



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2023 – 10:34 am GMT

PDB ID : 8B5L
EMDB ID : EMD-15860
Title : Cryo-EM structure of ribosome-Sec61-TRAP (TRanslocon Associated Protein) translocon complex
Authors : Pauwels, E.; Shewakramani, N.R.; De Wijngaert, B.; Vermeire, K.; Das, K.
Deposited on : 2022-09-23
Resolution : 2.86 Å (reported)
Based on initial models : 3J7Q, 6MTE

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

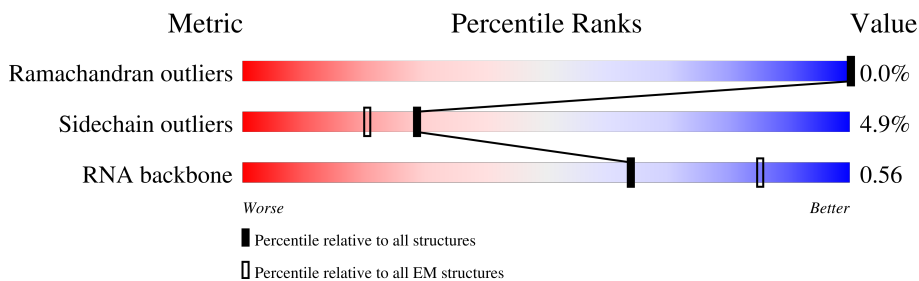
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

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 2.86 Å.

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




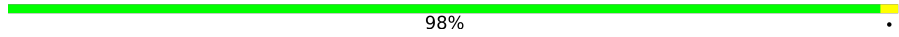
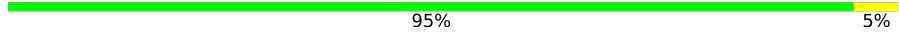

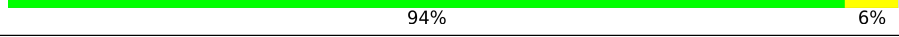



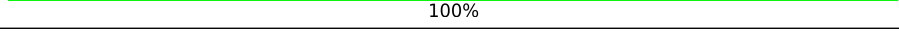
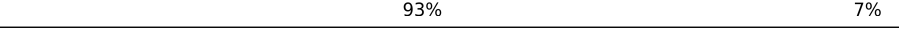
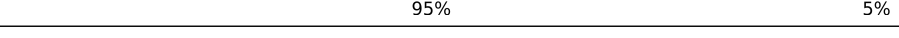
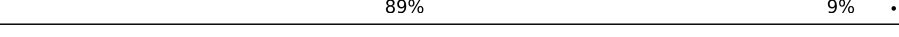
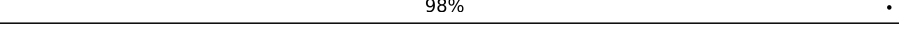
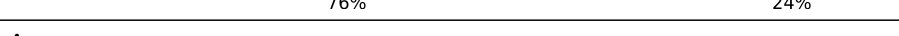
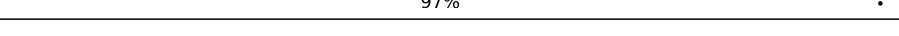
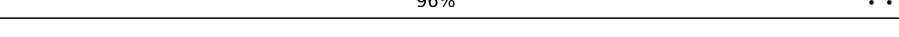
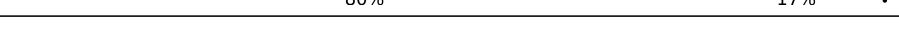
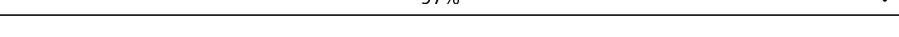
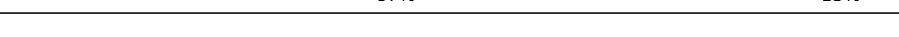






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	h	122	
2	P	153	
3	d	107	
4	5	4808	
5	G	319	
6	e	128	
7	t	185	
8	S	176	

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Mol	Chain	Length	Quality of chain
9	I	214	 91% 5%
10	D	293	 98%
11	V	131	 95% 5%
12	E	291	 72% 26%
13	J	170	 94% 6%
14	q	286	 24% 51% 47%
15	k	70	 90% 9%
16	b	245	 40% 58%
17	m	52	 100%
18	Z	135	 93% 7%
19	T	159	 95% 5%
20	i	105	 89% 9%
21	F	225	 98%
22	n	25	 76% 24%
23	L	211	 97%
24	O	203	 96%
25	8	156	 80% 17%
26	C	362	 97%
27	Y	134	 87% 13%
28	B	394	 97%
29	R	196	 85% 7% 8%
30	X	118	 95% 5%
31	p	91	 89% 11%
32	M	138	 98%
33	H	190	 96%

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Mol	Chain	Length	Quality of chain
34	7	120	90% 10%
35	r	124	94% 6%
36	Q	188	96% ..
37	f	109	96% .
38	a	147	98% ..
39	A	257	91% 5% .
40	g	114	92% 8%
41	K	173	42% 81% . 16%
42	u	68	97% ..
43	v	183	43% 83% . 14%
44	j	86	99% .
45	N	203	95% 5%
46	o	103	95% 5%
47	s	476	97% .
48	c	98	91% 9%
49	W	157	37% . 60%
50	l	50	88% 12%
51	U	99	88% 12%

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 145148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	h	122	1013	640	204	168	1	0	0

- Molecule 2 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	153	1242	777	241	215	9	0	0

- Molecule 3 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	107	888	560	171	155	2	0	0

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	5	3619	77665	34619	14204	25223	3619	0	0

- Molecule 5 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	233	1879	1199	361	315	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 6 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 7 is a protein called Signal sequence receptor subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	t	181	Total	C	N	O	S	0	0
			1459	951	241	264	3		

- Molecule 8 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 9 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 10 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 11 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 12 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	170	1362	861	254	241	6	0	0

- Molecule 14 is a protein called Translocon-associated protein subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	q	153	1222	795	196	228	3	0	0

- Molecule 15 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	k	69	569	366	103	99	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	24	LYS	ASN	conflict	UNP G1U001

- Molecule 16 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	b	104	848	527	189	129	3	0	0

- Molecule 17 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	m	52	430	267	90	67	6	0	0

- Molecule 18 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Z	135	1107	714	208	182	3	0	0

- Molecule 19 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 20 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 21 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

- Molecule 22 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 23 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	74	ARG	HIS	conflict	UNP G1TKB3
L	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 24 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 25 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	8	151	3208	1432	564	1062	150	0	0

- Molecule 26 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	C	362	2884	1813	577	480	14	0	0

- Molecule 27 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Y	134	1115	700	226	186	3	0	0

- Molecule 28 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	B	394	3172	2020	597	542	13	0	0

- Molecule 29 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	R	180	1508	933	328	238	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	HIS	conflict	UNP G1TYL6
R	151	ARG	HIS	conflict	UNP G1TYL6

- Molecule 30 is a protein called Ribosomal_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	X	118	967	618	181	167	1	0	0

- Molecule 31 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 32 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 33 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 34 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 35 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 36 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 37 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 38 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 39 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 40 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 41 is a protein called Translocon-associated protein subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	K	146	Total	C	N	O	S	0	0
			1159	739	195	223	2		

- Molecule 42 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	67	Total	C	N	O	S	0	0
			535	350	93	88	4		

- Molecule 43 is a protein called Translocon-associated protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	158	Total	C	N	O	S	0	0
			1229	792	207	228	2		

- Molecule 44 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 45 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 46 is a protein called 60S ribosomal protein L36a-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 47 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	464	Total	C	N	O	S	0	0
			3589	2355	578	632	24		

- Molecule 48 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 49 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 50 is a protein called 60S ribosomal protein L39-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 51 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
52	P	1	Total Mg 1 1	0
52	5	161	Total Mg 161 161	0
52	I	1	Total Mg 1 1	0
52	V	1	Total Mg 1 1	0
52	8	5	Total Mg 5 5	0
52	7	7	Total Mg 7 7	0
52	a	1	Total Mg 1 1	0
52	A	1	Total Mg 1 1	0

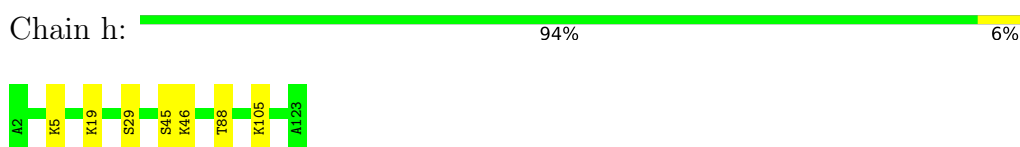
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
53	m	1	Total Zn 1 1	0
53	p	1	Total Zn 1 1	0
53	g	1	Total Zn 1 1	0
53	j	1	Total Zn 1 1	0
53	o	1	Total Zn 1 1	0

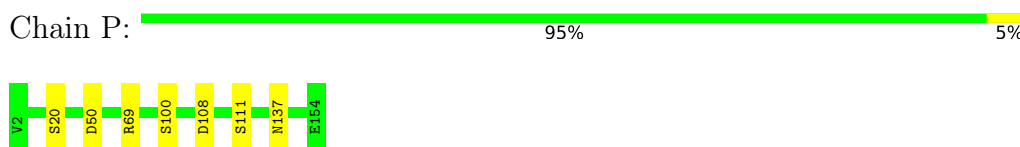
3 Residue-property plots [i](#)

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.

