



wwPDB EM Validation Summary Report ⓘ

Nov 21, 2023 – 04:44 pm GMT

PDB ID : 7A1G
EMDB ID : EMD-11608
Title : Structure of a crosslinked yeast ABCE1-bound 43S pre-initiation complex
Authors : Mackens-Kiani, T.; Kratzat, H.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2020-08-13
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

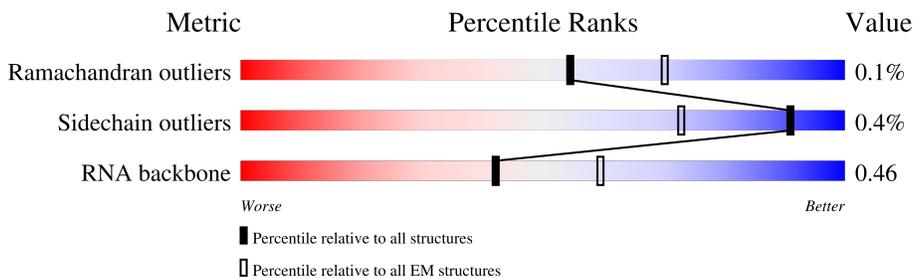
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	2	1771	
2	P	206	
3	Q	232	
4	R	216	
5	S	258	
6	T	228	
7	U	184	
8	V	200	

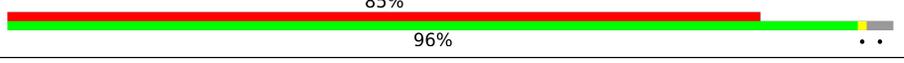
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Mol	Chain	Length	Quality of chain
9	W	184	32% 99%
10	X	142	24% 99%
11	Y	150	41% 99%
12	Z	127	72% 99%
13	a	87	46% 95% 5%
14	b	129	11% 98%
15	c	144	23% 99%
16	d	134	44% 99%
17	e	97	36% 100%
18	f	81	51% 99%
19	g	60	53% 98%
20	E	117	98% 98%
21	A	222	76% 99%
22	B	206	95% 100%
23	C	92	80% 98%
24	D	121	100% 97%
25	F	141	73% 98%
26	H	125	76% 94%
27	I	145	99% 97%
28	J	143	96% 99%
29	K	100	76% 99%
30	L	82	100% 98%
31	M	53	38% 98%
32	N	73	100% 81% 16%
33	O	312	99% 100%

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Mol	Chain	Length	Quality of chain
34	h	63	 <p>98% 100%</p>
35	y	265	 <p>30% 29% 70%</p>
35	z	265	 <p>45% 45% 55%</p>
36	x	601	 <p>85% 96%</p>

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 81866 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1771	37739	16872	6683	12413	1771	0	0

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	206	1603	1030	284	287	2	0	0

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Q	226	1798	1139	330	325	4	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	216	1626	1042	287	295	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	258	2056	1308	387	358	3	0	0

- Molecule 6 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	T	228	1815	1138	351	323	3	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	U	184	1473	946	263	264	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	V	187	1476	916	295	263	2	0	0

- Molecule 9 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	W	184	1479	935	285	258	1	0	0

- Molecule 10 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	142	1142	733	217	189	3	0	0

- Molecule 11 is a protein called 40S ribosomal protein S13.

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

- Molecule 12 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Z	127	923	568	185	167	3	0	0

- Molecule 13 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	a	87	673	415	125	131	2	0	0

- Molecule 14 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 15 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	c	144	1121	708	220	191	2	0	0

- Molecule 16 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	d	134	1073	676	208	189	0	0

- Molecule 17 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	e	97	765	473	160	127	5	0	0

- Molecule 18 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 19 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	g	60	472	298	97	76	1	0	0

- Molecule 20 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	E	117	916	583	171	155	7	0	0

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	A	222	1729	1098	312	313	6	0	0

- Molecule 22 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	B	206	1605	1005	299	298	3	0	0

- Molecule 23 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	C	92	754	489	122	141	2	0	0

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	D	121	875	551	153	169	2	0	0

- Molecule 25 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	F	141	1105	708	203	194	0	0

- Molecule 26 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	H	121	948	596	179	171	2	0	0

- Molecule 27 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	I	145	1188	741	237	208	2	0	0

- Molecule 28 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	J	143	1112	694	208	208	2	0	0

- Molecule 29 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	K	100	797	506	144	146	1	0	0

- Molecule 30 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	L	82	651	416	123	112	0	0

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	M	53	442	274	92	72	4	0	0

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	N	73	560	355	106	95	4	0	0

- Molecule 33 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	O	312	2383	1514	409	452	8	0	0

- Molecule 34 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	h	63	491	303	96	91	1	0	0

- Molecule 35 is a protein called Eukaryotic translation initiation factor 3 subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	120	Total	C	N	O	S	0	0
			896	556	172	166	2		
35	y	79	Total	C	N	O	S	0	0
			624	389	113	120	2		

- Molecule 36 is a protein called Translation initiation factor RLI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	x	582	Total	C	N	O	S	0	0
			4608	2951	795	839	23		

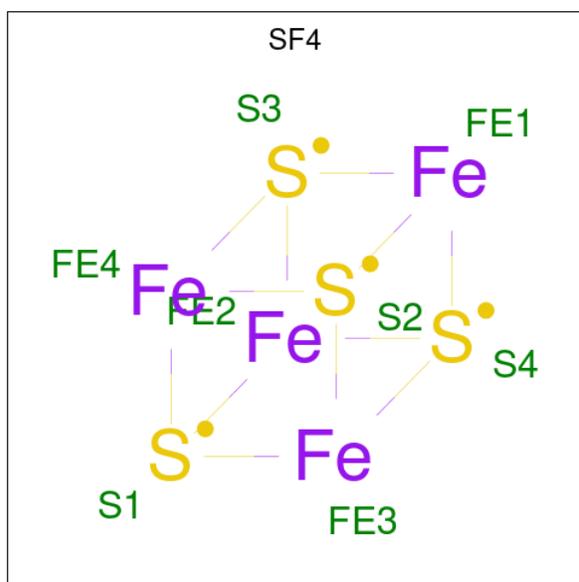
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	2	76	Total	Mg	0
			76	76	
37	R	1	Total	Mg	0
			1	1	
37	S	1	Total	Mg	0
			1	1	
37	B	1	Total	Mg	0
			1	1	
37	x	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

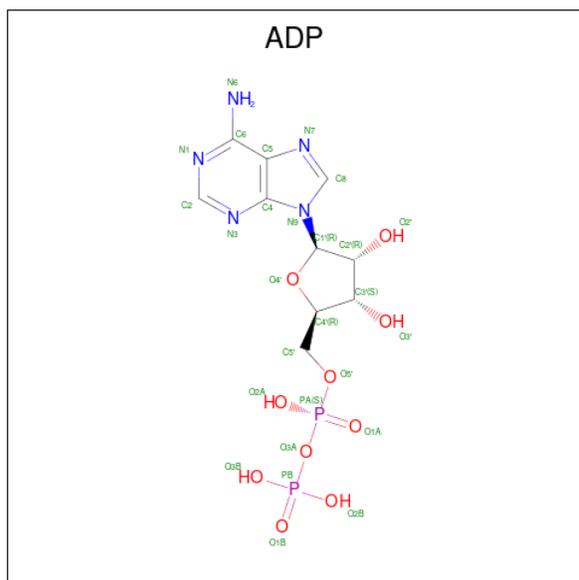
Mol	Chain	Residues	Atoms		AltConf
38	M	1	Total	Zn	0
			1	1	
38	N	1	Total	Zn	0
			1	1	

- Molecule 39 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms				AltConf
39	x	1	Total	Fe	S		0
			8	4	4		
39	x	1	Total	Fe	S		0
			8	4	4		

