



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 09:39 am BST

PDB ID : 6SW9 / pdb_00006sw9
EMDB ID : EMD-10320
Title : IC2A model of cryo-EM structure of a full archaeal ribosomal translation initiation complex devoid of aIF1 in *P. abyssi*
Authors : Coureux, P.-D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2019-09-20
Resolution : 4.20 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:

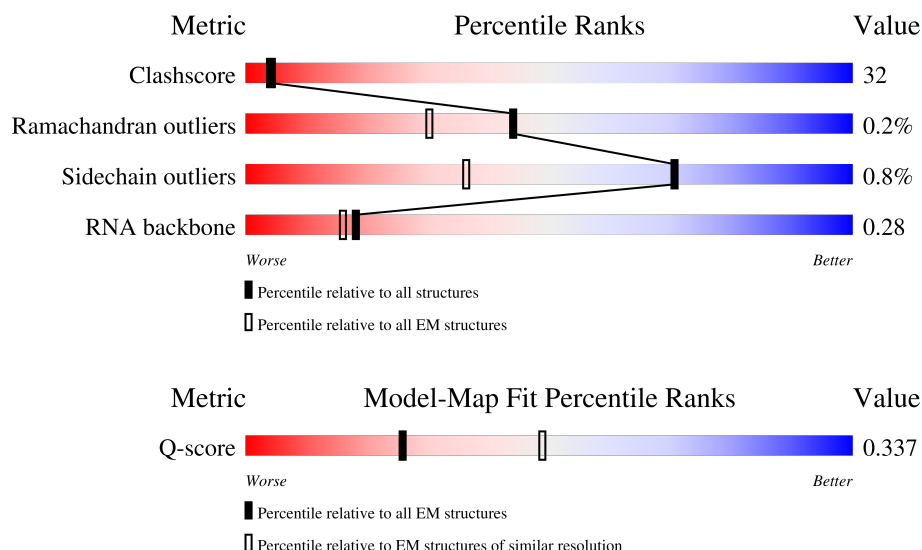
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 4.20 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.



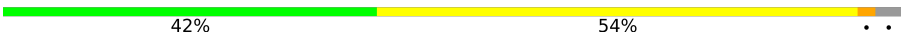
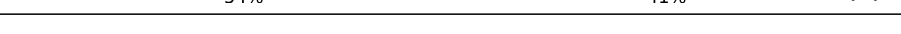
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	2	1497	
2	A	199	
3	B	202	

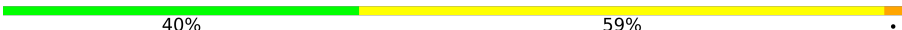
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Mol	Chain	Length	Quality of chain
4	C	63	
5	D	180	
6	E	243	
7	F	236	
8	G	125	
9	H	215	
10	I	130	
11	J	127	
12	K	135	
13	L	102	
14	M	137	
15	N	147	
16	O	148	
17	P	56	
18	Q	158	
19	R	113	
20	S	67	
21	T	132	
22	U	150	
23	V	99	
24	W	65	
25	X	71	
26	Y	51	
27	Z	210	
28	0	36	

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Mol	Chain	Length	Quality of chain
29	3	123	 40% 59%
30	5	20	 5% 60% 35%
31	4	76	 10% 53% 41%
32	6	113	 40% 44% 16%
33	7	414	 10% 36% 63%
34	8	129	 71% 65% 35%
35	9	254	 72% 65% 35%

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 70661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1497	Total	C	N	O	P	0	0
			32291	14394	5959	10441	1497		

- Molecule 2 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	188	Total	C	N	O	S	0	0
			1533	995	268	266	4		

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	196	Total	C	N	O	S	0	0
			1571	1017	269	281	4		

- Molecule 4 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	61	Total	C	N	O	S	0	0
			482	304	85	85	8		

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	175	Total	C	N	O	S	0	0
			1470	924	284	258	4		

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	242	Total	C	N	O	S	0	0
			1983	1281	358	339	5		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	124	Total	C	N	O	S	0	0
			977	621	178	176	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	213	Total	C	N	O	S	0	0
			1720	1092	322	299	7		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	129	Total	C	N	O	S	0	0
			1034	668	184	180	2		

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	J	126	Total	C	N	O	0	0
			996	617	206	173		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	134	Total	C	N	O	S	0	0
			1065	668	206	188	3		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	101	Total	C	N	O	S	0	0
			817	507	158	148	4		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	128	Total	C	N	O	S	0	0
			964	597	192	173	2		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	146	Total	C	N	O	S	0	0
			1148	727	224	194	3		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	138	Total	C	N	O	S	0	0
			1116	700	221	190	5		

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	55	Total	C	N	O	S	0	0
			455	288	95	67	5		

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	152	Total	C	N	O	S	0	0
			1262	804	240	214	4		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	109	Total	C	N	O	S	0	0
			900	572	174	151	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	66	Total	C	N	O	S	0	0
			558	355	106	96	1		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	125	Total	C	N	O	S	0	0
			1018	647	195	169	7		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	149	Total	C	N	O		0	0
			1223	790	221	212			

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	94	Total	C	N	O	S	0	0
			790	516	125	146	3		

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	63	Total	C	N	O	S	0	0
			481	303	93	80	5		

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	67	Total	C	N	O		0	0
			536	327	111	98			

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	50	Total	C	N	O	S	0	0
			408	262	77	63	6		

- Molecule 27 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	197	Total	C	N	O	S	0	0
			1550	989	286	271	4		

- Molecule 28 is a protein called 50S ribosomal protein L41e.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	0	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	123	Total	C	N	O	S	0	0
			941	599	157	181	4		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	20	Total	C	N	O	P	0	0
			430	192	78	140	20		

- Molecule 31 is a RNA chain called initiator Met-tRNA fMet from E. coli (A1U72 variant).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	76	Total	C	N	O	P	S	0	0
			1622	724	291	530	76	1		

- Molecule 32 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	95	Total	C	N	O	S	0	0
			777	496	148	130	3		

- Molecule 33 is a protein called Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	414	Total	C	N	O	S	0	0
			3213	2058	548	595	12		

- Molecule 34 is a protein called Translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	129	Total	C	N	O	S	0	0
			1032	659	171	192	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	?	-	GLU	deletion	UNP Q97W59
8	?	-	LYS	deletion	UNP Q97W59
8	?	-	GLY	deletion	UNP Q97W59
8	?	-	ARG	deletion	UNP Q97W59
8	?	-	LYS	deletion	UNP Q97W59
8	?	-	GLU	deletion	UNP Q97W59
8	?	-	GLY	deletion	UNP Q97W59
8	?	-	THR	deletion	UNP Q97W59

- Molecule 35 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	253	Total	C	N	O	S	0	0
			2025	1296	345	383	1		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	?	-	SER	deletion	UNP Q97Z79
9	?	-	LYS	deletion	UNP Q97Z79
9	?	-	TRP	deletion	UNP Q97Z79
9	?	-	VAL	deletion	UNP Q97Z79
9	?	-	LYS	deletion	UNP Q97Z79
9	?	-	LYS	deletion	UNP Q97Z79
9	?	-	HIS	deletion	UNP Q97Z79
9	?	-	ALA	deletion	UNP Q97Z79
9	?	-	GLU	deletion	UNP Q97Z79
9	?	-	GLU	deletion	UNP Q97Z79

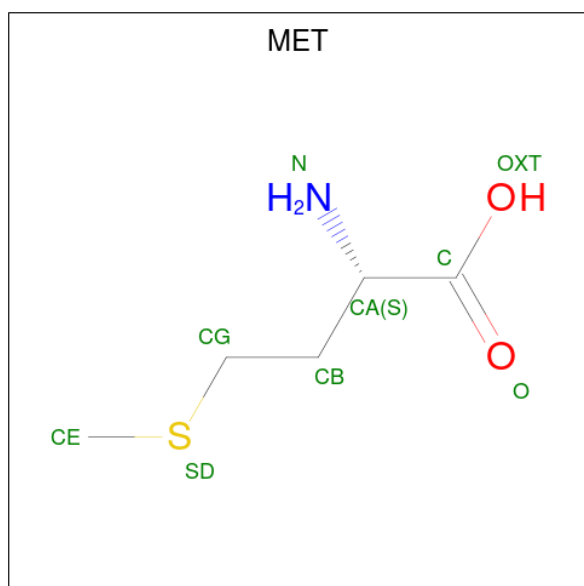
- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	2	31	Total	Mg	0
			31	31	
36	5	1	Total	Mg	0
			1	1	
36	4	1	Total	Mg	0
			1	1	
36	7	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

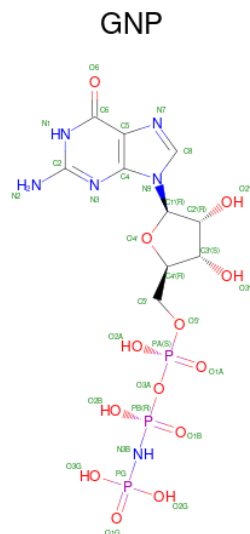
Mol	Chain	Residues	Atoms		AltConf
37	C	2	Total 2	Zn 2	0
37	F	1	Total 1	Zn 1	0
37	P	1	Total 1	Zn 1	0
37	R	1	Total 1	Zn 1	0
37	W	1	Total 1	Zn 1	0

- Molecule 38 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
38	7	1	Total 8	C 5	N 1	O 1	S 1	0

- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total 32	C 10	N 6	O 13	P 3	0

- Molecule 40 is water.

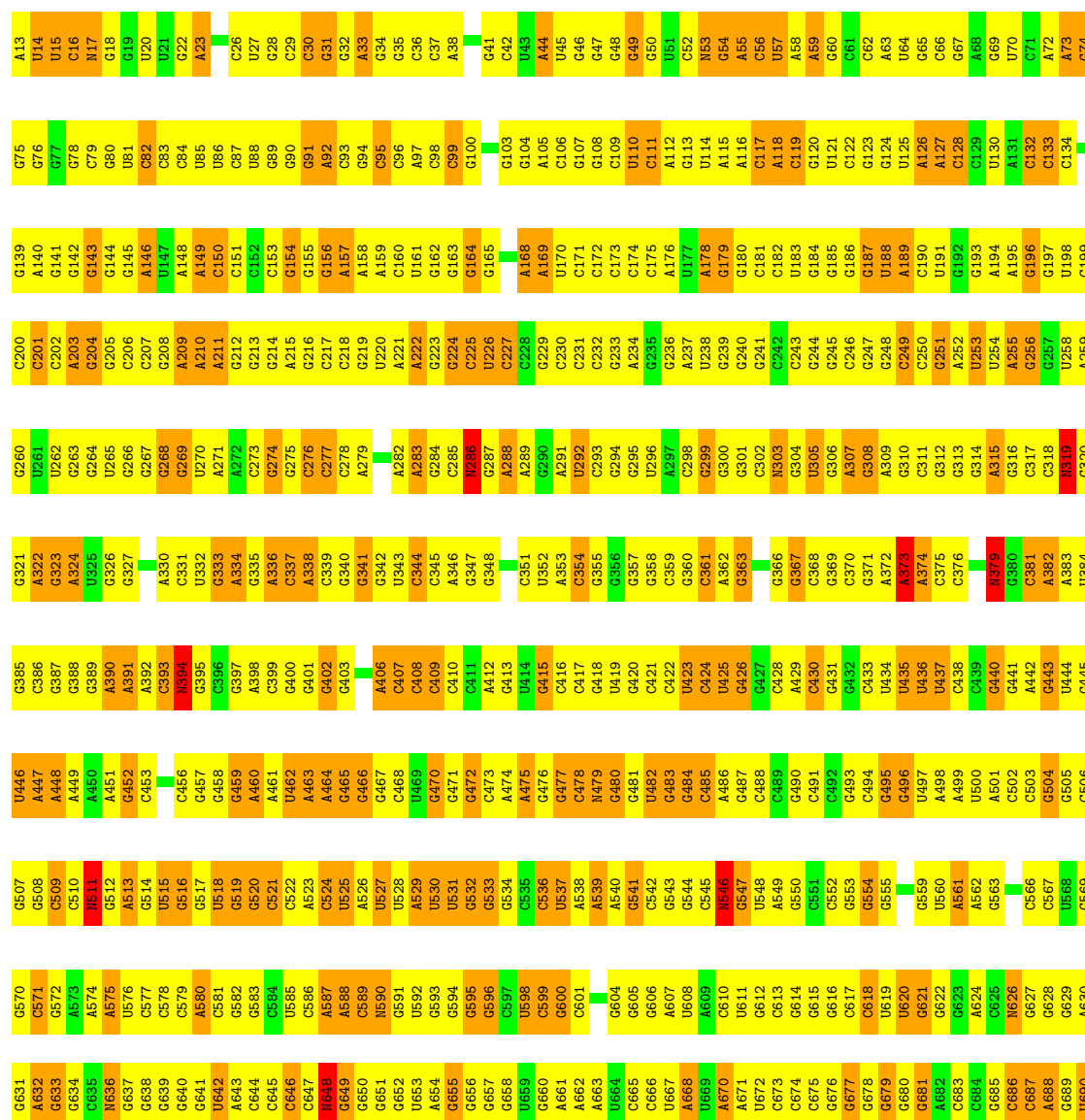
Mol	Chain	Residues	Atoms		AltConf
40	2	40	Total 40	O 40	0
40	K	1	Total 1	O 1	0
40	Q	1	Total 1	O 1	0

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.