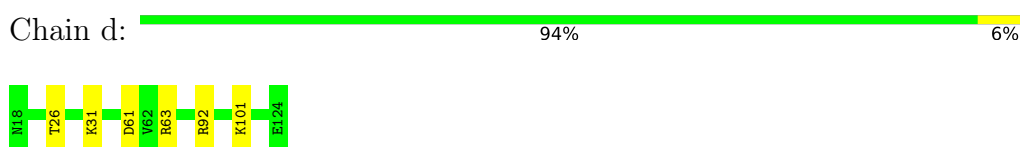
- Molecule 1: 60S ribosomal protein L35



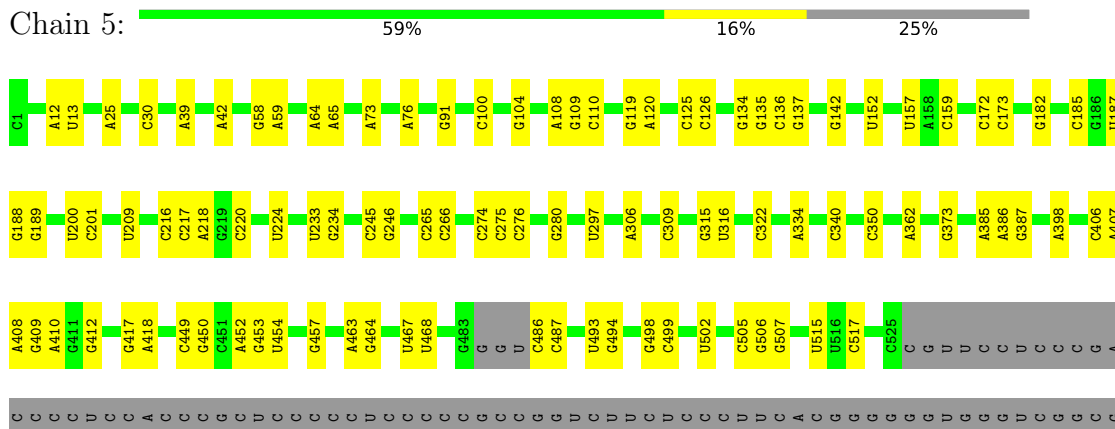
- Molecule 2: 60S ribosomal protein L17

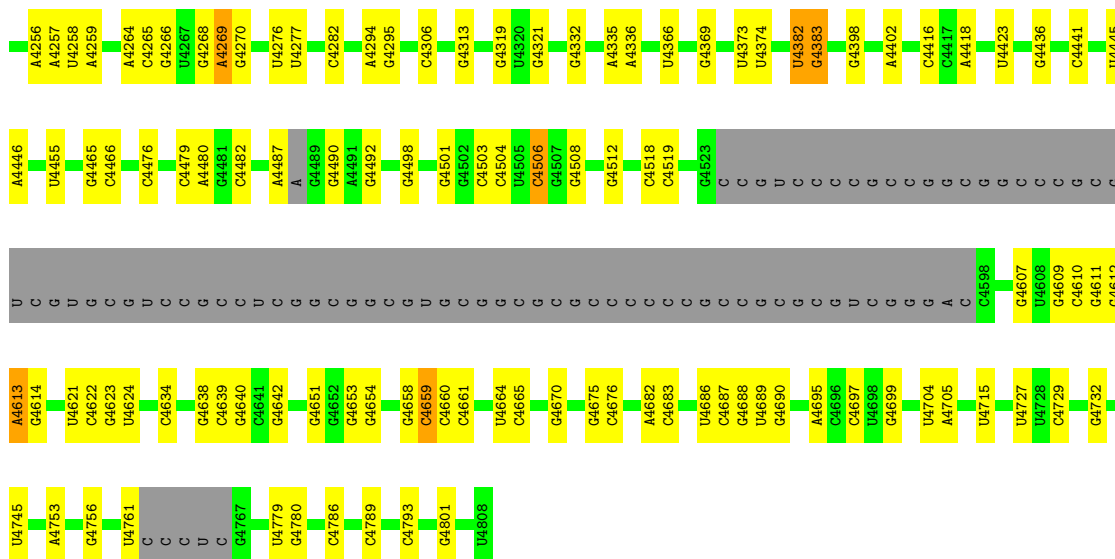


- Molecule 3: 60S ribosomal protein L31

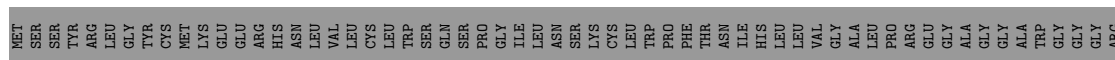


- Molecule 4: 28S rRNA





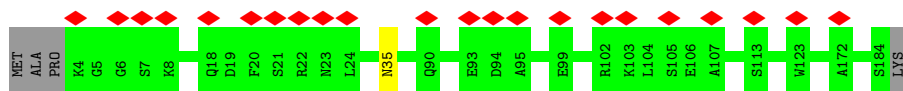
• Molecule 5: 60S ribosomal protein L7a



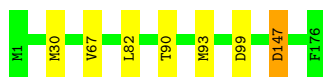
• Molecule 6: Ribosomal protein L32




• Molecule 7: Signal sequence receptor subunit 3

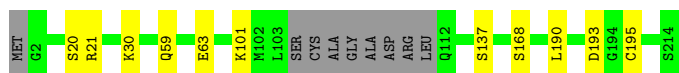


• Molecule 8: 60S ribosomal protein L18a



• Molecule 9: Ribosomal protein L10

Chain I:  91% 5%



- Molecule 10: Ribosomal_L18_c domain-containing protein

Chain D:  98%



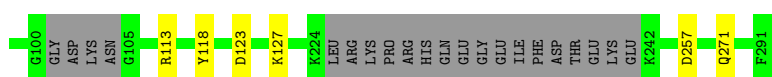
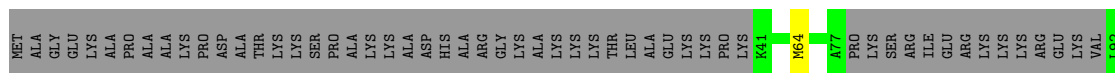
- Molecule 11: 60S ribosomal protein L23

Chain V:  95% 5%



- Molecule 12: 60S ribosomal protein L6

Chain E:  72% 26%



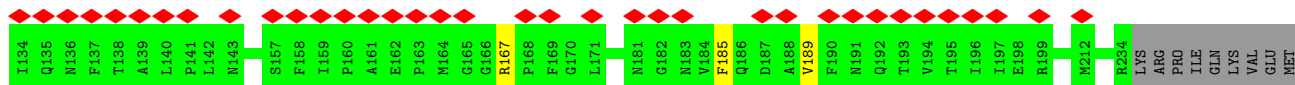
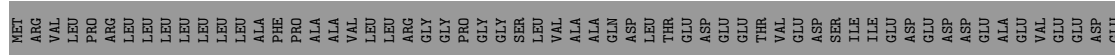
- Molecule 13: 60S ribosomal protein L11

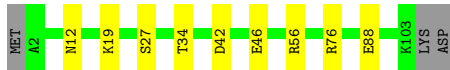
Chain J:  94% 6%



- Molecule 14: Translocon-associated protein subunit alpha

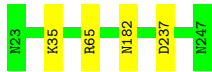
Chain q:  24% 51% 47%





- Molecule 21: 60S ribosomal protein L7

Chain F: 98%



- Molecule 22: 60S ribosomal protein L41

Chain n: 76%



- Molecule 23: 60S ribosomal protein L13

Chain L: 97%



- Molecule 24: 60S ribosomal protein L13a

Chain O: 96%



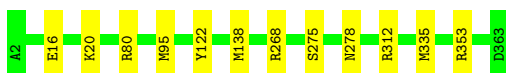
- Molecule 25: 5.8S rRNA

Chain 8: 80%



- Molecule 26: 60S ribosomal protein L4

Chain C: 97%



- Molecule 27: Ribosomal protein L26

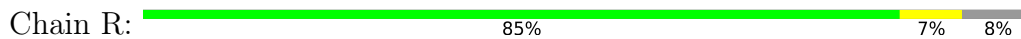
Chain Y: 87%



- Molecule 28: Ribosomal protein L3



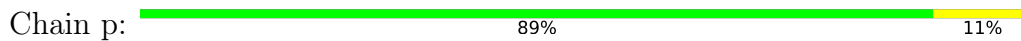
- Molecule 29: Ribosomal protein L19



- Molecule 30: Ribosomal_L23eN domain-containing protein



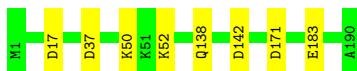
- Molecule 31: 60S ribosomal protein L37a



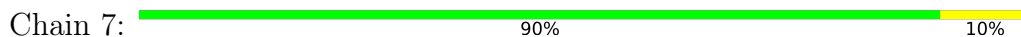
- Molecule 32: 60S ribosomal protein L14



- Molecule 33: 60S ribosomal protein L9



- Molecule 34: 5S rRNA





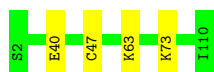
- Molecule 35: 60S ribosomal protein L28



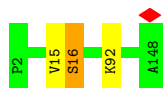
- Molecule 36: Ribosomal protein L18



- Molecule 37: 60S ribosomal protein L35a



- Molecule 38: 60S ribosomal protein L27a



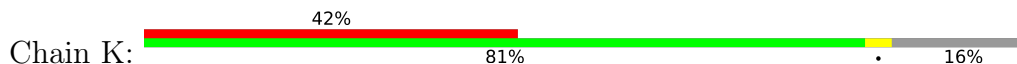
- Molecule 39: Ribosomal protein L8

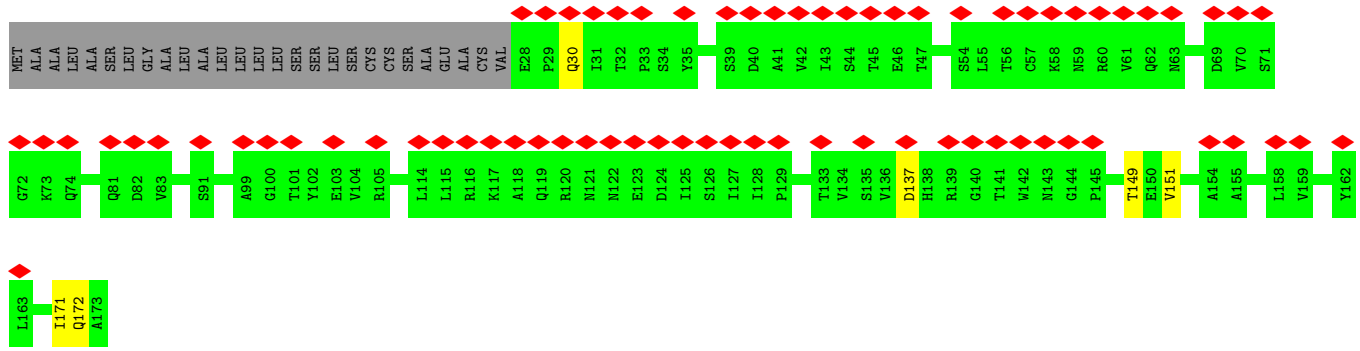


- Molecule 40: 60S ribosomal protein L34

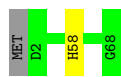


- Molecule 41: Translocon-associated protein subunit delta

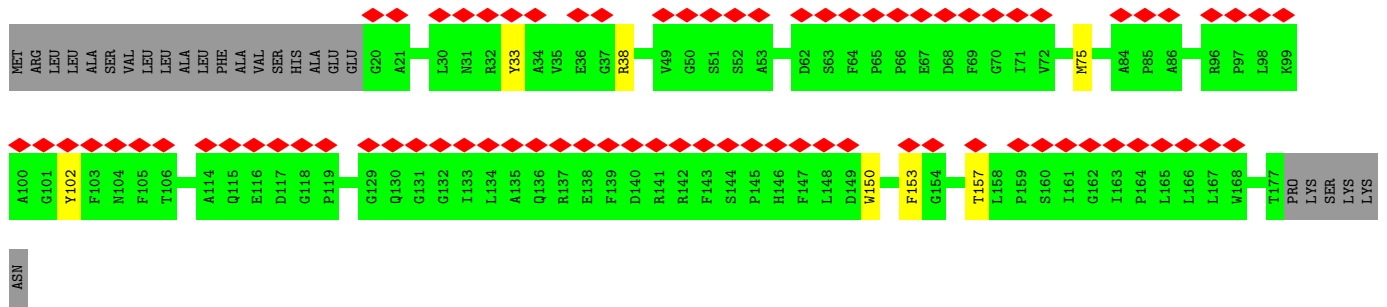
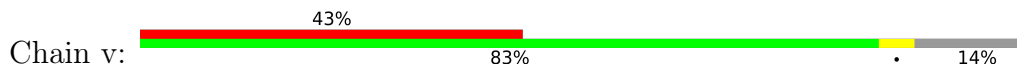




