



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2023 – 03:53 pm GMT

PDB ID : 8PV2
EMDB ID : EMD-17951
Title : Chaetomium thermophilum pre-60S State 10 - pre-5S rotation with Ytm1-Erb1
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on : 2023-07-17
Resolution : 2.63 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

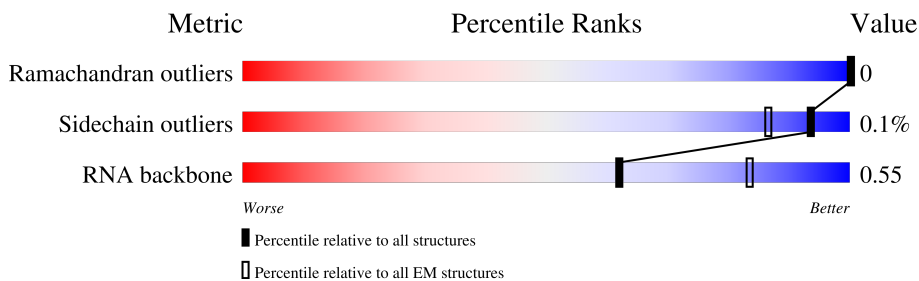
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.63 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.



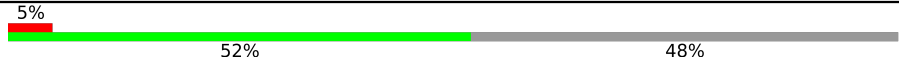
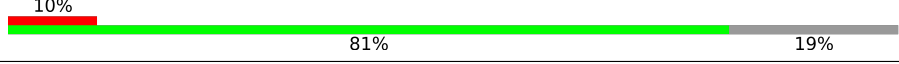
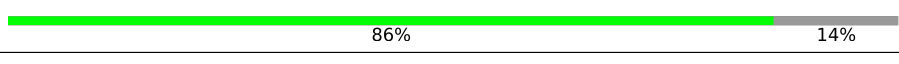


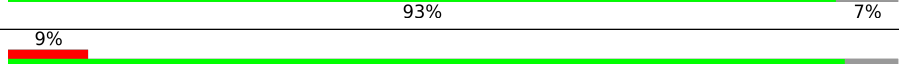
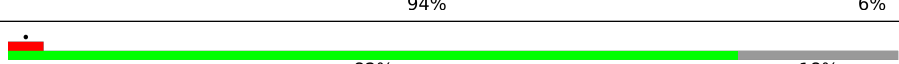
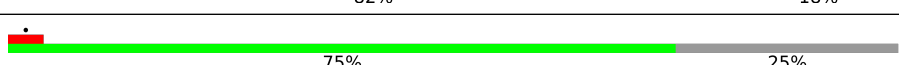
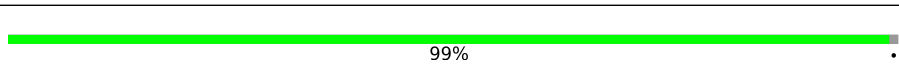
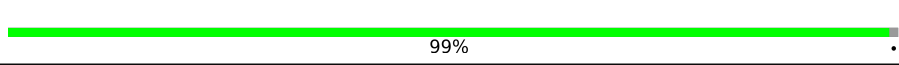
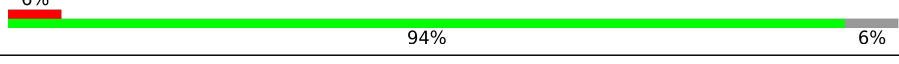
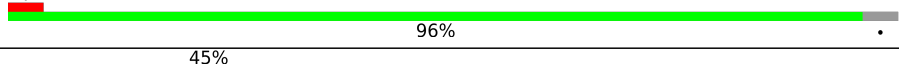
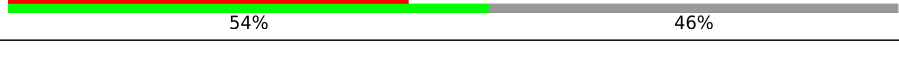
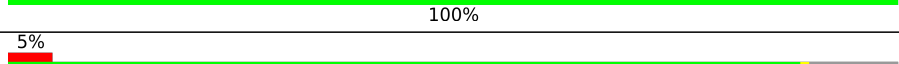
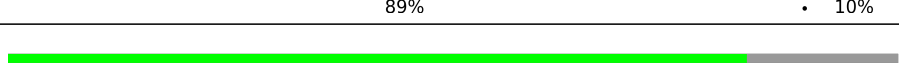
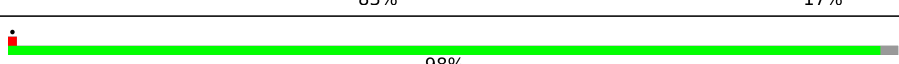
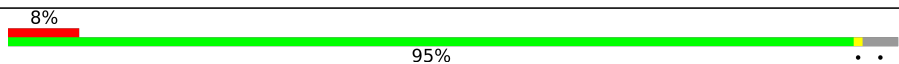
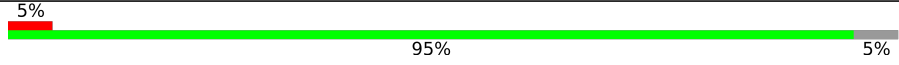
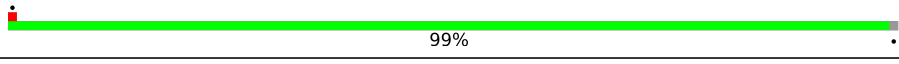
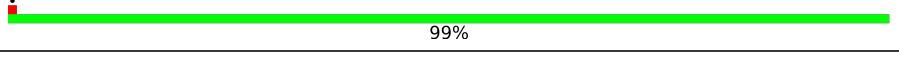
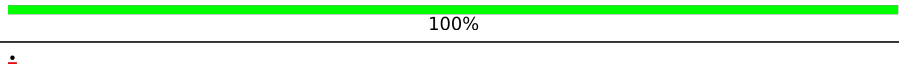
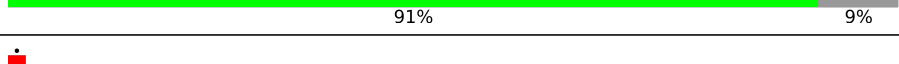



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	C1	3338	 8% 73% 17% 8%
2	C2	156	 85% 13%
3	C4	119	 8% 79% 20%
4	CF	270	 91% 9%
5	CH	661	 5% 95% 5%
6	CK	261	 91% 9%
7	CL	558	 14% 86%
8	CN	246	 100%

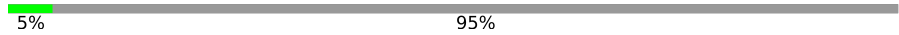
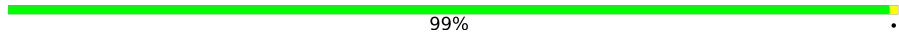


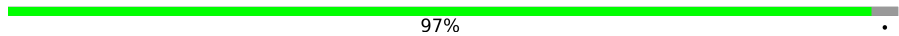

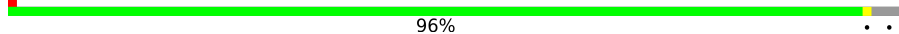
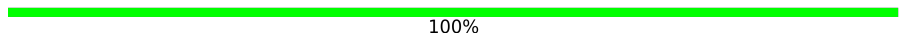



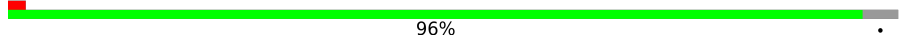




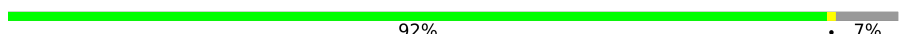

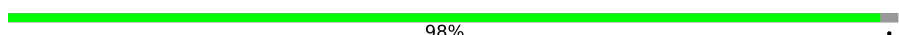
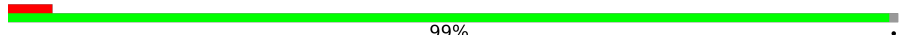
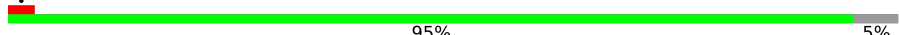



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Mol	Chain	Length	Quality of chain
9	CO	120	 5% 52% 48%
10	CQ	225	 10% 81% 19%
11	Cb	117	 86% 14%
12	Cd	627	 73% 26%
13	Cf	350	 81% 19%
14	Cg	202	 93% 7%
15	Ch	517	 9% 94% 6%
16	Cz	123	 82% 18%
17	LA	254	 75% 25%
18	LB	392	 99%
19	LC	365	 99%
20	LD	304	 6% 94% 6%
21	LE	200	 96%
22	CM	249	 45% 54% 46%
22	LF	249	 100%
23	LG	262	 5% 89% 10%
24	LH	229	 83% 17%
25	LJ	173	 98%
26	LK	165	 8% 95% 5%
27	LL	213	 5% 95% 5%
28	LM	142	 99%
29	LN	203	 99%
30	LO	204	 100%
31	LP	187	 91% 9%
32	LQ	213	 70% 30%

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Mol	Chain	Length	Quality of chain
33	LR	2898	 5% 95%
34	LS	174	 99%
35	LT	160	 11% 81% 19%
36	LU	127	 82% 17%
37	LV	139	 97%
38	LX	156	 78% 22%
39	LY	138	 96%
40	LZ	135	 100%
41	La	149	 72% 28%
42	Lc	108	 88% 12%
43	Ld	120	 92% 8%
44	Le	131	 96%
45	Lf	109	 99%
46	Lg	119	 8% 99%
47	Lh	935	 12% 88%
48	Li	110	 5% 92% 8%
49	Lj	95	 92% 7%
50	Lk	94	 81% 19%
51	Ll	51	 98%
52	Lp	92	 5% 99%
53	Lq	147	 95% 5%
54	CC	801	 6% 62% 38%
55	CD	495	 28% 91% 8%
56	CJ	679	 16% 72% 27%

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 155881 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 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C1	3056	65414	29219	11840	21299	3056	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	3338	C	-	insertion	GB XR_002966752

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C2	153	3259	1457	581	1068	153	0	0

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C4	119	2536	1131	453	833	119	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CF	245	1934	1215	350	360	9	0	0

- Molecule 5 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CH	627	5036	3167	914	936	19	0	0

- Molecule 6 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CK	237	1903	1198	368	333	4	0	0

- Molecule 7 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	CL	79	622	389	125	108		0	0

- Molecule 8 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	CN	246	1853	1156	322	368	7	0	0

- Molecule 9 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	CO	62	468	290	94	82	2	0	0

- Molecule 10 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	CQ	183	1480	925	304	241	10	0	0

- Molecule 11 is a protein called Zinc finger domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Cb	101	830	517	161	148	4	0	0

- Molecule 12 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Cd	462	3691	2350	671	659	11	0	0

- Molecule 13 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Cf	285	2282	1443	417	401	21	0	0

- Molecule 14 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Cg	188	1478	924	283	270	1	0	0

- Molecule 15 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Ch	485	3812	2396	696	710	10	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	117	ASP	GLU	insertion	UNP G0SC29

- Molecule 16 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Cz	101	869	541	180	144	4	0	0

- Molecule 17 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LA	191	1454	917	278	256	3	0	0

- Molecule 18 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	LB	389	3104	1973	579	539	13	0	0

- Molecule 19 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	LC	363	2751	1737	527	478	9	0	0

- Molecule 20 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	LD	286	2266	1434	407	422	3	0	0

- Molecule 21 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	LE	191	1477	944	267	263	3	0	0

- Molecule 22 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	LF	248	2023	1297	377	346	3	0	0
22	CM	134	685	414	137	134		0	0

- Molecule 23 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LG	235	1889	1210	350	324	5	0	0

- Molecule 24 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LH	190	1495	949	268	272	6	0	0

- Molecule 25 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LJ	169	1357	850	266	235	6	0	0

- Molecule 26 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LK	158	Total	C	N	O	S	0	0
			1184	743	215	224	2		

- Molecule 27 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LL	203	Total	C	N	O	S	0	0
			1587	989	325	271	2		

- Molecule 28 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LM	141	Total	C	N	O	S	0	0
			1126	714	216	195	1		

- Molecule 29 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LN	202	Total	C	N	O	S	0	0
			1704	1062	360	278	4		

- Molecule 30 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LO	203	Total	C	N	O	S	0	0
			1611	1034	305	267	5		

- Molecule 31 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LP	171	Total	C	N	O	S	0	0
			1343	834	274	232	3		

- Molecule 32 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LQ	150	Total	C	N	O	S	0	0
			1200	759	239	200	2		