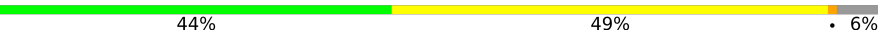
• Molecule 1: 16S ribosomal RNA

Chain 2: 

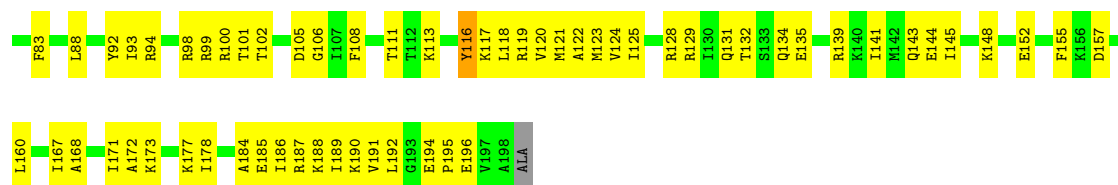


C1489	U1429	C1369	G1308	G1246	C1182	U1122	U1060	G1000	A940	G873	G813	G752	G691
C1490	C1430	C1370	C1309	C1247	C1183	U1123	C1081	A1001	A941	G874	A814	G753	G692
U1491	G1431	C1371	U1310	G1248	N1184	U1124	U1062	C1002	C942	C875	G815	A754	C693
A1492	G1432	A1372	G1311	A1249	G1185	G1063	G1064	G1003	G943	U876	C816	G755	G694
C1493	G1433	C1373	C1312	G1250	G1186	G1126	G1065	C1004	C944	G877	U817	U756	A695
G1494	U1434	C1374	A1313	G1251	A1187	G1127	U1065	G1005	C945	A878	C818	A757	A696

• Molecule 2: 30S ribosomal protein S3Ae

Chain A:  44% 49% 6%

NET	ALA	LYS	ARG	ARG	VAL	SER	ALA	ALA	K11	D12	K13	W14	K15	L16	K17	Q18	I22	Y23	A24	F27	V31	V32	V33	A38	D39	E42	K43	V44	L45	N46	R47	V48	V49	E50	T52	L53	K54	D55	G58	D59	F60	H64	F69	Q70	G71	Y72	D73	V74	K75
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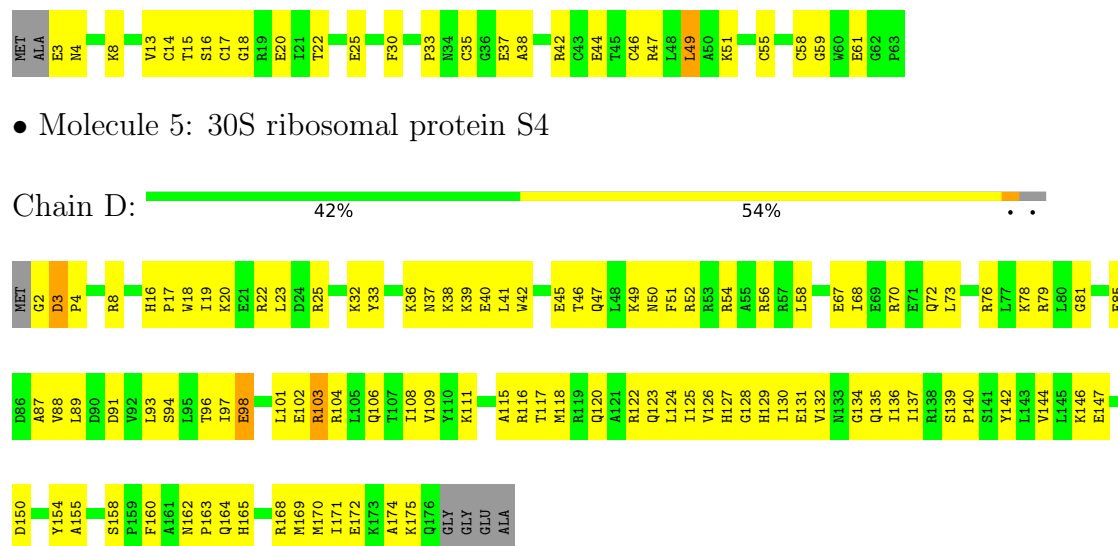
• Molecule 3: 30S ribosomal protein S2

Chain B: 56% 41%



• Molecule 4: Zn-ribbon RNA-binding protein involved in translation

Chain C: 54% 41%

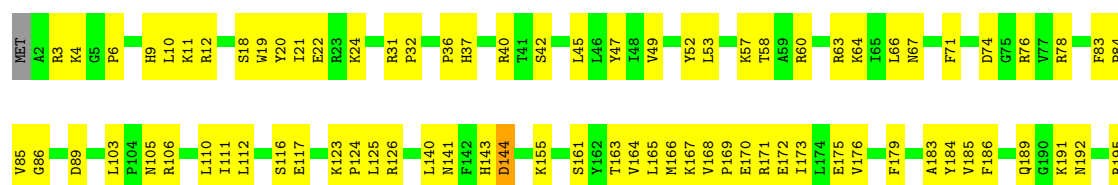


• Molecule 5: 30S ribosomal protein S4

Chain D: 42% 54%

• Molecule 6: 30S ribosomal protein S4e

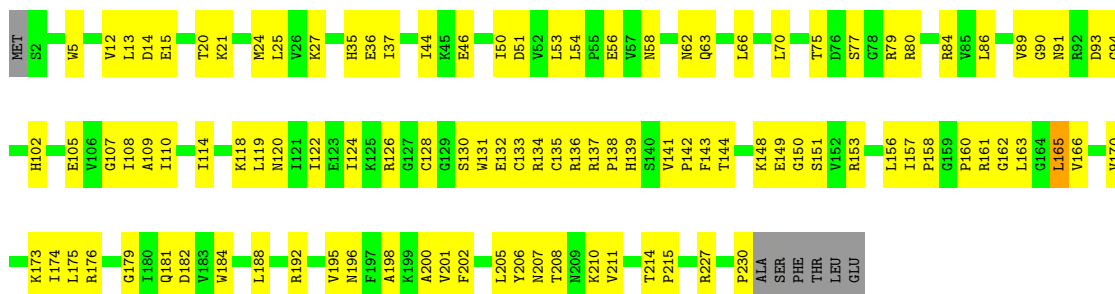
Chain E: 58% 42%





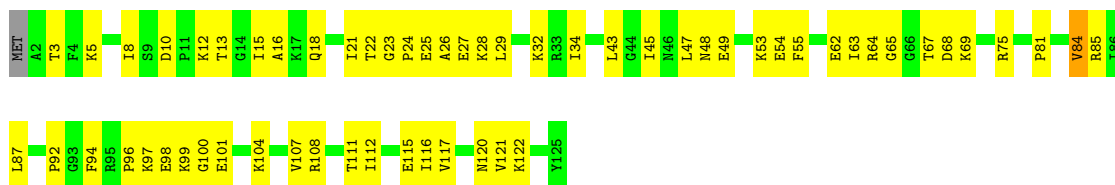
• Molecule 7: 30S ribosomal protein S5

Chain F: 53% 44%



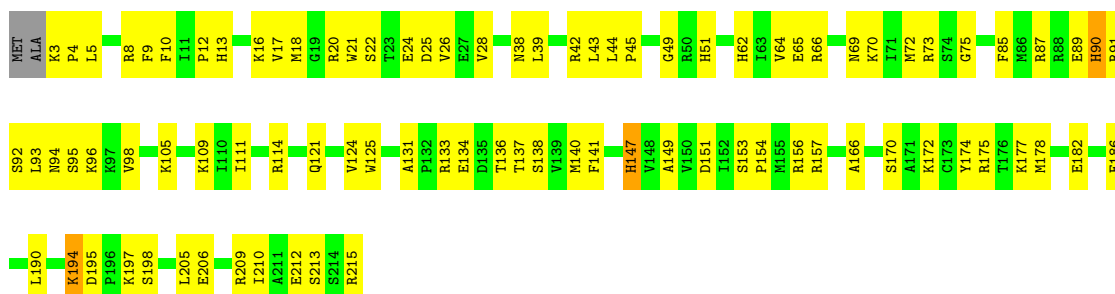
• Molecule 8: 30S ribosomal protein S6e

Chain G: 52% 46%



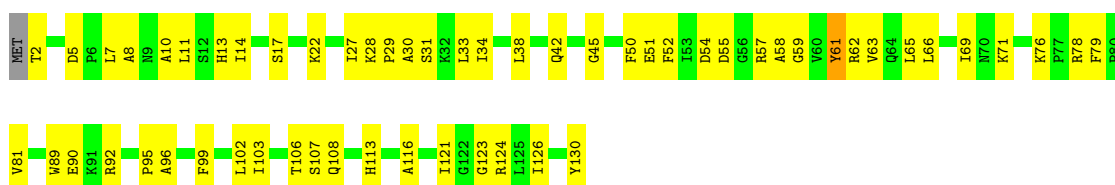
• Molecule 9: 30S ribosomal protein S7

Chain H: 58% 40%

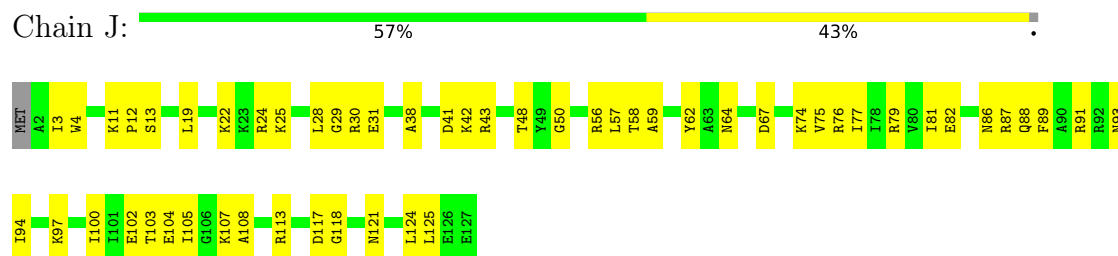


• Molecule 10: 30S ribosomal protein S8

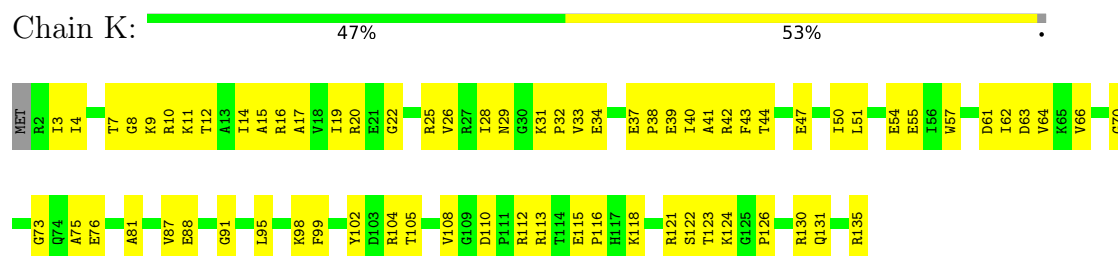
Chain I: 55% 43%



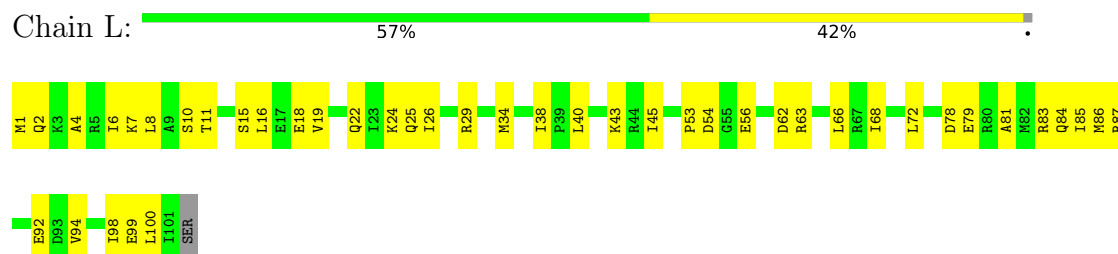
- Molecule 11: 30S ribosomal protein S8e



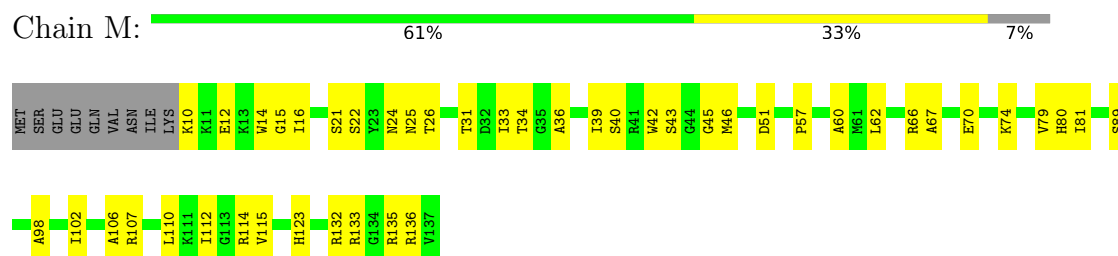
- Molecule 12: 30S ribosomal protein S9



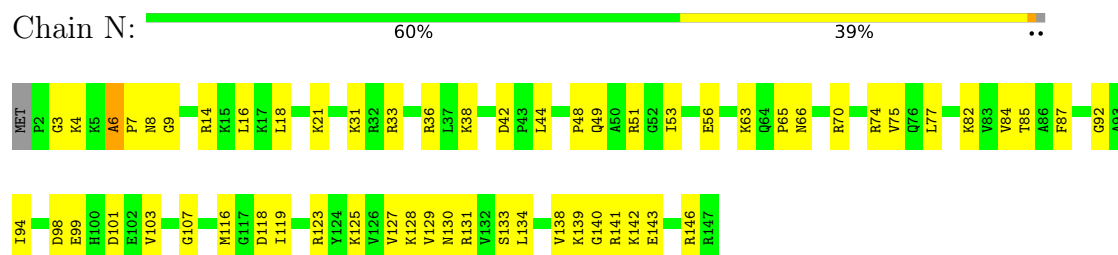
- Molecule 13: 30S ribosomal protein S10



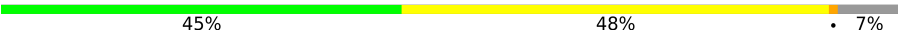
- Molecule 14: 30S ribosomal protein S11

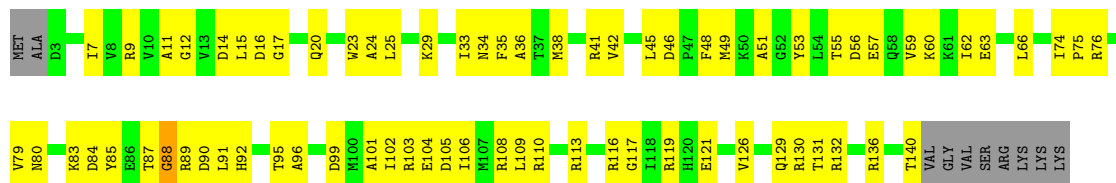


- Molecule 15: 30S ribosomal protein S12

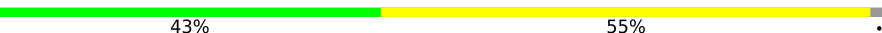


- Molecule 16: 30S ribosomal protein S13

Chain O:  45% 48% 7%



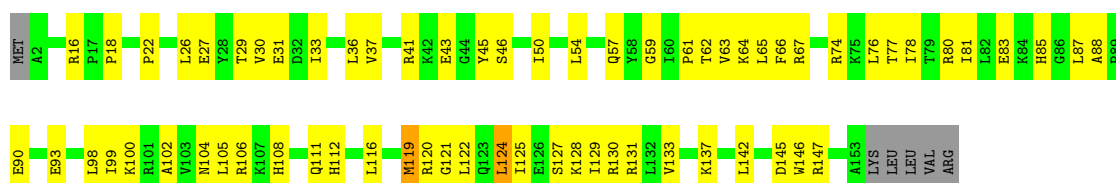
- Molecule 17: 30S ribosomal protein S14 type Z

