



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 10:54 pm GMT

PDB ID : 6ZQG
EMDB ID : EMD-11363
Title : Cryo-EM structure of the 90S pre-ribosome from *Saccharomyces cerevisiae*, state Dis-C
Authors : Cheng, J.; Lau, B.; Venuta, G.L.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on : 2020-07-09
Resolution : 3.50 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:

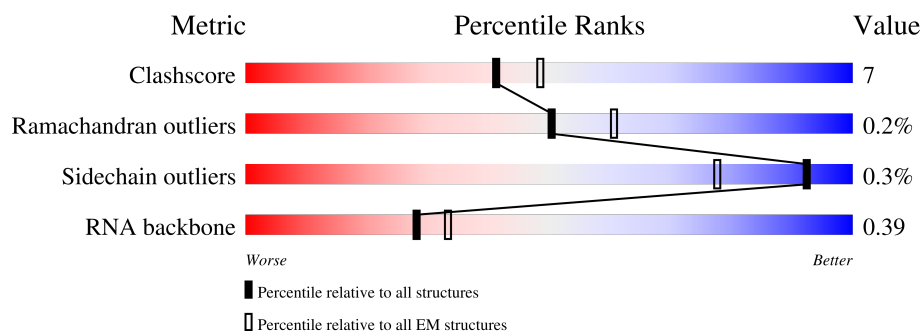
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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.





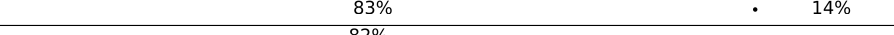




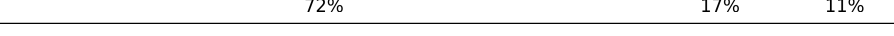




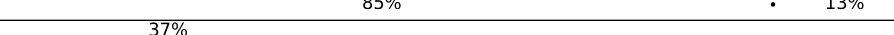




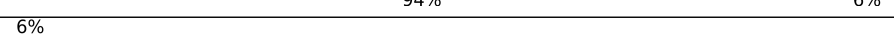
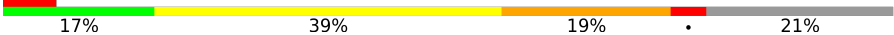



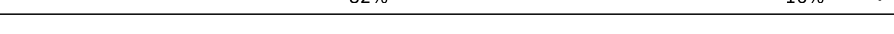






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	UB	810	
2	UC	610	
3	US	552	
4	UX	189	
5	CJ	290	
6	CK	593	
7	CL	1183	





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Mol	Chain	Length	Quality of chain
8	CM	367	
9	JF	252	
9	JG	252	
10	JH	483	
11	JL	318	
12	JJ	274	
13	DF	225	
14	DQ	143	
15	DS	147	
16	DT	144	
17	Dc	67	
18	D3	1758	
19	DA	255	
20	DE	261	
21	DG	236	
22	DH	190	
23	DI	200	
24	DJ	197	
25	DL	156	
26	DN	151	
27	DO	137	
28	DZ	108	
29	DW	130	
30	DX	145	
31	DY	135	
			
			
			
			

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Mol	Chain	Length	Quality of chain
32	Db	82	 <div>95%</div>
33	UN	899	 <div>11% 88%</div>
34	JD	1267	 <div>40% 60% 5% 35%</div>
35	D4	23	 <div>61% 30% 9%</div>
36	D5	9	 <div>33% 67%</div>

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 80072 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	UB	403	Total	C	N	O	S	0	0
			2207	1328	441	435	3		

- Molecule 2 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	UC	47	Total	C	N	O	0	0
			393	243	86	64		

- Molecule 3 is a protein called Noc4,Nucleolar complex protein 4,Noc4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	US	484	Total	C	N	O	0	0
			2411	1443	484	484		

- Molecule 4 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	UX	143	Total	C	N	O	S	0	0
			1132	729	199	194	10		

- Molecule 5 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	CJ	219	Total	C	N	O	0	0
			1083	645	219	219		

- Molecule 6 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	CK	92	Total	C	N	O	0	0
			645	398	116	131		

- Molecule 7 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CL	710	Total	C	N	O	S	0	0
			5758	3696	1019	1016	27		

- Molecule 8 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CM	360	Total	C	N	O	S	0	0
			2781	1781	473	516	11		

- Molecule 9 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	JF	216	Total	C	N	O	0	0
			1071	639	216	216		
9	JG	221	Total	C	N	O	0	0
			1096	654	221	221		

- Molecule 10 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	JH	261	Total	C	N	O	0	0
			1295	773	261	261		

- Molecule 11 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	JL	283	Total	C	N	O	S	0	0
			2262	1439	401	408	14		

- Molecule 12 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	JJ	181	Total	C	N	O	S	0	0
			1436	917	261	254	4		

- Molecule 13 is a protein called Rps5p.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	DF	196	Total	C	N	O	0	0
			970	578	196	196		

- Molecule 14 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	DQ	125	Total	C	N	O	0	0
			616	366	125	125		

- Molecule 15 is a protein called 40S ribosomal protein S18-A,40S ribosomal protein S18-A,Rps18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	DS	77	Total	C	N	O	S	0	0
			630	403	115	110	2		

- Molecule 16 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	DT	143	Total	C	N	O	0	0
			700	414	143	143		

- Molecule 17 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Dc	63	Total	C	N	O	0	0
			310	184	63	63		

- Molecule 18 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D3	1387	Total	C	N	O	P	0	0
			29536	13208	5223	9718	1387		

- Molecule 19 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	DA	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 20 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 21 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	DG	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 22 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DH	184	Total	C	N	O		0	0
			1481	951	265	265			

- Molecule 23 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	DI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 24 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	DJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 25 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	DL	143	Total	C	N	O	S	0	0
			1154	739	218	194	3		

- Molecule 26 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	DN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 27 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	DO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 28 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	DZ	67	Total	C	N	O	0	0
			332	198	67	67		

- Molecule 29 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	DW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 30 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	DX	143	Total	C	N	O	S	0	0
			1115	705	219	189	2		

- Molecule 31 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	DY	133	Total	C	N	O	0	0
			1067	673	207	187		

- Molecule 32 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Db	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 33 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	UN	108	Total	C	N	O	S	0	0
			920	561	184	165	10		

- Molecule 34 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	JD	829	Total	C	N	O	S	0	0
			4600	2795	916	887	2		

- Molecule 35 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	D4	23	Total	C	N	O	P	0	0
			496	220	87	165	24		

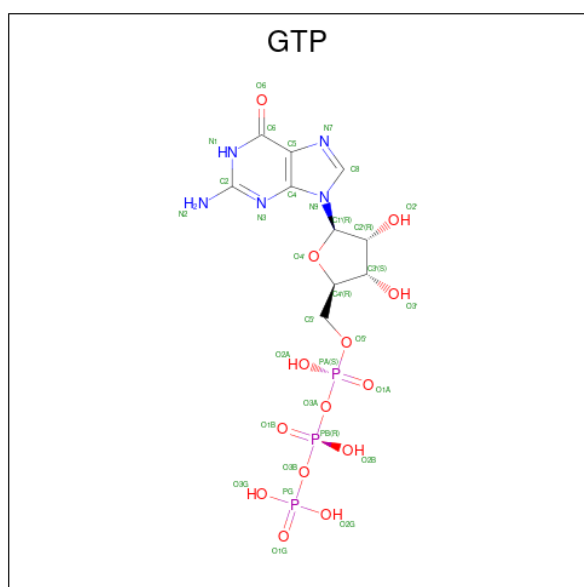
- Molecule 36 is a RNA chain called Poly-U RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	D5	9	Total	C	N	O	P	0	0
			180	81	18	72	9		

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	UX	1	Total	Zn	0
			1	1	

- Molecule 38 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
38	CL	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	CL	1	Total	Mg	0
			1	1	

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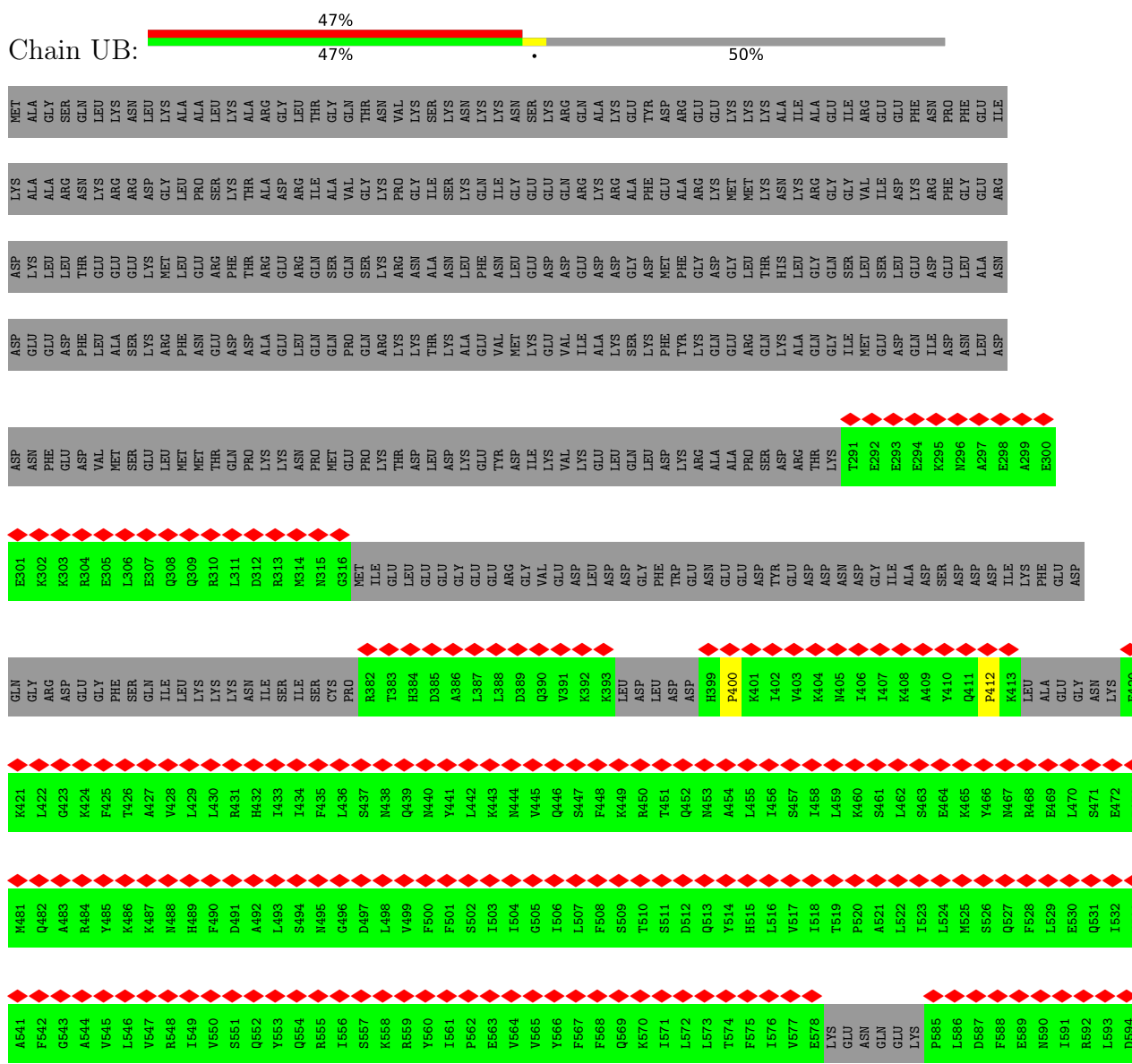
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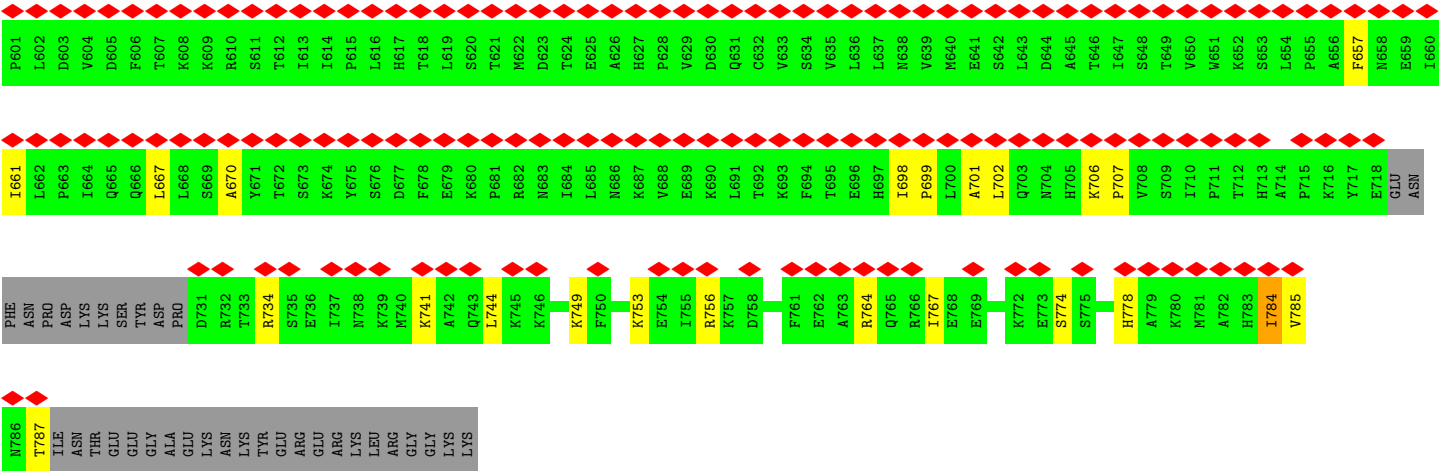
Mol	Chain	Residues	Atoms		AltConf
39	D3	37	Total	Mg	0
			37	37	
39	DG	1	Total	Mg	0
			1	1	

