



wwPDB EM Validation Summary Report

Mar 12, 2026 – 07:26 AM UTC


PDB ID : 6RXV / pdb_00006rxv
EMDB ID : EMD-10053
Title : Cryo-EM structure of the 90S pre-ribosome (Kre33-Noc4) from *Chaetomium thermophilum*, state B2
Authors : Cheng, J.; Kellner, N.; Griesel, S.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on : 2019-06-10
Resolution : 4.00 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:

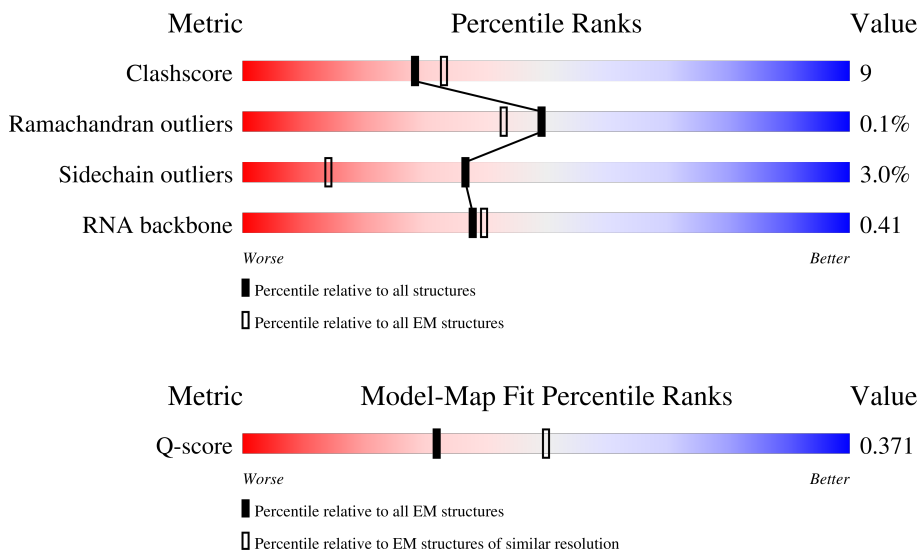
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	UA	904	 73% 20% 7%
2	UB	907	 47% 9% 44%
3	UC	648	 10% 89%

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Mol	Chain	Length	Quality of chain
4	UD	884	67% 20% 13%
5	UF	414	67% 13% 20%
6	UG	558	69% 16% 14%
7	UJ	1802	48% 13% 40%
8	UK	270	69% 12% 20%
9	UL	962	60% 21% 18%
10	UM	912	57% 22% 20%
11	UN	938	15% 81%
12	UO	557	70% 20% 10%
13	UQ	960	62% 19% 18%
14	UR	618	62% 10% 28%
15	UU	1049	70% 16% 14%
16	UX	193	72% 26% ..
17	UZ	391	50% 10% 40%
18	CA	313	64% 14% 23%
18	CB	313	56% 20% 24%
19	CC	523	65% 9% 26%
20	CD	582	58% 14% 28%
21	CE	127	76% 19% 5%
21	CF	127	72% 23% 6%
22	CG	630	50% 16% 34%
23	CH	411	72% 23% 5%
24	CI	1163	58% 12% 29%
25	CJ	183	78% 20% .
26	CK	297	77% 23%





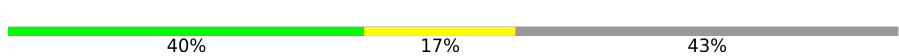





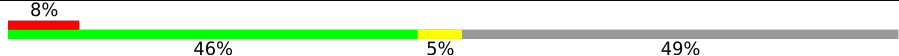
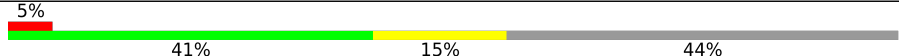
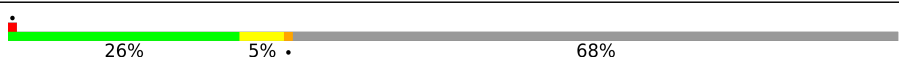
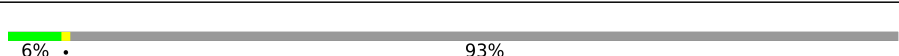
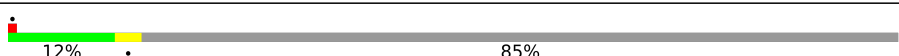
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Mol	Chain	Length	Quality of chain
27	CL	785	24% 6% 71%
28	CM	446	74% 26%
29	CN	252	73% 16% 10%
29	CO	252	72% 13% 15%
30	CP	322	59% 13% 28%
31	CQ	259	51% 17% 32%
32	CR	1073	36% 29% 6% 29%
32	CS	1073	11% 36% 28% 6% 29%
33	CT	203	55% 9% 35%
34	Ca	255	67% 21% 12%
35	Cb	264	62% 25% 12%
36	Cc	212	74% 17% 9%
37	Cd	239	72% 22% 5%
38	Ce	203	51% 27% 22%
39	Cf	202	65% 21% 14%
40	Cg	190	69% 15% 16%
41	Ch	151	37% 7% 56%
42	Ci	150	64% 13% 23%
43	Cj	143	78% 10% 12%
44	Ck	161	6% 63% 24% 13%
45	Cm	130	78% 18% 4%
46	Cn	145	57% 9% 34%
47	Co	136	43% 24% 32%
48	Cp	68	78% 12% 10%
49	CU	311	48% 8% 43%

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Mol	Chain	Length	Quality of chain
50	C1	2352	
51	C2	230	
52	UV	1171	
53	CV	322	
54	CW	668	
55	UT	2612	
56	UH	930	
57	UE	410	
57	UI	410	
58	US	549	
59	CI	156	
60	CX	480	
61	CY	381	
62	CZ	609	
63	UP	364	

2 Entry composition [i](#)

There are 66 unique types of molecules in this entry. The entry contains 221395 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 Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	UA	839	6366	4101	1136	1105	24	0	0

- Molecule 2 is a protein called Utp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	UB	512	4079	2576	781	711	11	0	0

- Molecule 3 is a protein called Utp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	UC	74	588	371	120	97	0	0

- Molecule 4 is a protein called Utp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	UD	772	6071	3851	1093	1103	24	0	0

- Molecule 5 is a protein called Utp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	UF	331	2591	1674	504	399	14	0	0

- Molecule 6 is a protein called Utp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	UG	479	3717	2369	700	636	12	0	0

- Molecule 7 is a protein called UTP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	UJ	1090	8416	5408	1452	1525	31	0	0

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	UK	217	1687	1062	351	269	5	0	0

- Molecule 9 is a protein called Utp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	UL	785	6175	3940	1088	1130	17	0	0

- Molecule 10 is a protein called Utp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	UM	729	5643	3590	995	1045	13	0	0

- Molecule 11 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	UN	177	1401	892	263	239	7	0	0

- Molecule 12 is a protein called Utp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	UO	504	3819	2422	699	684	14	0	0

- Molecule 13 is a protein called Utp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	UQ	789	6008	3831	1037	1119	21	0	0

- Molecule 14 is a protein called Utp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	UR	447	3491	2209	656	616	10	0	0

- Molecule 15 is a protein called Utp21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	UU	902	6734	4336	1236	1136	26	0	0

- Molecule 16 is a protein called Utp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	UX	190	1470	932	282	246	10	0	0

- Molecule 17 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	UZ	235	1815	1184	330	298	3	0	0

- Molecule 18 is a protein called Nop1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	CA	242	1778	1149	327	293	9	0	0
18	CB	237	1816	1154	318	335	9	0	0

- Molecule 19 is a protein called Nop56.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	CC	387	2866	1836	527	492	11	0	0

- Molecule 20 is a protein called Nop58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	CD	420	3150	2023	560	557	10	0	0

- Molecule 21 is a protein called Snu13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CE	121	Total	C	N	O	S	0	0
			879	557	165	154	3		
21	CF	120	Total	C	N	O	S	0	0
			864	550	161	150	3		

- Molecule 22 is a protein called Rrp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CG	416	Total	C	N	O	S	0	0
			3245	2065	587	580	13		

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CH	389	Total	C	N	O	S	0	0
			2888	1827	526	525	10		

- Molecule 24 is a protein called Bms1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CI	822	Total	C	N	O	S	0	0
			6486	4169	1213	1077	27		

- Molecule 25 is a protein called Imp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CJ	179	Total	C	N	O	S	0	0
			1434	918	283	226	7		

- Molecule 26 is a protein called Imp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CK	297	Total	C	N	O	S	0	0
			2329	1476	445	400	8		

- Molecule 27 is a protein called Mpp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CL	231	Total	C	N	O	S	0	0
			1786	1114	339	327	6		

- Molecule 28 is a protein called Sof1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	CM	445	3501	2195	672	619	15	0	0

- Molecule 29 is a protein called Emg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	CN	226	1762	1119	306	327	10	0	0
29	CO	215	1683	1067	293	313	10	0	0

- Molecule 30 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	CP	233	1893	1209	340	335	9	0	0

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	CQ	175	1361	862	250	242	7	0	0

- Molecule 32 is a protein called Kre33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	CR	760	5989	3851	1024	1087	27	0	0
32	CS	760	5989	3851	1024	1087	27	0	0

- Molecule 33 is a protein called Fcf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	CT	131	1035	656	197	178	4	0	0

- Molecule 34 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Ca	225	1821	1160	341	315	5	0	0

- Molecule 35 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Cb	232	1851	1179	340	325	7	0	0

- Molecule 36 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Cc	192	1464	926	278	253	7	0	0

- Molecule 37 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Cd	226	1819	1138	363	313	5	0	0

- Molecule 38 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	Ce	159	1279	810	237	232	0	0

- Molecule 39 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Cf	174	1398	872	283	242	1	0	0

- Molecule 40 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Cg	159	1242	801	255	184	2	0	0

- Molecule 41 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	Ch	66	546	355	101	90	0	0

- Molecule 42 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ci	115	Total	C	N	O	S	0	0
			808	506	156	141	5		

- Molecule 43 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Cj	126	Total	C	N	O	S	0	0
			943	613	177	151	2		

- Molecule 44 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ck	140	Total	C	N	O	S	0	0
			1163	750	224	184	5		

- Molecule 45 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Cm	126	Total	C	N	O	S	0	0
			985	632	184	164	5		

- Molecule 46 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Cn	96	Total	C	N	O	S	0	0
			702	456	134	110	2		

- Molecule 47 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Co	92	Total	C	N	O	S	0	0
			741	474	139	126	2		

- Molecule 48 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Cp	61	Total	C	N	O	0	0
			455	284	97	74		

- Molecule 49 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	CU	176	Total	C	N	O	S	0	0
			1337	822	265	244	6		

- Molecule 50 is a RNA chain called 35S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	C1	1575	Total	C	N	O	P	0	0
			33604	14992	6023	11014	1575		

- Molecule 51 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	C2	230	Total	C	N	O	P	0	0
			4891	2182	856	1623	230		

- Molecule 52 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	UV	1061	Total	C	N	O	S	0	0
			8424	5399	1480	1523	22		

- Molecule 53 is a protein called Rrp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	CV	148	Total	C	N	O	S	0	0
			1145	729	198	216	2		

- Molecule 54 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CW	382	Total	C	N	O	S	0	0
			2924	1857	530	524	13		

- Molecule 55 is a protein called Utp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	UT	2033	Total	C	N	O	S	0	0
			16049	10336	2819	2826	68		

- Molecule 56 is a protein called Utp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	UH	359	2809	1773	496	527	13	0	0

- Molecule 57 is a protein called Utp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	UE	125	972	608	183	175	6	0	0
57	UI	125	972	608	183	175	6	0	0

- Molecule 58 is a protein called Noc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	US	451	3672	2389	608	660	15	0	0

- Molecule 59 is a protein called Rps18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	CI	80	633	400	115	117	1	0	0

- Molecule 60 is a protein called Enp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	CX	267	2130	1384	374	362	10	0	0

- Molecule 61 is a protein called U3 small nucleolar ribonucleoprotein protein lcp5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	CY	123	979	592	195	189	3	0	0

- Molecule 62 is a protein called Bfr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	CZ	44	376	235	76	64	1	0	0

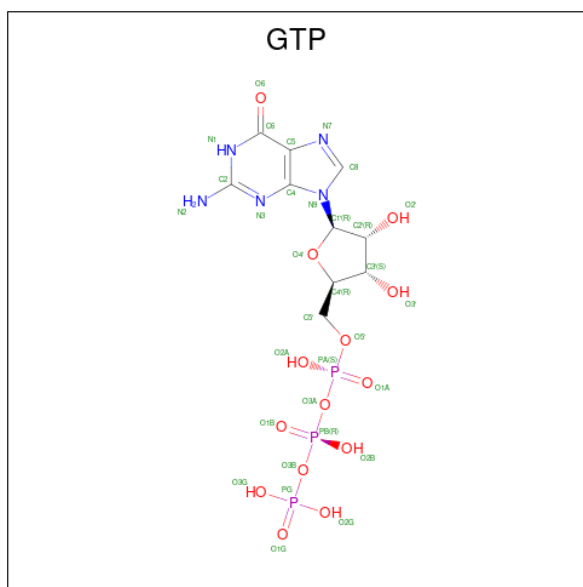
- Molecule 63 is a protein called Utp16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
63	UP	54	422	264	88	70	0	0

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 65 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

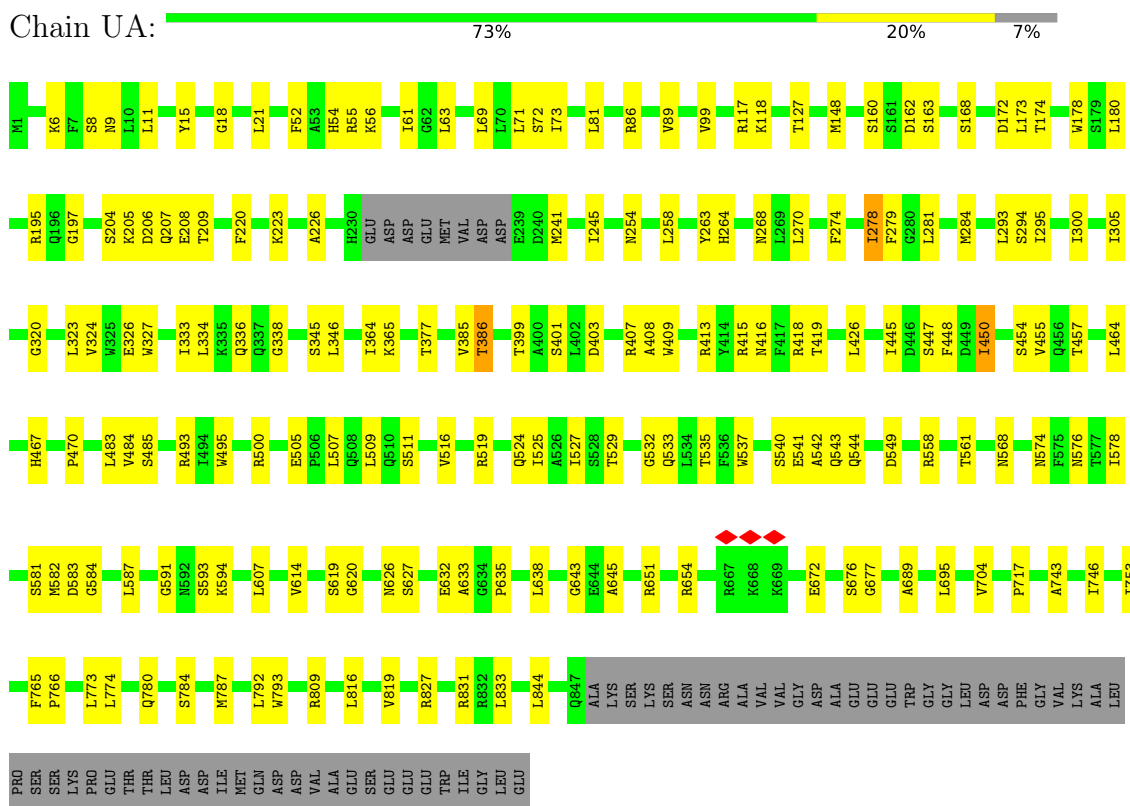
- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
66	CI	1	1	1	0

