above show the largest variance slices of the map in three orthogonal directions.

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

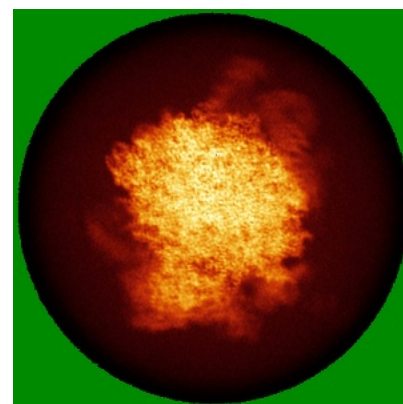
6.4.1 Primary map



X

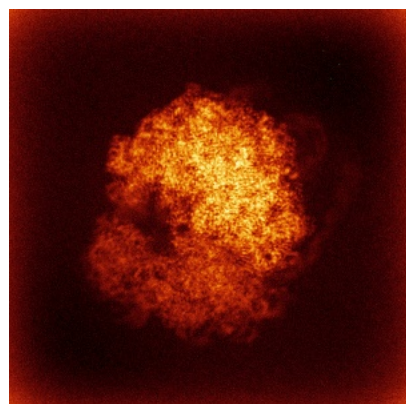


Y

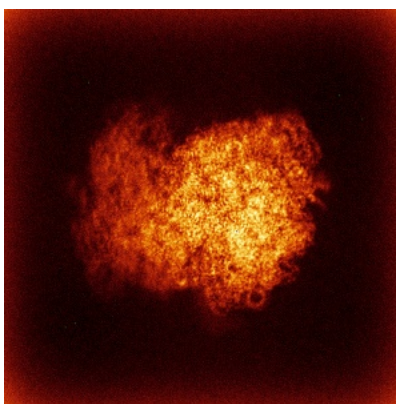


Z

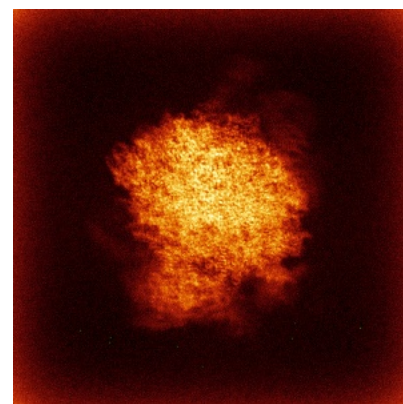
6.4.2 Raw map



X