3 Residue-property plots

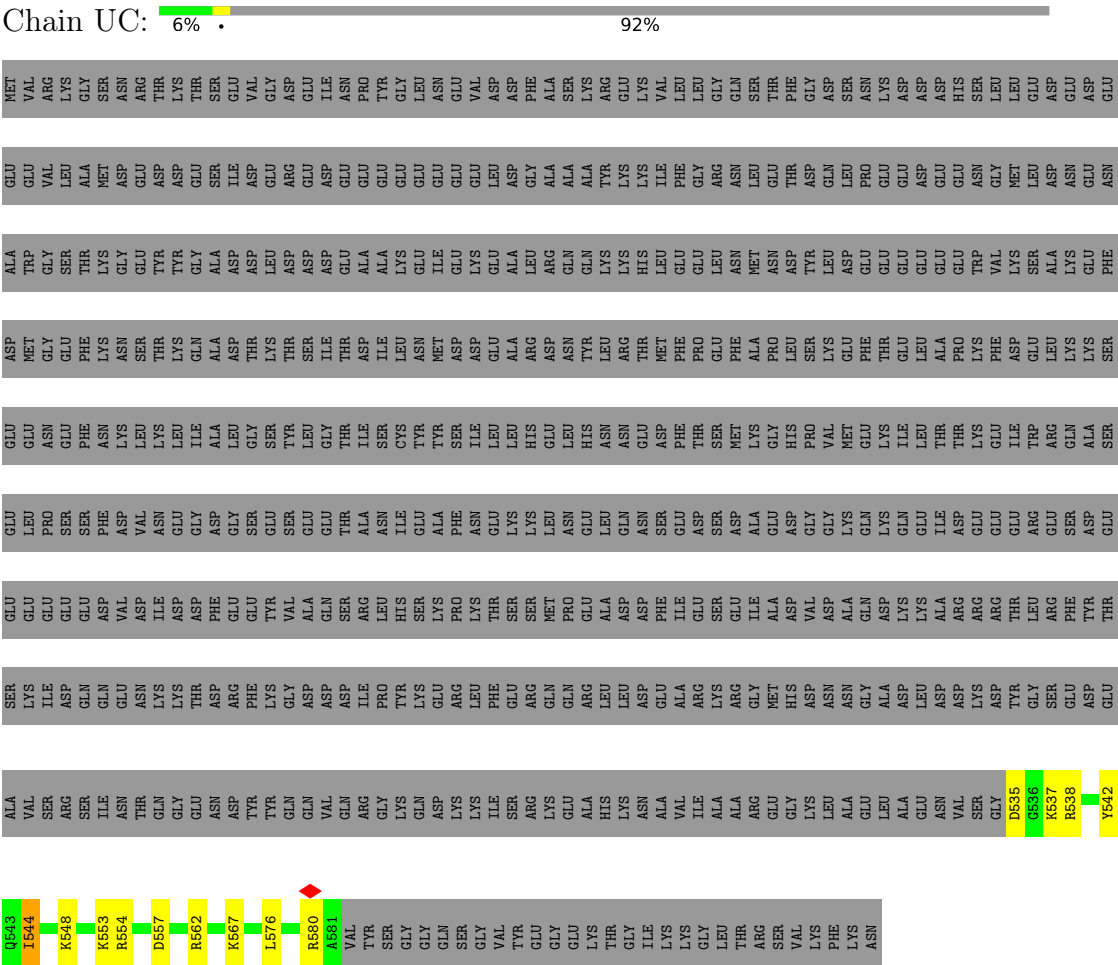
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Nucleolar complex protein 14

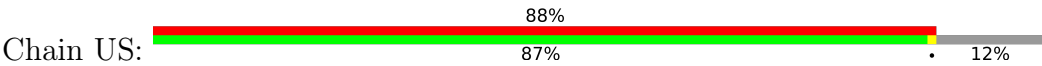


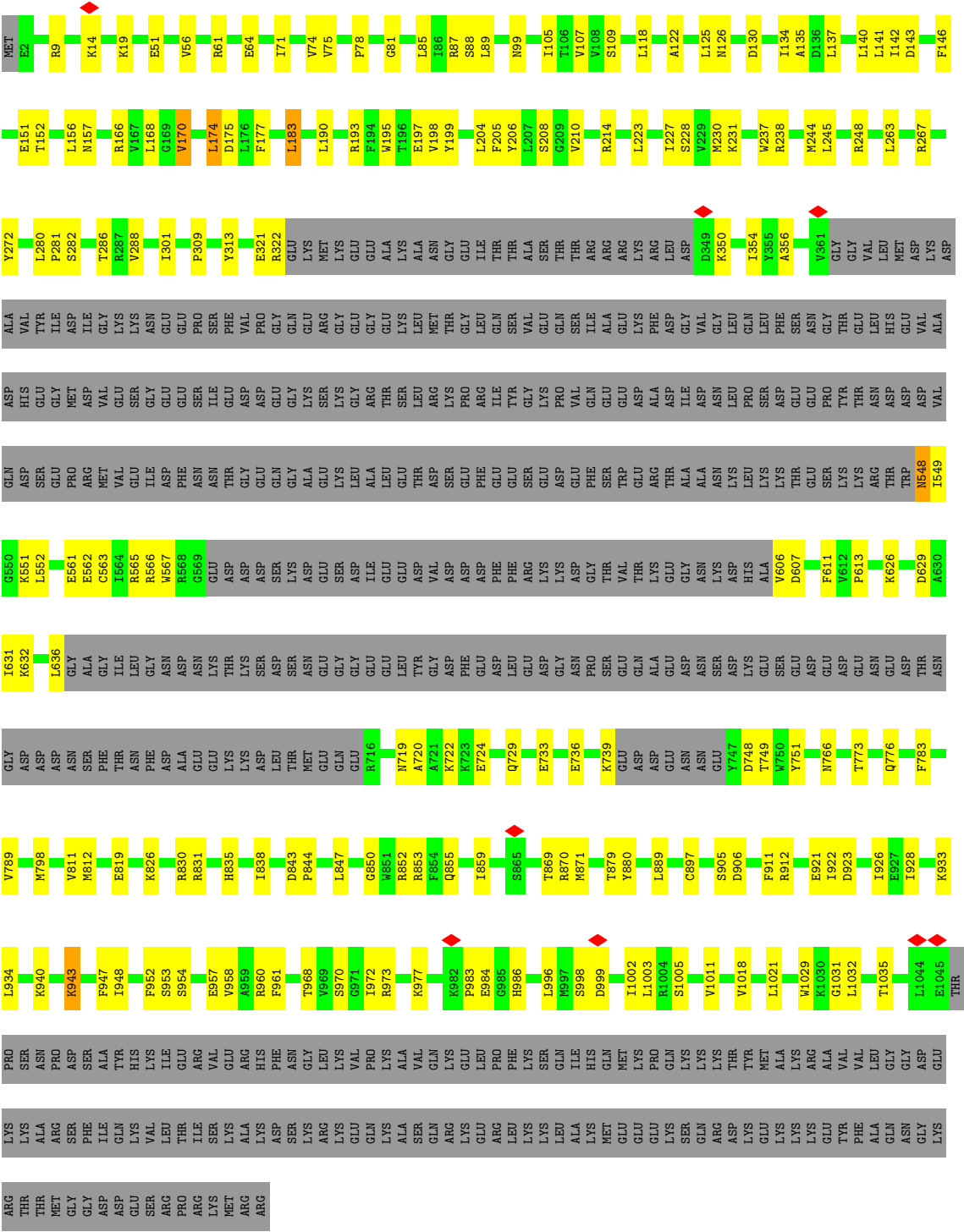


● Molecule 2: Something about silencing protein 10

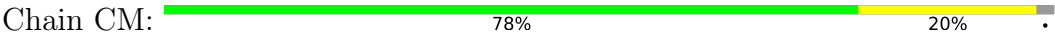


● Molecule 3: Noc4,Nucleolar complex protein 4,Noc4



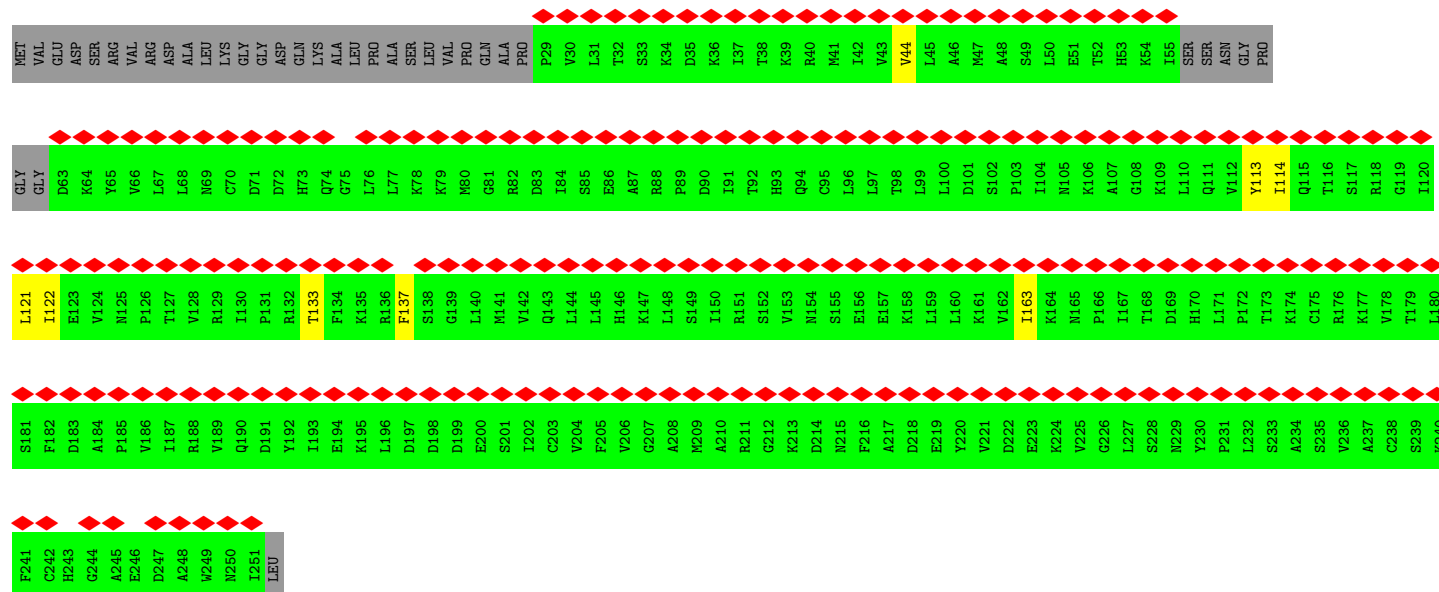
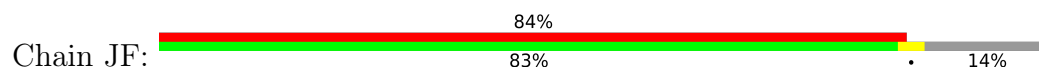