- Molecule 40 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

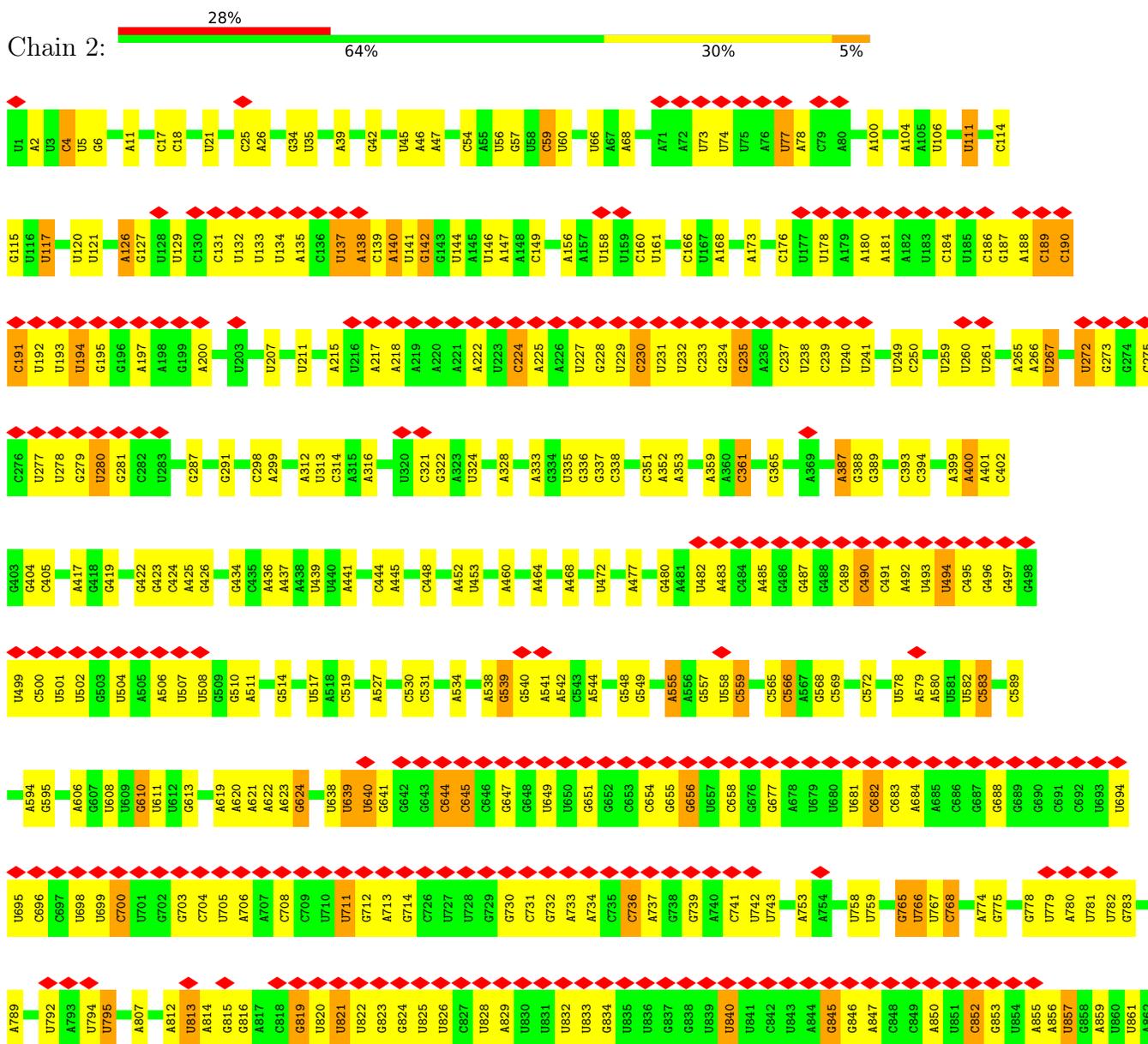


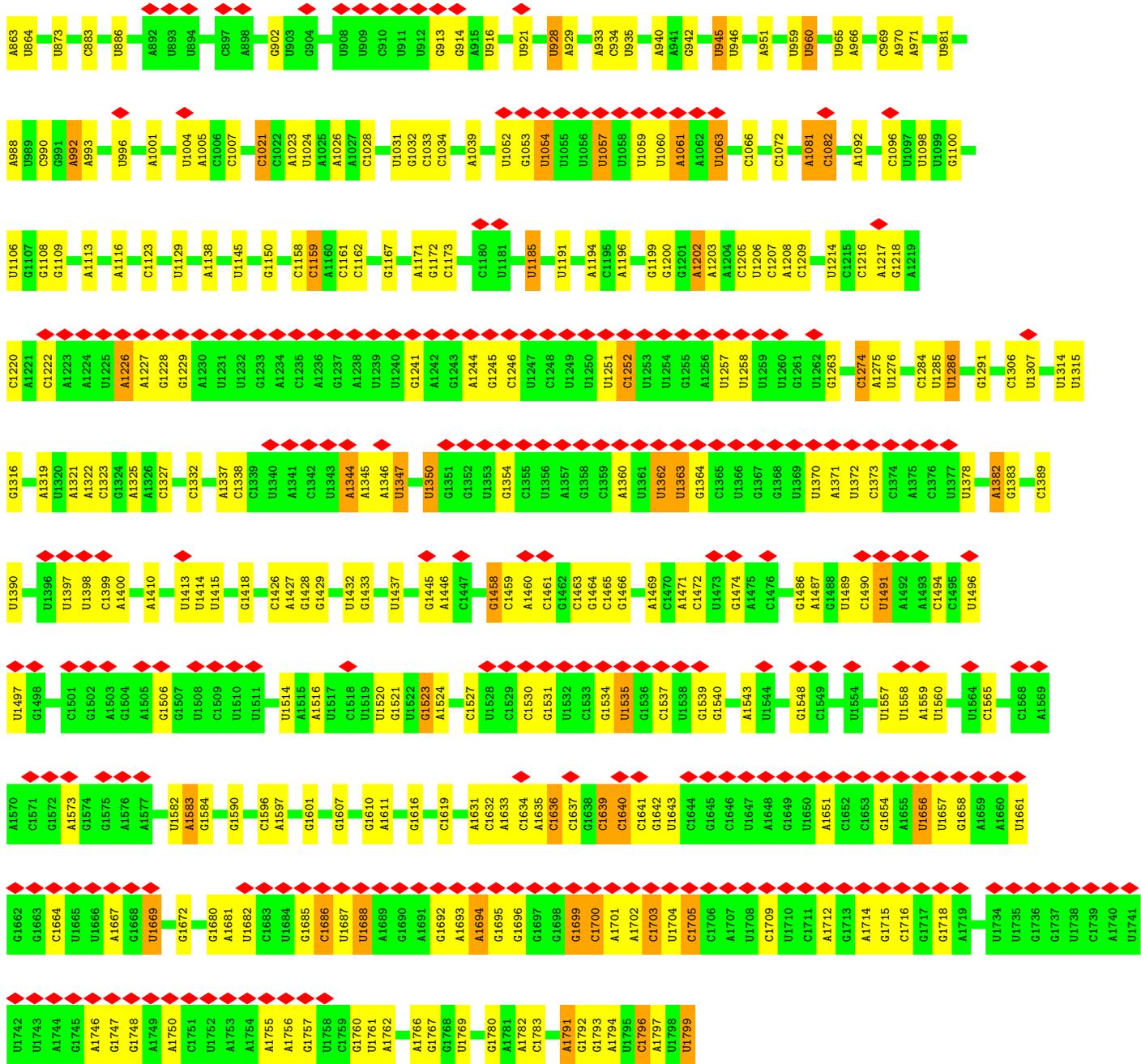
Mol	Chain	Residues	Atoms					AltConf	
40	x	1	Total	C	N	O	P		0
			27	10	5	10	2		

3 Residue-property plots

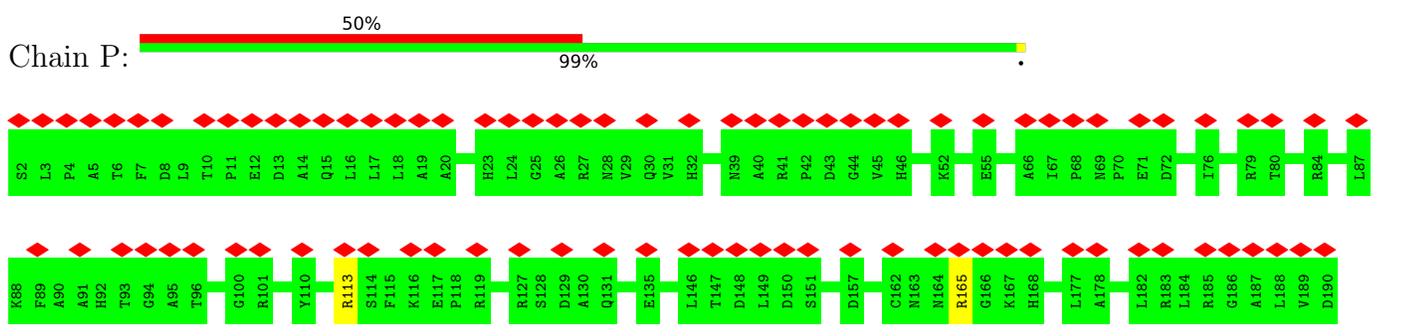
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 18S ribosomal RNA



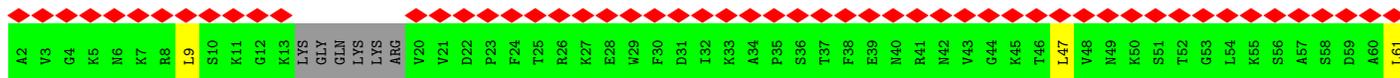


• Molecule 2: 40S ribosomal protein S0-A

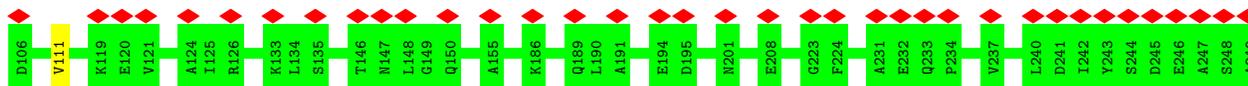
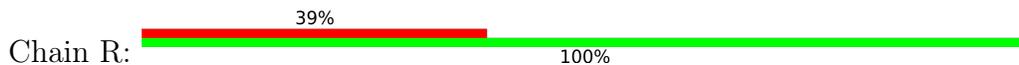




• Molecule 3: 40S ribosomal protein S1-A



• Molecule 4: 40S ribosomal protein S2



• Molecule 5: 40S ribosomal protein S4-A



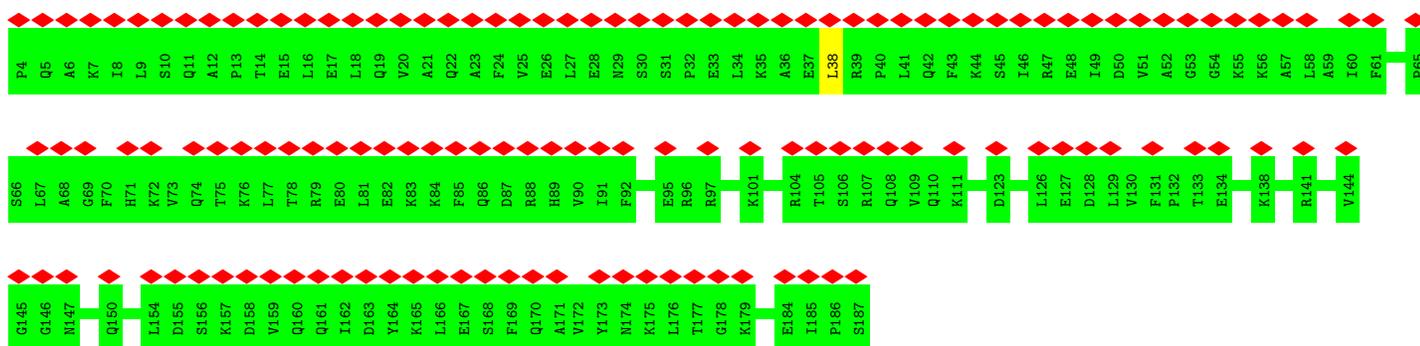
• Molecule 6: 40S ribosomal protein S6-A





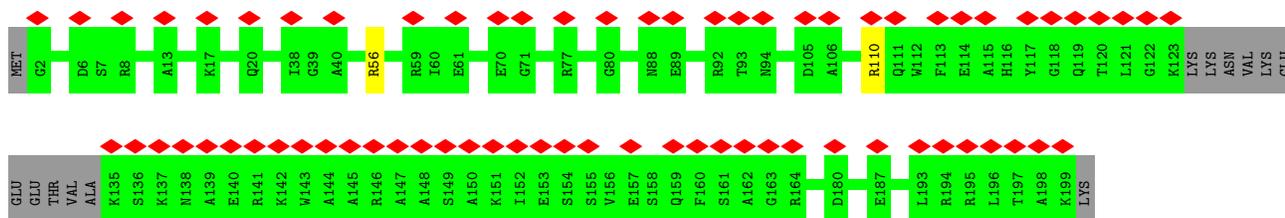
- Molecule 7: 40S ribosomal protein S7-A

Chain U: 74% 99%



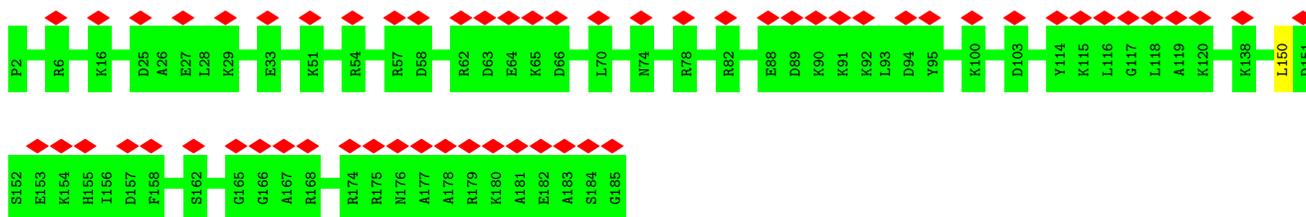
- Molecule 8: 40S ribosomal protein S8-A

Chain V: 35% 92% 6%

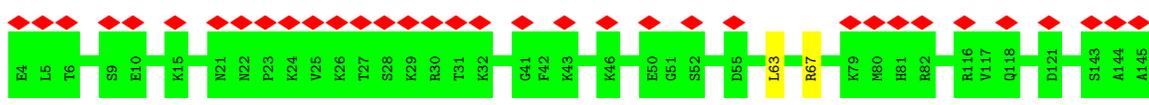


- Molecule 9: 40S ribosomal protein S9-A

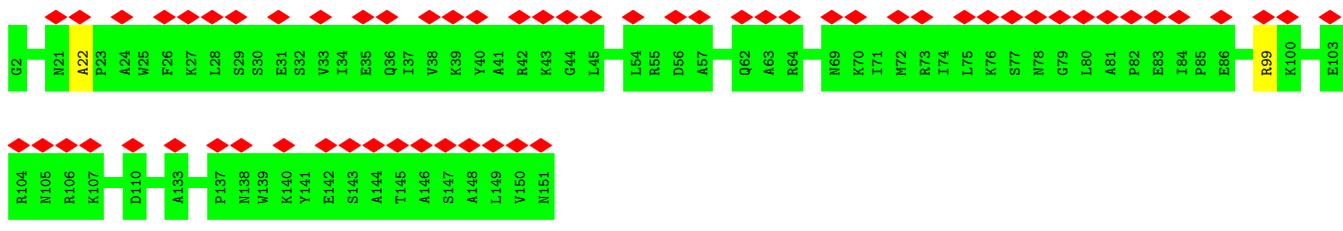
Chain W: 32% 99%



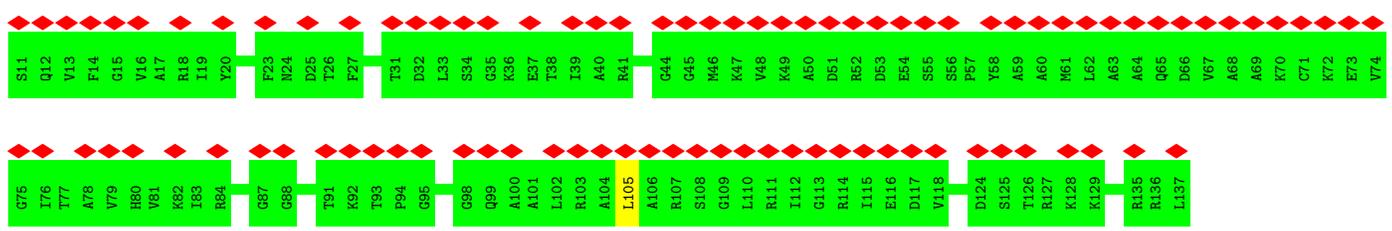
- Molecule 10: 40S ribosomal protein S11-A



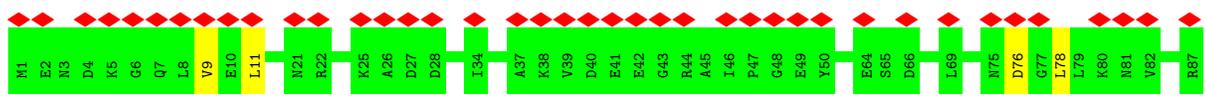
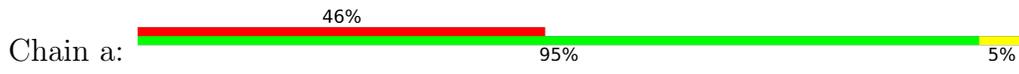
• Molecule 11: 40S ribosomal protein S13



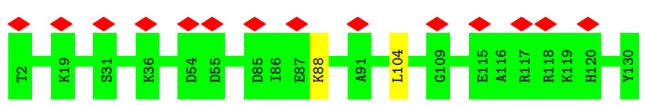
• Molecule 12: 40S ribosomal protein S14-B



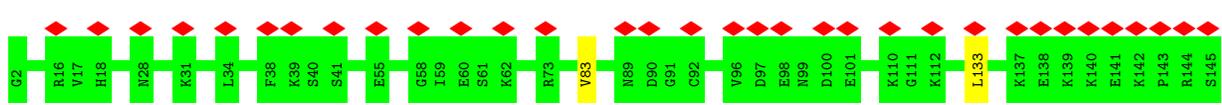
• Molecule 13: 40S ribosomal protein S21-A