Y

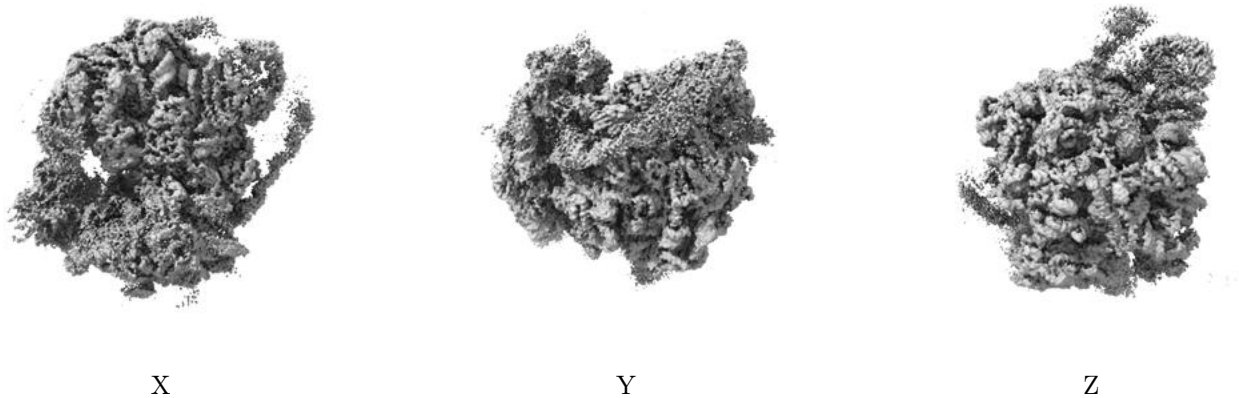


Z

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

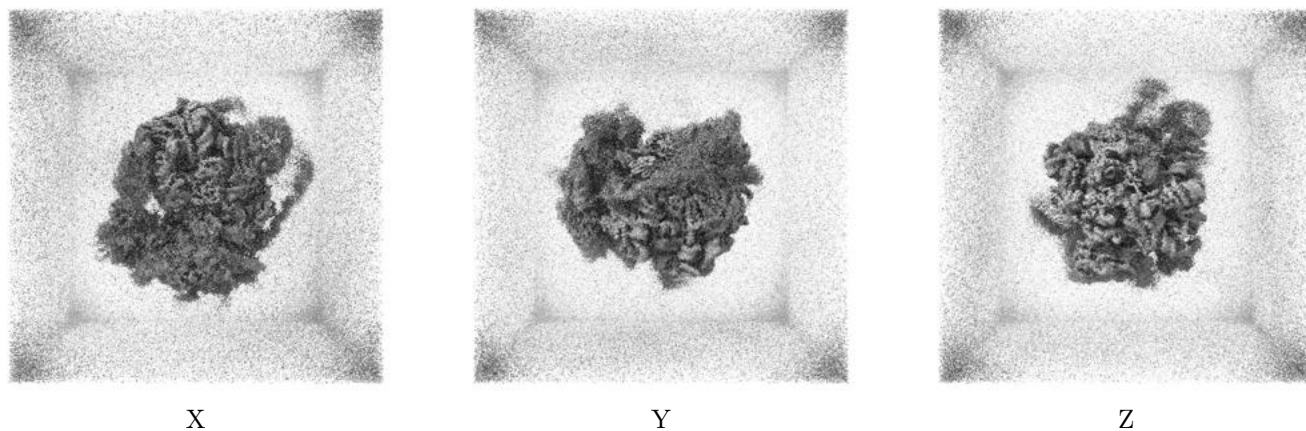
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.215. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

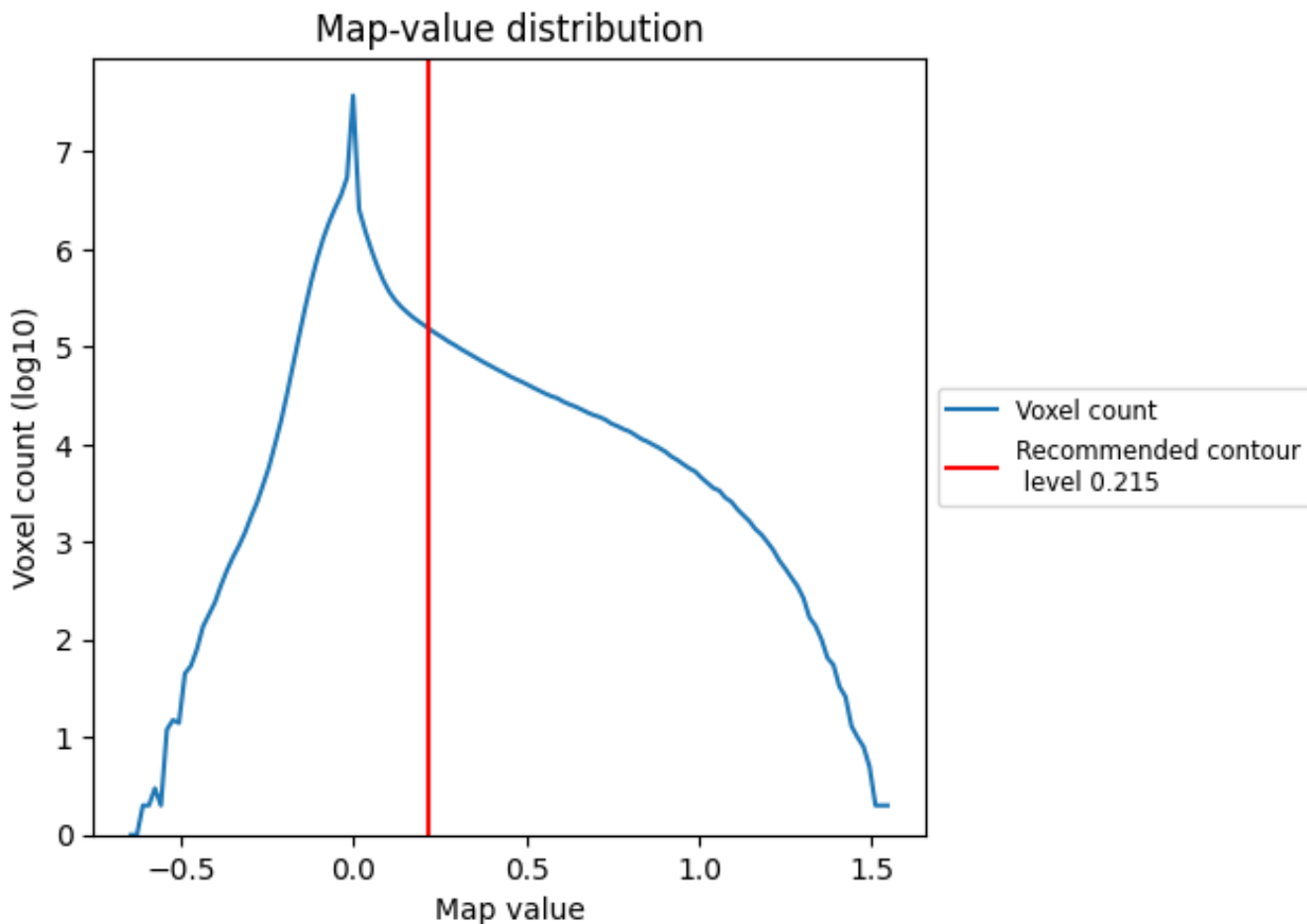
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