● Molecule 8: RNA 3'-terminal phosphate cyclase-like protein

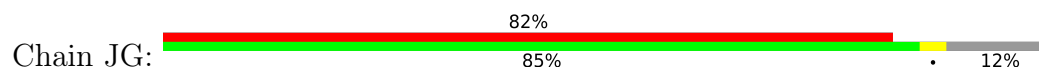




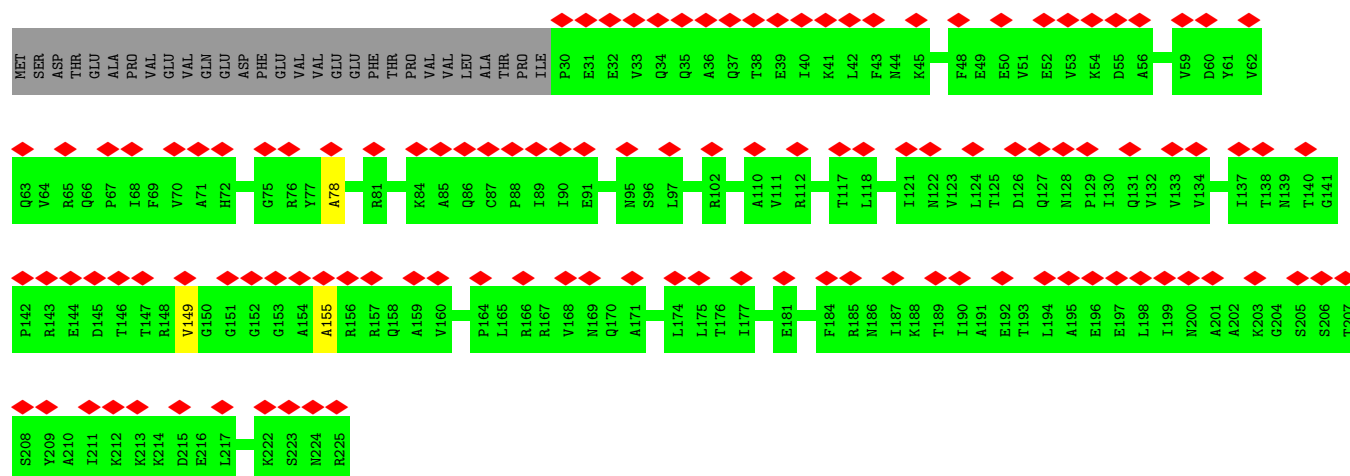
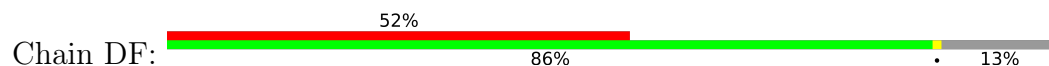
• Molecule 9: Ribosomal RNA small subunit methyltransferase NEP1



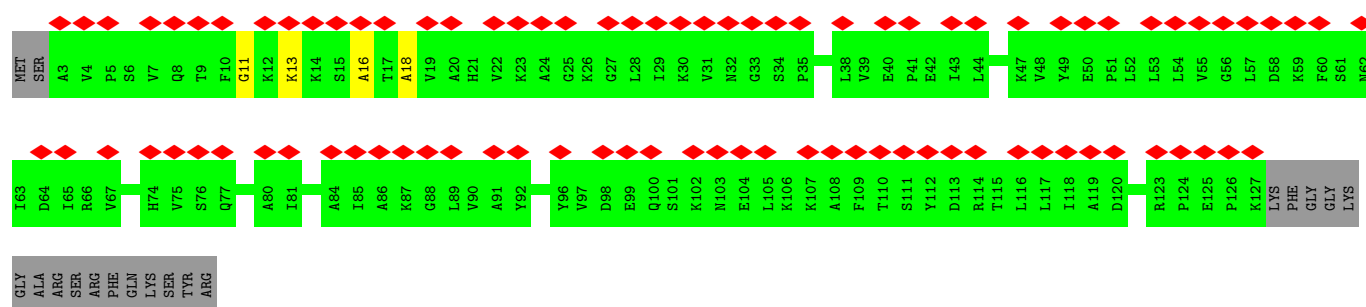
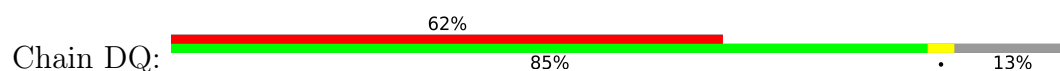
• Molecule 9: Ribosomal RNA small subunit methyltransferase NEP1



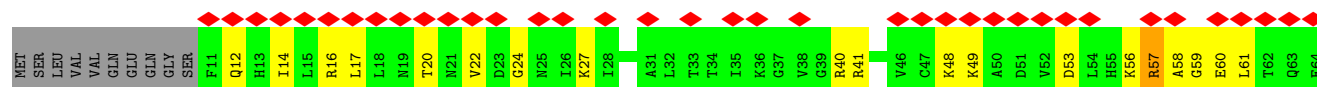
- Molecule 13: Rps5p

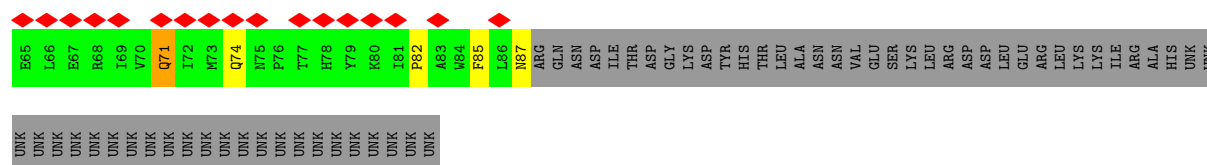


- Molecule 14: 40S ribosomal protein S16-A

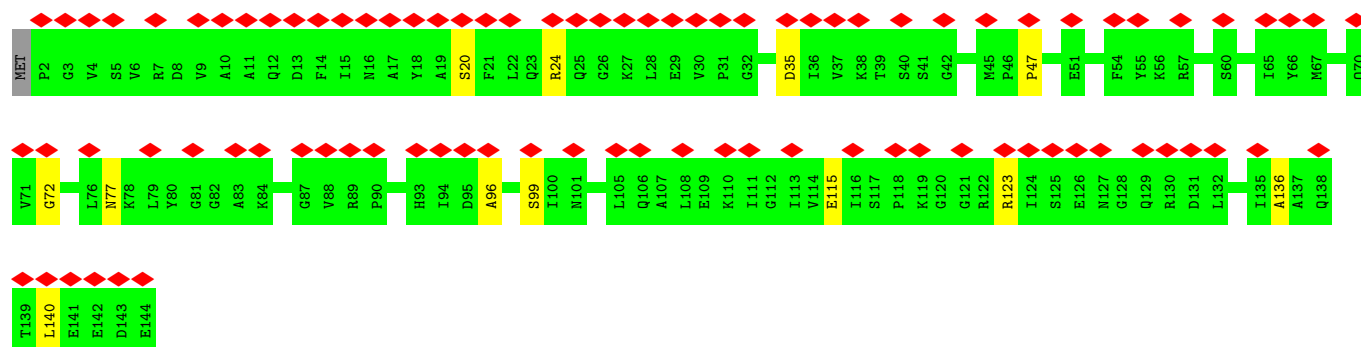


- Molecule 15: 40S ribosomal protein S18-A,40S ribosomal protein S18-A,Rps18

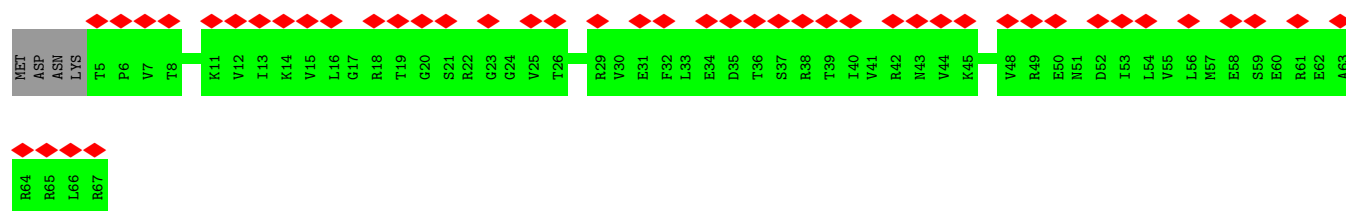




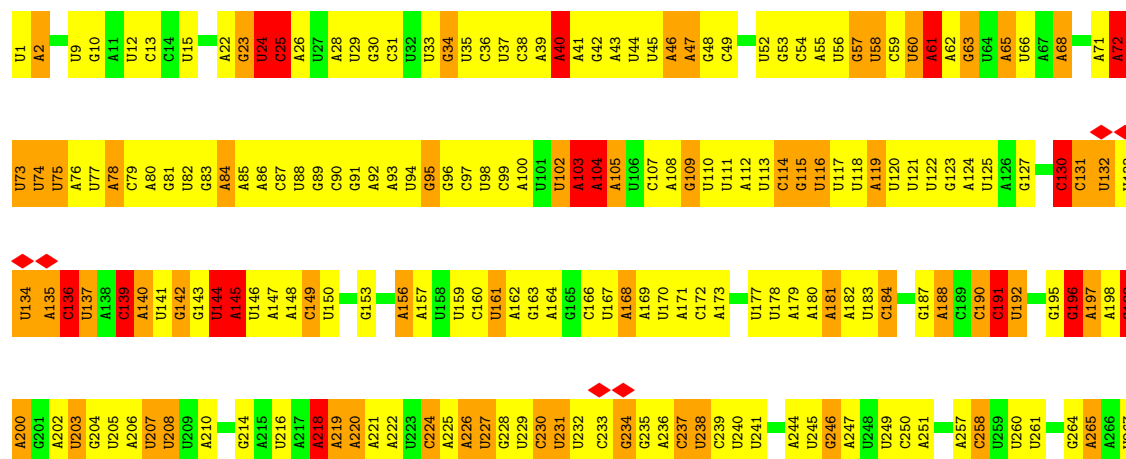
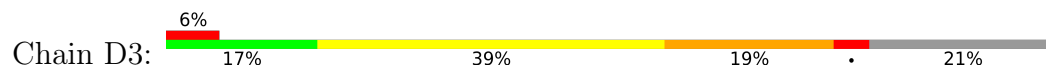
• Molecule 16: 40S ribosomal protein S19-A



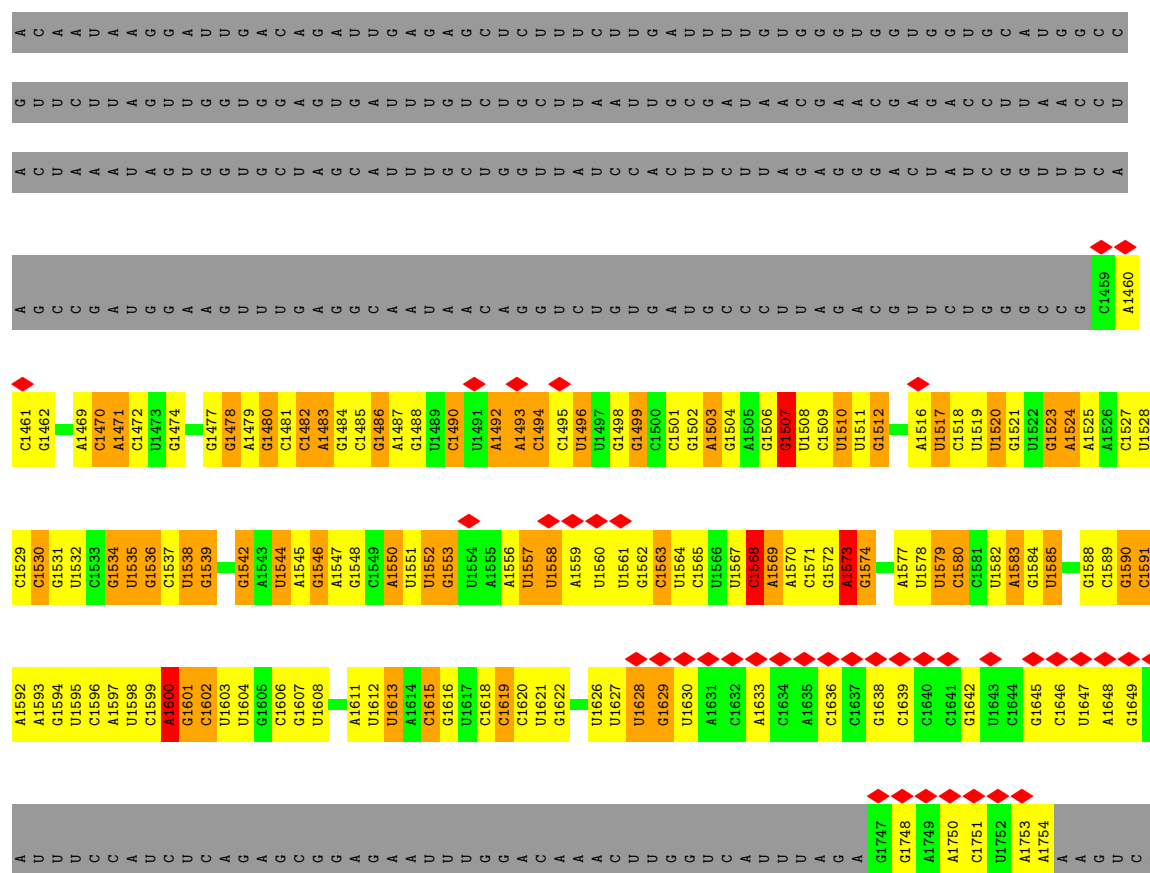
• Molecule 17: 40S ribosomal protein S28-A



