



## Full wwPDB EM Validation Report ⓘ

Jul 12, 2023 – 03:25 PM JST

PDB ID : 8I9X  
EMDB ID : EMD-35287  
Title : Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit - Ytm1-1  
Authors : Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.  
Deposited on : 2023-02-07  
Resolution : 2.80 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](mailto: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>.

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

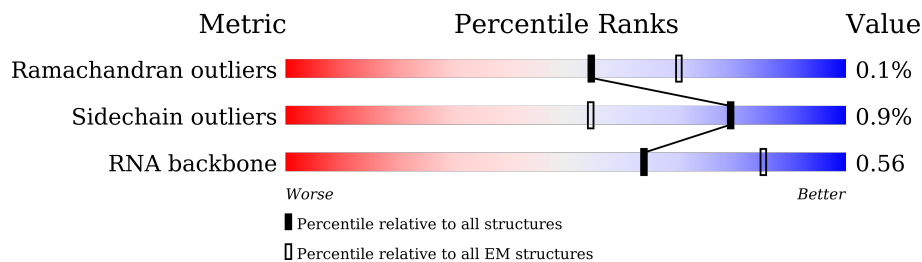
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.34

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

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



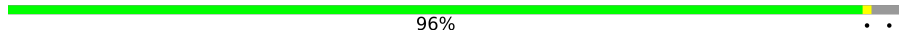












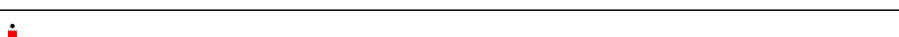
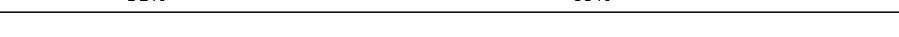
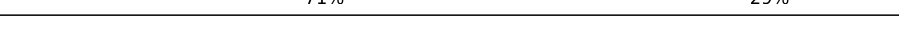

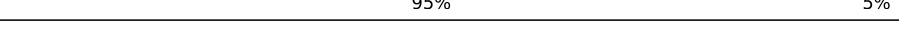

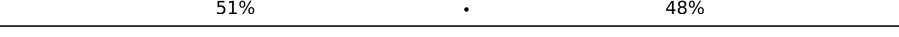



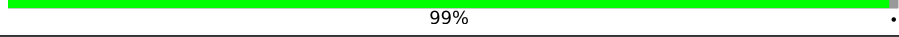

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	3341	
2	C2	319	
3	CA	316	
4	CB	391	
5	CC	801	
6	CD	495	
7	CE	598	
8	CF	270	

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Mol	Chain	Length	Quality of chain
9	CG	184	 96%
10	CH	661	 81% 18%
11	CI	414	 35% 65%
12	CJ	679	 72% 27%
13	CK	261	 90% 9%
14	CL	558	 50% 70% 29%
15	CM	249	 89% 10%
15	LF	249	 98%
16	CN	246	 100%
17	CO	120	 52% 48%
18	CP	751	 47% 53%
19	CQ	225	 79% 20%
20	CR	237	 70% 30%
21	CS	834	 31% 69%
22	CT	688	 71% 29%
23	CU	451	 39% 61%
24	CV	147	 95% 5%
25	CX	203	 43% 57%
26	CY	788	 51% 48%
27	Cb	924	 69% 31%
28	Cz	123	 9% 57% 43%
29	LB	392	 90% 9%
30	LC	365	 99%
31	LE	200	 90% 10%
32	LG	262	 77% 22%



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Mol	Chain	Length	Quality of chain
33	LH	192	98%
34	LK	165	85% 12%
35	LL	213	54% 45%
36	LM	142	96%
37	LN	203	89% 10%
38	LO	204	100%
39	LP	187	90% 10%
40	LQ	213	60% 39%
41	LR	2898	96%
42	LS	174	99%
43	LT	160	78% 21%
44	LU	127	83% 17%
45	LV	139	96%
46	LX	156	87% 12%
47	LY	138	97%
48	LZ	135	100%
49	Lc	108	91% 9%
50	Ld	120	91% 9%
51	Le	131	97%
52	Lf	109	99%
53	Lg	119	97%
54	Lh	935	13% 87%
55	Li	110	78% 20%
56	Lj	95	76% 22%
57	Lk	81	91% 7%

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Mol	Chain	Length	Quality of chain
58	Ll	51	 75% 25%
59	Lq	217	 12% 93% 5%

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 162633 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 RNA (3341-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C1	2658	56864	25379	10296	18531	2658	0	0

- Molecule 2 is a RNA chain called RNA (319-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C2	256	5456	2435	974	1791	256	0	0

- Molecule 3 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CA	251	2069	1324	381	357	7	0	0

- Molecule 4 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CB	260	2063	1322	367	371	3	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	CC	658	5297	3368	931	983	2	13	0	0

- Molecule 6 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CD	460	3468	2173	610	679	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CD	88	ASP	GLU	conflict	UNP G0SFB5

- Molecule 7 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	CE	462	3669	2350	642	666	11	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	543	LYS	-	insertion	UNP G0RYU9
CE	544	SER	-	insertion	UNP G0RYU9
CE	545	PHE	-	insertion	UNP G0RYU9
CE	546	GLY	-	insertion	UNP G0RYU9
CE	547	PHE	-	insertion	UNP G0RYU9
CE	548	SER	-	insertion	UNP G0RYU9
CE	549	THR	-	insertion	UNP G0RYU9
CE	550	PRO	-	insertion	UNP G0RYU9
CE	551	PRO	-	insertion	UNP G0RYU9
CE	552	ARG	-	insertion	UNP G0RYU9
CE	553	VAL	-	insertion	UNP G0RYU9
CE	554	ASP	-	insertion	UNP G0RYU9
CE	555	ILE	-	insertion	UNP G0RYU9
CE	556	THR	-	insertion	UNP G0RYU9
CE	557	LEU	-	insertion	UNP G0RYU9
CE	558	SER	-	insertion	UNP G0RYU9
CE	559	ALA	-	insertion	UNP G0RYU9
CE	560	SER	-	insertion	UNP G0RYU9
CE	561	LEU	-	insertion	UNP G0RYU9
CE	562	SER	-	insertion	UNP G0RYU9
CE	563	ARG	-	insertion	UNP G0RYU9
CE	564	ASP	-	insertion	UNP G0RYU9
CE	565	LYS	-	insertion	UNP G0RYU9
CE	566	LYS	-	insertion	UNP G0RYU9
CE	567	PRO	-	insertion	UNP G0RYU9
CE	568	GLN	-	insertion	UNP G0RYU9
CE	569	GLY	-	insertion	UNP G0RYU9
CE	570	ARG	-	insertion	UNP G0RYU9
CE	571	ARG	-	insertion	UNP G0RYU9
CE	572	ALA	-	insertion	UNP G0RYU9

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Chain	Residue	Modelled	Actual	Comment	Reference
CE	573	TYR	-	insertion	UNP G0RYU9
CE	574	GLY	-	insertion	UNP G0RYU9
CE	575	SER	-	insertion	UNP G0RYU9
CE	576	GLN	-	insertion	UNP G0RYU9
CE	577	PRO	-	insertion	UNP G0RYU9
CE	578	ARG	-	insertion	UNP G0RYU9
CE	579	GLN	-	insertion	UNP G0RYU9
CE	580	GLY	-	insertion	UNP G0RYU9
CE	581	GLY	-	insertion	UNP G0RYU9
CE	582	ARG	-	insertion	UNP G0RYU9
CE	583	TYR	-	insertion	UNP G0RYU9
CE	584	LYS	-	insertion	UNP G0RYU9

- Molecule 8 is a protein called Ribosome assembly factor mrt4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	CF	245	1945	1222	352	362	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CF	13	ILE	THR	conflict	UNP G0S616
CF	139	THR	PRO	conflict	UNP G0S616
CF	228	ASN	SER	conflict	UNP G0S616
CF	259	ILE	MET	conflict	UNP G0S616

- Molecule 9 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	CG	177	1396	884	247	253	12	0	0

- Molecule 10 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	CH	542	4388	2784	770	818	16	0	0

- Molecule 11 is a protein called Putative RNA-binding protein.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	CI	146	1196	763	224	204	5	0	0

- Molecule 12 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	CJ	494	4040	2575	719	734	12	0	0

- Molecule 13 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	CK	238	1908	1199	375	330	4	0	0

- Molecule 14 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	CL	397	2239	1350	459	430	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CL	69	ARG	ILE	conflict	UNP G0SEW3

- Molecule 15 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	CM	223	1820	1169	340	308	3	0	0
15	LF	247	2017	1294	376	344	3	0	0

- Molecule 16 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	CN	246	1856	1158	322	369	7	0	0

- Molecule 17 is a protein called DUF2423 domain-containing protein.

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

- Molecule 18 is a protein called RNA methyltransferase nop2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CP	356	Total	C	N	O	S	0	0
			2798	1777	495	510	16		

- Molecule 19 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CQ	179	Total	C	N	O	S	0	0
			1485	926	304	245	10		

- Molecule 20 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CR	167	Total	C	N	O	S	0	0
			1354	827	278	247	2		

- Molecule 21 is a protein called AdoMet-dependent rRNA methyltransferase SPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CS	262	Total	C	N	O	S	0	0
			2105	1322	399	377	7		

- Molecule 22 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CT	488	Total	C	N	O	S	0	0
			3911	2486	690	719	16		

- Molecule 23 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CU	178	Total	C	N	O	S	0	0
			1415	876	265	271	3		

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

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

- Molecule 25 is a protein called 60S ribosomal subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CX	88	Total	C	N	O	S	0	0
			701	435	128	135	3		

- Molecule 26 is a protein called Putative NOC2 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CY	410	Total	C	N	O	S	0	0
			3313	2127	597	577	12		

- Molecule 27 is a protein called ATP-dependent RNA helicase DBP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Cb	642	Total	C	N	O	S	0	0
			5058	3216	918	911	13		

- Molecule 28 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Cz	70	Total	C	N	O	S	0	0
			592	368	120	101	3		

- Molecule 29 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LB	356	Total	C	N	O	S	0	0
			2829	1798	518	501	12		

- Molecule 30 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LC	362	Total	C	N	O	S	0	0
			2752	1738	526	479	9		

- Molecule 31 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LE	179	Total	C	N	O	S	0	0
			1403	898	255	247	3		

- Molecule 32 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LG	204	Total	C	N	O	S	0	0
			1644	1060	297	282	5		

- Molecule 33 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LH	190	Total	C	N	O	S	0	0
			1496	950	268	272	6		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	TYR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5

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Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LEU	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5

- Molecule 34 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	LK	145	1103	695	201	205	2	0	0

- Molecule 35 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	LL	117	964	608	206	148	2	0	0

- Molecule 36 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	LM	137	1101	699	211	190	1	0	0

- Molecule 37 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	LN	183	1563	974	332	253	4	0	0

- Molecule 38 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	LO	204	1618	1039	306	267	6	0	0

- Molecule 39 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	LP	169	1345	835	273	234	3	0	0

- Molecule 40 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	LQ	129	1021	646	200	173	2	0	0

- Molecule 41 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	LR	118	964	607	195	158	4	0	0

- Molecule 42 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	LS	174	1433	922	267	239	5	0	0

- Molecule 43 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	LT	126	1014	643	196	173	2	0	0

- Molecule 44 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	LU	105	850	551	147	151	1	0	0

- Molecule 45 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	LV	135	995	633	185	170	7	0	0

- Molecule 46 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	LX	137	1062	678	194	190		0	0

- Molecule 47 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	LY	134	1065	664	215	184	2	0	0

- Molecule 48 is a protein called 60S ribosomal protein L27.

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

- Molecule 49 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Lc	98	731	463	126	137	5	0	0

- Molecule 50 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Ld	109	890	563	171	155	1	0	0

- Molecule 51 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Le	127	1025	645	209	164	7	0	0

- Molecule 52 is a protein called 60S ribosomal protein l33-like protein.

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

- Molecule 53 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Lg	117	930	578	189	159	4	0	0

- Molecule 54 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Lh	121	995	633	196	166		0	0

- Molecule 55 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Li	88	731	449	162	119	1	0	0

- Molecule 56 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	Lj	74	595	365	132	93	5	0	0

- Molecule 57 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	Lk	75	620	394	117	107	2	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lk	?	-	SER	deletion	UNP G0SG89
Lk	?	-	LYS	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89
Lk	?	-	THR	deletion	UNP G0SG89
Lk	?	-	ILE	deletion	UNP G0SG89

*Continued on next page...*



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Chain	Residue	Modelled	Actual	Comment	Reference
Lk	?	-	ALA	deletion	UNP G0SG89
Lk	?	-	PHE	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	PRO	deletion	UNP G0SG89
Lk	?	-	LEU	deletion	UNP G0SG89
Lk	?	-	THR	deletion	UNP G0SG89

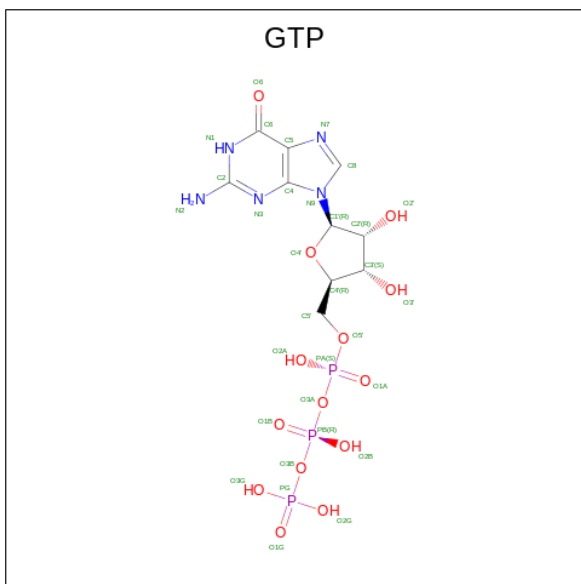
- Molecule 58 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	Ll	38	322	204	68	50	0	0

- Molecule 59 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	Lq	207	1600	1016	285	291	8	0	0

- Molecule 60 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	
60	CH	1	32	10	5	14	3	0

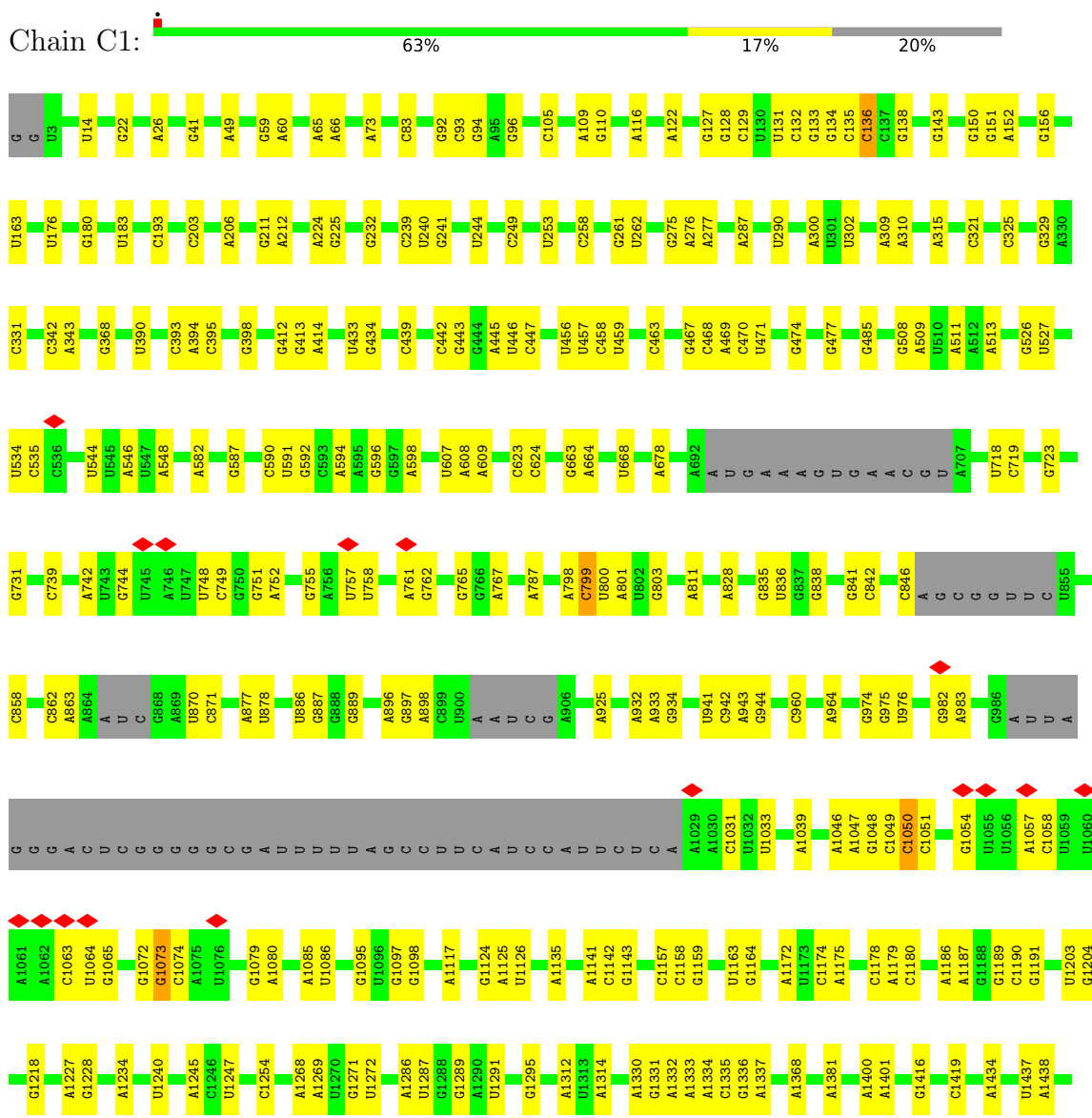
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	CQ	1	Total 1	Zn 1	0
61	Lj	1	Total 1	Zn 1	0