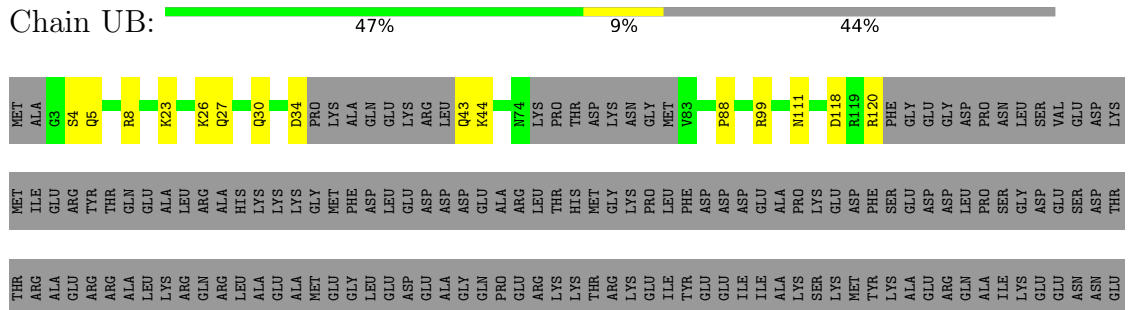
3 Residue-property plots

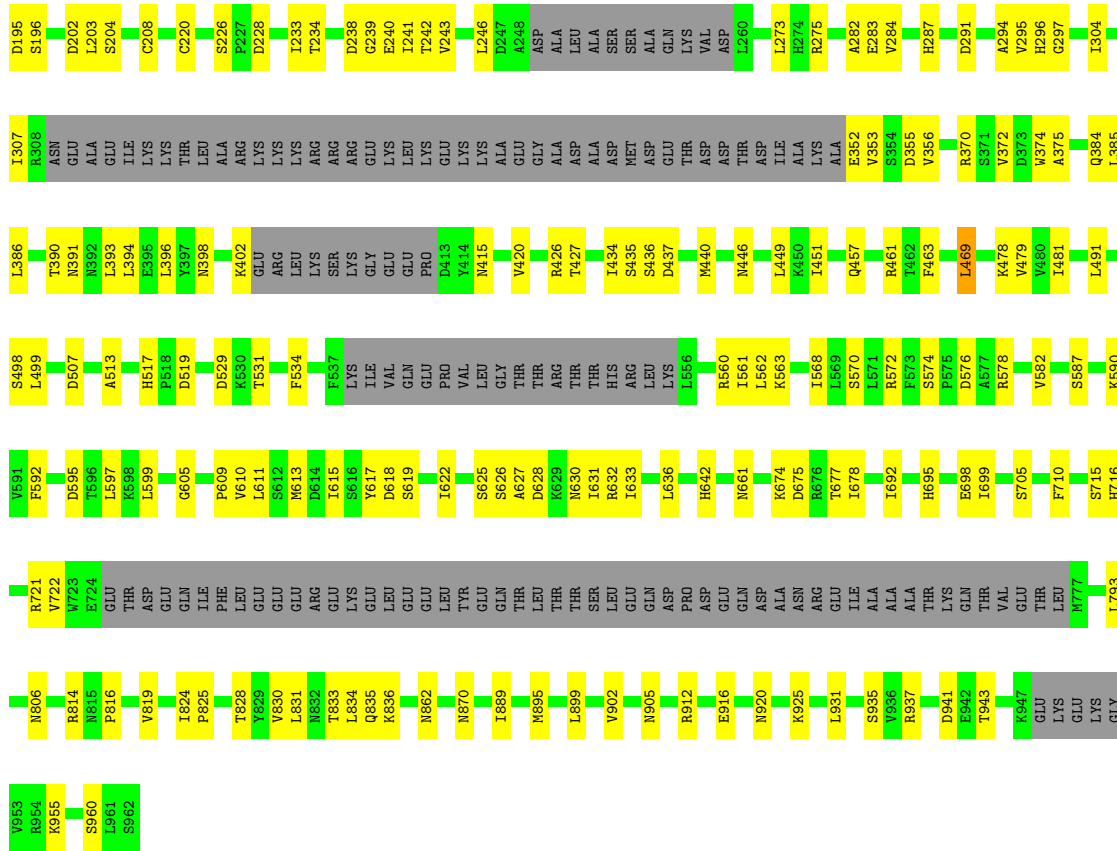
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Periodic tryptophan 2-like protein

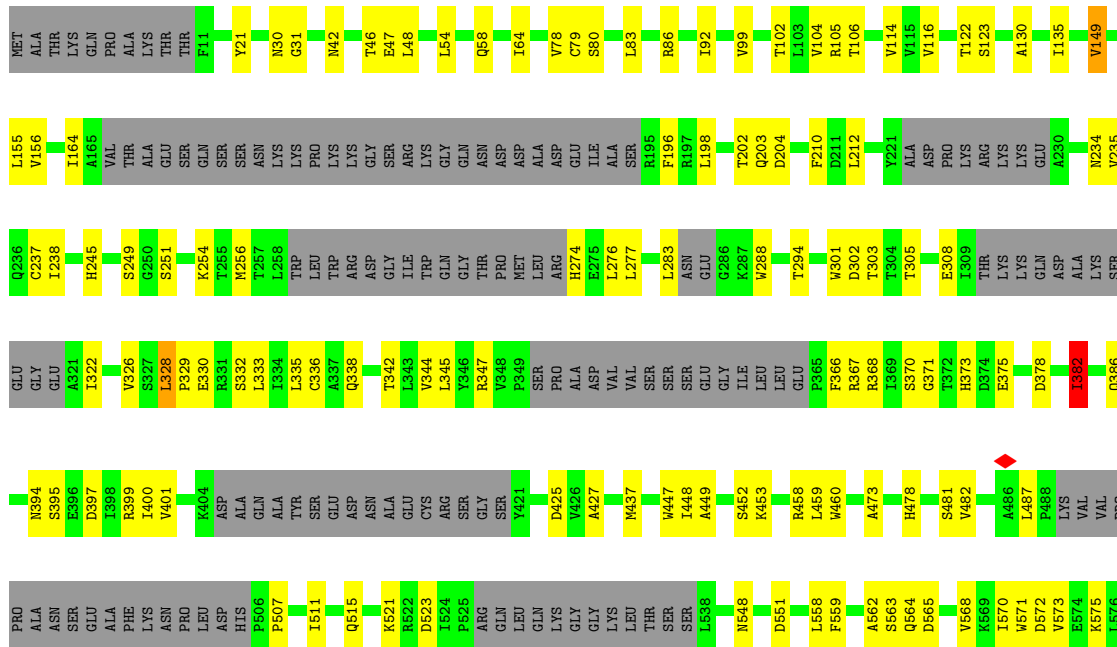


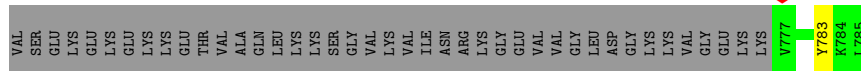
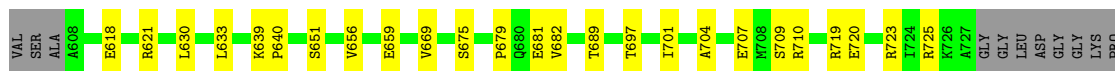
- Molecule 2: Utp2



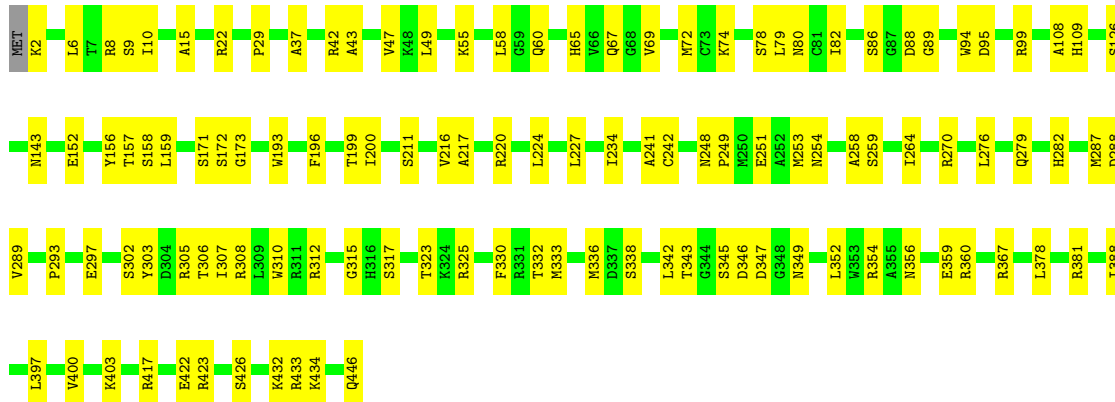
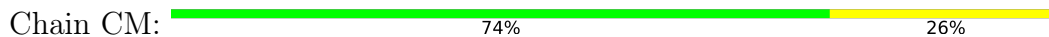