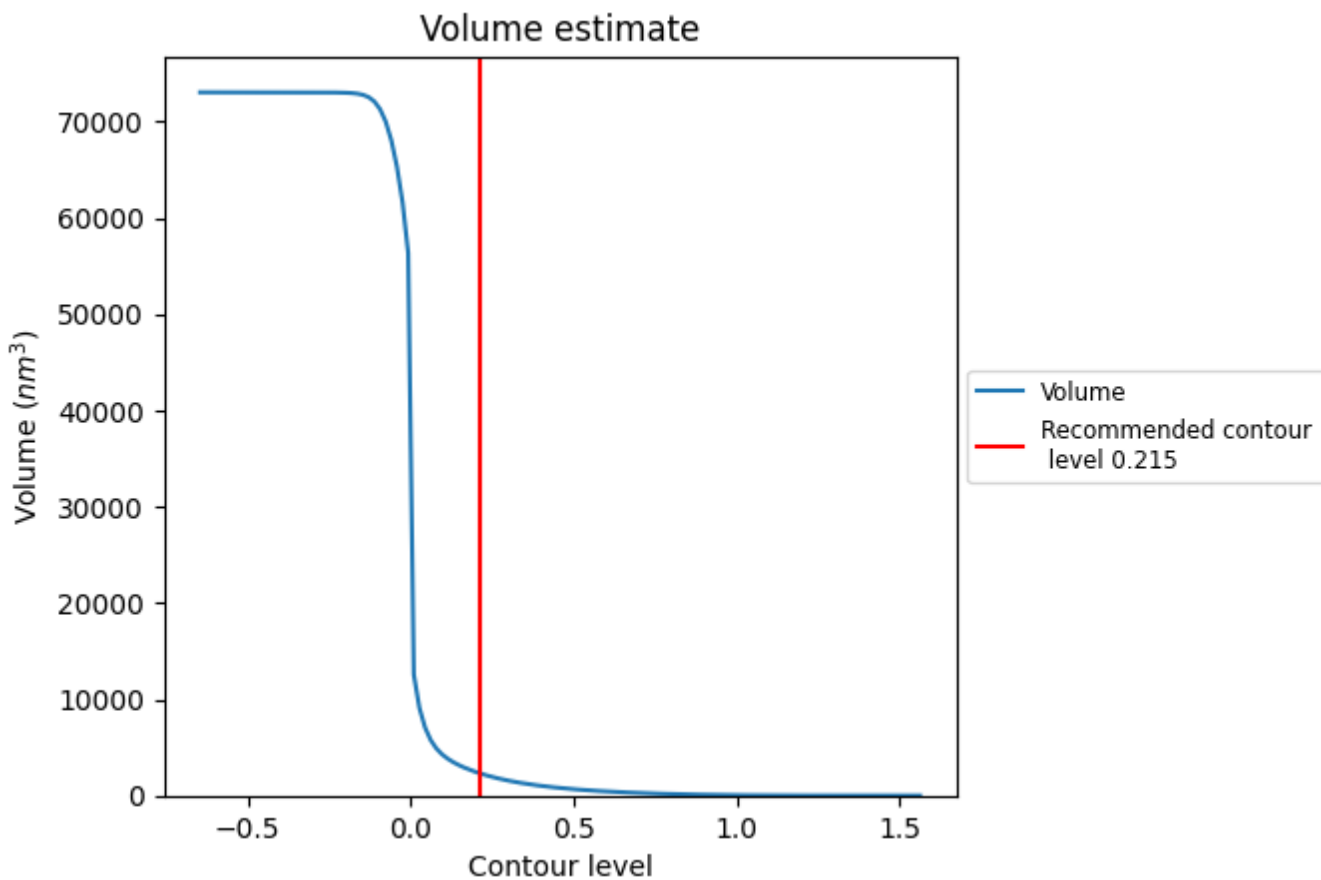
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