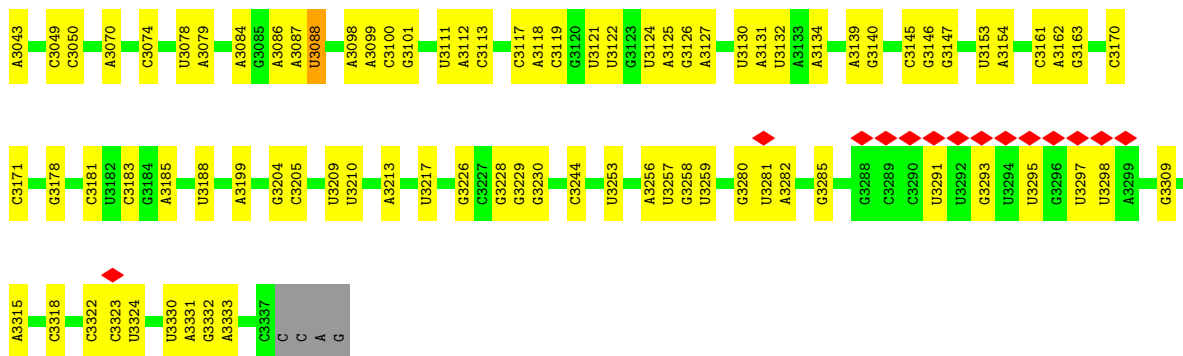
### 3 Residue-property plots

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.

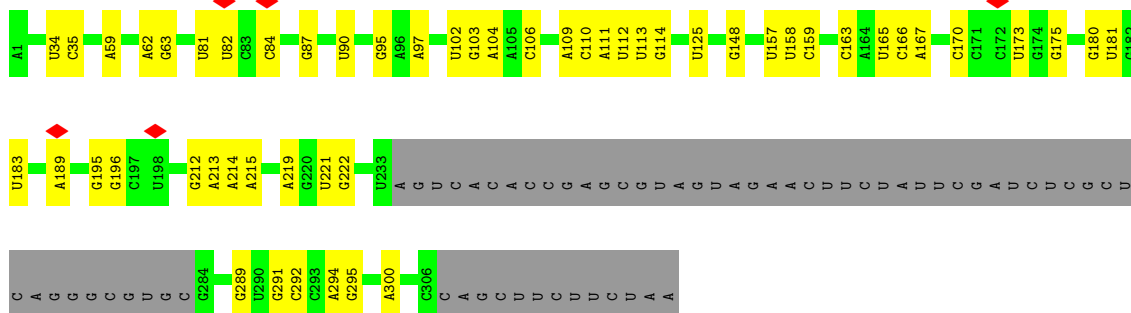
- Molecule 1: RNA (3341-MER)



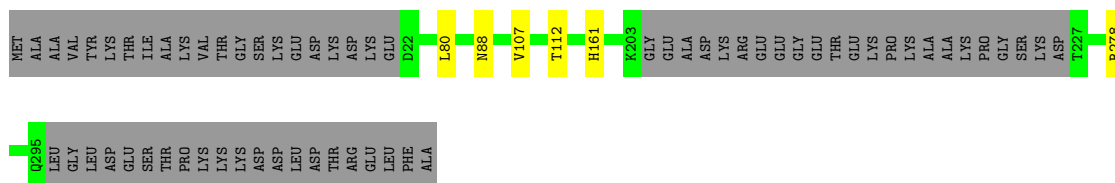
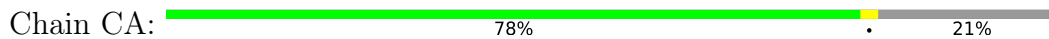




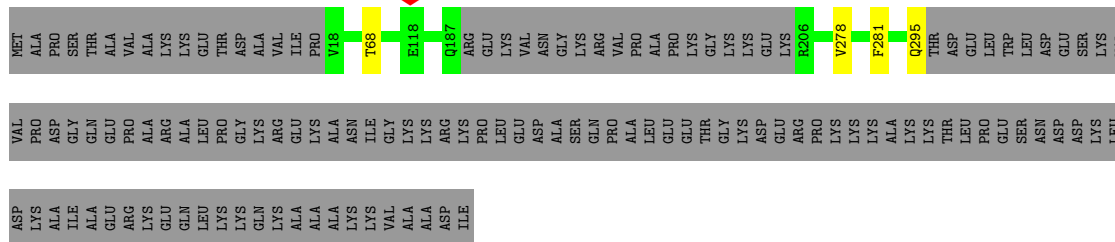
• Molecule 2: RNA (319-MER)



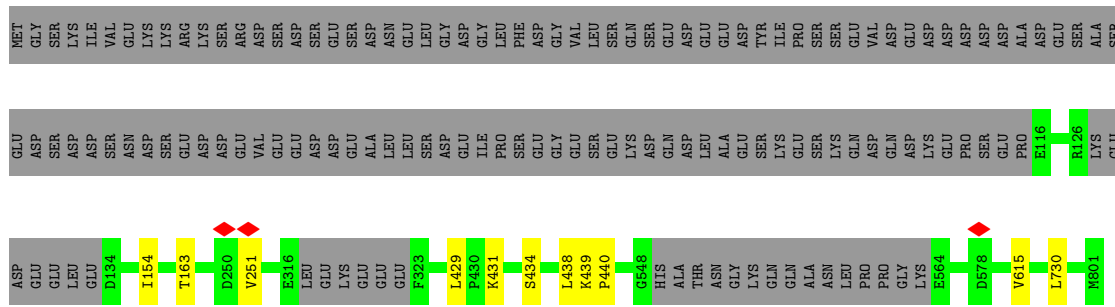
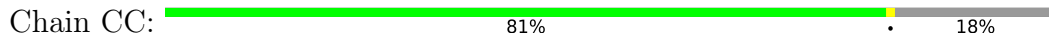
• Molecule 3: Brix domain-containing protein



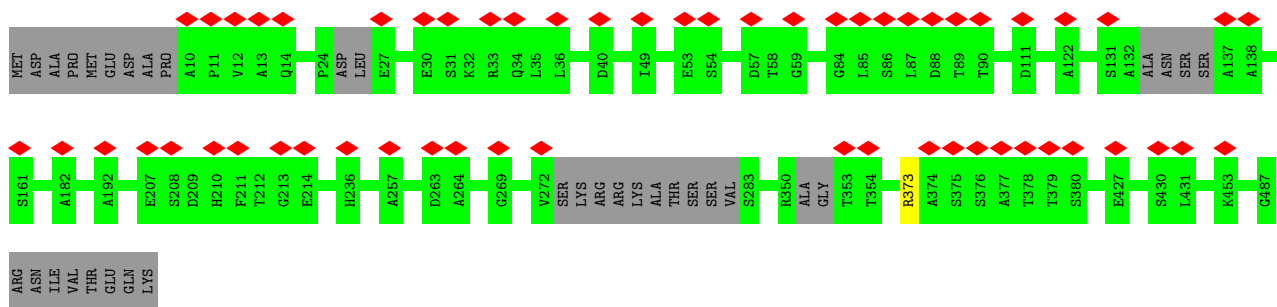
• Molecule 4: Ribosome biogenesis protein C8F11.04



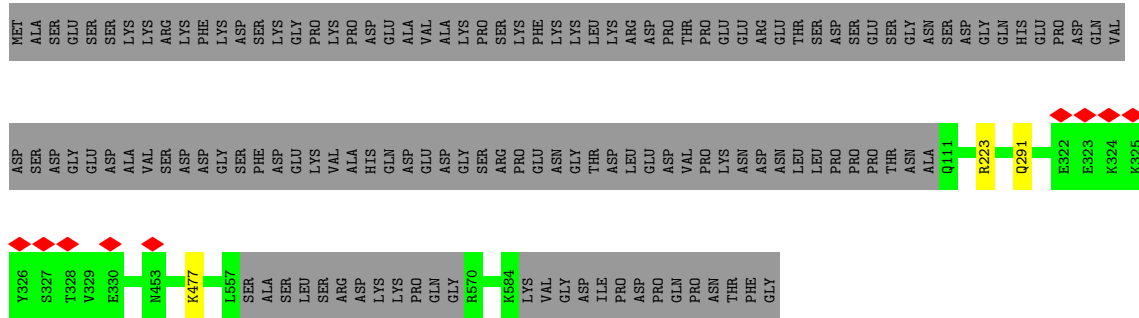
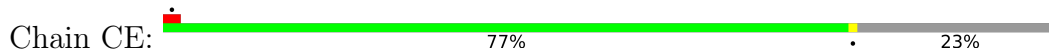
• Molecule 5: Ribosome biogenesis protein ERB1



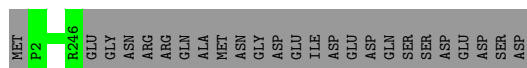
• Molecule 6: Ribosome biogenesis protein YTM1



• Molecule 7: RNA helicase



• Molecule 8: Ribosome assembly factor mrt4

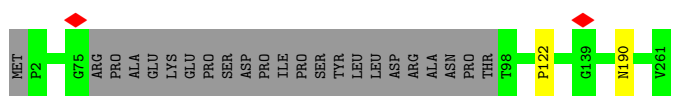
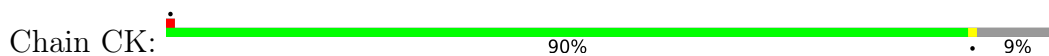


• Molecule 9: 60S ribosome subunit biogenesis protein NIP7

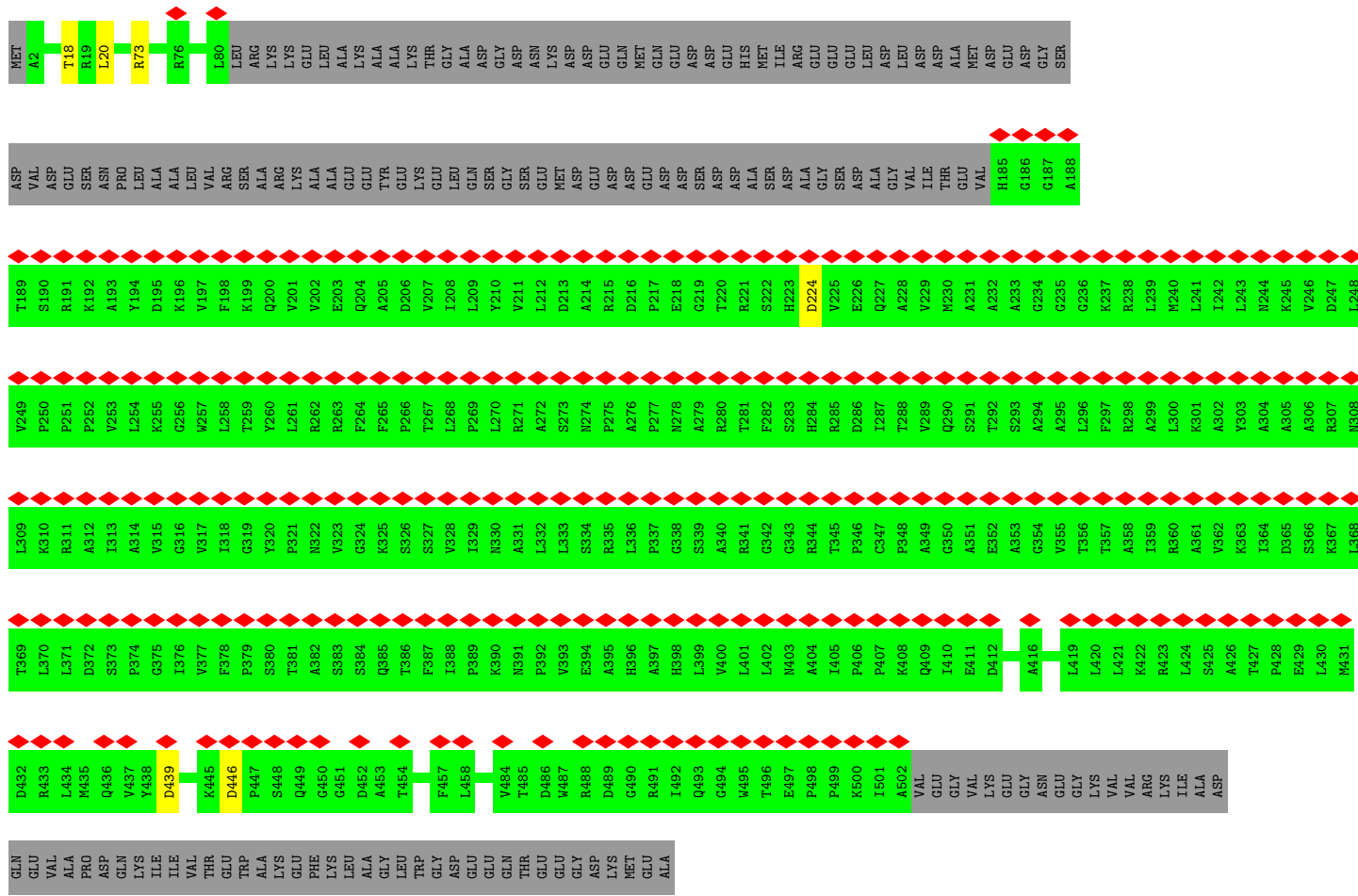




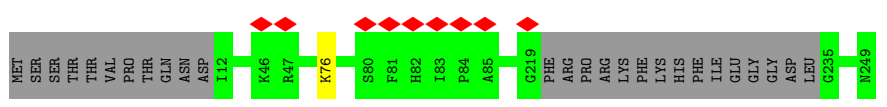
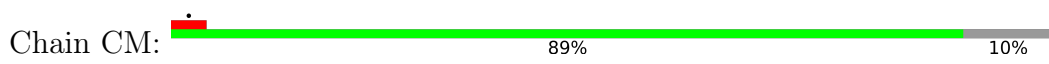
- Molecule 13: Ribosome biogenesis protein NSA2 homolog