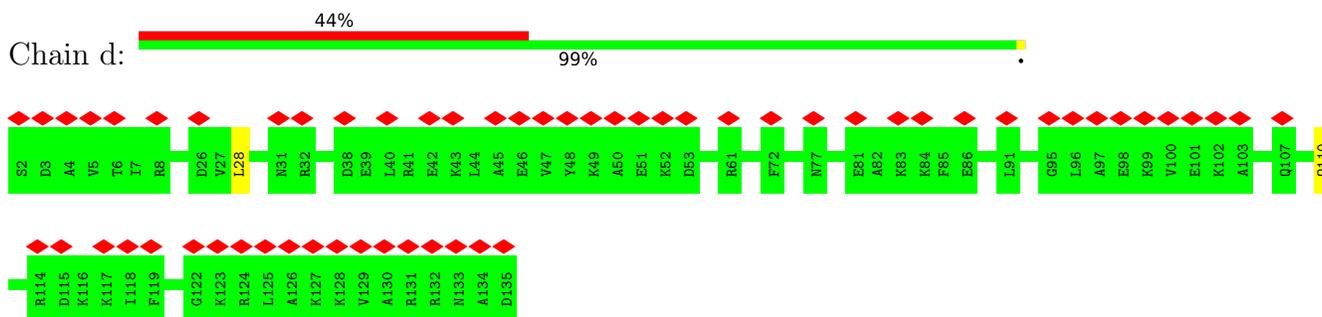
• Molecule 14: 40S ribosomal protein S22-A



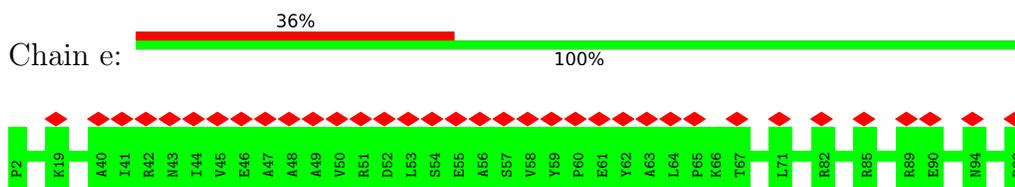
• Molecule 15: 40S ribosomal protein S23-A



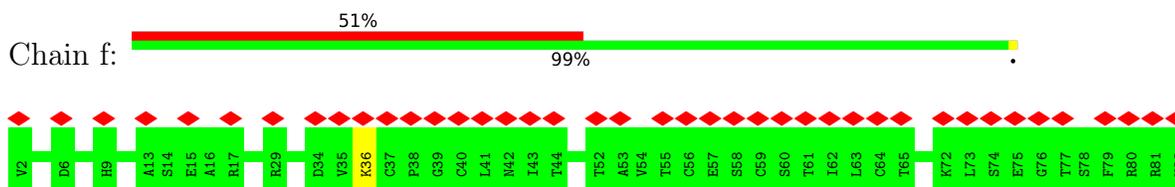
- Molecule 16: 40S ribosomal protein S24-A



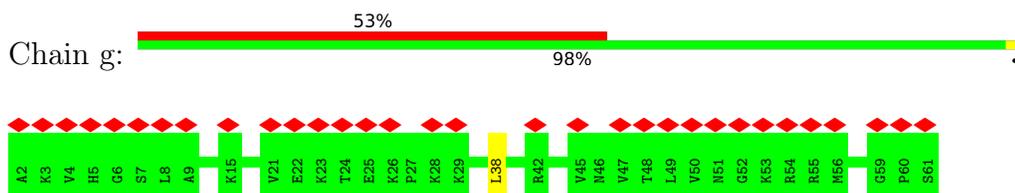
- Molecule 17: 40S ribosomal protein S26-B



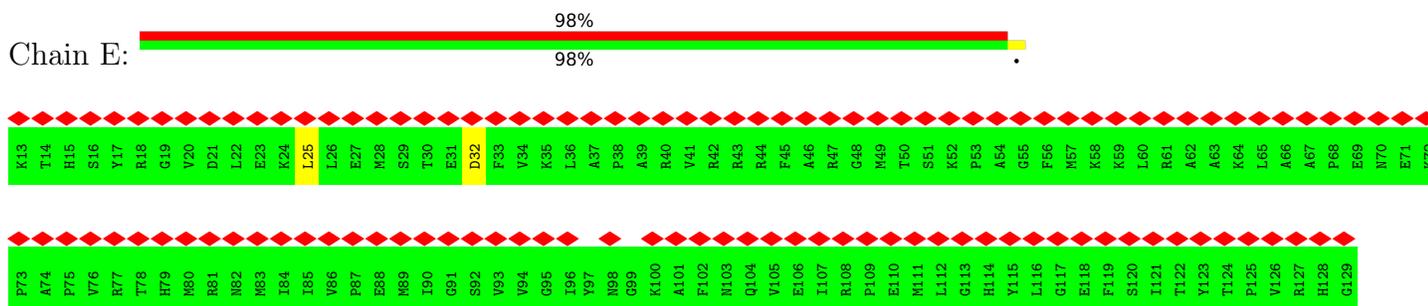
- Molecule 18: 40S ribosomal protein S27-A



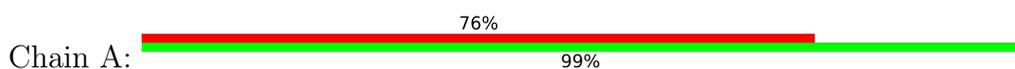
- Molecule 19: 40S ribosomal protein S30-A

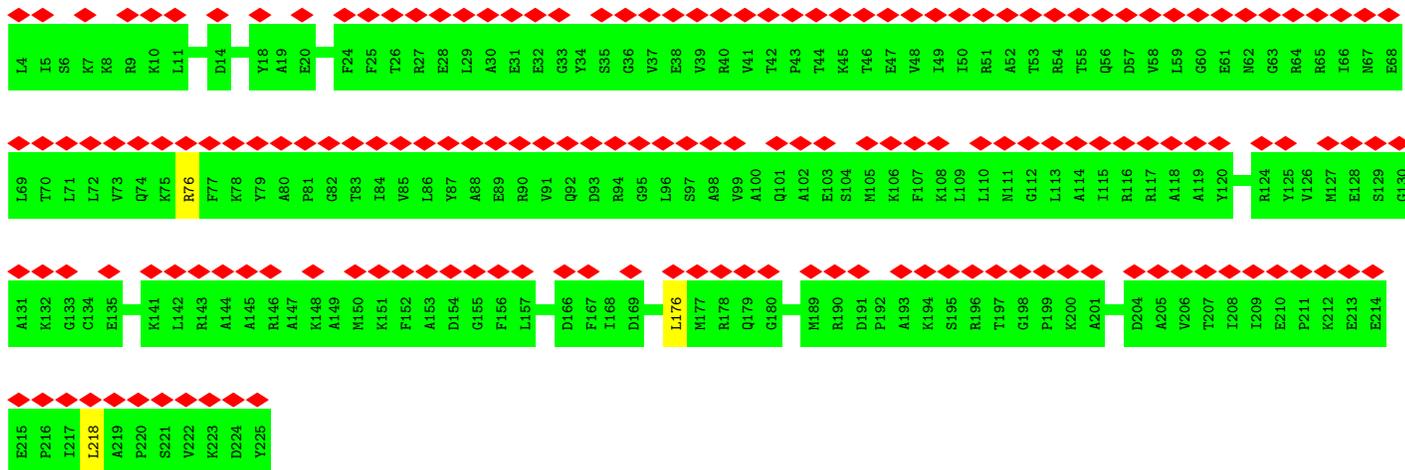


- Molecule 20: 40S ribosomal protein S15

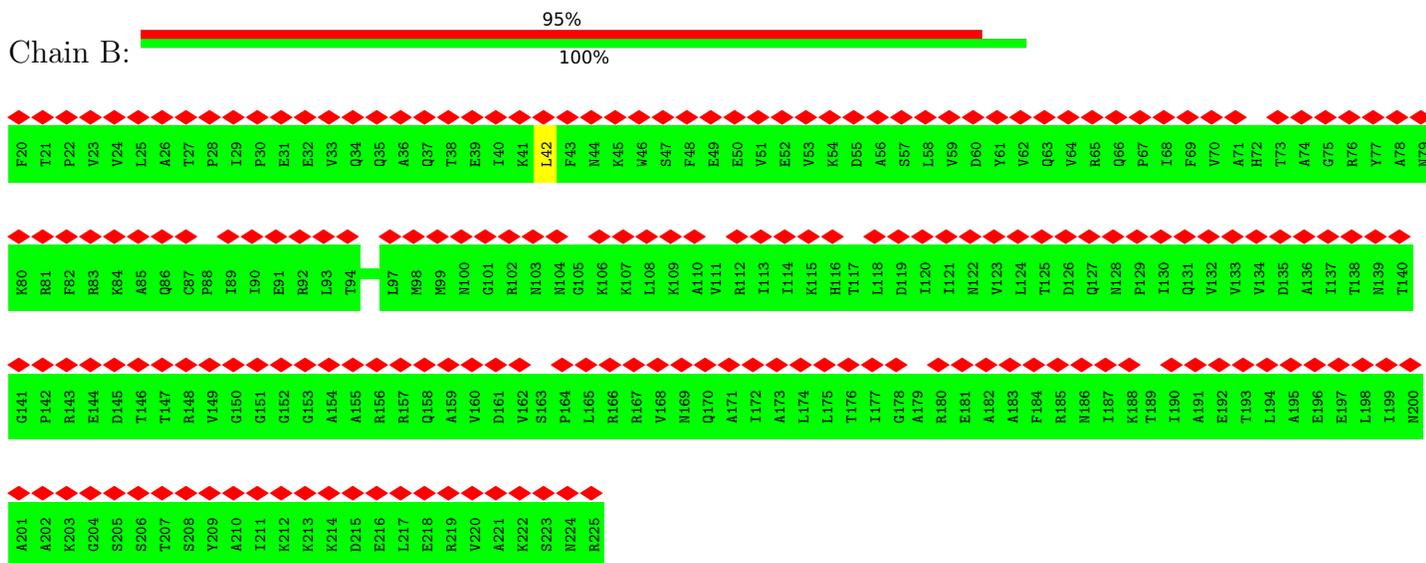


- Molecule 21: 40S ribosomal protein S3

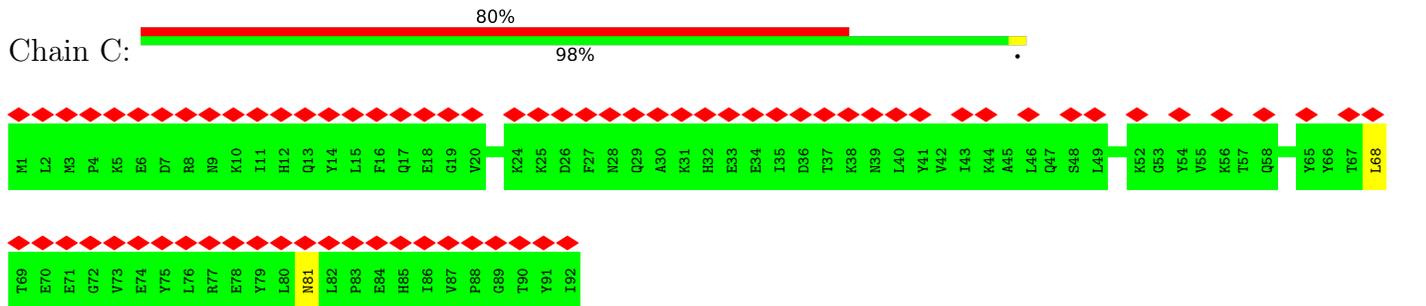




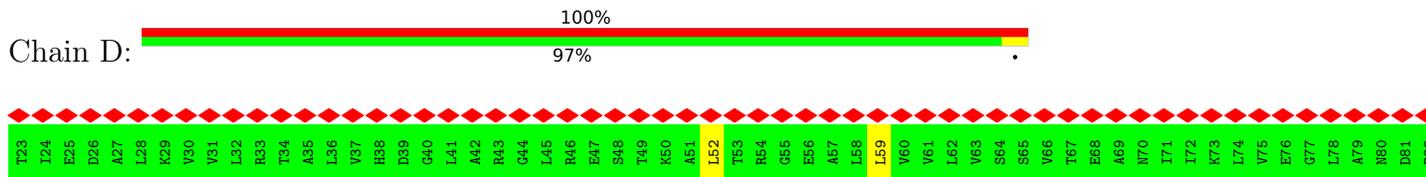
• Molecule 22: 40S ribosomal protein S5

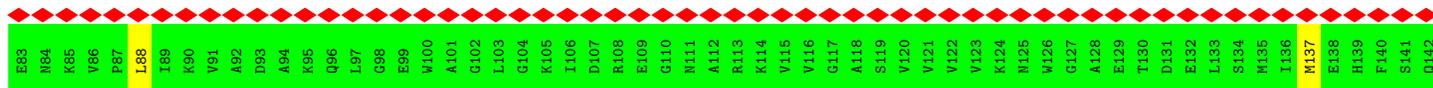


• Molecule 23: 40S ribosomal protein S10-A



• Molecule 24: 40S ribosomal protein S12



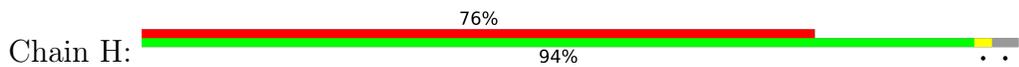


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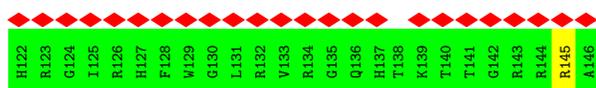
• Molecule 25: 40S ribosomal protein S16-A