• Molecule 18: 18S rRNA

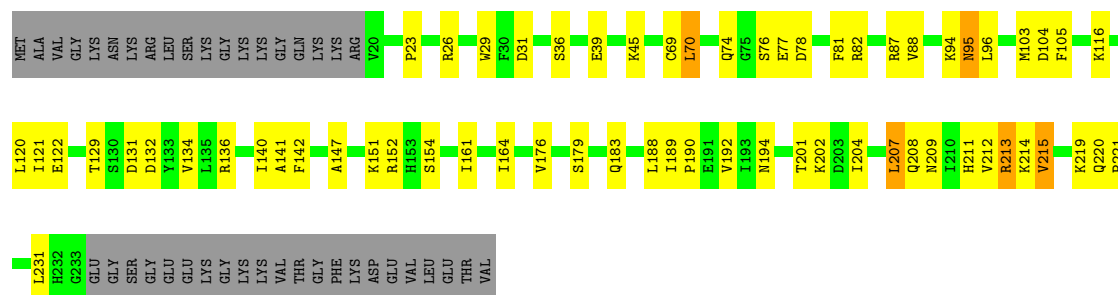






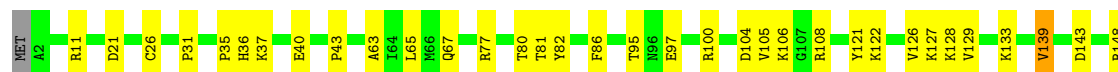
• Molecule 19: 40S ribosomal protein S1-A

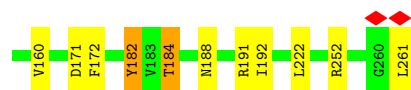
Chain DA: 59% 23% 16%



• Molecule 20: 40S ribosomal protein S4-A

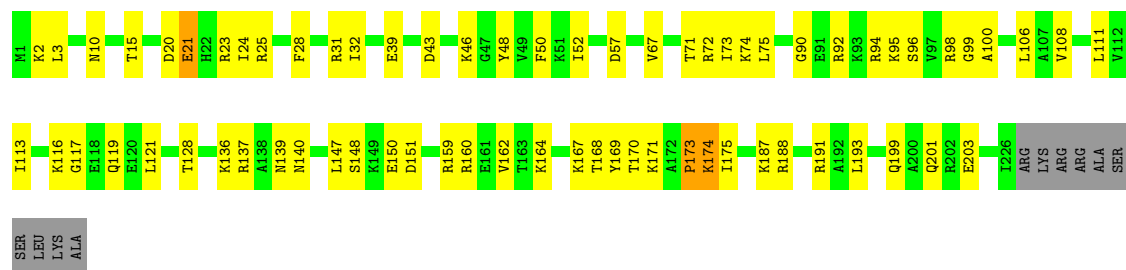
Chain DE: 82% 16% 2%





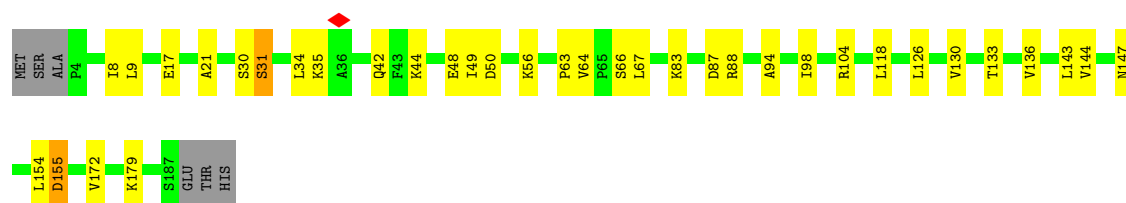
- Molecule 21: 40S ribosomal protein S6-A

Chain DG: 67% 28% . .



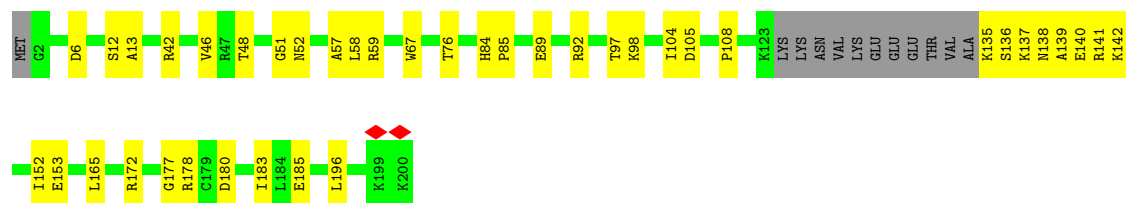
- Molecule 22: 40S ribosomal protein S7-A

Chain DH: 78% 18% . .



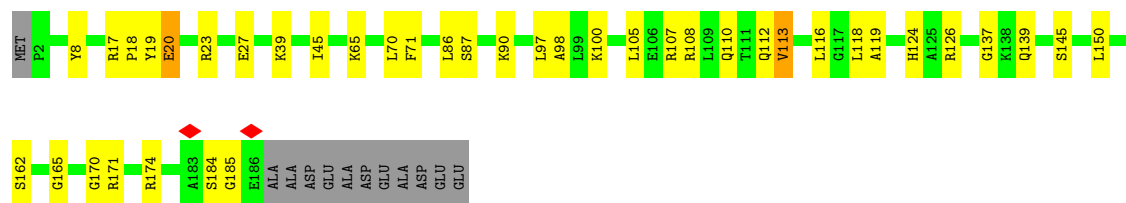
- Molecule 23: 40S ribosomal protein S8-A

Chain DI: 74% 20% 6%

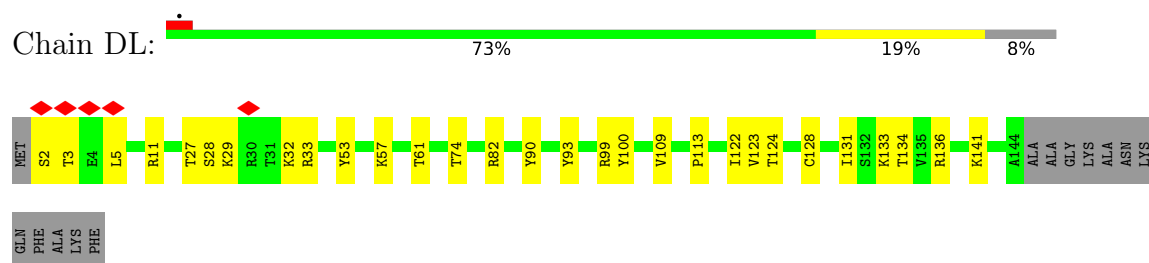


- Molecule 24: 40S ribosomal protein S9-A

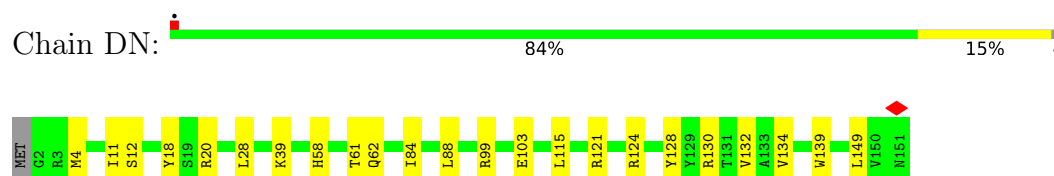
Chain DJ: 74% 19% 6%



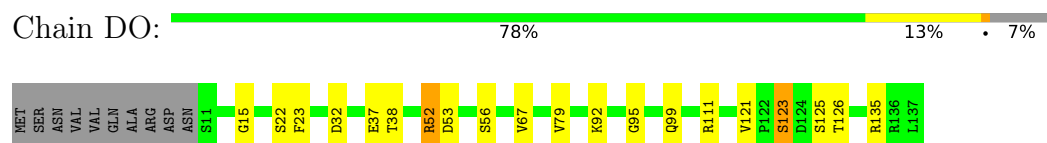
- Molecule 25: 40S ribosomal protein S11-A



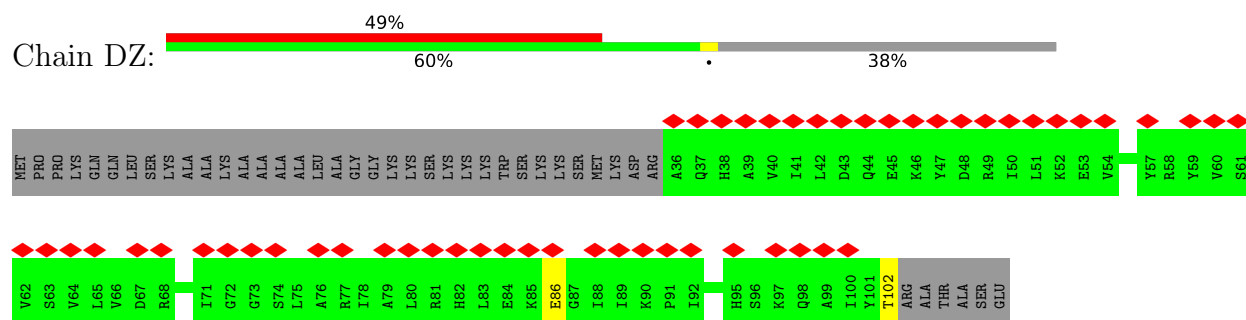
- Molecule 26: 40S ribosomal protein S13



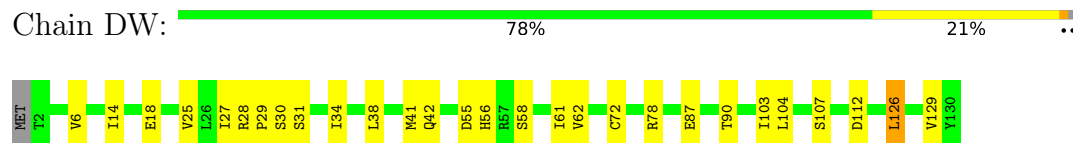
- Molecule 27: 40S ribosomal protein S14-A



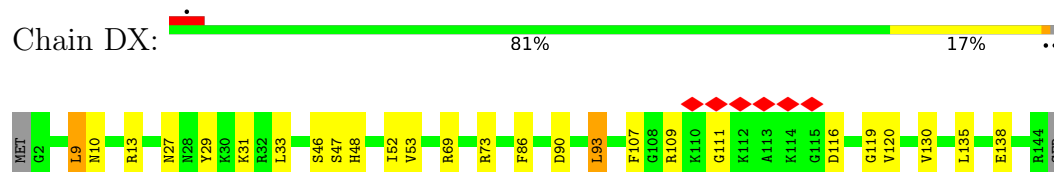
- Molecule 28: 40S ribosomal protein S25-A



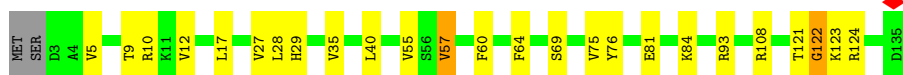
- Molecule 29: 40S ribosomal protein S22-A