• Molecule 10: Utp13

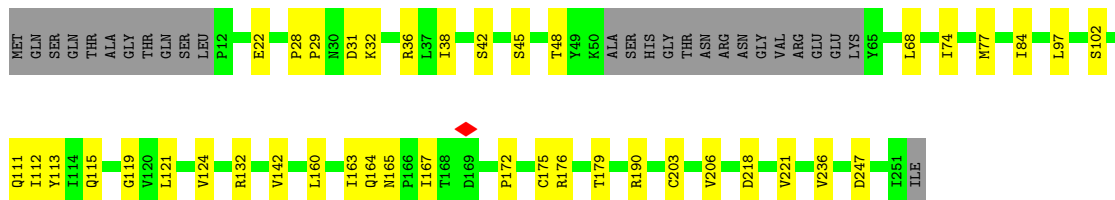




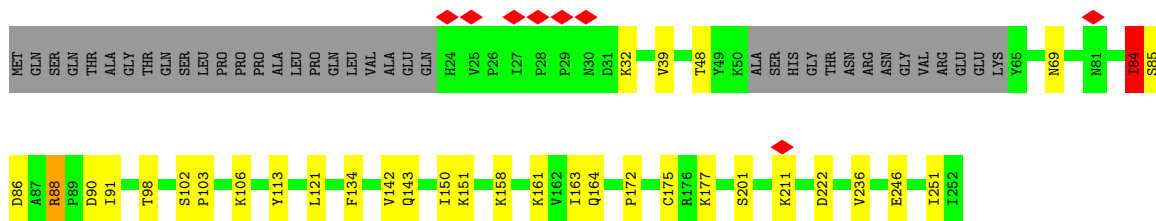
• Molecule 28: Sof1



• Molecule 29: Emg1

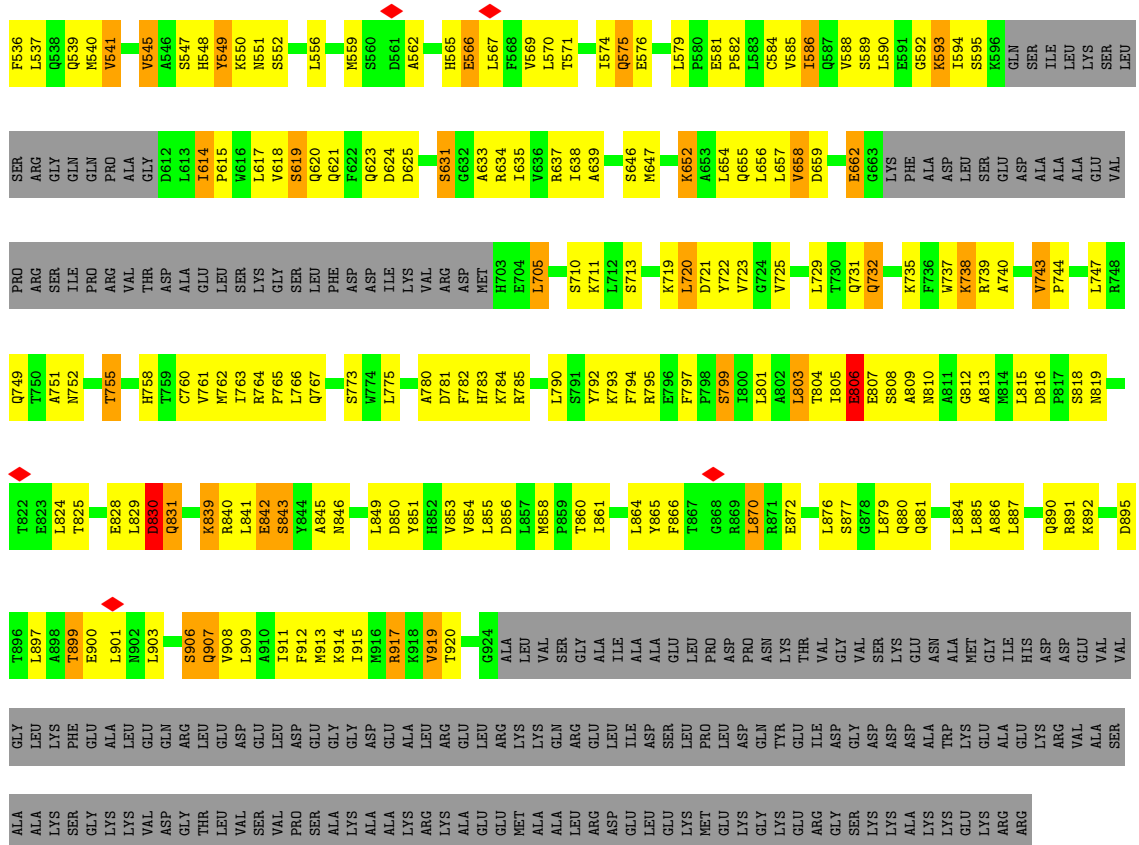


• Molecule 29: Emg1

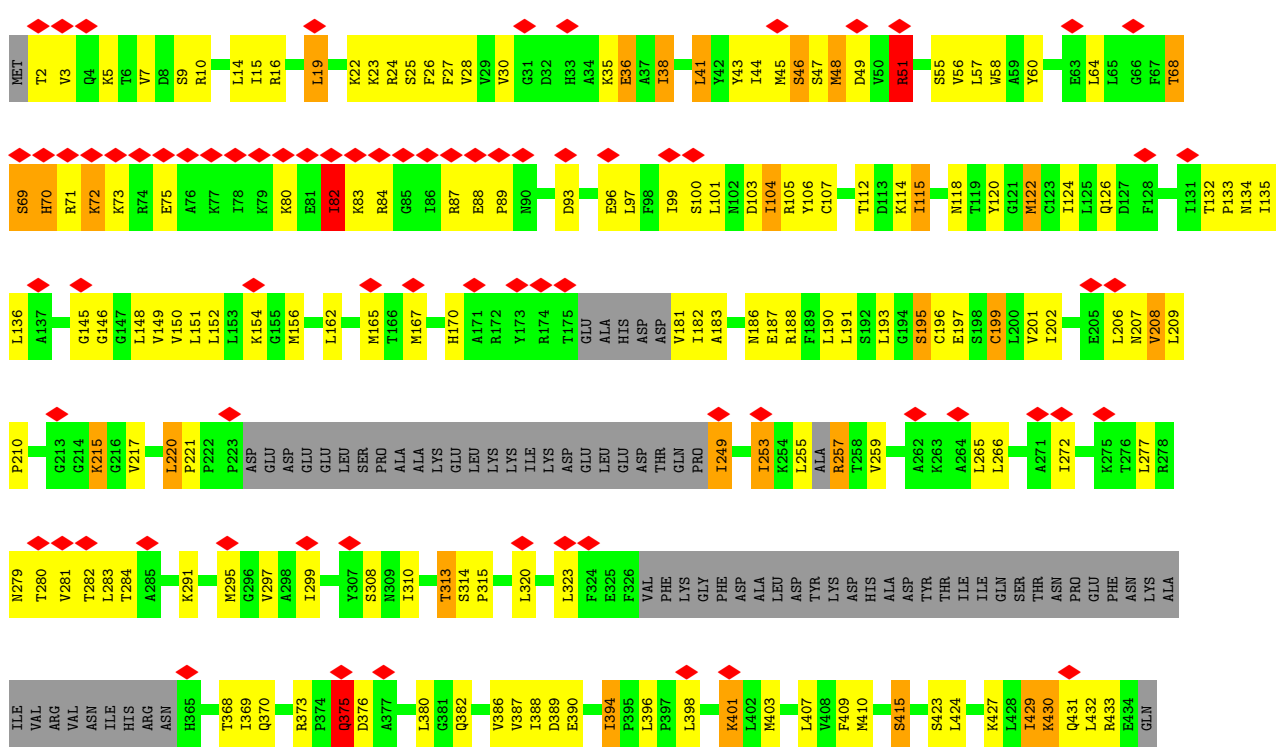


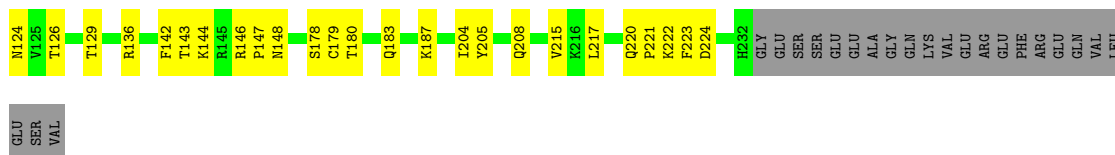
• Molecule 30: KRR1 small subunit processome component



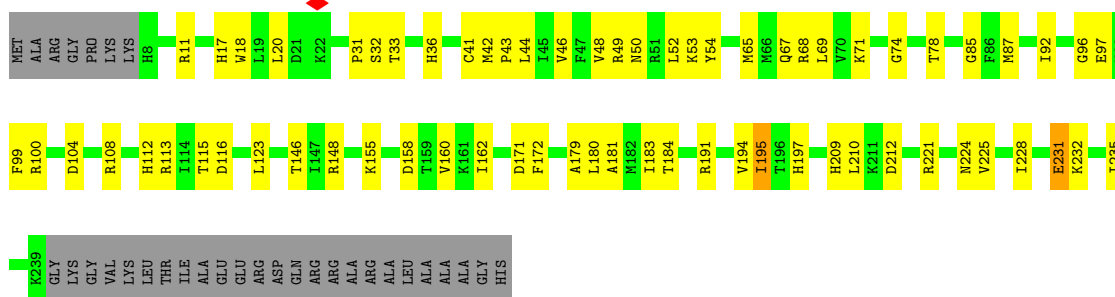


• Molecule 32: Kre33

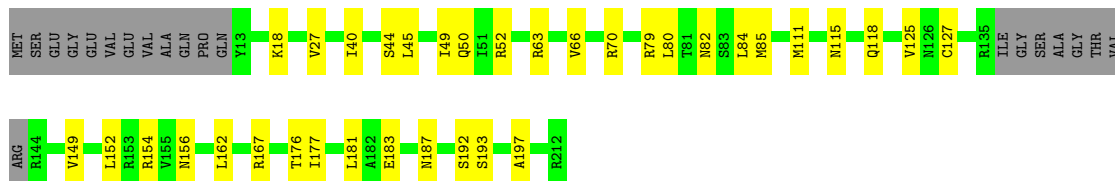




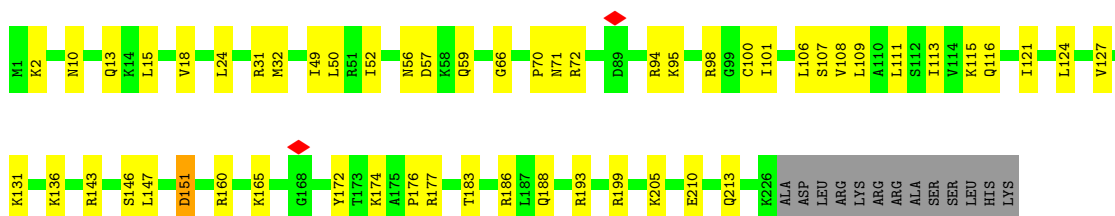
• Molecule 35: 40S ribosomal protein S4



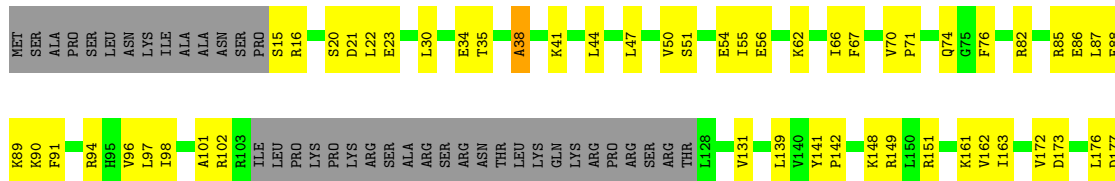
• Molecule 36: 40S ribosomal protein s5-like protein

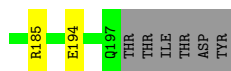


• Molecule 37: 40S ribosomal protein S6

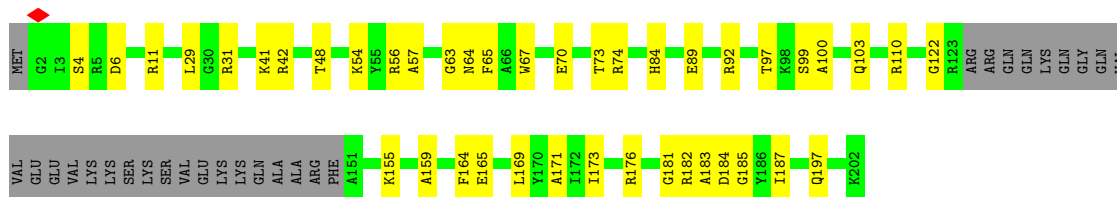


• Molecule 38: 40S ribosomal protein S7

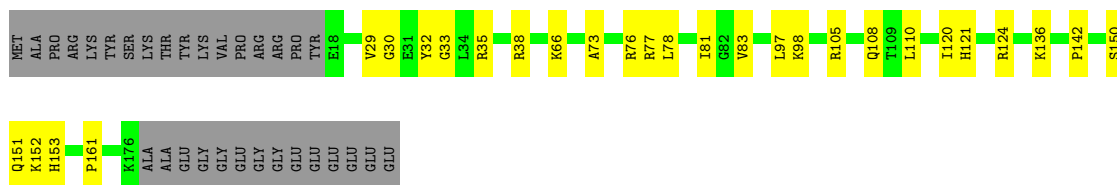




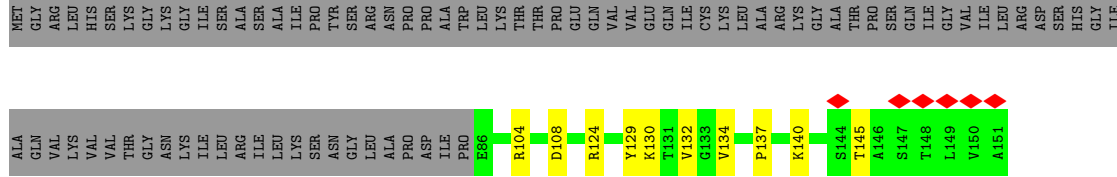
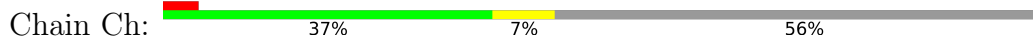
- Molecule 39: 40S ribosomal protein S8



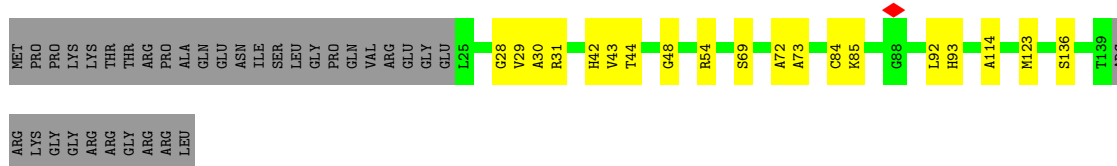
- Molecule 40: 40S ribosomal protein s9-like protein



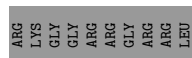
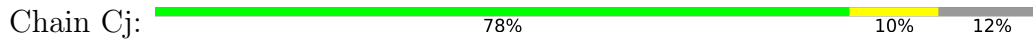
- Molecule 41: 40S ribosomal protein S13-like protein