• Molecule 26: 40S ribosomal protein S17-B

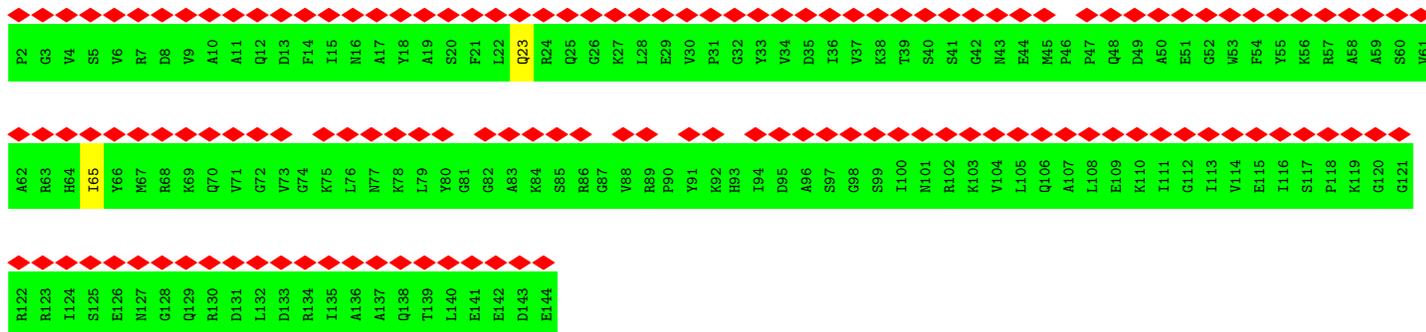


• Molecule 27: 40S ribosomal protein S18-A

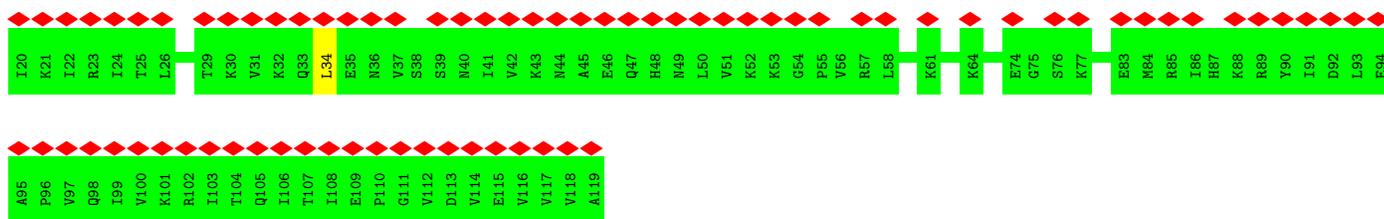
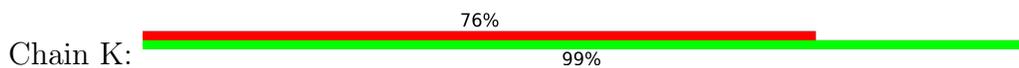


• Molecule 28: 40S ribosomal protein S19-A



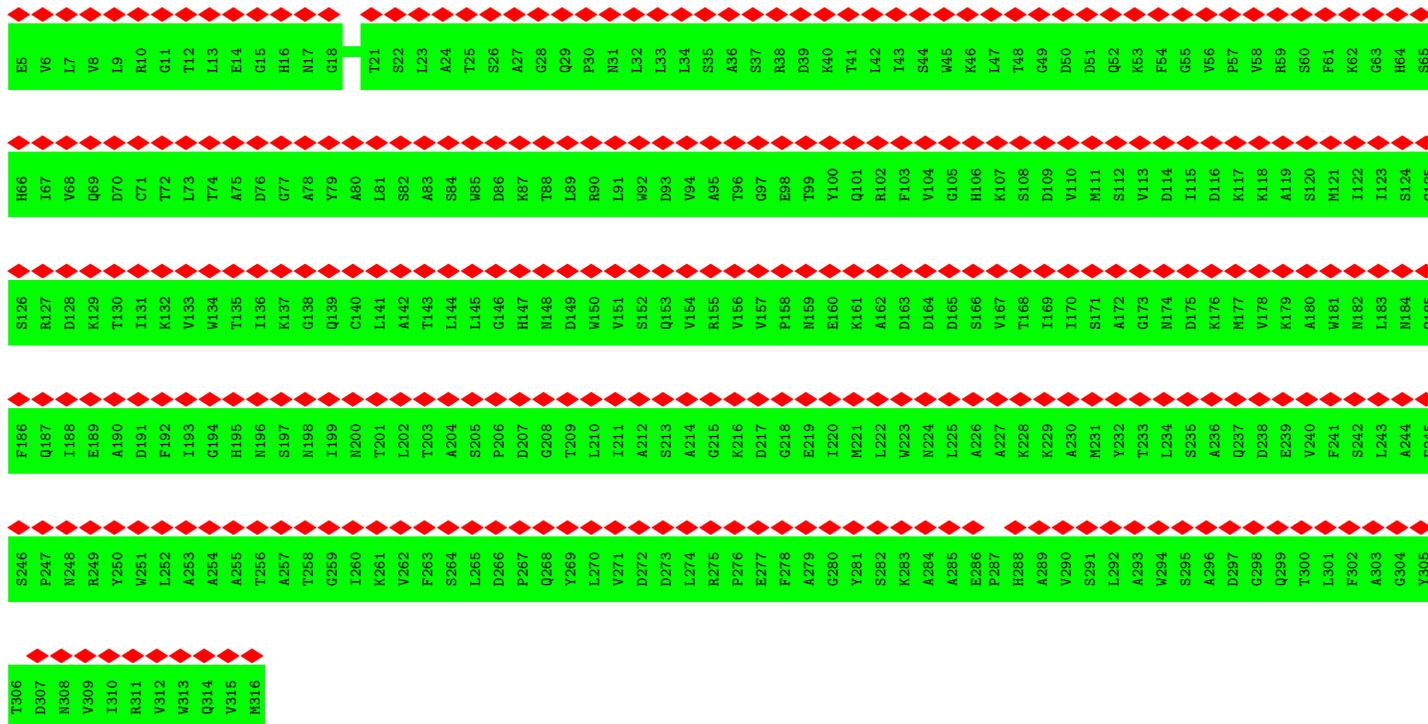


• Molecule 29: 40S ribosomal protein S20





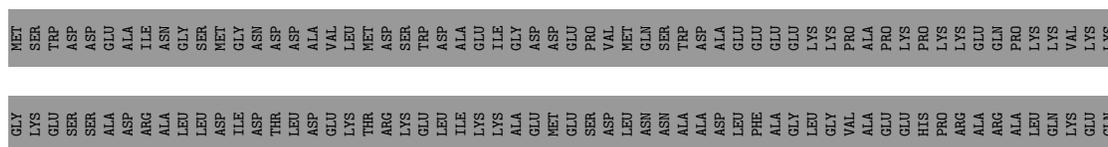
• Molecule 33: Guanine nucleotide-binding protein subunit beta-like protein



• Molecule 34: 40S ribosomal protein S28-A



• Molecule 35: Eukaryotic translation initiation factor 3 subunit J



Y273	V274	I275	C276	V277	E278	H279	D280	L281	S282	V283	L284	D285	Y286	L287	S288	D289	F290	V291	C292	I293	I294	Y295	G296	V297	P298	S299	V300	T305	L306	S309	V310	R311	E312	G313	I314	N315	I316	F317	L318	D319	G320	H321	A324	F329	R330	T331	E332	A333	L334	GLN	PHE	ARG	ILE	ALA	ASP				
ALA	THR	GLU	ASP	LEU	GLN	ASN	ASP	SER	ALA	SER	ARC	ALA	F354	S355	Y356	P357	S358	L359	K360	K361	T362	Q363	G364	D365	F366	V367	L368	N369	V370	E371	E372	G373	E374	F375	S376	D377	S378	E379	I380	L381	V382	M383	M384	G385	E386	N387	G388	T389	G390	K391	T392	T393	L394	I395	K396	L397	L398	A399	G400
A401	L402	K403	P404	D405	E406	G407	Q408	D409	I410	P411	K412	L413	N414	V415	S416	M417	K418	P419	Q420	K421	I422	A423	P424	K425	F426	P427	G428	T429	V430	R431	Q432	L433	F434	F435	K436	K437	I438	R439	G440	Q441	F442	L443	N444	P445	Q446	F447	Q448	T449	D450	V451	V452	K453	P454	L455	R456	I457	D458	D459	I460
I461	D462	Q463	E464	V465	Q466	H467	L468	S469	G470	G471	E472	L473	Q474	R475	V476	A477	I478	V479	L480	A481	L482	G483	I484	P485	A486	D487	I488	Y489	L490	I491	D492	E493	P494	S495	A496	Y497	L498	D499	S500	E501	Q502	R503	I504	I505	C506	S507	K508	V509	I510	R511	R512	F513	I514	L515	H516	N517	K518	K519	T520
A521	F522	I523	V524	E525	H526	D527	F528	I529	M530	A531	T532	Y533	L534	A535	D536	K537	V538	I539	V540	F541	E542	G543	I544	P545	S546	K547	N548	A549	H550	A551	R552	A553	P554	E555	S556	L557	L558	T559	G560	C561	N562	R563	F564	L565	K566	N567	L568	N569	V570	T571	F572	R573	L574	D575	P576	N577	S578	F579	R580
P581	R582	K585	L586	D587	M590	D591	K592	E593	Q594	K595	S596	S597	G598	N599	Y600	F601	F602	L603	D604																																								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25245	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	476.55002, 476.55002, 476.55002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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: SF4, ZN, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.91	3/42211 (0.0%)	1.23	404/65773 (0.6%)
2	P	0.46	0/1644	0.71	3/2249 (0.1%)
3	Q	0.45	0/1823	0.84	6/2447 (0.2%)
4	R	0.49	1/1656 (0.1%)	0.73	0/2251
5	S	0.53	0/2097	0.75	2/2823 (0.1%)
6	T	0.42	0/1839	0.72	0/2460
7	U	0.44	0/1498	0.71	1/2019 (0.0%)
8	V	0.50	0/1501	0.73	2/2006 (0.1%)
9	W	0.46	0/1504	0.75	1/2016 (0.0%)
10	X	0.54	0/1168	0.64	1/1575 (0.1%)
11	Y	0.49	0/1215	0.75	2/1638 (0.1%)
12	Z	0.44	0/934	0.77	1/1257 (0.1%)
13	a	0.51	0/682	0.89	4/921 (0.4%)
14	b	0.50	0/1038	0.76	1/1395 (0.1%)
15	c	0.53	0/1139	0.79	2/1518 (0.1%)
16	d	0.56	0/1087	0.76	2/1449 (0.1%)
17	e	0.46	0/778	0.71	0/1042
18	f	0.47	1/620 (0.2%)	0.74	0/838
19	g	0.43	0/480	0.76	1/639 (0.2%)
20	E	0.37	0/936	0.74	2/1259 (0.2%)
21	A	0.42	0/1754	0.71	2/2361 (0.1%)
22	B	0.39	0/1625	0.73	1/2197 (0.0%)
23	C	0.42	0/772	0.75	1/1044 (0.1%)
24	D	0.35	0/883	0.95	3/1199 (0.3%)
25	F	0.45	0/1125	0.83	3/1510 (0.2%)
26	H	0.41	0/957	0.83	2/1283 (0.2%)
27	I	0.34	0/1207	0.73	2/1623 (0.1%)
28	J	0.40	0/1130	0.73	2/1517 (0.1%)
29	K	0.43	0/807	0.76	1/1091 (0.1%)
30	L	0.38	0/661	0.81	3/888 (0.3%)
31	M	0.47	0/452	0.78	1/600 (0.2%)
32	N	0.36	0/571	0.87	2/768 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	O	0.38	0/2436	0.74	0/3318
34	h	0.45	0/493	0.75	0/663
35	y	0.35	0/631	0.81	2/851 (0.2%)
35	z	0.39	0/905	0.77	1/1213 (0.1%)
36	x	0.43	0/4695	0.78	7/6334 (0.1%)
All	All	0.71	5/86954 (0.0%)	1.03	468/126035 (0.4%)