Chain P:  43% 55%



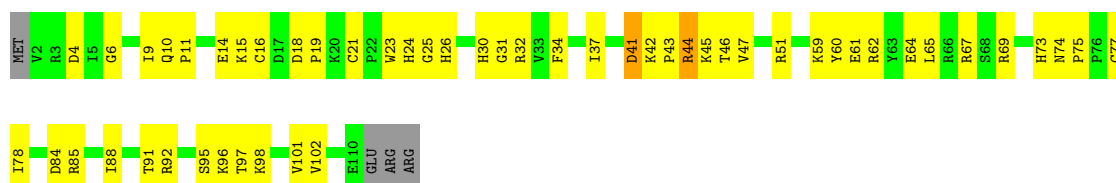
- Molecule 18: 30S ribosomal protein S15

Chain Q:  54% 41%



- Molecule 19: 30S ribosomal protein S17

Chain R:  50% 44%



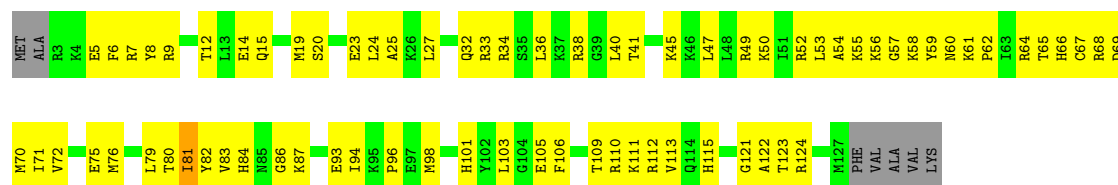
- Molecule 20: 30S ribosomal protein S17e

Chain S:  55% 43%



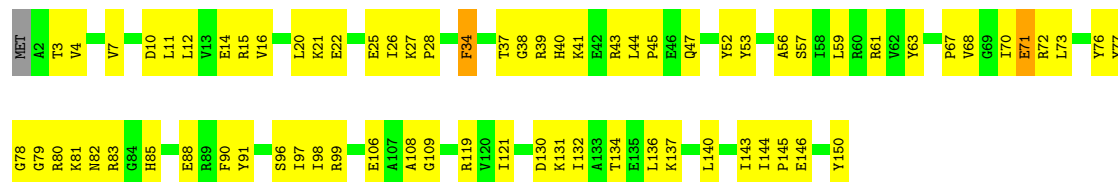
- Molecule 21: 30S ribosomal protein S19

Chain T:  39% 55% 6%



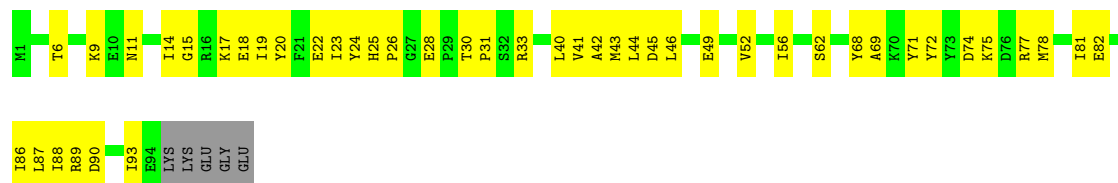
• Molecule 22: 30S ribosomal protein S19e

Chain U: 51% 47% ..



• Molecule 23: 30S ribosomal protein S24e

Chain V: 49% 45% 5%



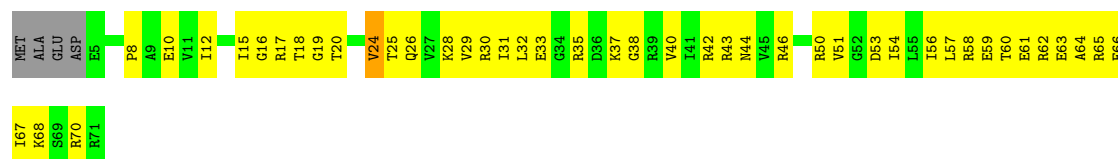
• Molecule 24: 30S ribosomal protein S27e

Chain W: 57% 40% .



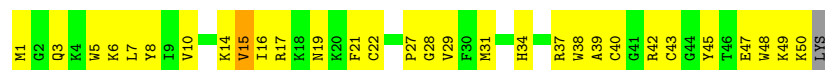
• Molecule 25: 30S ribosomal protein S28e

Chain X: 32% 61% . 6%

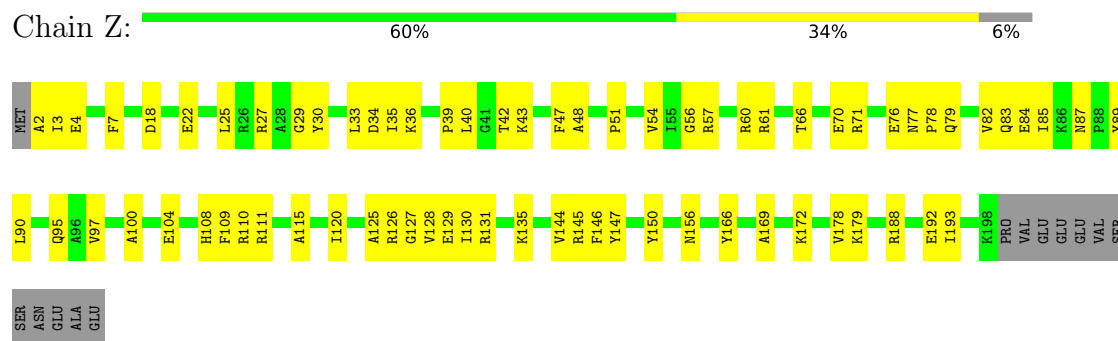


• Molecule 26: 30S ribosomal protein S27ae

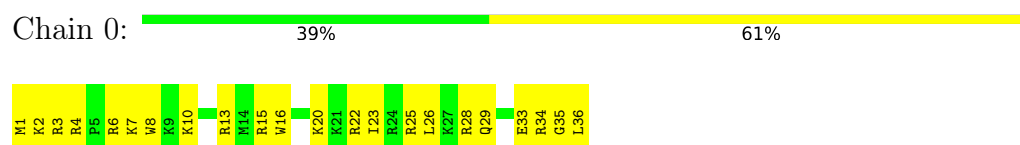
Chain Y: 39% 57% ..



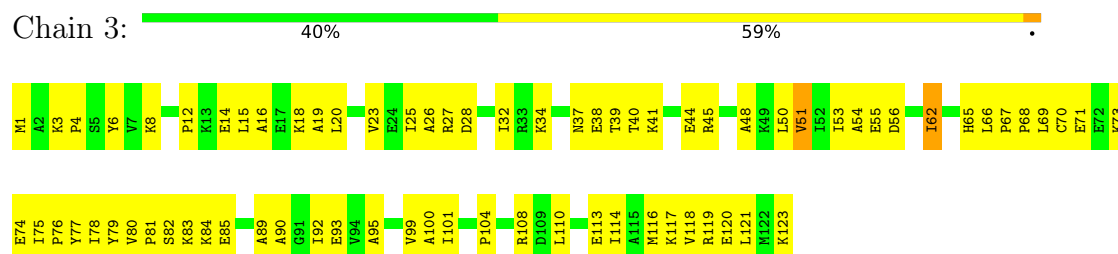
- Molecule 27: 30S ribosomal protein S3



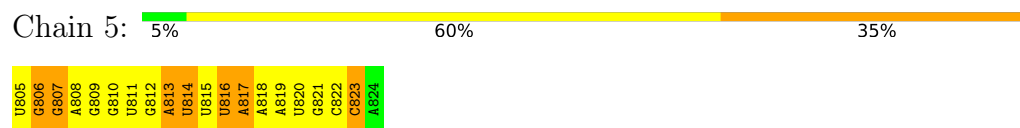
- Molecule 28: 50S ribosomal protein L41e



- Molecule 29: 50S ribosomal protein L7Ae



- Molecule 30: mRNA

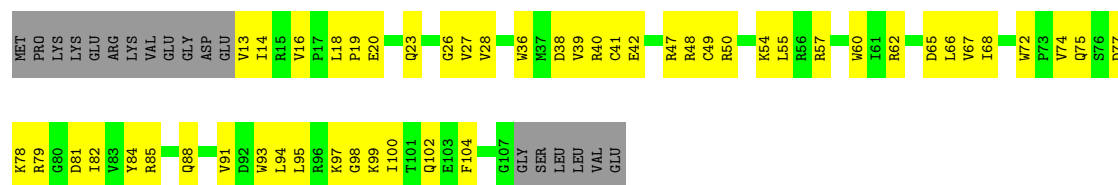


- Molecule 31: initiator Met-tRNA fMet from E. coli (A1U72 variant)

