



wwPDB EM Validation Summary Report ⓘ

Jun 19, 2026 – 02:03 am BST

PDB ID : 7O19 / pdb_00007o19
EMDB ID : EMD-12693
Title : Cryo-EM structure of an Escherichia coli TnaC-ribosome complex stalled in response to L-tryptophan
Authors : van der Stel, A.X.; Gordon, E.R.; Sengupta, A.; Martinez, A.K.; Klepacki, D.; Perry, T.N.; Herrero del Valle, A.; Vazquez-Laslop, N.; Sachs, M.S.; Cruz-Vera, L.R.; Innis, C.A.
Deposited on : 2021-03-29
Resolution : 2.90 Å(reported)
Based on initial model : 6TBV

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
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

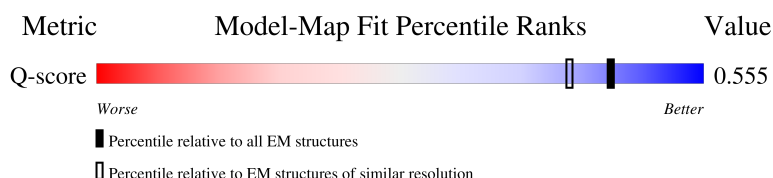
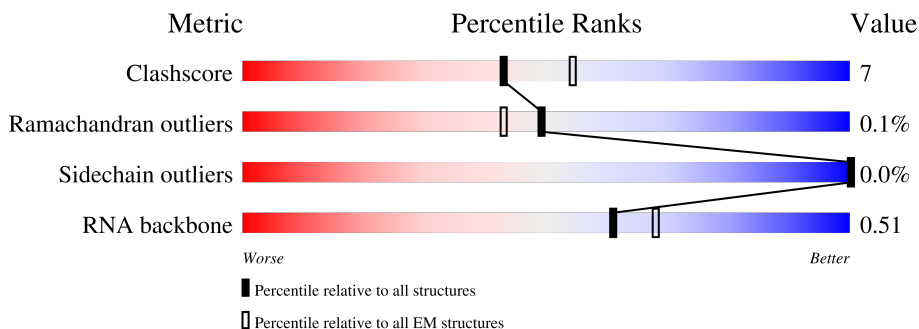
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	AA	1534	
2	AB	241	

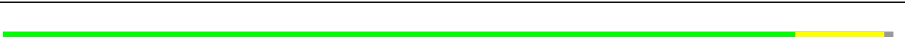
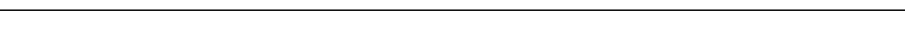
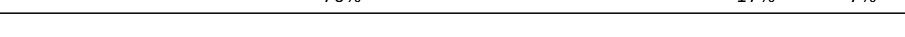
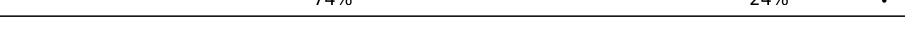
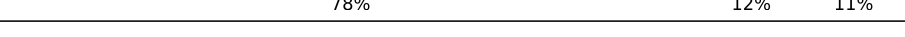
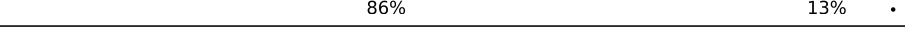
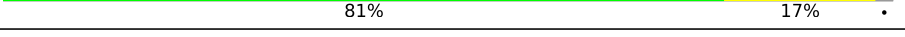
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Mol	Chain	Length	Quality of chain
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	BA	2897	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	

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Mol	Chain	Length	Quality of chain
28	BG	177	
29	BH	149	
30	BI	70	
31	BJ	142	
32	BK	123	
33	BL	144	
34	BM	136	
35	BN	127	
36	BO	117	
37	BP	115	
38	BQ	118	
39	BR	103	
40	BS	110	
41	BT	100	
42	BU	104	
43	BV	94	
44	BW	85	
45	BX	78	
46	BY	63	
47	BZ	59	
48	B0	57	
49	B1	55	
50	B2	46	
51	B3	65	
52	B4	38	

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Mol	Chain	Length	Quality of chain
53	B5	17	 76% 18% 6%
54	B7	7	 71% 29%
55	B8	77	 55% 30% 14% .

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 145019 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 Ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	82	Total	C	N	O	S	0	0
			656	419	125	110	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called Ribosomal RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0
			62209	27759	11446	20107	2897		

- Molecule 23 is a RNA chain called Ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BG	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BI	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BK	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BL	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BM	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BN	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BO	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	BQ	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BU	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BV	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BW	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BX	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BY	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BZ	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	51	Total	C	N	O		0	0
			414	266	76	72			

- Molecule 50 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called Tryptophanase leader peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B5	17	Total	C	N	O	0	0
			146	94	27	25		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B7	7	Total	C	N	O	P	0	0
			146	65	24	50	7		

- Molecule 55 is a RNA chain called P-site tRNA-Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B8	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		

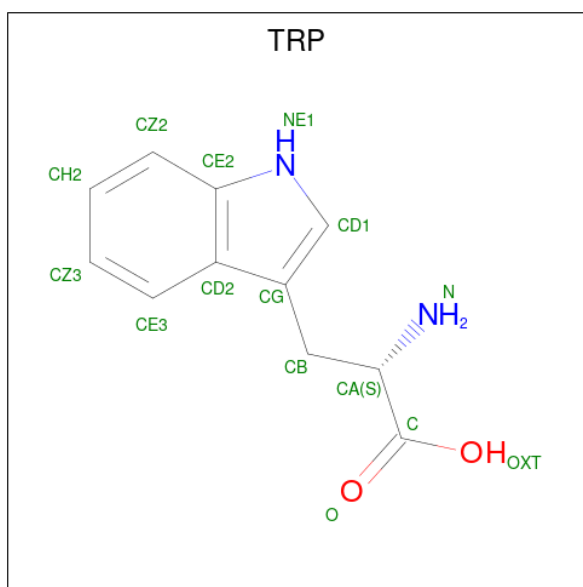
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	AA	35	Total	Mg	0
			35	35	
56	BA	132	Total	Mg	0
			132	132	
56	BC	1	Total	Mg	0
			1	1	
56	BD	1	Total	Mg	0
			1	1	
56	B8	1	Total	Mg	0
			1	1	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	AB	1	Total	Zn	0
			1	1	
57	BI	1	Total	Zn	0
			1	1	
57	B4	1	Total	Zn	0
			1	1	

- Molecule 58 is TRYPTOPHAN (CCD ID: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				AltConf
58	BA	1	Total	C	N	O	0
			15	11	2	2	

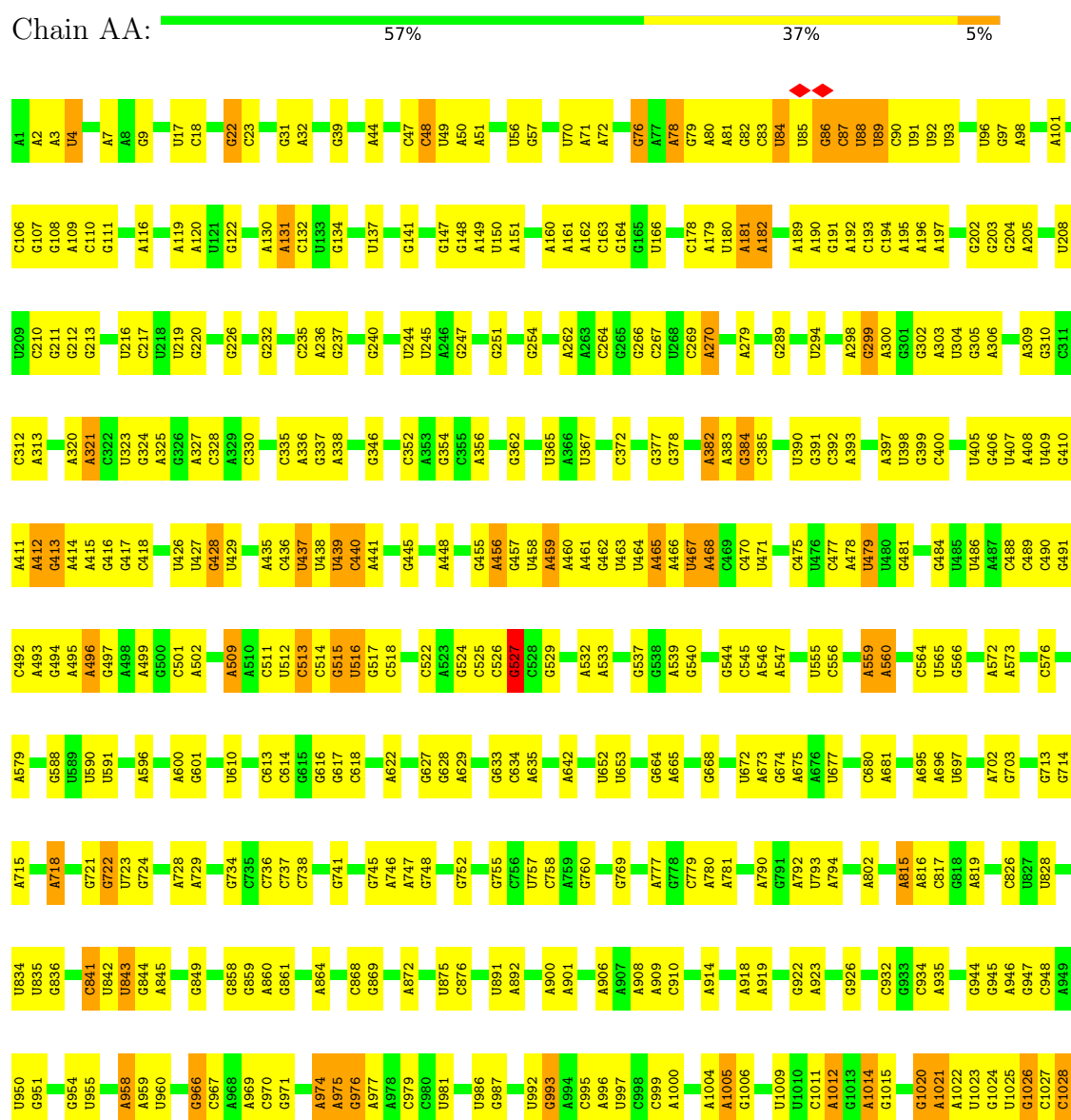
- Molecule 59 is water.

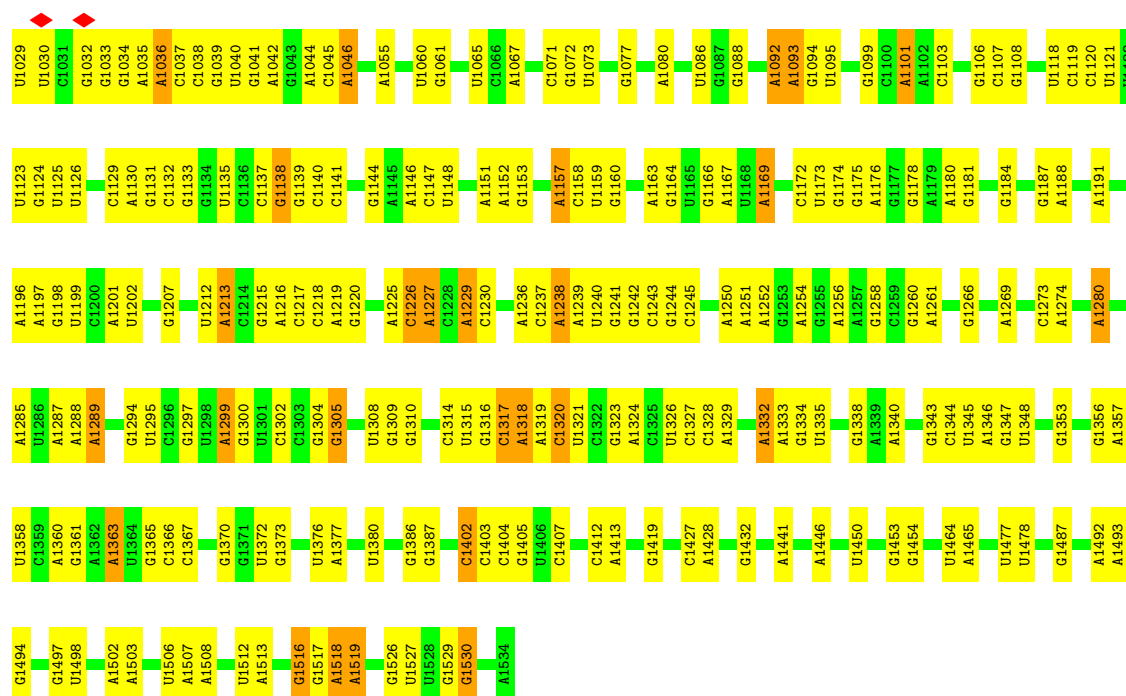
Mol	Chain	Residues	Atoms		AltConf
59	AA	168	Total	O	0
			168	168	
59	AK	1	Total	O	0
			1	1	
59	AM	1	Total	O	0
			1	1	
59	AN	2	Total	O	0
			2	2	
59	BA	608	Total	O	0
			608	608	
59	BC	7	Total	O	0
			7	7	
59	BD	1	Total	O	0
			1	1	
59	BE	1	Total	O	0
			1	1	
59	BL	2	Total	O	0
			2	2	
59	BN	1	Total	O	0
			1	1	
59	B8	1	Total	O	0
			1	1	