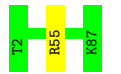
- Molecule 42: Protein transport protein Sec61 subunit gamma



- Molecule 43: Translocon-associated protein subunit beta



- Molecule 44: Ribosomal protein L37



- Molecule 45: Ribosomal protein L15

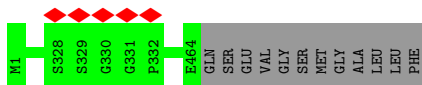


- Molecule 46: 60S ribosomal protein L36a-like

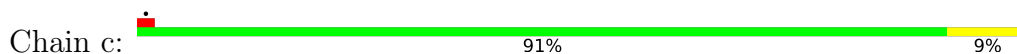




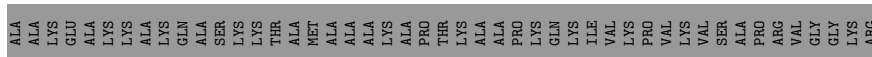
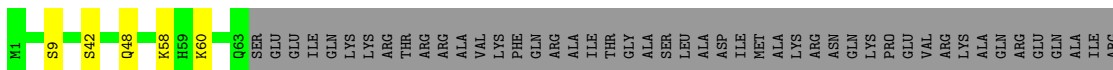
- Molecule 47: Protein transport protein Sec61 subunit alpha isoform 1



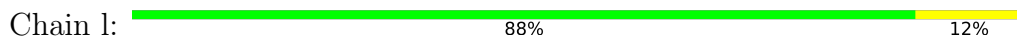
- Molecule 48: 60S ribosomal protein L30



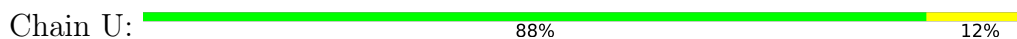
- Molecule 49: Ribosomal protein L24



- Molecule 50: 60S ribosomal protein L39-like



- Molecule 51: 60S ribosomal protein L22



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	119208	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.8	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.351	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.01527	Depositor
Map size (\AA)	432.96002, 432.96002, 432.96002	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.23, 1.23, 1.23	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, MLZ, OMC, E6G, 5MC, E7G, B8K, BGH, OMU, B8H, OMG, I4U, ZN, P4U, MG, A2M, PSU, 1MA, P7G, 7MG

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	h	0.28	0/1021	0.58	0/1348
2	P	0.33	0/1268	0.62	1/1700 (0.1%)
3	d	0.39	0/903	0.61	0/1216
4	5	0.41	2/85271 (0.0%)	0.78	11/132978 (0.0%)
5	G	0.33	0/1910	0.61	1/2569 (0.0%)
6	e	0.30	0/1071	0.57	0/1429
7	t	0.57	0/1489	0.65	0/2011
8	S	0.33	0/1501	0.61	2/2012 (0.1%)
9	I	0.36	0/1702	0.59	1/2272 (0.0%)
10	D	0.32	0/2437	0.56	0/3264
11	V	0.38	0/993	0.58	0/1332
12	E	0.30	0/1762	0.57	0/2362
13	J	0.33	0/1385	0.68	0/1852
14	q	0.38	0/1251	0.52	0/1699
15	k	0.35	0/575	0.70	0/761
16	b	0.31	0/861	0.68	1/1138 (0.1%)
17	m	0.33	0/425	0.64	0/561
18	Z	0.35	0/1130	0.61	2/1507 (0.1%)
19	T	0.34	0/1326	0.60	0/1770
20	i	0.29	0/841	0.62	0/1112
21	F	0.31	0/1911	0.54	0/2549
22	n	0.26	0/240	0.80	0/305
23	L	0.33	0/1733	0.62	0/2316
24	O	0.32	0/1662	0.57	0/2222
25	8	0.39	0/3581	0.74	0/5577
26	C	0.35	0/2927	0.58	0/3932
27	Y	0.32	0/1132	0.63	0/1504
28	B	0.30	0/3240	0.54	0/4339
29	R	0.29	0/1524	0.64	0/2013
30	X	0.31	0/984	0.68	1/1323 (0.1%)
31	p	0.34	0/718	0.57	0/953

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	M	0.33	0/1158	0.60	0/1547
33	H	0.31	0/1535	0.61	2/2063 (0.1%)
34	7	0.39	0/2858	0.75	0/4455
35	r	0.35	0/1010	0.60	0/1354
36	Q	0.31	0/1539	0.63	0/2054
37	f	0.32	0/895	0.61	0/1198
38	a	0.30	0/1191	0.77	3/1590 (0.2%)
39	A	0.37	0/1936	0.60	0/2596
40	g	0.31	0/916	0.63	0/1220
41	K	0.32	0/1188	0.51	0/1619
42	u	0.29	0/545	0.56	0/728
43	v	0.32	0/1261	0.52	0/1717
44	j	0.32	0/720	0.59	0/952
45	N	0.36	0/1746	0.62	0/2338
46	o	0.33	0/855	0.61	0/1128
47	s	0.30	0/3668	0.49	0/4974
48	c	0.31	0/771	0.61	1/1034 (0.1%)
49	W	0.32	0/541	0.58	0/720
50	l	0.27	0/459	0.59	0/608
51	U	0.37	0/823	0.82	1/1104 (0.1%)
All	All	0.38	2/154389 (0.0%)	0.72	27/226925 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	732	C	O3'-P	24.55	1.90	1.61
4	5	1390	G	O3'-P	23.25	1.89	1.61

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	a	16	SER	N-CA-CB	17.05	136.08	110.50
38	a	15	VAL	N-CA-C	-10.39	82.95	111.00
4	5	732	C	P-O3'-C3'	-9.70	108.06	119.70
4	5	732	C	C5'-C4'-O4'	-7.43	100.18	109.10
4	5	732	C	O3'-P-O5'	6.39	116.14	104.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
2	P	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
3	d	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
5	G	229/319 (72%)	219 (96%)	10 (4%)	0	100	100
6	e	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
7	t	179/185 (97%)	174 (97%)	5 (3%)	0	100	100
8	S	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
9	I	201/214 (94%)	193 (96%)	8 (4%)	0	100	100
10	D	291/293 (99%)	284 (98%)	7 (2%)	0	100	100
11	V	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
12	E	208/291 (72%)	198 (95%)	9 (4%)	1 (0%)	29	57
13	J	168/170 (99%)	159 (95%)	9 (5%)	0	100	100
14	q	151/286 (53%)	150 (99%)	1 (1%)	0	100	100
15	k	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
16	b	100/245 (41%)	97 (97%)	3 (3%)	0	100	100
17	m	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
18	Z	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
19	T	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
20	i	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
21	F	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
22	n	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	L	208/211 (99%)	201 (97%)	7 (3%)	0	100	100
24	O	197/203 (97%)	192 (98%)	5 (2%)	0	100	100
26	C	359/362 (99%)	343 (96%)	16 (4%)	0	100	100
27	Y	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
28	B	392/394 (100%)	382 (97%)	10 (3%)	0	100	100
29	R	178/196 (91%)	174 (98%)	4 (2%)	0	100	100
30	X	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
31	p	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
32	M	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
33	H	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
35	r	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
36	Q	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
37	f	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
38	a	145/147 (99%)	138 (95%)	6 (4%)	1 (1%)	22	50
39	A	246/257 (96%)	229 (93%)	17 (7%)	0	100	100
40	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
41	K	144/173 (83%)	143 (99%)	1 (1%)	0	100	100
42	u	65/68 (96%)	65 (100%)	0	0	100	100
43	v	156/183 (85%)	153 (98%)	3 (2%)	0	100	100
44	j	84/86 (98%)	84 (100%)	0	0	100	100
45	N	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
46	o	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
47	s	462/476 (97%)	454 (98%)	8 (2%)	0	100	100
48	c	96/98 (98%)	96 (100%)	0	0	100	100
49	W	61/157 (39%)	57 (93%)	4 (7%)	0	100	100
50	l	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
51	U	97/99 (98%)	88 (91%)	9 (9%)	0	100	100
All	All	7511/8263 (91%)	7267 (97%)	242 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	a	16	SER

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Mol	Chain	Res	Type
12	E	118	TYR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	h	109/109 (100%)	102 (94%)	7 (6%)	17 41
2	P	134/134 (100%)	128 (96%)	6 (4%)	27 57
3	d	98/98 (100%)	92 (94%)	6 (6%)	18 43
5	G	200/272 (74%)	189 (94%)	11 (6%)	21 49
6	e	114/114 (100%)	111 (97%)	3 (3%)	46 75
7	t	161/164 (98%)	160 (99%)	1 (1%)	86 95
8	S	157/157 (100%)	151 (96%)	6 (4%)	33 64
9	I	175/181 (97%)	165 (94%)	10 (6%)	20 47
10	D	247/247 (100%)	242 (98%)	5 (2%)	55 80
11	V	101/101 (100%)	94 (93%)	7 (7%)	15 38
12	E	190/251 (76%)	184 (97%)	6 (3%)	39 69
13	J	143/143 (100%)	133 (93%)	10 (7%)	15 37
14	q	133/249 (53%)	126 (95%)	7 (5%)	22 50
15	k	64/65 (98%)	58 (91%)	6 (9%)	8 23
16	b	84/184 (46%)	78 (93%)	6 (7%)	14 36
17	m	47/47 (100%)	47 (100%)	0	100 100
18	Z	117/117 (100%)	108 (92%)	9 (8%)	13 32
19	T	139/139 (100%)	131 (94%)	8 (6%)	20 46
20	i	86/89 (97%)	77 (90%)	9 (10%)	7 18
21	F	196/196 (100%)	192 (98%)	4 (2%)	55 80
22	n	24/24 (100%)	18 (75%)	6 (25%)	0 1
23	L	175/176 (99%)	170 (97%)	5 (3%)	42 72
24	O	171/173 (99%)	167 (98%)	4 (2%)	50 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	C	301/301 (100%)	289 (96%)	12 (4%)	31	62
27	Y	124/124 (100%)	106 (86%)	18 (14%)	3	8
28	B	342/342 (100%)	332 (97%)	10 (3%)	42	72
29	R	159/175 (91%)	146 (92%)	13 (8%)	11	29
30	X	106/106 (100%)	101 (95%)	5 (5%)	26	56
31	p	74/74 (100%)	64 (86%)	10 (14%)	4	9
32	M	117/117 (100%)	114 (97%)	3 (3%)	46	75
33	H	169/169 (100%)	163 (96%)	6 (4%)	35	66
35	r	108/108 (100%)	100 (93%)	8 (7%)	13	35
36	Q	164/165 (99%)	157 (96%)	7 (4%)	29	59
37	f	88/88 (100%)	84 (96%)	4 (4%)	27	57
38	a	119/119 (100%)	118 (99%)	1 (1%)	81	93
39	A	190/199 (96%)	177 (93%)	13 (7%)	16	38
40	g	98/98 (100%)	89 (91%)	9 (9%)	9	24
41	K	127/146 (87%)	121 (95%)	6 (5%)	26	56
42	u	58/59 (98%)	57 (98%)	1 (2%)	60	83
43	v	131/152 (86%)	124 (95%)	7 (5%)	22	50
44	j	73/73 (100%)	72 (99%)	1 (1%)	67	86
45	N	171/171 (100%)	161 (94%)	10 (6%)	20	46
46	o	91/91 (100%)	86 (94%)	5 (6%)	21	49
47	s	389/398 (98%)	389 (100%)	0	100	100
48	c	84/84 (100%)	76 (90%)	8 (10%)	8	23
49	W	55/126 (44%)	50 (91%)	5 (9%)	9	25
50	l	47/47 (100%)	41 (87%)	6 (13%)	4	11
51	U	89/89 (100%)	78 (88%)	11 (12%)	4	12
All	All	6539/7051 (93%)	6218 (95%)	321 (5%)	29	54