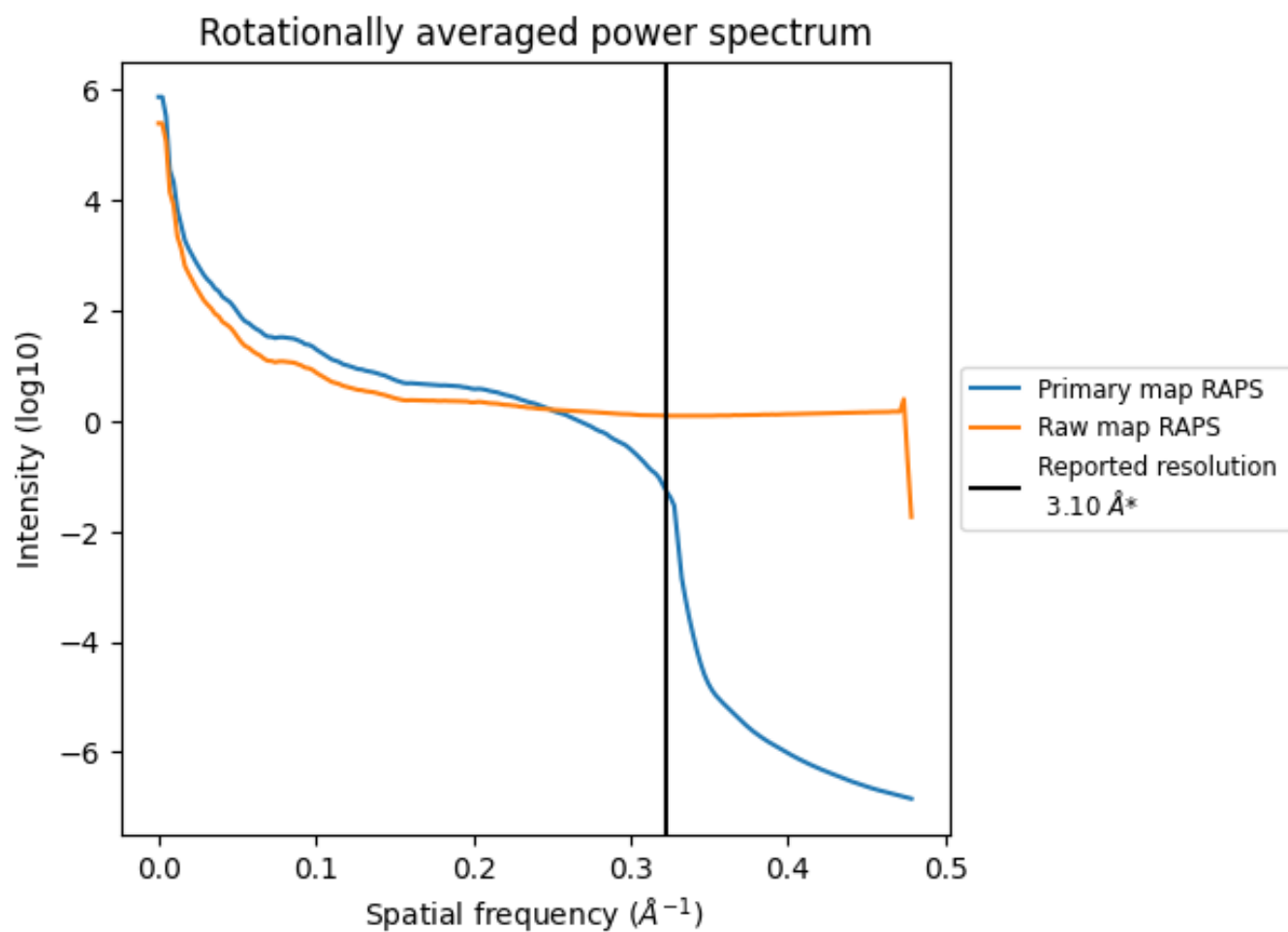
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2283 nm³; this corresponds to an approximate mass of 2062 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