3 Residue-property plots

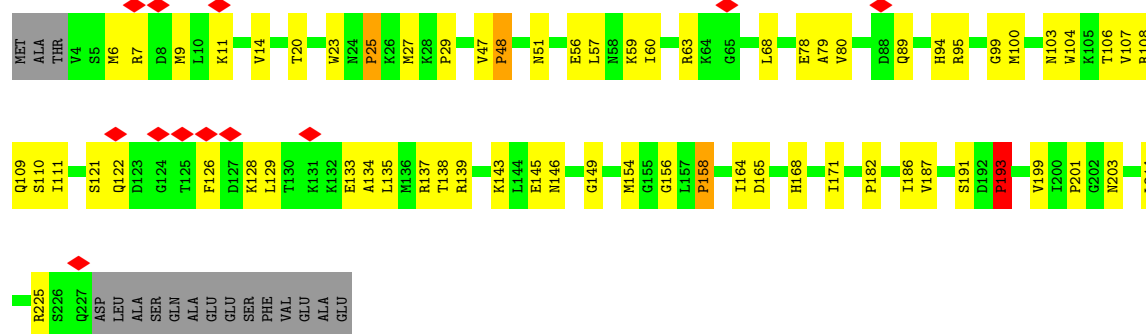
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ribosomal RNA 16S





• Molecule 2: 30S ribosomal protein S2

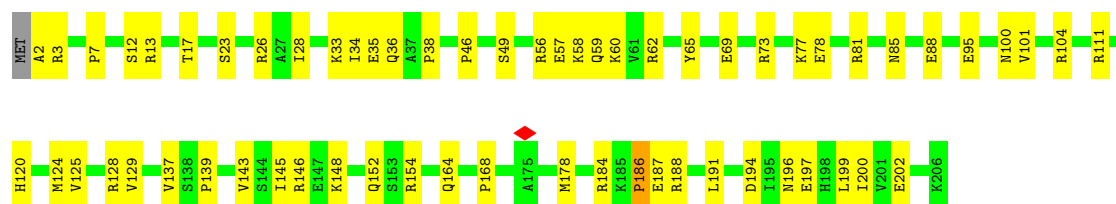


• Molecule 3: 30S ribosomal protein S3



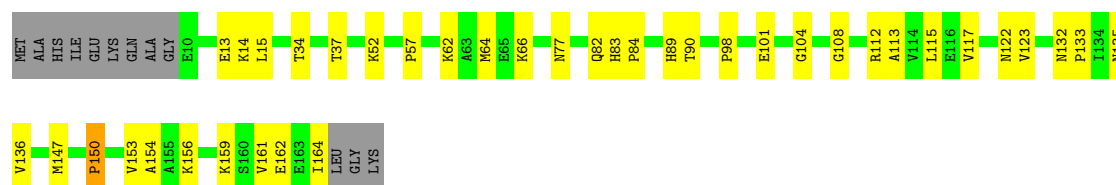
• Molecule 4: 30S ribosomal protein S4

Chain AD:  69% 30%



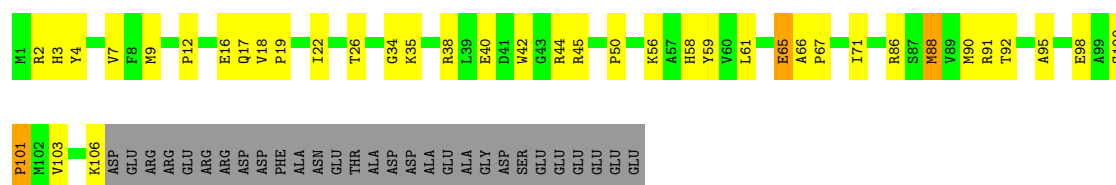
- Molecule 5: 30S ribosomal protein S5

Chain AE:  69% 23% 7%



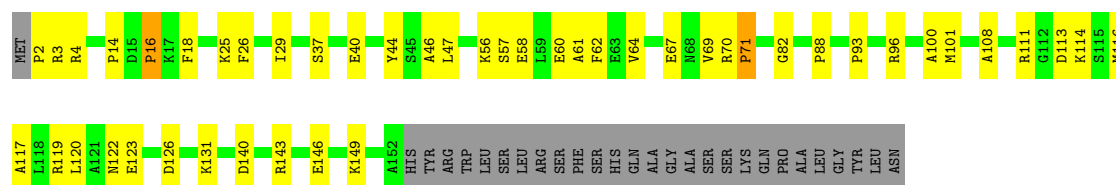
- Molecule 6: 30S ribosomal protein S6

Chain AF:  50% 27% 21%



- Molecule 7: 30S ribosomal protein S7

Chain AG:  58% 25% 16%

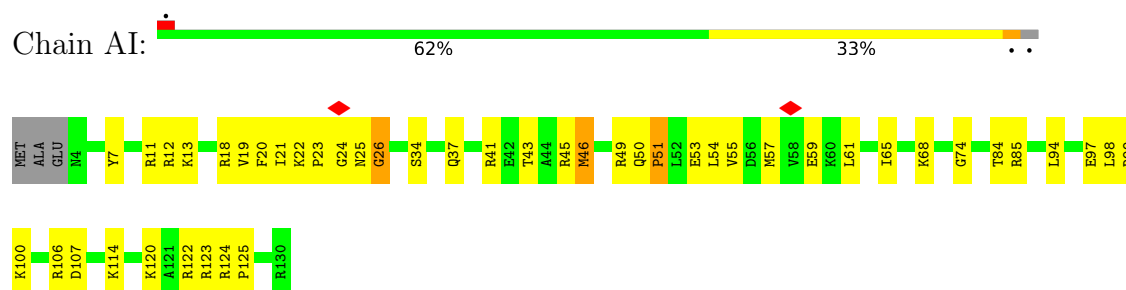


- Molecule 8: 30S ribosomal protein S8

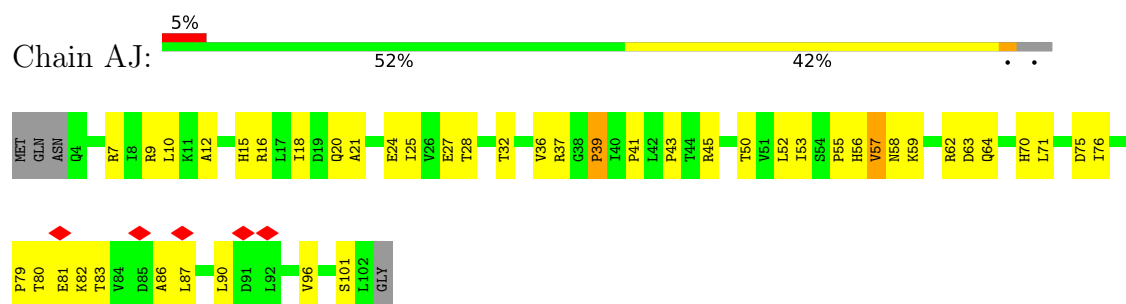
Chain AH:  64% 35%



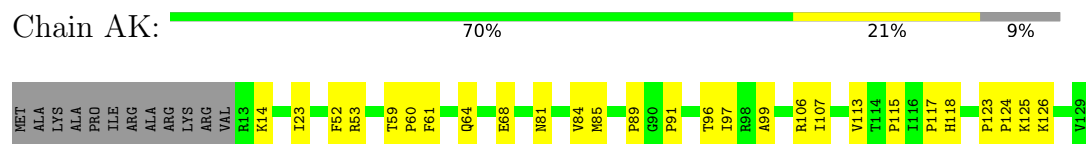
- Molecule 9: 30S ribosomal protein S9



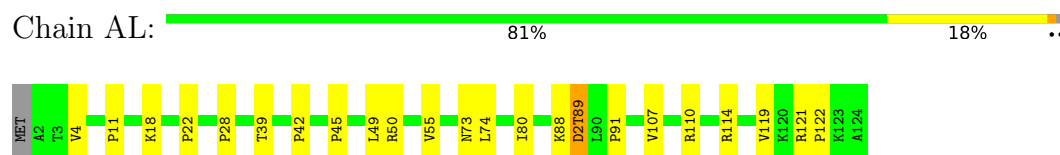
- Molecule 10: 30S ribosomal protein S10



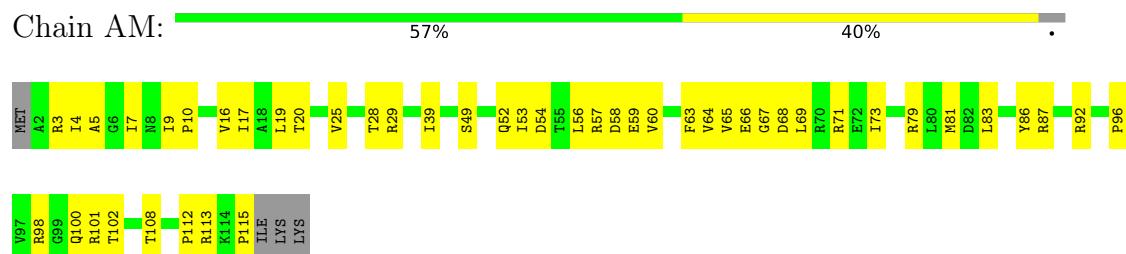
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

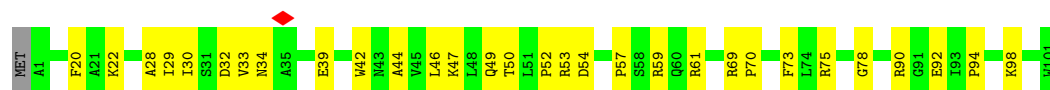


- Molecule 13: 30S ribosomal protein S13

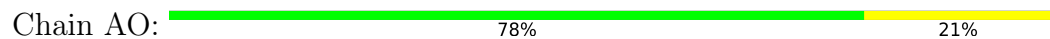


- Molecule 14: 30S ribosomal protein S14

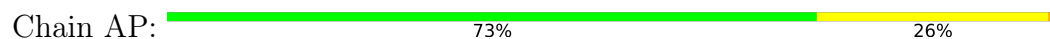




- Molecule 15: 30S ribosomal protein S15



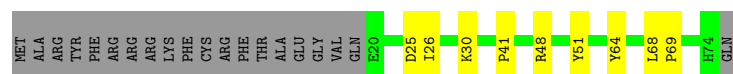
- Molecule 16: 30S ribosomal protein S16



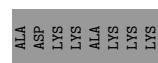
- Molecule 17: 30S ribosomal protein S17



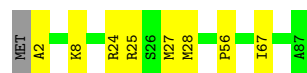
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



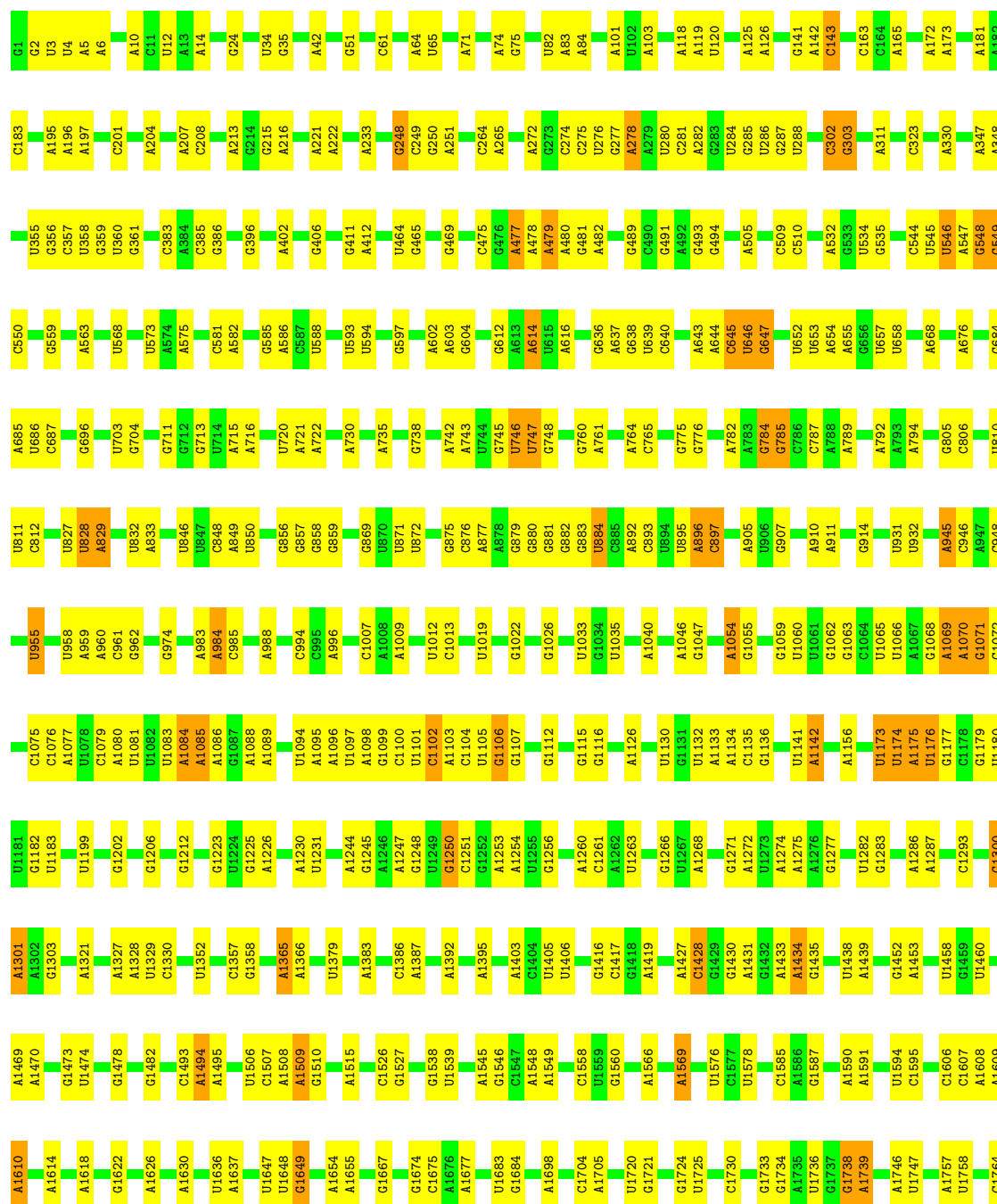
- Molecule 21: 30S ribosomal protein S21