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
35	y	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	111	VAL	CB-CG1	-6.11	1.40	1.52
1	2	142	G	C2-N3	-6.11	1.27	1.32
1	2	142	G	N3-C4	-5.50	1.31	1.35
1	2	555	A	N7-C5	-5.40	1.36	1.39
18	f	36	LYS	C-N	-5.17	1.22	1.34

The worst 5 of 468 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	453	U	C2-N1-C1'	12.85	133.12	117.70
1	2	453	U	N1-C2-O2	12.16	131.31	122.80
1	2	453	U	N3-C2-O2	-11.68	114.03	122.20
1	2	142	G	N3-C2-N2	-11.22	112.05	119.90
1	2	1639	C	N3-C2-O2	-10.89	114.28	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	y	213	GLN	Mainchain

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	
2	P	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
3	Q	222/232 (96%)	221 (100%)	1 (0%)	0	100	100
4	R	214/216 (99%)	213 (100%)	1 (0%)	0	100	100
5	S	256/258 (99%)	255 (100%)	1 (0%)	0	100	100
6	T	226/228 (99%)	223 (99%)	3 (1%)	0	100	100
7	U	182/184 (99%)	180 (99%)	2 (1%)	0	100	100
8	V	183/200 (92%)	183 (100%)	0	0	100	100
9	W	182/184 (99%)	181 (100%)	1 (0%)	0	100	100
10	X	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
11	Y	148/150 (99%)	148 (100%)	0	0	100	100
12	Z	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
13	a	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
14	b	127/129 (98%)	127 (100%)	0	0	100	100
15	c	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
16	d	132/134 (98%)	132 (100%)	0	0	100	100
17	e	95/97 (98%)	95 (100%)	0	0	100	100
18	f	79/81 (98%)	79 (100%)	0	0	100	100
19	g	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
20	E	115/117 (98%)	115 (100%)	0	0	100	100
21	A	220/222 (99%)	219 (100%)	1 (0%)	0	100	100
22	B	204/206 (99%)	204 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	C	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
24	D	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
25	F	139/141 (99%)	139 (100%)	0	0	100	100
26	H	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
27	I	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
28	J	141/143 (99%)	141 (100%)	0	0	100	100
29	K	98/100 (98%)	98 (100%)	0	0	100	100
30	L	80/82 (98%)	80 (100%)	0	0	100	100
31	M	51/53 (96%)	51 (100%)	0	0	100	100
32	N	71/73 (97%)	57 (80%)	10 (14%)	4 (6%)	2	10
33	O	310/312 (99%)	308 (99%)	2 (1%)	0	100	100
34	h	61/63 (97%)	61 (100%)	0	0	100	100
35	y	77/265 (29%)	76 (99%)	1 (1%)	0	100	100
35	z	118/265 (44%)	117 (99%)	1 (1%)	0	100	100
36	x	578/601 (96%)	577 (100%)	1 (0%)	0	100	100
All	All	5532/5985 (92%)	5484 (99%)	44 (1%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	N	140	TYR
32	N	141	CYS
32	N	120	GLU
32	N	98	VAL

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	
2	P	170/173 (98%)	169 (99%)	1 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	200/205 (98%)	200 (100%)	0	100	100
4	R	175/175 (100%)	175 (100%)	0	100	100
5	S	220/220 (100%)	219 (100%)	1 (0%)	88	96
6	T	189/195 (97%)	189 (100%)	0	100	100
7	U	163/165 (99%)	163 (100%)	0	100	100
8	V	148/161 (92%)	148 (100%)	0	100	100
9	W	156/157 (99%)	156 (100%)	0	100	100
10	X	126/127 (99%)	125 (99%)	1 (1%)	81	93
11	Y	127/127 (100%)	127 (100%)	0	100	100
12	Z	90/96 (94%)	90 (100%)	0	100	100
13	a	71/74 (96%)	71 (100%)	0	100	100
14	b	110/110 (100%)	109 (99%)	1 (1%)	78	92
15	c	119/119 (100%)	119 (100%)	0	100	100
16	d	112/112 (100%)	112 (100%)	0	100	100
17	e	82/83 (99%)	82 (100%)	0	100	100
18	f	70/70 (100%)	70 (100%)	0	100	100
19	g	50/51 (98%)	50 (100%)	0	100	100
20	E	95/98 (97%)	95 (100%)	0	100	100
21	A	182/182 (100%)	181 (100%)	1 (0%)	88	96
22	B	172/173 (99%)	172 (100%)	0	100	100
23	C	78/85 (92%)	77 (99%)	1 (1%)	69	89
24	D	88/98 (90%)	87 (99%)	1 (1%)	73	90
25	F	117/117 (100%)	117 (100%)	0	100	100
26	H	101/113 (89%)	100 (99%)	1 (1%)	76	91
27	I	127/128 (99%)	125 (98%)	2 (2%)	62	86
28	J	115/115 (100%)	115 (100%)	0	100	100
29	K	93/93 (100%)	93 (100%)	0	100	100
30	L	67/73 (92%)	67 (100%)	0	100	100
31	M	47/47 (100%)	47 (100%)	0	100	100
32	N	57/64 (89%)	47 (82%)	10 (18%)	2	10
33	O	250/257 (97%)	250 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	h	55/56 (98%)	55 (100%)	0	100	100
35	y	69/221 (31%)	69 (100%)	0	100	100
35	z	90/221 (41%)	89 (99%)	1 (1%)	73	90
36	x	516/531 (97%)	516 (100%)	0	100	100
All	All	4697/5092 (92%)	4676 (100%)	21 (0%)	91	97

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	N	125	THR
32	N	140	TYR
35	z	212	ARG
32	N	141	CYS
32	N	130	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
23	C	81	ASN
35	z	165	ASN
35	y	213	GLN
11	Y	36	GLN
13	a	7	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1768/1771 (99%)	521 (29%)	18 (1%)

5 of 521 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	6	G
1	2	11	A
1	2	25	C

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1382	A
1	2	1791	A
1	2	1694	A
1	2	711	U
1	2	1344	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 85 ligands modelled in this entry, 82 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
39	SF4	x	702	36	0,12,12	-	-	-		
40	ADP	x	703	37	24,29,29	0.94	1 (4%)	29,45,45	1.40	4 (13%)
39	SF4	x	701	36	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	SF4	x	701	36	-	-	0/6/5/5
39	SF4	x	702	36	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	ADP	x	703	37	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	x	703	ADP	C5-C4	2.45	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	x	703	ADP	PA-O3A-PB	-3.59	120.49	132.83
40	x	703	ADP	N3-C2-N1	-3.07	123.89	128.68
40	x	703	ADP	C4-C5-N7	-2.64	106.65	109.40
40	x	703	ADP	C3'-C2'-C1'	2.59	104.88	100.98

There are no chirality outliers.

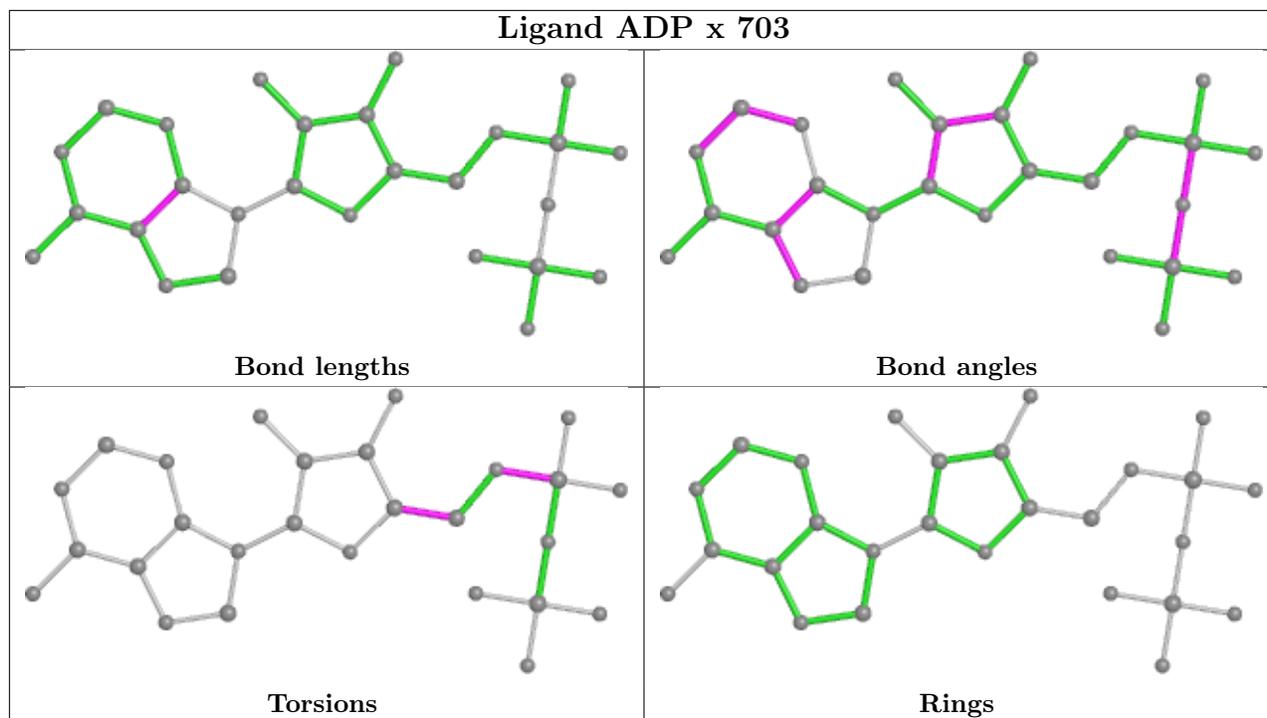
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	x	703	ADP	C5'-O5'-PA-O3A
40	x	703	ADP	C5'-O5'-PA-O1A
40	x	703	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	714:G	O3'	726:C	P	14.69
1	2	658:C	O3'	676:G	P	14.35

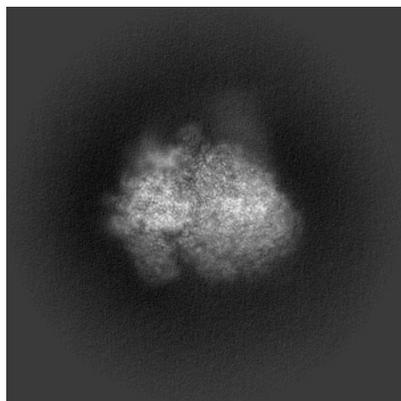
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11608. These allow visual inspection of the internal detail of the map and identification of artifacts.

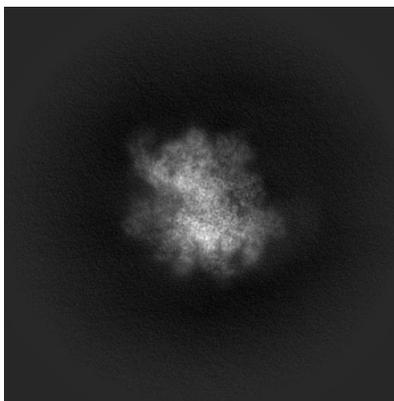
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

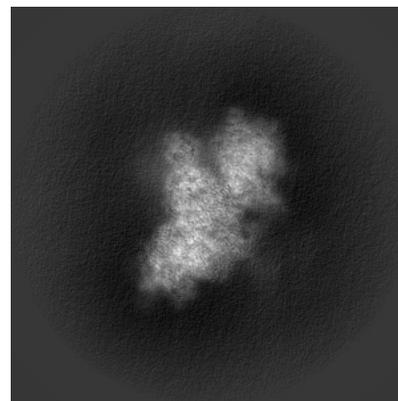
6.1.1 Primary map



X

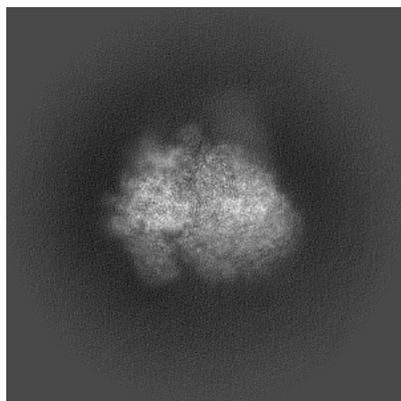


Y

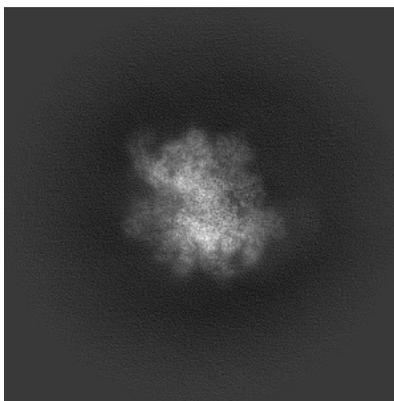


Z

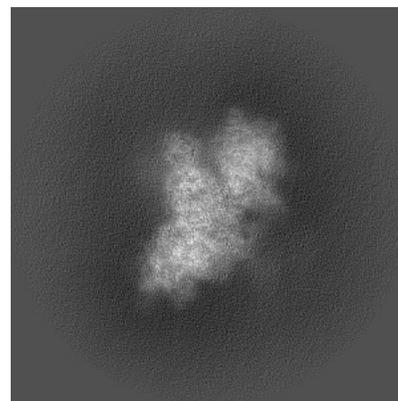
6.1.2 Raw map



X



Y

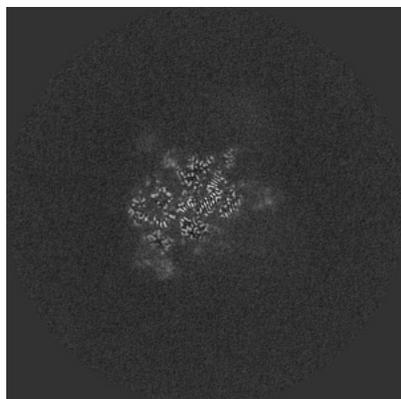


Z

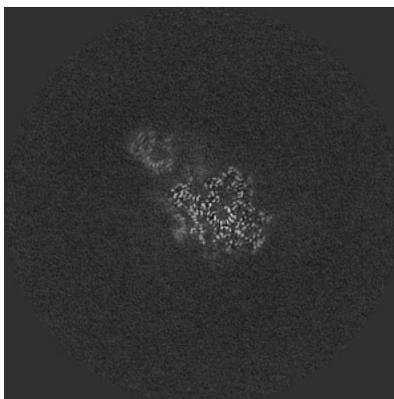
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