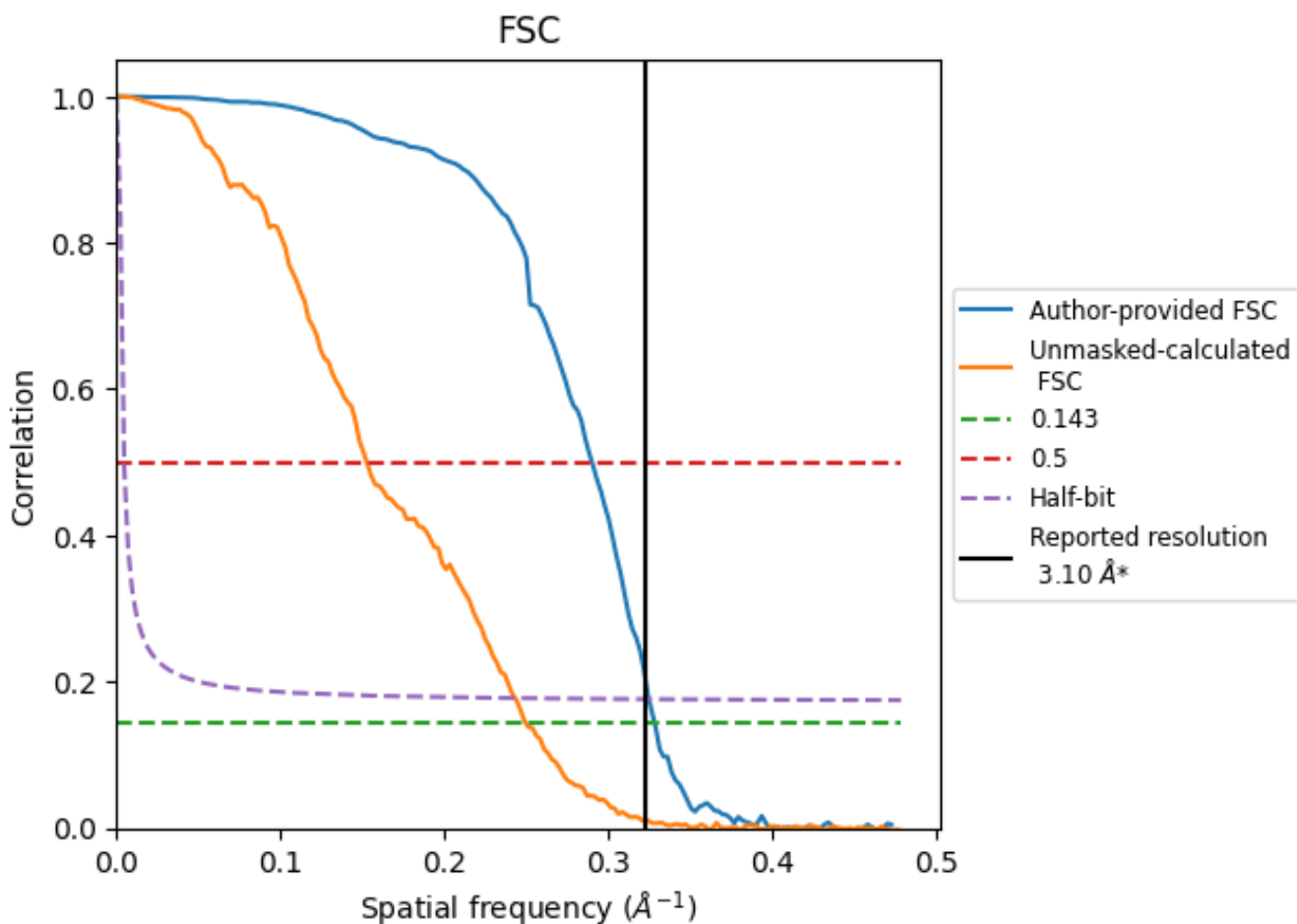


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

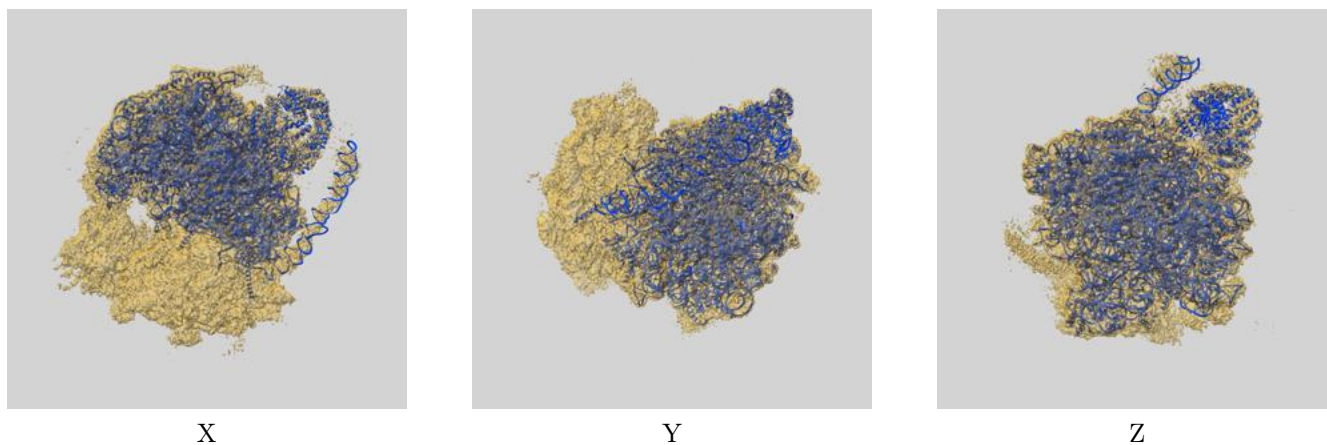
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.05	3.45	3.08
Unmasked-calculated*	4.00	6.55	4.11