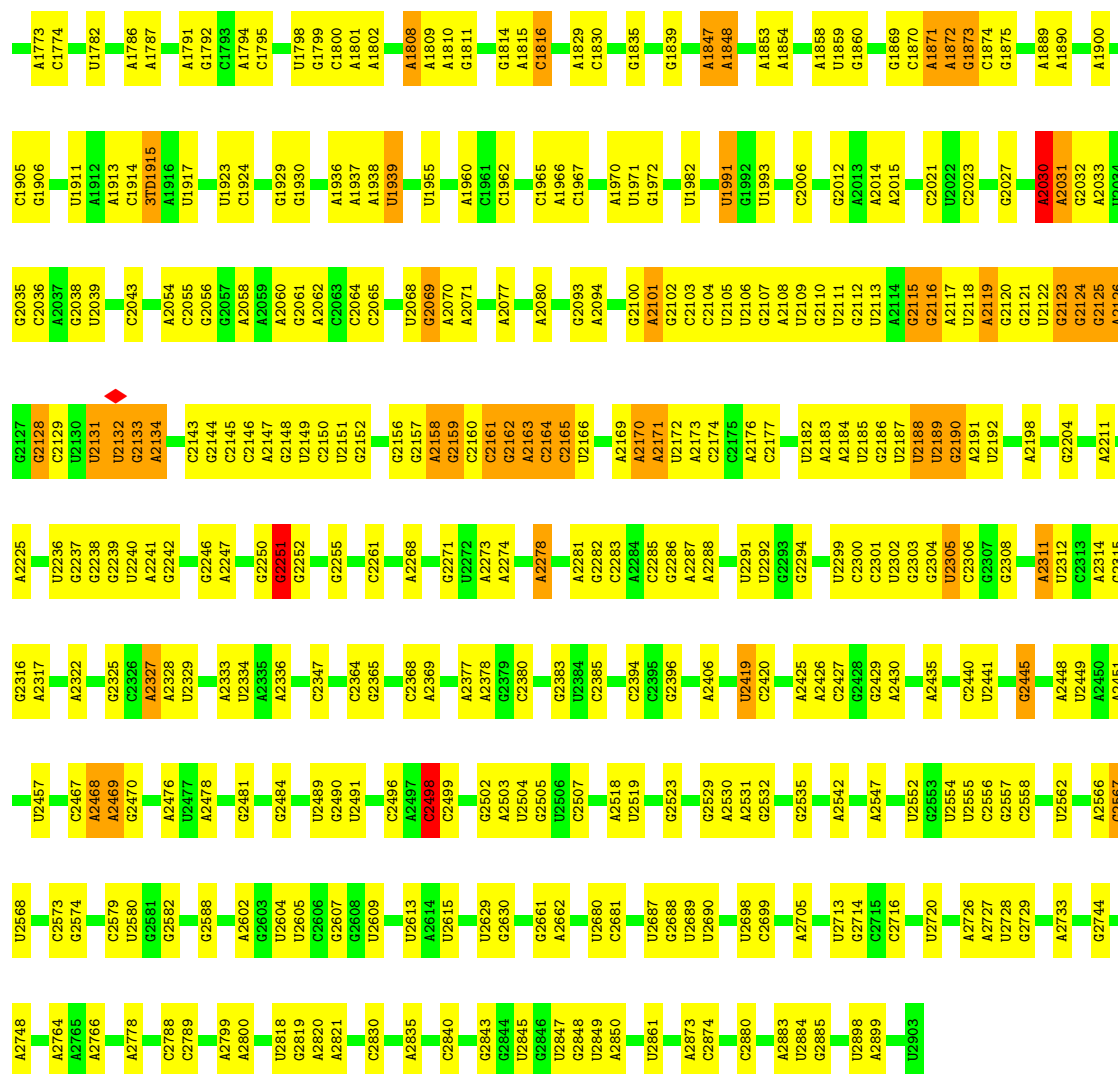
Chain AU:  56% 21% 21%



• Molecule 22: Ribosomal RNA 23S

Chain BA:  71% 25%





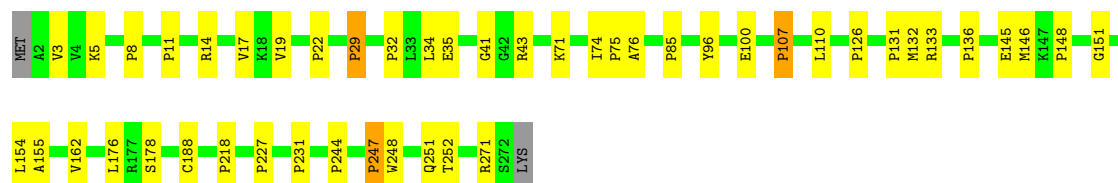
• Molecule 23: Ribosomal RNA 5S

Chain BB: 81% 16%



• Molecule 24: 50S ribosomal protein L2

Chain BC: 82% 16%



• Molecule 25: 50S ribosomal protein L3

Chain BD:  89% 11% .



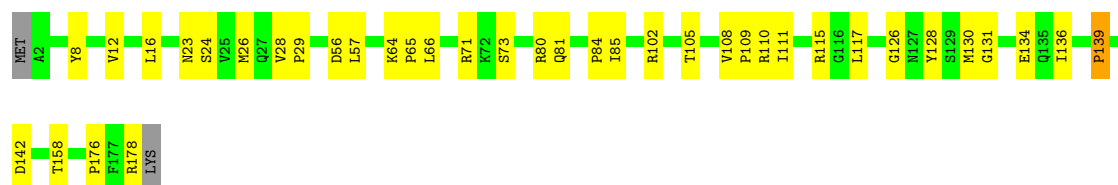
- Molecule 26: 50S ribosomal protein L4

Chain BE:  85% 15%



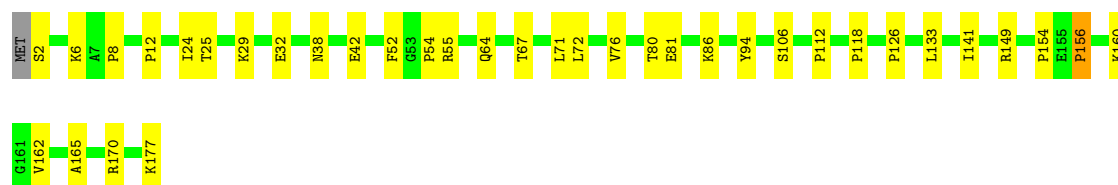
- Molecule 27: 50S ribosomal protein L5

Chain BF:  78% 21% ..



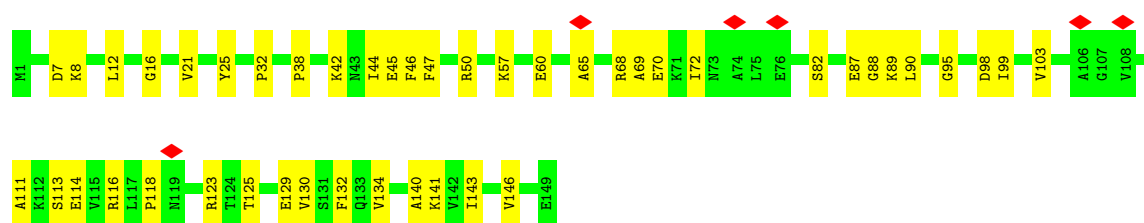
- Molecule 28: 50S ribosomal protein L6

Chain BG:  79% 20% ..



- Molecule 29: 50S ribosomal protein L9

Chain BH:  70% 30%



- Molecule 30: 50S ribosomal protein L31

Chain BI:  10% 66% 29% 6%





- Molecule 31: 50S ribosomal protein L13

Chain BJ: 85% 14%



- Molecule 32: 50S ribosomal protein L14

Chain BK: 82% 17%



- Molecule 33: 50S ribosomal protein L15

Chain BL: 81% 19%



- Molecule 34: 50S ribosomal protein L16

Chain BM: 84% 15%



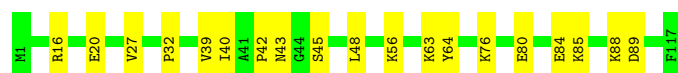
- Molecule 35: 50S ribosomal protein L17

Chain BN: 83% 10% 7%



- Molecule 36: 50S ribosomal protein L18

Chain BO: 84% 16%



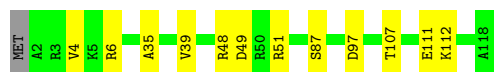
- Molecule 37: 50S ribosomal protein L19

Chain BP: 86% 13%



- Molecule 38: 50S ribosomal protein L20

Chain BQ: 89% 10%



- Molecule 39: 50S ribosomal protein L21

Chain BR: 82% 18%



- Molecule 40: 50S ribosomal protein L22

Chain BS: 83% 16%



- Molecule 41: 50S ribosomal protein L23

Chain BT: 76% 17% 7%



- Molecule 42: 50S ribosomal protein L24

Chain BU: 74% 24%



- Molecule 43: 50S ribosomal protein L25

Chain BV: 72% 27%



- Molecule 44: 50S ribosomal protein L27

Chain BW: 78% 12% 11%



- Molecule 45: 50S ribosomal protein L28

Chain BX: 90% 9% .



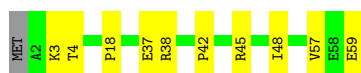
- Molecule 46: 50S ribosomal protein L29

Chain BY: 86% 13% .



- Molecule 47: 50S ribosomal protein L30

Chain BZ: 81% 17% .



- Molecule 48: 50S ribosomal protein L32

Chain B0: 86% 11% . .



- Molecule 49: 50S ribosomal protein L33

Chain B1: 64% 27% 7% .



- Molecule 50: 50S ribosomal protein L34

Chain B2: 85% 15%

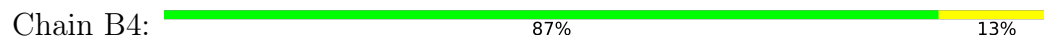


- Molecule 51: 50S ribosomal protein L35

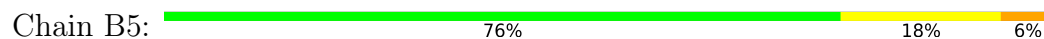
Chain B3: 78% 15% 5% .