- Molecule 14: Putative GTP binding protein



- Molecule 15: 60S ribosomal protein 17-like protein



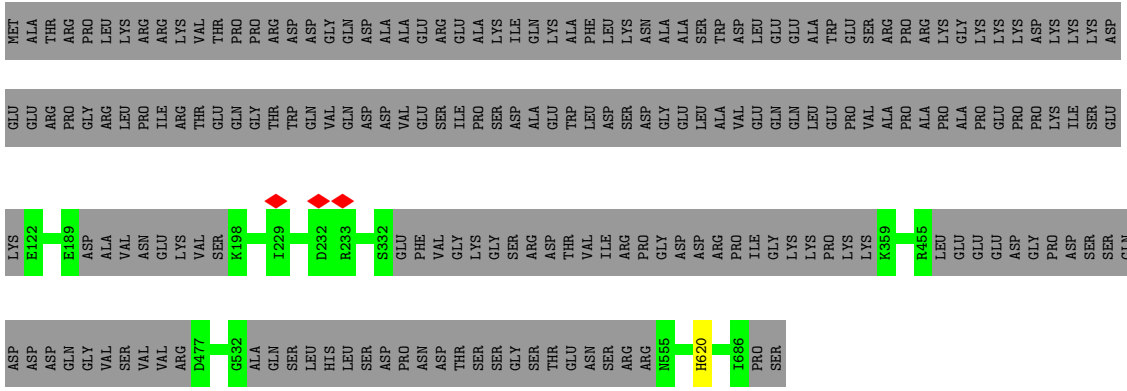
- Molecule 15: 60S ribosomal protein 17-like protein



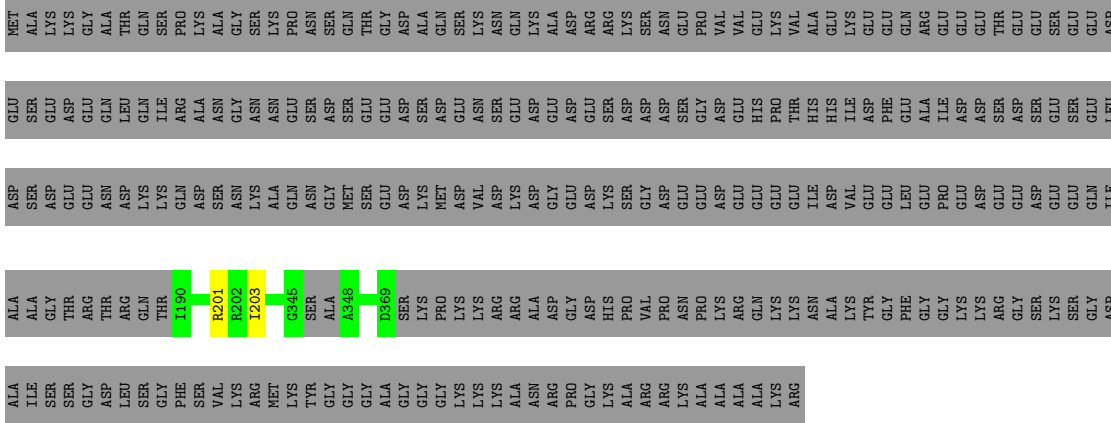




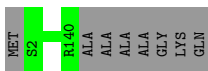




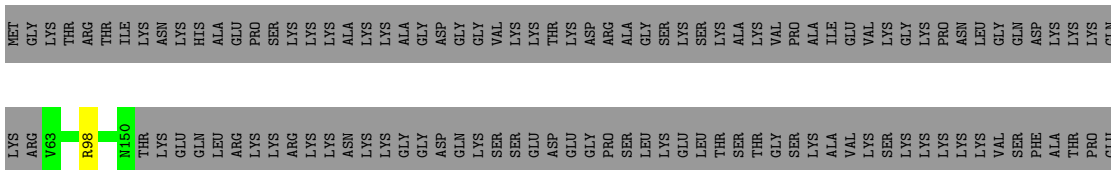
• Molecule 23: rRNA-processing protein EBP2



• Molecule 24: Putative 60S ribosomal protein

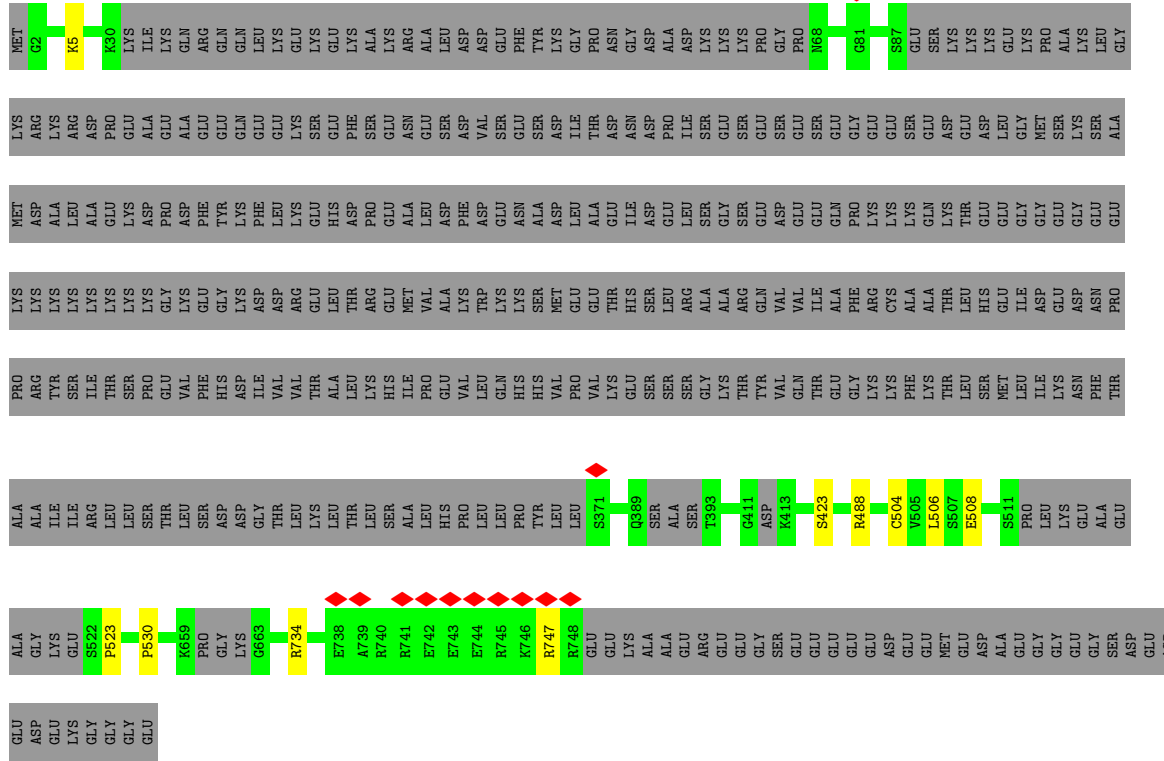


• Molecule 25: 60S ribosomal subunit-like protein

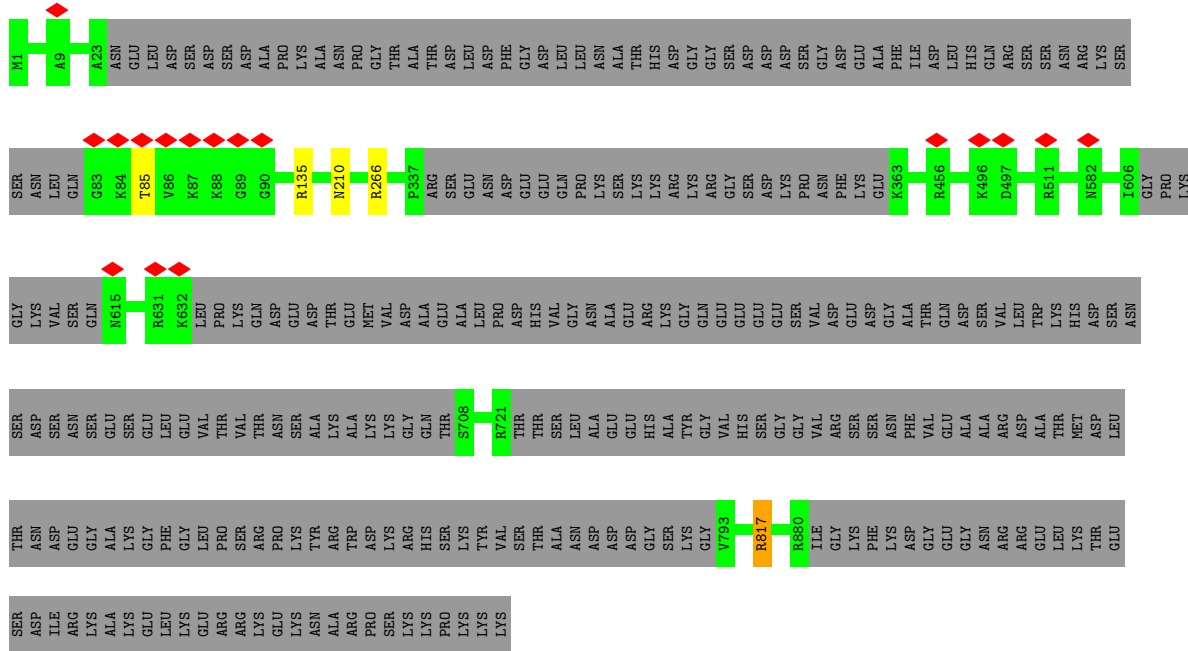


• Molecule 26: Putative NOC2 family protein



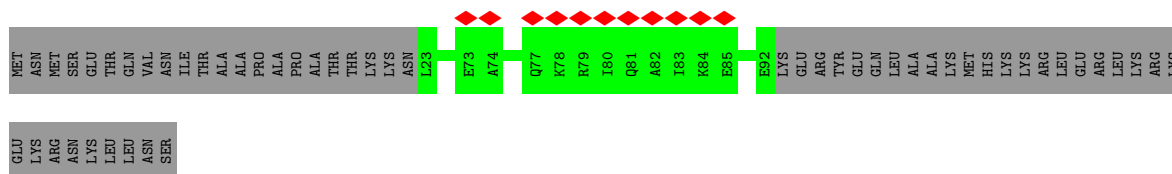


• Molecule 27: ATP-dependent RNA helicase DBP10

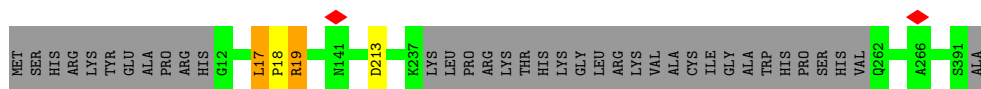
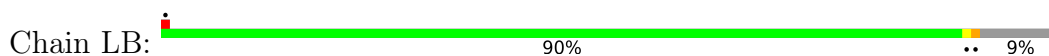


• Molecule 28: rRNA-processing protein

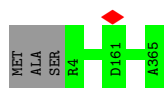




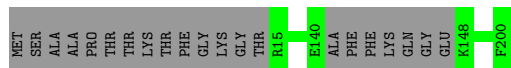
• Molecule 29: 60S ribosomal protein L3-like protein



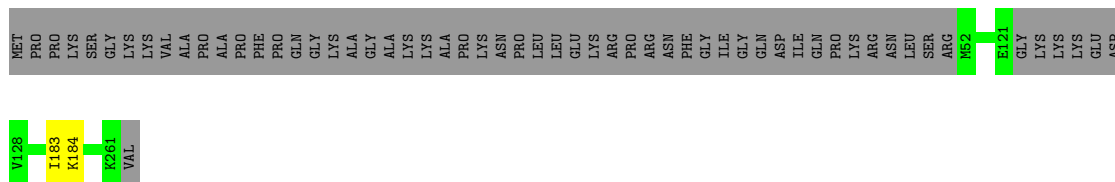
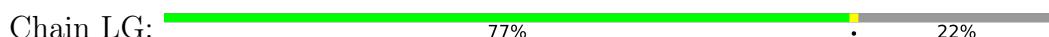
• Molecule 30: 60S ribosomal protein L4-like protein



• Molecule 31: 60S ribosomal protein L6



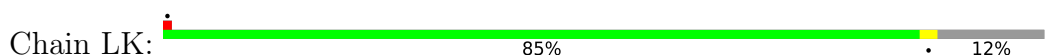
• Molecule 32: 60S ribosomal protein L8



• Molecule 33: 60S ribosomal protein 19-like protein



• Molecule 34: 60S ribosomal protein L12-like protein



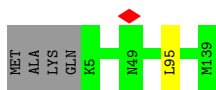




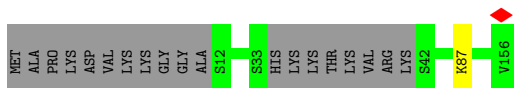
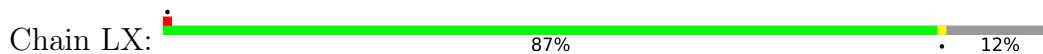




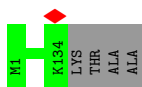




- Molecule 46: 60S ribosomal protein L25-like protein



- Molecule 47: 60S ribosomal protein L26-like protein

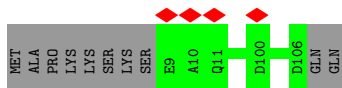


- Molecule 48: 60S ribosomal protein L27

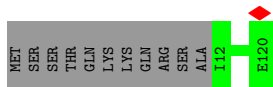
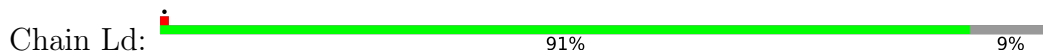


There are no outlier residues recorded for this chain.

- Molecule 49: 60S ribosomal protein l30-like protein



- Molecule 50: Putative 60S ribosomal protein



- Molecule 51: 60S ribosomal protein L32-like protein

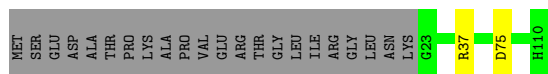
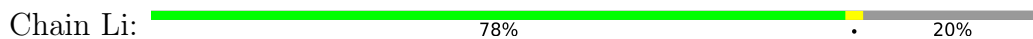


- Molecule 52: 60S ribosomal protein l33-like protein

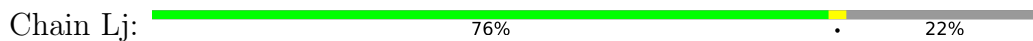




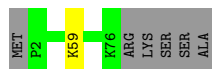
- Molecule 55: 60S ribosomal protein L36



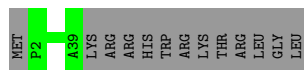
- Molecule 56: Ribosomal protein L37



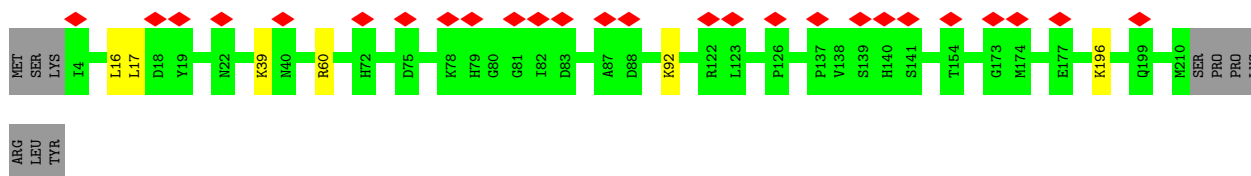
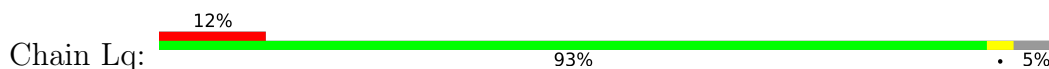
- Molecule 57: 60S ribosomal protein L38-like protein



- Molecule 58: 60S ribosomal protein L39



- Molecule 59: Ribosomal protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77844	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 ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.706	Depositor
Minimum map value	-0.294	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: SEP, GTP, ZN, TPO