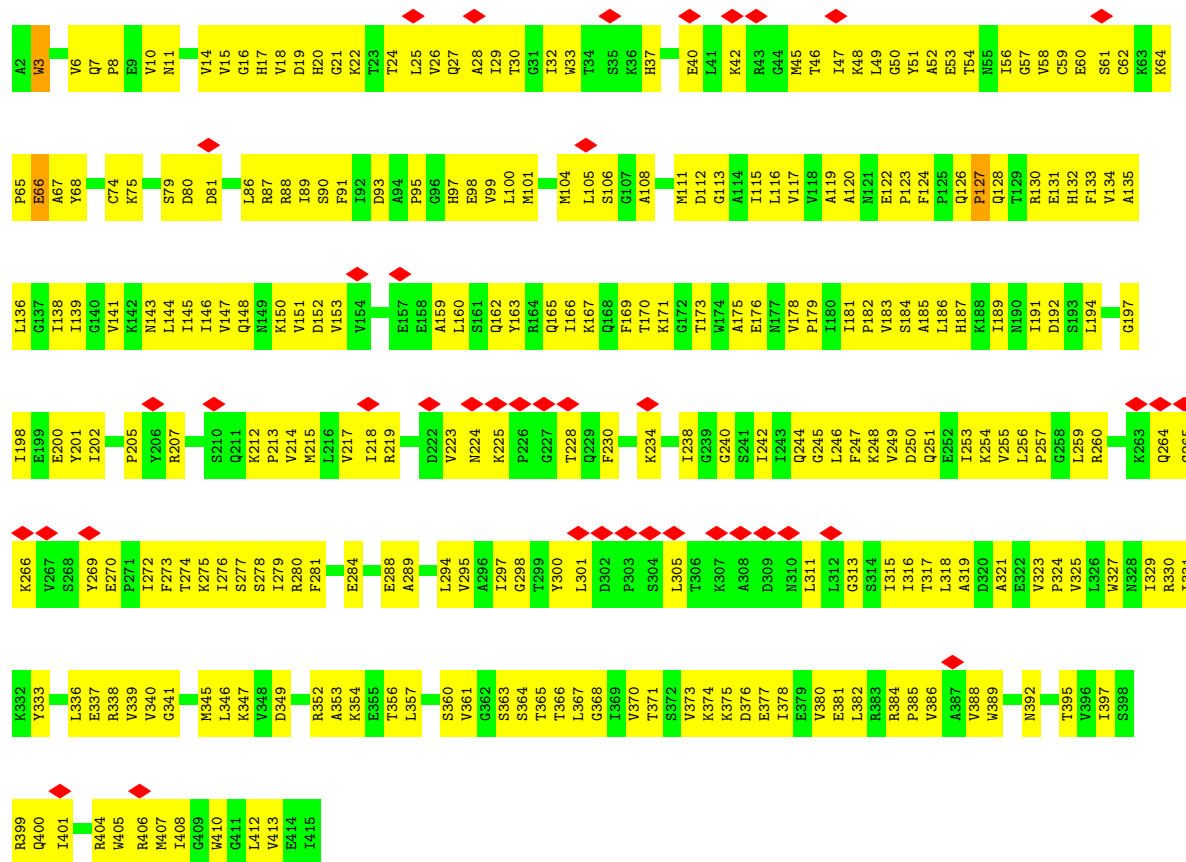


- Molecule 32: Translation initiation factor 1A

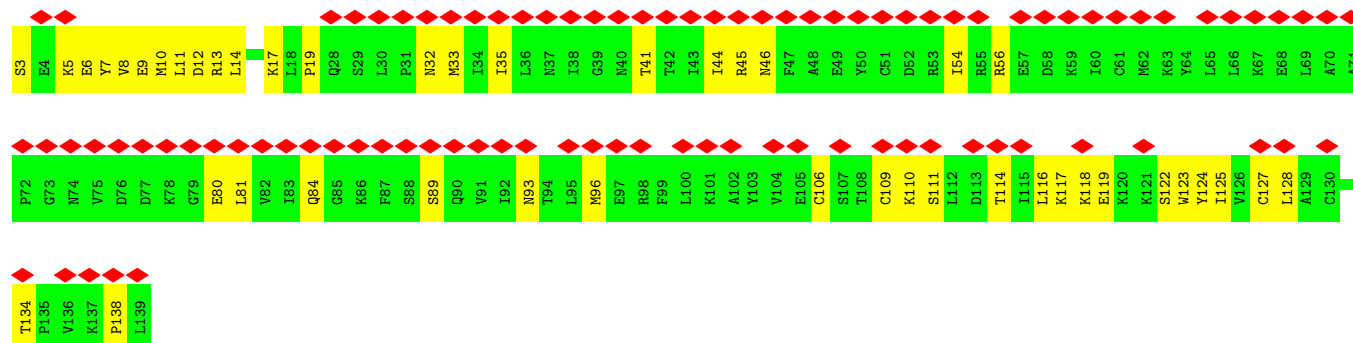




• Molecule 33: Translation initiation factor 2 subunit gamma

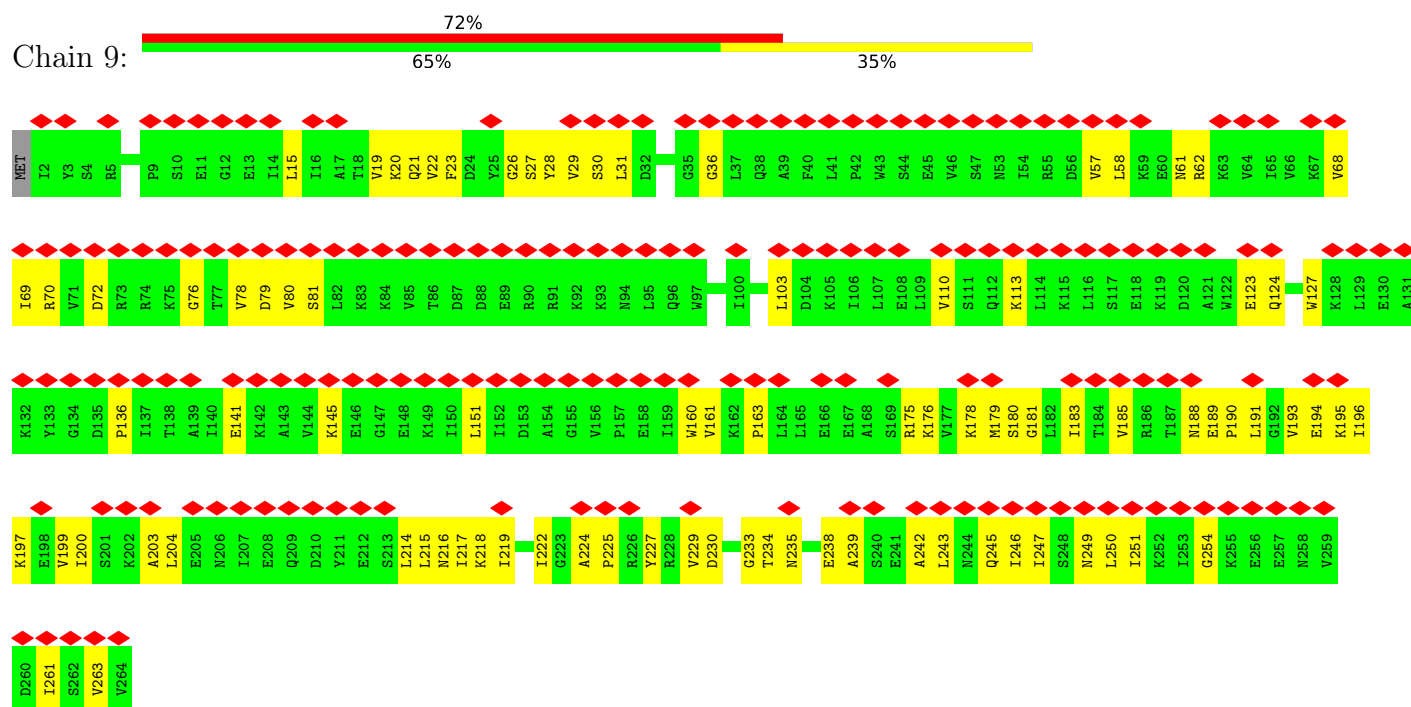


• Molecule 34: Translation initiation factor 2 subunit beta



● Molecule 35: Translation initiation factor 2 subunit alpha

Chain 9:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34000	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 ($e^-/\text{\AA}^2$)	2	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	0.044	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	379.32, 379.32, 379.32	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MA6, LHH, OMC, 5MC, A2M, PSU, 5HM, MG, 6MZ, 4AC, H2U, GNP, UR3, B8H, 4SU, 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	2	0.60	0/35019	0.59	0/54586
2	A	0.56	0/1559	0.72	0/2090
3	B	0.55	1/1602 (0.1%)	0.72	0/2165
4	C	0.51	0/496	0.64	0/673
5	D	0.60	1/1494 (0.1%)	0.72	0/2003
6	E	0.57	0/2032	0.74	2/2742 (0.1%)
7	F	0.64	0/1838	0.78	3/2478 (0.1%)
8	G	0.44	0/993	0.64	0/1329
9	H	0.52	1/1757 (0.1%)	0.71	0/2359
10	I	0.65	0/1055	0.85	0/1415
11	J	0.53	0/1005	0.76	0/1339
12	K	0.52	0/1081	0.73	0/1449
13	L	0.46	0/825	0.66	0/1107
14	M	0.53	0/982	0.72	0/1322
15	N	0.59	0/1165	0.78	2/1547 (0.1%)
16	O	0.49	0/1135	0.74	0/1526
17	P	0.50	0/465	0.77	1/613 (0.2%)
18	Q	0.53	0/1290	0.66	0/1734
19	R	0.61	1/923 (0.1%)	0.72	0/1247
20	S	0.46	0/565	0.60	0/747
21	T	0.49	0/1037	0.72	0/1385
22	U	0.49	0/1253	0.72	1/1689 (0.1%)
23	V	0.52	0/808	0.71	0/1086
24	W	0.47	0/488	0.73	0/659
25	X	0.46	0/538	0.68	0/719
26	Y	0.32	0/420	0.65	0/559
27	Z	0.49	0/1572	0.67	1/2110 (0.0%)
28	0	0.63	0/349	0.86	0/451
29	3	0.34	0/953	0.75	1/1284 (0.1%)
30	5	0.48	0/481	0.50	0/748
31	4	0.44	1/1699 (0.1%)	0.54	0/2648

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	6	0.41	0/793	0.73	0/1072
33	7	0.33	0/3272	0.66	0/4430
34	8	0.16	0/1045	0.39	0/1400
35	9	0.18	0/2050	0.42	1/2760 (0.0%)
All	All	0.54	5/74039 (0.0%)	0.64	12/107471 (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
7	F	0	1
18	Q	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	194	LYS	C-N	-8.22	1.20	1.33
19	R	41	ASP	CA-CB	-5.61	1.36	1.53
3	B	30	LYS	CA-C	-5.24	1.45	1.52
5	D	98	GLU	CA-C	-5.17	1.45	1.52
31	4	8	4SU	O3'-P	5.04	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	143	GLU	CA-C-N	-7.82	107.21	122.70
15	N	143	GLU	C-N-CA	-7.82	107.21	122.70
17	P	46	VAL	N-CA-C	-7.05	106.43	113.20
27	Z	3	ILE	N-CA-C	-6.35	107.06	113.47
7	F	165	LEU	CA-C-N	-6.26	117.02	122.96

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	F	5	TRP	Peptide
18	Q	106	ARG	Peptide

5.2 Too-close contacts ⓘ

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	2	32291	0	16316	2019	0
2	A	1533	0	1627	100	0
3	B	1571	0	1630	70	0
4	C	482	0	461	25	0
5	D	1470	0	1542	99	0
6	E	1983	0	2060	82	0
7	F	1808	0	1879	92	0
8	G	977	0	1037	58	0
9	H	1720	0	1775	92	0
10	I	1034	0	1069	58	0
11	J	996	0	1076	52	0
12	K	1065	0	1121	75	0
13	L	817	0	871	34	0
14	M	964	0	994	43	0
15	N	1148	0	1248	46	0
16	O	1116	0	1152	76	0
17	P	455	0	475	30	0
18	Q	1262	0	1331	54	0
19	R	900	0	921	54	0
20	S	558	0	595	33	0
21	T	1018	0	1086	74	0
22	U	1223	0	1263	63	0
23	V	790	0	806	40	0
24	W	481	0	512	21	0
25	X	536	0	571	44	0
26	Y	408	0	413	35	0
27	Z	1550	0	1637	58	0
28	0	343	0	407	24	0
29	3	941	0	994	91	0
30	5	430	0	215	41	0
31	4	1622	0	830	134	0
32	6	777	0	806	54	0
33	7	3213	0	3331	347	0
34	8	1032	0	1073	41	0
35	9	2025	0	2133	80	0
36	2	31	0	0	0	0
36	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	5	1	0	0	0	0
36	7	1	0	0	0	0
37	C	2	0	0	0	0
37	F	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	W	1	0	0	0	0
38	7	8	0	8	2	0
39	7	32	0	13	4	0
40	2	40	0	0	18	0
40	K	1	0	0	0	0
40	Q	1	0	0	0	0
All	All	70661	0	55278	3945	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 32.

The worst 5 of 3945 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)
1:2:140:A:N6	1:2:229:G:H1	1.36	1.23
33:7:213:PRO:HA	33:7:244:GLN:O	1.39	1.22
33:7:240:GLY:O	33:7:294:LEU:HA	1.57	1.04
31:4:74:C:H41	33:7:33:TRP:CD1	1.75	1.03
1:2:1300:C:OP1	22:U:39:ARG:NH2	1.96	0.97

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	
2	A	186/199 (94%)	157 (84%)	29 (16%)	0	100	100
3	B	194/202 (96%)	162 (84%)	32 (16%)	0	100	100
4	C	59/63 (94%)	43 (73%)	16 (27%)	0	100	100
5	D	173/180 (96%)	140 (81%)	32 (18%)	1 (1%)	21	58
6	E	240/243 (99%)	179 (75%)	60 (25%)	1 (0%)	30	66
7	F	227/236 (96%)	172 (76%)	55 (24%)	0	100	100
8	G	122/125 (98%)	97 (80%)	25 (20%)	0	100	100
9	H	211/215 (98%)	171 (81%)	40 (19%)	0	100	100
10	I	127/130 (98%)	96 (76%)	31 (24%)	0	100	100
11	J	124/127 (98%)	91 (73%)	33 (27%)	0	100	100
12	K	132/135 (98%)	107 (81%)	25 (19%)	0	100	100
13	L	99/102 (97%)	86 (87%)	13 (13%)	0	100	100
14	M	126/137 (92%)	105 (83%)	21 (17%)	0	100	100
15	N	144/147 (98%)	104 (72%)	39 (27%)	1 (1%)	18	54
16	O	136/148 (92%)	107 (79%)	28 (21%)	1 (1%)	18	54
17	P	53/56 (95%)	40 (76%)	13 (24%)	0	100	100
18	Q	150/158 (95%)	127 (85%)	23 (15%)	0	100	100
19	R	107/113 (95%)	80 (75%)	27 (25%)	0	100	100
20	S	64/67 (96%)	54 (84%)	10 (16%)	0	100	100
21	T	123/132 (93%)	94 (76%)	29 (24%)	0	100	100
22	U	147/150 (98%)	125 (85%)	22 (15%)	0	100	100
23	V	92/99 (93%)	69 (75%)	23 (25%)	0	100	100
24	W	61/65 (94%)	45 (74%)	16 (26%)	0	100	100
25	X	65/71 (92%)	48 (74%)	17 (26%)	0	100	100
26	Y	48/51 (94%)	28 (58%)	20 (42%)	0	100	100
27	Z	195/210 (93%)	152 (78%)	43 (22%)	0	100	100
28	0	34/36 (94%)	22 (65%)	12 (35%)	0	100	100
29	3	121/123 (98%)	96 (79%)	25 (21%)	0	100	100
32	6	93/113 (82%)	78 (84%)	15 (16%)	0	100	100
33	7	412/414 (100%)	363 (88%)	46 (11%)	3 (1%)	18	54
34	8	125/129 (97%)	113 (90%)	12 (10%)	0	100	100
35	9	247/254 (97%)	234 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4437/4630 (96%)	3585 (81%)	845 (19%)	7 (0%)	44	77

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	O	88	GLY
33	7	66	GLU
5	D	103	ARG
33	7	265	GLY
15	N	6	ALA

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	
2	A	161/167 (96%)	158 (98%)	3 (2%)	50	66
3	B	168/173 (97%)	167 (99%)	1 (1%)	78	80
4	C	54/55 (98%)	52 (96%)	2 (4%)	30	51
5	D	158/160 (99%)	157 (99%)	1 (1%)	78	80
6	E	213/214 (100%)	212 (100%)	1 (0%)	81	81
7	F	192/198 (97%)	190 (99%)	2 (1%)	68	75
8	G	107/108 (99%)	106 (99%)	1 (1%)	70	75
9	H	183/184 (100%)	181 (99%)	2 (1%)	65	73
10	I	106/107 (99%)	105 (99%)	1 (1%)	70	75
11	J	102/103 (99%)	101 (99%)	1 (1%)	68	75
12	K	110/111 (99%)	110 (100%)	0	100	100
13	L	90/91 (99%)	90 (100%)	0	100	100
14	M	95/104 (91%)	95 (100%)	0	100	100
15	N	120/121 (99%)	120 (100%)	0	100	100
16	O	115/123 (94%)	115 (100%)	0	100	100
17	P	45/46 (98%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Q	137/143 (96%)	135 (98%)	2 (2%)	57	70
19	R	98/102 (96%)	96 (98%)	2 (2%)	48	65
20	S	60/61 (98%)	60 (100%)	0	100	100
21	T	109/114 (96%)	108 (99%)	1 (1%)	70	75
22	U	126/127 (99%)	123 (98%)	3 (2%)	43	63
23	V	86/90 (96%)	86 (100%)	0	100	100
24	W	54/56 (96%)	54 (100%)	0	100	100
25	X	57/60 (95%)	55 (96%)	2 (4%)	32	53
26	Y	41/42 (98%)	39 (95%)	2 (5%)	22	45
27	Z	156/168 (93%)	154 (99%)	2 (1%)	61	71
28	0	34/34 (100%)	34 (100%)	0	100	100
29	3	99/99 (100%)	98 (99%)	1 (1%)	68	75
32	6	83/99 (84%)	83 (100%)	0	100	100
33	7	356/356 (100%)	355 (100%)	1 (0%)	86	84
34	8	117/118 (99%)	116 (99%)	1 (1%)	70	75
35	9	226/228 (99%)	226 (100%)	0	100	100
All	All	3858/3962 (97%)	3826 (99%)	32 (1%)	70	77

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	Z	178	VAL
29	3	51	VAL
9	H	147	HIS
9	H	90	HIS
33	7	3	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
11	J	64	ASN
33	7	143	ASN
17	P	34	HIS
33	7	97	HIS
27	Z	77	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1496/1497 (99%)	518 (34%)	19 (1%)
30	5	19/20 (95%)	9 (47%)	0
31	4	75/76 (98%)	33 (44%)	1 (1%)
All	All	1590/1593 (99%)	560 (35%)	20 (1%)