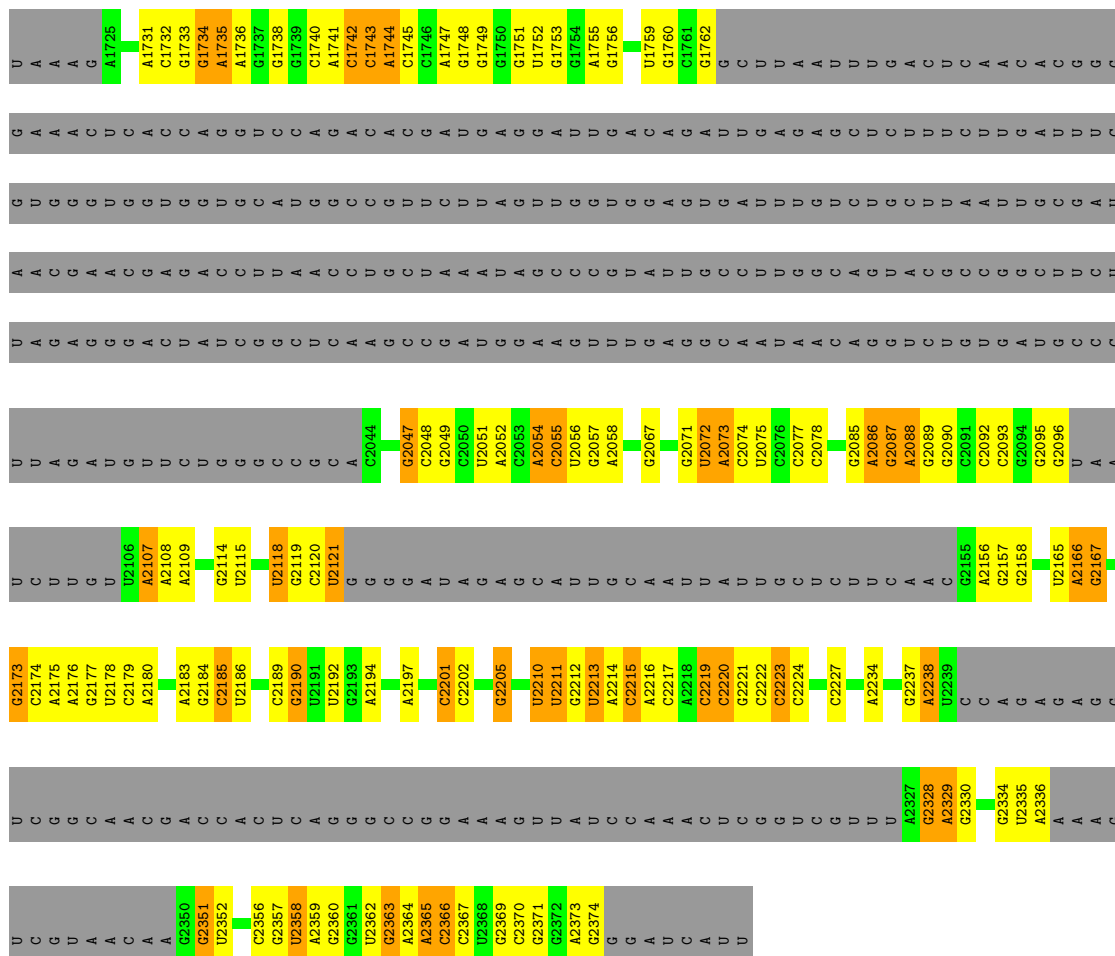


- Molecule 42: 40S ribosomal protein S14-like protein

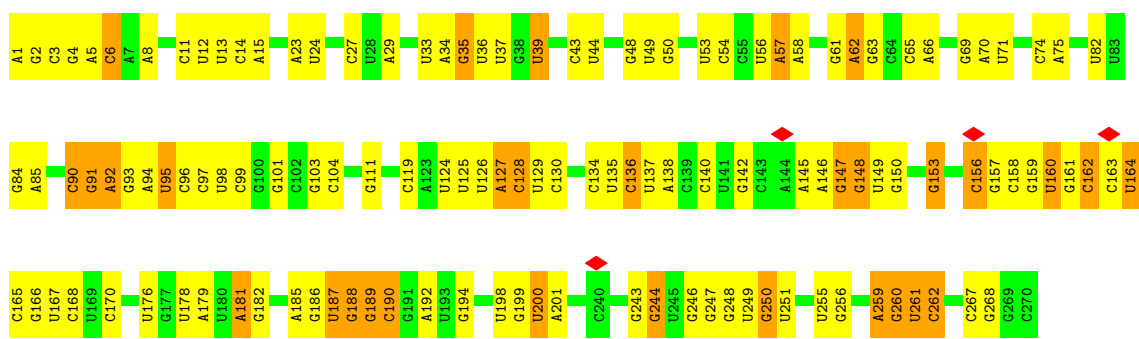


- Molecule 43: 40S ribosomal protein S16-like protein

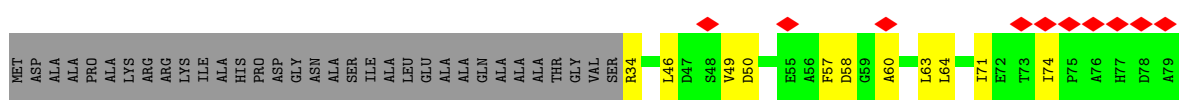




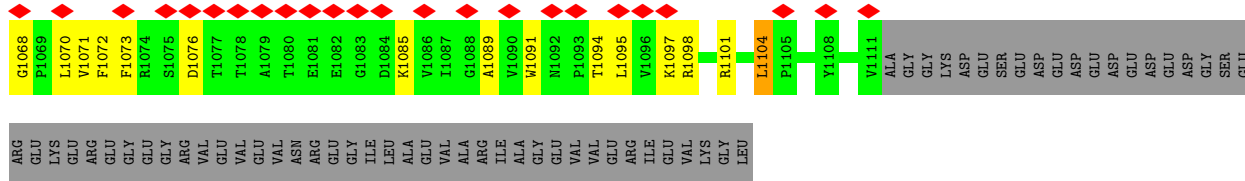
● Molecule 51: U3 snoRNA



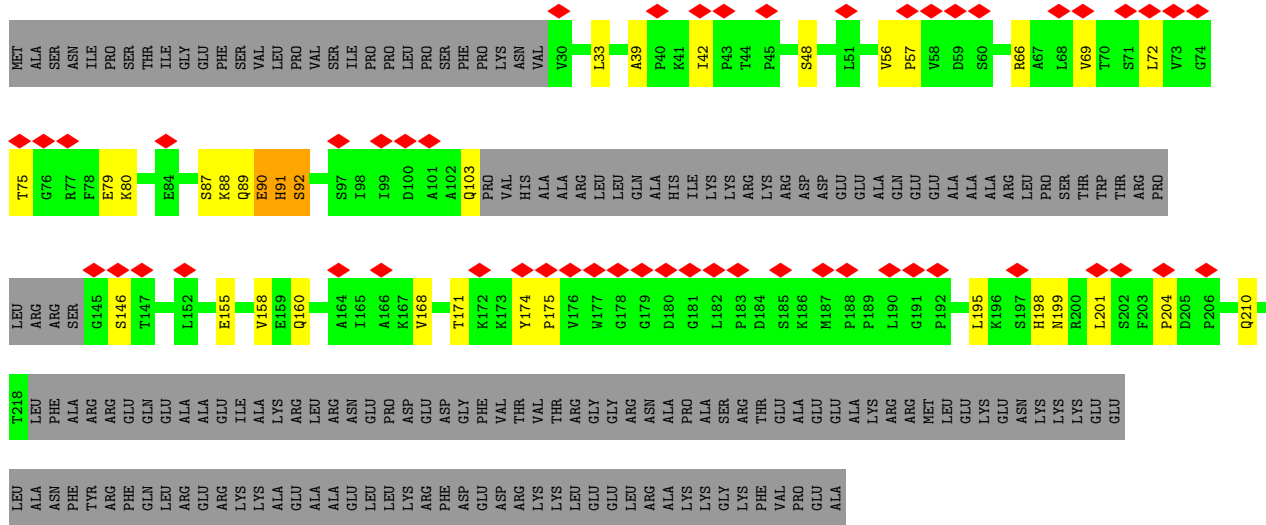
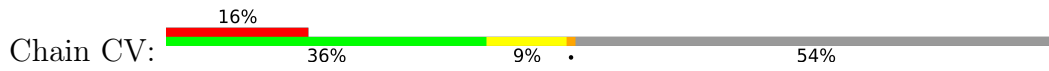
● Molecule 52: U3 small nucleolar RNA-associated protein 22



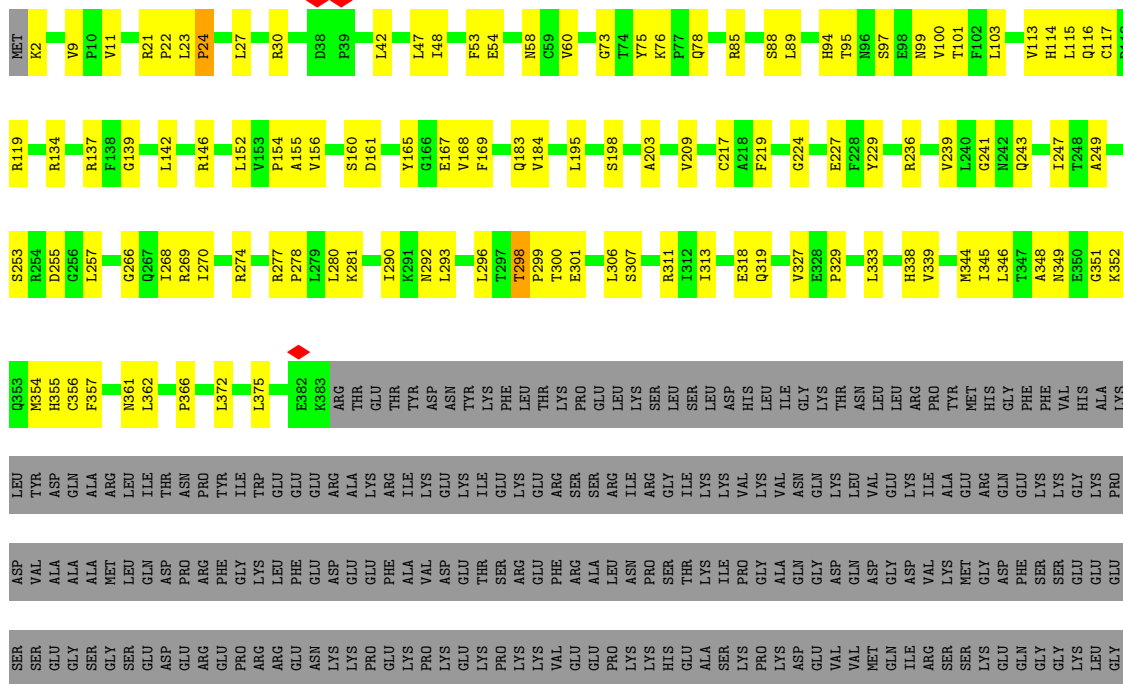


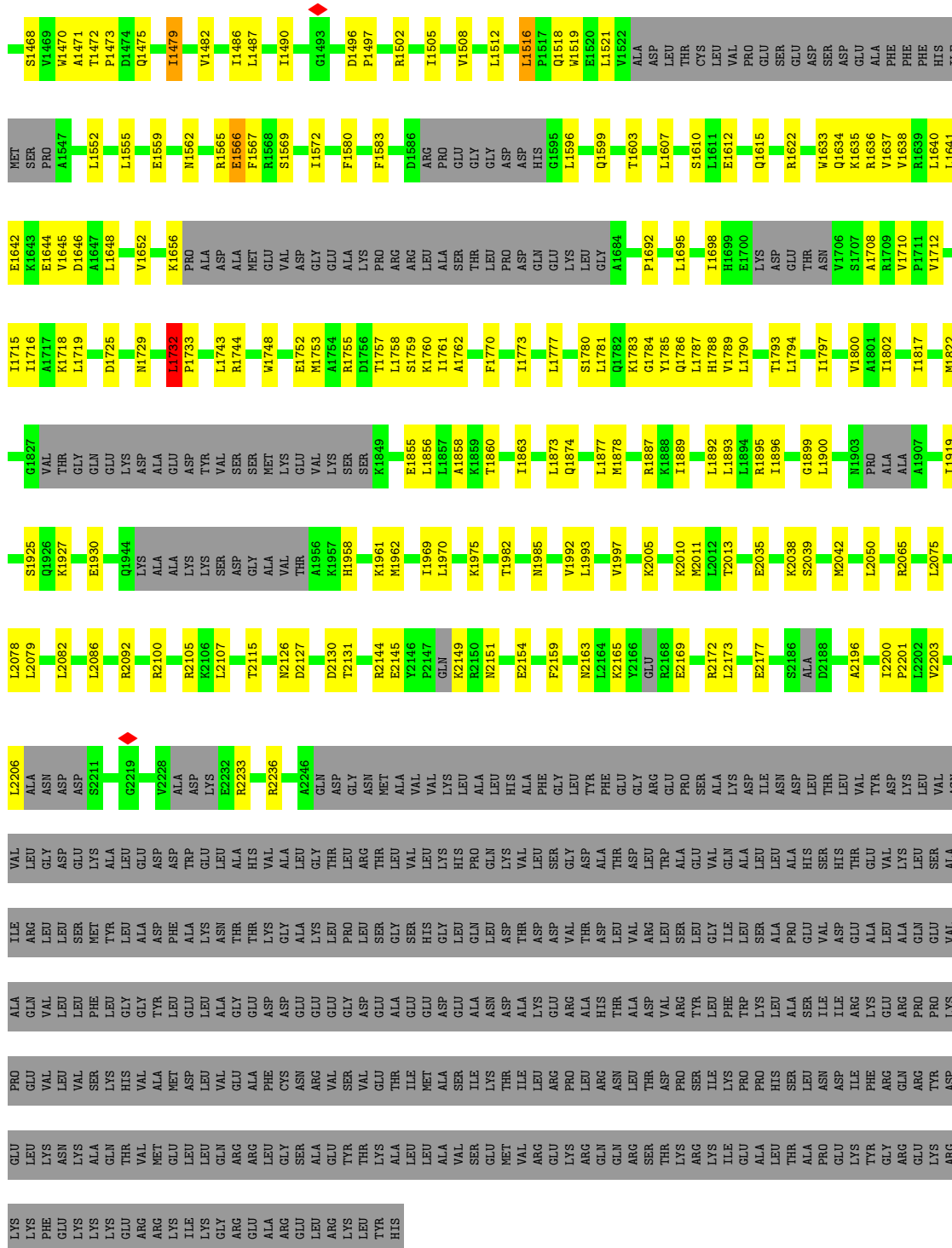


• Molecule 53: Rrp7

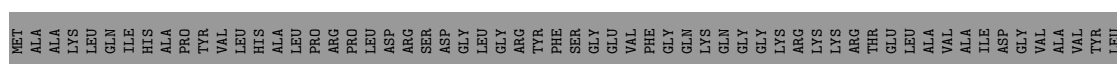


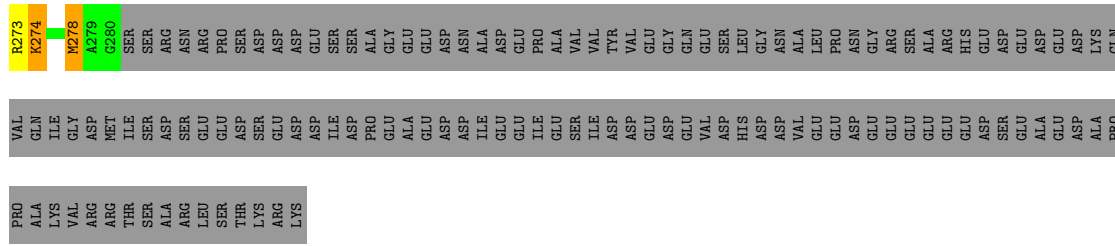
• Molecule 54: Ribosome biogenesis protein ENP2