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	0.32	0/63619	0.81	28/99165 (0.0%)
2	C2	0.28	0/6097	0.77	0/9499
3	CA	0.43	0/2115	0.72	0/2840
4	CB	0.31	0/2109	0.57	0/2866
5	CC	0.32	0/5423	0.58	0/7380
6	CD	0.26	0/3543	0.58	0/4824
7	CE	0.28	0/3739	0.53	0/5040
8	CF	0.31	0/1982	0.56	0/2671
9	CG	0.31	0/1422	0.56	0/1920
10	CH	0.32	0/4468	0.57	1/6029 (0.0%)
11	CI	0.29	0/1225	0.57	0/1645
12	CJ	0.30	0/4125	0.58	2/5548 (0.0%)
13	CK	0.28	0/1940	0.58	0/2601
14	CL	0.26	0/2247	0.51	0/3076
15	CM	0.29	0/1851	0.55	0/2481
15	LF	0.31	0/2055	0.58	1/2758 (0.0%)
16	CN	0.32	0/1881	0.58	0/2560
17	CO	0.27	0/470	0.55	0/619
18	CP	0.33	0/2859	0.60	1/3870 (0.0%)
19	CQ	0.28	0/1507	0.60	0/1996
20	CR	0.29	0/1369	0.58	0/1828
21	CS	0.27	0/2127	0.53	0/2817
22	CT	0.28	0/3974	0.54	0/5357
23	CU	0.37	0/1428	0.59	1/1910 (0.1%)
24	CV	0.36	0/1091	0.62	0/1468
25	CX	0.27	0/705	0.53	0/938
26	CY	0.33	0/3368	0.62	0/4525
27	Cb	0.27	0/5150	0.57	1/6936 (0.0%)
28	Cz	0.27	0/598	0.56	0/785
29	LB	0.35	0/2885	0.60	0/3872
30	LC	0.28	0/2809	0.53	0/3787
31	LE	0.34	0/1428	0.57	0/1921

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	LG	0.32	0/1667	0.57	0/2230
33	LH	0.29	0/1516	0.58	0/2038
34	LK	0.37	0/1115	0.61	0/1496
35	LL	0.36	0/983	0.67	0/1318
36	LM	0.28	0/1120	0.55	0/1507
37	LN	0.33	0/1595	0.62	0/2132
38	LO	0.35	0/1652	0.57	0/2215
39	LP	0.25	0/1367	0.57	0/1838
40	LQ	0.29	0/1033	0.58	0/1391
41	LR	0.27	0/980	0.55	0/1311
42	LS	0.30	0/1468	0.58	0/1975
43	LT	0.24	0/1033	0.54	0/1389
44	LU	0.29	0/863	0.52	0/1155
45	LV	0.29	0/1013	0.52	0/1361
46	LX	0.25	0/1078	0.49	0/1451
47	LY	0.26	0/1079	0.55	0/1443
48	LZ	0.27	0/1135	0.57	0/1519
49	Lc	0.25	0/740	0.51	0/995
50	Ld	0.27	0/904	0.55	0/1209
51	Le	0.28	0/1043	0.54	0/1389
52	Lf	0.37	0/883	0.64	0/1187
53	Lg	0.33	0/943	0.58	0/1258
54	Lh	0.25	0/1006	0.55	1/1338 (0.1%)
55	Li	0.28	0/738	0.61	0/971
56	Lj	0.33	0/606	0.64	0/803
57	Lk	0.27	0/628	0.59	0/835
58	Ll	0.24	0/329	0.57	0/440
59	Lq	0.28	0/1621	0.62	0/2180
All	All	0.31	0/171747	0.69	36/245906 (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
29	LB	0	1
59	Lq	0	1
All	All	0	2

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1050	C	N3-C2-O2	-12.22	113.34	121.90
1	C1	1050	C	N1-C2-O2	10.75	125.35	118.90
12	CJ	585	LEU	CA-CB-CG	8.98	135.96	115.30
1	C1	136	C	N3-C2-O2	-8.87	115.69	121.90
1	C1	2452	C	N3-C2-O2	-8.76	115.77	121.90
1	C1	2723	C	N3-C2-O2	-7.99	116.30	121.90
1	C1	1051	C	N3-C2-O2	-6.91	117.06	121.90
1	C1	83	C	C2-N3-C4	-6.50	116.65	119.90
1	C1	1051	C	C6-N1-C2	-6.43	117.73	120.30
1	C1	799	C	N3-C2-O2	-6.27	117.51	121.90
12	CJ	614	LEU	CA-CB-CG	6.18	129.53	115.30
1	C1	127	G	N3-C4-N9	6.05	129.63	126.00
1	C1	442	C	C2-N1-C1'	6.03	125.43	118.80
15	LF	13	LEU	CA-CB-CG	6.01	129.12	115.30
1	C1	83	C	N1-C2-N3	5.78	123.25	119.20
1	C1	136	C	N1-C2-O2	5.67	122.30	118.90
10	CH	299	PRO	CA-N-CD	-5.66	103.58	111.50
1	C1	3088	U	C2-N1-C1'	5.54	124.34	117.70
1	C1	249	C	N3-C2-O2	-5.53	118.03	121.90
1	C1	799	C	N1-C2-O2	5.43	122.16	118.90
18	CP	570	LEU	CA-CB-CG	5.41	127.74	115.30
1	C1	1050	C	C6-N1-C2	-5.40	118.14	120.30
1	C1	1073	G	N1-C2-N2	-5.26	111.47	116.20
1	C1	2752	G	C5-C6-O6	5.24	131.75	128.60
1	C1	398	G	O4'-C1'-N9	5.24	112.39	108.20
1	C1	2723	C	N1-C2-O2	5.23	122.04	118.90
23	CU	201	ARG	O-C-N	-5.22	114.34	122.70
1	C1	2752	G	N1-C6-O6	-5.21	116.77	119.90
27	Cb	817	ARG	CA-CB-CG	5.21	124.85	113.40
1	C1	136	C	C6-N1-C2	-5.14	118.24	120.30
1	C1	2745	G	N1-C6-O6	-5.14	116.82	119.90
1	C1	1072	G	N1-C2-N2	-5.12	111.60	116.20
1	C1	127	G	C4-N9-C1'	5.08	133.10	126.50
1	C1	127	G	C8-N9-C1'	-5.05	120.44	127.00
54	Lh	52	LEU	CA-CB-CG	5.03	126.86	115.30
1	C1	83	C	C6-N1-C1'	5.01	126.81	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	LB	17	LEU	Peptide
59	Lq	60	ARG	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	CA	247/316 (78%)	233 (94%)	14 (6%)	0	100	100
4	CB	256/391 (66%)	241 (94%)	15 (6%)	0	100	100
5	CC	648/801 (81%)	611 (94%)	35 (5%)	2 (0%)	41	72
6	CD	450/495 (91%)	426 (95%)	24 (5%)	0	100	100
7	CE	458/598 (77%)	441 (96%)	17 (4%)	0	100	100
8	CF	243/270 (90%)	232 (96%)	11 (4%)	0	100	100
9	CG	175/184 (95%)	168 (96%)	7 (4%)	0	100	100
10	CH	538/661 (81%)	514 (96%)	23 (4%)	1 (0%)	47	78
11	CI	144/414 (35%)	134 (93%)	10 (7%)	0	100	100
12	CJ	484/679 (71%)	470 (97%)	14 (3%)	0	100	100
13	CK	234/261 (90%)	222 (95%)	11 (5%)	1 (0%)	34	66
14	CL	393/558 (70%)	362 (92%)	28 (7%)	3 (1%)	19	49
15	CM	219/249 (88%)	209 (95%)	10 (5%)	0	100	100
15	LF	245/249 (98%)	239 (98%)	6 (2%)	0	100	100
16	CN	244/246 (99%)	230 (94%)	14 (6%)	0	100	100
17	CO	56/120 (47%)	54 (96%)	2 (4%)	0	100	100
18	CP	354/751 (47%)	336 (95%)	17 (5%)	1 (0%)	41	72
19	CQ	173/225 (77%)	165 (95%)	7 (4%)	1 (1%)	25	56
20	CR	159/237 (67%)	157 (99%)	2 (1%)	0	100	100
21	CS	246/834 (30%)	238 (97%)	8 (3%)	0	100	100
22	CT	478/688 (70%)	460 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	CU	174/451 (39%)	173 (99%)	1 (1%)	0	100	100
24	CV	137/147 (93%)	133 (97%)	4 (3%)	0	100	100
25	CX	86/203 (42%)	85 (99%)	1 (1%)	0	100	100
26	CY	396/788 (50%)	365 (92%)	29 (7%)	2 (0%)	29	61
27	Cb	630/924 (68%)	604 (96%)	25 (4%)	1 (0%)	47	78
28	Cz	68/123 (55%)	66 (97%)	2 (3%)	0	100	100
29	LB	352/392 (90%)	332 (94%)	18 (5%)	2 (1%)	25	56
30	LC	360/365 (99%)	342 (95%)	18 (5%)	0	100	100
31	LE	175/200 (88%)	165 (94%)	10 (6%)	0	100	100
32	LG	200/262 (76%)	191 (96%)	9 (4%)	0	100	100
33	LH	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
34	LK	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	22	53
35	LL	115/213 (54%)	107 (93%)	7 (6%)	1 (1%)	17	46
36	LM	135/142 (95%)	127 (94%)	8 (6%)	0	100	100
37	LN	179/203 (88%)	171 (96%)	8 (4%)	0	100	100
38	LO	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
39	LP	165/187 (88%)	161 (98%)	4 (2%)	0	100	100
40	LQ	127/213 (60%)	121 (95%)	6 (5%)	0	100	100
41	LR	114/2898 (4%)	114 (100%)	0	0	100	100
42	LS	172/174 (99%)	167 (97%)	5 (3%)	0	100	100
43	LT	124/160 (78%)	118 (95%)	5 (4%)	1 (1%)	19	49
44	LU	103/127 (81%)	101 (98%)	2 (2%)	0	100	100
45	LV	133/139 (96%)	128 (96%)	5 (4%)	0	100	100
46	LX	133/156 (85%)	129 (97%)	4 (3%)	0	100	100
47	LY	132/138 (96%)	127 (96%)	5 (4%)	0	100	100
48	LZ	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
49	Lc	96/108 (89%)	96 (100%)	0	0	100	100
50	Ld	107/120 (89%)	105 (98%)	2 (2%)	0	100	100
51	Le	125/131 (95%)	120 (96%)	5 (4%)	0	100	100
52	Lf	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
53	Lg	115/119 (97%)	112 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	Lh	119/935 (13%)	114 (96%)	5 (4%)	0	100	100
55	Li	86/110 (78%)	85 (99%)	1 (1%)	0	100	100
56	Lj	72/95 (76%)	70 (97%)	2 (3%)	0	100	100
57	Lk	73/81 (90%)	68 (93%)	5 (7%)	0	100	100
58	Ll	36/51 (71%)	34 (94%)	2 (6%)	0	100	100
59	Lq	205/217 (94%)	179 (87%)	26 (13%)	0	100	100
All	All	12458/20604 (60%)	11891 (95%)	550 (4%)	17 (0%)	54	81

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	CY	523	PRO
27	Cb	85	THR
26	CY	508	GLU
14	CL	224	ASP
14	CL	439	ASP
29	LB	18	PRO
29	LB	19	ARG
34	LK	159	GLU
35	LL	61	PRO
14	CL	446	ASP
18	CP	346	ASP
19	CQ	16	SER
10	CH	545	GLY
43	LT	44	VAL
5	CC	440	PRO
13	CK	122	PRO
5	CC	251	VAL

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CA	223/276 (81%)	217 (97%)	6 (3%)	44	78
4	CB	222/329 (68%)	218 (98%)	4 (2%)	59	86
5	CC	578/708 (82%)	570 (99%)	8 (1%)	67	90
6	CD	381/410 (93%)	380 (100%)	1 (0%)	92	98
7	CE	398/517 (77%)	395 (99%)	3 (1%)	81	94
8	CF	214/236 (91%)	214 (100%)	0	100	100
9	CG	150/155 (97%)	149 (99%)	1 (1%)	84	95
10	CH	481/575 (84%)	475 (99%)	6 (1%)	71	92
11	CI	121/336 (36%)	120 (99%)	1 (1%)	81	94
12	CJ	428/579 (74%)	426 (100%)	2 (0%)	88	96
13	CK	204/225 (91%)	203 (100%)	1 (0%)	88	96
14	CL	72/458 (16%)	69 (96%)	3 (4%)	30	63
15	CM	191/215 (89%)	190 (100%)	1 (0%)	88	96
15	LF	213/215 (99%)	212 (100%)	1 (0%)	88	96
16	CN	206/206 (100%)	205 (100%)	1 (0%)	88	96
17	CO	48/99 (48%)	48 (100%)	0	100	100
18	CP	302/632 (48%)	299 (99%)	3 (1%)	76	93
19	CQ	150/192 (78%)	150 (100%)	0	100	100
20	CR	144/206 (70%)	143 (99%)	1 (1%)	84	95
21	CS	209/716 (29%)	209 (100%)	0	100	100
22	CT	427/600 (71%)	426 (100%)	1 (0%)	93	98
23	CU	149/376 (40%)	148 (99%)	1 (1%)	84	95
24	CV	109/112 (97%)	109 (100%)	0	100	100
25	CX	76/172 (44%)	75 (99%)	1 (1%)	69	91
26	CY	355/686 (52%)	347 (98%)	8 (2%)	50	82
27	Cb	540/779 (69%)	536 (99%)	4 (1%)	84	95
28	Cz	60/107 (56%)	60 (100%)	0	100	100
29	LB	301/331 (91%)	298 (99%)	3 (1%)	76	93
30	LC	283/285 (99%)	283 (100%)	0	100	100
31	LE	151/166 (91%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	LG	175/222 (79%)	173 (99%)	2 (1%)	73	92
33	LH	167/169 (99%)	165 (99%)	2 (1%)	71	92
34	LK	120/136 (88%)	117 (98%)	3 (2%)	47	80
35	LL	99/176 (56%)	98 (99%)	1 (1%)	76	93
36	LM	115/117 (98%)	115 (100%)	0	100	100
37	LN	164/180 (91%)	162 (99%)	2 (1%)	71	92
38	LO	163/163 (100%)	162 (99%)	1 (1%)	86	96
39	LP	137/152 (90%)	137 (100%)	0	100	100
40	LQ	110/178 (62%)	109 (99%)	1 (1%)	78	94
41	LR	104/2396 (4%)	103 (99%)	1 (1%)	76	93
42	LS	154/154 (100%)	153 (99%)	1 (1%)	86	96
43	LT	109/135 (81%)	108 (99%)	1 (1%)	78	94
44	LU	93/108 (86%)	93 (100%)	0	100	100
45	LV	99/102 (97%)	98 (99%)	1 (1%)	76	93
46	LX	114/129 (88%)	113 (99%)	1 (1%)	78	94
47	LY	117/119 (98%)	117 (100%)	0	100	100
48	LZ	121/121 (100%)	121 (100%)	0	100	100
49	Lc	79/88 (90%)	79 (100%)	0	100	100
50	Ld	95/105 (90%)	95 (100%)	0	100	100
51	Le	110/114 (96%)	110 (100%)	0	100	100
52	Lf	89/90 (99%)	89 (100%)	0	100	100
53	Lg	101/102 (99%)	99 (98%)	2 (2%)	55	84
54	Lh	108/781 (14%)	108 (100%)	0	100	100
55	Li	75/93 (81%)	73 (97%)	2 (3%)	44	78
56	Lj	61/78 (78%)	59 (97%)	2 (3%)	38	72
57	Lk	71/76 (93%)	70 (99%)	1 (1%)	67	90
58	Ll	34/46 (74%)	34 (100%)	0	100	100
59	Lq	179/189 (95%)	174 (97%)	5 (3%)	43	77
All	All	10549/17418 (61%)	10459 (99%)	90 (1%)	79	94