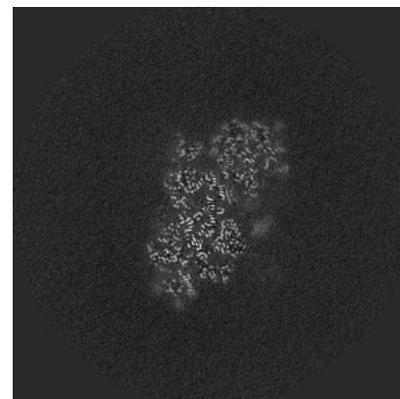
6.2.1 Primary map



X Index: 225

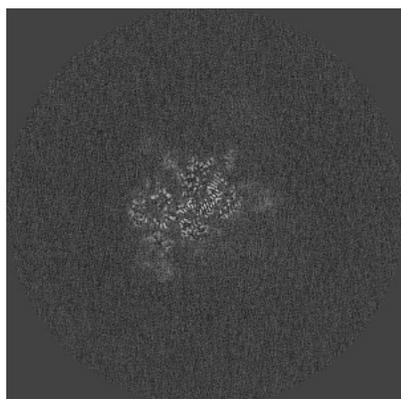


Y Index: 225

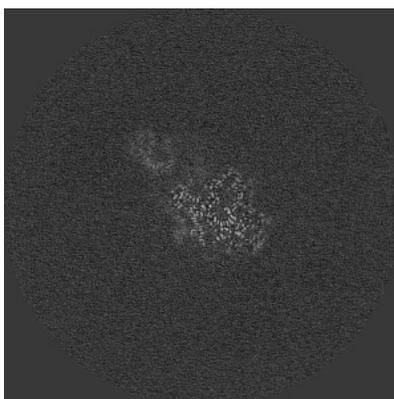


Z Index: 225

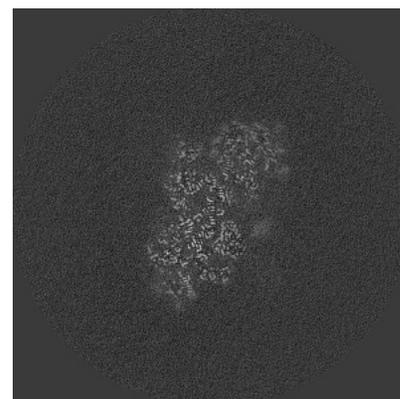
6.2.2 Raw map



X Index: 225



Y Index: 225

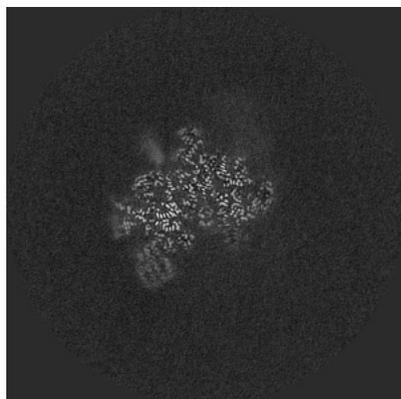


Z Index: 225

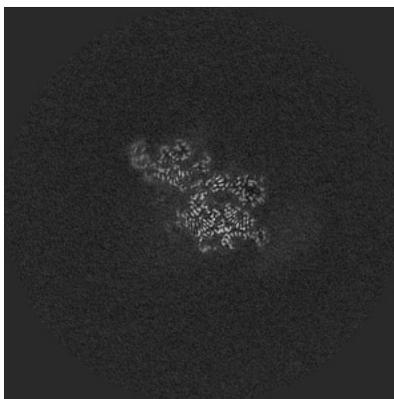
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

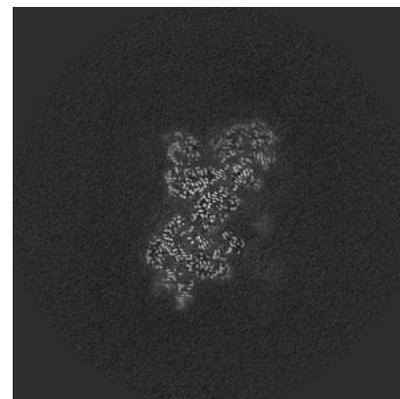
6.3.1 Primary map



X Index: 204

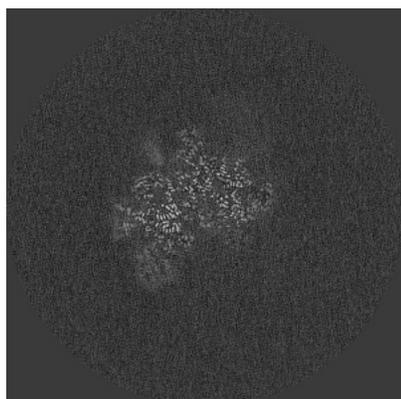


Y Index: 247

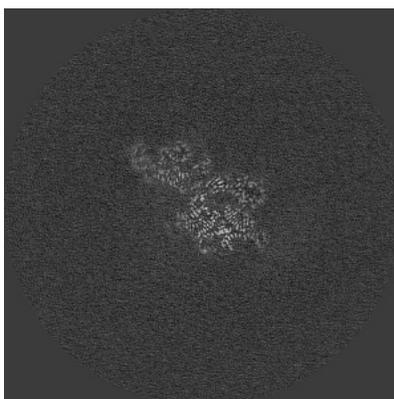


Z Index: 231

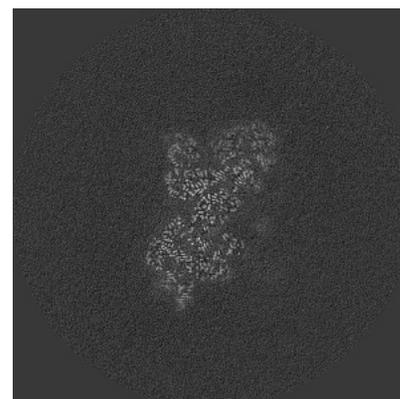
6.3.2 Raw map



X Index: 204



Y Index: 247

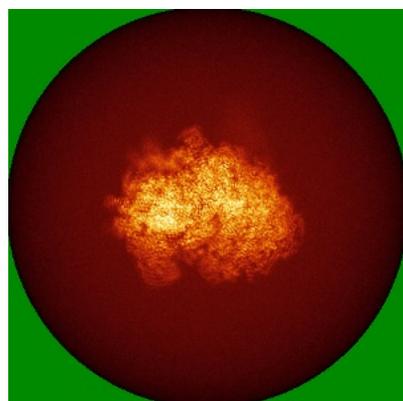


Z Index: 231

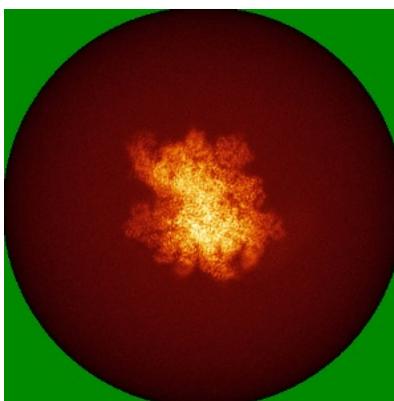
The images above show the largest variance slices of the map in three orthogonal directions.

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

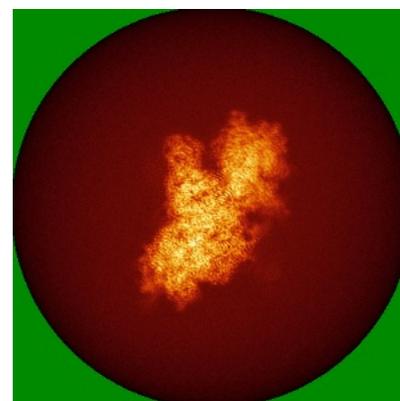
6.4.1 Primary map



X

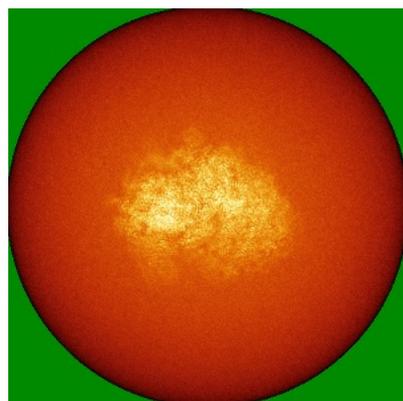


Y

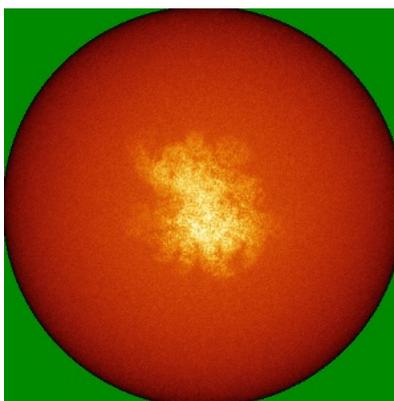


Z

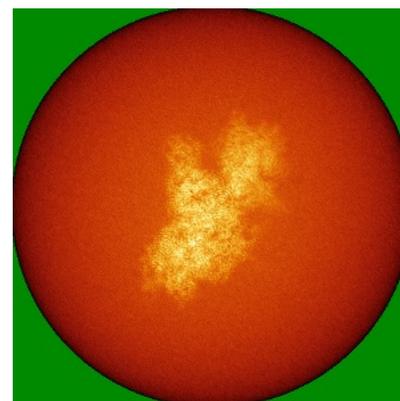
6.4.2 Raw map



X



Y

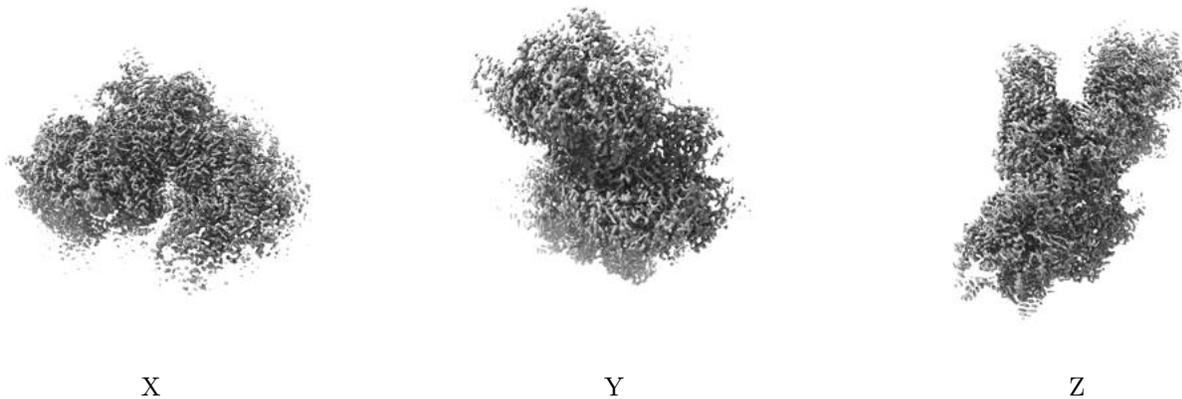


Z

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.