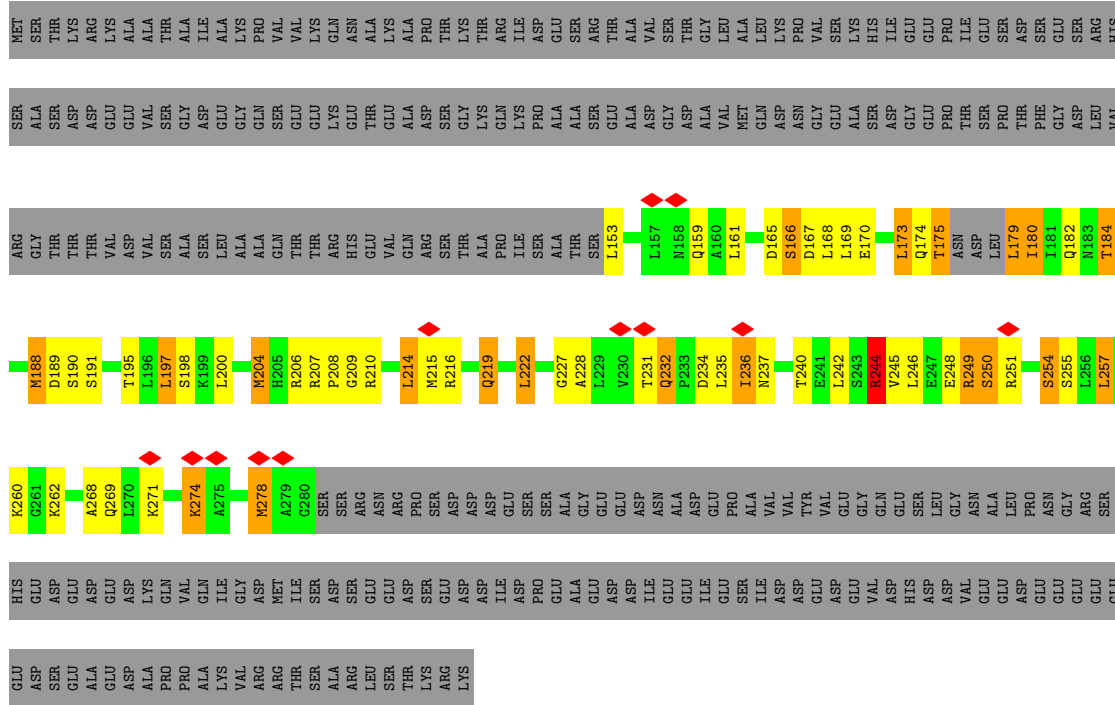


• Molecule 56: Utp8

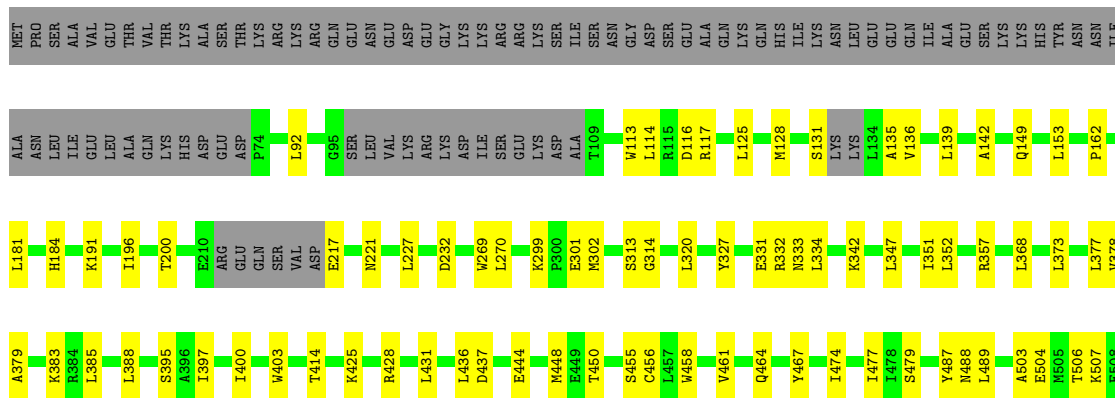




• Molecule 57: Utp5



• Molecule 58: Noc4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48335	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.418	Depositor
Minimum map value	-0.315	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	520.32, 520.32, 520.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	UA	0.49	0/6521	0.67	3/8867 (0.0%)
2	UB	0.31	0/4154	0.54	0/5583
3	UC	0.40	0/595	0.56	0/786
4	UD	0.39	0/6211	0.59	2/8408 (0.0%)
5	UF	0.36	0/2657	0.57	0/3596
6	UG	0.48	0/3790	0.65	2/5120 (0.0%)
7	UJ	0.32	0/8567	0.61	0/11619
8	UK	0.38	0/1701	0.51	0/2251
9	UL	0.37	0/6299	0.64	0/8531
10	UM	0.33	0/5755	0.62	4/7827 (0.1%)
11	UN	0.39	0/1425	0.56	0/1913
12	UO	0.41	0/3903	0.63	0/5312
13	UQ	0.40	0/6136	0.64	0/8348
14	UR	0.47	0/3564	0.62	0/4816
15	UU	0.47	1/6903 (0.0%)	0.63	0/9392
16	UX	0.43	0/1493	0.59	1/2011 (0.0%)
17	UZ	0.32	0/1857	0.70	6/2526 (0.2%)
18	CA	0.45	0/1814	0.63	0/2456
18	CB	0.32	0/1853	0.56	0/2511
19	CC	0.36	0/2911	0.54	0/3937
20	CD	0.34	0/3205	0.59	0/4338
21	CE	0.42	0/891	0.66	2/1214 (0.2%)
21	CF	0.39	0/876	0.63	0/1195
22	CG	0.36	0/3307	0.61	0/4462
23	CH	0.40	0/2939	0.57	0/3988
24	CI	0.42	0/6631	0.62	4/8943 (0.0%)
25	CJ	0.50	0/1462	0.63	0/1967
26	CK	0.45	0/2376	0.61	2/3214 (0.1%)
27	CL	0.38	0/1812	0.56	0/2437
28	CM	0.49	0/3573	0.63	0/4829
29	CN	0.36	0/1797	0.59	0/2443
29	CO	0.32	0/1714	0.66	2/2325 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	CP	0.37	0/1923	0.56	0/2577
31	CQ	0.32	0/1379	0.57	0/1850
32	CR	0.36	0/6108	0.80	9/8266 (0.1%)
32	CS	0.36	0/6108	0.80	9/8266 (0.1%)
33	CT	0.36	0/1053	0.57	0/1413
34	Ca	0.37	0/1850	0.61	0/2486
35	Cb	0.33	0/1890	0.60	0/2548
36	Cc	0.40	0/1485	0.56	0/2008
37	Cd	0.32	0/1850	0.56	0/2474
38	Ce	0.35	0/1298	0.71	2/1750 (0.1%)
39	Cf	0.34	0/1429	0.57	0/1915
40	Cg	0.41	0/1259	0.53	0/1687
41	Ch	0.27	0/557	0.46	0/749
42	Ci	0.38	0/819	0.60	0/1107
43	Cj	0.44	0/958	0.59	0/1293
44	Ck	0.28	0/1190	0.56	0/1592
45	Cm	0.37	0/1001	0.55	0/1345
46	Cn	0.46	0/712	0.57	0/954
47	Co	0.32	0/754	0.64	0/1011
48	Cp	0.40	0/458	0.64	0/617
49	CU	0.34	0/1350	0.61	0/1810
50	C1	0.35	0/37546	0.47	4/58475 (0.0%)
51	C2	0.36	0/5459	0.54	5/8498 (0.1%)
52	UV	0.30	2/8638 (0.0%)	0.66	3/11725 (0.0%)
53	CV	0.37	1/1172 (0.1%)	0.73	4/1592 (0.3%)
54	CW	0.35	0/2996	0.67	2/4075 (0.0%)
55	UT	0.31	2/16367 (0.0%)	0.61	2/22149 (0.0%)
56	UH	0.33	0/2852	0.60	2/3846 (0.1%)
57	UE	0.38	0/980	0.86	5/1316 (0.4%)
57	UI	0.38	0/980	0.86	5/1316 (0.4%)
58	US	0.33	0/3765	0.59	0/5100
59	Cl	0.28	0/638	0.65	0/857
60	CX	0.27	0/2180	0.63	0/2956
61	CY	0.40	0/986	0.69	0/1303
62	CZ	0.29	0/384	0.68	0/511
63	UP	0.32	0/428	0.53	0/570
All	All	0.37	6/229494 (0.0%)	0.60	80/319172 (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
1	UA	0	1
5	UF	0	1
6	UG	0	1
10	UM	0	2
12	UO	0	2
13	UQ	0	3
15	UU	0	3
18	CB	0	1
21	CF	0	1
24	CI	0	1
29	CO	0	2
31	CQ	0	1
32	CR	0	3
32	CS	0	3
35	Cb	0	1
37	Cd	0	1
38	Ce	0	1
52	UV	0	4
53	CV	0	1
54	CW	0	1
55	UT	0	9
58	US	0	1
61	CY	0	1
All	All	0	45

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	UV	1058	TYR	N-CA	6.82	1.54	1.46
15	UU	191	ASN	C-N	-5.86	1.24	1.33
52	UV	372	LYS	C-N	5.65	1.38	1.33
55	UT	1732	LEU	C-N	5.61	1.39	1.34
53	CV	91	HIS	N-CA	5.22	1.52	1.46

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	C2	2	G	OP1-P-OP2	-13.25	79.84	119.60
52	UV	1058	TYR	CA-CB-CG	11.26	134.17	113.90
51	C2	1	A	OP2-P-O3'	-11.19	74.43	108.00
51	C2	2	G	O5'-P-OP1	-11.11	74.66	108.00
29	CO	164	GLN	CA-C-N	10.37	134.81	120.39

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	UA	386	THR	Peptide
5	UF	120	VAL	Peptide
6	UG	227	TYR	Peptide
10	UM	328	LEU	Peptide
10	UM	382	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	UA	6366	0	6273	124	0
2	UB	4079	0	4201	63	0
3	UC	588	0	647	11	0
4	UD	6071	0	6080	118	0
5	UF	2591	0	2642	37	0
6	UG	3717	0	3756	75	0
7	UJ	8416	0	8591	151	0
8	UK	1687	0	1820	31	0
9	UL	6175	0	6188	143	0
10	UM	5643	0	5643	141	0
11	UN	1401	0	1455	29	0
12	UO	3819	0	3873	78	0
13	UQ	6008	0	6033	132	0
14	UR	3491	0	3507	51	0
15	UU	6734	0	6745	110	0
16	UX	1470	0	1532	34	0
17	UZ	1815	0	1896	25	0
18	CA	1778	0	1830	27	0
18	CB	1816	0	1847	41	0
19	CC	2866	0	2960	32	0
20	CD	3150	0	3262	58	0
21	CE	879	0	918	19	0
21	CF	864	0	900	16	0
22	CG	3245	0	3262	66	0
23	CH	2888	0	2979	63	0
24	CI	6486	0	6648	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	CJ	1434	0	1482	30	0
26	CK	2329	0	2373	51	0
27	CL	1786	0	1826	39	0
28	CM	3501	0	3498	87	0
29	CN	1762	0	1807	29	0
29	CO	1683	0	1726	21	0
30	CP	1893	0	1993	29	0
31	CQ	1361	0	1431	27	0
32	CR	5989	0	6130	163	0
32	CS	5989	0	6130	157	0
33	CT	1035	0	1063	19	0
34	Ca	1821	0	1936	40	0
35	Cb	1851	0	1905	44	0
36	Cc	1464	0	1504	24	0
37	Cd	1819	0	1920	46	0
38	Ce	1279	0	1322	33	0
39	Cf	1398	0	1401	32	0
40	Cg	1242	0	1354	26	0
41	Ch	546	0	580	7	0
42	Ci	808	0	831	11	0
43	Cj	943	0	1002	13	0
44	Ck	1163	0	1230	26	0
45	Cm	985	0	1021	15	0
46	Cn	702	0	750	11	0
47	Co	741	0	785	26	0
48	Cp	455	0	482	5	0
49	CU	1337	0	1376	23	0
50	C1	33604	0	17014	582	0
51	C2	4891	0	2476	81	0
52	UV	8424	0	8502	211	0
53	CV	1145	0	1155	28	0
54	CW	2924	0	2854	92	0
55	UT	16049	0	16453	344	0
56	UH	2809	0	2843	83	0
57	UE	972	0	1032	30	0
57	UI	972	0	1032	48	0
58	US	3672	0	3679	67	0
59	Cl	633	0	676	7	0
60	CX	2130	0	2219	44	0
61	CY	979	0	995	40	0
62	CZ	376	0	371	5	0
63	UP	422	0	457	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	UX	1	0	0	0	0
65	CI	32	0	12	1	0
66	CI	1	0	0	0	0
All	All	221395	0	206116	4006	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 9.

The worst 5 of 4006 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)
50:C1:471:C:N4	61:CY:377:ARG:O	1.74	1.18
54:CW:23:LEU:HB3	54:CW:24:PRO:CD	1.75	1.17
56:UH:555:GLY:O	56:UH:567:LEU:HA	1.44	1.16
50:C1:1029:A:H62	50:C1:1045:G:N2	1.43	1.15
56:UH:557:GLU:O	56:UH:565:GLY:HA2	1.53	1.08

There are no symmetry-related clashes.

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	
1	UA	835/904 (92%)	753 (90%)	82 (10%)	0	100	100
2	UB	502/907 (55%)	469 (93%)	33 (7%)	0	100	100
3	UC	72/648 (11%)	67 (93%)	5 (7%)	0	100	100
4	UD	754/884 (85%)	705 (94%)	49 (6%)	0	100	100
5	UF	325/414 (78%)	309 (95%)	16 (5%)	0	100	100
6	UG	475/558 (85%)	439 (92%)	33 (7%)	3 (1%)	21	57
7	UJ	1062/1802 (59%)	1007 (95%)	55 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	UK	211/270 (78%)	207 (98%)	4 (2%)	0	100	100
9	UL	767/962 (80%)	694 (90%)	73 (10%)	0	100	100
10	UM	705/912 (77%)	645 (92%)	59 (8%)	1 (0%)	48	81
11	UN	171/938 (18%)	161 (94%)	9 (5%)	1 (1%)	21	57
12	UO	498/557 (89%)	465 (93%)	33 (7%)	0	100	100
13	UQ	775/960 (81%)	707 (91%)	67 (9%)	1 (0%)	48	81
14	UR	437/618 (71%)	407 (93%)	30 (7%)	0	100	100
15	UU	890/1049 (85%)	814 (92%)	76 (8%)	0	100	100
16	UX	188/193 (97%)	176 (94%)	12 (6%)	0	100	100
17	UZ	229/391 (59%)	213 (93%)	16 (7%)	0	100	100
18	CA	238/313 (76%)	221 (93%)	17 (7%)	0	100	100
18	CB	235/313 (75%)	217 (92%)	18 (8%)	0	100	100
19	CC	383/523 (73%)	362 (94%)	21 (6%)	0	100	100
20	CD	416/582 (72%)	385 (92%)	31 (8%)	0	100	100
21	CE	119/127 (94%)	112 (94%)	7 (6%)	0	100	100
21	CF	118/127 (93%)	110 (93%)	8 (7%)	0	100	100
22	CG	402/630 (64%)	369 (92%)	33 (8%)	0	100	100
23	CH	383/411 (93%)	351 (92%)	31 (8%)	1 (0%)	36	70
24	CI	812/1163 (70%)	742 (91%)	69 (8%)	1 (0%)	48	81
25	CJ	177/183 (97%)	169 (96%)	8 (4%)	0	100	100
26	CK	295/297 (99%)	272 (92%)	23 (8%)	0	100	100
27	CL	225/785 (29%)	209 (93%)	15 (7%)	1 (0%)	30	65
28	CM	443/446 (99%)	406 (92%)	37 (8%)	0	100	100
29	CN	222/252 (88%)	207 (93%)	15 (7%)	0	100	100
29	CO	211/252 (84%)	192 (91%)	17 (8%)	2 (1%)	14	48
30	CP	227/322 (70%)	216 (95%)	11 (5%)	0	100	100
31	CQ	171/259 (66%)	164 (96%)	7 (4%)	0	100	100
32	CR	746/1073 (70%)	687 (92%)	58 (8%)	1 (0%)	48	81
32	CS	746/1073 (70%)	687 (92%)	58 (8%)	1 (0%)	48	81
33	CT	127/203 (63%)	113 (89%)	14 (11%)	0	100	100
34	Ca	223/255 (88%)	206 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Cb	230/264 (87%)	209 (91%)	21 (9%)	0	100	100
36	Cc	188/212 (89%)	177 (94%)	11 (6%)	0	100	100
37	Cd	224/239 (94%)	209 (93%)	15 (7%)	0	100	100
38	Ce	155/203 (76%)	138 (89%)	17 (11%)	0	100	100
39	Cf	170/202 (84%)	162 (95%)	8 (5%)	0	100	100
40	Cg	157/190 (83%)	150 (96%)	7 (4%)	0	100	100
41	Ch	64/151 (42%)	62 (97%)	2 (3%)	0	100	100
42	Ci	113/150 (75%)	108 (96%)	5 (4%)	0	100	100
43	Cj	124/143 (87%)	117 (94%)	7 (6%)	0	100	100
44	Ck	136/161 (84%)	127 (93%)	9 (7%)	0	100	100
45	Cm	122/130 (94%)	114 (93%)	8 (7%)	0	100	100
46	Cn	92/145 (63%)	89 (97%)	3 (3%)	0	100	100
47	Co	90/136 (66%)	80 (89%)	10 (11%)	0	100	100
48	Cp	59/68 (87%)	53 (90%)	6 (10%)	0	100	100
49	CU	168/311 (54%)	154 (92%)	14 (8%)	0	100	100
52	UV	1057/1171 (90%)	966 (91%)	89 (8%)	2 (0%)	43	75
53	CV	144/322 (45%)	129 (90%)	14 (10%)	1 (1%)	18	54
54	CW	380/668 (57%)	337 (89%)	43 (11%)	0	100	100
55	UT	1987/2612 (76%)	1877 (94%)	103 (5%)	7 (0%)	30	65
56	UH	349/930 (38%)	328 (94%)	21 (6%)	0	100	100
57	UE	121/410 (30%)	113 (93%)	8 (7%)	0	100	100
57	UI	121/410 (30%)	113 (93%)	8 (7%)	0	100	100
58	US	443/549 (81%)	407 (92%)	36 (8%)	0	100	100
59	Cl	78/156 (50%)	74 (95%)	4 (5%)	0	100	100
60	CX	265/480 (55%)	251 (95%)	14 (5%)	0	100	100
61	CY	119/381 (31%)	112 (94%)	6 (5%)	1 (1%)	16	52
62	CZ	42/609 (7%)	36 (86%)	6 (14%)	0	100	100
63	UP	52/364 (14%)	43 (83%)	8 (15%)	1 (2%)	6	34
All	All	23065/34323 (67%)	21370 (93%)	1670 (7%)	25 (0%)	49	81