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CA	80	LEU
3	CA	88	ASN
3	CA	107	VAL
3	CA	112	THR
3	CA	161	HIS
3	CA	278	ARG
4	CB	68	THR
4	CB	278	VAL
4	CB	281	PHE
4	CB	295	GLN
5	CC	154	ILE
5	CC	429	LEU
5	CC	431	LYS
5	CC	434	SER
5	CC	438	LEU
5	CC	439	LYS
5	CC	615	VAL
5	CC	730	LEU
6	CD	373	ARG
7	CE	223	ARG
7	CE	291	GLN
7	CE	477	LYS
9	CG	40	MET
10	CH	53	GLN
10	CH	78	ARG
10	CH	388	LYS
10	CH	509	ARG
10	CH	518	ILE
10	CH	544	ILE
11	CI	319	LYS
12	CJ	93	ARG
12	CJ	644	LYS
13	CK	190	ASN
14	CL	18	THR
14	CL	20	LEU
14	CL	73	ARG
15	CM	76	LYS
16	CN	216	SER
18	CP	303	PRO
18	CP	309	ARG
18	CP	402	MET
20	CR	8	ARG
22	CT	620	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	CU	203	ILE
25	CX	98	ARG
26	CY	5	LYS
26	CY	423	SER
26	CY	488	ARG
26	CY	504	CYS
26	CY	506	LEU
26	CY	530	PRO
26	CY	734	ARG
26	CY	747	ARG
27	Cb	135	ARG
27	Cb	210	ASN
27	Cb	266	ARG
27	Cb	817	ARG
29	LB	17	LEU
29	LB	19	ARG
29	LB	213	ASP
15	LF	222	PRO
32	LG	183	ILE
32	LG	184	LYS
33	LH	179	GLN
33	LH	205	LYS
34	LK	32	ILE
34	LK	35	LEU
34	LK	37	LEU
35	LL	59	ARG
37	LN	60	VAL
37	LN	61	ILE
38	LO	102	GLU
40	LQ	119	ARG
41	LR	146	LYS
42	LS	119	ARG
43	LT	92	ARG
45	LV	95	LEU
46	LX	87	LYS
53	Lg	56	PRO
53	Lg	115	LYS
55	Li	37	ARG
55	Li	75	ASP
56	Lj	20	ARG
56	Lj	27	LEU
57	Lk	59	LYS

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Mol	Chain	Res	Type
59	Lq	16	LEU
59	Lq	17	LEU
59	Lq	39	LYS
59	Lq	92	LYS
59	Lq	196	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
3	CA	48	HIS
3	CA	118	GLN
3	CA	119	ASN
3	CA	161	HIS
3	CA	246	GLN
4	CB	87	HIS
5	CC	166	ASN
5	CC	446	GLN
5	CC	618	HIS
6	CD	409	HIS
7	CE	472	HIS
10	CH	53	GLN
13	CK	186	HIS
15	CM	119	ASN
16	CN	82	GLN
16	CN	86	ASN
18	CP	343	GLN
20	CR	136	GLN
22	CT	215	HIS
23	CU	204	GLN
26	CY	509	HIS
26	CY	615	GLN
27	Cb	820	HIS
27	Cb	852	GLN
15	LF	119	ASN
15	LF	178	ASN
32	LG	212	ASN
33	LH	179	GLN
39	LP	34	GLN
39	LP	118	GLN
39	LP	120	ASN
42	LS	5	GLN
42	LS	114	HIS

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Mol	Chain	Res	Type
58	Ll	19	GLN
59	Lq	200	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2640/3341 (79%)	535 (20%)	36 (1%)
2	C2	254/319 (79%)	52 (20%)	1 (0%)
All	All	2894/3660 (79%)	587 (20%)	37 (1%)

All (587) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	14	U
1	C1	22	G
1	C1	26	A
1	C1	41	G
1	C1	49	A
1	C1	59	G
1	C1	60	A
1	C1	65	A
1	C1	66	A
1	C1	73	A
1	C1	92	G
1	C1	93	C
1	C1	94	G
1	C1	96	G
1	C1	105	C
1	C1	109	A
1	C1	110	G
1	C1	116	A
1	C1	122	A
1	C1	128	G
1	C1	129	C
1	C1	131	U
1	C1	132	C
1	C1	133	G
1	C1	134	G
1	C1	135	C
1	C1	136	C
1	C1	138	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	143	G
1	C1	150	G
1	C1	151	G
1	C1	152	A
1	C1	156	G
1	C1	163	U
1	C1	176	U
1	C1	180	G
1	C1	183	U
1	C1	193	C
1	C1	203	C
1	C1	206	A
1	C1	211	G
1	C1	212	A
1	C1	224	A
1	C1	225	G
1	C1	232	G
1	C1	239	C
1	C1	240	U
1	C1	244	U
1	C1	253	U
1	C1	258	C
1	C1	261	G
1	C1	262	U
1	C1	275	G
1	C1	276	A
1	C1	277	A
1	C1	287	A
1	C1	290	U
1	C1	300	A
1	C1	302	U
1	C1	309	A
1	C1	310	A
1	C1	315	A
1	C1	321	C
1	C1	325	C
1	C1	329	G
1	C1	331	C
1	C1	342	C
1	C1	343	A
1	C1	368	G
1	C1	390	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	393	C
1	C1	394	A
1	C1	395	C
1	C1	412	G
1	C1	413	G
1	C1	414	A
1	C1	433	U
1	C1	434	G
1	C1	439	C
1	C1	443	G
1	C1	445	A
1	C1	446	U
1	C1	447	C
1	C1	456	U
1	C1	457	U
1	C1	458	C
1	C1	459	U
1	C1	463	C
1	C1	467	G
1	C1	468	C
1	C1	469	A
1	C1	470	C
1	C1	471	U
1	C1	474	G
1	C1	477	G
1	C1	485	G
1	C1	508	G
1	C1	509	A
1	C1	511	A
1	C1	513	A
1	C1	526	G
1	C1	527	U
1	C1	534	U
1	C1	535	C
1	C1	544	U
1	C1	546	A
1	C1	548	A
1	C1	582	A
1	C1	587	G
1	C1	590	C
1	C1	591	U
1	C1	592	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	594	A
1	C1	596	G
1	C1	598	A
1	C1	607	U
1	C1	608	A
1	C1	609	A
1	C1	623	C
1	C1	624	C
1	C1	663	G
1	C1	664	A
1	C1	668	U
1	C1	678	A
1	C1	718	U
1	C1	719	C
1	C1	723	G
1	C1	731	G
1	C1	739	C
1	C1	742	A
1	C1	744	G
1	C1	748	U
1	C1	749	C
1	C1	751	G
1	C1	752	A
1	C1	755	G
1	C1	757	U
1	C1	758	U
1	C1	761	A
1	C1	762	G
1	C1	765	G
1	C1	767	A
1	C1	787	A
1	C1	798	A
1	C1	799	C
1	C1	800	U
1	C1	801	A
1	C1	803	G
1	C1	811	A
1	C1	828	A
1	C1	835	G
1	C1	836	U
1	C1	838	G
1	C1	841	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	842	C
1	C1	846	C
1	C1	858	C
1	C1	862	C
1	C1	863	A
1	C1	871	C
1	C1	877	A
1	C1	878	U
1	C1	887	G
1	C1	889	G
1	C1	896	A
1	C1	898	A
1	C1	925	A
1	C1	932	A
1	C1	933	A
1	C1	934	G
1	C1	941	U
1	C1	942	C
1	C1	943	A
1	C1	944	G
1	C1	960	C
1	C1	964	A
1	C1	974	G
1	C1	975	G
1	C1	976	U
1	C1	982	G
1	C1	983	A
1	C1	1031	C
1	C1	1033	U
1	C1	1039	A
1	C1	1046	A
1	C1	1047	A
1	C1	1048	G
1	C1	1049	C
1	C1	1050	C
1	C1	1054	G
1	C1	1057	A
1	C1	1058	C
1	C1	1063	C
1	C1	1064	U
1	C1	1065	G
1	C1	1073	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	1074	C
1	C1	1079	G
1	C1	1080	A
1	C1	1085	A
1	C1	1086	U
1	C1	1095	G
1	C1	1097	G
1	C1	1098	G
1	C1	1117	A
1	C1	1125	A
1	C1	1126	U
1	C1	1135	A
1	C1	1141	A
1	C1	1142	C
1	C1	1143	G
1	C1	1157	C
1	C1	1158	C
1	C1	1159	G
1	C1	1163	U
1	C1	1164	G
1	C1	1172	A
1	C1	1174	C
1	C1	1175	A
1	C1	1178	C
1	C1	1179	A
1	C1	1180	C
1	C1	1186	A
1	C1	1187	A
1	C1	1189	G
1	C1	1190	C
1	C1	1191	G
1	C1	1203	U
1	C1	1204	G
1	C1	1218	G
1	C1	1227	A
1	C1	1228	G
1	C1	1234	A
1	C1	1240	U
1	C1	1245	A
1	C1	1247	U
1	C1	1254	C
1	C1	1268	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	1269	A
1	C1	1271	G
1	C1	1272	U
1	C1	1286	A
1	C1	1287	U
1	C1	1289	G
1	C1	1291	U
1	C1	1295	G
1	C1	1312	A
1	C1	1314	A
1	C1	1330	A
1	C1	1331	G
1	C1	1332	A
1	C1	1333	A
1	C1	1334	A
1	C1	1335	C
1	C1	1336	G
1	C1	1337	A
1	C1	1368	A
1	C1	1381	A
1	C1	1400	A
1	C1	1401	A
1	C1	1416	G
1	C1	1419	C
1	C1	1434	A
1	C1	1437	U
1	C1	1438	A
1	C1	1457	G
1	C1	1463	A
1	C1	1465	G
1	C1	1466	U
1	C1	1470	G
1	C1	1489	G
1	C1	1490	C
1	C1	1535	U
1	C1	1537	U
1	C1	1538	C
1	C1	1541	A
1	C1	1548	C
1	C1	1549	U
1	C1	1551	G
1	C1	1552	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	1553	G
1	C1	1556	C
1	C1	1560	G
1	C1	1561	U
1	C1	1562	G
1	C1	1566	A
1	C1	1568	A
1	C1	1575	C
1	C1	1584	A
1	C1	1607	U
1	C1	1608	U
1	C1	1609	G
1	C1	1610	C
1	C1	1618	C
1	C1	1621	A
1	C1	1622	A
1	C1	1623	C
1	C1	1624	U
1	C1	1637	G
1	C1	1662	C
1	C1	1693	A
1	C1	1695	A
1	C1	1696	C
1	C1	1709	G
1	C1	1715	G
1	C1	1722	G
1	C1	1729	A
1	C1	1730	G
1	C1	1741	U
1	C1	1742	U
1	C1	1744	U
1	C1	1749	G
1	C1	1759	G
1	C1	1760	C
1	C1	1774	U
1	C1	1775	G
1	C1	1776	A
1	C1	1791	G
1	C1	1794	U
1	C1	1795	A
1	C1	1798	U
1	C1	1800	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	1813	U
1	C1	1819	U
1	C1	1820	A
1	C1	1821	A
1	C1	1822	C
1	C1	1825	C
1	C1	1828	C
1	C1	1829	A
1	C1	1837	A
1	C1	1842	G
1	C1	1843	A
1	C1	1845	C
1	C1	1857	G
1	C1	1858	A
1	C1	1859	U
1	C1	1861	G
1	C1	1864	C
1	C1	1865	A
1	C1	1866	A
1	C1	1867	U
1	C1	1874	A
1	C1	1875	A
1	C1	1883	C
1	C1	1886	C
1	C1	1897	C
1	C1	1900	A
1	C1	1901	A
1	C1	2075	A
1	C1	2088	A
1	C1	2287	G
1	C1	2288	A
1	C1	2292	C
1	C1	2294	A
1	C1	2297	G
1	C1	2302	U
1	C1	2310	A
1	C1	2311	U
1	C1	2325	A
1	C1	2327	C
1	C1	2332	G
1	C1	2335	A
1	C1	2338	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	2339	G
1	C1	2342	U
1	C1	2343	G
1	C1	2347	A
1	C1	2355	G
1	C1	2356	G
1	C1	2359	A
1	C1	2361	A
1	C1	2362	G
1	C1	2363	A
1	C1	2364	A
1	C1	2396	U
1	C1	2397	G
1	C1	2399	G
1	C1	2407	A
1	C1	2409	A
1	C1	2414	G
1	C1	2415	U
1	C1	2419	G
1	C1	2422	U
1	C1	2424	G
1	C1	2425	G
1	C1	2428	G
1	C1	2430	A
1	C1	2432	C
1	C1	2433	U
1	C1	2434	U
1	C1	2435	C
1	C1	2436	G
1	C1	2437	G
1	C1	2438	C
1	C1	2439	G
1	C1	2443	G
1	C1	2444	U
1	C1	2449	U
1	C1	2453	A
1	C1	2456	A
1	C1	2464	U
1	C1	2465	G
1	C1	2467	U
1	C1	2484	G
1	C1	2551	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	2560	G
1	C1	2564	G
1	C1	2730	C
1	C1	2738	A
1	C1	2740	U
1	C1	2749	G
1	C1	2758	G
1	C1	2759	A
1	C1	2760	A
1	C1	2761	A
1	C1	2767	C
1	C1	2775	A
1	C1	2777	A
1	C1	2778	A
1	C1	2782	G
1	C1	2783	C
1	C1	2784	U
1	C1	2786	G
1	C1	2806	G
1	C1	2818	U
1	C1	2819	U
1	C1	2820	U
1	C1	2845	A
1	C1	2846	U
1	C1	2847	C
1	C1	2856	G
1	C1	2857	C
1	C1	2862	U
1	C1	2869	A
1	C1	2874	U
1	C1	2875	G
1	C1	2876	G
1	C1	2889	C
1	C1	2893	U
1	C1	2894	A
1	C1	2899	A
1	C1	2902	U
1	C1	2917	C
1	C1	2925	A
1	C1	2926	G
1	C1	2936	U
1	C1	2942	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	2948	G
1	C1	2954	C
1	C1	2955	U
1	C1	2956	C
1	C1	2969	A
1	C1	3006	A
1	C1	3016	G
1	C1	3035	G
1	C1	3043	A
1	C1	3049	C
1	C1	3050	C
1	C1	3070	A
1	C1	3074	C
1	C1	3079	A
1	C1	3084	A
1	C1	3086	A
1	C1	3087	A
1	C1	3088	U
1	C1	3098	A
1	C1	3099	A
1	C1	3100	C
1	C1	3101	G
1	C1	3111	U
1	C1	3112	A
1	C1	3113	C
1	C1	3117	C
1	C1	3118	A
1	C1	3119	C
1	C1	3121	U
1	C1	3122	U
1	C1	3124	U
1	C1	3125	A
1	C1	3126	G
1	C1	3127	A
1	C1	3130	U
1	C1	3131	A
1	C1	3132	U
1	C1	3134	A
1	C1	3139	A
1	C1	3140	G
1	C1	3145	C
1	C1	3146	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	3147	G
1	C1	3153	U
1	C1	3154	A
1	C1	3161	C
1	C1	3162	A
1	C1	3163	G
1	C1	3170	C
1	C1	3171	C
1	C1	3178	G
1	C1	3181	C
1	C1	3183	C
1	C1	3185	A
1	C1	3188	U
1	C1	3199	A
1	C1	3205	C
1	C1	3210	U
1	C1	3213	A
1	C1	3217	U
1	C1	3226	G
1	C1	3228	G
1	C1	3229	G
1	C1	3230	G
1	C1	3244	C
1	C1	3253	U
1	C1	3256	A
1	C1	3258	G
1	C1	3259	U
1	C1	3280	G
1	C1	3281	U
1	C1	3282	A
1	C1	3285	G
1	C1	3291	U
1	C1	3293	G
1	C1	3295	U
1	C1	3298	U
1	C1	3309	G
1	C1	3315	A
1	C1	3318	C
1	C1	3322	C
1	C1	3323	C
1	C1	3324	U
1	C1	3330	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	3331	A
1	C1	3332	G
1	C1	3333	A
2	C2	34	U
2	C2	35	C
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	81	U
2	C2	82	U
2	C2	84	C
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	97	A
2	C2	103	G
2	C2	104	A
2	C2	106	C
2	C2	109	A
2	C2	110	C
2	C2	111	A
2	C2	112	U
2	C2	113	U
2	C2	114	G
2	C2	125	U
2	C2	148	G
2	C2	157	U
2	C2	158	U
2	C2	159	C
2	C2	163	C
2	C2	165	U
2	C2	166	C
2	C2	167	A
2	C2	170	C
2	C2	173	U
2	C2	175	G
2	C2	180	G
2	C2	181	U
2	C2	183	U
2	C2	189	A
2	C2	195	G
2	C2	196	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C2	212	G
2	C2	213	A
2	C2	214	A
2	C2	215	A
2	C2	219	A
2	C2	221	U
2	C2	222	G
2	C2	289	G
2	C2	291	G
2	C2	292	C
2	C2	294	A
2	C2	295	G
2	C2	300	A

All (37) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C1	150	G
1	C1	241	G
1	C1	467	G
1	C1	468	C
1	C1	526	G
1	C1	590	C
1	C1	835	G
1	C1	862	C
1	C1	870	U
1	C1	886	U
1	C1	897	G
1	C1	1063	C
1	C1	1085	A
1	C1	1124	G
1	C1	1142	C
1	C1	1475	G
1	C1	1584	A
1	C1	1820	A
1	C1	2301	C
1	C1	2333	G
1	C1	2360	A
1	C1	2777	A
1	C1	2817	U
1	C1	2898	A
1	C1	2925	A

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Mol	Chain	Res	Type
1	C1	3005	A
1	C1	3078	U
1	C1	3124	U
1	C1	3125	A
1	C1	3131	A
1	C1	3162	A
1	C1	3204	G
1	C1	3209	U
1	C1	3229	G
1	C1	3257	U
1	C1	3297	U
2	C2	102	U

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

2 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	$\# Z  > 2$
5	SEP	CC	160	5	8,9,10	0.62	0	8,12,14	0.70	0
5	TPO	CC	163	5	8,10,11	0.67	0	10,14,16	1.03	1 (10%)

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
5	SEP	CC	160	5	-	0/5/8/10	-
5	TPO	CC	163	5	-	1/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	CC	163	TPO	O-C-CA	-2.51	118.19	124.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	CC	163	TPO	O-C-CA-CB

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	GTP	CH	1001	-	26,34,34	0.97	2 (7%)	32,54,54	0.86	0

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
60	GTP	CH	1001	-	-	3/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CH	1001	GTP	C5-C6	-2.63	1.42	1.47
60	CH	1001	GTP	C8-N7	-2.11	1.31	1.35

There are no bond angle outliers.