5 of 560 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	14	U
1	2	15	U
1	2	16	C
1	2	23	A
1	2	30	C

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1155	G
1	2	1435	C
31	4	73	A
1	2	1448	C
1	2	599	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	4AC	2	319	1	21,24,25	1.20	3 (14%)	29,34,37	1.48	4 (13%)
1	4AC	2	53	1	21,24,25	1.06	2 (9%)	29,34,37	1.48	5 (17%)
1	4AC	2	868	1	21,24,25	1.23	3 (14%)	29,34,37	1.37	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	2	1488	1	23,26,27	1.43	4 (17%)	34,38,41	2.01	7 (20%)
1	LHH	2	250	1	22,25,26	2.45	8 (36%)	29,35,38	1.20	2 (6%)
1	4AC	2	479	1	21,24,25	1.13	3 (14%)	29,34,37	1.59	5 (17%)
1	4AC	2	1233	1	21,24,25	1.09	2 (9%)	29,34,37	1.53	4 (13%)
1	A2M	2	373	1	22,25,26	1.61	4 (18%)	31,36,39	2.80	12 (38%)
1	4AC	2	1239	1	21,24,25	1.15	2 (9%)	29,34,37	1.87	4 (13%)
1	4AC	2	1479	1	21,24,25	1.10	3 (14%)	29,34,37	1.50	4 (13%)
1	4AC	2	394	1	21,24,25	1.02	2 (9%)	29,34,37	1.66	5 (17%)
1	4AC	2	851	1	21,24,25	1.24	3 (14%)	29,34,37	1.57	4 (13%)
1	4AC	2	303	1	21,24,25	1.16	3 (14%)	29,34,37	1.44	3 (10%)
1	4AC	2	1041	1	21,24,25	1.01	2 (9%)	29,34,37	1.98	4 (13%)
1	4AC	2	590	1,36	21,24,25	1.15	3 (14%)	29,34,37	1.47	4 (13%)
1	4AC	2	636	1	21,24,25	1.12	3 (14%)	29,34,37	1.60	4 (13%)
31	OMC	4	32	31	19,22,23	0.99	2 (10%)	26,31,34	1.13	2 (7%)
31	H2U	4	20	31	18,21,22	1.10	2 (11%)	21,30,33	2.24	1 (4%)
1	4AC	2	828	1	21,24,25	1.01	1 (4%)	29,34,37	1.64	4 (13%)
1	4AC	2	17	1	21,24,25	1.06	2 (9%)	29,34,37	1.77	5 (17%)
1	4AC	2	648	1	21,24,25	1.20	3 (14%)	29,34,37	1.85	7 (24%)
1	4AC	2	751	1	21,24,25	1.13	3 (14%)	29,34,37	1.26	4 (13%)
1	4AC	2	839	1	21,24,25	1.13	2 (9%)	29,34,37	1.80	6 (20%)
1	6MZ	2	1469	1,36	22,25,26	1.39	3 (13%)	30,36,39	2.26	8 (26%)
1	4AC	2	848	1	21,24,25	1.12	2 (9%)	29,34,37	1.75	4 (13%)
1	4AC	2	1193	1	21,24,25	1.13	2 (9%)	29,34,37	2.00	5 (17%)
1	5HM	2	1378	1	19,23,24	2.94	7 (36%)	25,33,36	0.64	0
1	UR3	2	1467	1	19,22,23	1.10	2 (10%)	26,32,35	1.50	5 (19%)
31	5MU	4	54	31	19,22,23	1.44	6 (31%)	28,32,35	2.05	8 (28%)
1	4AC	2	1147	1	21,24,25	1.12	3 (14%)	29,34,37	2.24	6 (20%)
1	4AC	2	703	1	21,24,25	1.07	2 (9%)	29,34,37	1.82	6 (20%)
1	4AC	2	731	1	21,24,25	1.16	3 (14%)	29,34,37	1.37	5 (17%)
31	4SU	4	8	31	18,21,22	1.79	5 (27%)	26,30,33	2.15	4 (15%)
1	OMC	2	1376	1	19,22,23	0.90	2 (10%)	26,31,34	0.76	0
1	4AC	2	626	1	21,24,25	1.05	3 (14%)	29,34,37	1.41	4 (13%)
1	4AC	2	1184	1	21,24,25	1.06	3 (14%)	29,34,37	1.39	4 (13%)
1	4AC	2	546	1	21,24,25	1.03	2 (9%)	29,34,37	1.44	3 (10%)
1	5MC	2	939	1	18,22,23	1.05	2 (11%)	26,32,35	1.25	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	B8H	2	938	1	19,22,23	0.82	0	22,32,35	1.52	3 (13%)
1	4AC	2	1028	1	21,24,25	1.05	3 (14%)	29,34,37	1.62	4 (13%)
1	4AC	2	718	1	21,24,25	1.08	2 (9%)	29,34,37	1.18	3 (10%)
1	4AC	2	957	1	21,24,25	1.12	1 (4%)	29,34,37	2.29	7 (24%)
31	PSU	4	55	31	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
1	4AC	2	511	1	21,24,25	1.15	3 (14%)	29,34,37	1.87	6 (20%)
1	MA6	2	1487	1	23,26,27	1.49	4 (17%)	34,38,41	2.06	10 (29%)
1	4AC	2	379	1	21,24,25	1.08	3 (14%)	29,34,37	1.55	5 (17%)
1	5MC	2	1202	1	18,22,23	1.00	1 (5%)	26,32,35	1.21	1 (3%)
1	4AC	2	286	1	21,24,25	1.11	2 (9%)	29,34,37	1.64	7 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	319	1	-	4/11/29/30	0/2/2/2
1	4AC	2	53	1	-	0/11/29/30	0/2/2/2
1	4AC	2	868	1	-	2/11/29/30	0/2/2/2
1	MA6	2	1488	1	-	0/11/29/30	0/3/3/3
1	LHH	2	250	1	-	1/13/31/32	0/2/2/2
1	4AC	2	479	1	-	3/11/29/30	0/2/2/2
1	4AC	2	1233	1	-	0/11/29/30	0/2/2/2
1	A2M	2	373	1	-	1/9/27/28	0/3/3/3
1	4AC	2	1239	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1479	1	-	0/11/29/30	0/2/2/2
1	4AC	2	394	1	-	2/11/29/30	0/2/2/2
1	4AC	2	851	1	-	4/11/29/30	0/2/2/2
1	4AC	2	303	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1041	1	-	0/11/29/30	0/2/2/2
1	4AC	2	590	1,36	-	2/11/29/30	0/2/2/2
1	4AC	2	636	1	-	0/11/29/30	0/2/2/2
31	OMC	4	32	31	-	2/9/27/28	0/2/2/2
31	H2U	4	20	31	-	4/7/38/39	0/2/2/2
1	4AC	2	828	1	-	0/11/29/30	0/2/2/2
1	4AC	2	17	1	-	0/11/29/30	0/2/2/2
1	4AC	2	648	1	-	2/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	751	1	-	0/11/29/30	0/2/2/2
1	4AC	2	839	1	-	1/11/29/30	0/2/2/2
1	6MZ	2	1469	1,36	-	2/9/27/28	0/3/3/3
1	4AC	2	848	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1193	1	-	0/11/29/30	0/2/2/2
1	5HM	2	1378	1	-	2/9/27/28	0/2/2/2
1	UR3	2	1467	1	-	6/7/25/26	0/2/2/2
31	5MU	4	54	31	-	1/7/25/26	0/2/2/2
1	4AC	2	1147	1	-	2/11/29/30	0/2/2/2
1	4AC	2	703	1	-	0/11/29/30	0/2/2/2
1	4AC	2	731	1	-	3/11/29/30	0/2/2/2
31	4SU	4	8	31	-	5/7/25/26	0/2/2/2
1	OMC	2	1376	1	-	2/9/27/28	0/2/2/2
1	4AC	2	626	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1184	1	-	2/11/29/30	0/2/2/2
1	4AC	2	546	1	-	2/11/29/30	0/2/2/2
1	5MC	2	939	1	-	0/7/25/26	0/2/2/2
1	B8H	2	938	1	-	3/7/25/26	0/2/2/2
1	4AC	2	1028	1	-	2/11/29/30	0/2/2/2
1	4AC	2	718	1	-	0/11/29/30	0/2/2/2
1	4AC	2	957	1	-	1/11/29/30	0/2/2/2
31	PSU	4	55	31	-	0/7/25/26	0/2/2/2
1	4AC	2	511	1	-	2/11/29/30	0/2/2/2
1	MA6	2	1487	1	-	1/11/29/30	0/3/3/3
1	4AC	2	379	1	-	2/11/29/30	0/2/2/2
1	5MC	2	1202	1	-	2/7/25/26	0/2/2/2
1	4AC	2	286	1	-	5/11/29/30	0/2/2/2

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1378	5HM	C4-N3	6.29	1.44	1.34
1	2	250	LHH	C4-N4	6.05	1.48	1.39
1	2	250	LHH	C7-N4	5.67	1.47	1.37
1	2	1378	5HM	C2-N3	5.46	1.47	1.36
1	2	1378	5HM	C4-N4	5.36	1.48	1.34

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	4	20	H2U	C4-N3-C2	-9.61	117.82	125.79
1	2	373	A2M	C2'-C1'-N9	-8.09	99.91	113.53
1	2	373	A2M	C5-C4-N3	-7.03	117.58	126.75
31	4	8	4SU	C4-N3-C2	-6.85	120.68	127.34
1	2	1469	6MZ	C5-C4-N3	-6.58	118.16	126.75

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	250	LHH	C1'-C2'-O2'-C1
1	2	286	4AC	C3'-C4'-C5'-O5'
1	2	373	A2M	C1'-C2'-O2'-CM'
1	2	379	4AC	C3'-C4'-C5'-O5'
1	2	511	4AC	O4'-C4'-C5'-O5'

There are no ring outliers.

47 monomers are involved in 148 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	319	4AC	3	0
1	2	53	4AC	1	0
1	2	868	4AC	3	0
1	2	1488	MA6	3	0
1	2	479	4AC	4	0
1	2	1233	4AC	6	0
1	2	373	A2M	7	0
1	2	1239	4AC	5	0
1	2	1479	4AC	5	0
1	2	394	4AC	4	0
1	2	851	4AC	6	0
1	2	303	4AC	3	0
1	2	1041	4AC	4	0
1	2	590	4AC	2	0
1	2	636	4AC	2	0
31	4	32	OMC	3	0
31	4	20	H2U	1	0
1	2	828	4AC	3	0
1	2	17	4AC	3	0
1	2	648	4AC	5	0
1	2	751	4AC	1	0
1	2	839	4AC	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1469	6MZ	2	0
1	2	848	4AC	2	0
1	2	1193	4AC	3	0
1	2	1378	5HM	4	0
1	2	1467	UR3	3	0
31	4	54	5MU	3	0
1	2	1147	4AC	5	0
1	2	703	4AC	6	0
1	2	731	4AC	4	0
31	4	8	4SU	2	0
1	2	1376	OMC	2	0
1	2	626	4AC	1	0
1	2	1184	4AC	4	0
1	2	546	4AC	2	0
1	2	939	5MC	2	0
1	2	938	B8H	1	0
1	2	1028	4AC	2	0
1	2	718	4AC	4	0
1	2	957	4AC	3	0
31	4	55	PSU	4	0
1	2	511	4AC	1	0
1	2	1487	MA6	4	0
1	2	379	4AC	2	0
1	2	1202	5MC	3	0
1	2	286	4AC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 40 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	GNP	7	502	36	33,34,34	1.27	5 (15%)	46,54,54	0.76	2 (4%)
38	MET	7	501	-	6,7,8	0.50	0	2,7,9	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GNP	7	502	36	-	7/18/38/38	0/3/3/3
38	MET	7	501	-	-	2/5/6/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	502	GNP	PB-O3A	4.26	1.64	1.59
39	7	502	GNP	PB-O1B	3.18	1.51	1.46
39	7	502	GNP	PG-N3B	2.80	1.70	1.63
39	7	502	GNP	PG-O1G	2.60	1.50	1.46
39	7	502	GNP	PB-O2B	-2.07	1.51	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	7	502	GNP	PB-O3A-PA	-2.95	122.22	132.62
39	7	502	GNP	O3G-PG-O1G	-2.32	107.63	113.45

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

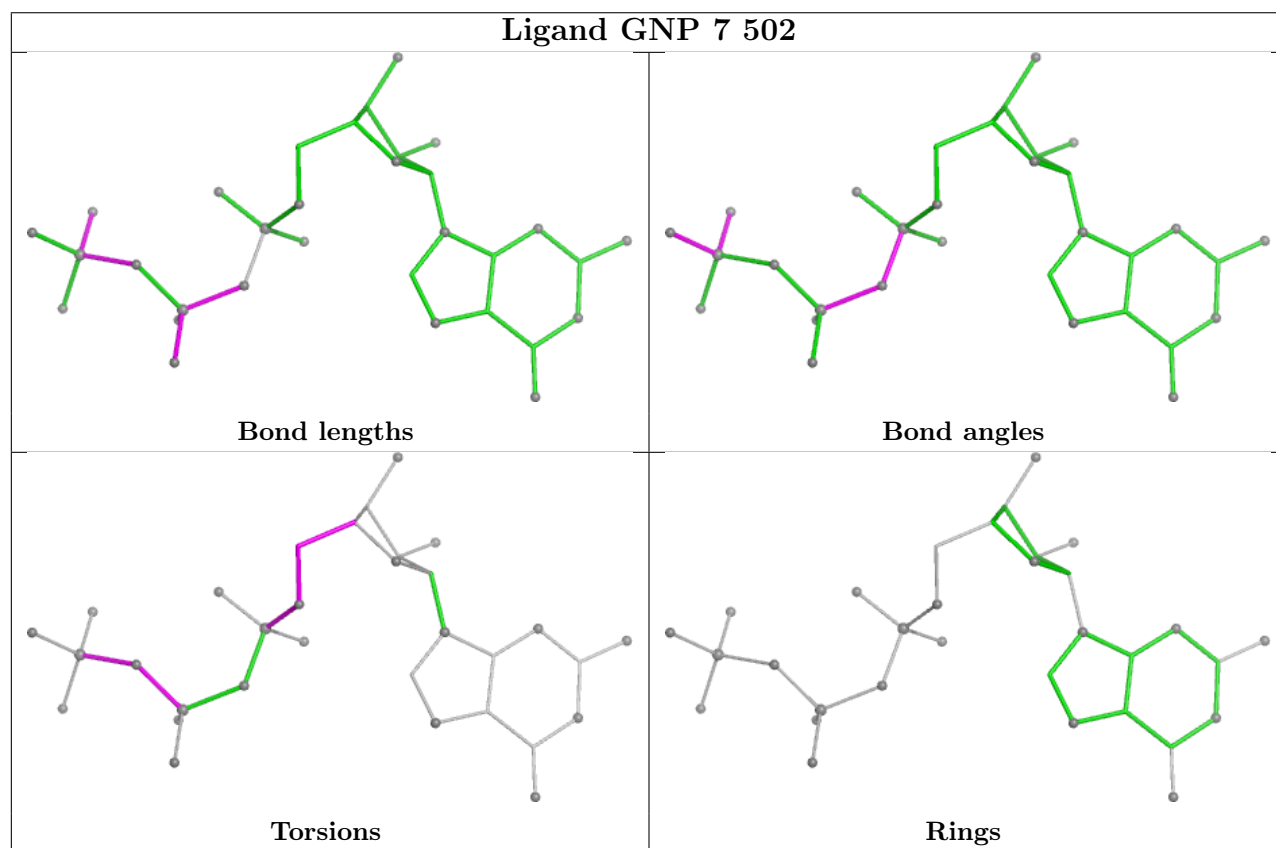
Mol	Chain	Res	Type	Atoms
39	7	502	GNP	PB-N3B-PG-O1G
39	7	502	GNP	PG-N3B-PB-O1B
39	7	502	GNP	C5'-O5'-PA-O3A
39	7	502	GNP	O4'-C4'-C5'-O5'
38	7	501	MET	CA-CB-CG-SD