- Molecule 52: 50S ribosomal protein L36



- Molecule 53: Tryptophanase leader peptide



- Molecule 54: mRNA



- Molecule 55: P-site tRNA-Pro



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	55127	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0075	Depositor
Map size (Å)	370.056, 370.056, 370.056	wwPDB
Map dimensions	408, 408, 408	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.907, 0.907, 0.907	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, ZN, G7M, OMC, 4OC, OMG, OMU, 3TD, UR3, MEQ, D2T, 6MZ, PSU, MA6, MG, 4D4, 2MG, 5MC, 2MA, 5MU

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	AA	0.61	0/36593	0.71	0/57081
2	AB	0.79	7/1784 (0.4%)	0.54	1/2403 (0.0%)
3	AC	0.81	7/1651 (0.4%)	0.51	0/2225
4	AD	0.75	6/1665 (0.4%)	0.42	0/2227
5	AE	0.84	5/1157 (0.4%)	0.53	0/1557
6	AF	0.99	6/881 (0.7%)	0.58	1/1189 (0.1%)
7	AG	0.92	7/1195 (0.6%)	0.53	1/1602 (0.1%)
8	AH	0.89	5/989 (0.5%)	0.53	0/1326
9	AI	0.72	3/1034 (0.3%)	0.68	2/1375 (0.1%)
10	AJ	1.02	7/805 (0.9%)	0.57	0/1089
11	AK	1.08	7/893 (0.8%)	0.55	0/1205
12	AL	1.10	9/960 (0.9%)	0.56	0/1286
13	AM	0.91	5/892 (0.6%)	0.59	0/1193
14	AN	0.86	4/811 (0.5%)	0.52	0/1081
15	AO	0.33	0/722	0.42	0/964
16	AP	0.73	2/659 (0.3%)	0.53	0/884
17	AQ	0.72	2/657 (0.3%)	0.53	0/881
18	AR	0.84	2/462 (0.4%)	0.49	0/621
19	AS	1.07	5/672 (0.7%)	0.58	0/904
20	AT	0.52	1/676 (0.1%)	0.38	0/895
21	AU	1.07	4/472 (0.8%)	0.59	1/627 (0.2%)
22	BA	0.80	5/69120 (0.0%)	0.77	1/107824 (0.0%)
23	BB	0.66	0/2872	0.65	0/4478
24	BC	1.18	18/2121 (0.8%)	0.61	0/2852
25	BD	0.92	8/1576 (0.5%)	0.53	0/2119
26	BE	0.83	5/1571 (0.3%)	0.53	0/2113
27	BF	0.83	6/1434 (0.4%)	0.49	0/1926
28	BG	0.98	8/1343 (0.6%)	0.54	0/1816
29	BH	0.67	3/1121 (0.3%)	0.55	0/1515
30	BI	0.78	2/531 (0.4%)	0.59	0/709
31	BJ	0.99	6/1152 (0.5%)	0.53	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BK	0.99	5/955 (0.5%)	0.63	1/1279 (0.1%)
33	BL	0.90	4/1062 (0.4%)	0.60	0/1413
34	BM	1.07	7/1081 (0.6%)	0.55	0/1443
35	BN	0.96	4/958 (0.4%)	0.57	0/1281
36	BO	0.70	2/910 (0.2%)	0.51	1/1219 (0.1%)
37	BP	0.85	3/929 (0.3%)	0.57	0/1242
38	BQ	0.65	0/960	0.48	0/1278
39	BR	0.76	3/829 (0.4%)	0.54	0/1107
40	BS	0.76	2/864 (0.2%)	0.50	0/1156
41	BT	0.64	1/744 (0.1%)	0.51	0/994
42	BU	0.86	3/787 (0.4%)	0.54	0/1051
43	BV	0.98	4/766 (0.5%)	0.54	0/1025
44	BW	0.77	1/587 (0.2%)	0.56	0/776
45	BX	0.86	2/635 (0.3%)	0.56	0/848
46	BY	0.43	0/502	0.40	0/667
47	BZ	0.92	2/453 (0.4%)	0.52	0/605
48	B0	0.78	1/450 (0.2%)	0.57	0/599
49	B1	1.15	5/421 (1.2%)	0.72	1/561 (0.2%)
50	B2	0.86	1/380 (0.3%)	0.62	0/498
51	B3	1.13	4/513 (0.8%)	0.74	0/676
52	B4	0.87	1/303 (0.3%)	0.50	0/397
53	B5	1.64	3/150 (2.0%)	0.80	0/203
54	B7	0.18	0/161	0.45	0/248
55	B8	0.79	14/1839 (0.8%)	0.65	0/2866
All	All	0.79	227/155710 (0.1%)	0.70	10/232950 (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
10	AJ	0	1
27	BF	0	1
51	B3	0	1
All	All	0	3

The worst 5 of 227 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	C2'-C1'	-16.08	1.29	1.53
22	BA	892	A	O4'-C1'	14.13	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	B5	24	PRO	N-CD	13.62	1.66	1.47
2	AB	48	PRO	N-CD	11.71	1.64	1.47
5	AE	57	PRO	N-CD	11.69	1.64	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BK	102	PRO	CA-N-CD	-7.57	101.40	112.00
22	BA	2251	OMG	P-O3'-C3'	6.13	129.40	120.20
21	AU	2	PRO	CA-N-CD	-5.96	103.66	112.00
9	AI	46	MET	CB-CG-SD	-5.87	95.08	112.70
2	AB	193	PRO	CA-N-CD	-5.84	103.82	112.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	AJ	81	GLU	Peptide
51	B3	31	HIS	Peptide
27	BF	142	ASP	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	AA	32930	0	16591	434	0
2	AB	1753	0	1780	45	0
3	AC	1624	0	1696	39	0
4	AD	1643	0	1707	43	0
5	AE	1144	0	1185	28	0
6	AF	862	0	864	30	0
7	AG	1181	0	1238	38	0
8	AH	979	0	1031	33	0
9	AI	1022	0	1070	46	0
10	AJ	795	0	836	34	0
11	AK	877	0	887	25	0
12	AL	957	0	1017	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AM	883	0	941	50	0
14	AN	799	0	841	26	0
15	AO	714	0	734	14	0
16	AP	649	0	666	16	0
17	AQ	648	0	691	13	0
18	AR	455	0	478	7	0
19	AS	656	0	680	34	0
20	AT	670	0	719	5	0
21	AU	465	0	491	17	0
22	BA	62209	0	31308	393	0
23	BB	2569	0	1301	15	0
24	BC	2082	0	2154	22	0
25	BD	1566	0	1618	14	0
26	BE	1552	0	1619	16	0
27	BF	1410	0	1444	32	0
28	BG	1323	0	1371	19	0
29	BH	1110	0	1148	32	0
30	BI	522	0	520	20	0
31	BJ	1129	0	1162	12	0
32	BK	946	0	1023	13	0
33	BL	1053	0	1129	20	0
34	BM	1075	0	1155	11	0
35	BN	945	0	989	8	0
36	BO	900	0	935	11	0
37	BP	917	0	962	12	0
38	BQ	947	0	1019	12	0
39	BR	816	0	839	12	0
40	BS	857	0	922	11	0
41	BT	738	0	807	13	0
42	BU	779	0	831	16	0
43	BV	753	0	780	14	0
44	BW	580	0	594	6	0
45	BX	625	0	652	4	0
46	BY	501	0	531	5	0
47	BZ	449	0	488	5	0
48	B0	444	0	458	5	0
49	B1	414	0	442	11	0
50	B2	377	0	418	7	0
51	B3	504	0	572	11	0
52	B4	302	0	340	3	0
53	B5	146	0	143	2	0
54	B7	146	0	77	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	B8	1646	0	831	19	0
56	AA	35	0	0	0	0
56	B8	1	0	0	0	0
56	BA	132	0	0	1	0
56	BC	1	0	0	0	0
56	BD	1	0	0	0	0
57	AB	1	0	0	0	0
57	B4	1	0	0	0	0
57	BI	1	0	0	0	0
58	BA	15	0	9	1	0
59	AA	168	0	0	3	0
59	AK	1	0	0	0	0
59	AM	1	0	0	0	0
59	AN	2	0	0	0	0
59	B8	1	0	0	1	0
59	BA	608	0	0	4	0
59	BC	7	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BL	2	0	0	0	0
59	BN	1	0	0	0	0
All	All	145019	0	96734	1567	0

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

The worst 5 of 1567 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)
22:BA:962:G:OP1	59:BA:3201:HOH:O	1.58	1.19
22:BA:2107:G:H1	22:BA:2182:U:H3	1.03	1.01
22:BA:2133:G:N2	22:BA:2158:A:N6	2.12	0.98
13:AM:53:ILE:HG22	13:AM:57:ARG:HH21	1.26	0.97
22:BA:2133:G:N2	22:BA:2158:A:C6	2.35	0.94

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/241 (92%)	209 (94%)	13 (6%)	0	100	100
3	AC	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
4	AD	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
5	AE	153/167 (92%)	148 (97%)	5 (3%)	0	100	100
6	AF	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	AG	149/179 (83%)	143 (96%)	6 (4%)	0	100	100
8	AH	127/130 (98%)	127 (100%)	0	0	100	100
9	AI	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
10	AJ	97/103 (94%)	89 (92%)	6 (6%)	2 (2%)	5	21
11	AK	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
12	AL	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
13	AM	112/118 (95%)	104 (93%)	8 (7%)	0	100	100
14	AN	99/102 (97%)	88 (89%)	11 (11%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	AP	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
17	AQ	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
18	AR	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
19	AS	80/92 (87%)	74 (92%)	6 (8%)	0	100	100
20	AT	84/87 (97%)	84 (100%)	0	0	100	100
21	AU	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
24	BC	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
25	BD	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	24	54
26	BE	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
27	BF	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
28	BG	174/177 (98%)	173 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BH	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
30	BI	64/70 (91%)	58 (91%)	6 (9%)	0	100	100
31	BJ	140/142 (99%)	140 (100%)	0	0	100	100
32	BK	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	BL	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
34	BM	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
35	BN	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
36	BO	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
37	BP	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	BS	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	BT	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
42	BU	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
43	BV	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
44	BW	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
45	BX	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
46	BY	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
47	BZ	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	B0	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
49	B1	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
50	B2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
51	B3	62/65 (95%)	57 (92%)	3 (5%)	2 (3%)	3	13
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	B5	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
All	All	5590/5931 (94%)	5378 (96%)	207 (4%)	5 (0%)	49	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	BD	149	ASN
51	B3	32	ILE
51	B3	33	LEU

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Mol	Chain	Res	Type
10	AJ	57	VAL
10	AJ	58	ASN

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	AB	186/199 (94%)	185 (100%)	1 (0%)	81	93
3	AC	170/190 (90%)	170 (100%)	0	100	100
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	118/126 (94%)	118 (100%)	0	100	100
6	AF	92/116 (79%)	92 (100%)	0	100	100
7	AG	124/147 (84%)	124 (100%)	0	100	100
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	105 (100%)	0	100	100
10	AJ	87/90 (97%)	87 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	102/103 (99%)	102 (100%)	0	100	100
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	79 (100%)	0	100	100
15	AO	76/77 (99%)	76 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	71/79 (90%)	71 (100%)	0	100	100
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	48/61 (79%)	48 (100%)	0	100	100
24	BC	216/218 (99%)	216 (100%)	0	100	100
25	BD	163/163 (100%)	163 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BE	165/165 (100%)	165 (100%)	0	100	100
27	BF	148/150 (99%)	148 (100%)	0	100	100
28	BG	137/138 (99%)	137 (100%)	0	100	100
29	BH	114/114 (100%)	114 (100%)	0	100	100
30	BI	59/62 (95%)	59 (100%)	0	100	100
31	BJ	116/116 (100%)	116 (100%)	0	100	100
32	BK	104/104 (100%)	104 (100%)	0	100	100
33	BL	103/103 (100%)	103 (100%)	0	100	100
34	BM	108/108 (100%)	108 (100%)	0	100	100
35	BN	98/103 (95%)	98 (100%)	0	100	100
36	BO	87/87 (100%)	87 (100%)	0	100	100
37	BP	99/100 (99%)	99 (100%)	0	100	100
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	84 (100%)	0	100	100
40	BS	93/93 (100%)	93 (100%)	0	100	100
41	BT	80/84 (95%)	80 (100%)	0	100	100
42	BU	83/85 (98%)	83 (100%)	0	100	100
43	BV	78/78 (100%)	78 (100%)	0	100	100
44	BW	57/63 (90%)	57 (100%)	0	100	100
45	BX	67/68 (98%)	67 (100%)	0	100	100
46	BY	54/55 (98%)	54 (100%)	0	100	100
47	BZ	48/49 (98%)	48 (100%)	0	100	100
48	B0	47/48 (98%)	47 (100%)	0	100	100
49	B1	45/49 (92%)	45 (100%)	0	100	100
50	B2	38/38 (100%)	38 (100%)	0	100	100
51	B3	51/52 (98%)	51 (100%)	0	100	100
52	B4	34/34 (100%)	34 (100%)	0	100	100
53	B5	17/17 (100%)	16 (94%)	1 (6%)	18	48
All	All	4650/4844 (96%)	4648 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	193	PRO
53	B5	24	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
31	BJ	86	GLN
52	B4	35	GLN
32	BK	93	GLN
53	B5	17	ASN
43	BV	87	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	238 (15%)	7 (0%)
22	BA	2894/2897 (99%)	422 (14%)	23 (0%)
23	BB	119/120 (99%)	13 (10%)	1 (0%)
54	B7	6/7 (85%)	3 (50%)	1 (16%)
55	B8	76/77 (98%)	12 (15%)	2 (2%)
All	All	4628/4635 (99%)	688 (14%)	34 (0%)

5 of 688 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	7	A
1	AA	9	G
1	AA	22	G
1	AA	32	A

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2518	A
22	BA	2873	A
55	B8	2	G
22	BA	984	A
22	BA	784	G