5 of 321 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	Q	108	ARG
46	o	27	LYS
38	a	92	LYS

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Mol	Chain	Res	Type
40	g	114	GLN
49	W	42	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
43	v	115	GLN
50	l	20	ASN
47	s	259	GLN
35	r	83	ASN
41	K	30	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	8	149/156 (95%)	26 (17%)	1 (0%)
34	7	119/120 (99%)	12 (10%)	0
4	5	3590/4808 (74%)	696 (19%)	56 (1%)
All	All	3858/5084 (75%)	734 (19%)	57 (1%)

5 of 734 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	5	12	A
4	5	13	U
4	5	25	A
4	5	30	C
4	5	39	A

5 of 57 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	5	1985	G
4	5	4786	C
4	5	2597	G
4	5	4686	U
4	5	4465	G

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

66 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$
4	OMC	5	3619	4	19,22,23	2.26	5 (26%)	26,31,34	0.95	3 (11%)
4	E7G	5	1736	4	24,27,28	5.35	7 (29%)	30,40,43	2.21	10 (33%)
4	P7G	5	1848	4	24,28,29	6.31	6 (25%)	27,41,44	1.35	3 (11%)
4	5MC	5	3514	4	18,22,23	1.99	4 (22%)	26,32,35	1.37	3 (11%)
4	PSU	5	4188	4	18,21,22	2.01	6 (33%)	22,30,33	1.95	5 (22%)
4	A2M	5	398	4	18,25,26	4.08	5 (27%)	18,36,39	1.22	1 (5%)
4	OMG	5	2616	4	18,26,27	2.83	4 (22%)	19,38,41	1.25	3 (15%)
4	OMG	5	2267	4	18,26,27	1.06	1 (5%)	19,38,41	1.14	2 (10%)
4	A2M	5	1489	52,4	18,25,26	4.07	5 (27%)	18,36,39	1.22	1 (5%)
4	A2M	5	1810	52,4	18,25,26	0.98	0	18,36,39	1.25	2 (11%)
4	P7G	5	3612	4	24,28,29	6.43	6 (25%)	27,41,44	1.38	3 (11%)
4	OMG	5	1477	4	18,26,27	2.84	5 (27%)	19,38,41	1.25	3 (15%)
4	1MA	5	1266	4	16,25,26	2.25	4 (25%)	18,37,40	1.50	3 (16%)
4	OMG	5	3524	4	18,26,27	2.84	4 (22%)	19,38,41	1.23	3 (15%)
4	7MG	5	2365	4	22,26,27	1.45	4 (18%)	29,39,42	2.67	8 (27%)
4	OMC	5	4282	4	19,22,23	0.96	1 (5%)	26,31,34	1.04	1 (3%)
4	PSU	5	2351	4	18,21,22	1.98	5 (27%)	22,30,33	1.82	4 (18%)
4	PSU	5	4039	4	18,21,22	1.98	5 (27%)	22,30,33	1.91	4 (18%)
4	PSU	5	4374	4	18,21,22	2.00	6 (33%)	22,30,33	1.93	4 (18%)
4	A2M	5	1479	4	18,25,26	4.05	5 (27%)	18,36,39	1.34	2 (11%)
4	BGH	5	3631	4	25,29,30	6.33	13 (52%)	31,43,46	2.34	9 (29%)
4	PSU	5	4149	4	18,21,22	1.59	5 (27%)	22,30,33	2.11	5 (22%)
4	OMU	5	4366	4	19,22,23	3.09	7 (36%)	26,31,34	1.84	6 (23%)
4	OMG	5	4383	4	18,26,27	2.84	5 (27%)	19,38,41	1.27	3 (15%)
17	MLZ	m	72	17	8,9,10	0.48	0	4,9,11	0.52	0
4	B8H	5	4042	4	19,22,23	2.01	7 (36%)	22,32,35	2.05	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMC	5	2265	52,4	19,22,23	2.24	5 (26%)	26,31,34	0.94	2 (7%)
4	OMG	5	1260	4	18,26,27	2.82	4 (22%)	19,38,41	1.21	3 (15%)
4	P4U	5	1292	4	21,24,25	2.43	7 (33%)	27,33,36	1.14	2 (7%)
4	7MG	5	1560	4	22,26,27	5.21	6 (27%)	29,39,42	2.10	8 (27%)
4	A2M	5	3455	4	18,25,26	4.07	5 (27%)	18,36,39	1.23	1 (5%)
4	OMG	5	4116	4	18,26,27	1.06	1 (5%)	19,38,41	1.23	3 (15%)
4	PSU	5	1632	4	18,21,22	1.95	5 (27%)	22,30,33	1.97	4 (18%)
4	PSU	5	1537	4	18,21,22	2.02	6 (33%)	22,30,33	1.85	4 (18%)
4	B8H	5	3494	4	19,22,23	1.99	7 (36%)	22,32,35	1.92	3 (13%)
4	A2M	5	3557	4	18,25,26	4.04	5 (27%)	18,36,39	1.21	1 (5%)
4	OMG	5	1580	52,4	18,26,27	1.16	1 (5%)	19,38,41	1.15	2 (10%)
4	OMG	5	4240	4	18,26,27	2.83	4 (22%)	19,38,41	1.23	3 (15%)
4	PSU	5	4246	4	18,21,22	1.98	5 (27%)	22,30,33	1.94	5 (22%)
4	OMG	5	4369	4	18,26,27	2.83	4 (22%)	19,38,41	1.24	3 (15%)
4	PSU	5	4196	52,4	18,21,22	1.95	5 (27%)	22,30,33	1.91	4 (18%)
4	I4U	5	1614	4	21,24,25	2.55	7 (33%)	27,34,37	1.07	1 (3%)
4	OMC	5	2704	4	19,22,23	2.24	5 (26%)	26,31,34	0.95	2 (7%)
4	PSU	5	3461	4	18,21,22	2.00	5 (27%)	22,30,33	1.81	4 (18%)
26	MLZ	C	333	26	8,9,10	0.47	0	4,9,11	0.64	0
4	B8K	5	4436	4	24,28,29	5.80	7 (29%)	30,42,45	2.30	7 (23%)
4	OMU	5	4052	4	19,22,23	3.10	7 (36%)	26,31,34	1.80	6 (23%)
4	A2M	5	1270	4	18,25,26	0.97	1 (5%)	18,36,39	1.23	2 (11%)
4	B8H	5	1799	4	19,22,23	2.01	7 (36%)	22,32,35	2.05	3 (13%)
4	PSU	5	3496	4	18,21,22	1.98	6 (33%)	22,30,33	1.78	5 (22%)
4	E6G	5	4101	4	20,27,28	1.98	3 (15%)	22,39,42	2.09	5 (22%)
4	1MA	5	4161	4	16,25,26	2.26	3 (18%)	18,37,40	1.42	3 (16%)
4	PSU	5	1638	4	18,21,22	2.00	6 (33%)	22,30,33	1.89	4 (18%)
4	PSU	5	3447	4	18,21,22	1.95	5 (27%)	22,30,33	1.83	4 (18%)
4	OMC	5	2647	4	19,22,23	2.26	5 (26%)	26,31,34	0.93	2 (7%)
4	OMC	5	3601	4	19,22,23	2.25	5 (26%)	26,31,34	0.94	2 (7%)
4	5MC	5	4193	4	18,22,23	1.01	2 (11%)	26,32,35	1.37	3 (11%)
4	OMC	5	2208	4	19,22,23	2.26	5 (26%)	26,31,34	0.94	2 (7%)
4	A2M	5	3450	4	18,25,26	4.08	5 (27%)	18,36,39	1.22	1 (5%)
4	OMC	5	3433	4	19,22,23	2.24	5 (26%)	26,31,34	0.95	2 (7%)
4	A2M	5	4269	52,4	18,25,26	4.05	6 (33%)	18,36,39	1.21	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	B8K	5	3629	4	24,28,29	5.87	7 (29%)	30,42,45	2.26	7 (23%)
4	PSU	5	4382	4	18,21,22	1.97	5 (27%)	22,30,33	1.95	5 (22%)
4	UR3	5	4276	4	19,22,23	1.01	1 (5%)	26,32,35	1.52	2 (7%)
4	PSU	5	4277	4	18,21,22	1.92	4 (22%)	22,30,33	1.87	4 (18%)
4	OMG	5	2207	4	18,26,27	2.83	4 (22%)	19,38,41	1.20	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMC	5	3619	4	-	1/9/27/28	0/2/2/2
4	E7G	5	1736	4	-	3/9/39/40	0/3/3/3
4	P7G	5	1848	4	-	0/10/40/41	0/3/3/3
4	5MC	5	3514	4	-	0/7/25/26	0/2/2/2
4	PSU	5	4188	4	-	0/7/25/26	0/2/2/2
4	A2M	5	398	4	-	1/5/27/28	0/3/3/3
4	OMG	5	2616	4	-	1/5/27/28	0/3/3/3
4	OMG	5	2267	4	-	2/5/27/28	0/3/3/3
4	A2M	5	1489	52,4	-	3/5/27/28	0/3/3/3
4	A2M	5	1810	52,4	-	0/5/27/28	0/3/3/3
4	P7G	5	3612	4	-	3/10/40/41	0/3/3/3
4	OMG	5	1477	4	-	0/5/27/28	0/3/3/3
4	1MA	5	1266	4	-	0/3/25/26	0/3/3/3
4	OMG	5	3524	4	-	2/5/27/28	0/3/3/3
4	7MG	5	2365	4	-	0/7/37/38	0/3/3/3
4	OMC	5	4282	4	-	2/9/27/28	0/2/2/2
4	PSU	5	2351	4	-	0/7/25/26	0/2/2/2
4	PSU	5	4039	4	-	2/7/25/26	0/2/2/2
4	PSU	5	4374	4	-	0/7/25/26	0/2/2/2
4	A2M	5	1479	4	-	2/5/27/28	0/3/3/3
4	BGH	5	3631	4	-	2/13/43/44	0/3/3/3
4	PSU	5	4149	4	-	2/7/25/26	0/2/2/2
4	OMU	5	4366	4	-	1/9/27/28	0/2/2/2
4	OMG	5	4383	4	-	3/5/27/28	0/3/3/3
17	MLZ	m	72	17	-	1/7/8/10	-
4	B8H	5	4042	4	-	2/7/25/26	0/2/2/2
4	OMC	5	2265	52,4	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	5	1260	4	-	1/5/27/28	0/3/3/3
4	P4U	5	1292	4	-	4/10/29/30	0/2/2/2
4	7MG	5	1560	4	-	0/7/37/38	0/3/3/3
4	A2M	5	3455	4	-	0/5/27/28	0/3/3/3
4	OMG	5	4116	4	-	1/5/27/28	0/3/3/3
4	PSU	5	1632	4	-	2/7/25/26	0/2/2/2
4	PSU	5	1537	4	-	2/7/25/26	0/2/2/2
4	B8H	5	3494	4	-	2/7/25/26	0/2/2/2
4	A2M	5	3557	4	-	1/5/27/28	0/3/3/3
4	OMG	5	1580	52,4	-	0/5/27/28	0/3/3/3
4	OMG	5	4240	4	-	3/5/27/28	0/3/3/3
4	PSU	5	4246	4	-	5/7/25/26	0/2/2/2
4	OMG	5	4369	4	-	1/5/27/28	0/3/3/3
4	PSU	5	4196	52,4	-	5/7/25/26	0/2/2/2
4	I4U	5	1614	4	-	1/9/29/30	0/2/2/2
4	OMC	5	2704	4	-	1/9/27/28	0/2/2/2
4	PSU	5	3461	4	-	2/7/25/26	0/2/2/2
26	MLZ	C	333	26	-	0/7/8/10	-
4	B8K	5	4436	4	-	0/11/41/42	0/3/3/3
4	OMU	5	4052	4	-	3/9/27/28	0/2/2/2
4	A2M	5	1270	4	-	3/5/27/28	0/3/3/3
4	B8H	5	1799	4	-	0/7/25/26	0/2/2/2
4	PSU	5	3496	4	-	3/7/25/26	0/2/2/2
4	E6G	5	4101	4	-	3/6/28/29	0/3/3/3
4	1MA	5	4161	4	-	1/3/25/26	0/3/3/3
4	PSU	5	1638	4	-	0/7/25/26	0/2/2/2
4	PSU	5	3447	4	-	0/7/25/26	0/2/2/2
4	OMC	5	2647	4	-	1/9/27/28	0/2/2/2
4	OMC	5	3601	4	-	0/9/27/28	0/2/2/2
4	5MC	5	4193	4	-	4/7/25/26	0/2/2/2
4	OMC	5	2208	4	-	0/9/27/28	0/2/2/2
4	A2M	5	3450	4	-	0/5/27/28	0/3/3/3
4	OMC	5	3433	4	-	4/9/27/28	0/2/2/2
4	A2M	5	4269	52,4	-	3/5/27/28	0/3/3/3
4	B8K	5	3629	4	-	3/11/41/42	0/3/3/3
4	PSU	5	4382	4	-	3/7/25/26	0/2/2/2
4	UR3	5	4276	4	-	0/7/25/26	0/2/2/2
4	PSU	5	4277	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	5	2207	4	-	3/5/27/28	0/3/3/3