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	CO	85	SER
52	UV	1059	ASP
13	UQ	708	SER
55	UT	457	TRP
55	UT	487	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	651/775 (84%)	648 (100%)	3 (0%)	81	82
2	UB	425/788 (54%)	422 (99%)	3 (1%)	76	79
3	UC	61/536 (11%)	61 (100%)	0	100	100
4	UD	653/738 (88%)	648 (99%)	5 (1%)	73	77
5	UF	248/341 (73%)	248 (100%)	0	100	100
6	UG	373/474 (79%)	368 (99%)	5 (1%)	61	72
7	UJ	898/1526 (59%)	897 (100%)	1 (0%)	88	89
8	UK	159/227 (70%)	158 (99%)	1 (1%)	78	81
9	UL	667/821 (81%)	665 (100%)	2 (0%)	86	85
10	UM	606/770 (79%)	603 (100%)	3 (0%)	81	82
11	UN	146/765 (19%)	145 (99%)	1 (1%)	76	79
12	UO	404/456 (89%)	400 (99%)	4 (1%)	68	76
13	UQ	650/817 (80%)	646 (99%)	4 (1%)	78	81
14	UR	360/524 (69%)	359 (100%)	1 (0%)	86	85
15	UU	672/863 (78%)	668 (99%)	4 (1%)	78	81
16	UX	150/167 (90%)	148 (99%)	2 (1%)	61	72
17	UZ	186/329 (56%)	184 (99%)	2 (1%)	65	74
18	CA	175/228 (77%)	174 (99%)	1 (1%)	78	81
18	CB	195/228 (86%)	195 (100%)	0	100	100
19	CC	287/435 (66%)	286 (100%)	1 (0%)	86	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	CD	319/489 (65%)	318 (100%)	1 (0%)	86	85
21	CE	91/108 (84%)	91 (100%)	0	100	100
21	CF	88/108 (82%)	86 (98%)	2 (2%)	44	64
22	CG	331/525 (63%)	328 (99%)	3 (1%)	70	76
23	CH	303/320 (95%)	300 (99%)	3 (1%)	68	76
24	CI	661/1009 (66%)	658 (100%)	3 (0%)	81	82
25	CJ	147/169 (87%)	145 (99%)	2 (1%)	59	71
26	CK	245/266 (92%)	243 (99%)	2 (1%)	73	77
27	CL	181/642 (28%)	181 (100%)	0	100	100
28	CM	364/383 (95%)	363 (100%)	1 (0%)	86	85
29	CN	202/223 (91%)	201 (100%)	1 (0%)	81	82
29	CO	193/223 (86%)	192 (100%)	1 (0%)	81	82
30	CP	202/287 (70%)	202 (100%)	0	100	100
31	CQ	145/215 (67%)	145 (100%)	0	100	100
32	CR	654/916 (71%)	445 (68%)	209 (32%)	0	2
32	CS	654/916 (71%)	445 (68%)	209 (32%)	0	2
33	CT	108/167 (65%)	108 (100%)	0	100	100
34	Ca	198/223 (89%)	197 (100%)	1 (0%)	81	82
35	Cb	199/221 (90%)	198 (100%)	1 (0%)	81	82
36	Cc	149/178 (84%)	147 (99%)	2 (1%)	61	72
37	Cd	192/204 (94%)	192 (100%)	0	100	100
38	Ce	137/177 (77%)	135 (98%)	2 (2%)	57	70
39	Cf	139/164 (85%)	139 (100%)	0	100	100
40	Cg	122/162 (75%)	122 (100%)	0	100	100
41	Ch	58/130 (45%)	58 (100%)	0	100	100
42	Ci	78/117 (67%)	78 (100%)	0	100	100
43	Cj	92/115 (80%)	92 (100%)	0	100	100
44	Ck	126/143 (88%)	125 (99%)	1 (1%)	73	77
45	Cm	103/113 (91%)	101 (98%)	2 (2%)	50	67
46	Cn	70/116 (60%)	70 (100%)	0	100	100
47	Co	79/115 (69%)	78 (99%)	1 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	Cp	46/61 (75%)	46 (100%)	0	100	100
49	CU	137/260 (53%)	137 (100%)	0	100	100
52	UV	908/989 (92%)	906 (100%)	2 (0%)	87	87
53	CV	129/276 (47%)	127 (98%)	2 (2%)	55	70
54	CW	309/587 (53%)	308 (100%)	1 (0%)	86	85
55	UT	1731/2276 (76%)	1727 (100%)	4 (0%)	87	87
56	UH	301/788 (38%)	301 (100%)	0	100	100
57	UE	105/346 (30%)	69 (66%)	36 (34%)	0	2
57	UI	105/346 (30%)	69 (66%)	36 (34%)	0	2
58	US	404/493 (82%)	404 (100%)	0	100	100
59	Cl	71/135 (53%)	70 (99%)	1 (1%)	59	71
60	CX	227/411 (55%)	227 (100%)	0	100	100
61	CY	100/322 (31%)	95 (95%)	5 (5%)	22	45
62	CZ	38/519 (7%)	38 (100%)	0	100	100
63	UP	44/314 (14%)	44 (100%)	0	100	100
All	All	19251/29075 (66%)	18674 (97%)	577 (3%)	37	57

5 of 577 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	CS	861	ILE
57	UI	255	SER
32	CS	911	ILE
32	CS	860	THR
57	UE	219	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 328 such sidechains are listed below:

Mol	Chain	Res	Type
42	Ci	102	ASN
55	UT	495	GLN
45	Cm	8	HIS
52	UV	752	ASN
55	UT	1741	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	C1	1550/2352 (65%)	482 (31%)	31 (2%)
51	C2	226/230 (98%)	67 (29%)	3 (1%)
All	All	1776/2582 (68%)	549 (30%)	34 (1%)

5 of 549 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	C1	4	G
50	C1	5	G
50	C1	7	A
50	C1	13	G
50	C1	14	G

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	C1	2156	A
50	C1	2177	G
51	C2	35	G
50	C1	771	G
50	C1	684	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 oligosaccharides 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$
65	GTP	CI	1201	-	33,34,34	1.01	3 (9%)	50,54,54	1.64	8 (16%)

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
65	GTP	CI	1201	-	-	4/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	CI	1201	GTP	C5-N7	-2.23	1.34	1.39
65	CI	1201	GTP	PA-O3A	2.13	1.61	1.59
65	CI	1201	GTP	C2-N3	2.11	1.38	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	CI	1201	GTP	C5-C4-N3	-5.15	120.19	128.39
65	CI	1201	GTP	C2-N3-C4	4.51	120.08	112.30
65	CI	1201	GTP	N9-C4-N3	3.48	132.91	125.95
65	CI	1201	GTP	C2-N1-C6	-3.33	119.08	125.11
65	CI	1201	GTP	C5-C6-N1	2.74	120.23	113.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

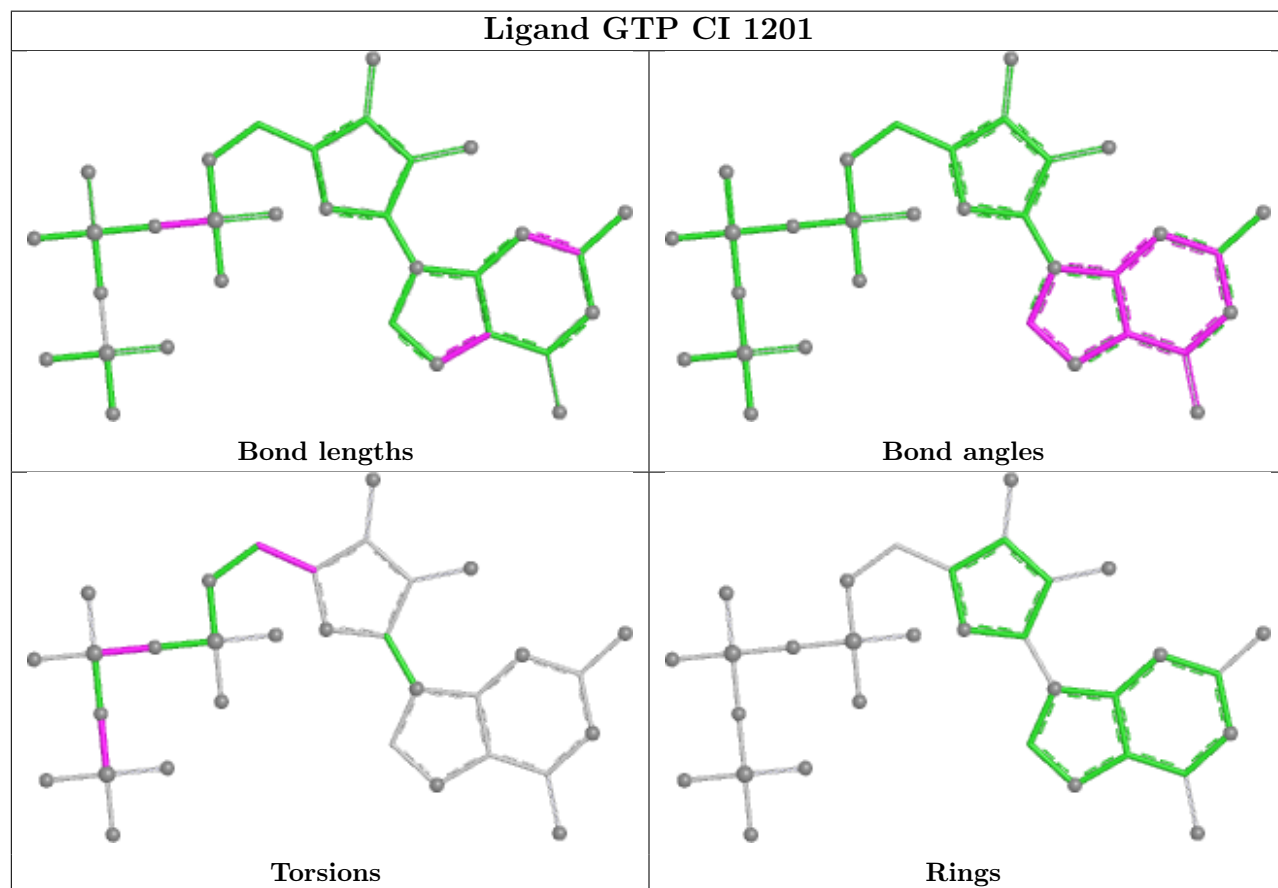
Mol	Chain	Res	Type	Atoms
65	CI	1201	GTP	PB-O3B-PG-O3G
65	CI	1201	GTP	PB-O3B-PG-O1G
65	CI	1201	GTP	PA-O3A-PB-O1B
65	CI	1201	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	CI	1201	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 [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
51	C2	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C2	206:G	O3'	240:C	P	19.22
1	C2	105:C	O3'	110:A	P	16.33
1	C2	119:C	O3'	123:A	P	11.75

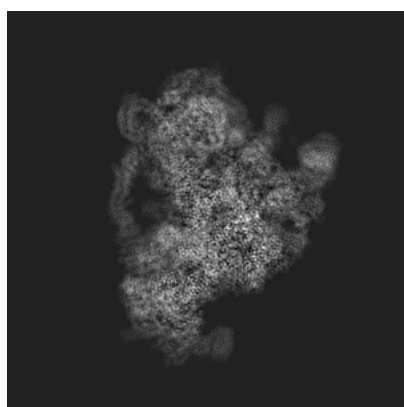
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10053. These allow visual inspection of the internal detail of the map and identification of artifacts.

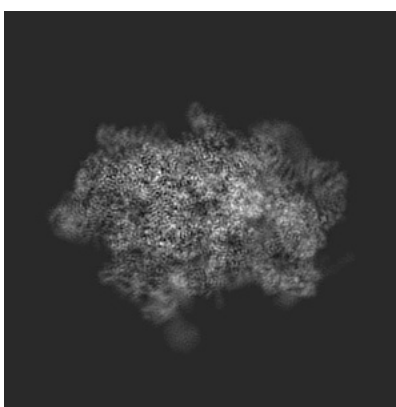
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

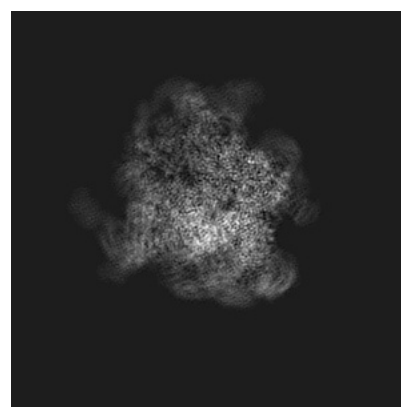
6.1.1 Primary map



X



Y

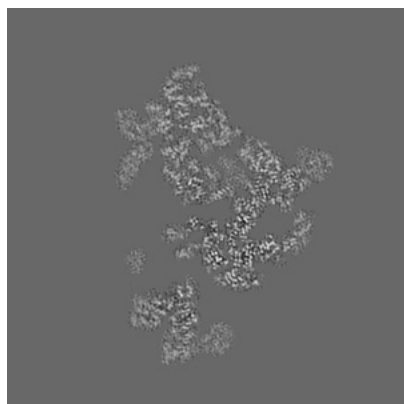


Z

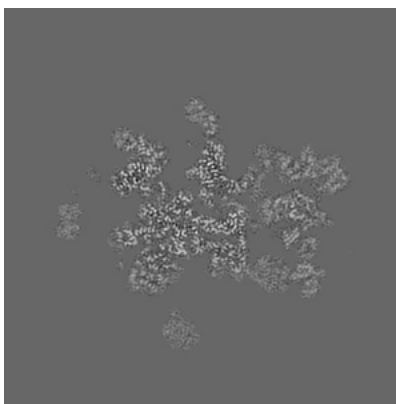
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

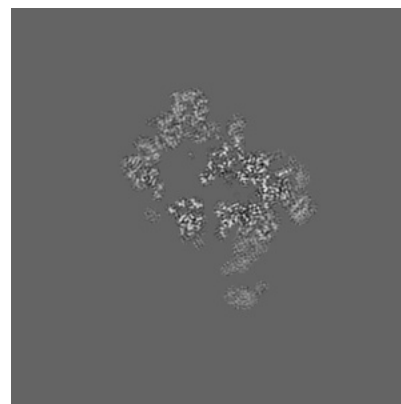
6.2.1 Primary map



X Index: 240



Y Index: 240

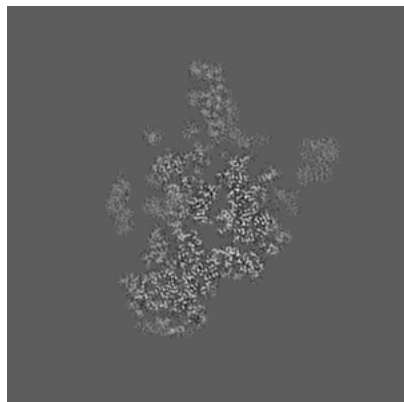


Z Index: 240

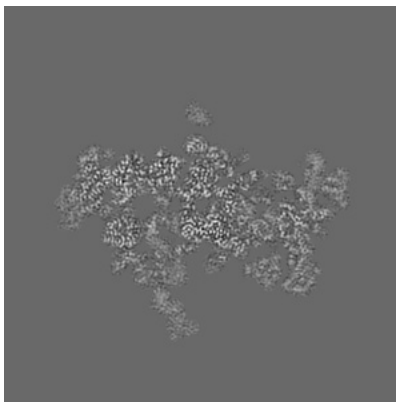
The images above show central slices of the map in three orthogonal directions.