- Molecule 33 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	LR	155	1241	772	262	203	4	0	0

- Molecule 34 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	LS	174	1426	917	266	238	5	0	0

- Molecule 35 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	LT	129	1027	651	195	179	2	0	0

- Molecule 36 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	LU	105	846	548	146	151	1	0	0

- Molecule 37 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	LV	135	991	630	184	170	7	0	0

- Molecule 38 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	LX	122	967	620	175	172	0	0

- Molecule 39 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	LY	133	1056	658	213	183	2	0	0

- Molecule 40 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	LZ	135	1112	713	207	188	4	0	0

- Molecule 41 is a protein called 60S ribosomal protein L28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	La	108	872	556	168	147	1	0	0

- Molecule 42 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Lc	95	705	449	122	129	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Ld	110	875	555	171	148	1	0	0

- Molecule 44 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Le	126	1017	640	208	163	6	0	0

- Molecule 45 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Lf	108	862	546	171	144	1	0	0

- Molecule 46 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Lg	118	914	567	186	157	4	0	0

- Molecule 47 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	Lh	115	Total	C	N	O	0	0
			951	605	189	157		

- Molecule 48 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Li	101	Total	C	N	O	S	0	0
			827	509	181	136	1		

- Molecule 49 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lj	88	Total	C	N	O	S	0	0
			698	427	154	112	5		

- Molecule 50 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lk	76	Total	C	N	O	S	0	0
			632	400	121	109	2		

- Molecule 51 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	Ll	50	Total	C	N	O	0	0
			436	275	97	64		

- Molecule 52 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lp	91	Total	C	N	O	S	0	0
			698	430	138	124	6		

- Molecule 53 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Lq	139	Total	C	N	O	0	0
			1073	672	213	188		

- Molecule 54 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	CC	499	3890	2492	697	691	10	0	0

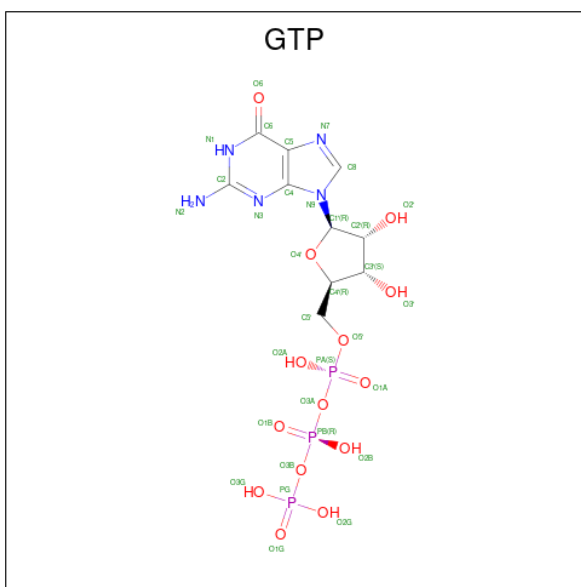
- Molecule 55 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	CD	453	3390	2126	598	660	6	0	0

- Molecule 56 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	CJ	493	3577	2274	659	633	11	0	0

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	CH	1	32	10	5	14	3	0
57	Cd	1	32	10	5	14	3	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

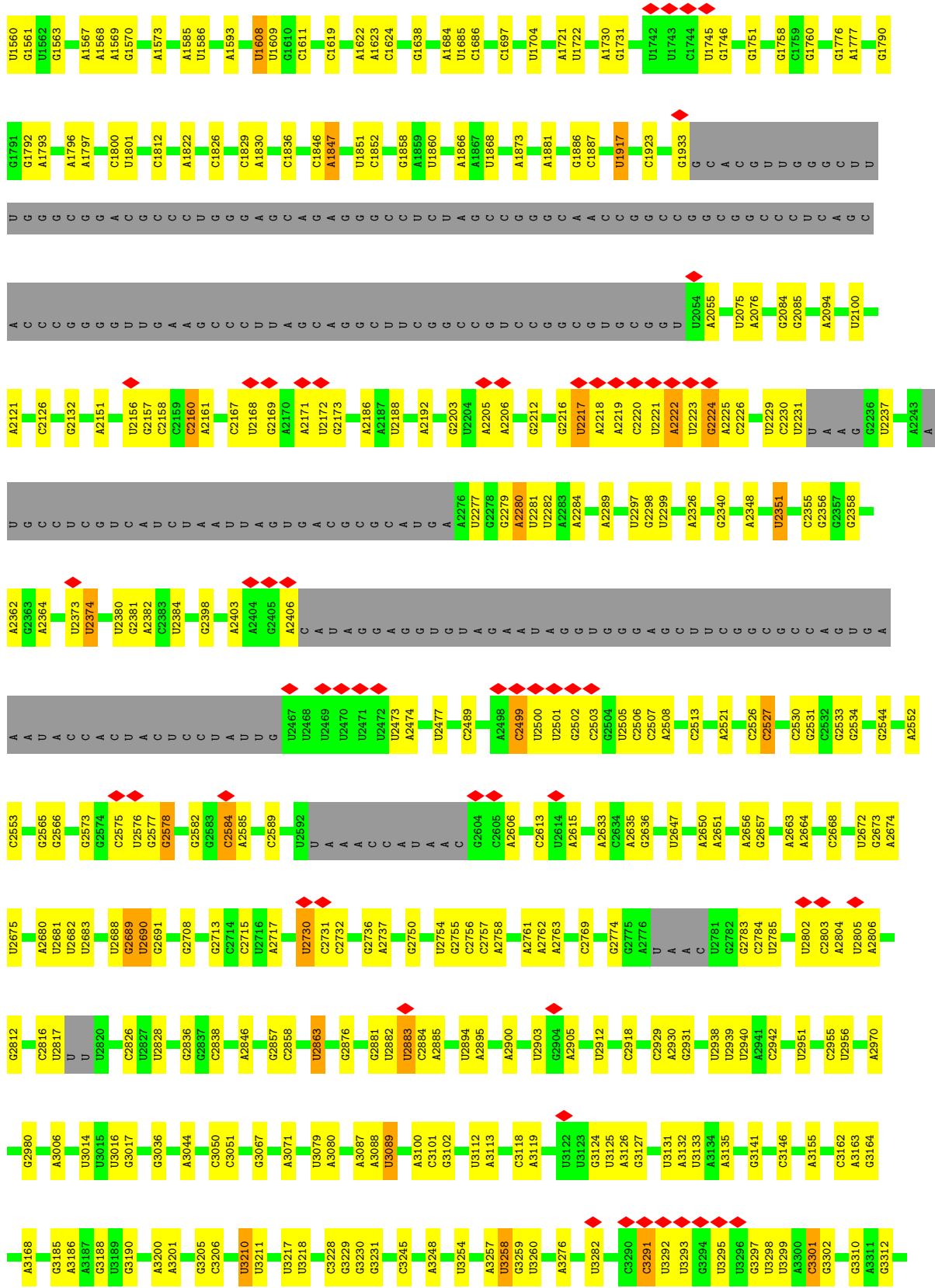
Mol	Chain	Residues	Atoms	AltConf
58	CH	1	Total Mg 1 1	0
58	Cd	2	Total Mg 2 2	0

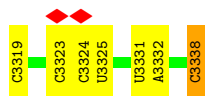
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
59	CQ	1	Total Zn 1 1	0
59	Cb	1	Total Zn 1 1	0
59	Lg	1	Total Zn 1 1	0
59	Lj	1	Total Zn 1 1	0
59	Lp	1	Total Zn 1 1	0

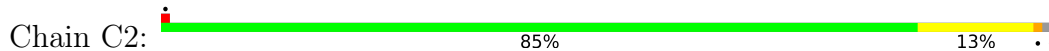
- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	CH	1	Total O 1 1	0
60	Cd	2	Total O 2 2	0

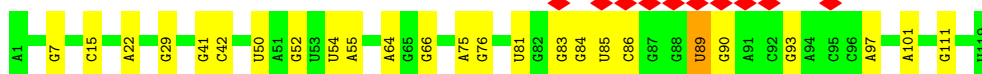
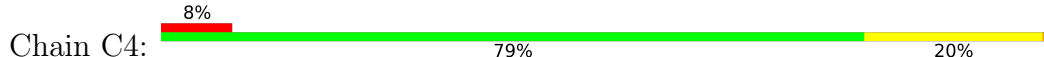




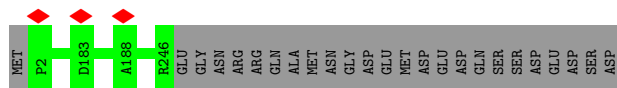
- Molecule 2: 5.8S rRNA



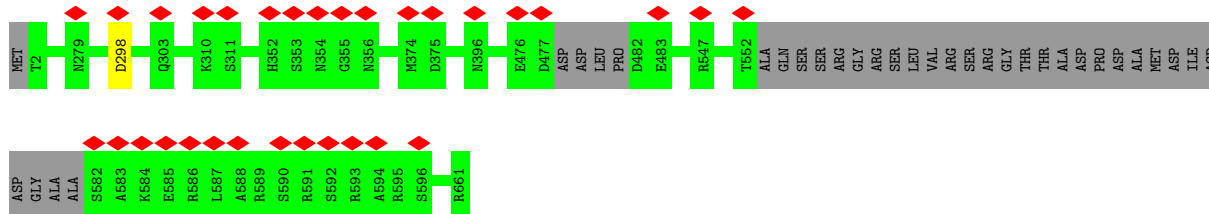
- Molecule 3: 5S rRNA



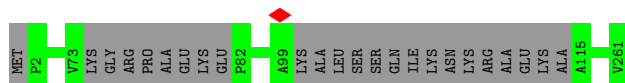
- Molecule 4: Large ribosomal subunit protein uL10



- Molecule 5: Nucleolar GTP-binding protein 1




- Molecule 6: Ribosome biogenesis protein NSA2 homolog

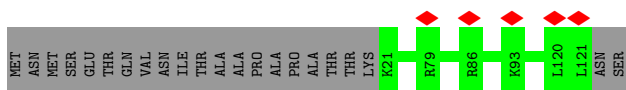


- Molecule 7: Putative GTP binding protein




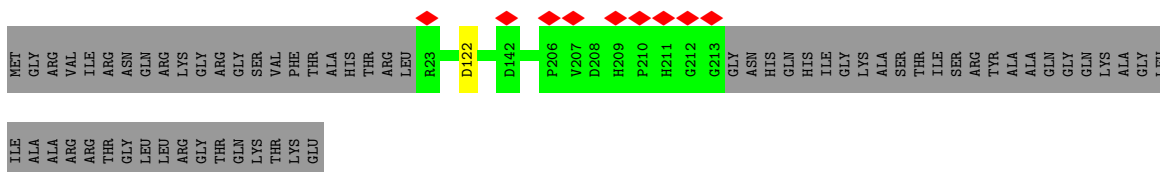
- Molecule 16: rRNA-processing protein

Chain Cz:  82% 18%



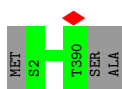
- Molecule 17: 60S ribosomal protein L2-like protein

Chain LA:  75% 25%



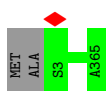
- Molecule 18: 60S ribosomal protein L3-like protein

Chain LB:  99%



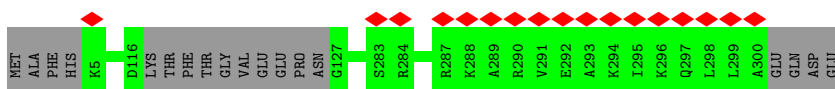
- Molecule 19: 60S ribosomal protein L4-like protein

Chain LC:  99%



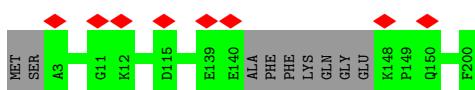
- Molecule 20: 60S ribosomal protein l5-like protein

Chain LD:  6% 94% 6%

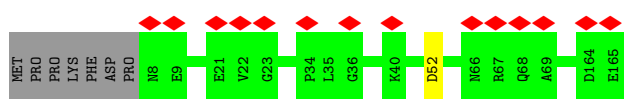


- Molecule 21: 60S ribosomal protein L6

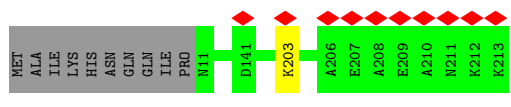
Chain LE:  96%



- Molecule 22: 60S ribosomal protein l7-like protein



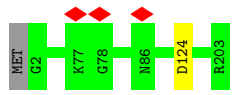
• Molecule 27: 60S ribosomal protein L13