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	7	502	GNP	4	0
38	7	501	MET	2	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
35	9	2
34	8	1
9	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	8	19:PRO	C	28:GLN	N	14.63
1	9	47:SER	C	53:ASN	N	11.57
1	9	169:SER	C	175:ARG	N	8.00
1	H	194:LYS	C	195:ASP	N	1.20

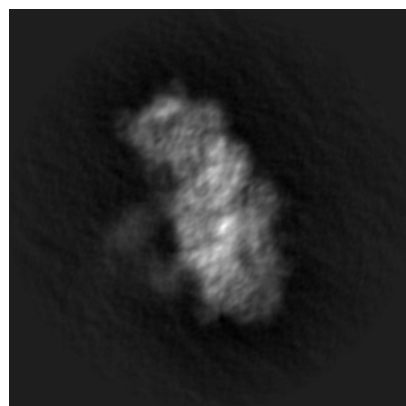
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10320. These allow visual inspection of the internal detail of the map and identification of artifacts.

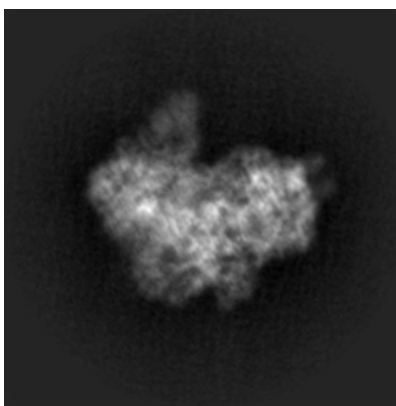
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

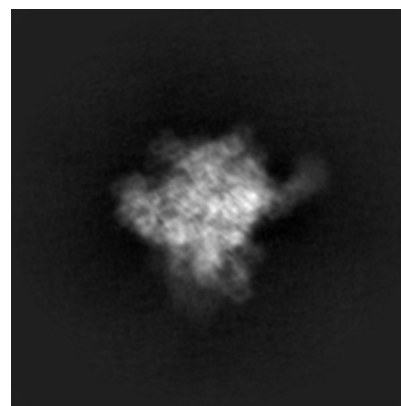
6.1.1 Primary map



X

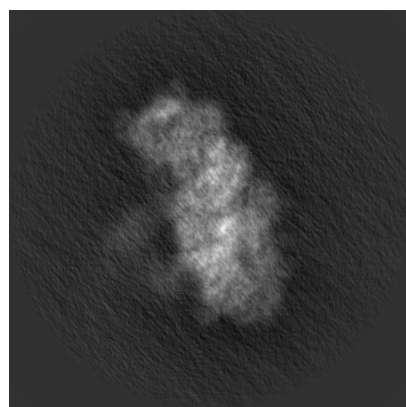


Y

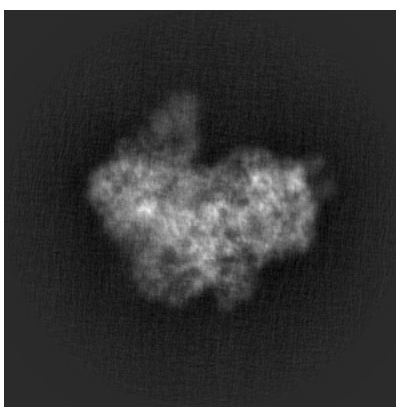


Z

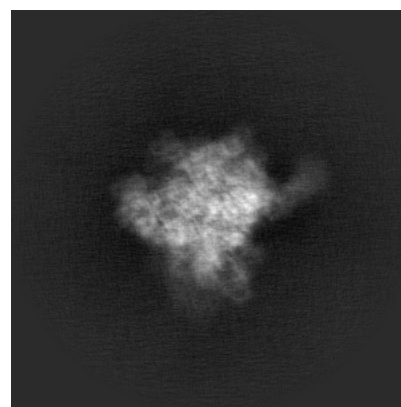
6.1.2 Raw map



X



Y

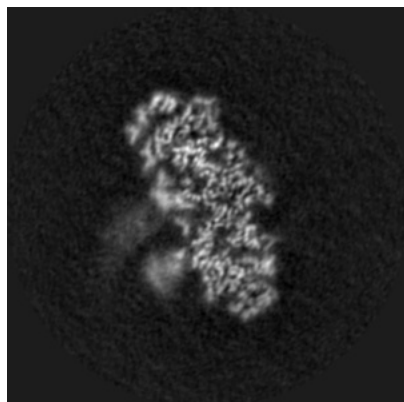


Z

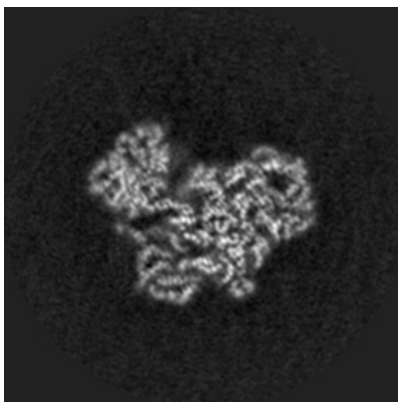
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

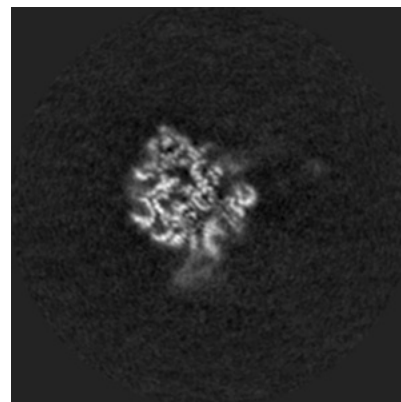
6.2.1 Primary map



X Index: 174

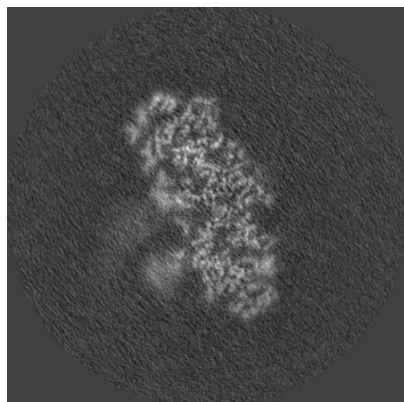


Y Index: 174

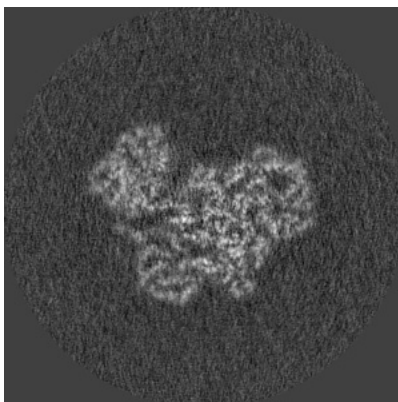


Z Index: 174

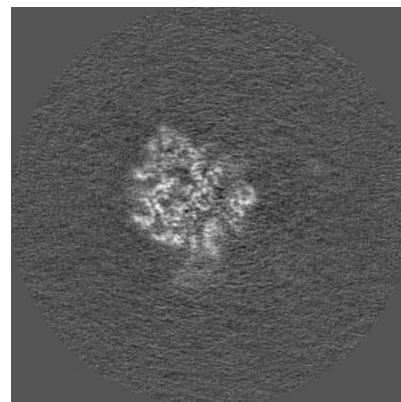
6.2.2 Raw map



X Index: 174



Y Index: 174

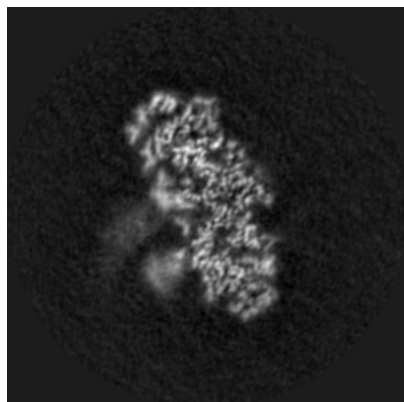


Z Index: 174

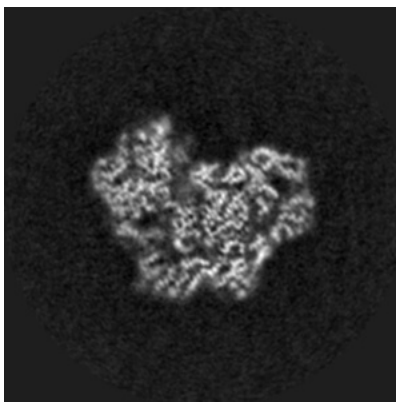
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

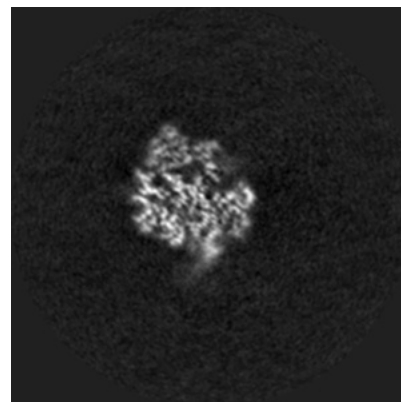
6.3.1 Primary map



X Index: 174

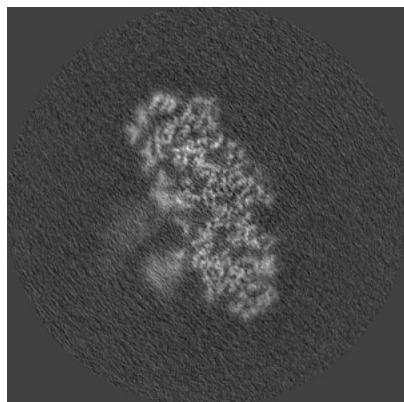


Y Index: 178

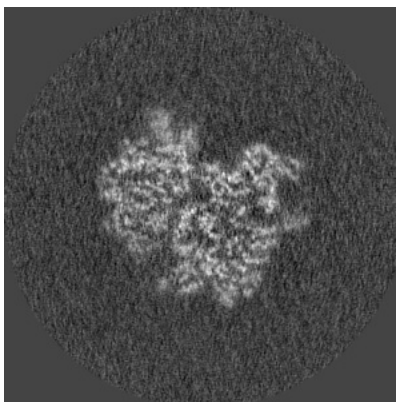


Z Index: 180

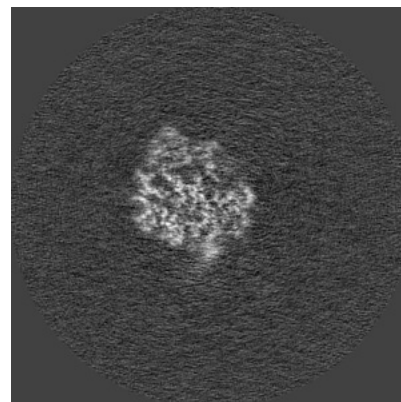
6.3.2 Raw map



X Index: 174



Y Index: 185

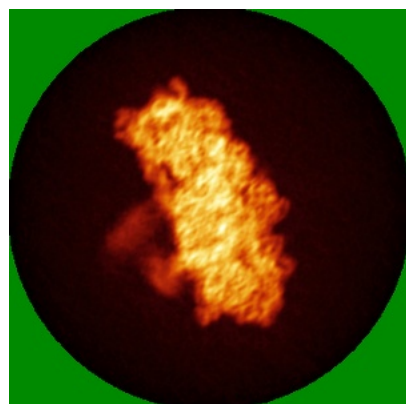


Z Index: 180

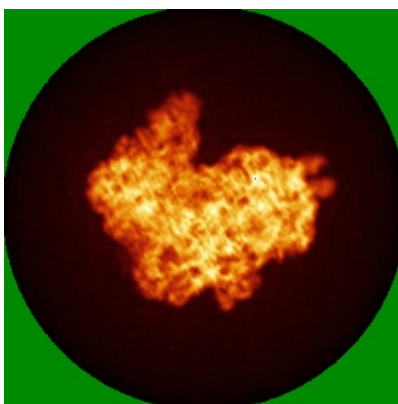
The images above show the largest variance slices of the map in three orthogonal directions.