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

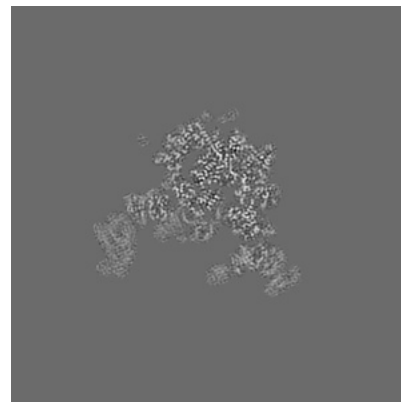
6.3.1 Primary map



X Index: 279



Y Index: 224

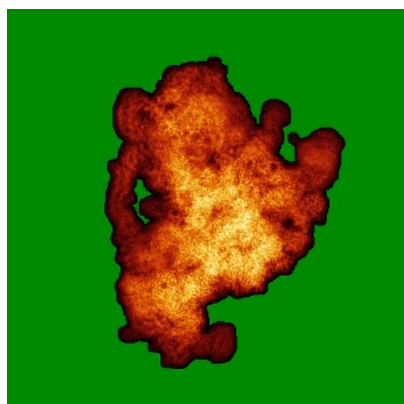


Z Index: 183

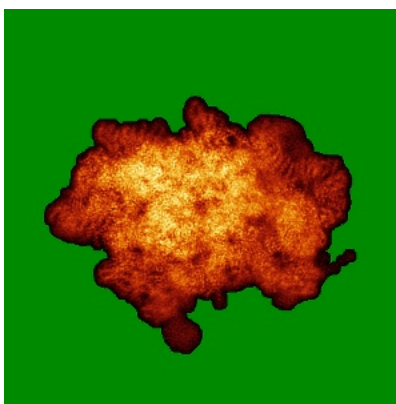
The images above show the largest variance slices of the map in three orthogonal directions.

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

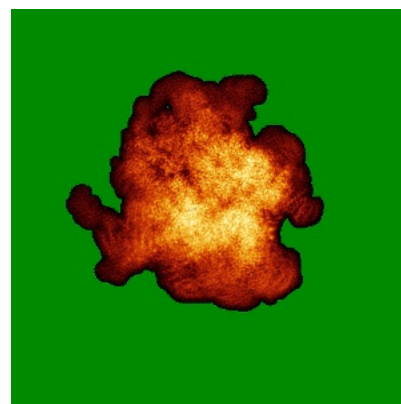
6.4.1 Primary map



X



Y

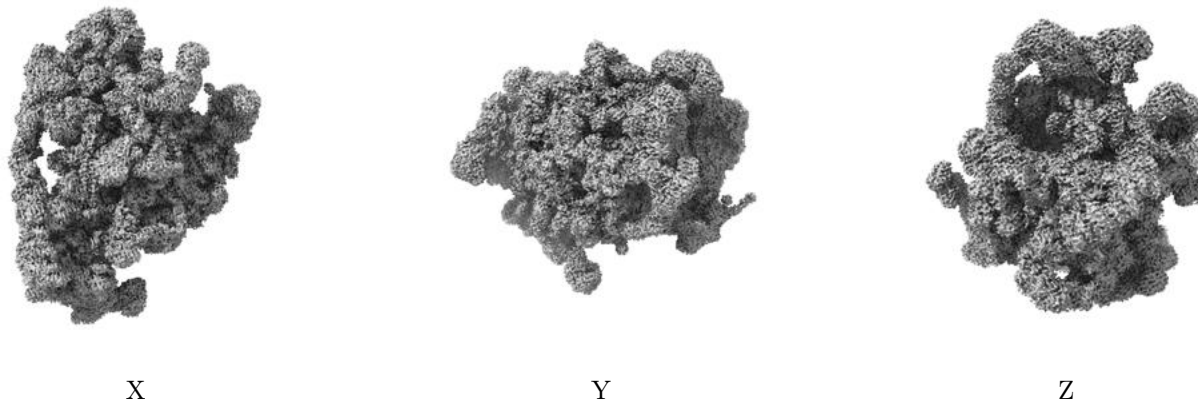


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

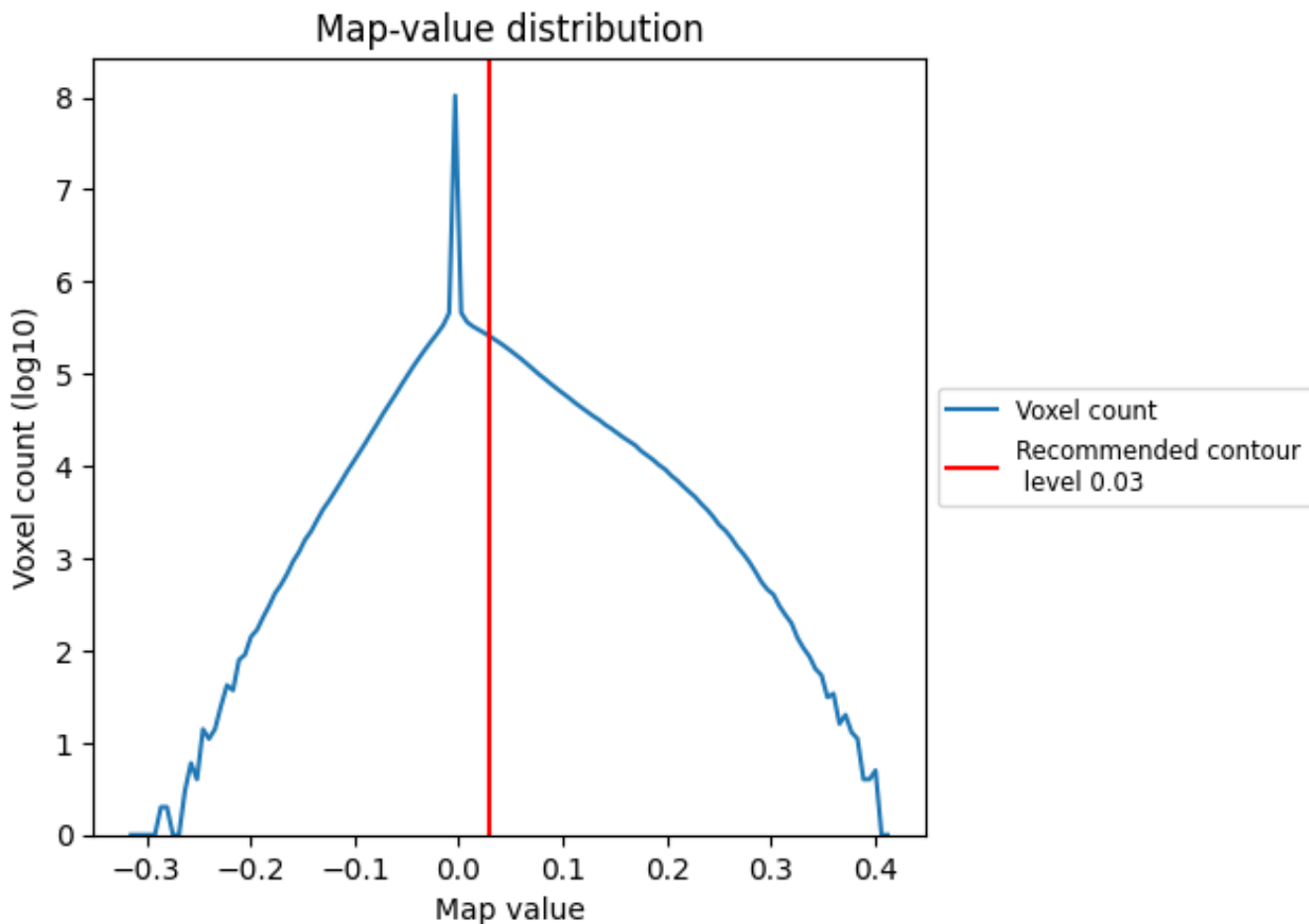
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

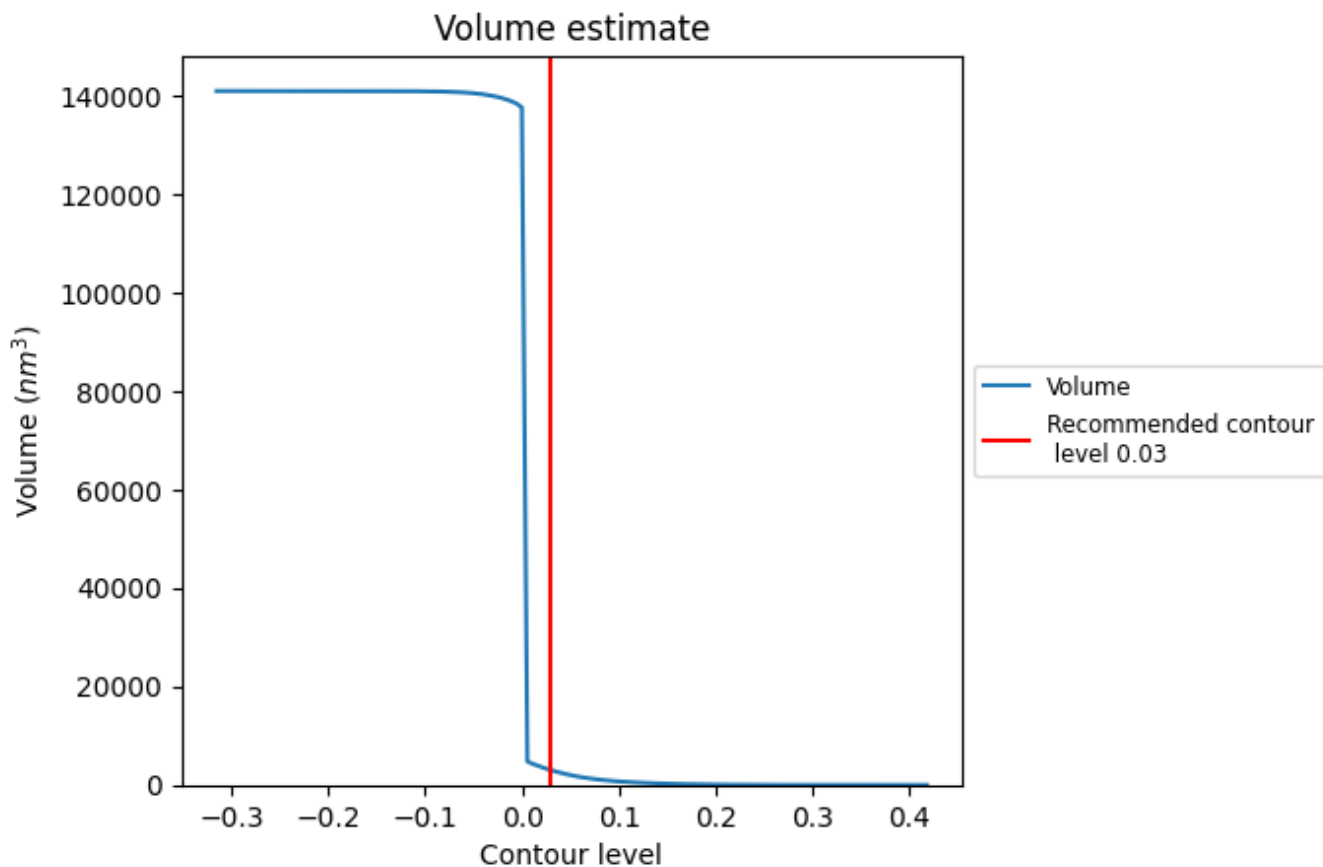
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

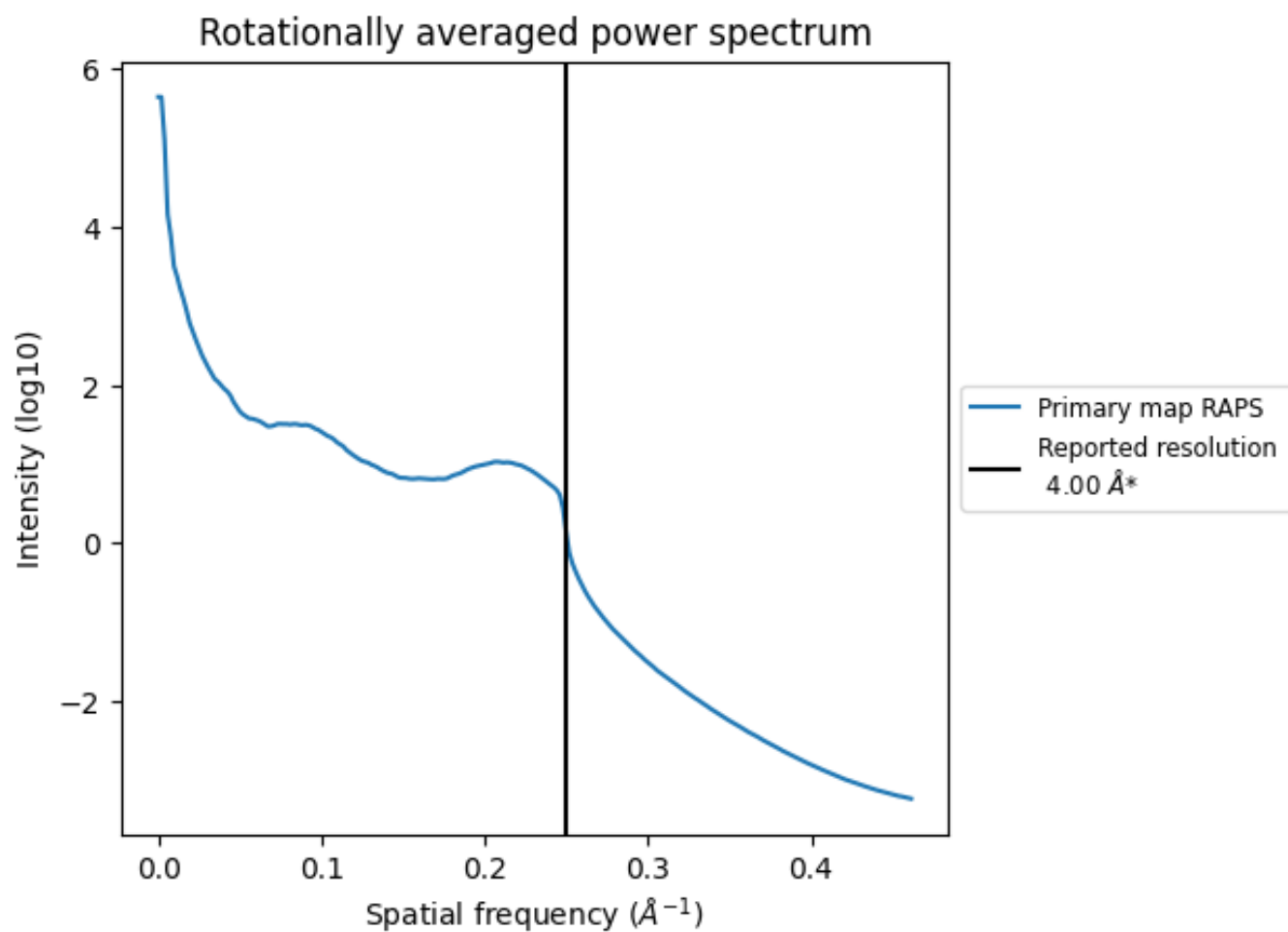
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3004 nm³; this corresponds to an approximate mass of 2713 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](#)