• Molecule 28: 60S ribosomal protein L14-like protein



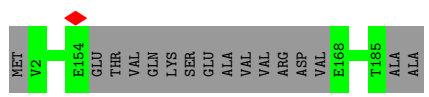
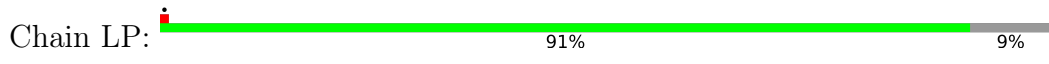
• Molecule 29: Ribosomal protein L15



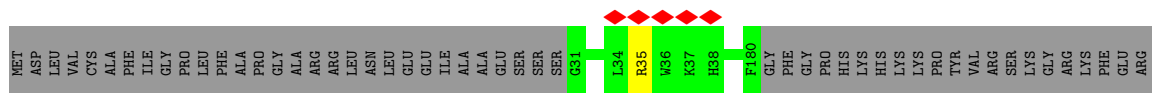
• Molecule 30: 60S ribosomal protein L16-like protein



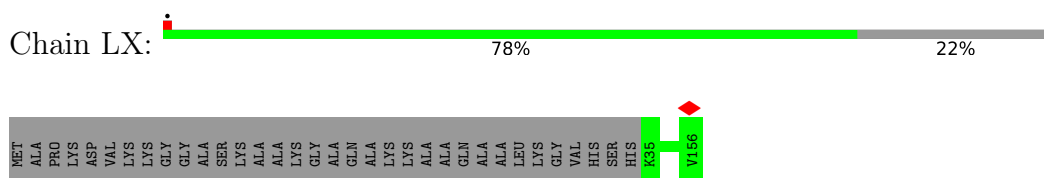
• Molecule 31: 60S ribosomal protein l17-like protein



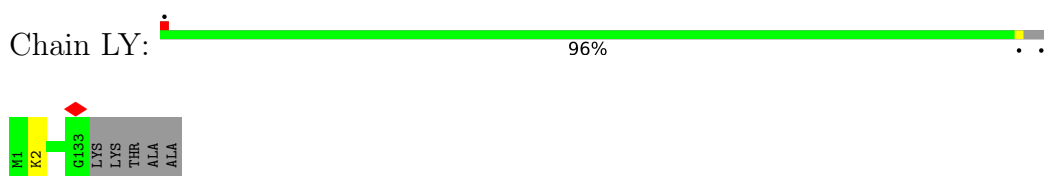
• Molecule 32: Ribosomal protein L18-like protein



- Molecule 38: 60S ribosomal protein L25-like protein



- Molecule 39: 60S ribosomal protein L26-like protein

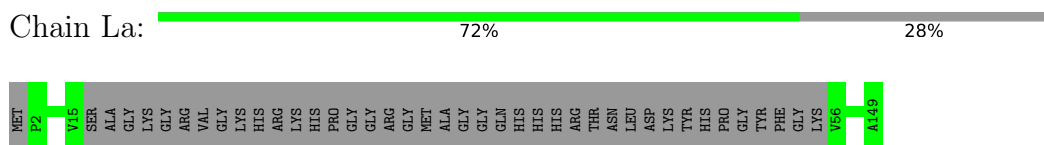


- Molecule 40: 60S ribosomal protein L27

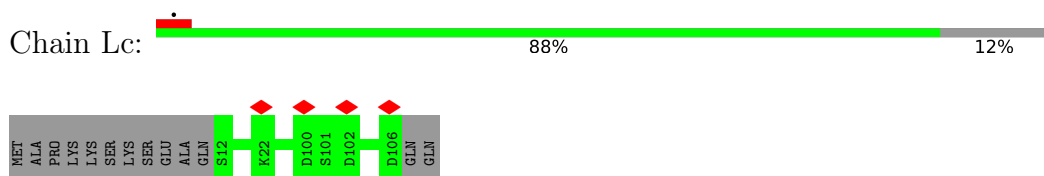


There are no outlier residues recorded for this chain.

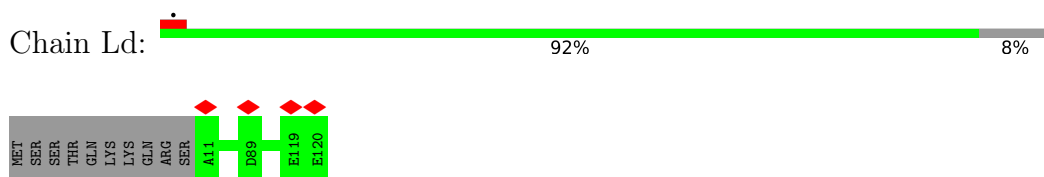
- Molecule 41: 60S ribosomal protein L28-like protein



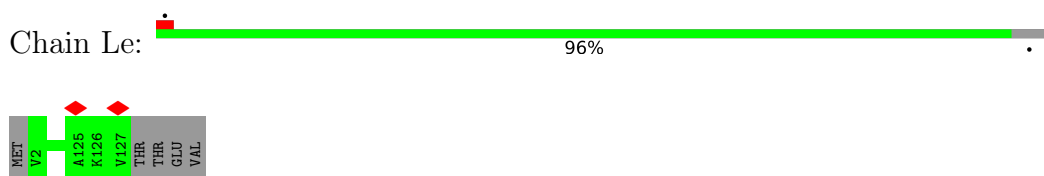
- Molecule 42: 60S ribosomal protein l30-like protein



- Molecule 43: Putative 60S ribosomal protein



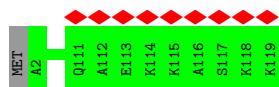
- Molecule 44: 60S ribosomal protein L32-like protein



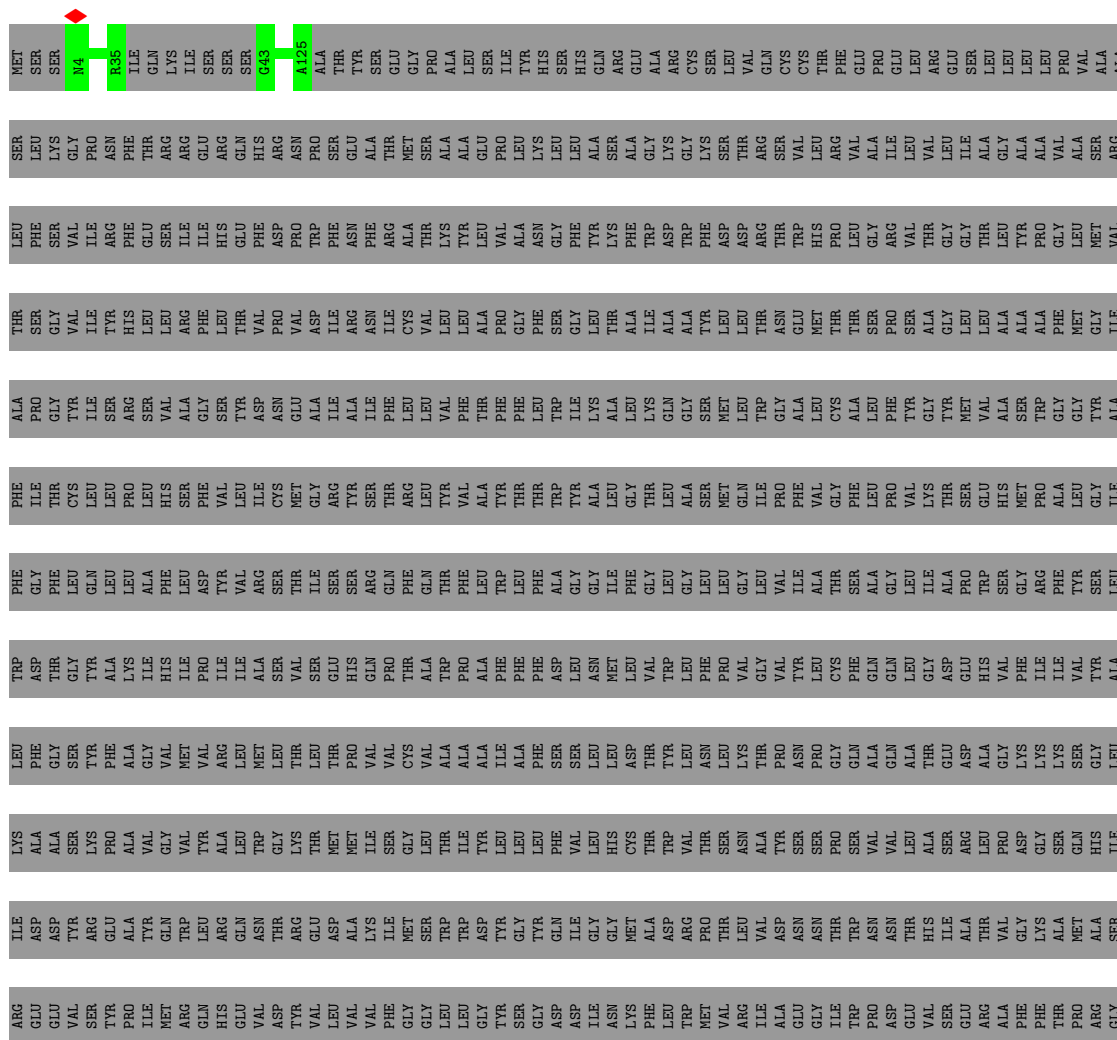
- Molecule 45: 60S ribosomal protein l33-like protein



- Molecule 46: Ribosomal protein l34-like protein



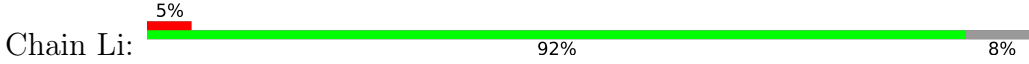
- Molecule 47: dolichyl-diphosphooligosaccharide--protein glycotransferase



GLU TYR ARG VAL ASP ALA ALA THR THR MET LYS ASN ASN SER LEU LEU MET TYR LYS MET TYR TYR ASN ASN ASN PHE LEU PHE PRO GLY ALA VAL THR VAL ARG MET ARG VAL ARG LEU PRO GLU VAL VAL GLY THR THR LEU ASN THR THR LEU GLU GLU ALA PHE THR SER SER GLU

ASN TRP ILE ILE ARG ILE THR LYS VAL ASP THR MET LYS ASN ASN LEU LEU ARG MET TYR HIS ALA SER ALA TYR ALA ALA TYR PHE GLU ARG HIS LYS LYS LYS LYS THR VAL THR LYS ARG MET ARG PRO VAL VAL LEU PRO ARG VAL VAL GLU