The worst 5 of 311 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	3629	B8K	C8-N9	-26.25	1.31	1.46
4	5	3631	BGH	C8-N9	-26.13	1.31	1.46
4	5	4436	B8K	C8-N9	-25.90	1.31	1.46
4	5	3612	P7G	C8-N9	-25.18	1.31	1.46
4	5	1848	P7G	C8-N9	-24.68	1.32	1.46

The worst 5 of 222 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	2365	7MG	N9-C4-N3	9.33	139.42	125.47
4	5	4149	PSU	N1-C2-N3	6.52	122.52	115.13
4	5	1799	B8H	N3-C2-N1	6.08	121.71	115.14
4	5	4042	B8H	N3-C2-N1	6.02	121.65	115.14
4	5	3494	B8H	N3-C2-N1	5.83	121.44	115.14

There are no chirality outliers.

5 of 100 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	5	1260	OMG	C1'-C2'-O2'-CM2
4	5	1270	A2M	C1'-C2'-O2'-CM'
4	5	1292	P4U	N3-C4-O4-C41
4	5	1292	P4U	C3'-C4'-C5'-O5'
4	5	1292	P4U	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 183 ligands modelled in this entry, 183 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

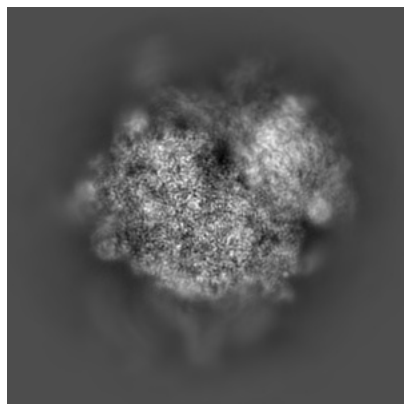
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15860. These allow visual inspection of the internal detail of the map and identification of artifacts.

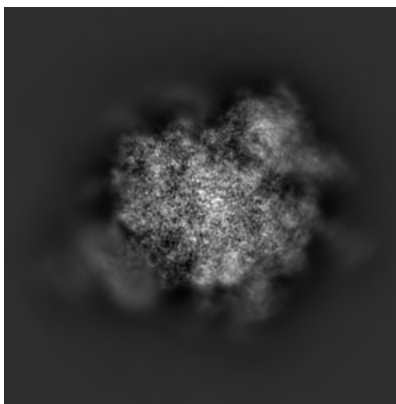
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

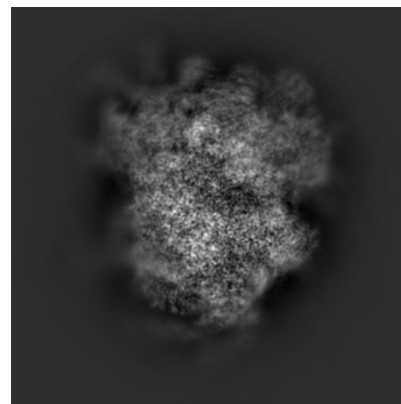
6.1.1 Primary map



X

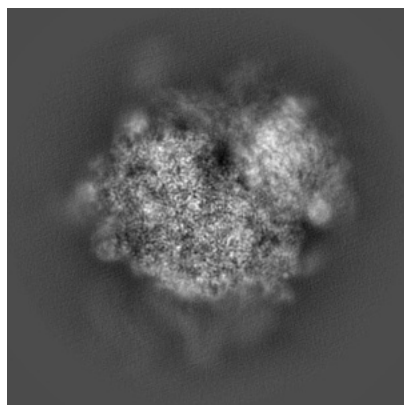


Y

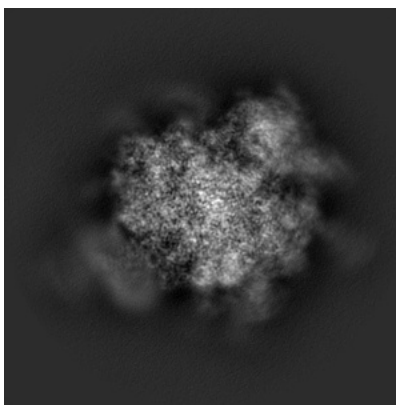


Z

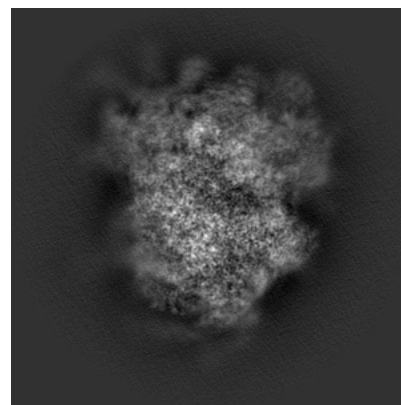
6.1.2 Raw map



X



Y

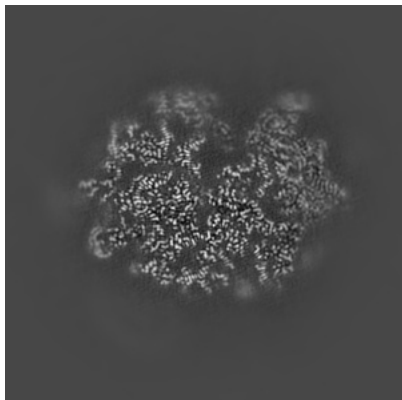


Z

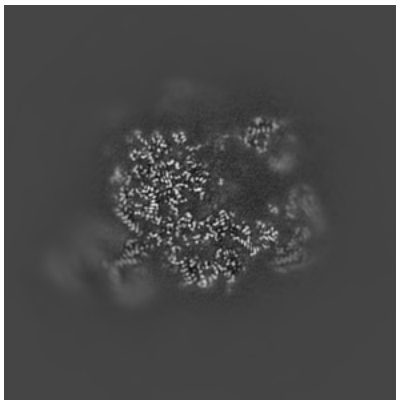
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

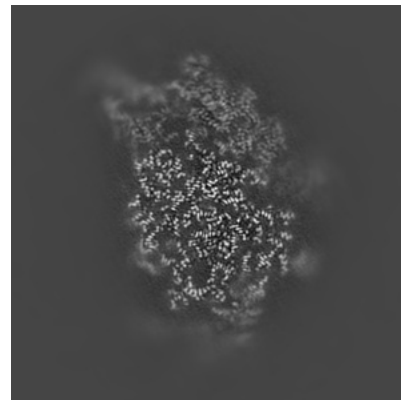
6.2.1 Primary map



X Index: 176

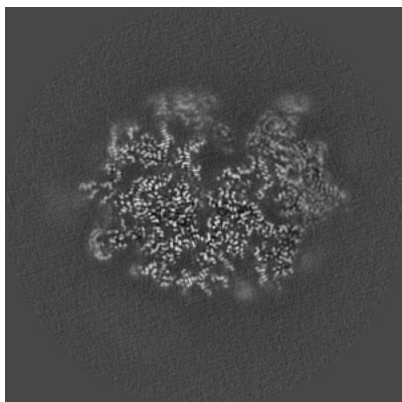


Y Index: 176

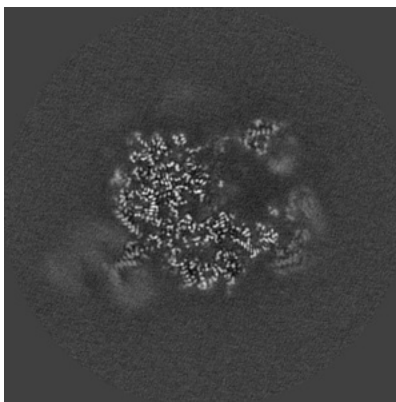


Z Index: 176

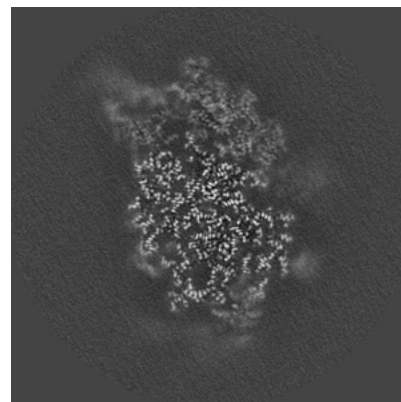
6.2.2 Raw map



X Index: 176



Y Index: 176

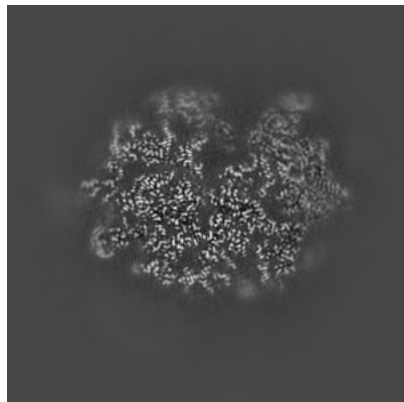


Z Index: 176

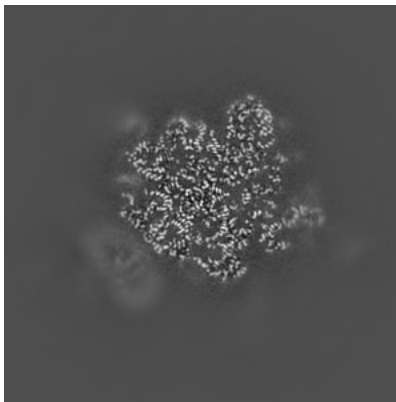
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