*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 4.00 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

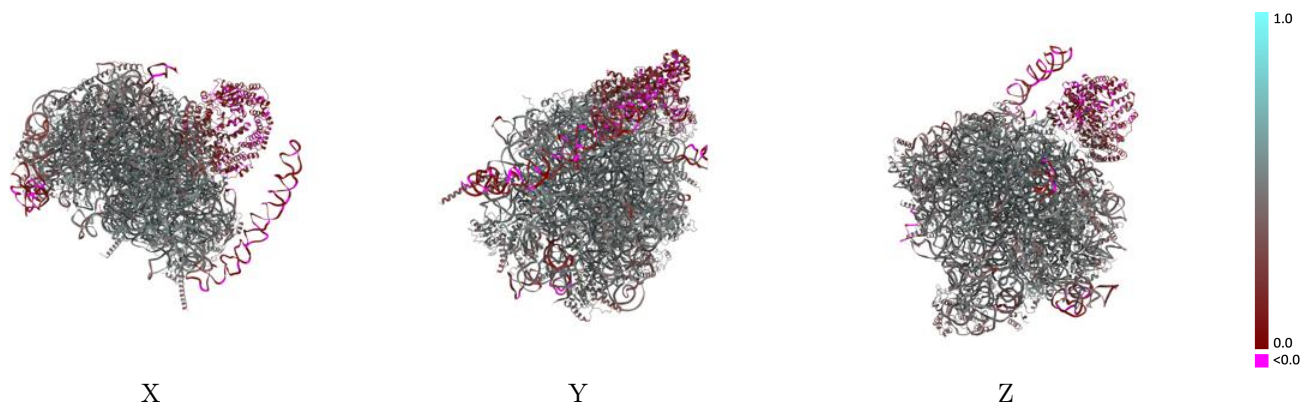
This section contains information regarding the fit between EMDB map EMD-16086 and PDB model 8BIP. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