• Molecule 48: 60S ribosomal protein L36



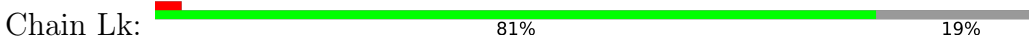
MET SER GLU ASP THR PRO LYS ALA P10 R101 E105 S106 R107 R108 A109 H110

• Molecule 49: Ribosomal protein L37



MET F2 K57 F89 ALA VAL SER SER SER

• Molecule 50: 60S ribosomal protein L38-like protein



MET F2 S22 LYS ILE LEU THR ILE ALA PHE PRO PRO PRO LEU THR ALA A23 D51 S52 S53 D67 R77 LYS SER SER ALA

• Molecule 51: Ribosomal protein eL39



MET P2 L51

• Molecule 52: 60S ribosomal protein L43-like protein



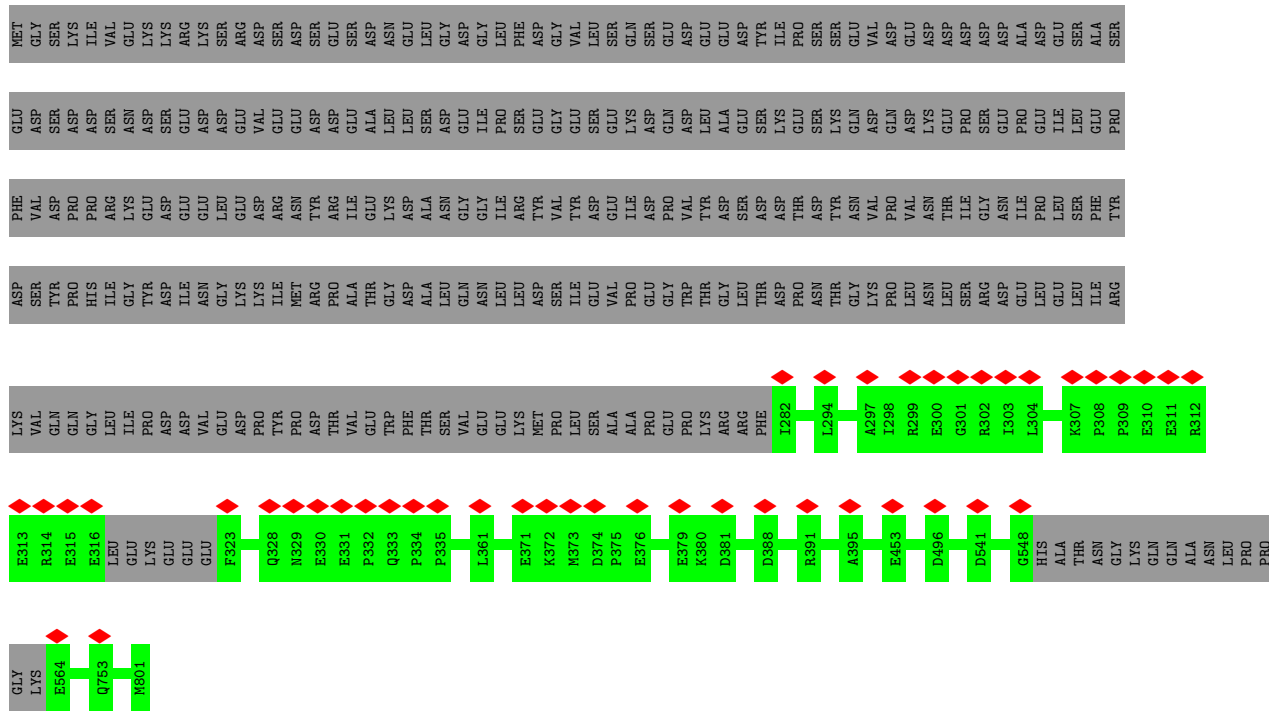
MET S2 R85 I89 T90 E91 A92

• Molecule 53: Putative 60S ribosomal protein

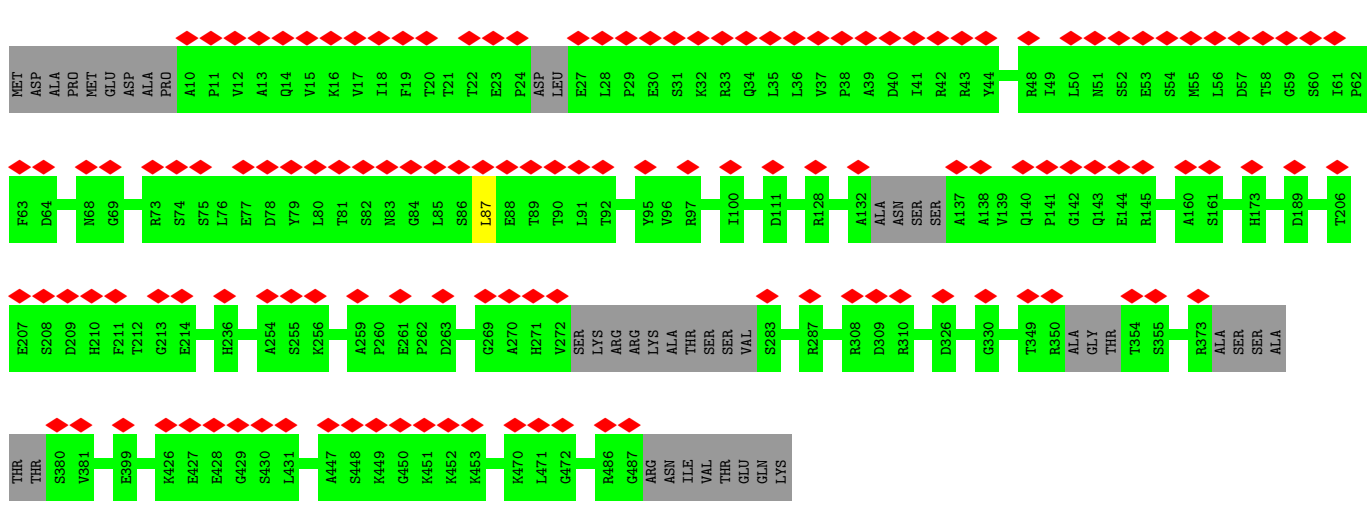
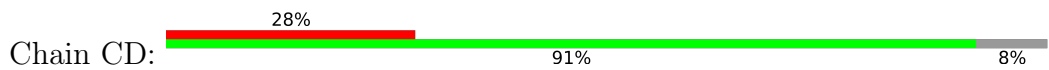


MET S2 E128 A136 A137 A138 R139 ALA ALA ALA ALA GLY LYS GLN

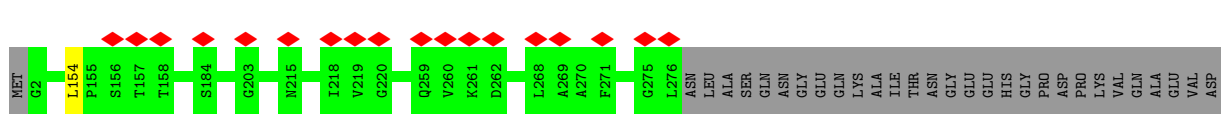
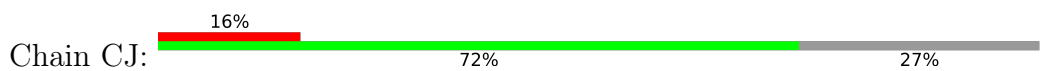
• Molecule 54: Ribosome biogenesis protein ERB1



• Molecule 55: Ribosome biogenesis protein YTM1



• Molecule 56: Pescadillo homolog



LYS	LEU	VAL	ALA	LYS	LEU	ARG	GLU	GLU	GLN	GLN	ALA	ASN	GLY	ASP	LYS	THR	ASP	GLU	LYS	GLY	GLU	ASN	GLU	GLY	ASP	LYS	PRO	SER	ASP	ALA	ILE	ASP	LYS	PHE	PRO	VAL	ALA	PRO	GLY	ASP	VAL	LEU	PRO	GLN	PRO	SER	TYR	SER	SER	SER	D362	P363	S364	Q365					
A368	R376	E377	T378	P379	R380	Q381	G391	C392	K393	A399	V400	L401	G402	E403	G404	A405	F406	T407	T408	D409	E410	S411	D412	P413	R414	I415	T416	D421	R422	P423	VAL	ILE	ARG	ALA	ALA	VAL	SER	GLU	ASP	GLY	ASP	GLY	GLN	GLU	ASP	ASN	GLN	THR	SER	GLN	LYS	LEU	ALA	PRO	ASN				
G448	R449	Y450	P451	G452	R453	I454	Y455	V456	Q457	V461	W462	I465	N466	D467	E468	E469	E474	G479	A480	Q481	L486	K491	P492	T493	Q494	G495	T500	E504	A515	E518	D519	A520	Q521	A522	GLN	GLN	GLU	GLY	SER	ASP	GLU	SER	GLY	SER	GLY	VAL	ASN												
ASP	MET	SER	VAL	ALA	LYS	SER	ASP	GLU	GLU	ASP	GLN	GLU	ASP	ASP	PHE	GLY	GLY	PHE	SER	ASP	GLU	ASP	GLU	GLU	GLN	GLN	SER	ASP	GLU	GLY	SER	GLU	GLU	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	E582	A583	T584	L585	E586	R587	Q588	R589	E590	L591	E592	A593	E594	LEU	ALA	GLY
LYS	ALA	VAL	SER	LYS	GLY	LYS	PRO	L606	D607	P608	K609	V610	K611	A612	E615	R622	E659	I670	E671	K672	E673	MET	ALA	ALA	LYS	LYS	ALA																																

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66943	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 ($e^-/\text{\AA}^2$)	45.6	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	8.046	Depositor
Minimum map value	0.000	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, OMG, ZN, A2M, OMC, GTP, 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	C1	0.51	0/72351	0.94	101/112799 (0.1%)
2	C2	0.53	0/3643	0.88	3/5672 (0.1%)
3	C4	0.48	0/2833	0.99	6/4414 (0.1%)
4	CF	0.29	0/1972	0.56	0/2660
5	CH	0.30	0/5120	0.56	1/6895 (0.0%)
6	CK	0.32	0/1939	0.55	0/2608
7	CL	0.27	0/631	0.56	0/843
8	CN	0.30	0/1878	0.59	0/2555
9	CO	0.29	0/470	0.57	0/619
10	CQ	0.31	0/1504	0.61	0/2000
11	Cb	0.30	0/845	0.61	0/1128
12	Cd	0.30	0/3770	0.55	1/5082 (0.0%)
13	Cf	0.31	0/2326	0.57	0/3113
14	Cg	0.28	0/1508	0.54	0/2051
15	Ch	0.32	0/3914	0.59	0/5319
16	Cz	0.27	0/877	0.54	0/1148
17	LA	0.32	0/1488	0.59	1/2009 (0.0%)
18	LB	0.33	0/3172	0.57	0/4260
19	LC	0.30	0/2808	0.53	0/3785
20	LD	0.34	0/2308	0.53	0/3105
21	LE	0.30	0/1504	0.53	0/2027
22	CM	0.24	0/692	0.41	0/966
22	LF	0.33	0/2061	0.56	0/2765
23	LG	0.31	0/1918	0.54	0/2565
24	LH	0.31	0/1515	0.55	1/2037 (0.0%)
25	LJ	0.29	0/1379	0.60	0/1844
26	LK	0.29	0/1198	0.59	1/1611 (0.1%)
27	LL	0.28	0/1614	0.58	0/2168
28	LM	0.33	0/1145	0.56	0/1539
29	LN	0.32	0/1741	0.62	1/2332 (0.0%)
30	LO	0.34	0/1645	0.56	0/2205
31	LP	0.32	0/1364	0.59	0/1835

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LQ	0.28	0/1218	0.58	0/1639
33	LR	0.30	0/1260	0.57	0/1683
34	LS	0.32	0/1461	0.56	0/1966
35	LT	0.31	0/1046	0.56	0/1409
36	LU	0.31	0/859	0.56	1/1151 (0.1%)
37	LV	0.31	0/1009	0.55	0/1357
38	LX	0.30	0/983	0.55	0/1327
39	LY	0.29	0/1070	0.61	0/1432
40	LZ	0.36	0/1135	0.60	0/1519
41	La	0.29	0/892	0.52	0/1200
42	Lc	0.32	0/714	0.55	0/960
43	Ld	0.30	0/889	0.58	0/1192
44	Le	0.29	0/1035	0.57	0/1379
45	Lf	0.33	0/883	0.59	0/1187
46	Lg	0.33	0/927	0.61	0/1244
47	Lh	0.28	0/961	0.54	0/1277
48	Li	0.28	0/834	0.64	0/1099
49	Lj	0.33	0/712	0.65	0/944
50	Lk	0.34	0/640	0.62	0/850
51	Ll	0.28	0/446	0.58	0/593
52	Lp	0.33	0/706	0.64	0/940
53	Lq	0.31	0/1091	0.57	0/1468
54	CC	0.29	0/4005	0.55	0/5466
55	CD	0.26	0/3464	0.57	1/4720 (0.0%)
56	CJ	0.29	0/3651	0.53	1/4951 (0.0%)
All	All	0.42	0/165024	0.78	119/238912 (0.0%)

There are no bond length outliers.