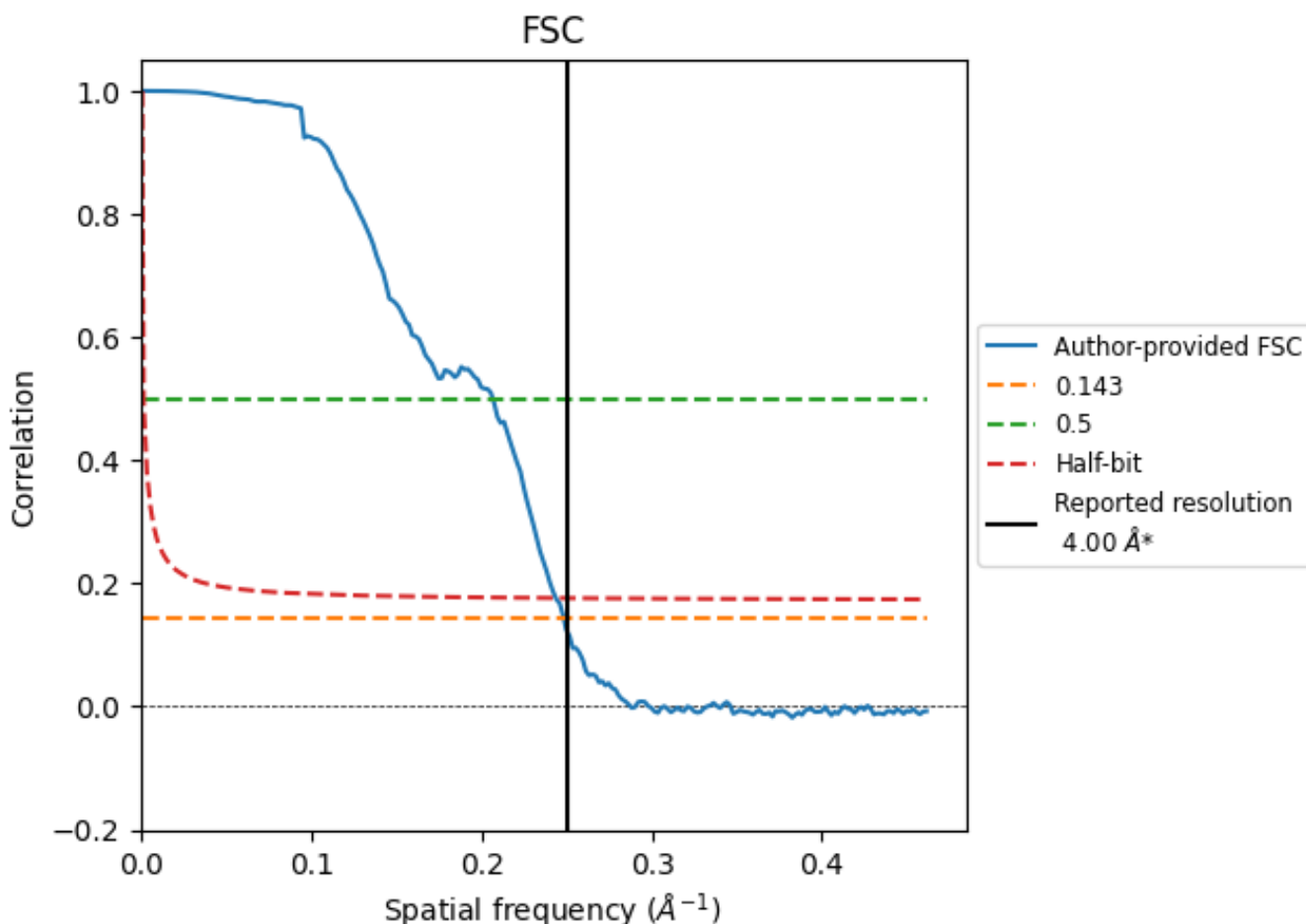


*Reported resolution corresponds to spatial frequency of 0.250\AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

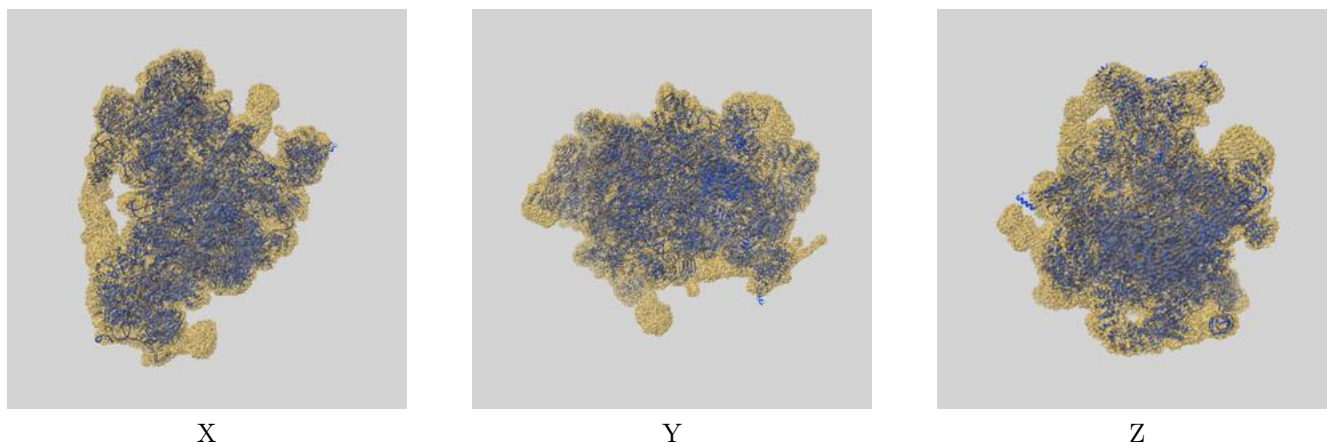
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.03	4.84	4.10
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

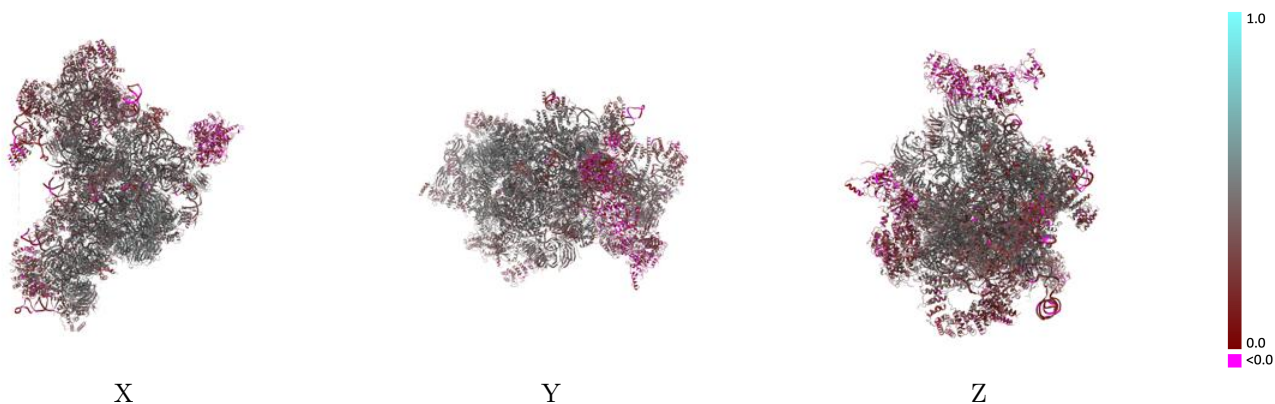
This section contains information regarding the fit between EMDB map EMD-10053 and PDB model 6RXV. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



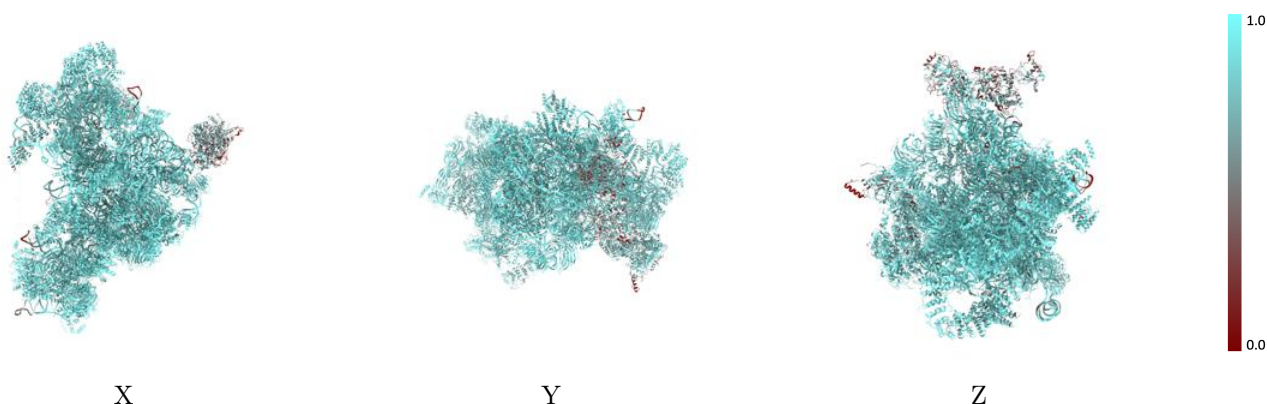
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



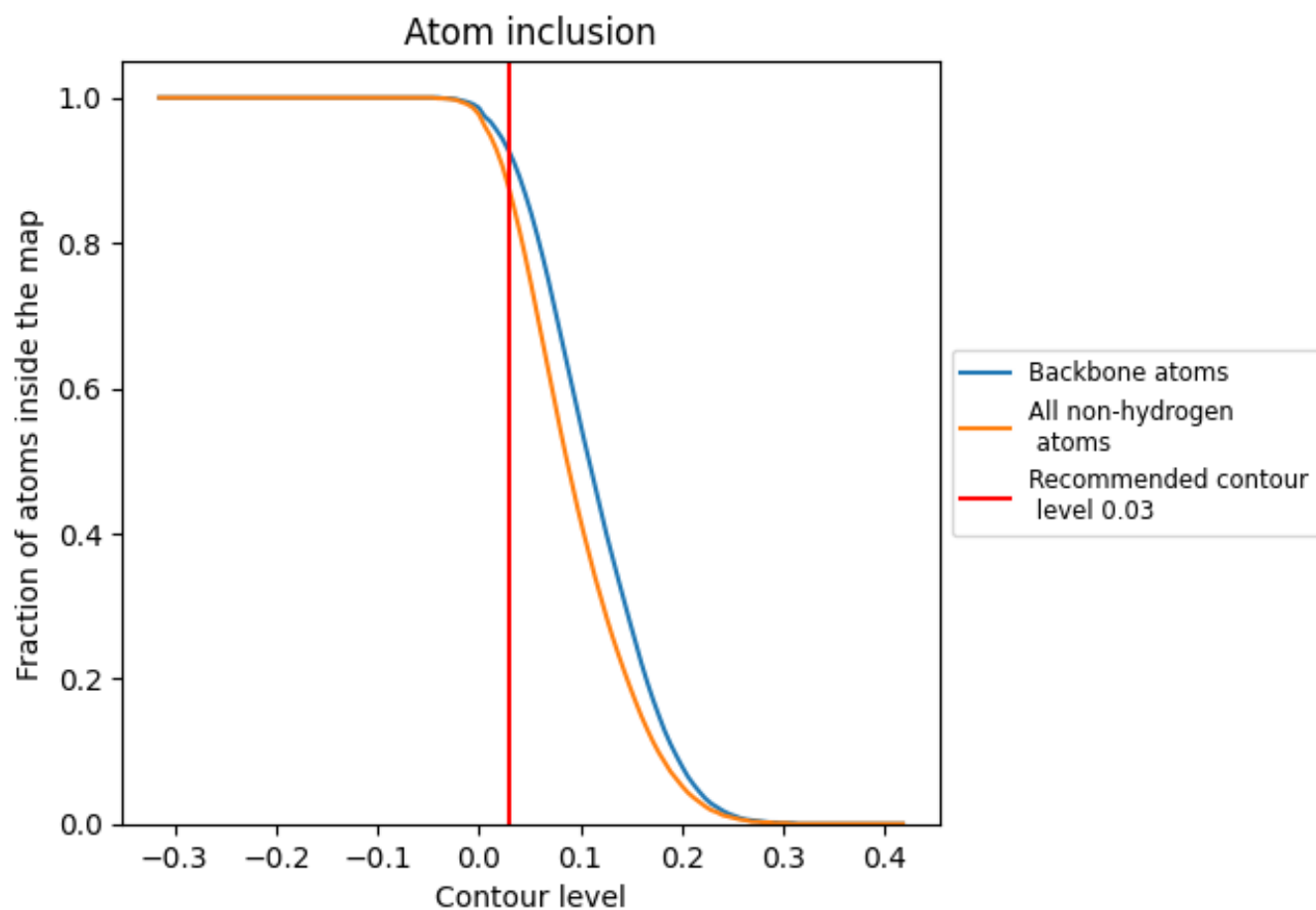
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8730	 0.3710
C1	 0.9240	 0.3580
C2	 0.8880	 0.3120
CA	 0.9110	 0.4790
CB	 0.8660	 0.4000
CC	 0.9000	 0.4040
CD	 0.8810	 0.3870
CE	 0.8970	 0.4530
CF	 0.8840	 0.4180
CG	 0.8980	 0.4110
CH	 0.8990	 0.4440
CI	 0.9140	 0.4450
CJ	 0.9220	 0.4780
CK	 0.8940	 0.4650
CL	 0.8870	 0.4480
CM	 0.9170	 0.4780
CN	 0.8720	 0.4190
CO	 0.8240	 0.3410
CP	 0.8690	 0.4140
CQ	 0.8740	 0.3620
CR	 0.8250	 0.2970
CS	 0.6750	 0.1460
CT	 0.8760	 0.4520
CU	 0.8770	 0.4340
CV	 0.5100	 0.1010
CW	 0.8810	 0.3900
CX	 0.7570	 0.1610
CY	 0.8340	 0.3890
CZ	 0.8420	 0.3030
Ca	 0.8810	 0.4080
Cb	 0.8750	 0.3870
Cc	 0.8970	 0.4520
Cd	 0.9020	 0.4070
Ce	 0.8620	 0.3540
Cf	 0.8940	 0.3970



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Chain	Atom inclusion	Q-score
Cg	 0.9150	 0.4580
Ch	 0.8460	 0.3570
Ci	 0.9330	 0.4560
Cj	 0.9160	 0.4800
Ck	 0.8270	 0.3540
Cl	 0.7020	 0.3080
Cm	 0.8720	 0.4330
Cn	 0.9130	 0.4790
Co	 0.8700	 0.3840
Cp	 0.9380	 0.4770
UA	 0.9200	 0.4790
UB	 0.9030	 0.3770
UC	 0.8930	 0.4820
UD	 0.9070	 0.4290
UE	 0.8270	 0.3370
UF	 0.9150	 0.3730
UG	 0.9240	 0.4680
UH	 0.9010	 0.3480
UI	 0.7320	 0.1790
UJ	 0.8560	 0.3080
UK	 0.9010	 0.4490
UL	 0.9120	 0.4210
UM	 0.9030	 0.3870
UN	 0.9230	 0.4390
UO	 0.9150	 0.4550
UP	 0.8720	 0.4220
UQ	 0.9200	 0.4420
UR	 0.9250	 0.4670
US	 0.8890	 0.3600
UT	 0.8750	 0.3070
UU	 0.9330	 0.4710
UV	 0.5090	 0.1100
UX	 0.8860	 0.4590
UZ	 0.8930	 0.3920