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

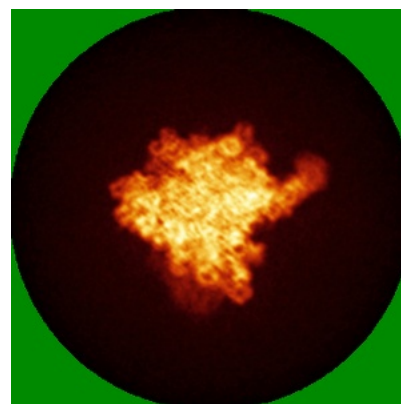
6.4.1 Primary map



X

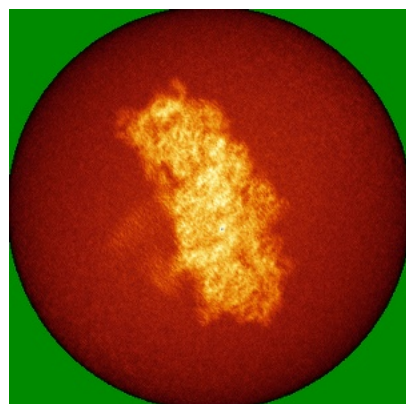


Y

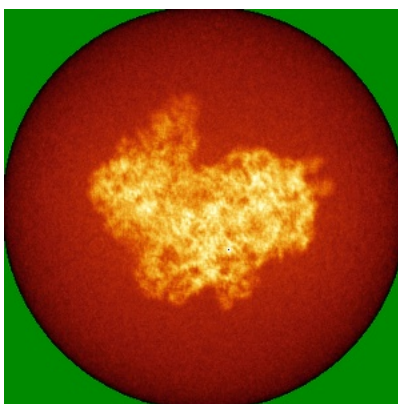


Z

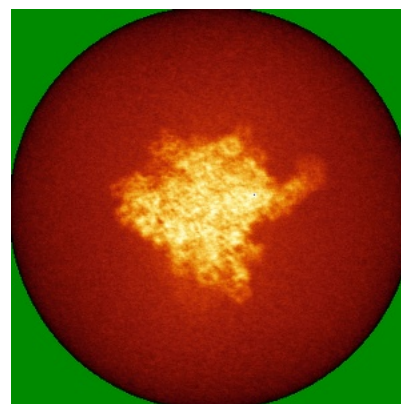
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



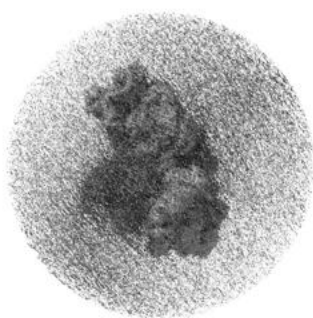
Y



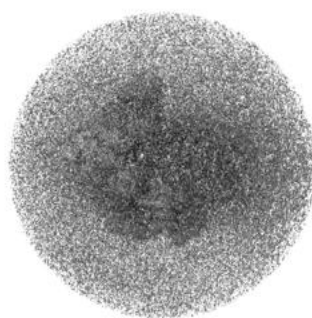
Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

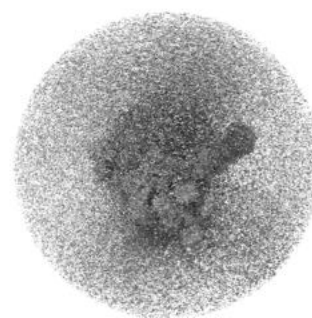
6.5.2 Raw map



X



Y



Z

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

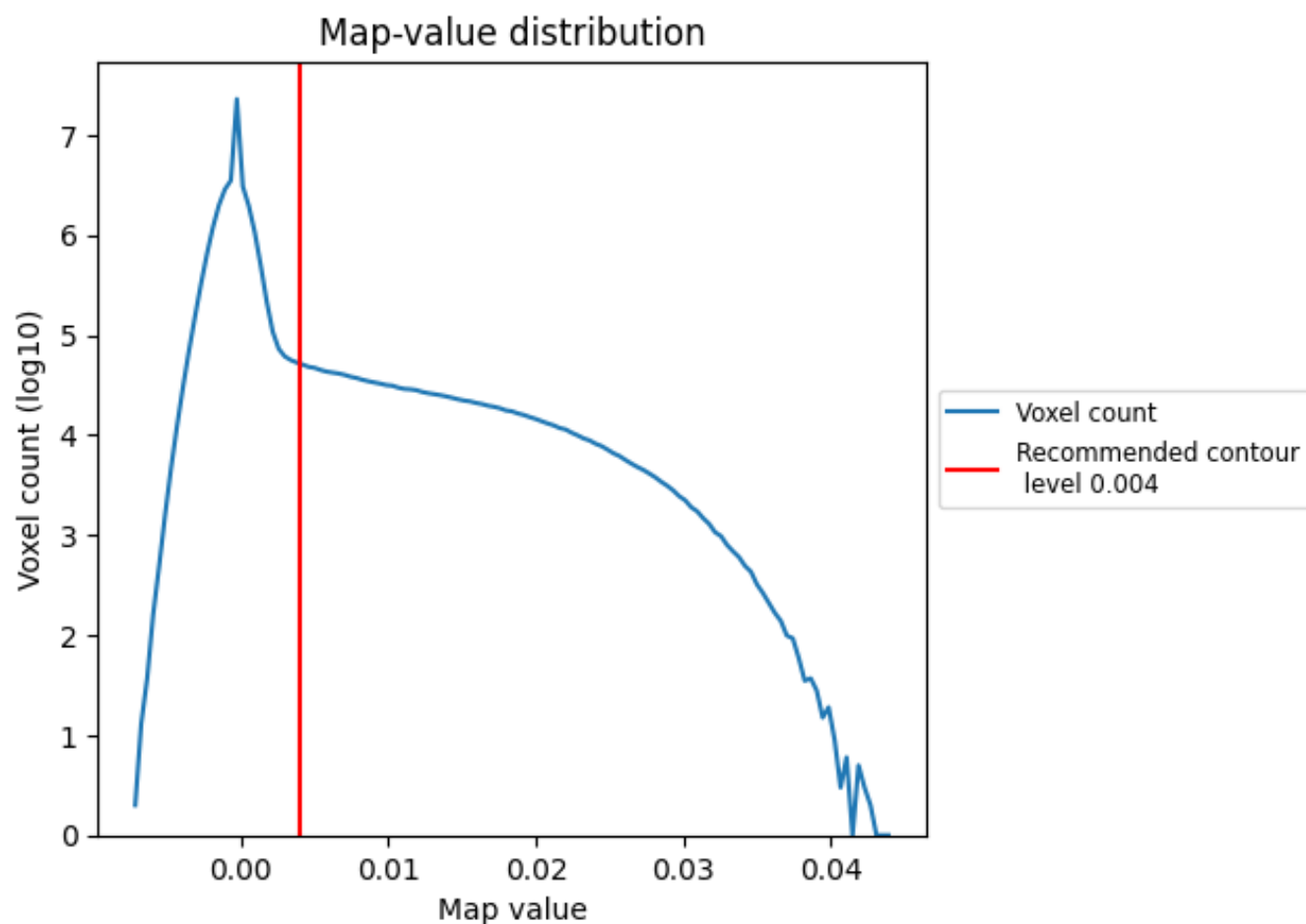
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

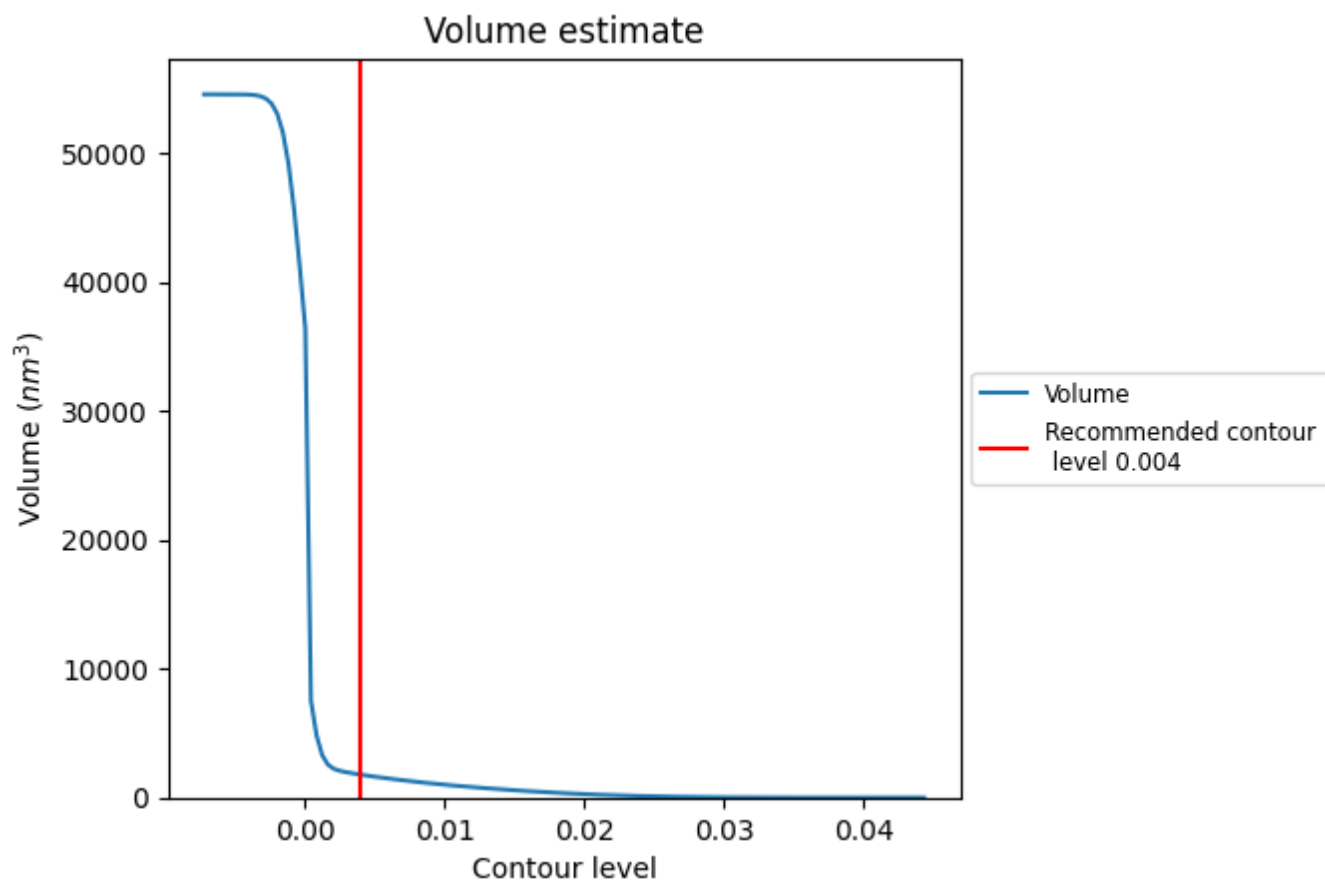
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

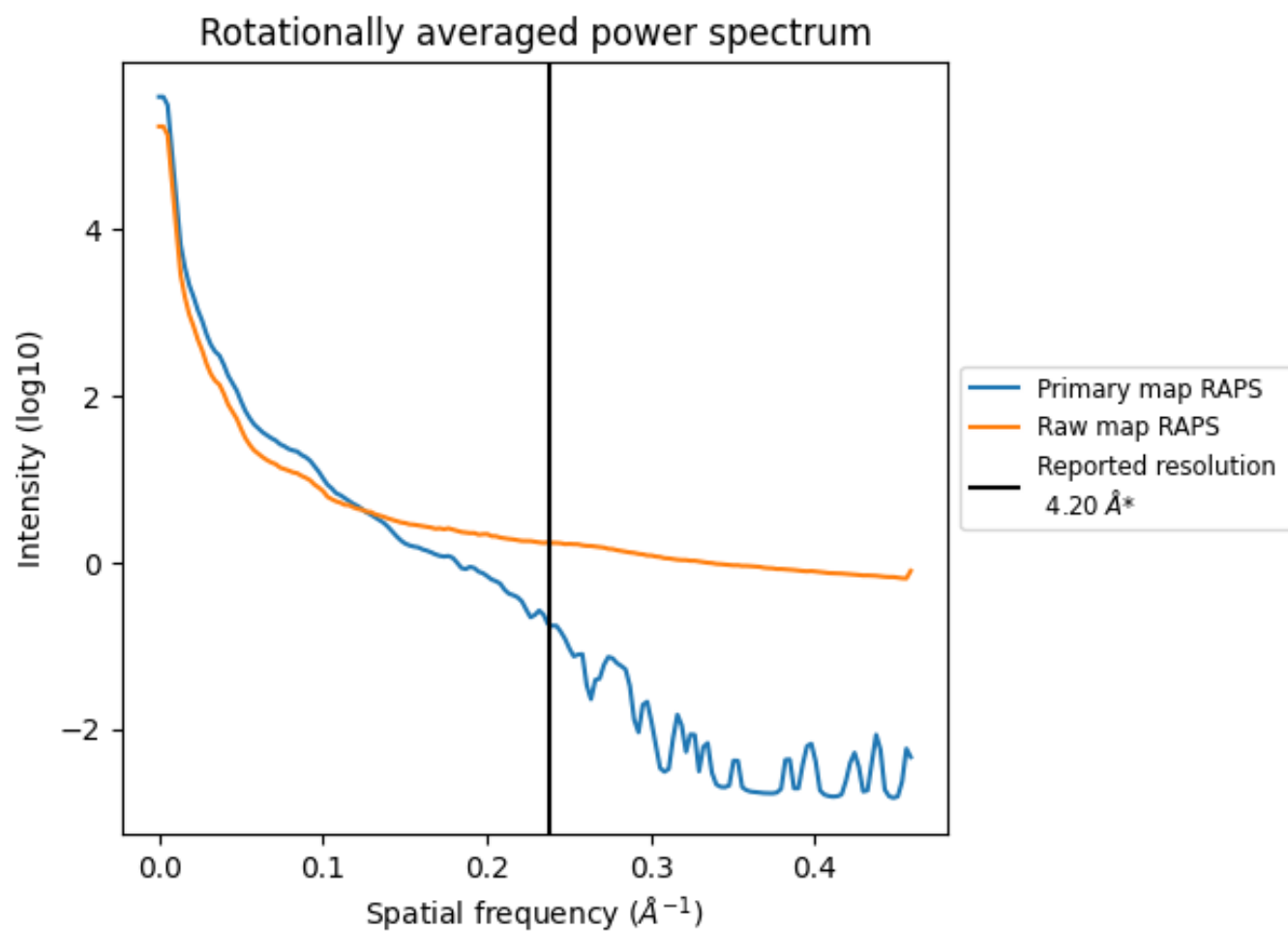
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1784 nm^3 ; this corresponds to an approximate mass of 1611 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 ⓘ