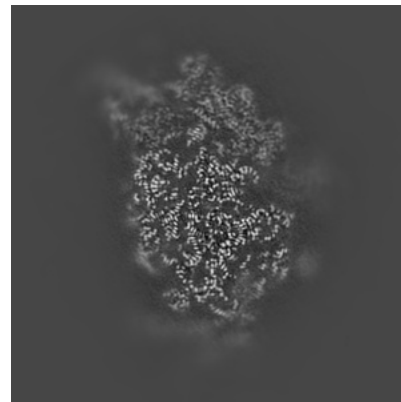
6.3.1 Primary map



X Index: 176

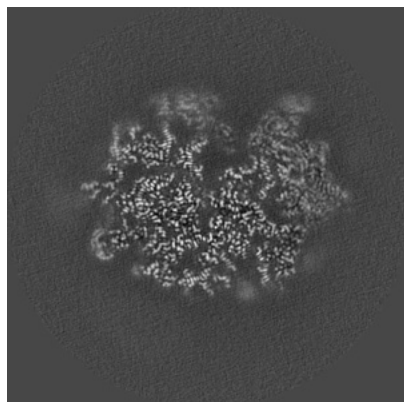


Y Index: 147

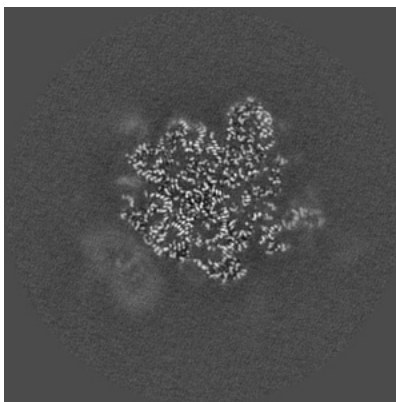


Z Index: 179

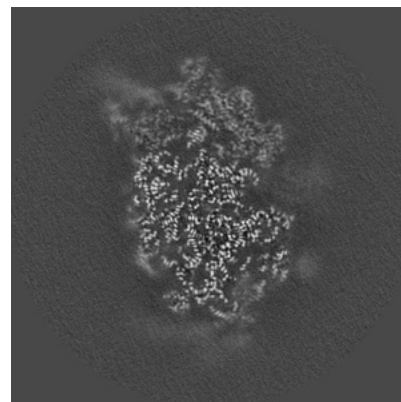
6.3.2 Raw map



X Index: 176



Y Index: 147

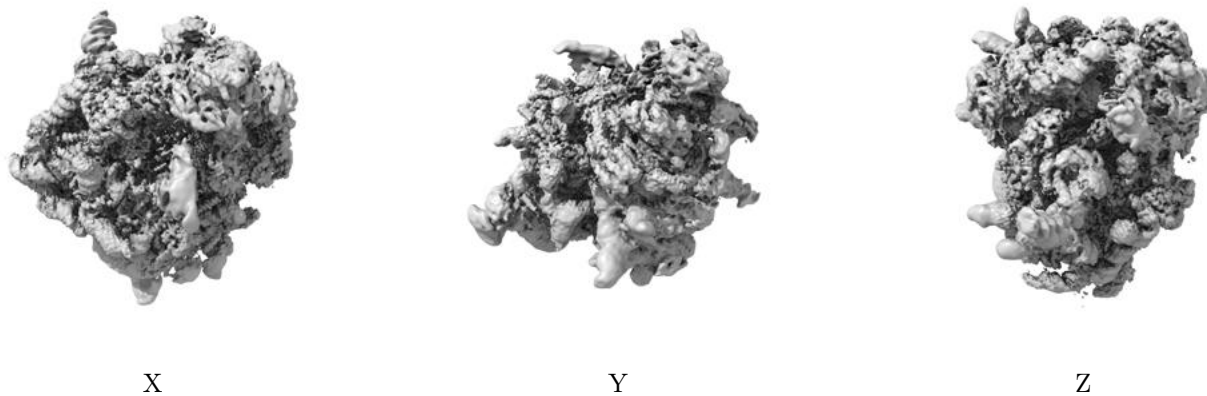


Z Index: 179

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

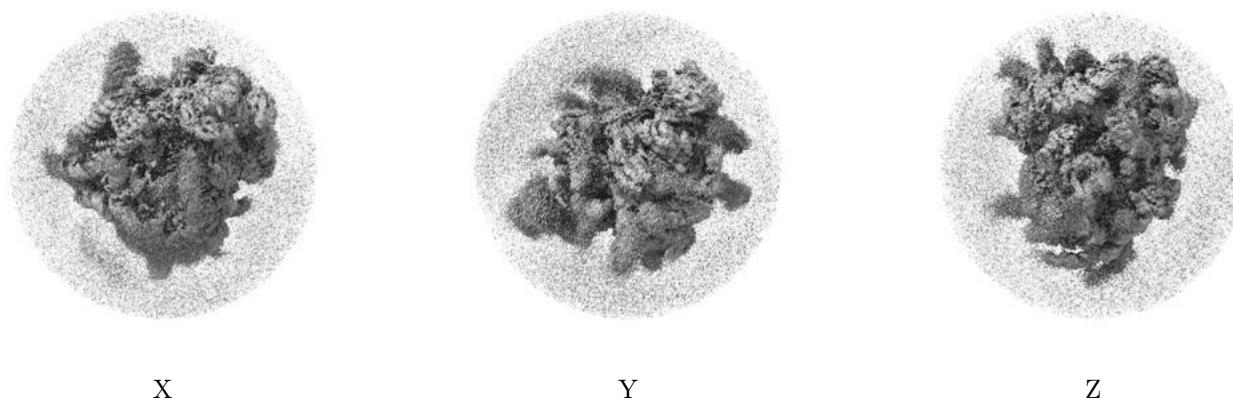
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01527. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

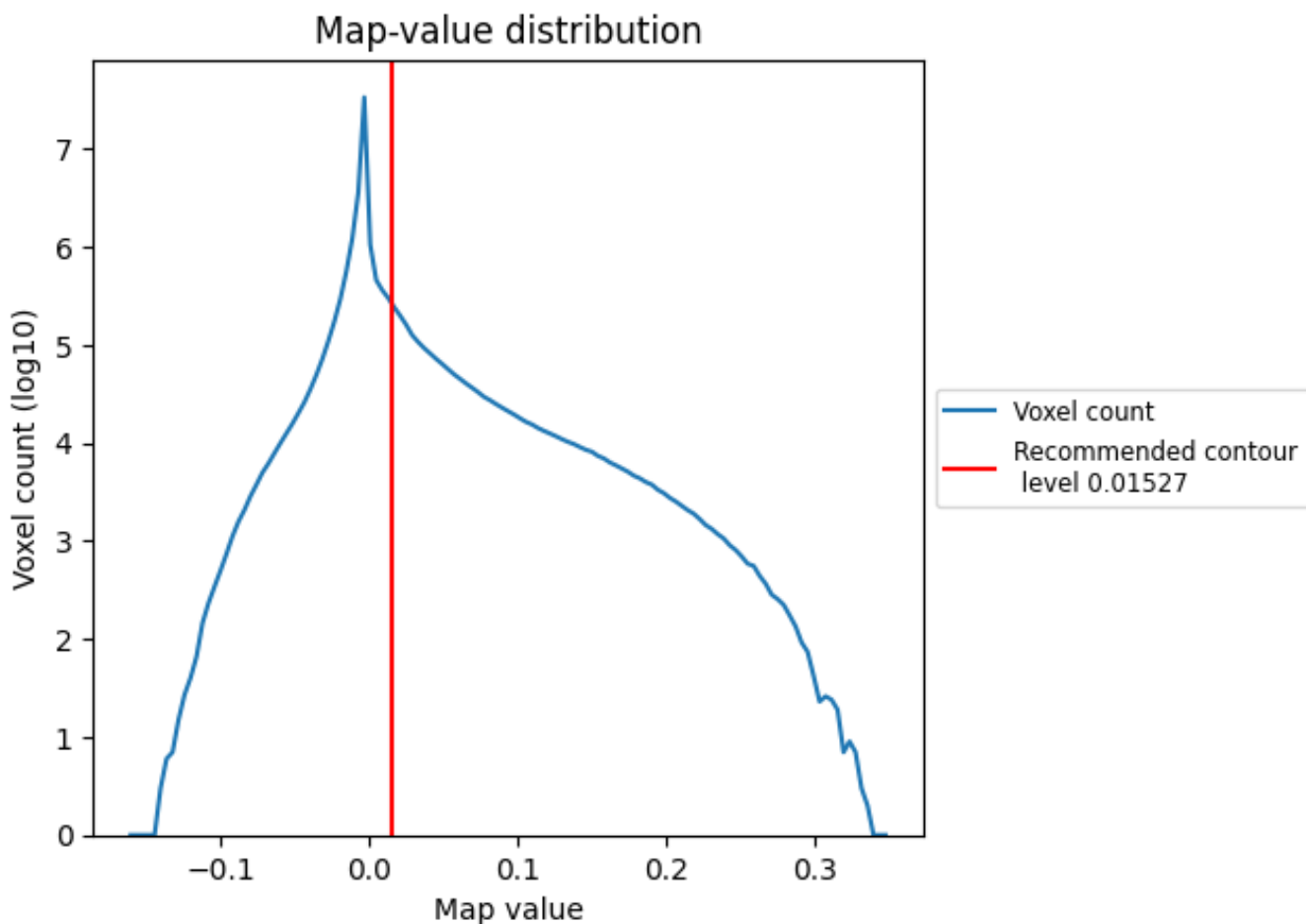
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