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

37 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
22	5MU	BA	747	22	19,22,23	0.82	1 (5%)	28,32,35	1.26	3 (10%)
22	OMU	BA	2552	22	19,22,23	2.64	7 (36%)	26,31,34	1.92	5 (19%)
1	MA6	AA	1518	1	23,26,27	1.86	6 (26%)	34,38,41	3.27	11 (32%)
22	5MU	BA	1939	22	19,22,23	0.76	0	28,32,35	1.17	3 (10%)
22	1MG	BA	745	22	22,26,27	2.47	8 (36%)	33,39,42	1.79	8 (24%)
1	G7M	AA	527	1	23,26,27	2.66	8 (34%)	35,39,42	2.40	11 (31%)
22	PSU	BA	2457	22	18,21,22	3.66	7 (38%)	22,30,33	2.28	5 (22%)
22	PSU	BA	1917	22	18,21,22	4.07	7 (38%)	22,30,33	1.88	5 (22%)
22	2MA	BA	2503	22,56	22,25,26	3.53	8 (36%)	33,37,40	2.09	7 (21%)
22	PSU	BA	2605	22	18,21,22	3.73	7 (38%)	22,30,33	1.88	4 (18%)
22	G7M	BA	2069	22	23,26,27	2.55	8 (34%)	35,39,42	2.17	11 (31%)
1	2MG	AA	966	1	23,26,27	2.80	9 (39%)	32,38,41	2.19	11 (34%)
1	4OC	AA	1402	1	20,23,24	2.90	8 (40%)	26,32,35	0.97	2 (7%)
22	OMC	BA	2498	22,56	19,22,23	2.64	7 (36%)	26,31,34	1.05	1 (3%)
1	5MC	AA	967	1	18,22,23	3.43	7 (38%)	26,32,35	1.06	2 (7%)
22	PSU	BA	2580	22	18,21,22	3.77	7 (38%)	22,30,33	2.14	6 (27%)
22	PSU	BA	746	22,56	18,21,22	1.47	3 (16%)	22,30,33	2.42	5 (22%)
34	4D4	BM	81	34	9,11,12	2.44	3 (33%)	8,13,15	1.06	0
22	6MZ	BA	1618	22	22,25,26	3.97	6 (27%)	30,36,39	2.42	10 (33%)
1	UR3	AA	1498	1	19,22,23	3.03	8 (42%)	26,32,35	1.40	3 (11%)
1	2MG	AA	1516	1	23,26,27	2.63	8 (34%)	32,38,41	2.12	11 (34%)
22	PSU	BA	955	22	18,21,22	3.80	6 (33%)	22,30,33	2.17	5 (22%)
1	5MC	AA	1407	1	18,22,23	3.26	7 (38%)	26,32,35	1.00	1 (3%)
1	MA6	AA	1519	1	23,26,27	1.84	5 (21%)	34,38,41	3.40	11 (32%)
22	PSU	BA	2604	22	18,21,22	3.82	6 (33%)	22,30,33	2.05	5 (22%)
1	2MG	AA	1207	1	23,26,27	2.74	9 (39%)	32,38,41	2.12	11 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	5MC	BA	1962	22	18,22,23	3.07	7 (38%)	26,32,35	1.26	5 (19%)
22	PSU	BA	1911	22	18,21,22	4.12	6 (33%)	22,30,33	2.00	5 (22%)
22	PSU	BA	2504	22	18,21,22	3.88	6 (33%)	22,30,33	1.72	4 (18%)
1	PSU	AA	516	56,1	18,21,22	4.19	6 (33%)	22,30,33	1.95	6 (27%)
22	OMG	BA	2251	55,22	23,26,27	2.29	8 (34%)	33,38,41	2.09	11 (33%)
25	MEQ	BD	150	25	8,9,10	1.37	2 (25%)	5,10,12	1.46	1 (20%)
22	2MG	BA	2445	22	23,26,27	2.63	8 (34%)	32,38,41	2.36	12 (37%)
22	2MG	BA	1835	22	23,26,27	2.56	7 (30%)	32,38,41	2.32	11 (34%)
22	6MZ	BA	2030	22	22,25,26	4.00	7 (31%)	30,36,39	2.40	11 (36%)
22	3TD	BA	1915	22	18,22,23	4.06	8 (44%)	22,32,35	1.97	4 (18%)
12	D2T	AL	89	12	7,9,10	1.07	0	6,11,13	2.56	2 (33%)

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
22	5MU	BA	747	22	-	0/7/25/26	0/2/2/2
22	OMU	BA	2552	22	-	0/9/27/28	0/2/2/2
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
22	5MU	BA	1939	22	-	2/7/25/26	0/2/2/2
22	1MG	BA	745	22	-	0/7/25/26	0/3/3/3
1	G7M	AA	527	1	-	2/7/25/26	0/3/3/3
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	1917	22	-	0/7/25/26	0/2/2/2
22	2MA	BA	2503	22,56	-	1/7/25/26	0/3/3/3
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
22	G7M	BA	2069	22	-	1/7/25/26	0/3/3/3
1	2MG	AA	966	1	-	2/9/27/28	0/3/3/3
1	4OC	AA	1402	1	-	1/9/29/30	0/2/2/2
22	OMC	BA	2498	22,56	-	2/9/27/28	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
22	PSU	BA	2580	22	-	1/7/25/26	0/2/2/2
22	PSU	BA	746	22,56	-	2/7/25/26	0/2/2/2
34	4D4	BM	81	34	-	2/11/12/14	-
22	6MZ	BA	1618	22	-	0/9/27/28	0/3/3/3
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/11/29/30	0/3/3/3
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	0/9/27/28	0/3/3/3
22	5MC	BA	1962	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	1911	22	-	2/7/25/26	0/2/2/2
22	PSU	BA	2504	22	-	2/7/25/26	0/2/2/2
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
22	OMG	BA	2251	55,22	-	3/9/27/28	0/3/3/3
25	MEQ	BD	150	25	-	2/8/9/11	-
22	2MG	BA	2445	22	-	2/9/27/28	0/3/3/3
22	2MG	BA	1835	22	-	0/9/27/28	0/3/3/3
22	6MZ	BA	2030	22	-	2/9/27/28	0/3/3/3
22	3TD	BA	1915	22	-	2/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/7/12/14	-

The worst 5 of 231 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1618	6MZ	C6-N6	17.25	1.52	1.34
22	BA	2030	6MZ	C6-N6	17.14	1.52	1.34
22	BA	1915	3TD	C6-C5	11.67	1.48	1.35
1	AA	516	PSU	C6-C5	11.19	1.48	1.35
22	BA	1911	PSU	C6-C5	10.95	1.48	1.35

The worst 5 of 229 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	MA6	N1-C6-N6	-13.45	102.37	117.08
1	AA	1518	MA6	N1-C6-N6	-12.89	103.00	117.08
22	BA	746	PSU	N1-C2-N3	7.79	123.96	115.13
1	AA	527	G7M	C1'-N9-C8	-7.10	102.78	126.74
1	AA	527	G7M	C1'-N9-C4	6.87	146.92	126.50

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	O4'-C4'-C5'-O5'
34	BM	81	4D4	NE-CD-CG-CB
22	BA	746	PSU	C2'-C1'-C5-C4
22	BA	1915	3TD	C3'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	1	0
1	AA	527	G7M	1	0
1	AA	1402	4OC	1	0
22	BA	2498	OMC	1	0
22	BA	746	PSU	1	0
1	AA	1516	2MG	1	0
22	BA	955	PSU	1	0
1	AA	1519	MA6	1	0
22	BA	2251	OMG	1	0
25	BD	150	MEQ	1	0
22	BA	2030	6MZ	3	0
12	AL	89	D2T	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 173 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	$\# Z > 2$
58	TRP	BA	3001	-	14,16,16	0.72	1 (7%)	20,22,22	0.85	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	TRP	BA	3001	-	-	0/8/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	3001	TRP	OXT-C	-2.20	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	TRP	OXT-C-O	-2.59	118.21	124.09
58	BA	3001	TRP	OXT-C-CA	2.15	120.71	113.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	BA	3001	TRP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	BA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	P	13.83
1	BA	2099:U	O3'	2100:G	P	3.52

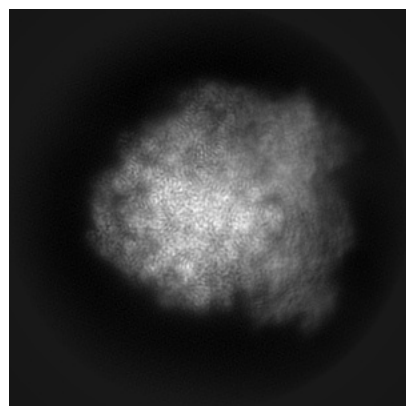
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12693. These allow visual inspection of the internal detail of the map and identification of artifacts.

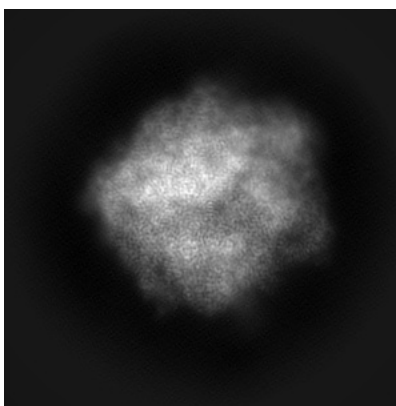
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

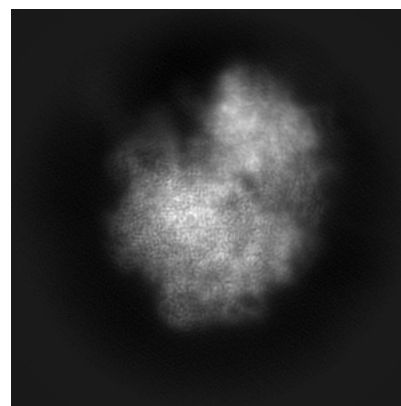
6.1.1 Primary map



X

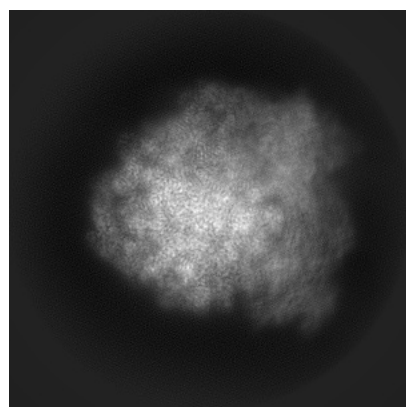


Y

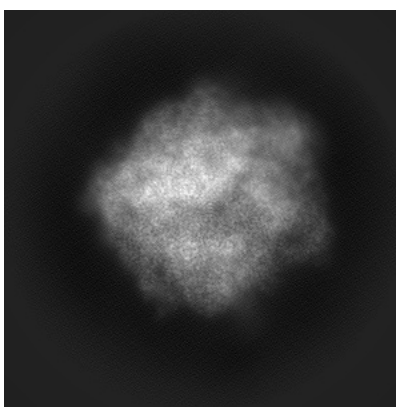


Z

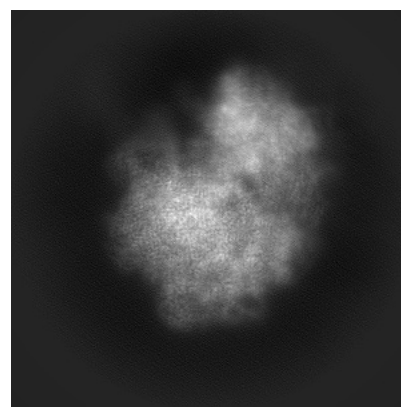
6.1.2 Raw map



X



Y

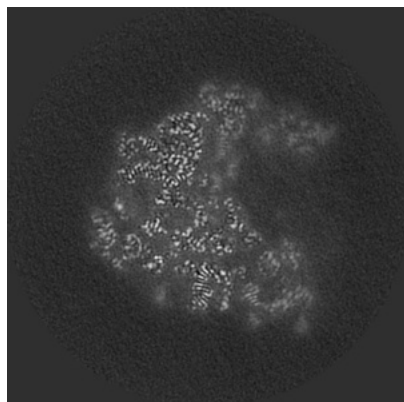


Z

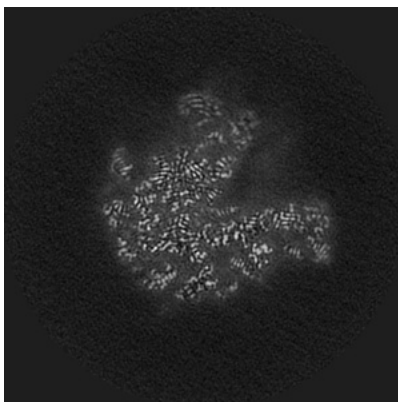
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