- Molecule 30: 40S ribosomal protein S23-A



- Molecule 31: 40S ribosomal protein S24-A



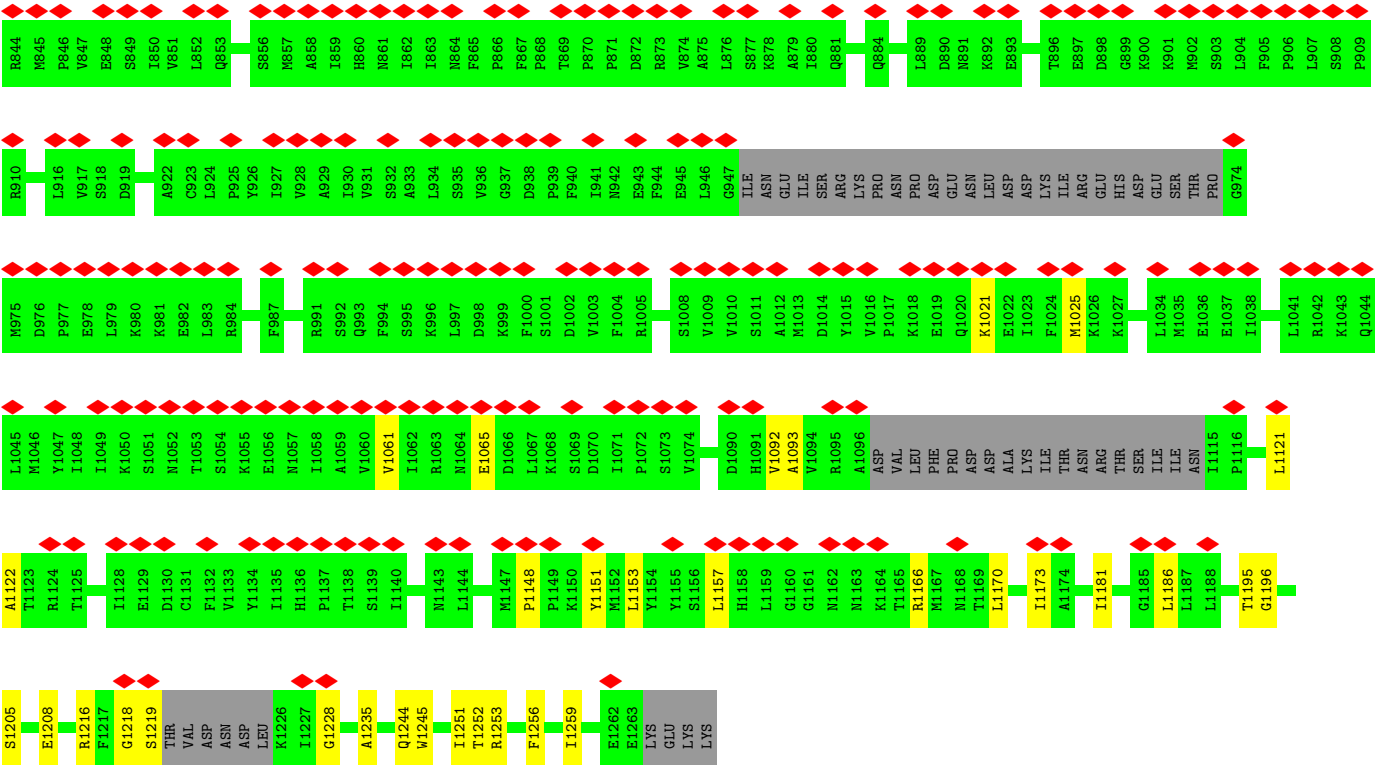
-

- Chain UN:  11% . 88%

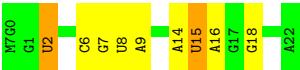


Chain JD:

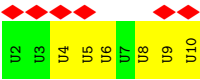




• Molecule 35: U3 snoRNA



• Molecule 36: Poly-U RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102097	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	508.32, 508.32, 508.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, M7G, MG, ZN

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	UB	0.27	0/2206	0.47	3/3035 (0.1%)
2	UC	0.85	0/395	0.83	1/517 (0.2%)
3	US	0.23	0/2406	0.38	2/3355 (0.1%)
4	UX	0.91	3/1154 (0.3%)	0.82	2/1557 (0.1%)
5	CJ	0.30	0/1082	0.62	0/1506
6	CK	0.47	0/649	0.67	0/877
7	CL	0.99	12/5887 (0.2%)	0.85	13/7931 (0.2%)
8	CM	0.92	0/2832	0.76	1/3825 (0.0%)
9	JF	0.24	0/1069	0.44	0/1488
9	JG	0.23	0/1094	0.45	0/1523
10	JH	0.24	0/1293	0.37	0/1801
11	JL	0.96	4/2305 (0.2%)	0.77	0/3116
12	JJ	0.86	0/1462	0.83	1/1969 (0.1%)
13	DF	0.24	0/969	0.44	0/1349
14	DQ	0.24	0/615	0.46	0/854
15	DS	0.26	0/641	0.56	0/866
16	DT	0.25	0/699	0.40	0/968
17	Dc	0.25	0/309	0.49	0/428
18	D3	2.08	1291/33028 (3.9%)	1.51	628/51447 (1.2%)
19	DA	0.91	1/1735 (0.1%)	0.84	2/2335 (0.1%)
20	DE	1.27	10/2109 (0.5%)	0.90	1/2839 (0.0%)
21	DG	0.78	0/1823	0.77	1/2439 (0.0%)
22	DH	0.74	1/1506 (0.1%)	0.77	1/2028 (0.0%)
23	DI	1.01	1/1514 (0.1%)	0.86	3/2021 (0.1%)
24	DJ	1.10	4/1519 (0.3%)	0.93	3/2035 (0.1%)
25	DL	1.38	8/1180 (0.7%)	0.85	1/1591 (0.1%)
26	DN	1.03	2/1215 (0.2%)	0.90	3/1638 (0.2%)
27	DO	0.94	1/952 (0.1%)	0.91	0/1279
28	DZ	0.27	0/331	0.56	0/460
29	DW	1.27	1/1038 (0.1%)	0.96	4/1395 (0.3%)
30	DX	1.17	3/1133 (0.3%)	0.94	3/1510 (0.2%)
31	DY	1.21	3/1081 (0.3%)	0.85	1/1441 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Db	0.92	0/620	0.83	1/838 (0.1%)
33	UN	0.78	0/926	0.78	1/1213 (0.1%)
34	JD	0.45	0/4616	0.63	2/6348 (0.0%)
35	D4	1.78	2/521 (0.4%)	1.21	0/809
36	D5	0.28	0/197	1.00	0/302
All	All	1.46	1347/84111 (1.6%)	1.14	678/120933 (0.6%)

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
1	UB	0	1
7	CL	0	1
11	JL	0	1
19	DA	0	3
22	DH	0	4
23	DI	0	1
24	DJ	0	2
25	DL	0	1
26	DN	0	1
27	DO	0	2
31	DY	0	2
32	Db	0	2
33	UN	0	1
34	JD	0	3
All	All	0	25

The worst 5 of 1347 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	621	A	N9-C4	-10.39	1.31	1.37
18	D3	387	A	N9-C4	-10.38	1.31	1.37
18	D3	387	A	N7-C5	-10.18	1.33	1.39
18	D3	621	A	N3-C4	-9.77	1.28	1.34
18	D3	1103	U	C2-N3	-9.54	1.31	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	44	U	N3-C4-O4	-13.16	110.19	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	453	U	N1-C2-O2	12.13	131.29	122.80
18	D3	507	U	N3-C2-O2	-11.72	113.99	122.20
18	D3	44	U	C5-C4-O4	11.71	132.93	125.90
18	D3	453	U	C2-N1-C1'	11.62	131.64	117.70

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	CL	51	GLU	Peptide
19	DA	147	ALA	Peptide
19	DA	69	CYS	Peptide
11	JL	233	ARG	Peptide
1	UB	784	ILE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	UB	2207	0	1231	22	0
2	UC	393	0	444	10	0
3	US	2411	0	1035	7	0
4	UX	1132	0	1186	16	0
5	CJ	1083	0	478	11	0
6	CK	645	0	541	18	0
7	CL	5758	0	5885	119	0
8	CM	2781	0	2878	49	0
9	JF	1071	0	467	5	0
9	JG	1096	0	478	4	0
10	JH	1295	0	570	0	0
11	JL	2262	0	2330	30	0
12	JJ	1436	0	1515	22	0
13	DF	970	0	462	2	0
14	DQ	616	0	285	3	0
15	DS	630	0	652	16	0
16	DT	700	0	334	8	0
17	Dc	310	0	134	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	D3	29536	0	14872	424	0
19	DA	1709	0	1784	42	0
20	DE	2068	0	2154	26	0
21	DG	1799	0	1879	49	0
22	DH	1481	0	1572	23	0
23	DI	1489	0	1525	25	0
24	DJ	1494	0	1573	23	0
25	DL	1154	0	1220	14	0
26	DN	1192	0	1255	10	0
27	DO	941	0	979	13	0
28	DZ	332	0	149	1	0
29	DW	1021	0	1060	22	0
30	DX	1115	0	1191	16	0
31	DY	1067	0	1127	19	0
32	Db	610	0	633	0	0
33	UN	920	0	972	6	0
34	JD	4600	0	2789	36	0
35	D4	496	0	253	2	0
36	D5	180	0	91	0	0
37	UX	1	0	0	0	0
38	CL	32	0	12	1	0
39	CL	1	0	0	0	0
39	D3	37	0	0	0	0
39	DG	1	0	0	0	0
All	All	80072	0	57995	973	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 973 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UB:701:ALA:HB2	3:US:417:HIS:HA	1.27	1.14
18:D3:187:G:N2	18:D3:198:A:N7	2.04	1.06
18:D3:736:C:H6	18:D3:736:C:H5'	1.24	1.02
1:UB:701:ALA:CB	3:US:417:HIS:HA	1.91	1.00
18:D3:895:G:H1	18:D3:917:U:H3	1.02	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UB	391/810 (48%)	372 (95%)	14 (4%)	5 (1%)	12	48
2	UC	45/610 (7%)	40 (89%)	5 (11%)	0	100	100
3	US	474/552 (86%)	463 (98%)	11 (2%)	0	100	100
4	UX	141/189 (75%)	124 (88%)	17 (12%)	0	100	100
5	CJ	217/290 (75%)	195 (90%)	22 (10%)	0	100	100
6	CK	90/593 (15%)	83 (92%)	7 (8%)	0	100	100
7	CL	698/1183 (59%)	633 (91%)	64 (9%)	1 (0%)	51	84
8	CM	358/367 (98%)	326 (91%)	32 (9%)	0	100	100
9	JF	212/252 (84%)	211 (100%)	1 (0%)	0	100	100
9	JG	217/252 (86%)	209 (96%)	8 (4%)	0	100	100
10	JH	257/483 (53%)	252 (98%)	5 (2%)	0	100	100
11	JL	281/318 (88%)	260 (92%)	21 (8%)	0	100	100
12	JJ	179/274 (65%)	167 (93%)	12 (7%)	0	100	100
13	DF	194/225 (86%)	185 (95%)	9 (5%)	0	100	100
14	DQ	123/143 (86%)	114 (93%)	9 (7%)	0	100	100
15	DS	75/147 (51%)	67 (89%)	8 (11%)	0	100	100
16	DT	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
17	Dc	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
19	DA	212/255 (83%)	170 (80%)	40 (19%)	2 (1%)	17	56
20	DE	258/261 (99%)	229 (89%)	29 (11%)	0	100	100
21	DG	224/236 (95%)	202 (90%)	19 (8%)	3 (1%)	12	48
22	DH	182/190 (96%)	158 (87%)	23 (13%)	1 (0%)	29	68
23	DI	184/200 (92%)	154 (84%)	30 (16%)	0	100	100
24	DJ	183/197 (93%)	163 (89%)	19 (10%)	1 (0%)	29	68
25	DL	141/156 (90%)	125 (89%)	16 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	DN	148/151 (98%)	129 (87%)	18 (12%)	1 (1%)	22	61
27	DO	125/137 (91%)	102 (82%)	23 (18%)	0	100	100
28	DZ	65/108 (60%)	51 (78%)	14 (22%)	0	100	100
29	DW	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
30	DX	141/145 (97%)	123 (87%)	18 (13%)	0	100	100
31	DY	131/135 (97%)	120 (92%)	11 (8%)	0	100	100
32	Db	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
33	UN	104/899 (12%)	100 (96%)	4 (4%)	0	100	100
34	JD	815/1267 (64%)	743 (91%)	72 (9%)	0	100	100
All	All	7273/11448 (64%)	6654 (92%)	605 (8%)	14 (0%)	50	81

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	UB	698	ILE
1	UB	699	PRO
1	UB	706	LYS
19	DA	213	ARG
21	DG	173	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UB	52/732 (7%)	51 (98%)	1 (2%)	57	80
2	UC	42/538 (8%)	41 (98%)	1 (2%)	49	76
4	UX	126/169 (75%)	126 (100%)	0	100	100
6	CK	51/535 (10%)	51 (100%)	0	100	100
7	CL	624/1039 (60%)	619 (99%)	5 (1%)	81	91
8	CM	307/312 (98%)	307 (100%)	0	100	100
11	JL	255/283 (90%)	253 (99%)	2 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	JJ	158/238 (66%)	158 (100%)	0	100	100
15	DS	69/110 (63%)	67 (97%)	2 (3%)	42	71
19	DA	191/224 (85%)	190 (100%)	1 (0%)	88	94
20	DE	221/222 (100%)	221 (100%)	0	100	100
21	DG	188/201 (94%)	187 (100%)	1 (0%)	88	94
22	DH	165/170 (97%)	165 (100%)	0	100	100
23	DI	150/161 (93%)	150 (100%)	0	100	100
24	DJ	158/166 (95%)	158 (100%)	0	100	100
25	DL	129/137 (94%)	129 (100%)	0	100	100
26	DN	127/128 (99%)	127 (100%)	0	100	100
27	DO	96/105 (91%)	96 (100%)	0	100	100
29	DW	110/111 (99%)	110 (100%)	0	100	100
30	DX	118/120 (98%)	118 (100%)	0	100	100
31	DY	111/113 (98%)	111 (100%)	0	100	100
32	Db	70/71 (99%)	70 (100%)	0	100	100
33	UN	98/808 (12%)	98 (100%)	0	100	100
34	JD	133/1140 (12%)	133 (100%)	0	100	100
All	All	3749/7833 (48%)	3736 (100%)	13 (0%)	92	97