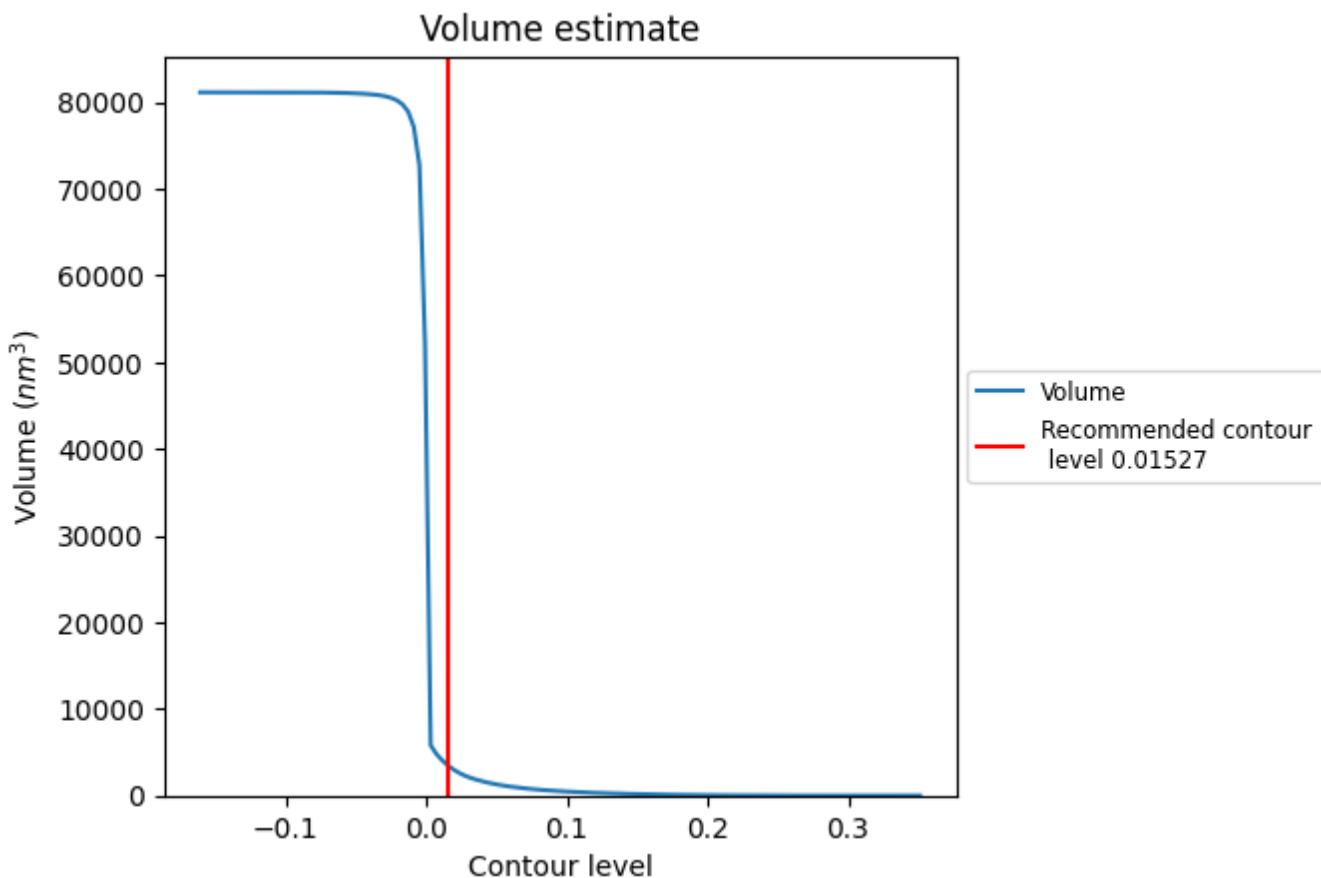
This section contains the results of statistical analysis of the map.

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.

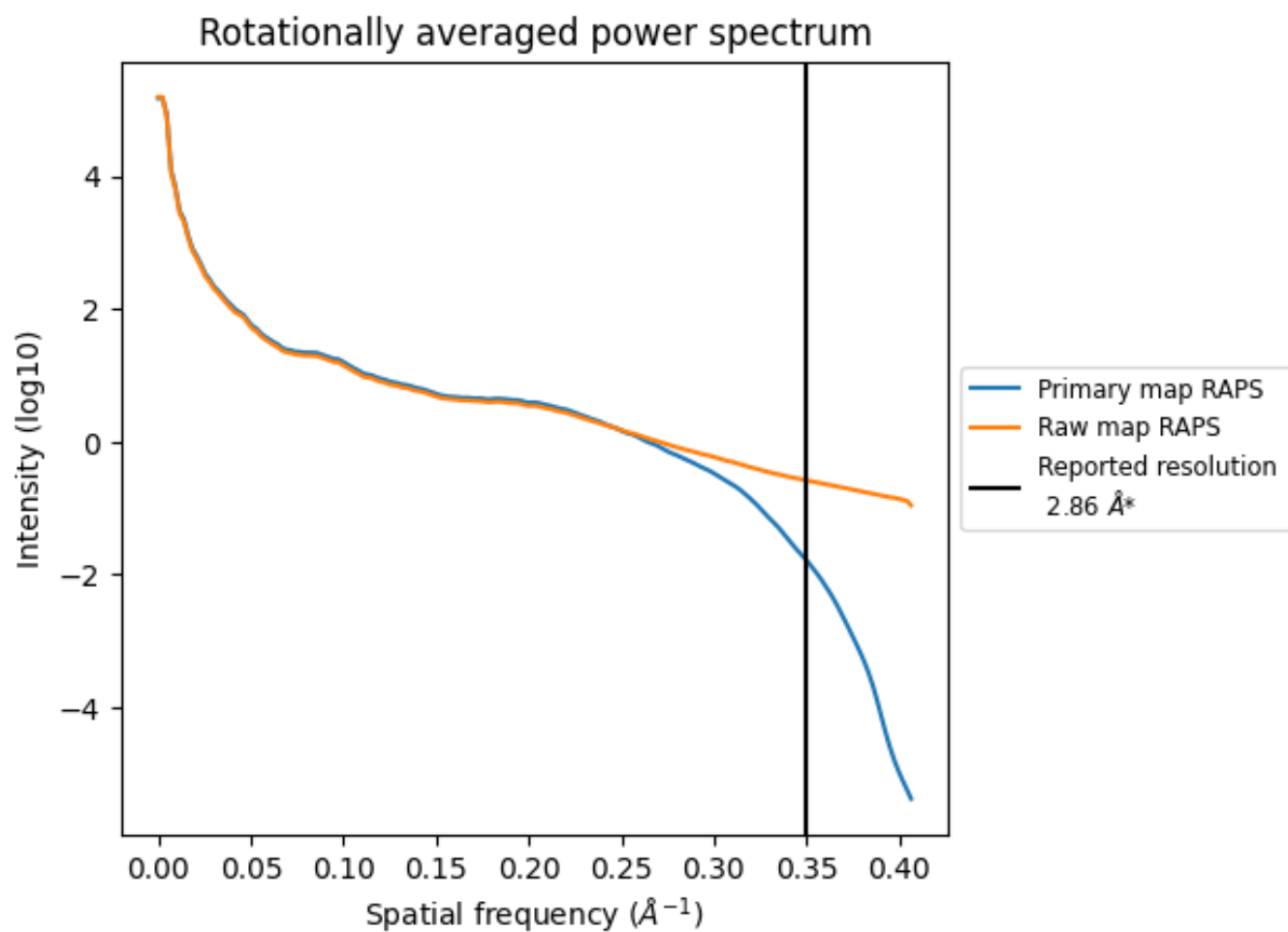
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3499 nm³; this corresponds to an approximate mass of 3161 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