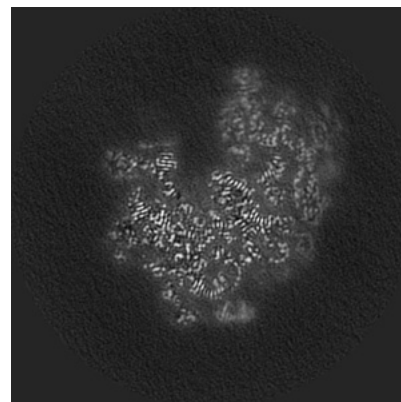
6.2.1 Primary map



X Index: 204

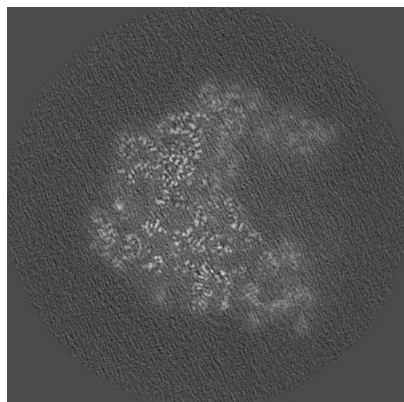


Y Index: 204

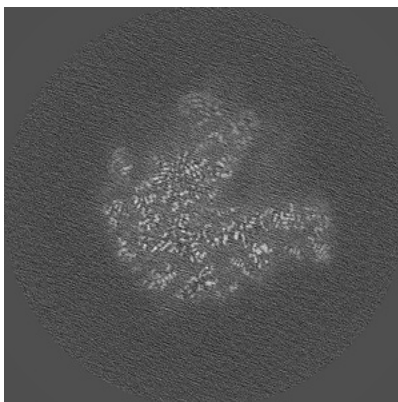


Z Index: 204

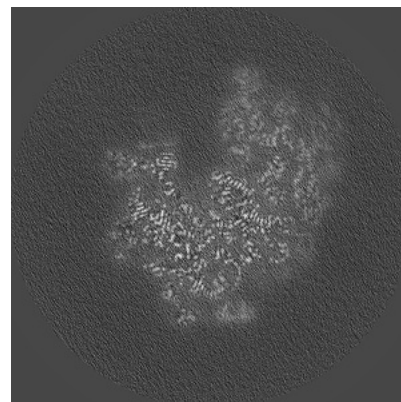
6.2.2 Raw map



X Index: 204



Y Index: 204

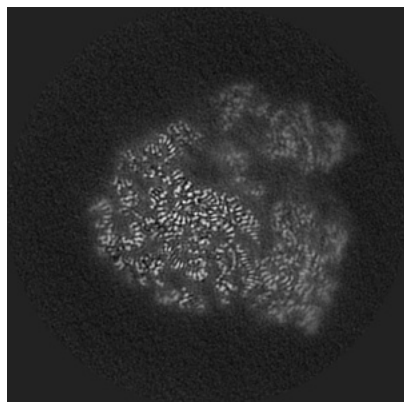


Z Index: 204

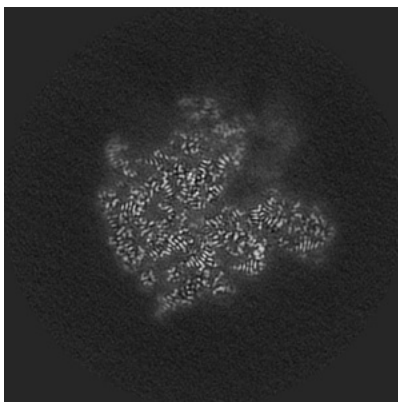
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

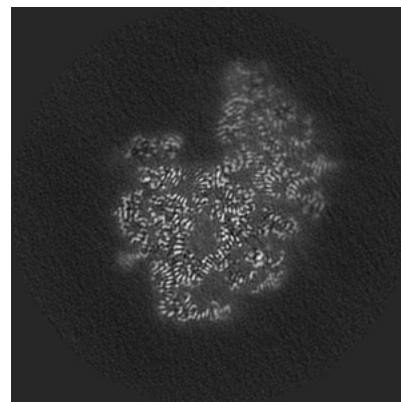
6.3.1 Primary map



X Index: 219

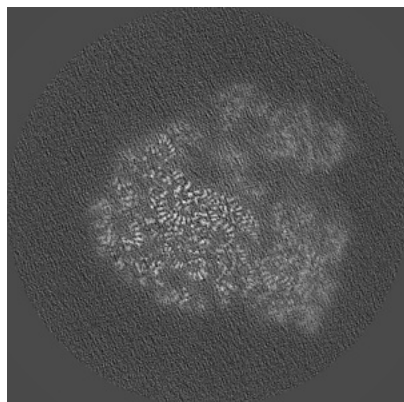


Y Index: 196

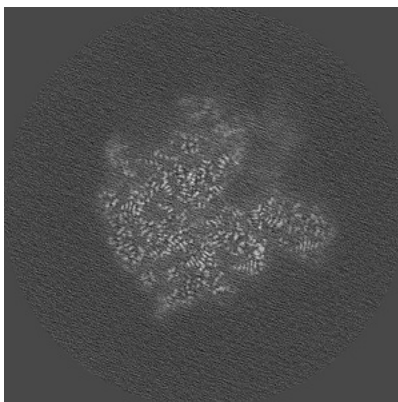


Z Index: 188

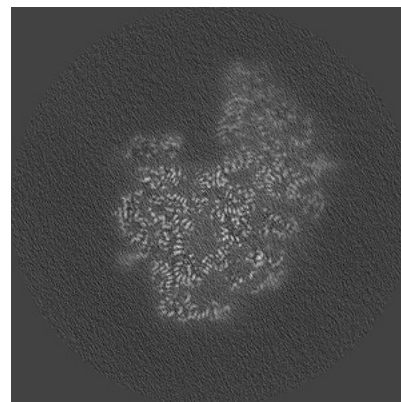
6.3.2 Raw map



X Index: 219



Y Index: 196

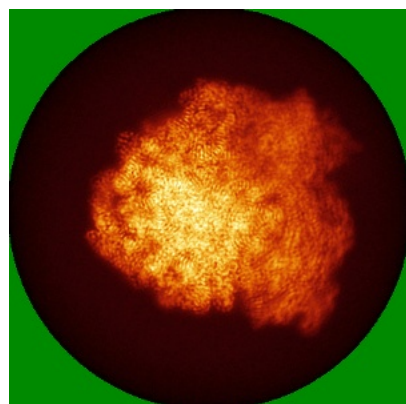


Z Index: 188

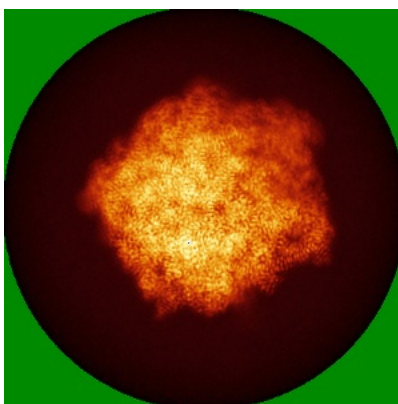
The images above show the largest variance slices of the map in three orthogonal directions.

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

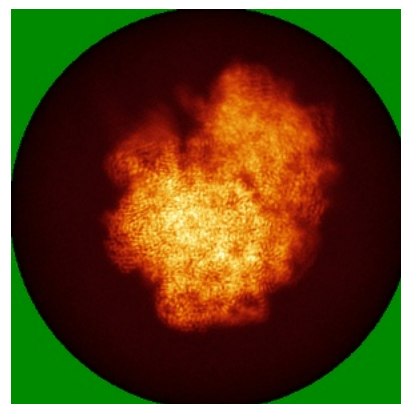
6.4.1 Primary map



X

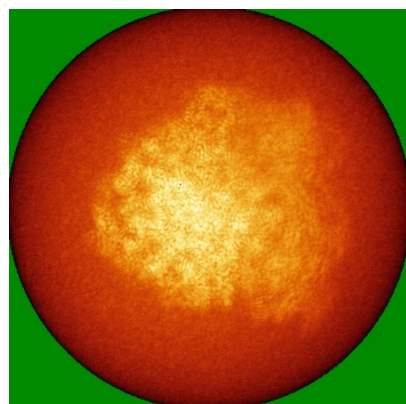


Y

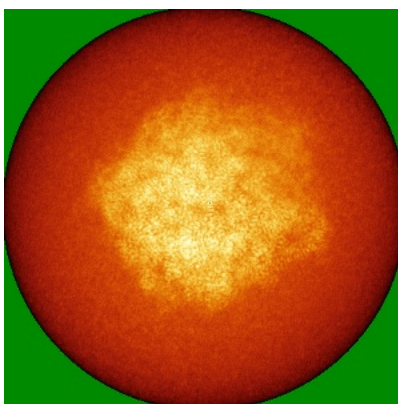


Z

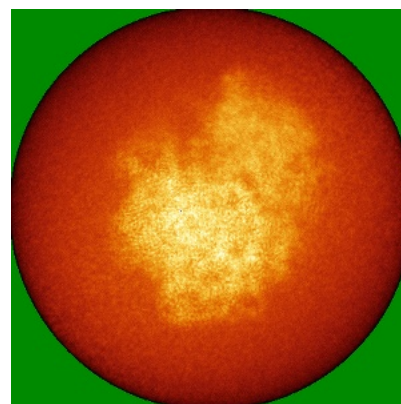
6.4.2 Raw map



X



Y

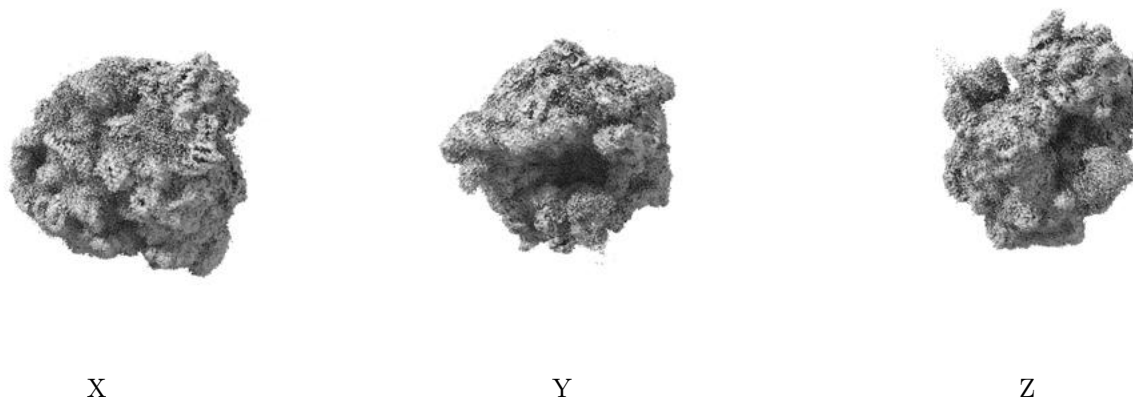


Z

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.

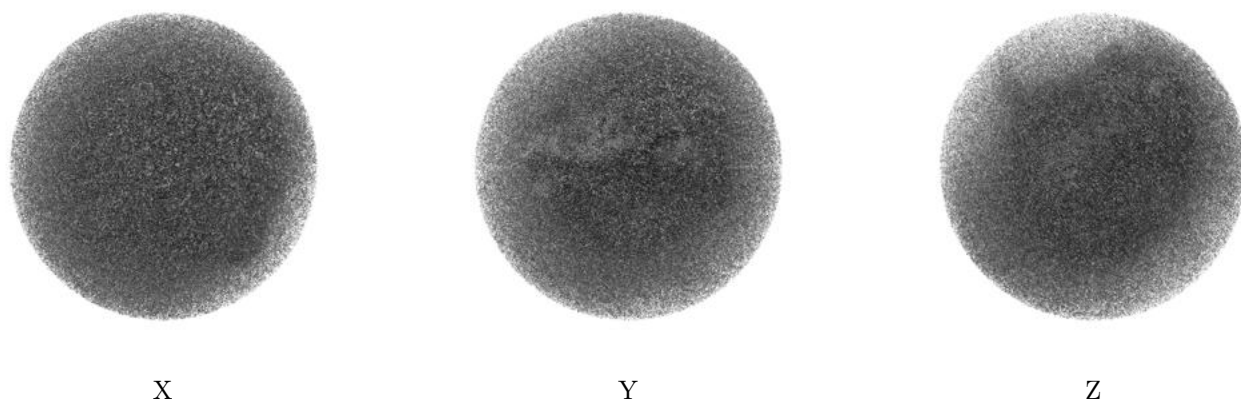
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

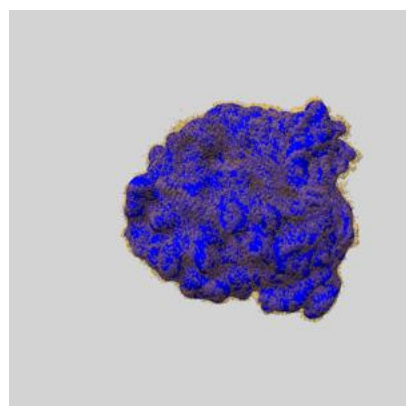
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

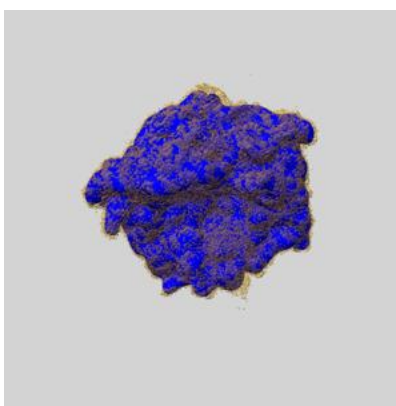
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

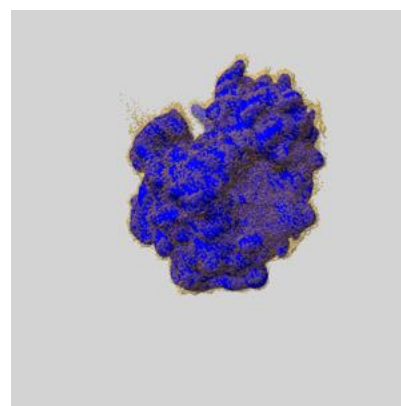
6.6.1 emd_12693_msk_1.map [i](#)