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	JL	164	LEU
11	JL	166	ARG
21	DG	98	ARG
15	DS	71	GLN
19	DA	95	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
29	DW	24	GLN
21	DG	139	ASN
19	DA	232	HIS
19	DA	95	ASN

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Mol	Chain	Res	Type
20	DE	36	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	D3	1380/1758 (78%)	492 (35%)	34 (2%)
35	D4	21/23 (91%)	7 (33%)	0
36	D5	8/9 (88%)	6 (75%)	1 (12%)
All	All	1409/1790 (78%)	505 (35%)	35 (2%)

5 of 505 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	D3	2	A
18	D3	9	U
18	D3	10	G
18	D3	12	U
18	D3	15	U

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	D3	1535	U
18	D3	1568	C
18	D3	1800	A
18	D3	417	A
18	D3	280	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 40 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	$\# Z > 2$
38	GTP	CL	2001	39	26,34,34	0.94	1 (3%)	32,54,54	1.50	5 (15%)

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
38	GTP	CL	2001	39	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	CL	2001	GTP	C6-N1	-2.55	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	CL	2001	GTP	PB-O3B-PG	-4.35	117.91	132.83
38	CL	2001	GTP	C3'-C2'-C1'	3.06	105.58	100.98
38	CL	2001	GTP	PA-O3A-PB	-3.00	122.54	132.83
38	CL	2001	GTP	C5-C6-N1	2.36	118.11	113.95
38	CL	2001	GTP	C8-N7-C5	2.31	107.39	102.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

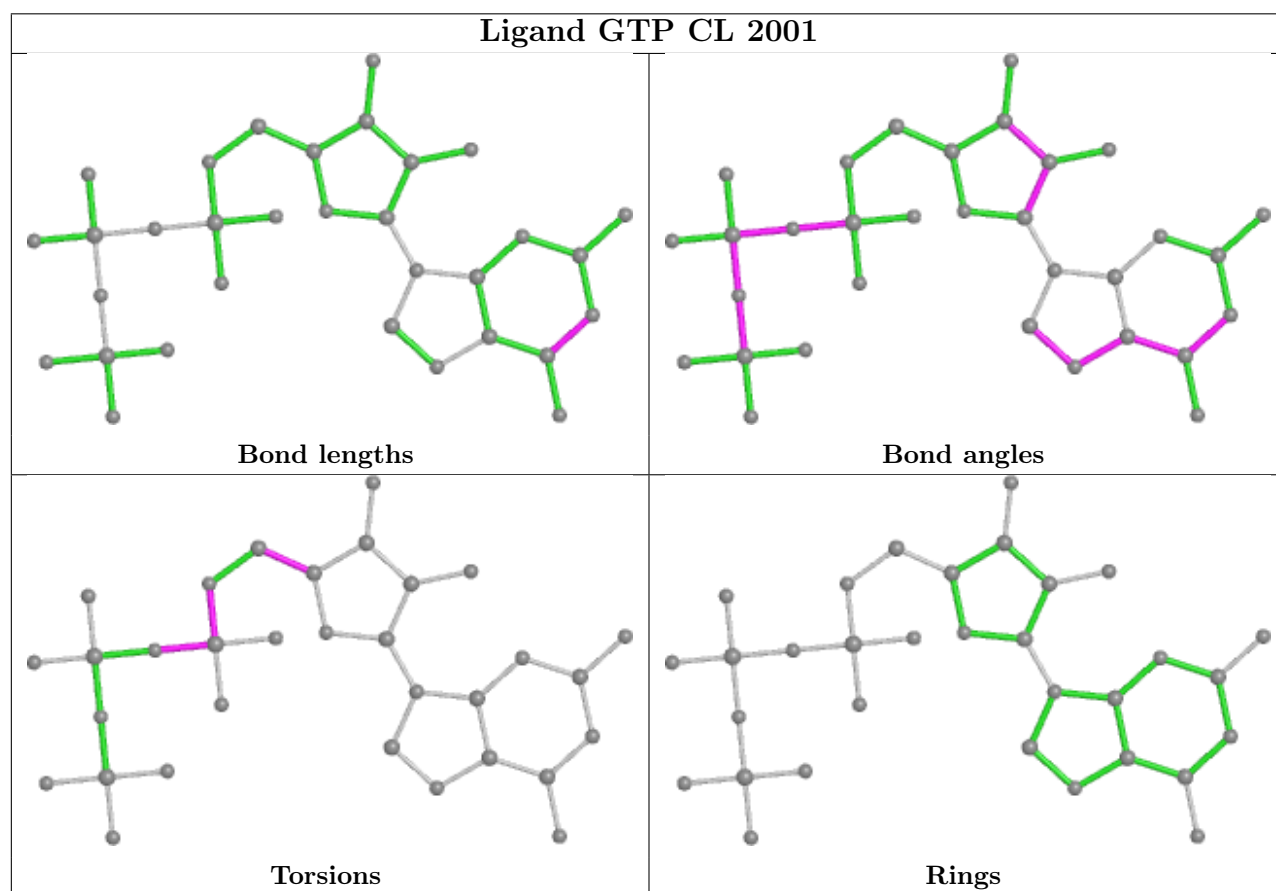
Mol	Chain	Res	Type	Atoms
38	CL	2001	GTP	O4'-C4'-C5'-O5'
38	CL	2001	GTP	C3'-C4'-C5'-O5'
38	CL	2001	GTP	PB-O3A-PA-O2A
38	CL	2001	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	CL	2001	GTP	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

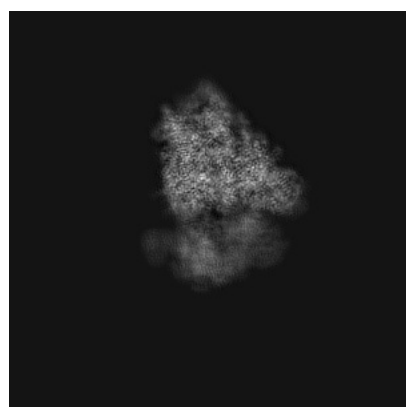
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11363. These allow visual inspection of the internal detail of the map and identification of artifacts.

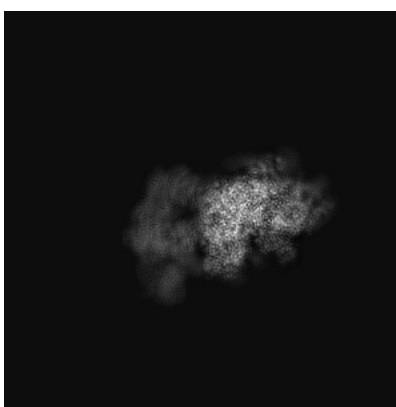
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

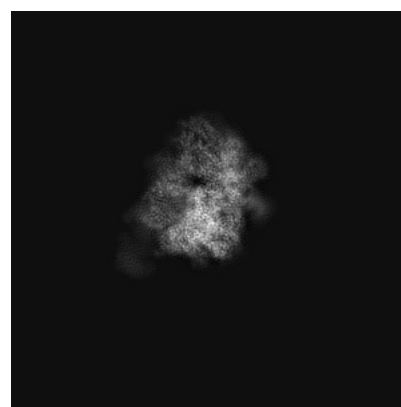
6.1.1 Primary map



X



Y

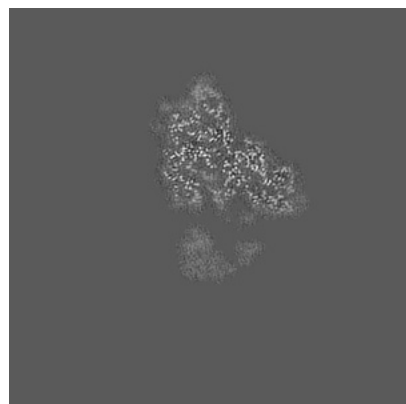


Z

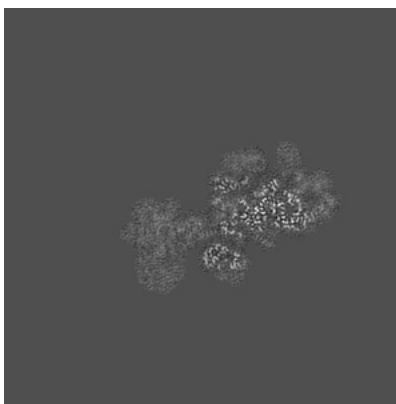
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

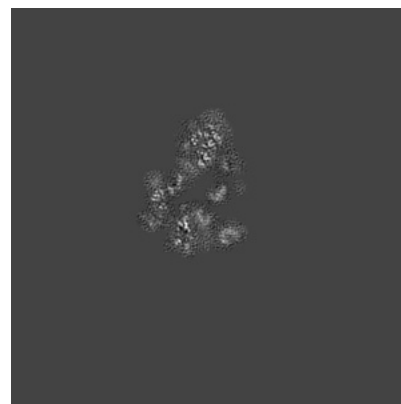
6.2.1 Primary map



X Index: 240



Y Index: 240

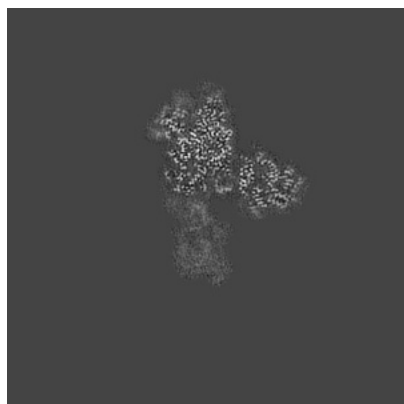


Z Index: 240

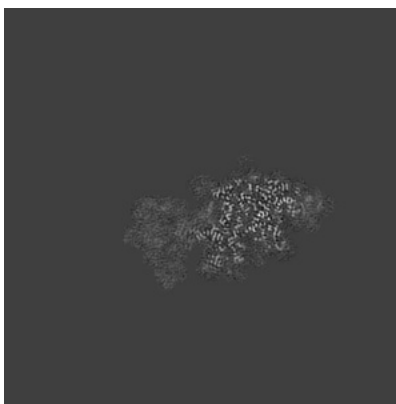
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

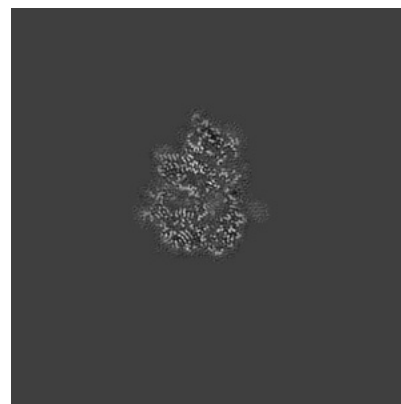
6.3.1 Primary map



X Index: 226



Y Index: 219



Z Index: 278

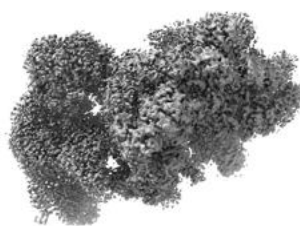
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

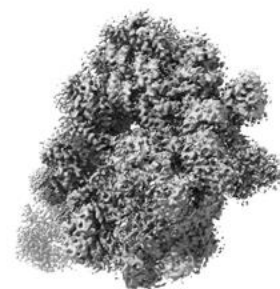
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