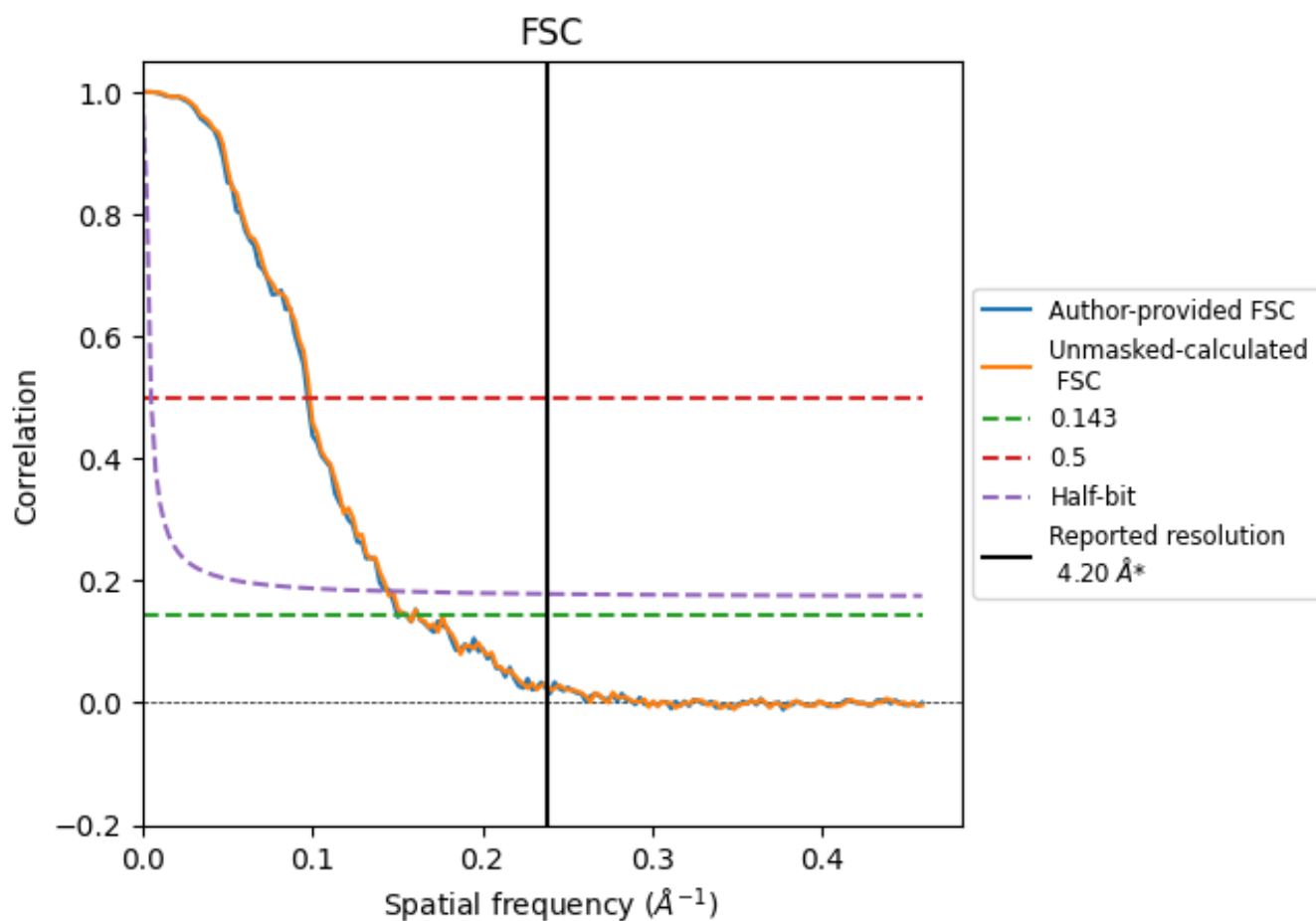


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 $0.238 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	6.67	10.29	6.87
Unmasked-calculated*	6.41	10.14	6.93

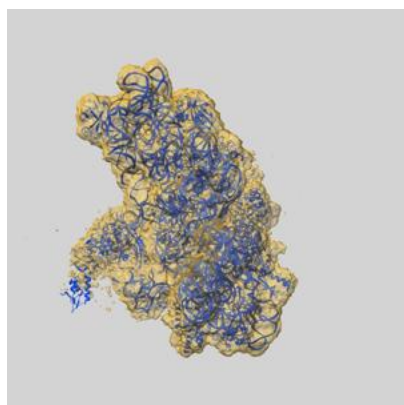
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.67 differs from the reported value 4.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 4.2 by more than 10 %

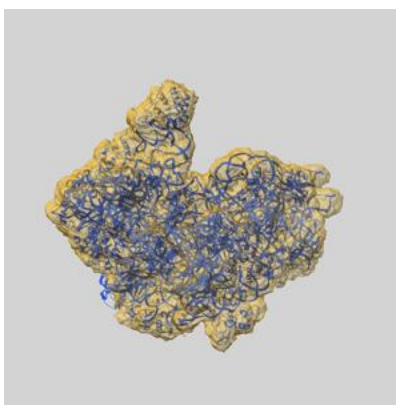
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10320 and PDB model 6SW9. Per-residue inclusion information can be found in section [3](#) on page [13](#).

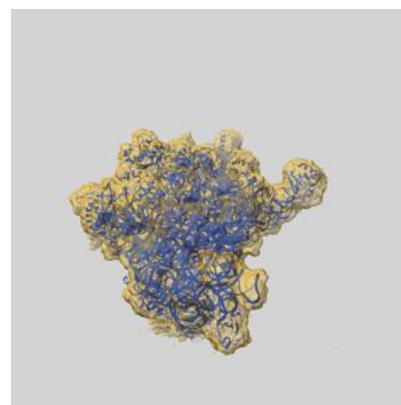
9.1 Map-model overlay [i](#)



X



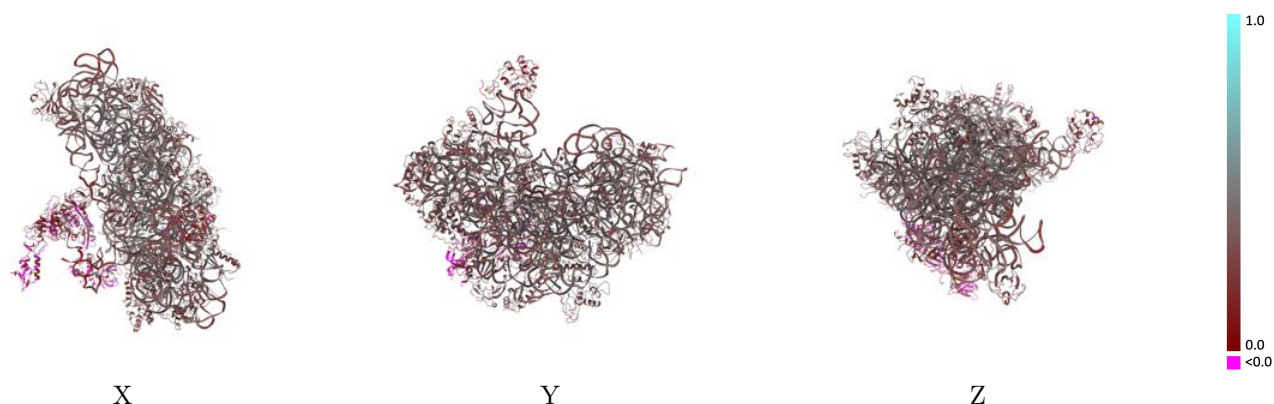
Y



Z

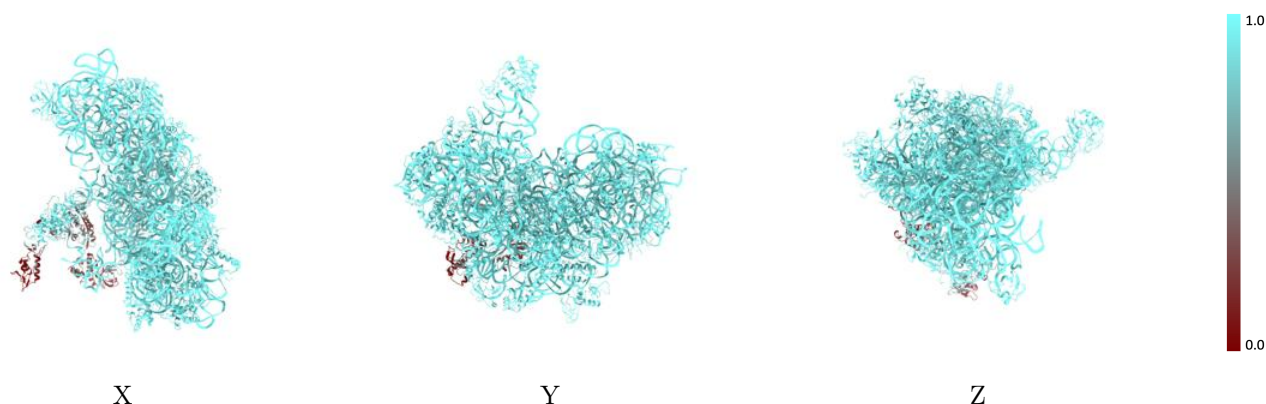
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



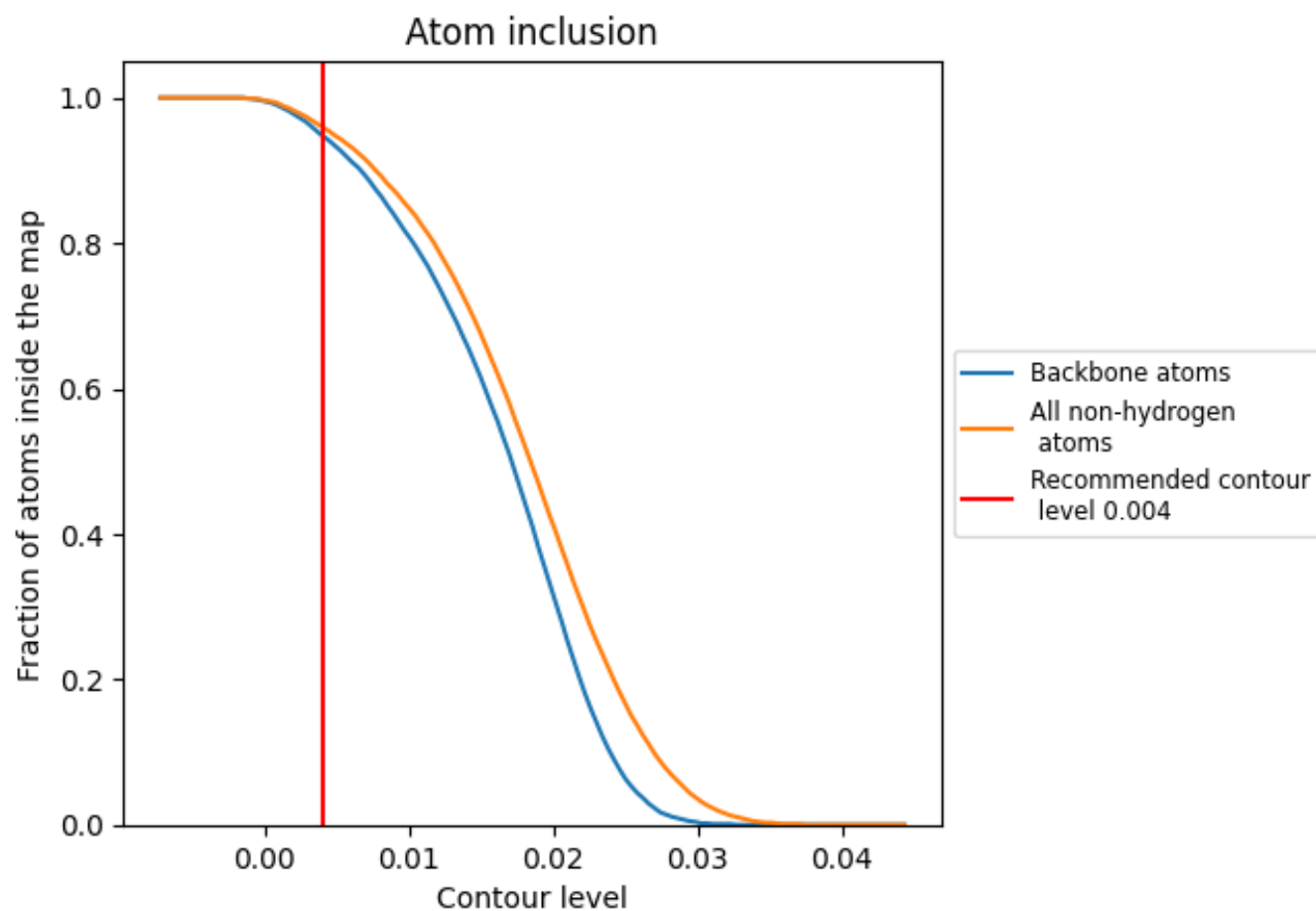
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.3370
0	 0.9970	 0.3730
2	 1.0000	 0.3830
3	 1.0000	 0.2200
4	 0.9870	 0.2310
5	 0.9980	 0.3390
6	 1.0000	 0.2490
7	 0.8600	 0.1420
8	 0.2740	 0.0540
9	 0.2580	 0.0380
A	 0.9960	 0.3430
B	 0.9970	 0.3580
C	 0.9940	 0.3660
D	 1.0000	 0.3580
E	 0.9990	 0.3700
F	 0.9930	 0.3750
G	 0.9980	 0.3170
H	 0.9960	 0.3410
I	 0.9980	 0.3770
J	 0.9980	 0.3550
K	 0.9980	 0.3510
L	 0.9980	 0.3520
M	 1.0000	 0.3570
N	 0.9980	 0.3830
O	 0.9980	 0.3280
P	 1.0000	 0.3630
Q	 0.9980	 0.3450
R	 0.9990	 0.3900
S	 0.9850	 0.3060
T	 0.9930	 0.3340
U	 0.9980	 0.3410
V	 0.9990	 0.3440
W	 0.9960	 0.3620
X	 1.0000	 0.3480
Y	 0.9900	 0.2050
Z	 0.9950	 0.3530