X



Y

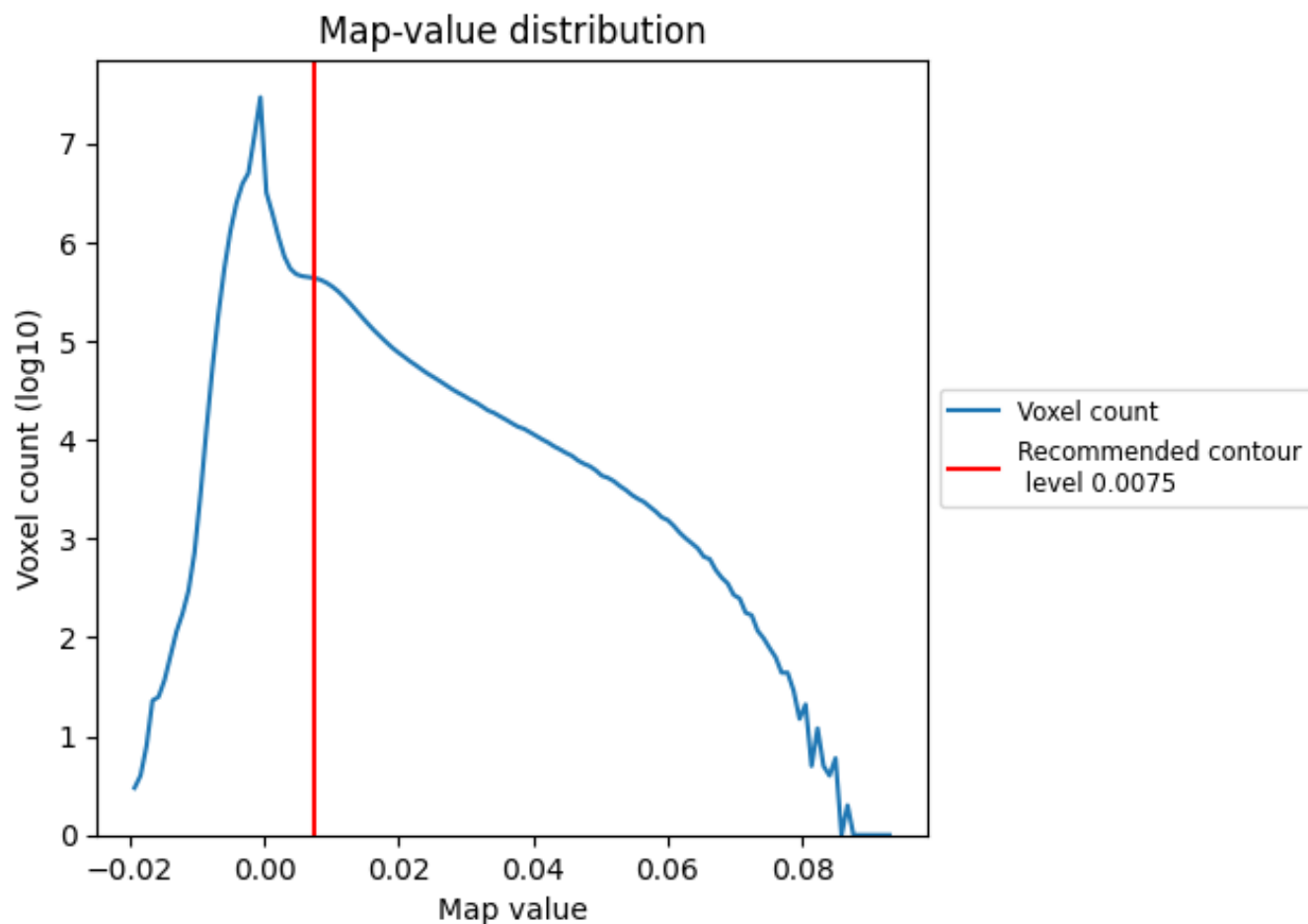


Z

7 Map analysis [i](#)

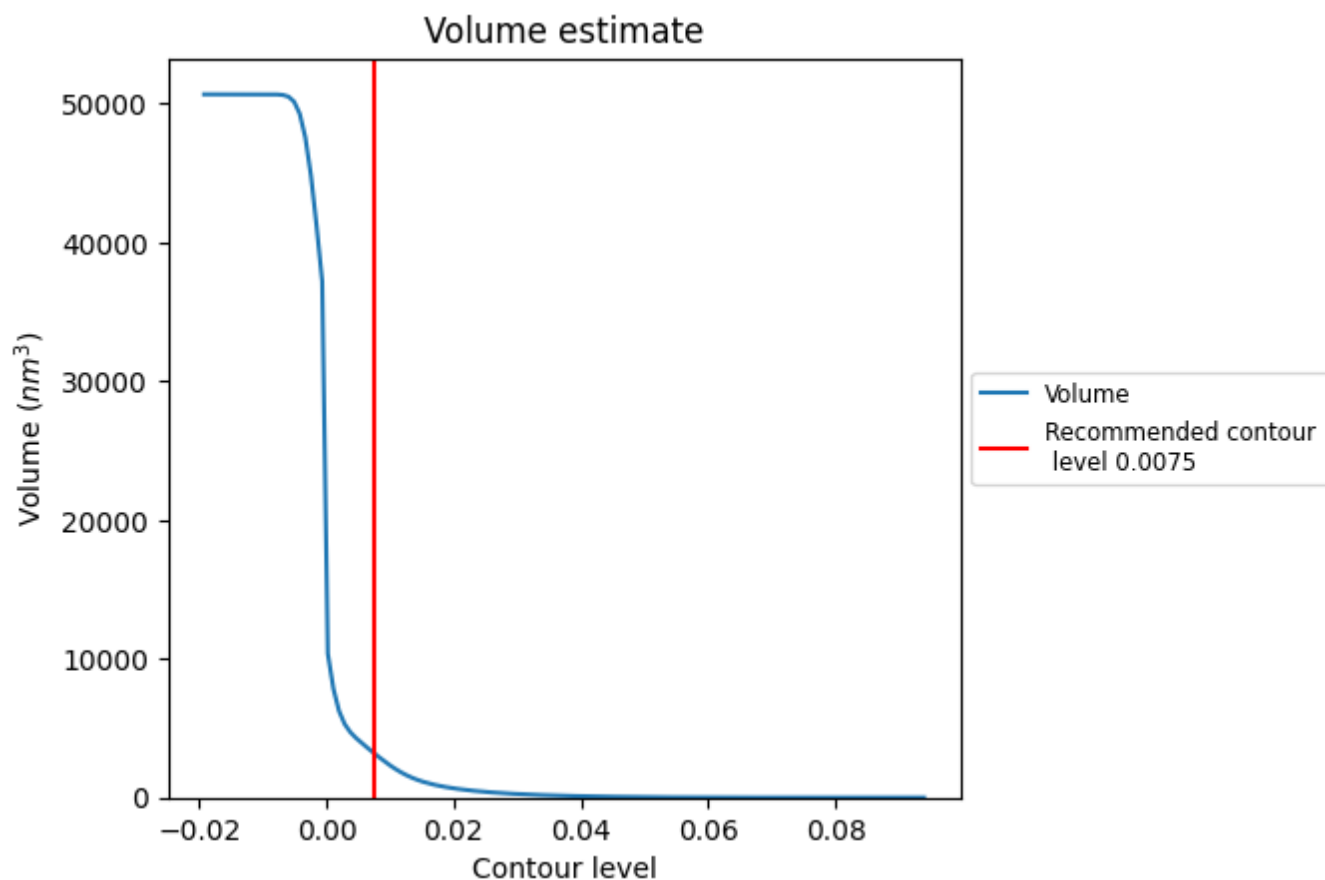
This section contains the results of statistical analysis of the map.

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.

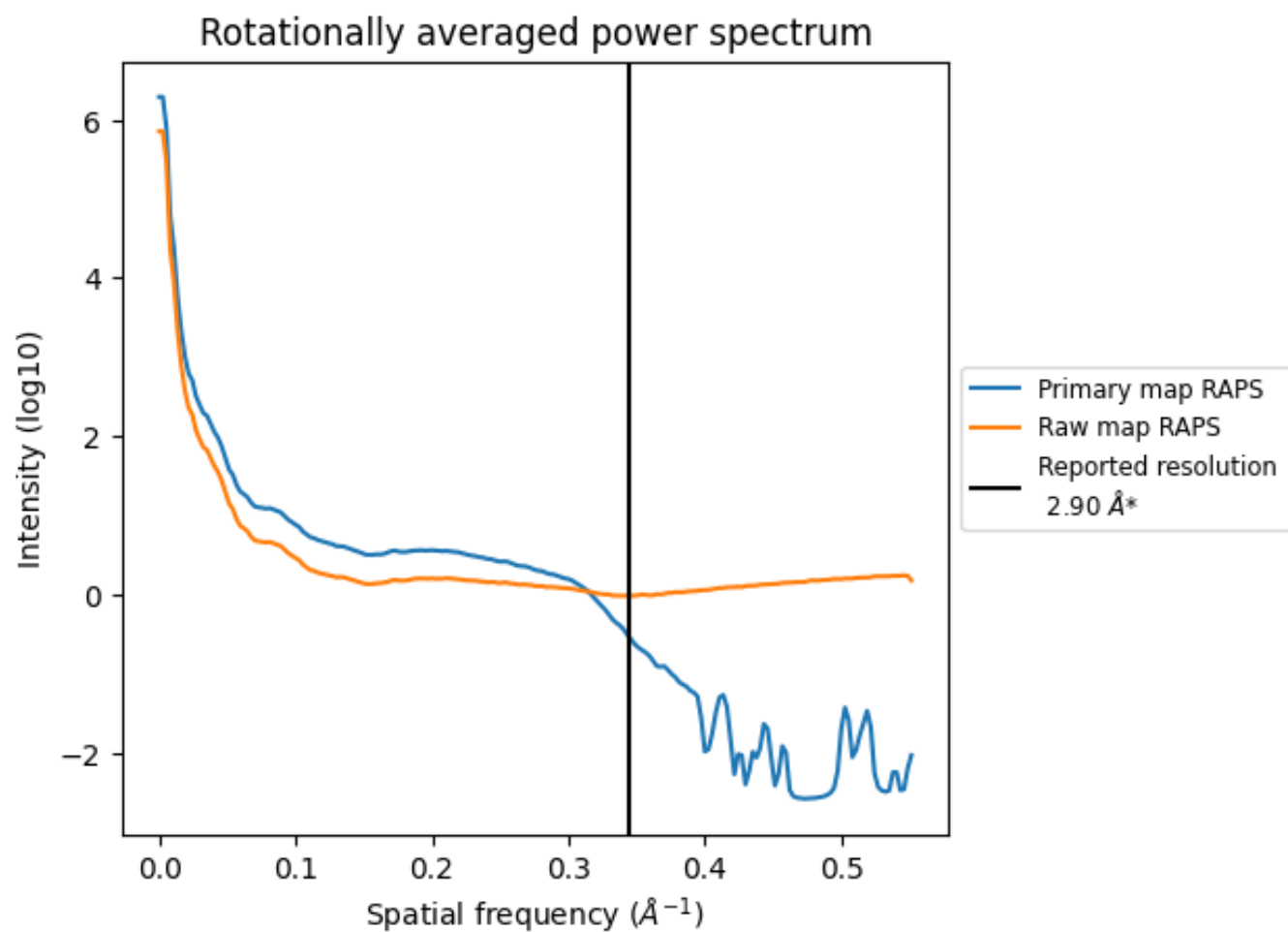
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3192 nm³; this corresponds to an approximate mass of 2883 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 ⓘ