There are no chirality outliers.

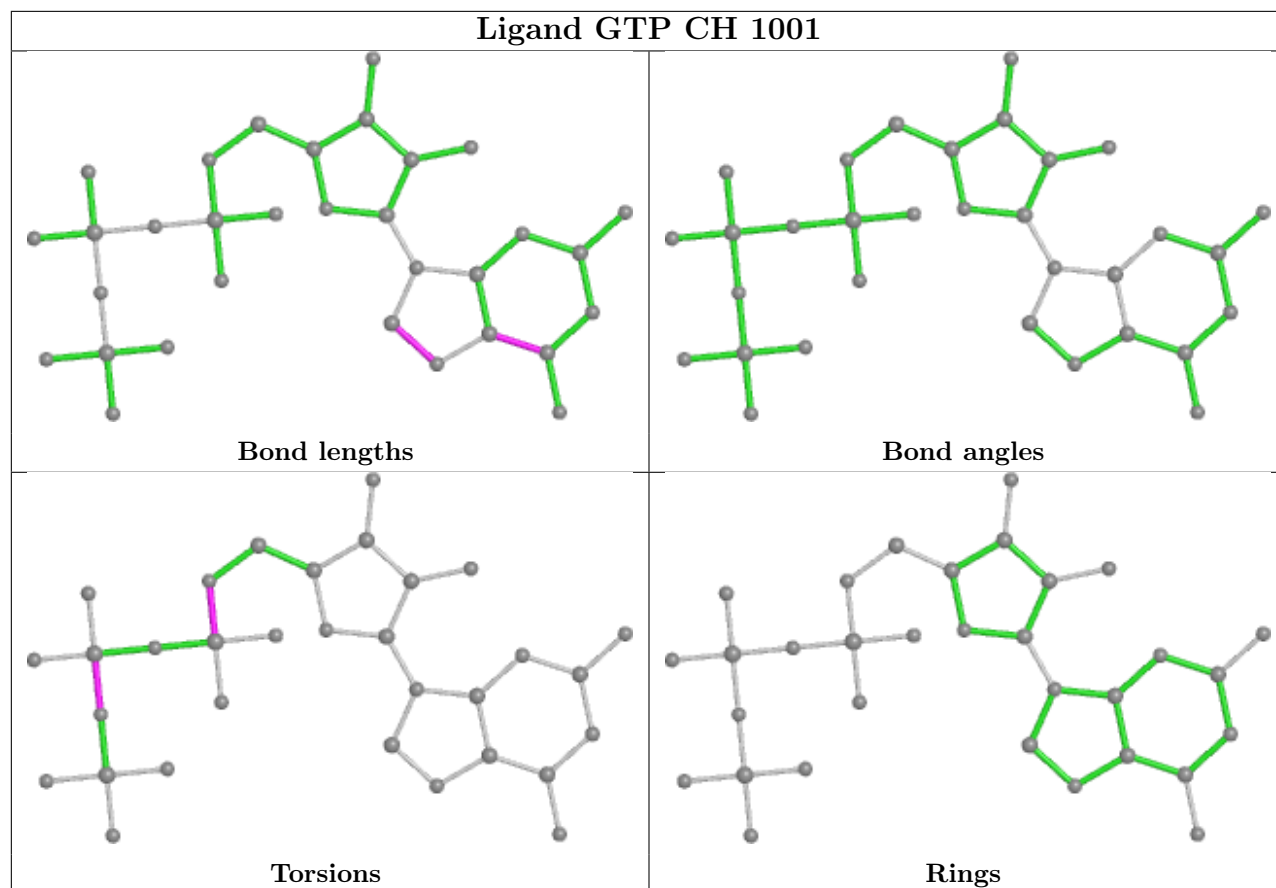
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	CH	1001	GTP	PG-O3B-PB-O1B
60	CH	1001	GTP	PG-O3B-PB-O2B
60	CH	1001	GTP	C5'-O5'-PA-O1A

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.

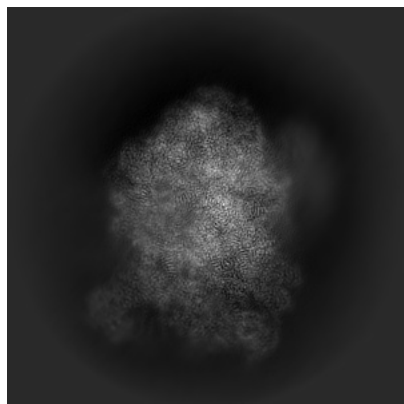
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35287. These allow visual inspection of the internal detail of the map and identification of artifacts.

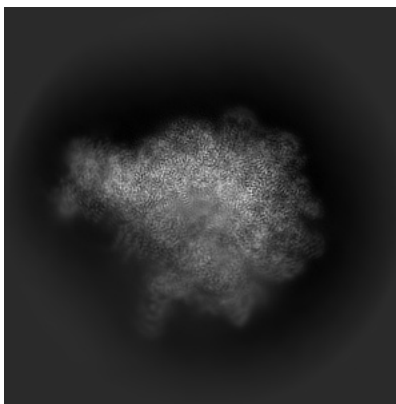
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

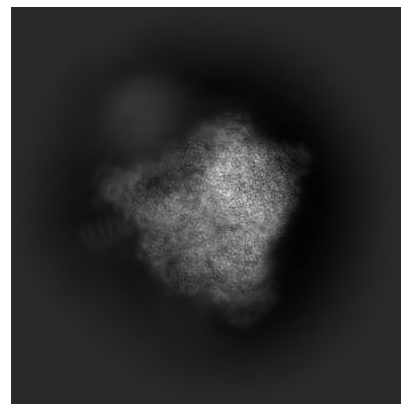
#### 6.1.1 Primary map



X

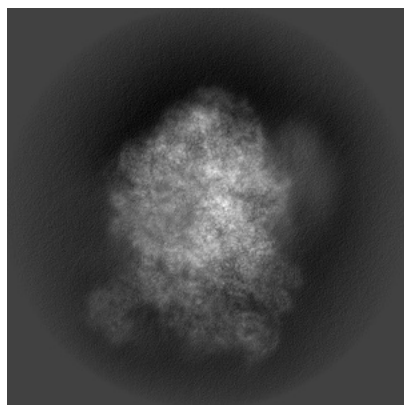


Y

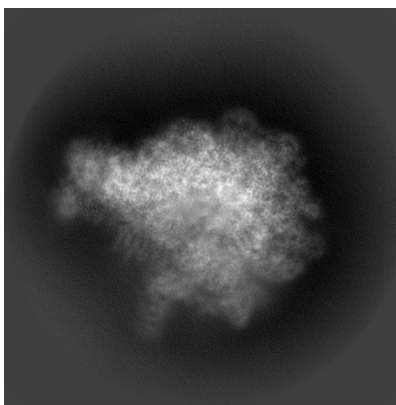


Z

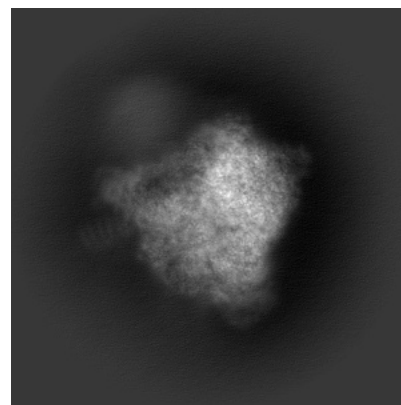
#### 6.1.2 Raw map



X



Y

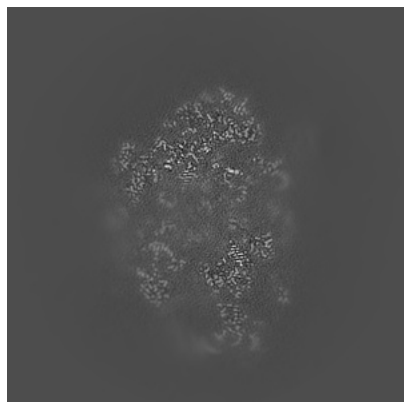


Z

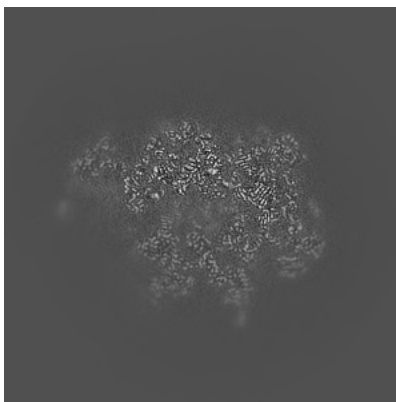
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

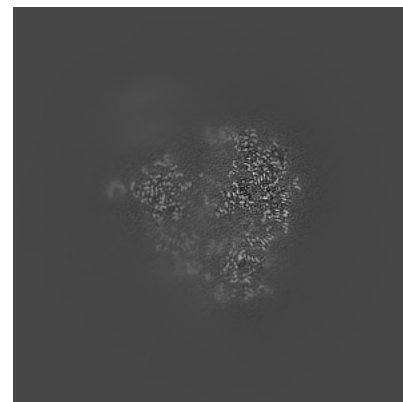
### 6.2.1 Primary map



X Index: 210

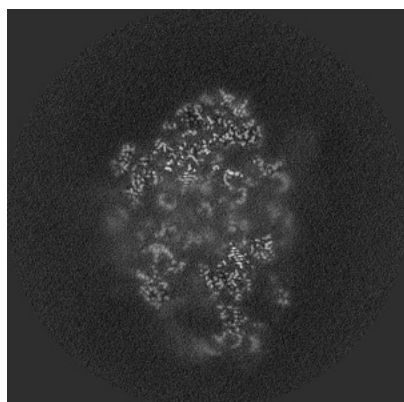


Y Index: 210

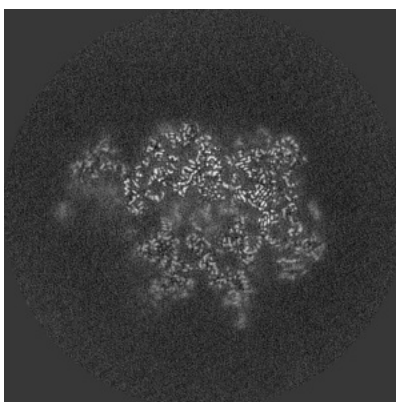


Z Index: 210

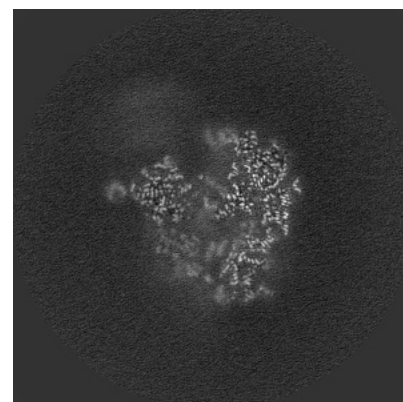
### 6.2.2 Raw map



X Index: 210



Y Index: 210

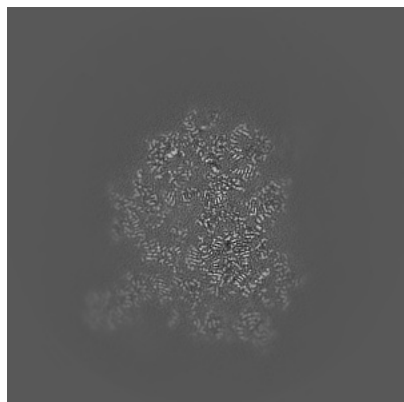


Z Index: 210

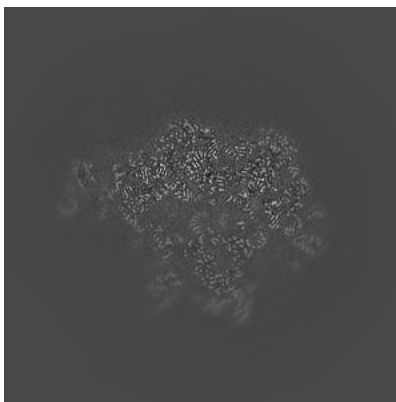
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