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1538	U	N3-C2-O2	-9.48	115.56	122.20
1	C1	1179	C	N1-C2-O2	9.48	124.59	118.90
1	C1	1538	U	N1-C2-O2	9.41	129.39	122.80
1	C1	1478	U	C2-N1-C1'	9.20	128.74	117.70
1	C1	1179	C	C2-N1-C1'	9.20	128.92	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CF	243/270 (90%)	241 (99%)	2 (1%)	0	100	100
5	CH	621/661 (94%)	612 (99%)	9 (1%)	0	100	100
6	CK	231/261 (88%)	225 (97%)	6 (3%)	0	100	100
7	CL	77/558 (14%)	77 (100%)	0	0	100	100
8	CN	244/246 (99%)	238 (98%)	6 (2%)	0	100	100
9	CO	56/120 (47%)	56 (100%)	0	0	100	100
10	CQ	181/225 (80%)	180 (99%)	1 (1%)	0	100	100
11	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100
12	Cd	458/627 (73%)	449 (98%)	9 (2%)	0	100	100
13	Cf	281/350 (80%)	279 (99%)	2 (1%)	0	100	100
14	Cg	186/202 (92%)	184 (99%)	2 (1%)	0	100	100
15	Ch	484/517 (94%)	469 (97%)	15 (3%)	0	100	100
16	Cz	99/123 (80%)	98 (99%)	1 (1%)	0	100	100
17	LA	189/254 (74%)	186 (98%)	3 (2%)	0	100	100
18	LB	387/392 (99%)	380 (98%)	7 (2%)	0	100	100
19	LC	361/365 (99%)	355 (98%)	6 (2%)	0	100	100
20	LD	282/304 (93%)	280 (99%)	2 (1%)	0	100	100
21	LE	187/200 (94%)	183 (98%)	4 (2%)	0	100	100
22	CM	130/249 (52%)	126 (97%)	4 (3%)	0	100	100
22	LF	246/249 (99%)	241 (98%)	5 (2%)	0	100	100
23	LG	233/262 (89%)	230 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	LH	188/229 (82%)	185 (98%)	3 (2%)	0	100	100
25	LJ	167/173 (96%)	166 (99%)	1 (1%)	0	100	100
26	LK	156/165 (94%)	153 (98%)	3 (2%)	0	100	100
27	LL	201/213 (94%)	200 (100%)	1 (0%)	0	100	100
28	LM	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
29	LN	200/203 (98%)	194 (97%)	6 (3%)	0	100	100
30	LO	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
31	LP	167/187 (89%)	164 (98%)	3 (2%)	0	100	100
32	LQ	148/213 (70%)	145 (98%)	3 (2%)	0	100	100
33	LR	153/2898 (5%)	152 (99%)	1 (1%)	0	100	100
34	LS	172/174 (99%)	169 (98%)	3 (2%)	0	100	100
35	LT	127/160 (79%)	124 (98%)	3 (2%)	0	100	100
36	LU	103/127 (81%)	100 (97%)	3 (3%)	0	100	100
37	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
38	LX	120/156 (77%)	119 (99%)	1 (1%)	0	100	100
39	LY	131/138 (95%)	125 (95%)	6 (5%)	0	100	100
40	LZ	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
41	La	104/149 (70%)	104 (100%)	0	0	100	100
42	Lc	93/108 (86%)	93 (100%)	0	0	100	100
43	Ld	108/120 (90%)	107 (99%)	1 (1%)	0	100	100
44	Le	124/131 (95%)	123 (99%)	1 (1%)	0	100	100
45	Lf	106/109 (97%)	106 (100%)	0	0	100	100
46	Lg	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
47	Lh	111/935 (12%)	110 (99%)	1 (1%)	0	100	100
48	Li	99/110 (90%)	99 (100%)	0	0	100	100
49	Lj	86/95 (90%)	84 (98%)	2 (2%)	0	100	100
50	Lk	74/94 (79%)	71 (96%)	3 (4%)	0	100	100
51	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
52	Lp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
53	Lq	137/147 (93%)	133 (97%)	4 (3%)	0	100	100
54	CC	493/801 (62%)	481 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	CD	441/495 (89%)	430 (98%)	11 (2%)	0	100	100
56	CJ	483/679 (71%)	471 (98%)	12 (2%)	0	100	100
All	All	10626/16443 (65%)	10439 (98%)	187 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	CF	212/236 (90%)	212 (100%)	0	100	100
5	CH	543/575 (94%)	543 (100%)	0	100	100
6	CK	206/225 (92%)	206 (100%)	0	100	100
7	CL	61/458 (13%)	61 (100%)	0	100	100
8	CN	205/206 (100%)	205 (100%)	0	100	100
9	CO	48/99 (48%)	48 (100%)	0	100	100
10	CQ	144/192 (75%)	144 (100%)	0	100	100
11	Cb	85/101 (84%)	85 (100%)	0	100	100
12	Cd	403/541 (74%)	402 (100%)	1 (0%)	93	97
13	Cf	250/310 (81%)	250 (100%)	0	100	100
14	Cg	158/176 (90%)	158 (100%)	0	100	100
15	Ch	408/436 (94%)	408 (100%)	0	100	100
16	Cz	89/107 (83%)	89 (100%)	0	100	100
17	LA	150/198 (76%)	150 (100%)	0	100	100
18	LB	329/331 (99%)	329 (100%)	0	100	100
19	LC	282/285 (99%)	282 (100%)	0	100	100
20	LD	221/253 (87%)	221 (100%)	0	100	100
21	LE	157/166 (95%)	157 (100%)	0	100	100
22	CM	10/215 (5%)	10 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	LF	213/215 (99%)	213 (100%)	0	100	100
23	LG	200/222 (90%)	198 (99%)	2 (1%)	76	86
24	LH	167/200 (84%)	167 (100%)	0	100	100
25	LJ	140/150 (93%)	140 (100%)	0	100	100
26	LK	127/136 (93%)	127 (100%)	0	100	100
27	LL	158/176 (90%)	157 (99%)	1 (1%)	86	93
28	LM	116/117 (99%)	116 (100%)	0	100	100
29	LN	179/180 (99%)	179 (100%)	0	100	100
30	LO	162/163 (99%)	162 (100%)	0	100	100
31	LP	133/152 (88%)	133 (100%)	0	100	100
32	LQ	128/178 (72%)	127 (99%)	1 (1%)	81	89
33	LR	125/2396 (5%)	125 (100%)	0	100	100
34	LS	152/154 (99%)	151 (99%)	1 (1%)	84	91
35	LT	110/135 (82%)	110 (100%)	0	100	100
36	LU	92/108 (85%)	92 (100%)	0	100	100
37	LV	98/102 (96%)	98 (100%)	0	100	100
38	LX	107/129 (83%)	107 (100%)	0	100	100
39	LY	116/119 (98%)	115 (99%)	1 (1%)	78	88
40	LZ	121/121 (100%)	121 (100%)	0	100	100
41	La	93/122 (76%)	93 (100%)	0	100	100
42	Lc	76/88 (86%)	76 (100%)	0	100	100
43	Ld	90/105 (86%)	90 (100%)	0	100	100
44	Le	109/114 (96%)	109 (100%)	0	100	100
45	Lf	89/90 (99%)	89 (100%)	0	100	100
46	Lg	95/102 (93%)	95 (100%)	0	100	100
47	Lh	102/781 (13%)	102 (100%)	0	100	100
48	Li	85/93 (91%)	85 (100%)	0	100	100
49	Lj	72/78 (92%)	71 (99%)	1 (1%)	67	80
50	Lk	73/88 (83%)	73 (100%)	0	100	100
51	Ll	45/46 (98%)	45 (100%)	0	100	100
52	Lp	73/74 (99%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	Lq	109/112 (97%)	109 (100%)	0	100	100
54	CC	408/710 (58%)	408 (100%)	0	100	100
55	CD	365/410 (89%)	365 (100%)	0	100	100
56	CJ	301/579 (52%)	301 (100%)	0	100	100
All	All	8790/13855 (63%)	8782 (100%)	8 (0%)	93	97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	Lj	57	LYS
39	LY	2	LYS
32	LQ	35	ARG
27	LL	203	LYS
34	LS	115	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
23	LG	62	GLN
23	LG	158	ASN
31	LP	75	GLN
25	LJ	166	GLN
23	LG	36	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	3046/3338 (91%)	554 (18%)	24 (0%)
2	C2	151/156 (96%)	20 (13%)	0
3	C4	118/119 (99%)	22 (18%)	0
All	All	3315/3613 (91%)	596 (17%)	24 (0%)

5 of 596 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	6	G
1	C1	27	A
1	C1	50	A

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Mol	Chain	Res	Type
1	C1	60	G
1	C1	61	A

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	2883	U
1	C1	3205	G
1	C1	3132	A
1	C1	3210	U
1	C1	1267	C

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

34 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	C1	1433	1	18,26,27	1.21	2 (11%)	19,38,41	0.80	1 (5%)
1	OMG	C1	2774	1	18,26,27	1.21	2 (11%)	19,38,41	0.89	1 (5%)
1	OMU	C1	2277	1	19,22,23	3.02	6 (31%)	26,31,34	1.66	4 (15%)
1	A2M	C1	1847	1	18,25,26	4.33	8 (44%)	18,36,39	4.00	4 (22%)
1	OMG	C1	2358	1	18,26,27	1.25	2 (11%)	19,38,41	0.91	1 (5%)
1	OMU	C1	2690	1	19,22,23	2.93	7 (36%)	26,31,34	1.73	5 (19%)
1	OMU	C1	2384	1	19,22,23	3.05	6 (31%)	26,31,34	1.72	5 (19%)
1	A2M	C1	1223	1	18,25,26	4.30	8 (44%)	18,36,39	3.86	5 (27%)
1	OMG	C1	787	1	18,26,27	1.21	3 (16%)	19,38,41	0.90	1 (5%)
1	OMC	C1	1812	1	19,22,23	0.64	0	26,31,34	1.45	2 (7%)
1	A2M	C1	848	1	18,25,26	4.32	9 (50%)	18,36,39	3.76	4 (22%)
1	OMU	C1	1868	1	19,22,23	3.00	6 (31%)	26,31,34	1.81	5 (19%)
1	A2M	C1	389	1	18,25,26	4.32	7 (38%)	18,36,39	3.97	4 (22%)
1	OMG	C1	2876	1	18,26,27	1.24	2 (11%)	19,38,41	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	C1	2289	1	18,25,26	4.39	7 (38%)	18,36,39	3.80	4 (22%)
1	OMG	C1	385	1	18,26,27	1.19	2 (11%)	19,38,41	0.83	1 (5%)
1	OMC	C1	1836	1	19,22,23	0.66	0	26,31,34	0.77	1 (3%)
1	A2M	C1	1432	1	18,25,26	4.32	8 (44%)	18,36,39	3.90	4 (22%)
1	OMU	C1	2688	1	19,22,23	3.01	6 (31%)	26,31,34	1.68	5 (19%)
1	OMC	C1	778	1	19,22,23	0.60	0	26,31,34	0.90	1 (3%)
1	A2M	C1	858	1	18,25,26	4.39	8 (44%)	18,36,39	4.05	4 (22%)
1	OMC	C1	1491	1	19,22,23	0.68	0	26,31,34	0.72	0
1	OMC	C1	2300	1	19,22,23	0.63	0	26,31,34	0.79	0
1	OMU	C1	2683	1	19,22,23	2.99	6 (31%)	26,31,34	1.69	4 (15%)
1	A2M	C1	637	1	18,25,26	4.29	7 (38%)	18,36,39	3.90	4 (22%)
1	OMU	C1	1917	1	19,22,23	3.00	6 (31%)	26,31,34	1.73	5 (19%)
1	OMG	C1	2578	1	18,26,27	1.19	2 (11%)	19,38,41	0.91	1 (5%)
1	OMG	C1	627	1	18,26,27	1.24	3 (16%)	19,38,41	0.91	1 (5%)
1	OMU	C1	2380	1	19,22,23	3.00	6 (31%)	26,31,34	1.66	4 (15%)
1	OMC	C1	1420	1	19,22,23	0.71	0	26,31,34	1.32	2 (7%)
1	OMC	C1	2838	1	19,22,23	0.76	1 (5%)	26,31,34	1.50	4 (15%)
1	OMG	C1	646	1	18,26,27	1.26	3 (16%)	19,38,41	0.88	1 (5%)
1	OMG	C1	2881	1	18,26,27	1.13	2 (11%)	19,38,41	0.85	1 (5%)
1	OMC	C1	2918	1	19,22,23	0.63	0	26,31,34	0.86	1 (3%)

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
1	OMG	C1	1433	1	-	2/5/27/28	0/3/3/3
1	OMG	C1	2774	1	-	0/5/27/28	0/3/3/3
1	OMU	C1	2277	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	1847	1	-	3/5/27/28	0/3/3/3
1	OMG	C1	2358	1	-	0/5/27/28	0/3/3/3
1	OMU	C1	2690	1	-	2/9/27/28	0/2/2/2
1	OMU	C1	2384	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	1223	1	-	1/5/27/28	0/3/3/3
1	OMG	C1	787	1	-	2/5/27/28	0/3/3/3
1	OMC	C1	1812	1	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	C1	848	1	-	1/5/27/28	0/3/3/3
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	389	1	-	3/5/27/28	0/3/3/3
1	OMG	C1	2876	1	-	0/5/27/28	0/3/3/3
1	A2M	C1	2289	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	385	1	-	0/5/27/28	0/3/3/3
1	OMC	C1	1836	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	1432	1	-	0/5/27/28	0/3/3/3
1	OMU	C1	2688	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	778	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	858	1	-	0/5/27/28	0/3/3/3
1	OMC	C1	1491	1	-	1/9/27/28	0/2/2/2
1	OMC	C1	2300	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2683	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	637	1	-	1/5/27/28	0/3/3/3
1	OMU	C1	1917	1	-	2/9/27/28	0/2/2/2
1	OMG	C1	2578	1	-	3/5/27/28	0/3/3/3
1	OMG	C1	627	1	-	0/5/27/28	0/3/3/3
1	OMU	C1	2380	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1420	1	-	4/9/27/28	0/2/2/2
1	OMC	C1	2838	1	-	2/9/27/28	0/2/2/2
1	OMG	C1	646	1	-	0/5/27/28	0/3/3/3
1	OMG	C1	2881	1	-	0/5/27/28	0/3/3/3
1	OMC	C1	2918	1	-	0/9/27/28	0/2/2/2