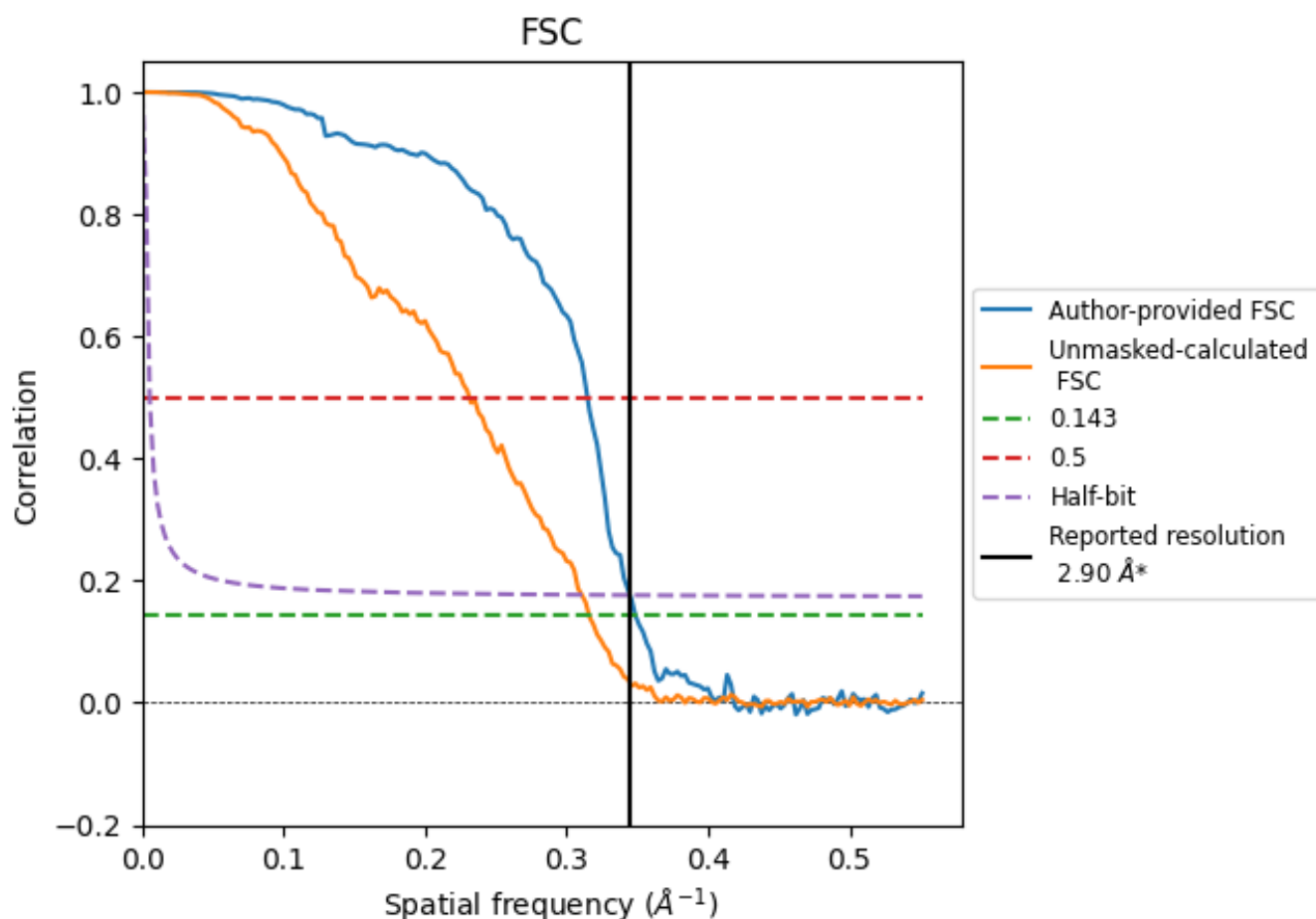


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

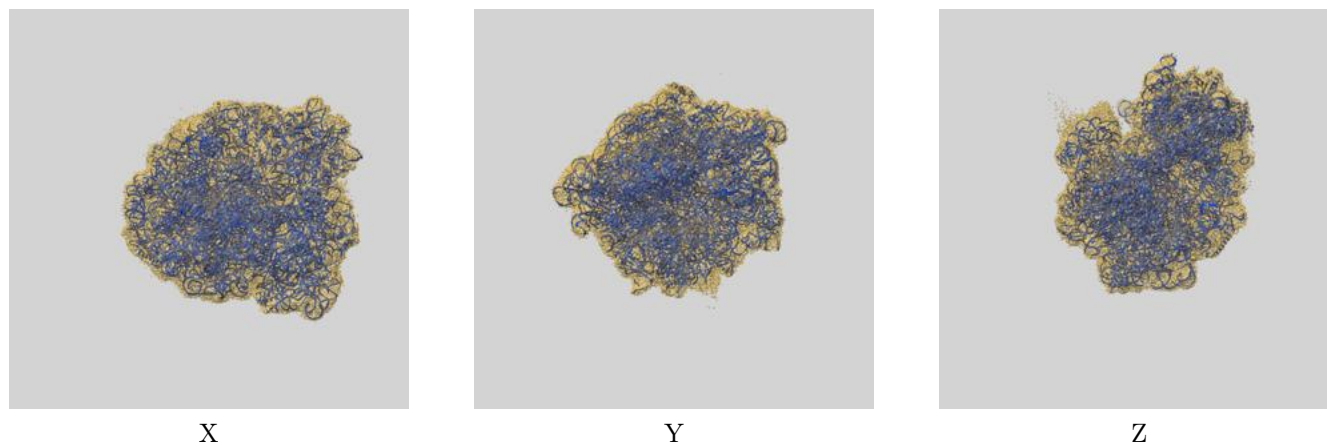
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.18	2.90
Unmasked-calculated*	3.17	4.33	3.22

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

9 Map-model fit [i](#)

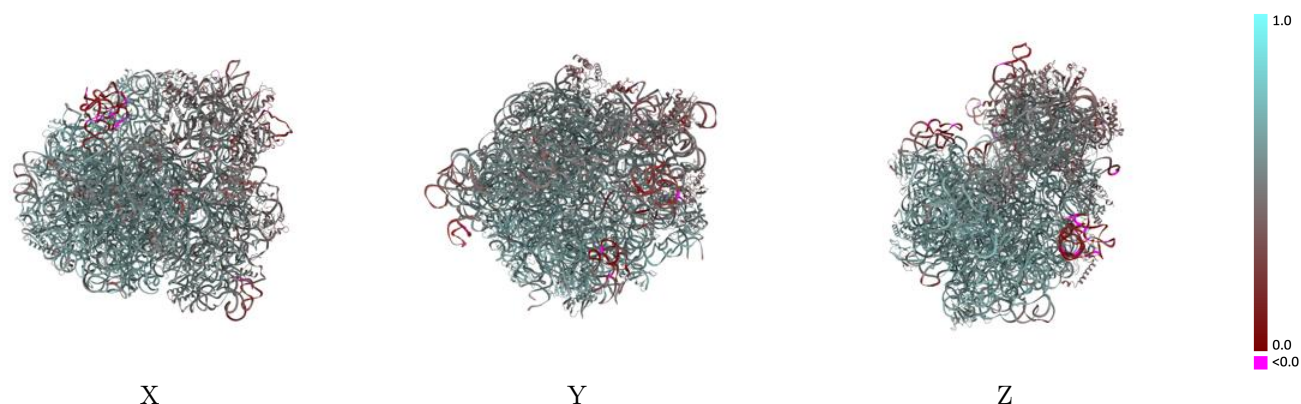
This section contains information regarding the fit between EMDB map EMD-12693 and PDB model 7O19. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



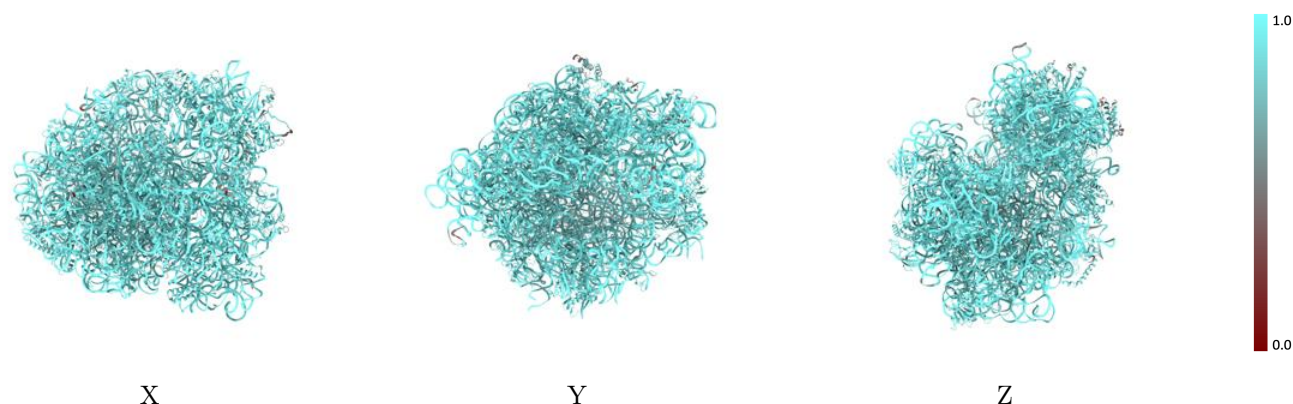
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



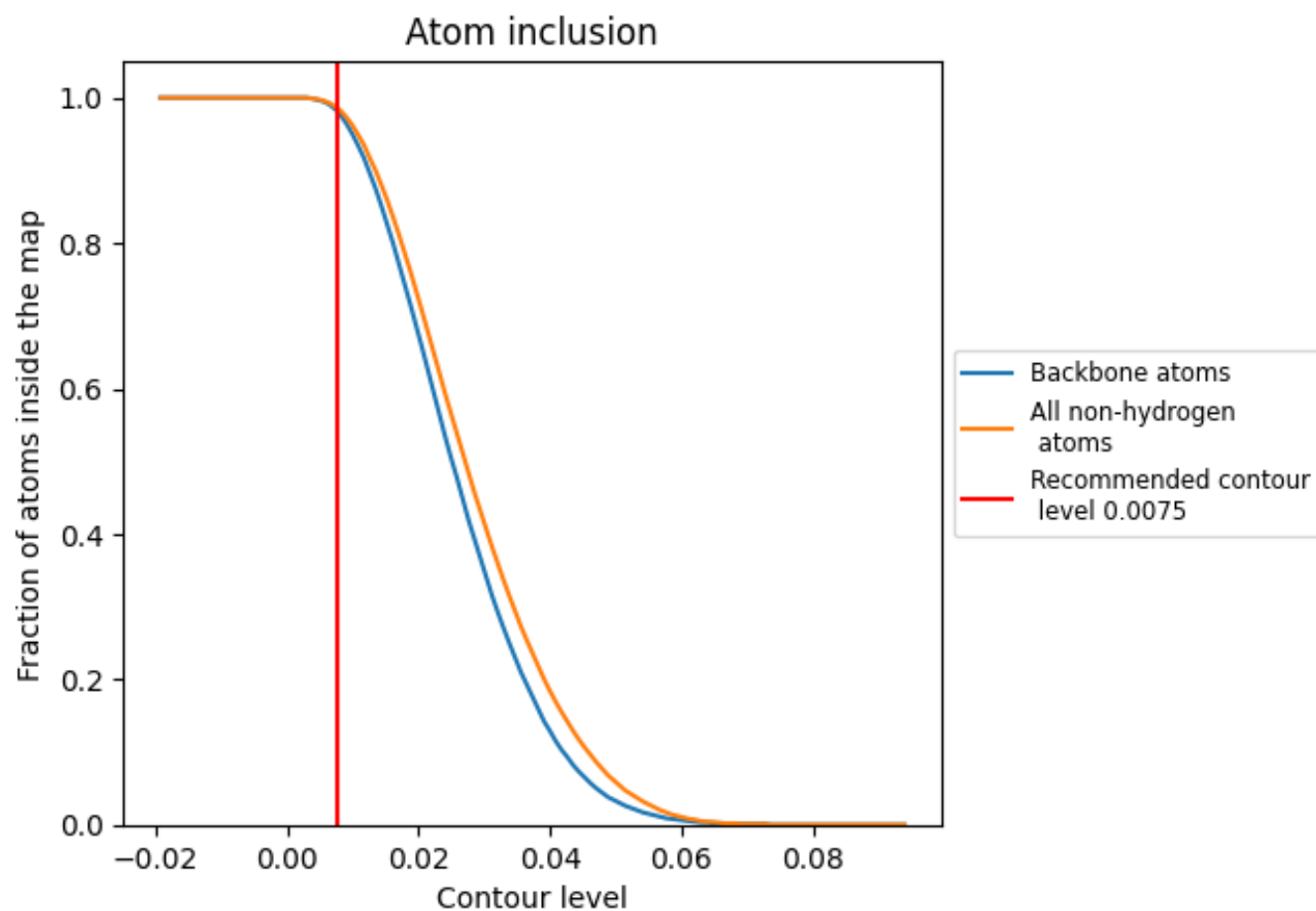
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 99% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9870	 0.5550
AA	 0.9920	 0.5160
AB	 0.8310	 0.4000
AC	 0.9560	 0.4400
AD	 0.9540	 0.4560
AE	 0.9950	 0.5140
AF	 0.9680	 0.4860
AG	 0.9600	 0.4210
AH	 0.9840	 0.5180
AI	 0.9600	 0.4200
AJ	 0.8910	 0.3800
AK	 0.9930	 0.5200
AL	 0.9970	 0.5400
AM	 0.9690	 0.4510
AN	 0.9810	 0.4340
AO	 0.9870	 0.5240
AP	 0.9940	 0.5160
AQ	 0.9980	 0.5170
AR	 1.0000	 0.5170
AS	 0.9610	 0.4170
AT	 0.9800	 0.5330
AU	 0.9120	 0.4360
B0	 0.9930	 0.6040
B1	 1.0000	 0.5900
B2	 1.0000	 0.6400
B3	 1.0000	 0.6290
B4	 1.0000	 0.6250
B5	 1.0000	 0.4990
B7	 1.0000	 0.4410
B8	 0.9990	 0.4470
BA	 0.9950	 0.5930
BB	 0.9980	 0.5930
BC	 1.0000	 0.6240
BD	 0.9930	 0.6170
BE	 0.9780	 0.5860



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Chain	Atom inclusion	Q-score
BF	 0.9910	 0.5010
BG	 0.9760	 0.5380
BH	 0.8620	 0.4080
BI	 0.8560	 0.3820
BJ	 0.9950	 0.6200
BK	 0.9990	 0.6120
BL	 0.9850	 0.6040
BM	 0.9930	 0.6100
BN	 1.0000	 0.6330
BO	 0.9840	 0.5800
BP	 0.9980	 0.6020
BQ	 0.9980	 0.6300
BR	 0.9600	 0.5950
BS	 0.9890	 0.6120
BT	 0.9900	 0.5810
BU	 0.9880	 0.5730
BV	 0.9730	 0.5840
BW	 0.9860	 0.6090
BX	 0.9980	 0.6040
BY	 0.9860	 0.5660
BZ	 0.9770	 0.5990