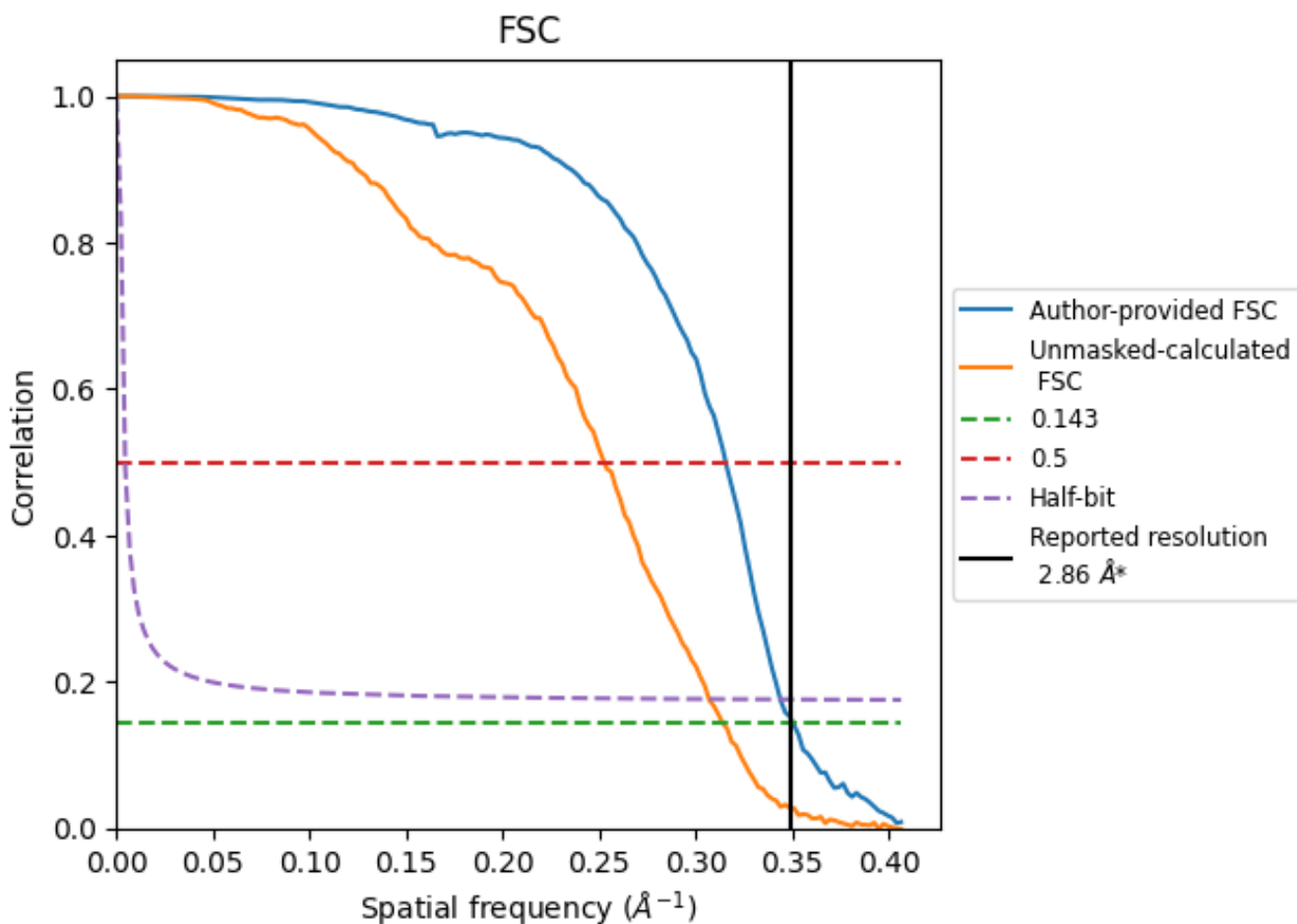


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

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 0.350 Å⁻¹

8.2 Resolution estimates [i](#)

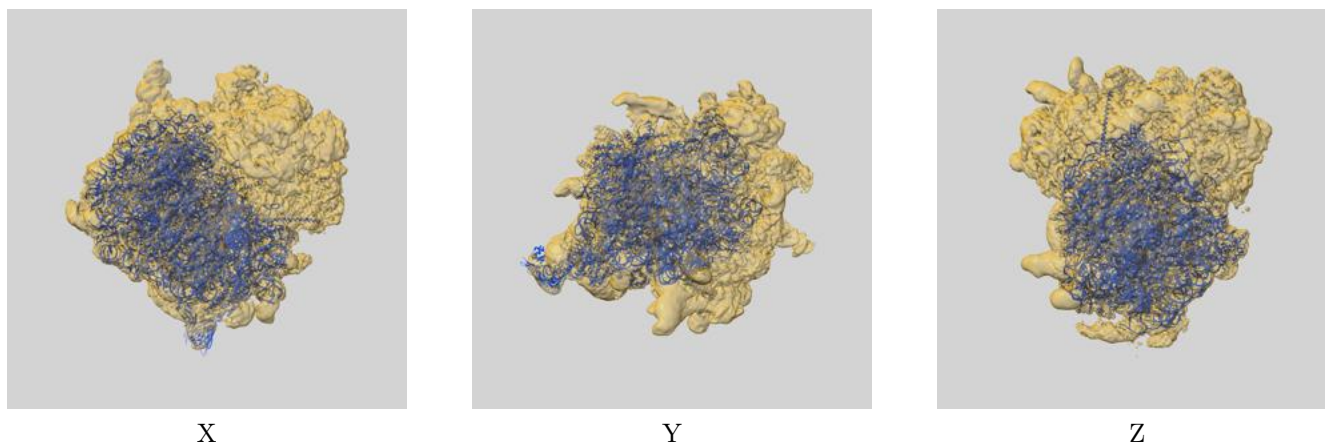
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.85	3.17	2.91
Unmasked-calculated*	3.18	3.96	3.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.18 differs from the reported value 2.86 by more than 10 %

9 Map-model fit [i](#)

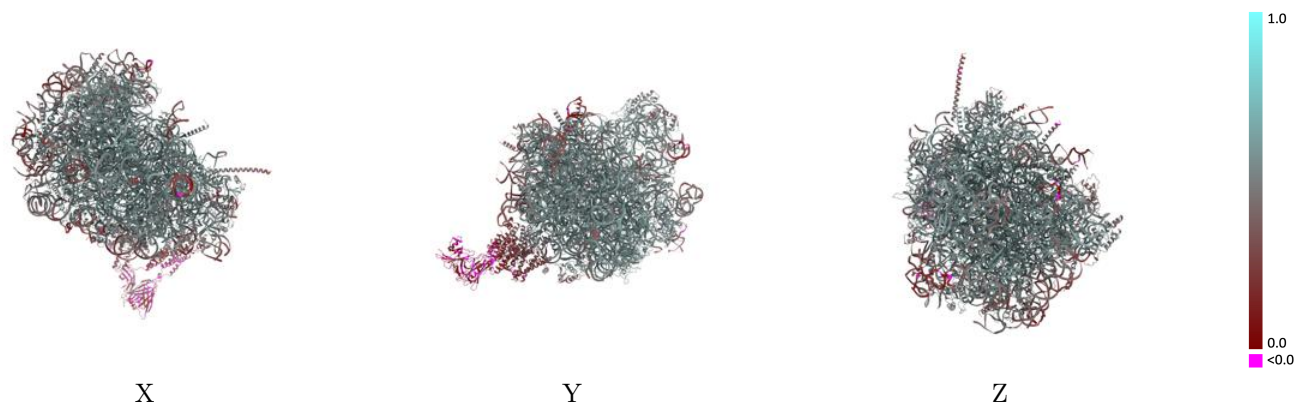
This section contains information regarding the fit between EMDB map EMD-15860 and PDB model 8B5L. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



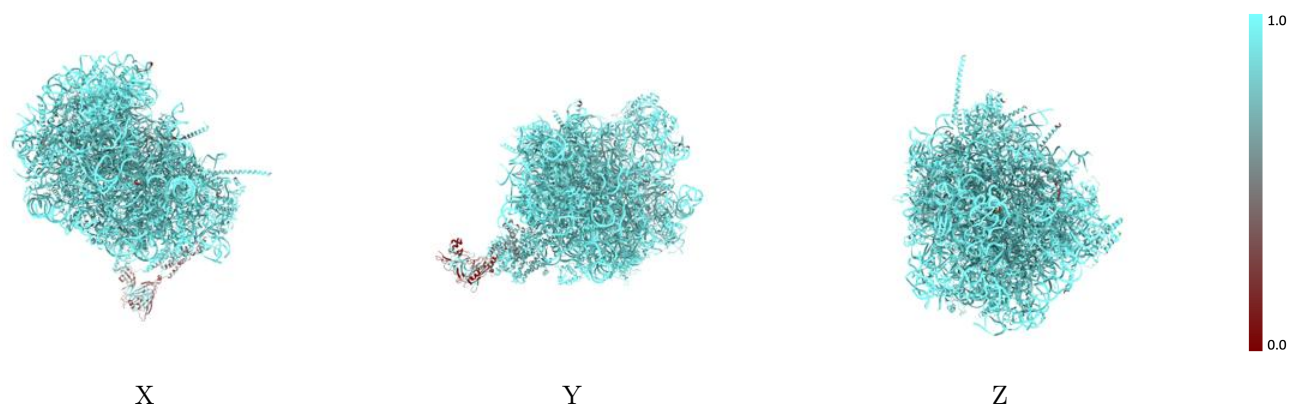
The images above show the 3D surface view of the map at the recommended contour level 0.01527 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



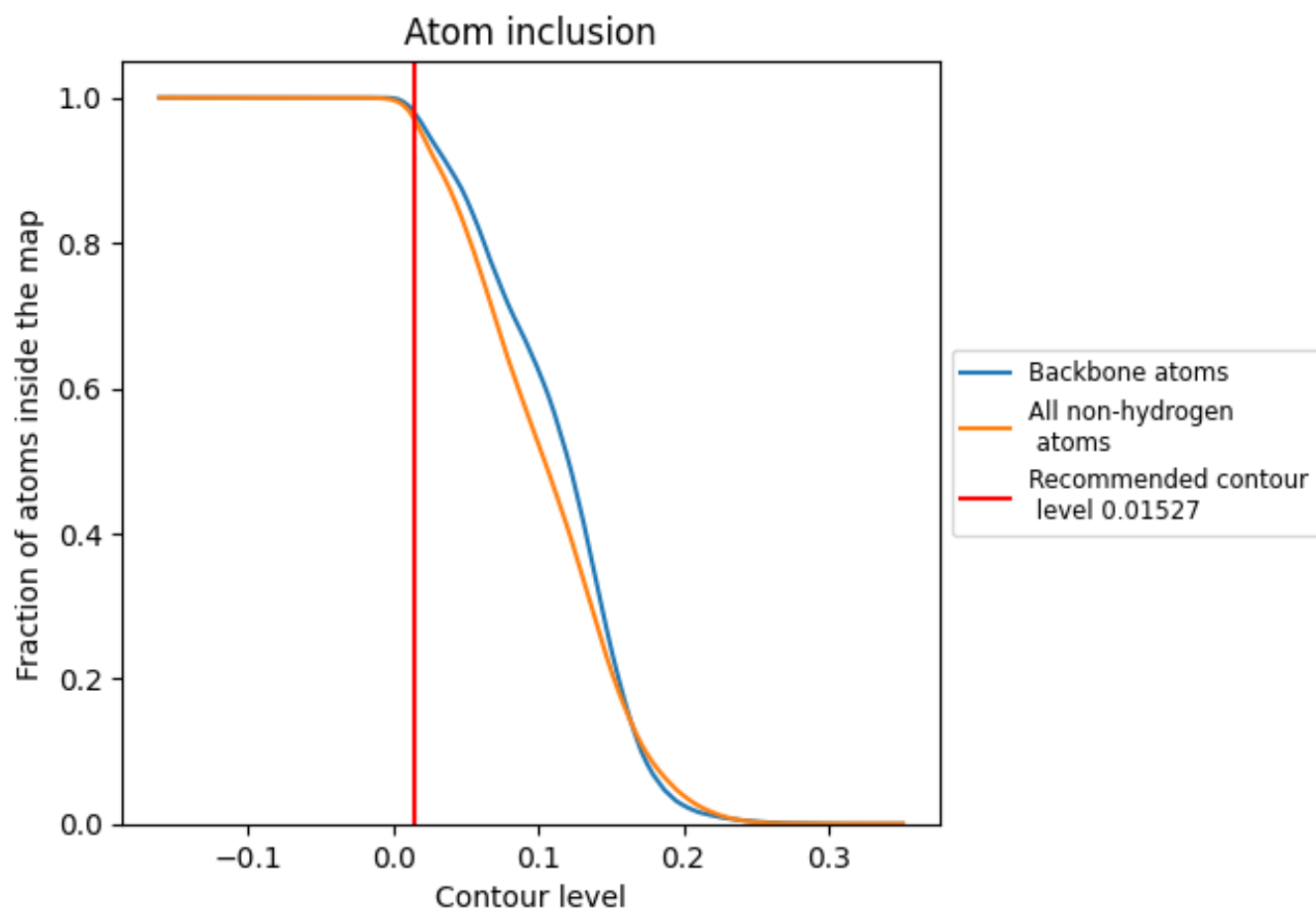
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01527).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.01527) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9682	 0.5050
5	 0.9935	 0.5160
7	 0.9992	 0.5490
8	 0.9947	 0.5370
A	 0.9777	 0.5760
B	 0.9845	 0.5590
C	 0.9799	 0.5560
D	 0.9862	 0.5150
E	 0.9839	 0.5230
F	 0.9713	 0.5520
G	 0.9721	 0.4900
H	 0.9824	 0.5390
I	 0.9752	 0.5550
J	 0.9727	 0.4730
K	 0.4630	 0.0490
L	 0.9547	 0.5200
M	 0.9873	 0.5320
N	 0.9858	 0.5850
O	 0.9873	 0.5570
P	 0.9760	 0.5630
Q	 0.9710	 0.5660
R	 0.9598	 0.5060
S	 0.9815	 0.5610
T	 0.9715	 0.5440
U	 0.9722	 0.4550
V	 0.9791	 0.5710
W	 0.9764	 0.5550
X	 0.9511	 0.5350
Y	 0.9731	 0.5310
Z	 0.9851	 0.5230
a	 0.9752	 0.5690
b	 0.9460	 0.4790
c	 0.9556	 0.5170
d	 0.9673	 0.5430
e	 0.9764	 0.5790



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Chain	Atom inclusion	Q-score
f	 0.9786	 0.5840
g	 0.9598	 0.5530
h	 0.9632	 0.5290
i	 0.9724	 0.5190
j	 0.9822	 0.5800
k	 0.9461	 0.4820
l	 0.9625	 0.5570
m	 0.9688	 0.5630
n	 0.9128	 0.5070
o	 0.9804	 0.5620
p	 0.9623	 0.5610
q	 0.5000	 0.0890
r	 0.9864	 0.5540
s	 0.8718	 0.2790
t	 0.7413	 0.2090
u	 0.8956	 0.3230
v	 0.4588	 0.0720