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2289	A2M	C3'-C2'	-12.98	1.24	1.52
1	C1	858	A2M	C3'-C2'	-12.96	1.24	1.52
1	C1	848	A2M	C3'-C2'	-12.70	1.24	1.52
1	C1	637	A2M	C3'-C2'	-12.69	1.24	1.52
1	C1	1223	A2M	C3'-C2'	-12.69	1.24	1.52

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1432	A2M	C1'-N9-C4	10.85	145.70	126.64
1	C1	1847	A2M	C1'-N9-C4	10.72	145.47	126.64
1	C1	858	A2M	C1'-N9-C4	10.47	145.03	126.64
1	C1	637	A2M	C1'-N9-C4	10.46	145.03	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	389	A2M	C1'-N9-C4	10.42	144.95	126.64

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C1	389	A2M	O4'-C4'-C5'-O5'
1	C1	389	A2M	C1'-C2'-O2'-CM'
1	C1	637	A2M	C1'-C2'-O2'-CM'
1	C1	1433	OMG	O4'-C4'-C5'-O5'
1	C1	1433	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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
57	GTP	Cd	1000	58	26,34,34	1.23	1 (3%)	32,54,54	1.51	5 (15%)
57	GTP	CH	701	58	26,34,34	1.18	1 (3%)	32,54,54	1.58	7 (21%)

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
57	GTP	Cd	1000	58	-	1/18/38/38	0/3/3/3
57	GTP	CH	701	58	-	7/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	Cd	1000	GTP	C5-C6	-4.31	1.38	1.47
57	CH	701	GTP	C5-C6	-4.20	1.38	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	Cd	1000	GTP	PB-O3B-PG	-4.05	118.92	132.83
57	CH	701	GTP	PB-O3B-PG	-3.53	120.71	132.83
57	CH	701	GTP	PA-O3A-PB	-3.34	121.38	132.83
57	CH	701	GTP	C5-C6-N1	3.24	119.67	113.95
57	Cd	1000	GTP	C5-C6-N1	3.14	119.50	113.95

There are no chirality outliers.

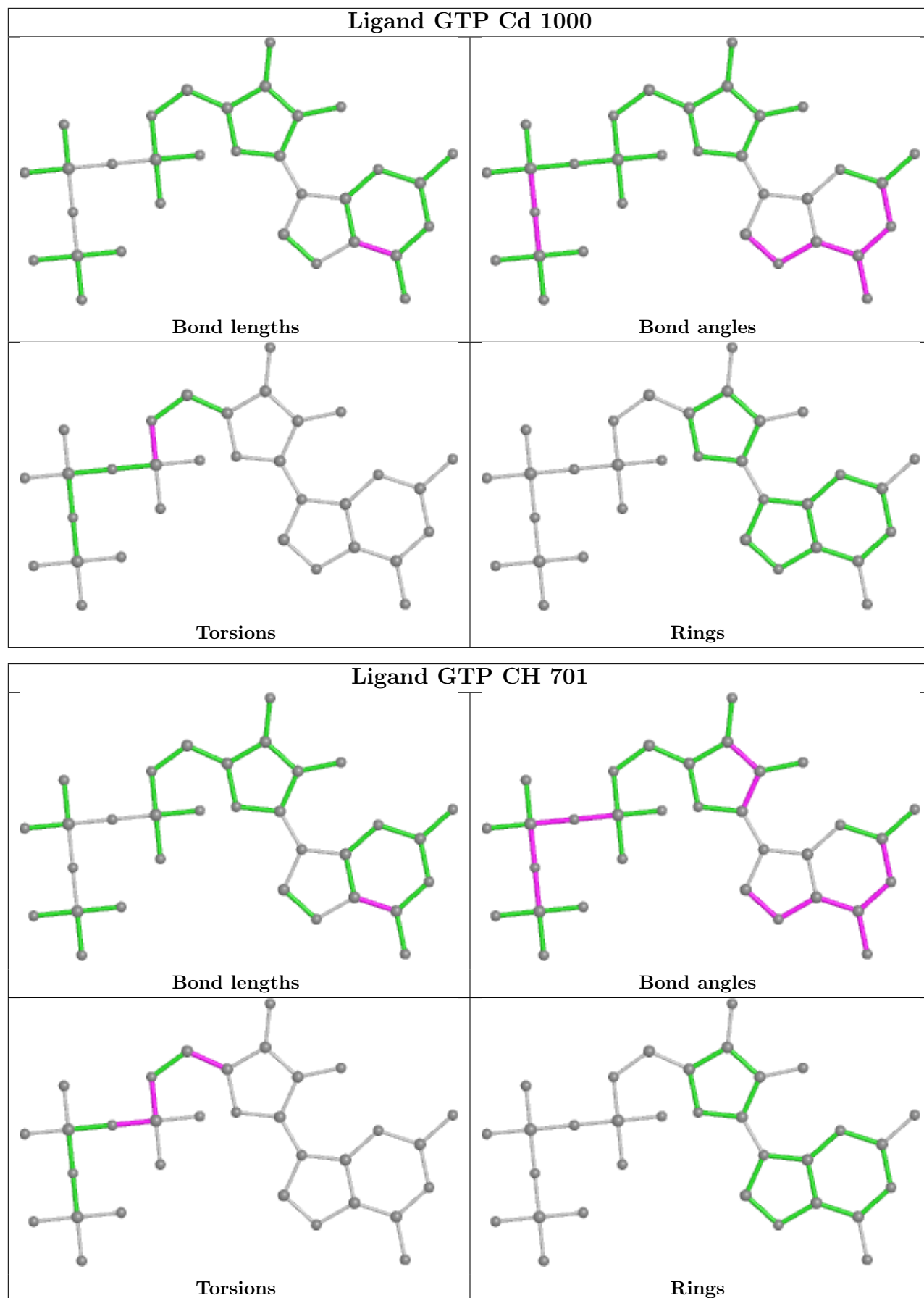
5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	CH	701	GTP	C5'-O5'-PA-O3A
57	CH	701	GTP	O4'-C4'-C5'-O5'
57	CH	701	GTP	C3'-C4'-C5'-O5'
57	CH	701	GTP	C5'-O5'-PA-O1A
57	CH	701	GTP	C5'-O5'-PA-O2A

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.

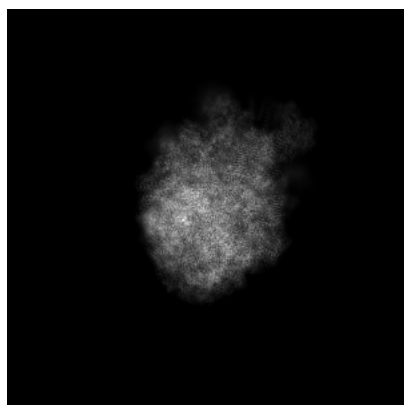
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17951. These allow visual inspection of the internal detail of the map and identification of artifacts.

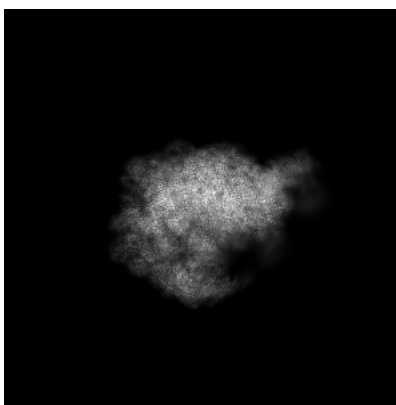
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

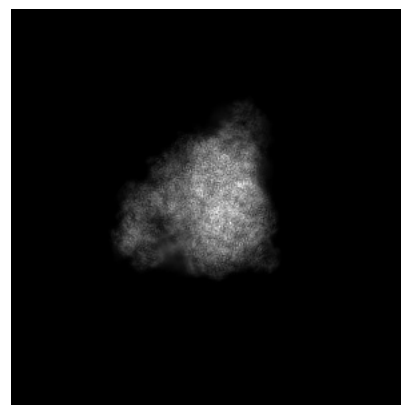
6.1.1 Primary map



X



Y

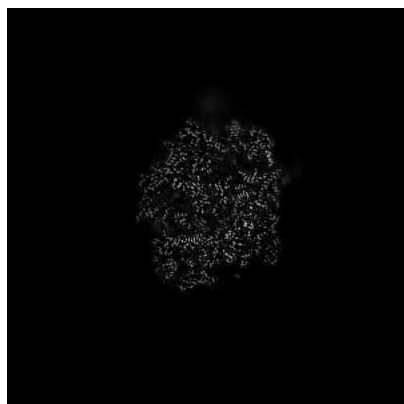


Z

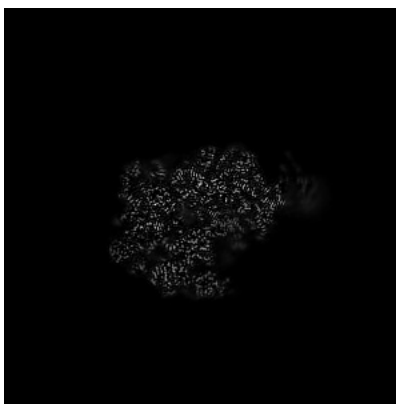
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

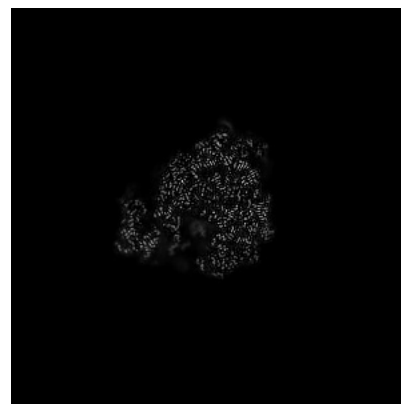
6.2.1 Primary map



X Index: 250



Y Index: 250

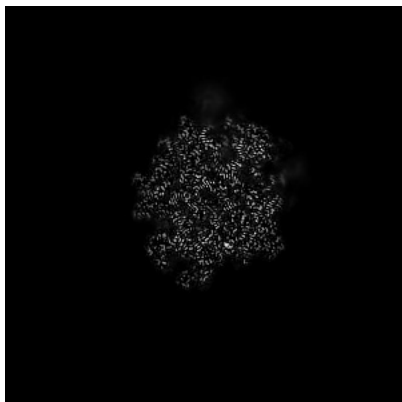


Z Index: 250

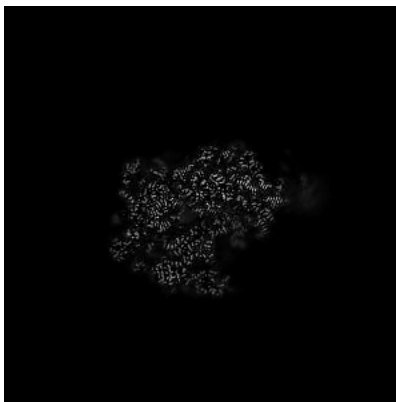
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

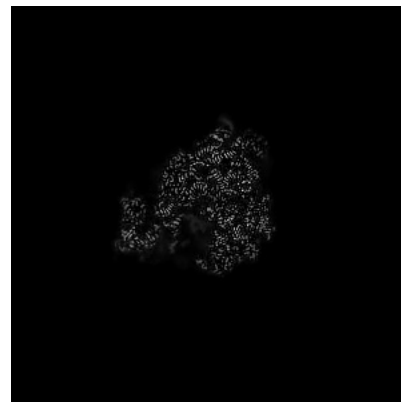
6.3.1 Primary map



X Index: 259



Y Index: 248

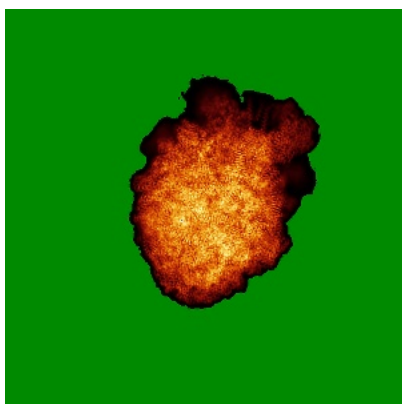


Z Index: 252

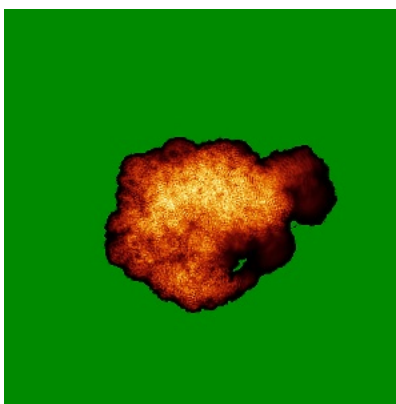
The images above show the largest variance slices of the map in three orthogonal directions.