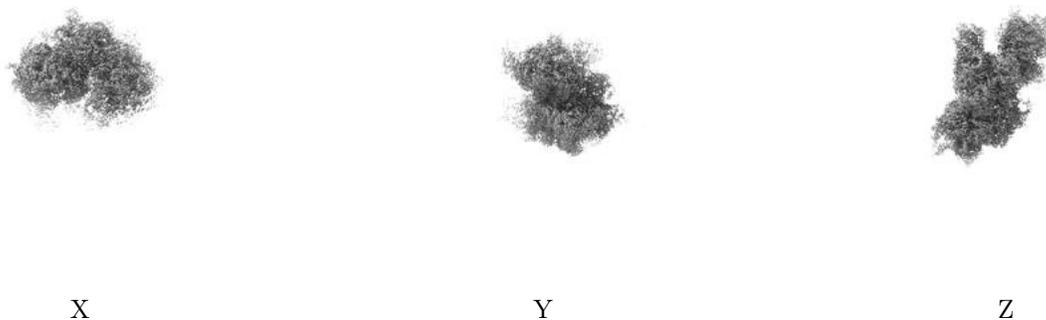
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

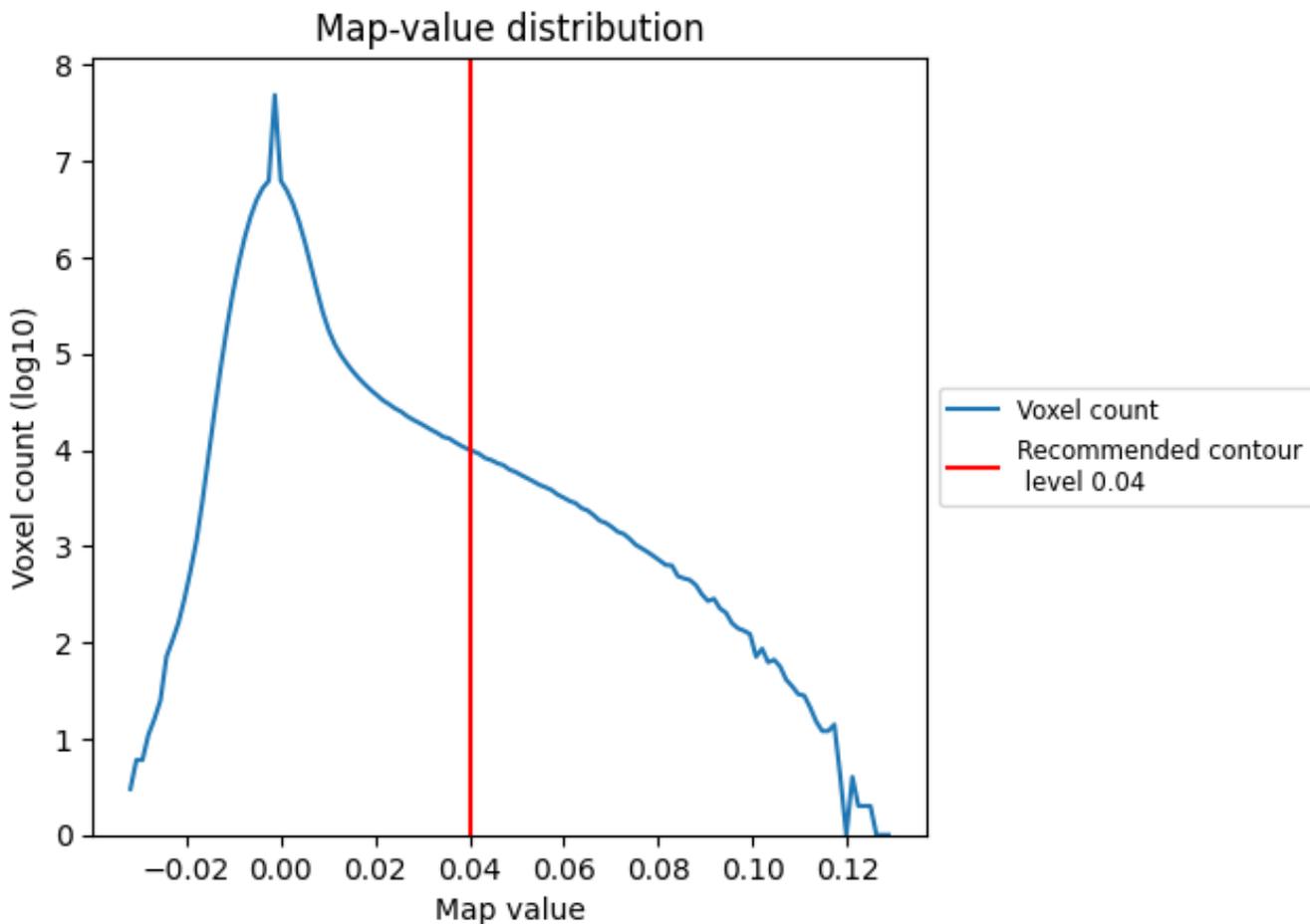
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

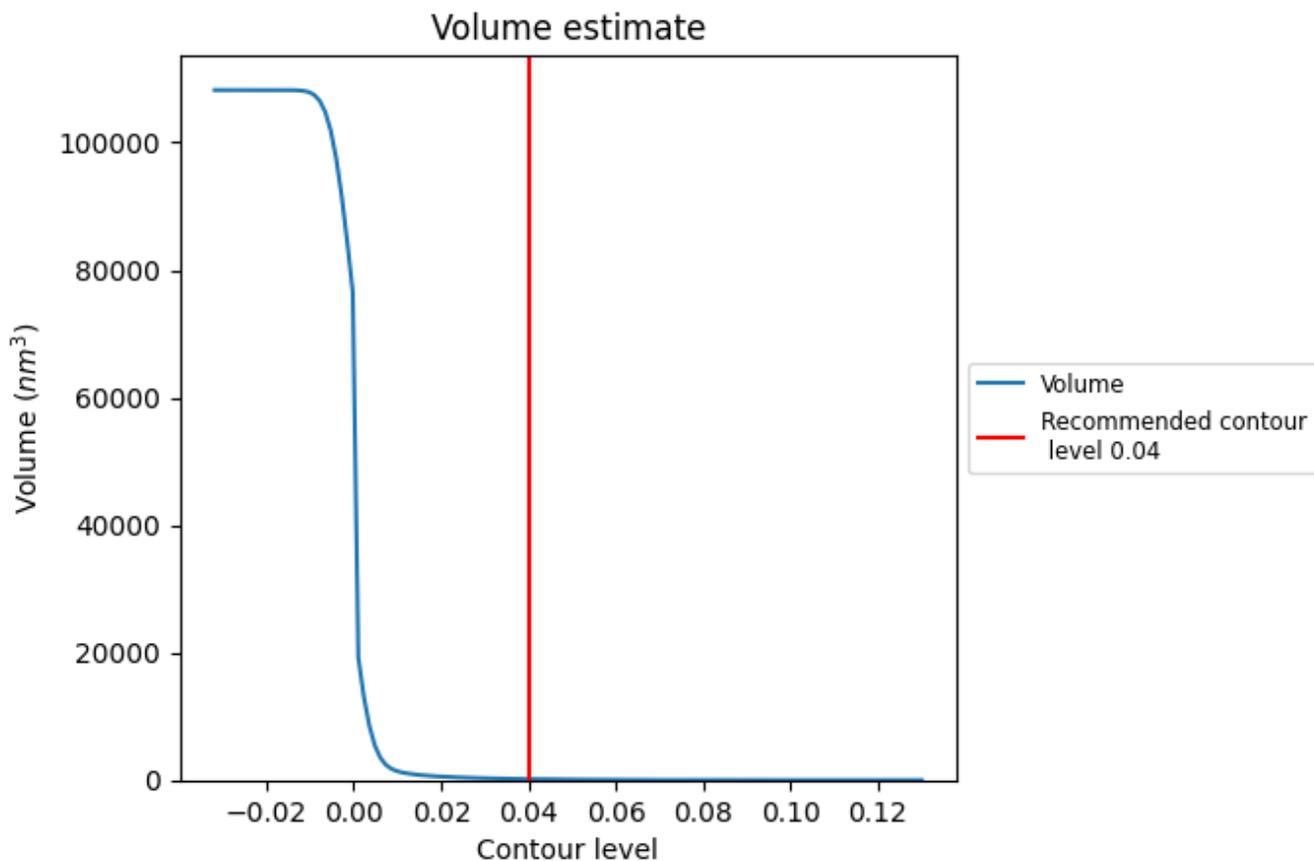
This section contains the results of statistical analysis of the map.

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.

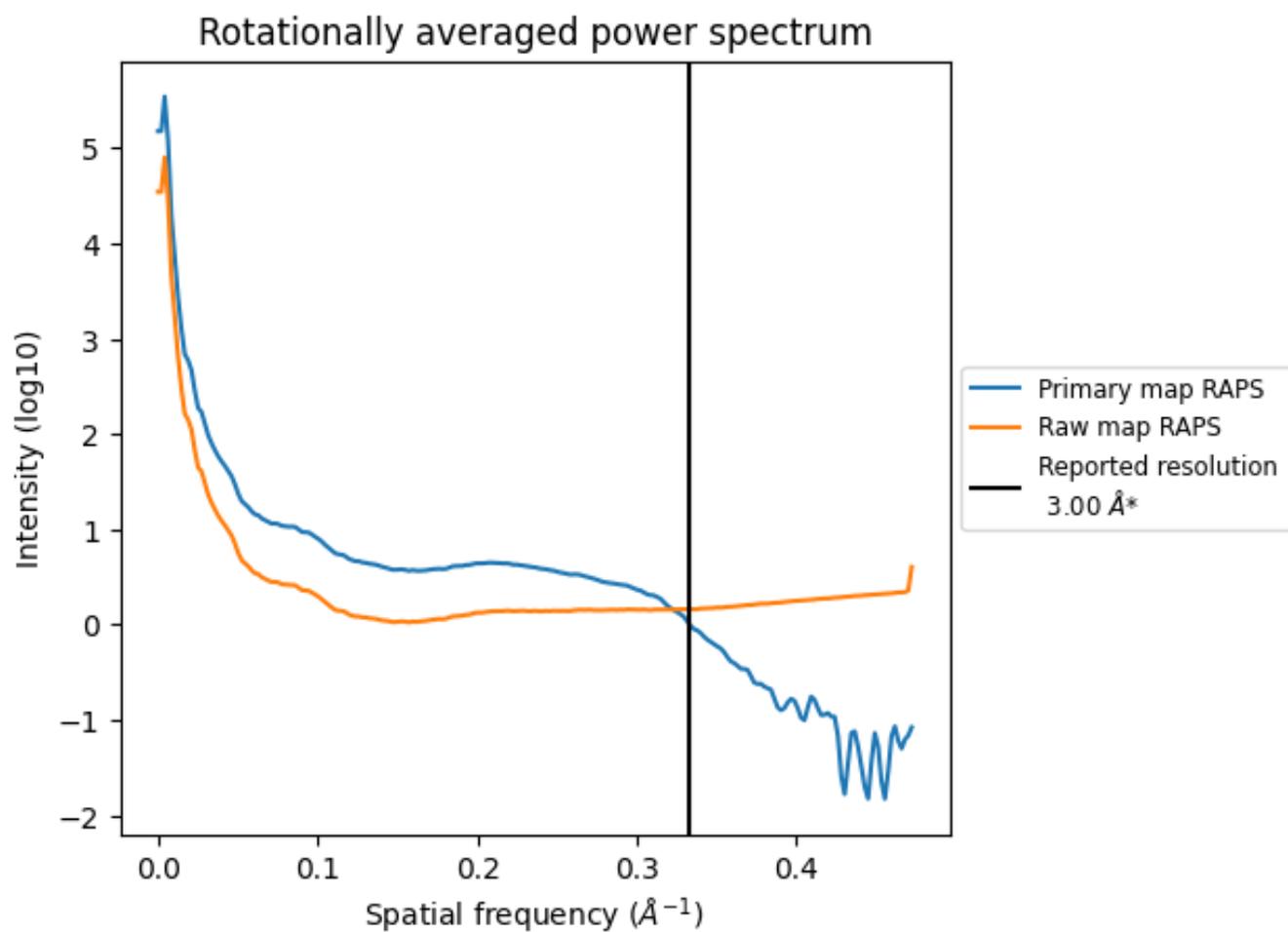
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 158 nm^3 ; this corresponds to an approximate mass of 143 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](#)