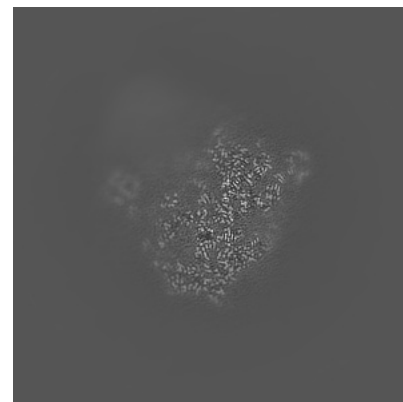
### 6.3.1 Primary map



X Index: 244

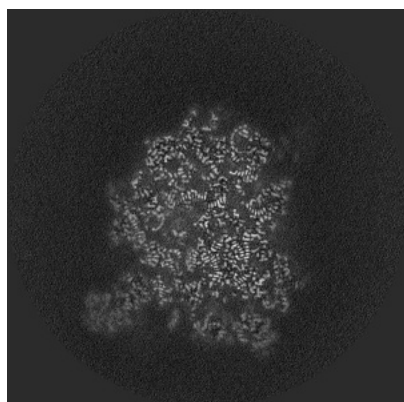


Y Index: 220

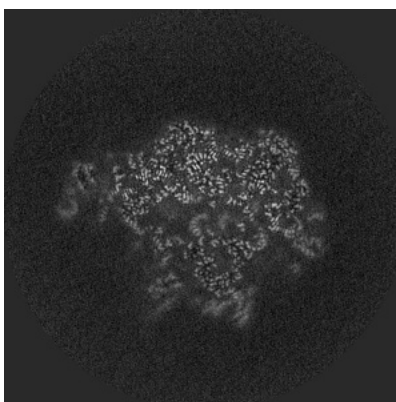


Z Index: 259

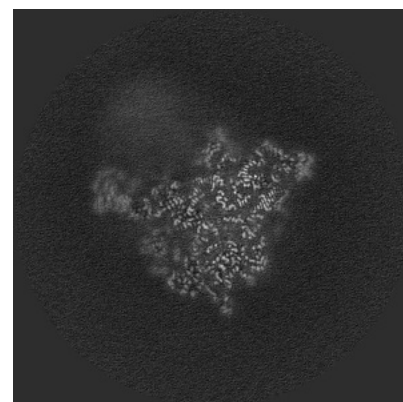
### 6.3.2 Raw map



X Index: 243



Y Index: 220

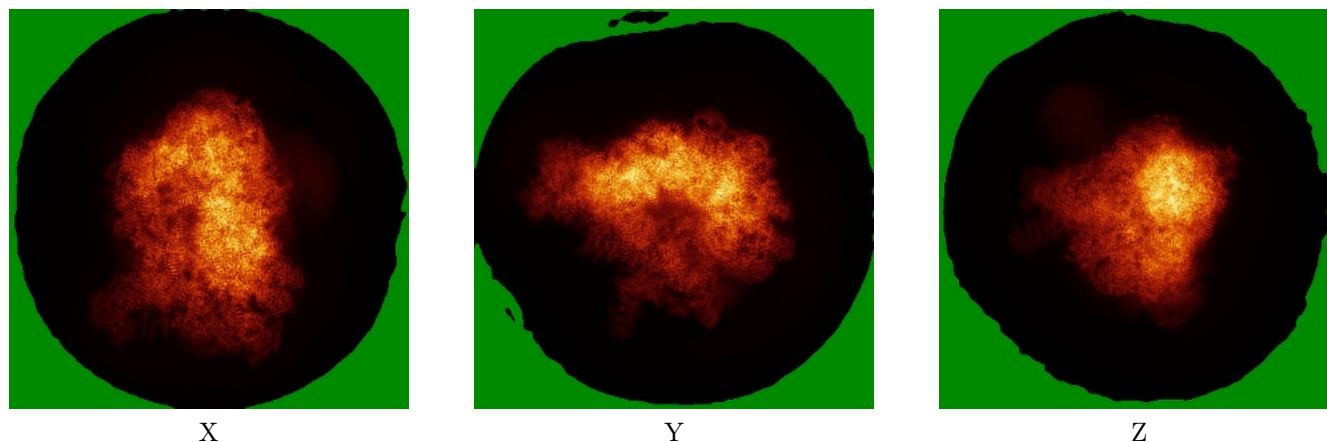


Z Index: 248

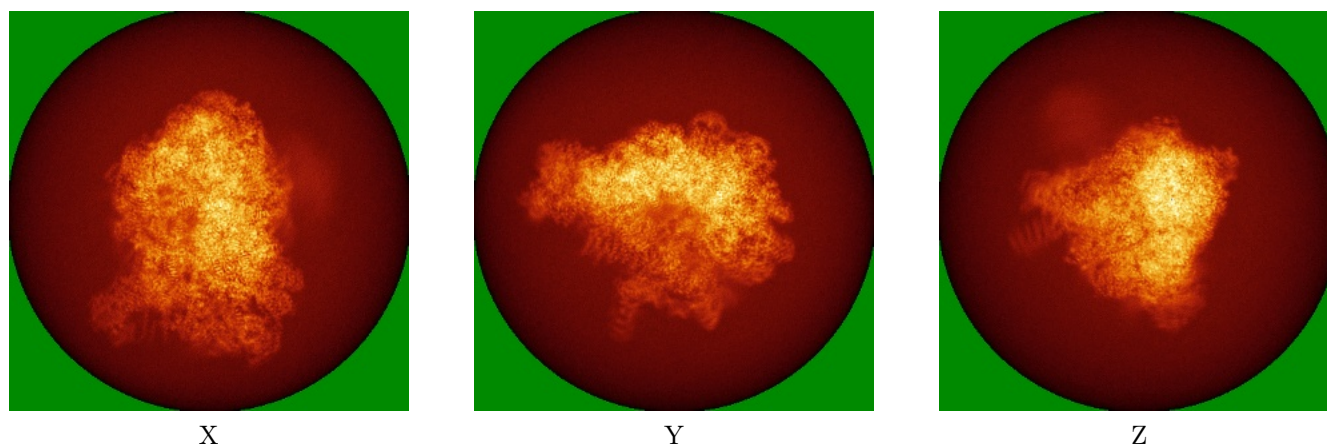
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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.

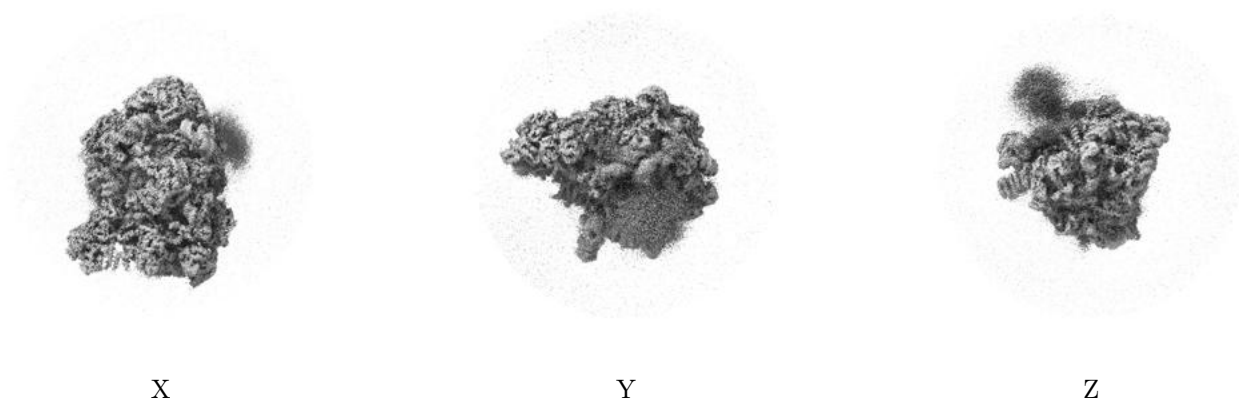
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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](#)

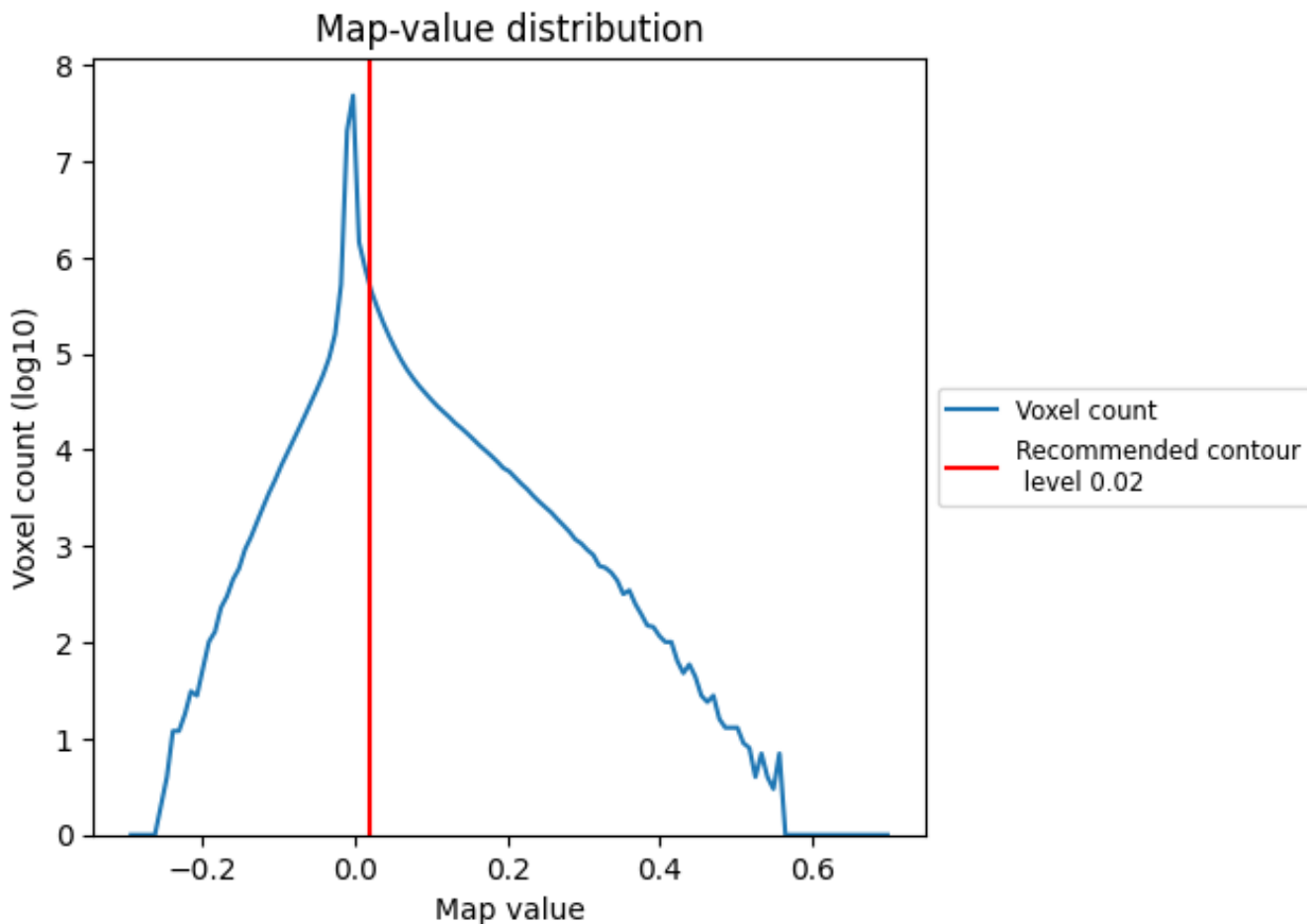
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

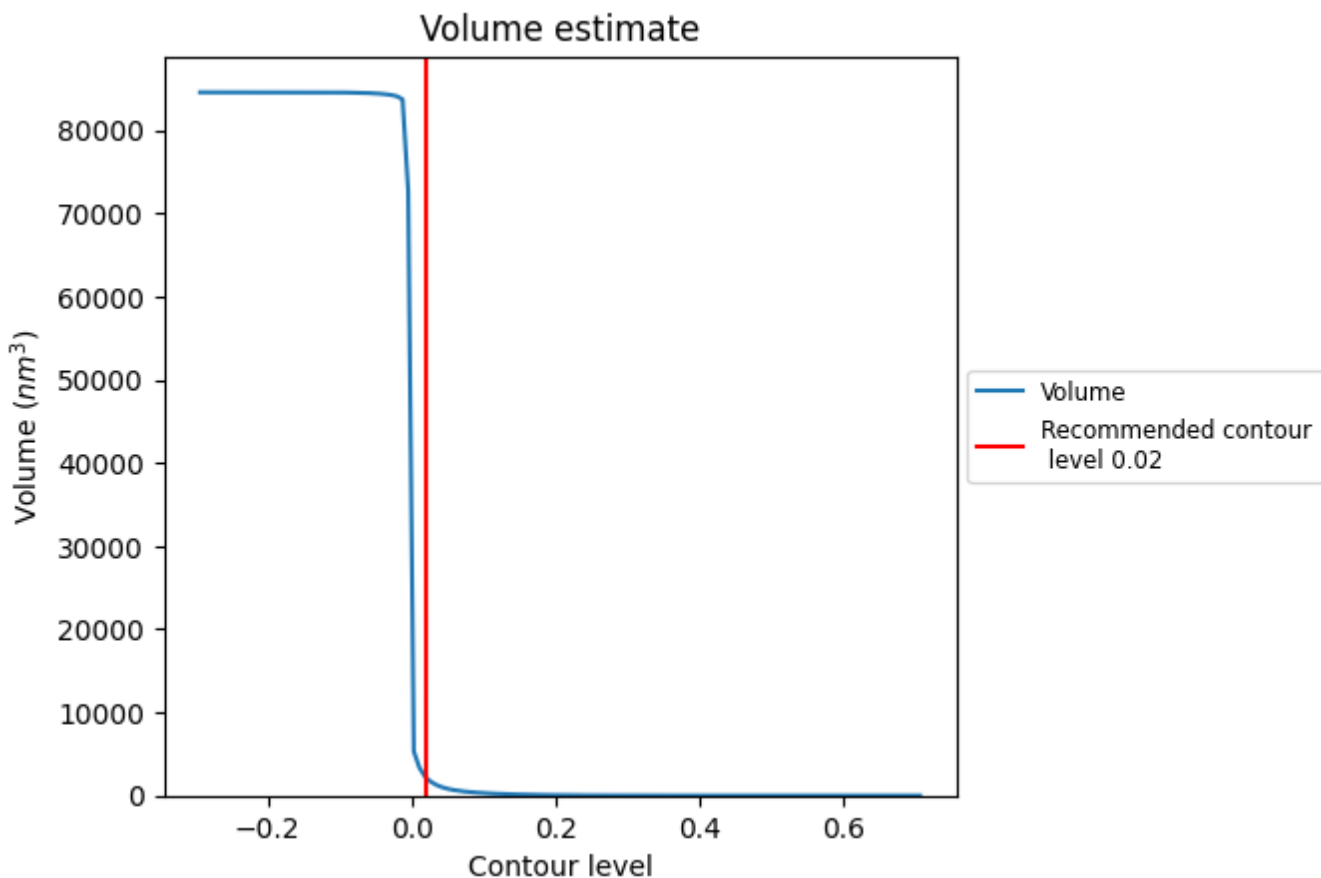
This section contains the results of statistical analysis of the map.

### 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.

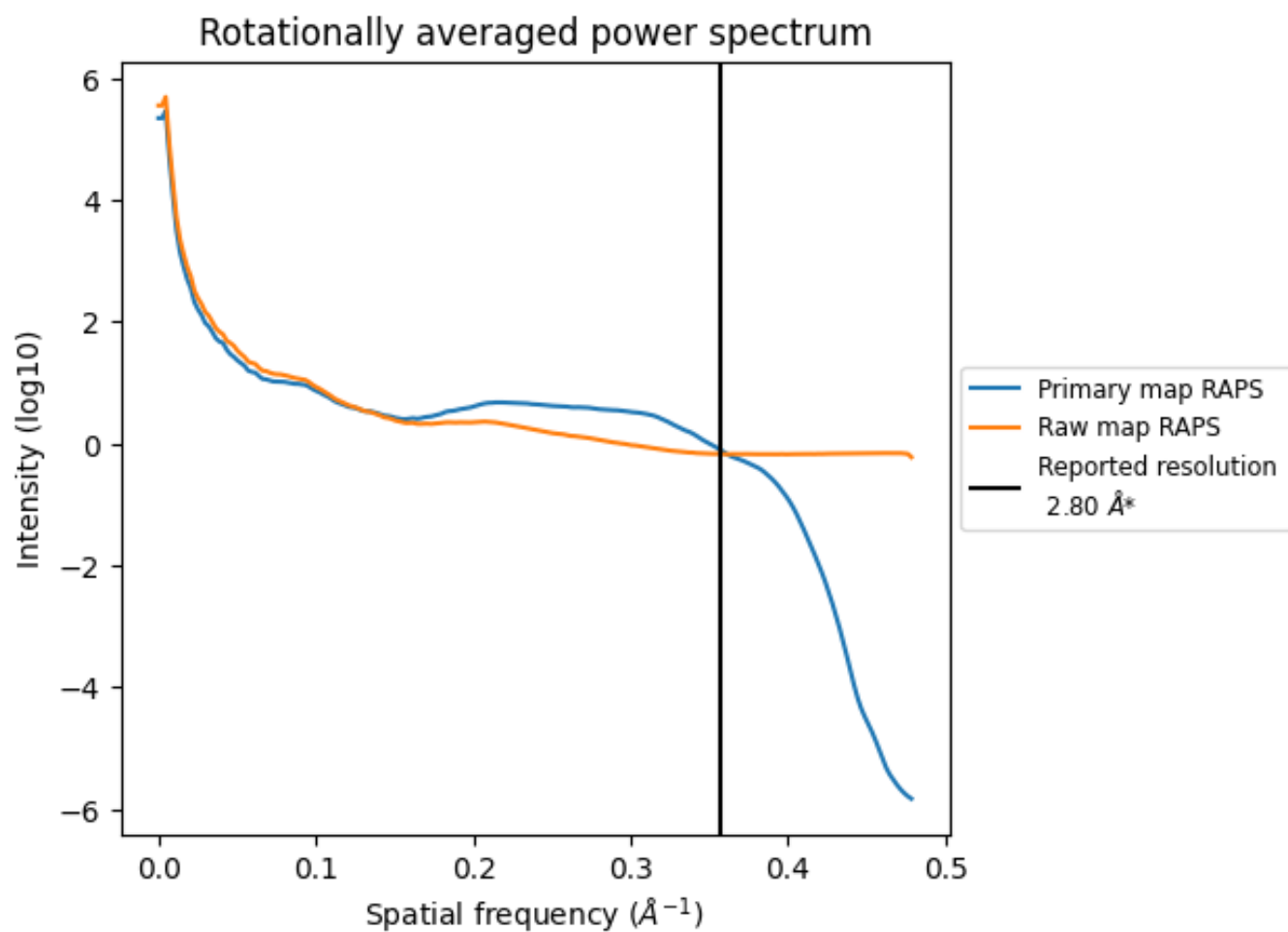
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2160  $\text{nm}^3$ ; this corresponds to an approximate mass of 1951 kDa.