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

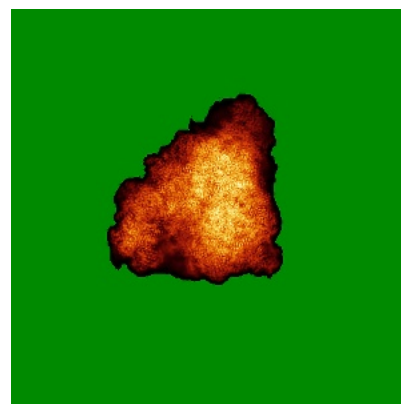
6.4.1 Primary map



X



Y

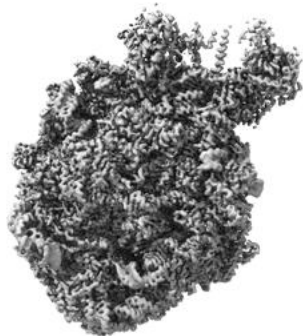


Z

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](#)

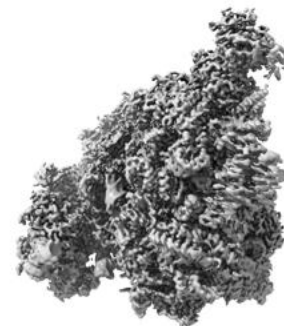
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

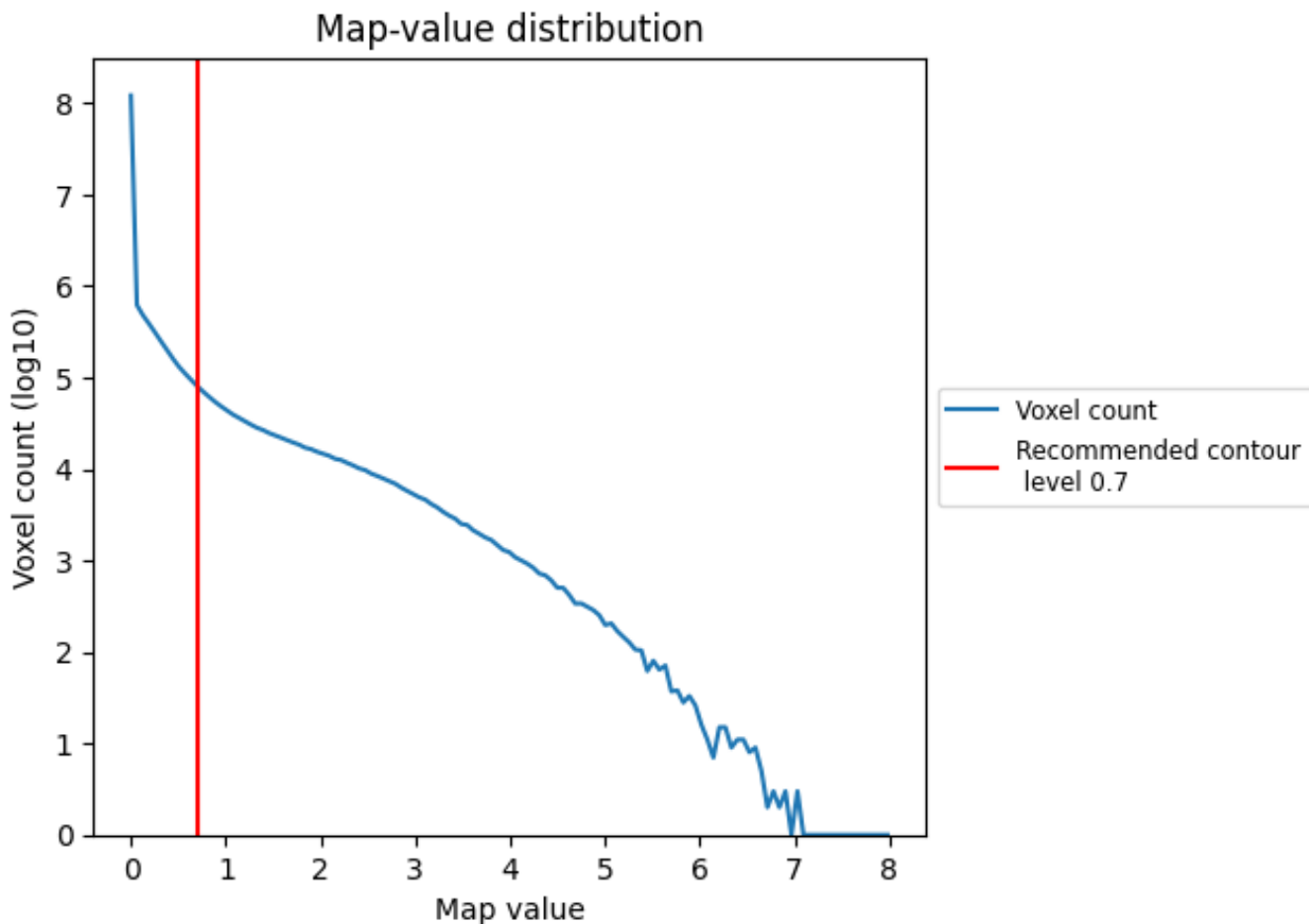
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

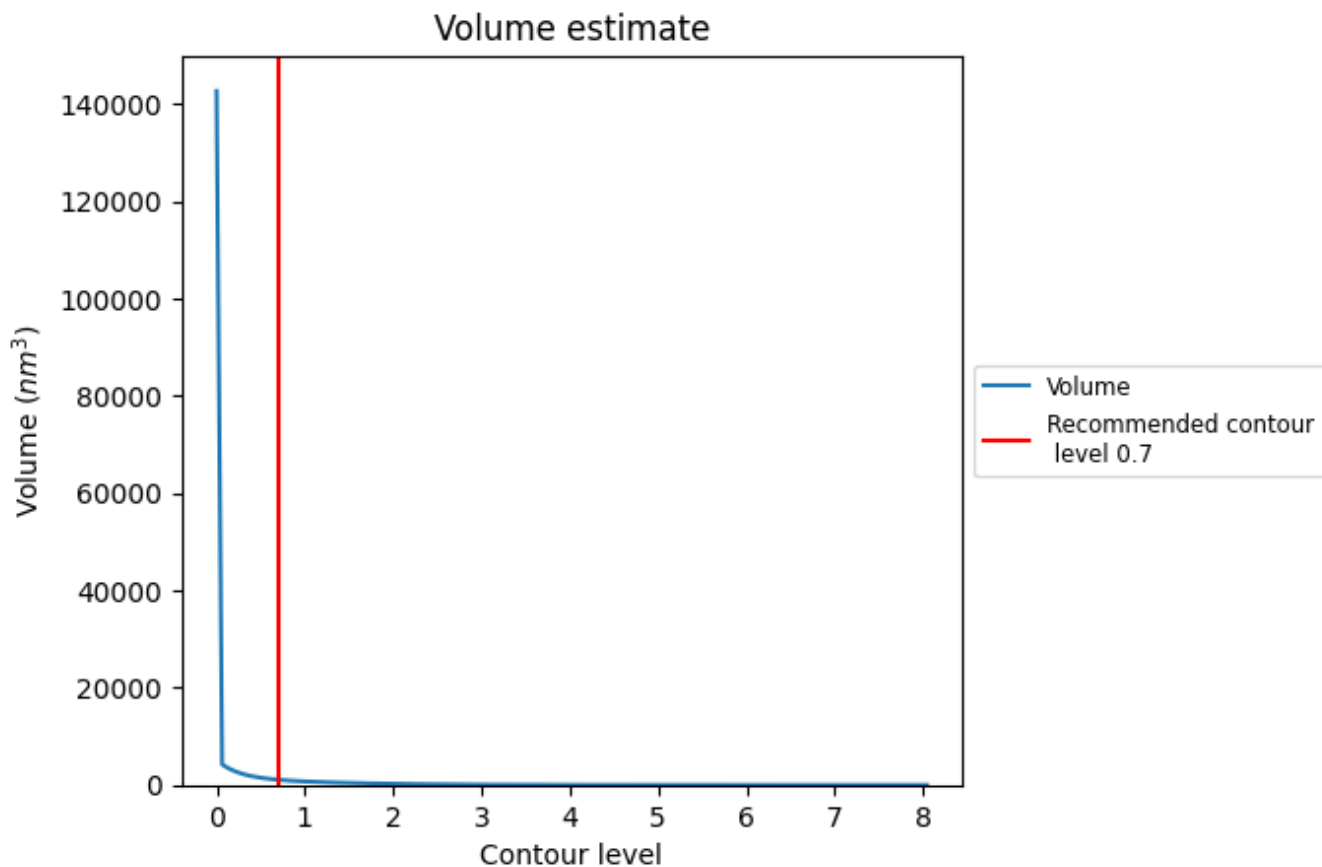
This section contains the results of statistical analysis of the map.

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.

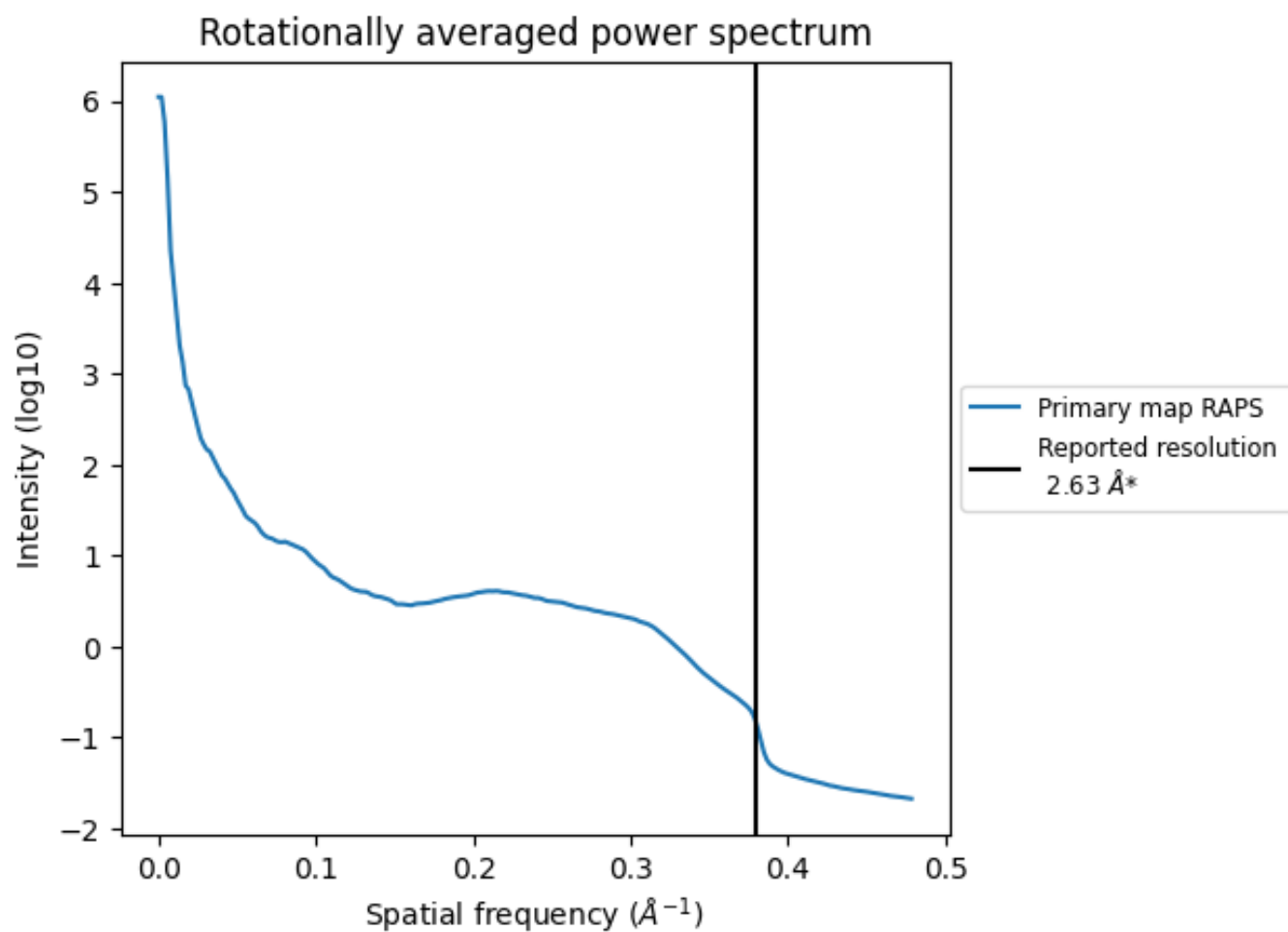
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1068 nm^3 ; this corresponds to an approximate mass of 965 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 0.380 Å⁻¹