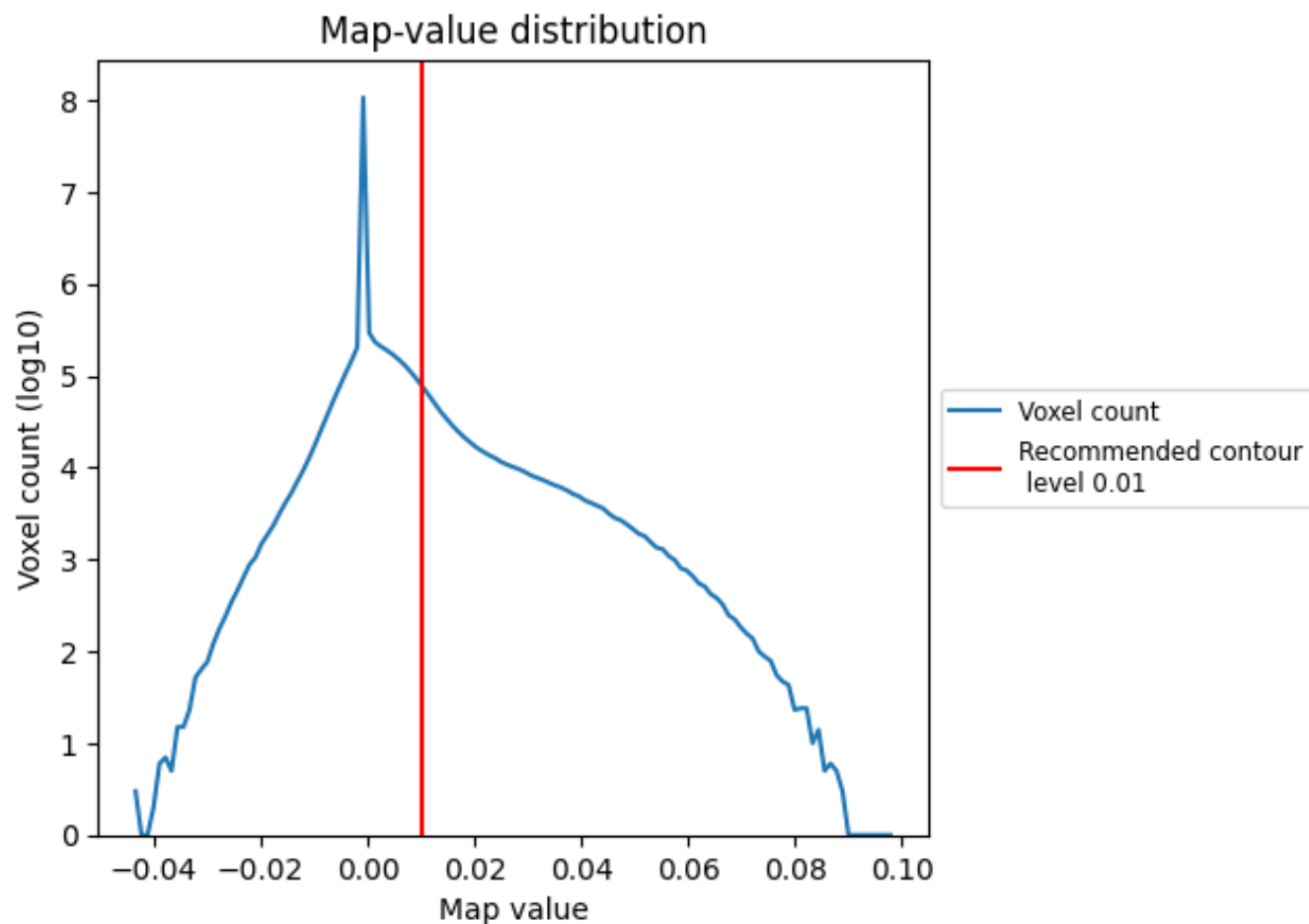
6.5 Mask visualisation

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

7 Map analysis [i](#)

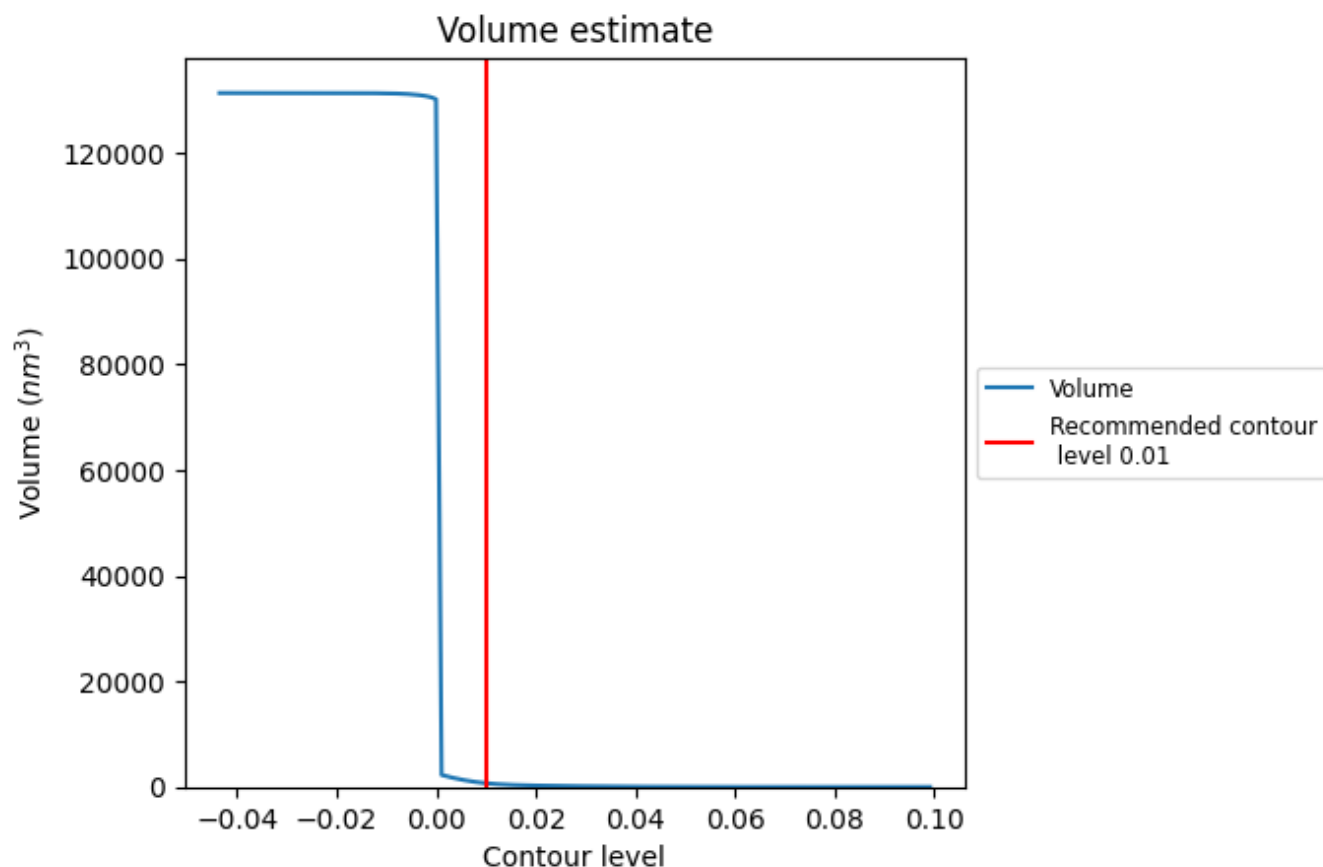
This section contains the results of statistical analysis of the map.

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.

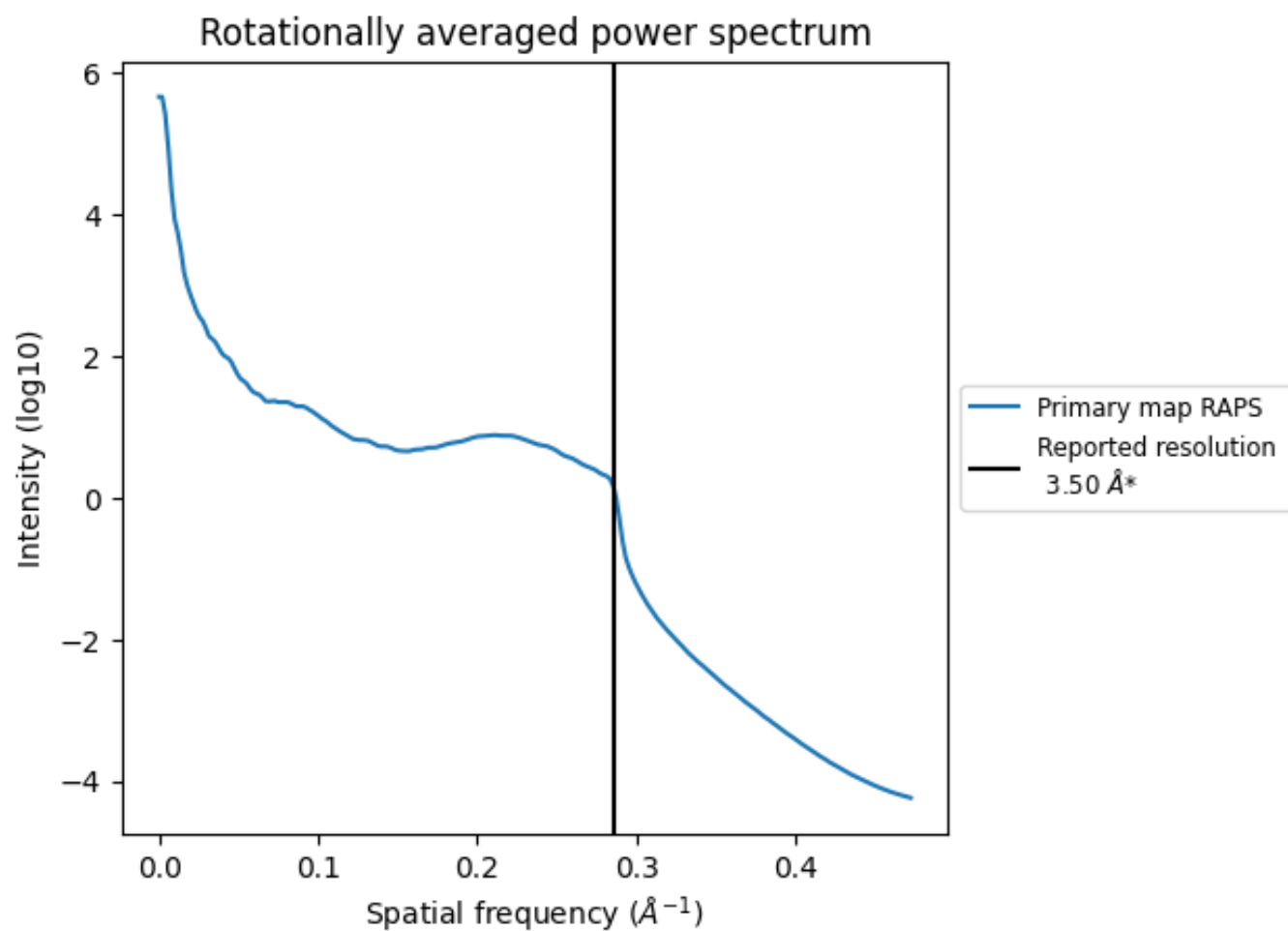
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 707 nm^3 ; this corresponds to an approximate mass of 638 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 ⓘ