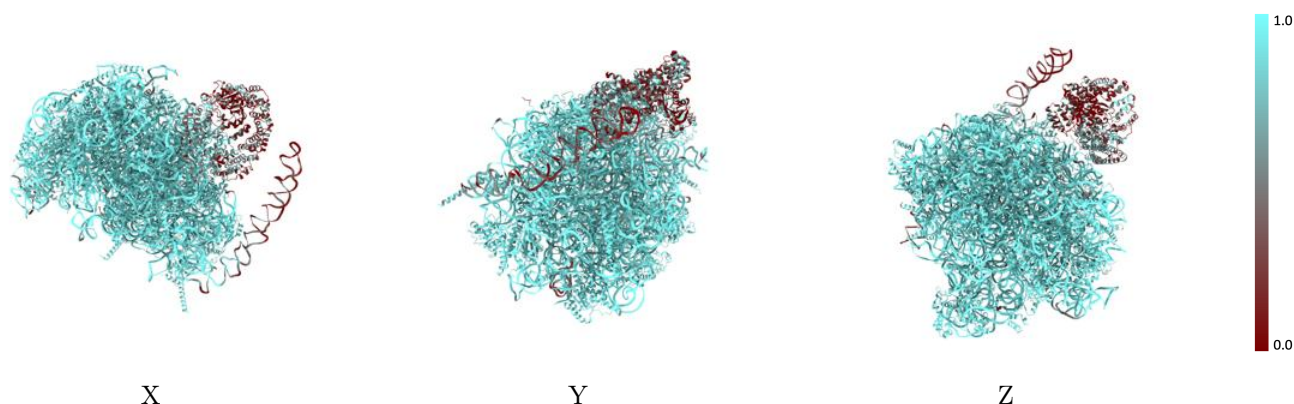
The images above show the 3D surface view of the map at the recommended contour level 0.215 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