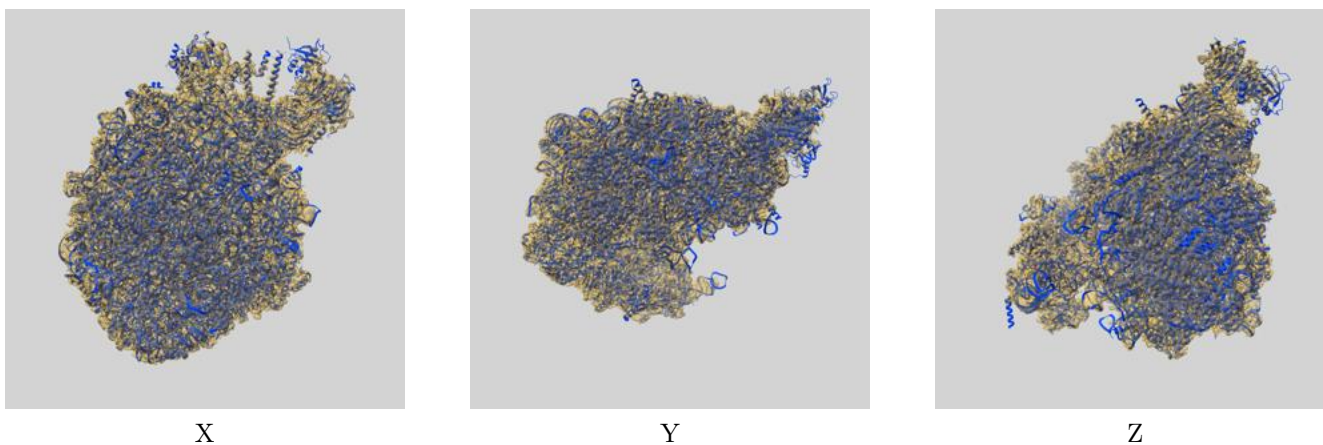
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

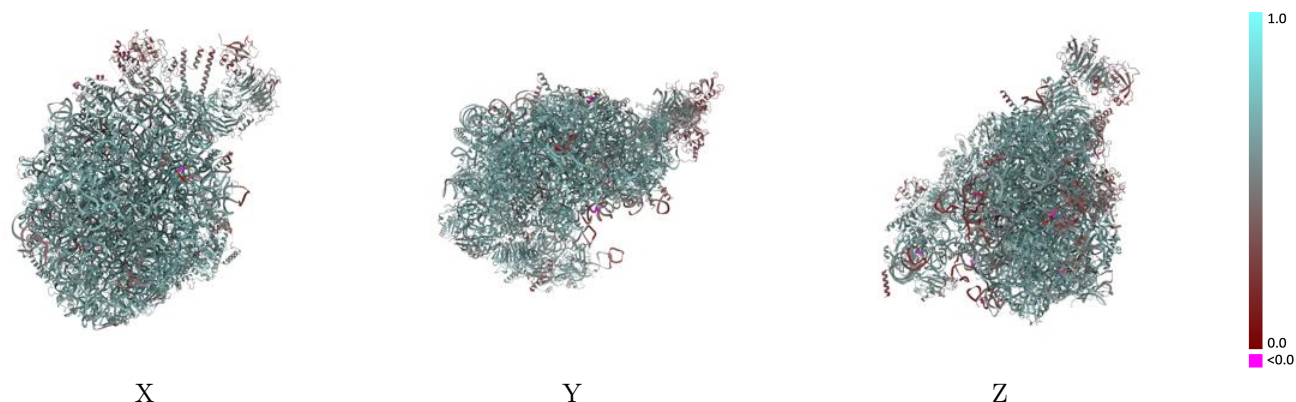
This section contains information regarding the fit between EMDB map EMD-17951 and PDB model 8PV2. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



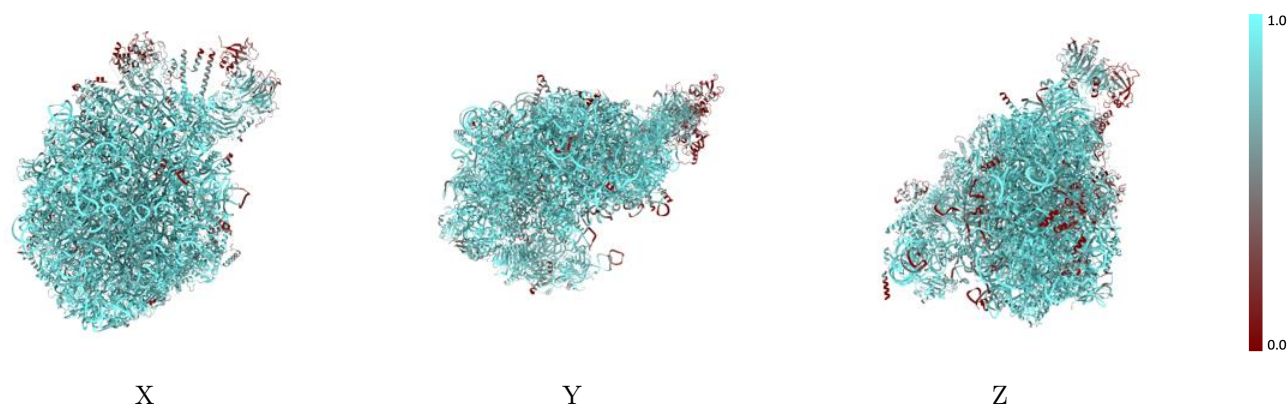
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



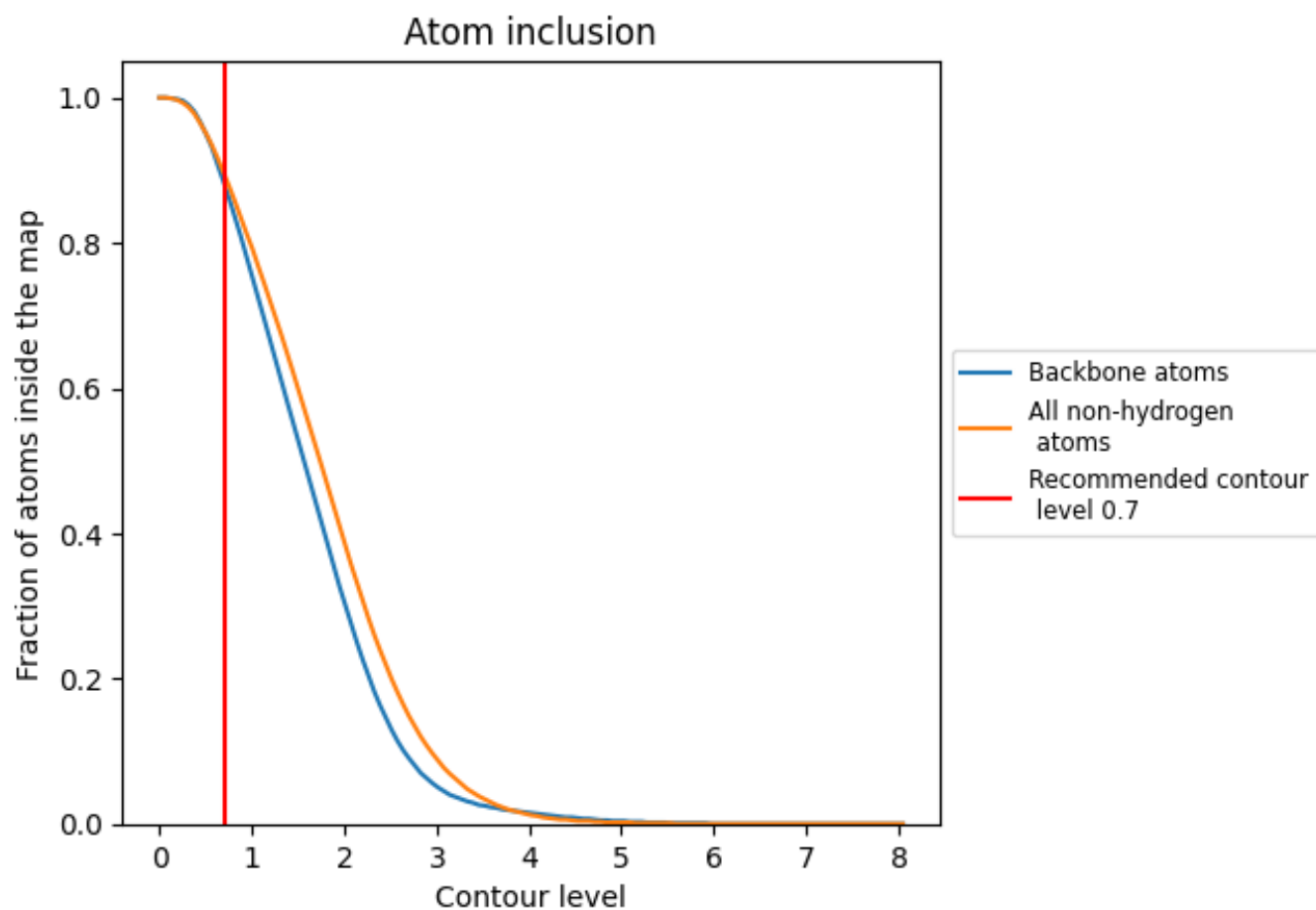
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).







































































9.4 Atom inclusion [i](#)

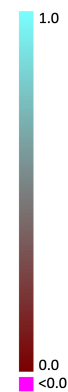


At the recommended contour level, 88% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary















































The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8950	 0.6000
C1	 0.9400	 0.6070
C2	 0.9850	 0.6490
C4	 0.8850	 0.5460
CC	 0.8020	 0.5510
CD	 0.5410	 0.4540
CF	 0.8550	 0.5830
CH	 0.8550	 0.6040
CJ	 0.6710	 0.4640
CK	 0.9490	 0.6510
CL	 0.8040	 0.5690
CM	 0.2020	 0.2870
CN	 0.9210	 0.6280
CO	 0.8270	 0.6100
CQ	 0.8340	 0.6030
Cb	 0.9210	 0.6280
Cd	 0.9140	 0.6220
Cf	 0.9090	 0.5990
Cg	 0.8630	 0.5730
Ch	 0.8510	 0.5820
Cz	 0.7610	 0.5310
LA	 0.9100	 0.6250
LB	 0.9560	 0.6650
LC	 0.9470	 0.6460
LD	 0.8810	 0.5830
LE	 0.8510	 0.5890
LF	 0.9110	 0.6310
LG	 0.8580	 0.5820
LH	 0.9150	 0.6360
LJ	 0.8540	 0.5390
LK	 0.7600	 0.5280
LL	 0.8740	 0.6080
LM	 0.9230	 0.6290
LN	 0.9550	 0.6540
LO	 0.9670	 0.6630



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Chain	Atom inclusion	Q-score
LP	 0.9510	 0.6540
LQ	 0.9050	 0.6200
LR	 0.9280	 0.6290
LS	 0.9410	 0.6380
LT	 0.7370	 0.5190
LU	 0.8560	 0.5800
LV	 0.9600	 0.6610
LX	 0.9240	 0.6150
LY	 0.9150	 0.6260
LZ	 0.9320	 0.6090
La	 0.9210	 0.6240
Lc	 0.8820	 0.5940
Ld	 0.9210	 0.6520
Le	 0.9550	 0.6590
Lf	 0.9760	 0.6700
Lg	 0.9000	 0.6120
Lh	 0.8860	 0.6000
Li	 0.8190	 0.5650
Lj	 0.9810	 0.6780
Lk	 0.8190	 0.5470
Ll	 0.9880	 0.6830
Lp	 0.8750	 0.6000
Lq	 0.9180	 0.6140