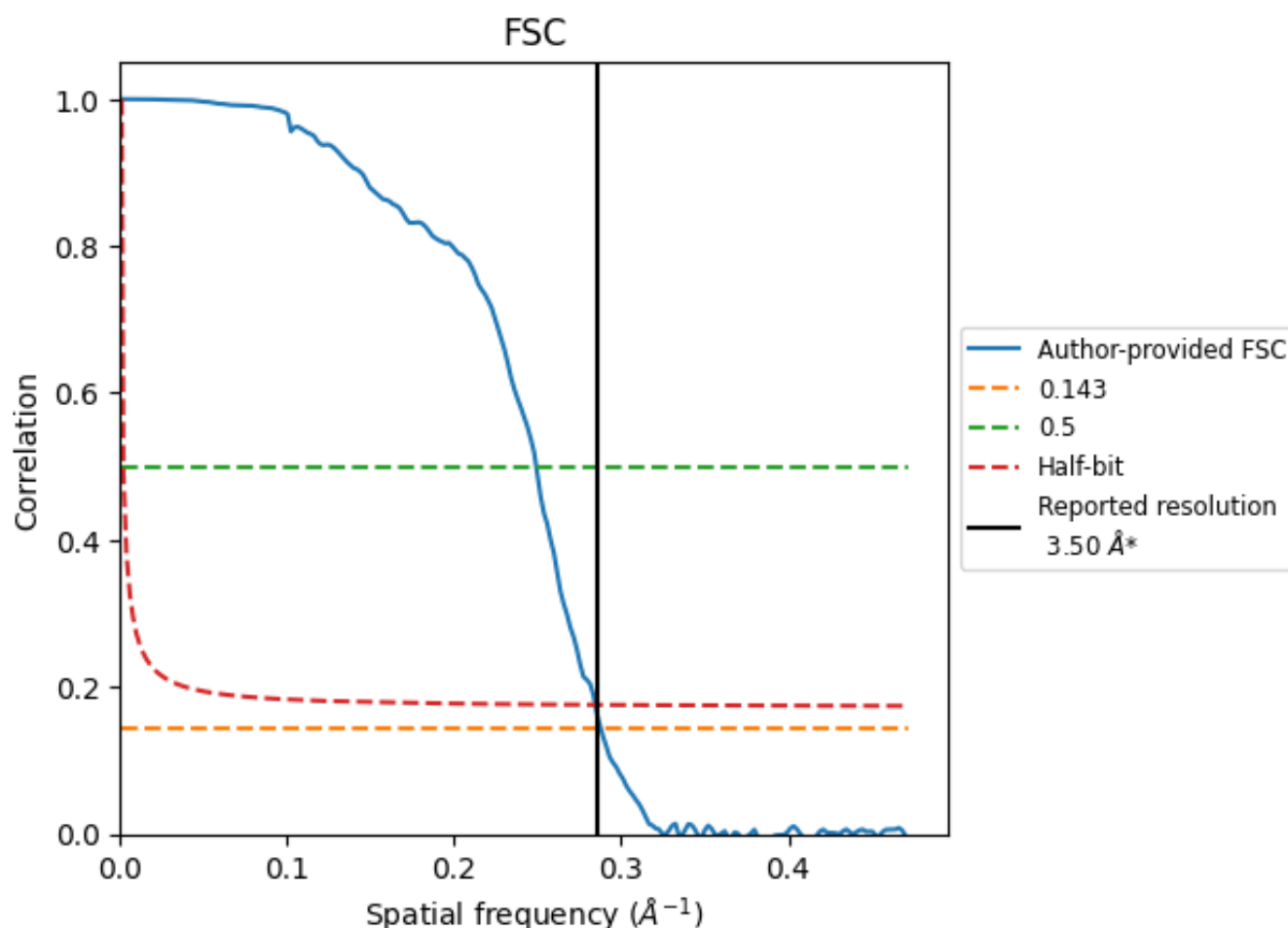


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

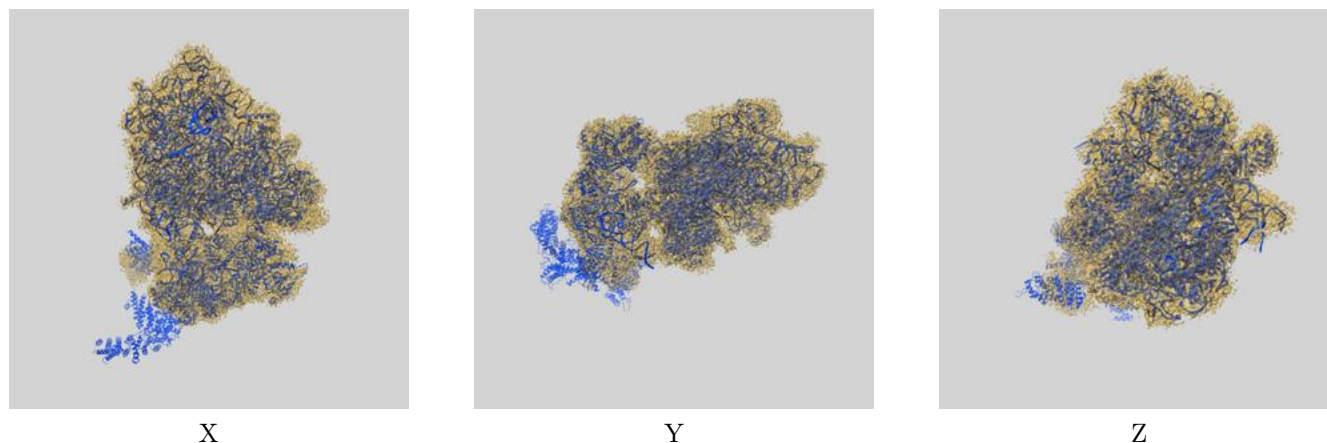
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	4.01	3.52
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

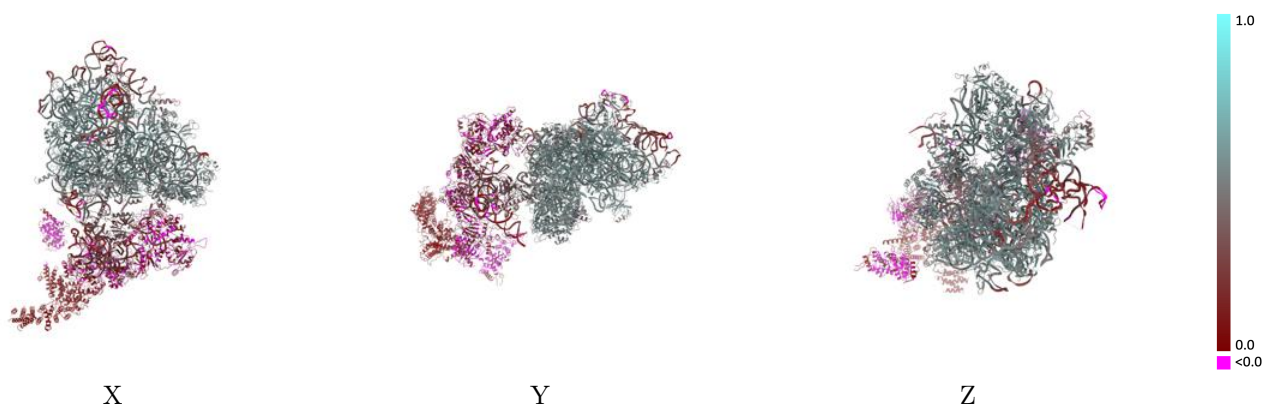
This section contains information regarding the fit between EMDB map EMD-11363 and PDB model 6ZQG. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



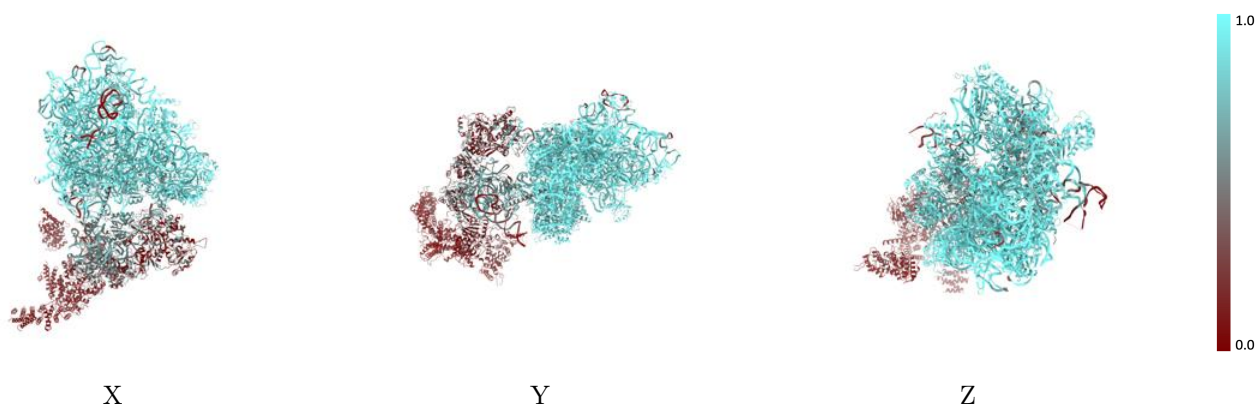
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



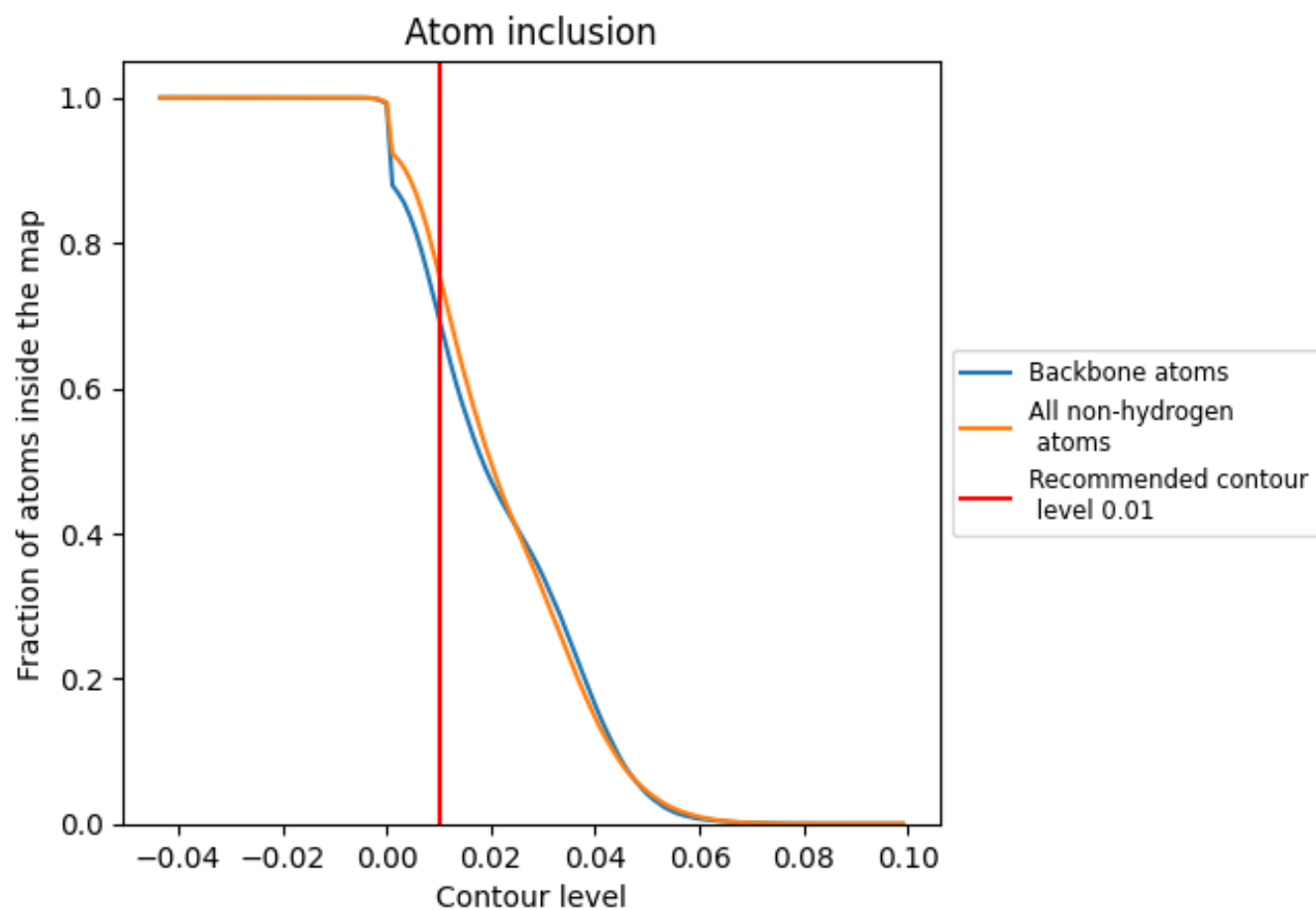
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 70% of all backbone atoms, 76% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.4050
CJ	 0.6030	 0.3060
CK	 0.7461	 0.4080
CL	 0.9182	 0.5250
CM	 0.9408	 0.5440
D3	 0.8655	 0.4250
D4	 0.9798	 0.4900
D5	 0.3833	 0.2000
DA	 0.9428	 0.5380
DE	 0.9618	 0.5680
DF	 0.4186	 0.1550
DG	 0.9428	 0.5120
DH	 0.9132	 0.4860
DI	 0.9575	 0.5480
DJ	 0.9438	 0.5550
DL	 0.9314	 0.5520
DN	 0.9567	 0.5520
DO	 0.9594	 0.5380
DQ	 0.3506	 0.1660
DS	 0.3247	 0.1450
DT	 0.4186	 0.1510
DW	 0.9679	 0.5730
DX	 0.9035	 0.5490
DY	 0.9440	 0.5520
DZ	 0.2620	 0.1620
Db	 0.9301	 0.5260
Dc	 0.3161	 0.1410
JD	 0.4491	 0.2300
JF	 0.0738	 0.0360
JG	 0.1515	 0.1140
JH	 0.0456	 -0.0270
JJ	 0.9158	 0.5250
JL	 0.9143	 0.5300
UB	 0.0757	 0.0720
UC	 0.9129	 0.5480



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Chain	Atom inclusion	Q-score
UN	 0.8739	 0.5350
US	 0.0000	 -0.0000
UX	 0.9100	 0.5380