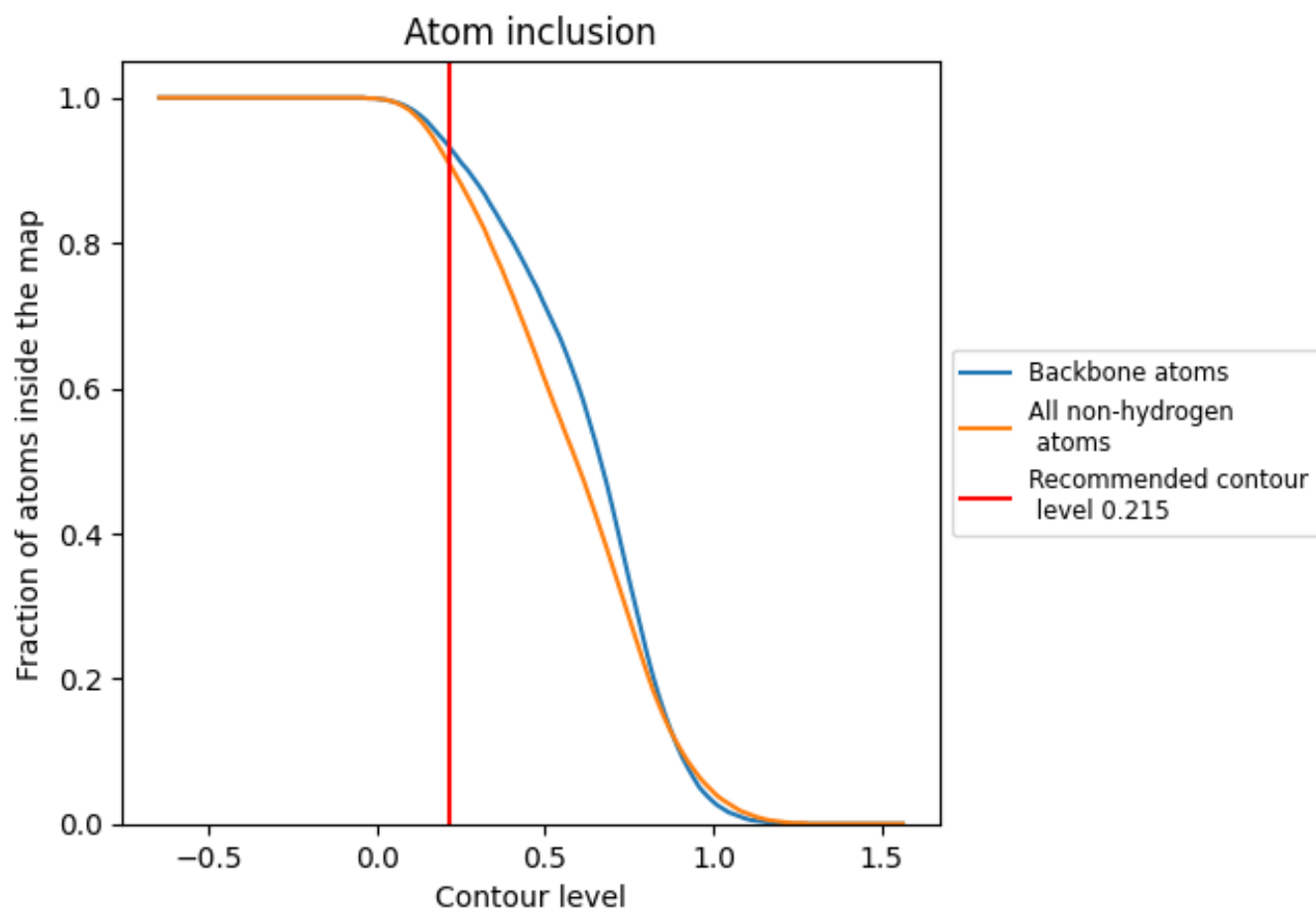
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.215).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% 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 (0.215) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.4510
1	 0.9540	 0.4550
8	 0.7220	 0.4130
A	 0.0550	 0.0950
B	 0.4360	 0.1860
C3	 0.9930	 0.4860
C4	 0.9980	 0.4740
LA	 0.9140	 0.5230
LB	 0.9420	 0.5050
LC	 0.9430	 0.5040
LD	 0.9270	 0.4260
LE	 0.9280	 0.4510
LF	 0.9450	 0.4930
LG	 0.9090	 0.4540
LH	 0.9280	 0.4700
LI	 0.9030	 0.4810
LJ	 0.8540	 0.4040
LL	 0.9380	 0.4750
LM	 0.9240	 0.4630
LN	 0.9430	 0.5170
LO	 0.9390	 0.4950
LP	 0.9040	 0.5080
LQ	 0.9530	 0.5080
LR	 0.9110	 0.4920
LS	 0.9250	 0.5000
LT	 0.9260	 0.5040
LU	 0.9010	 0.4630
LV	 0.8790	 0.5080
LW	 0.8850	 0.4970
LX	 0.9040	 0.5050
LY	 0.9440	 0.5030
LZ	 0.9390	 0.4740
La	 0.9540	 0.5110
Lb	 0.9140	 0.4700
Lc	 0.9320	 0.4800



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Chain	Atom inclusion	Q-score
Ld	 0.9170	 0.5130
Le	 0.9300	 0.5220
Lf	 0.9390	 0.5150
Lg	 0.9300	 0.5130
Lh	 0.9400	 0.4760
Li	 0.8920	 0.4520
Lj	 0.9740	 0.5340
Lk	 0.9130	 0.4740
Ll	 0.9420	 0.5140
Lm	 0.9080	 0.4920
Ln	 0.8410	 0.4580
Lo	 0.9340	 0.4970
Lp	 0.9060	 0.5050