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

### 7.3 Rotationally averaged power spectrum i

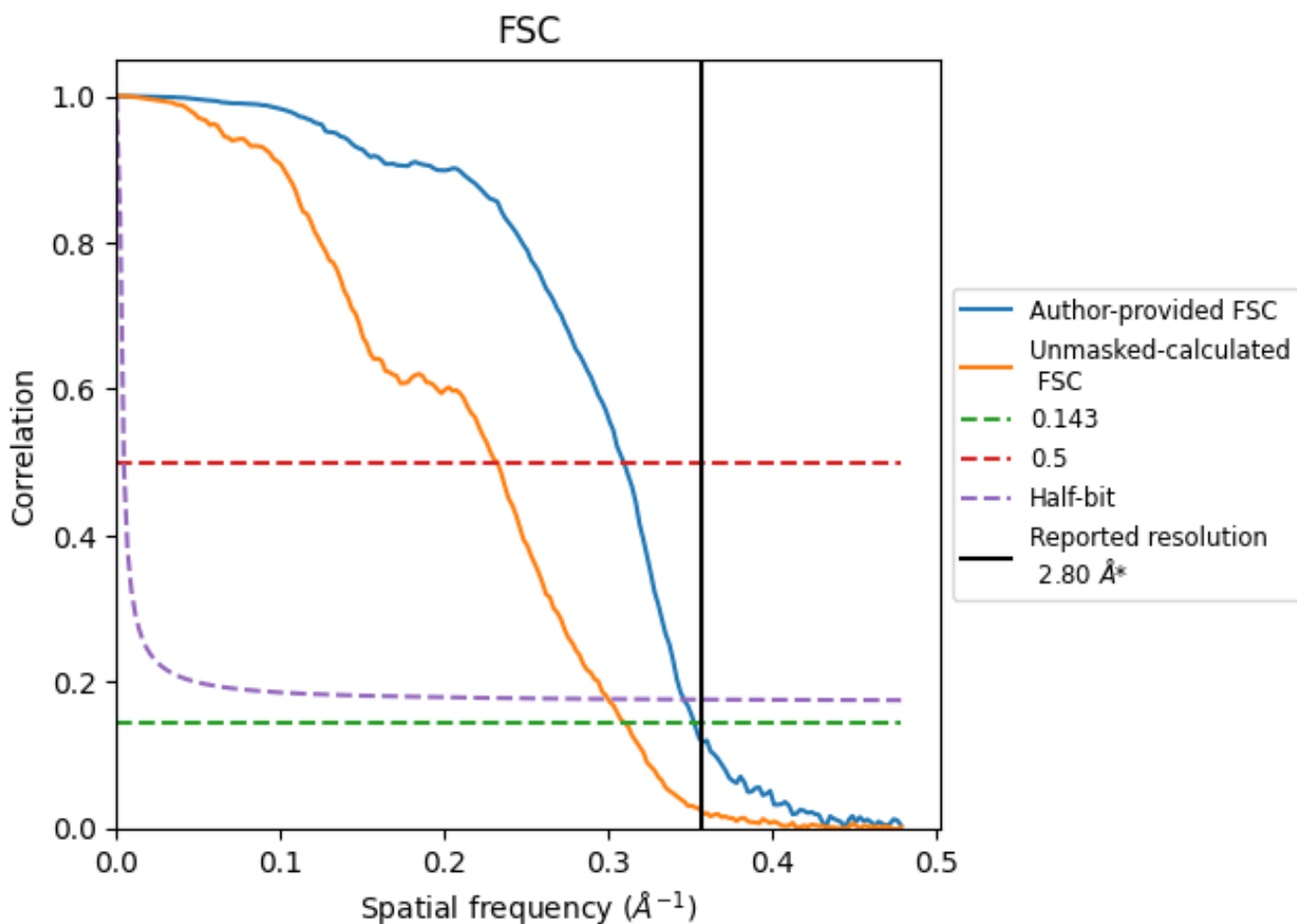


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

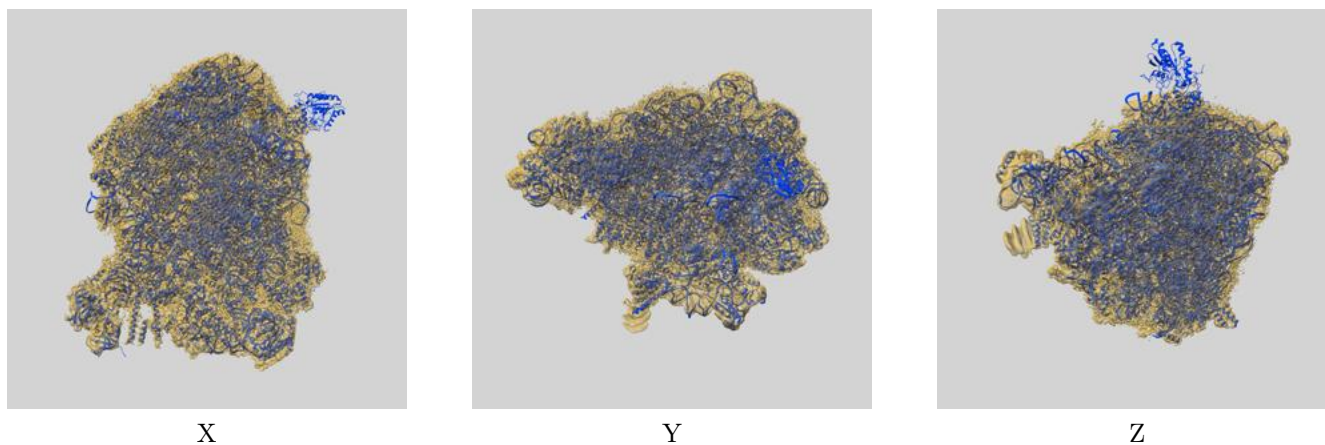
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.84	3.23	2.89
Unmasked-calculated*	3.22	4.31	3.34

\*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 3.22 differs from the reported value 2.8 by more than 10 %

## 9 Map-model fit [i](#)

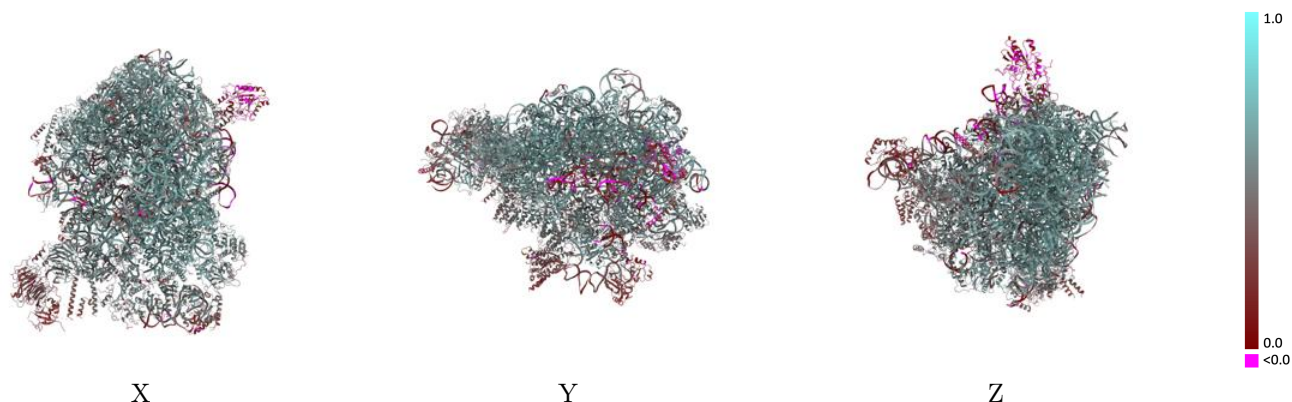
This section contains information regarding the fit between EMDB map EMD-35287 and PDB model 8I9X. Per-residue inclusion information can be found in section 3 on page 19.

### 9.1 Map-model overlay [i](#)



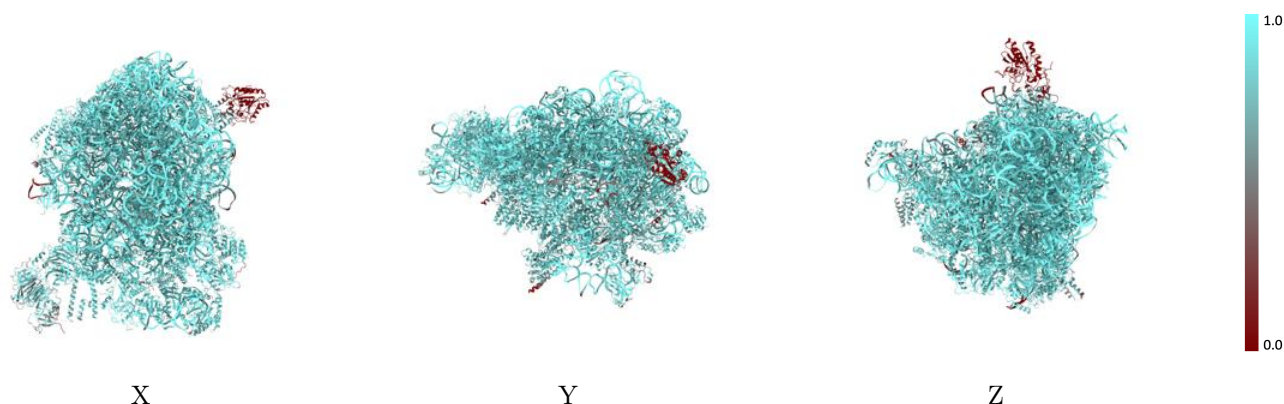
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



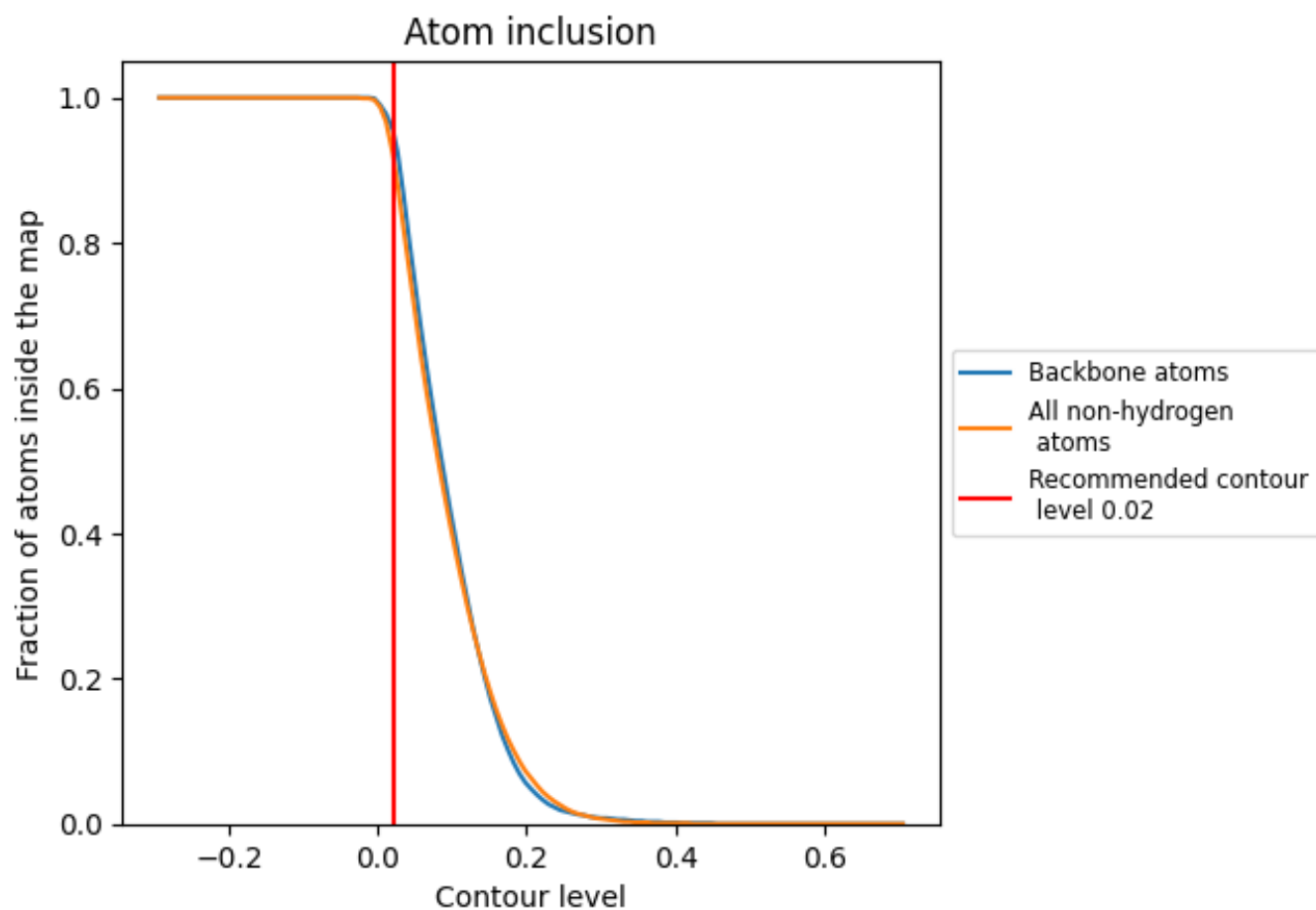
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9230	 0.5100
C1	 0.9620	 0.5330
C2	 0.9560	 0.5250
CA	 0.9650	 0.5880
CB	 0.8770	 0.4350
CC	 0.9190	 0.4980
CD	 0.7160	 0.2940
CE	 0.9120	 0.5220
CF	 0.9180	 0.4920
CG	 0.9590	 0.5500
CH	 0.9210	 0.5160
CI	 0.8830	 0.4590
CJ	 0.9080	 0.4920
CK	 0.9420	 0.5280
CL	 0.3510	 0.2110
CM	 0.8870	 0.4600
CN	 0.9580	 0.5610
CO	 0.9630	 0.5830
CP	 0.9490	 0.5390
CQ	 0.9110	 0.5060
CR	 0.9460	 0.5800
CS	 0.8710	 0.4630
CT	 0.9210	 0.4850
CU	 0.9440	 0.5460
CV	 0.9680	 0.6000
CX	 0.9210	 0.5140
CY	 0.8150	 0.3390
Cb	 0.8500	 0.3790
Cz	 0.7450	 0.3270
LB	 0.9520	 0.5710
LC	 0.9640	 0.6040
LE	 0.9470	 0.5630
LF	 0.9600	 0.5880
LG	 0.9470	 0.5890
LH	 0.9480	 0.5600



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Chain	Atom inclusion	Q-score
LK	 0.8580	 0.3800
LL	 0.9830	 0.6150
LM	 0.9690	 0.5910
LN	 0.9850	 0.6500
LO	 0.9760	 0.6200
LP	 0.9550	 0.5550
LQ	 0.9570	 0.5560
LR	 0.9330	 0.4670
LS	 0.9640	 0.5760
LT	 0.8440	 0.3240
LU	 0.9140	 0.4990
LV	 0.9420	 0.5230
LX	 0.9430	 0.5510
LY	 0.9470	 0.5760
LZ	 0.9240	 0.4980
Lc	 0.8540	 0.4250
Ld	 0.9380	 0.5570
Le	 0.9720	 0.6150
Lf	 0.9830	 0.6290
Lg	 0.9060	 0.5300
Lh	 0.9410	 0.5440
Li	 0.9520	 0.5620
Lj	 0.9820	 0.6330
Lk	 0.8810	 0.4580
Ll	 0.9480	 0.4850
Lq	 0.7320	 0.2120