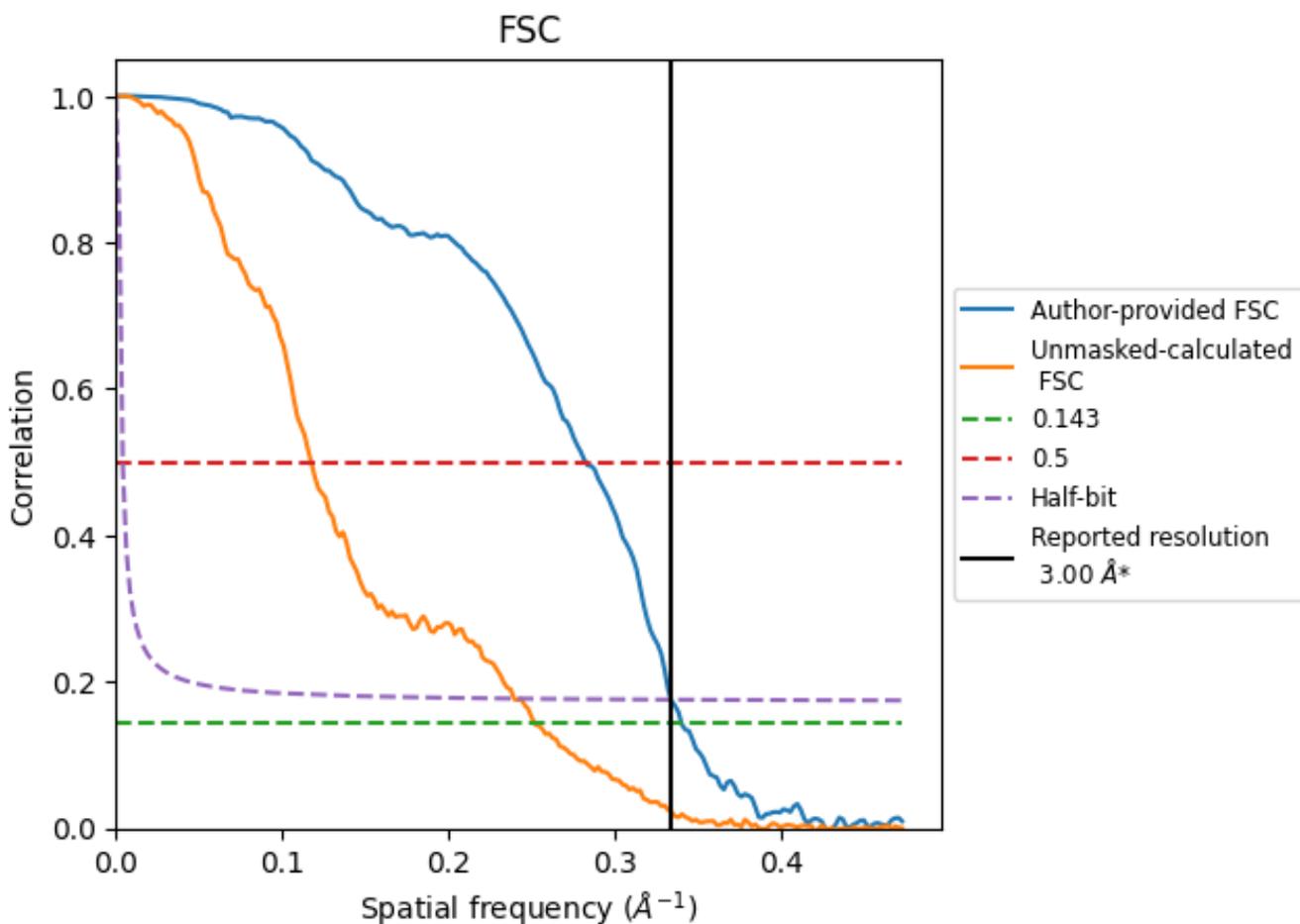


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates

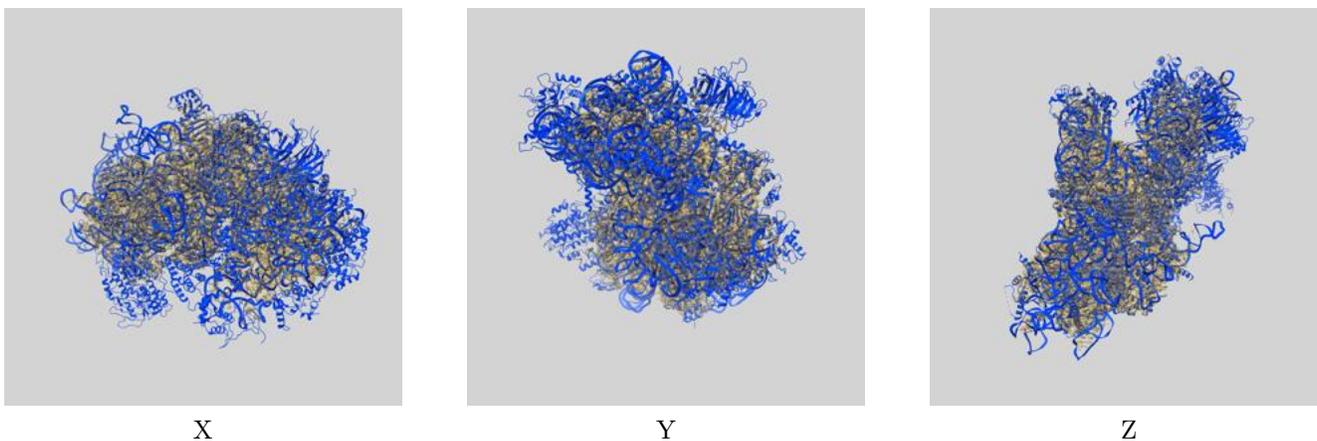
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.94	3.55	3.00
Unmasked-calculated*	3.98	8.53	4.18

*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 3.98 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

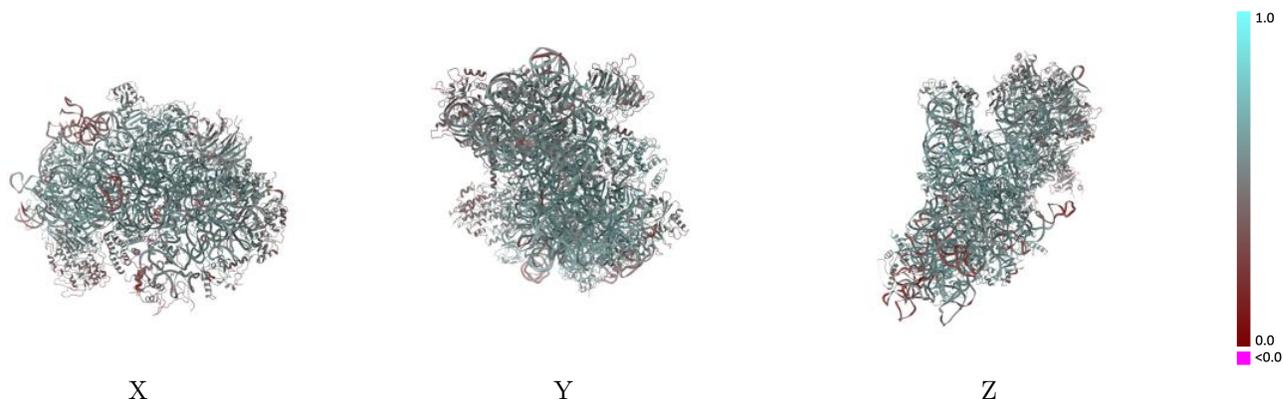
This section contains information regarding the fit between EMDB map EMD-11608 and PDB model 7A1G. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



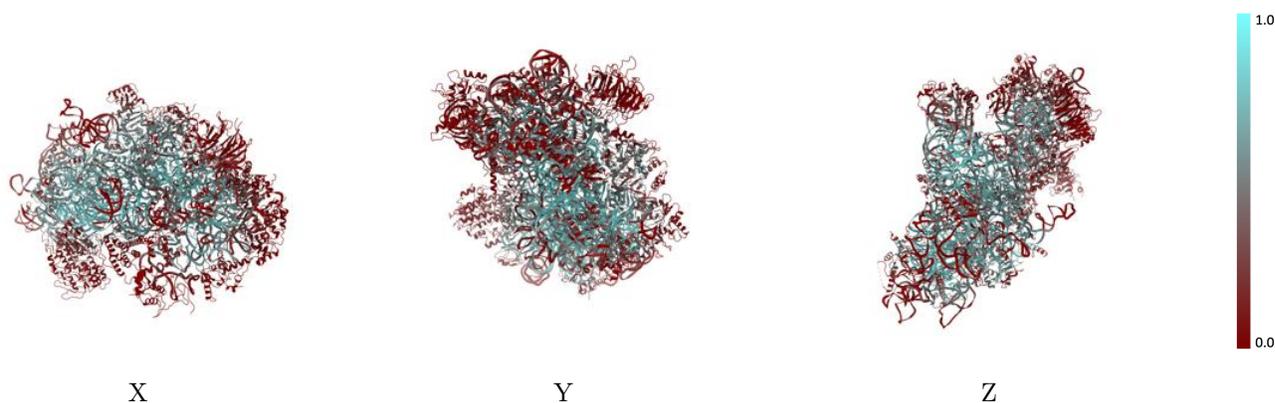
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



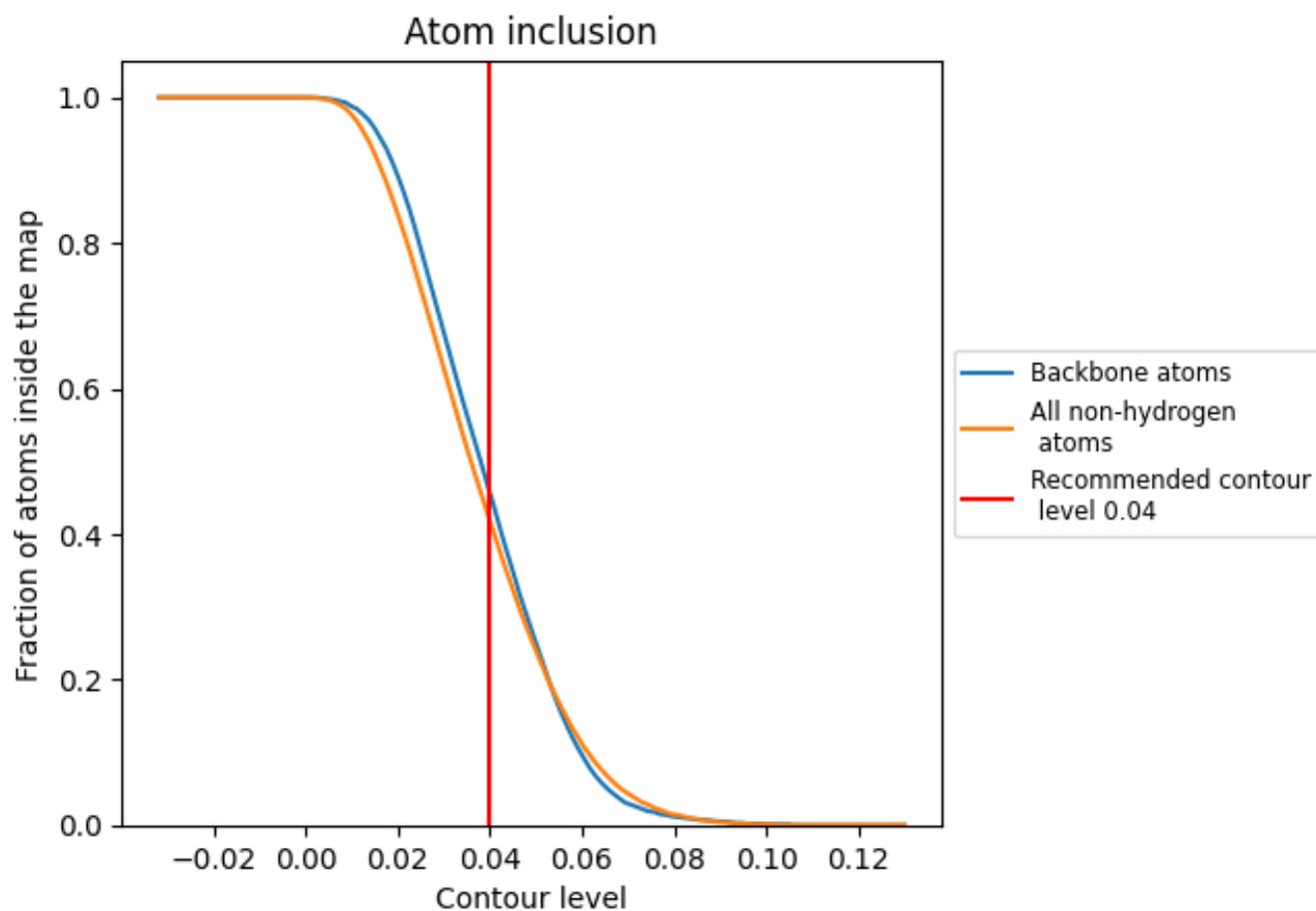
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)

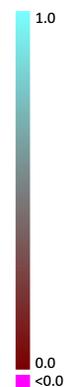


At the recommended contour level, 46% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4180	 0.5470
2	 0.5790	 0.5630
A	 0.2410	 0.5320
B	 0.1190	 0.5070
C	 0.1950	 0.5040
D	 0.0000	 0.3700
E	 0.0610	 0.4790
F	 0.2510	 0.5580
H	 0.2200	 0.5180
I	 0.0320	 0.4750
J	 0.1160	 0.5140
K	 0.2280	 0.5180
L	 0.0080	 0.4330
M	 0.4810	 0.6070
N	 0.0040	 0.3590
O	 0.0370	 0.4870
P	 0.4100	 0.5840
Q	 0.2670	 0.5460
R	 0.4640	 0.5970
S	 0.5300	 0.6030
T	 0.2970	 0.5510
U	 0.2290	 0.5190
V	 0.4880	 0.5850
W	 0.5070	 0.5900
X	 0.5770	 0.6060
Y	 0.4490	 0.5790
Z	 0.3000	 0.5650
a	 0.4330	 0.5830
b	 0.6070	 0.6170
c	 0.5580	 0.6020
d	 0.4390	 0.5600
e	 0.4670	 0.5970
f	 0.3780	 0.5760
g	 0.3640	 0.5370
h	 0.0590	 0.4960



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Chain	Atom inclusion	Q-score
x	 0.1330	 0.4760
y	 0.0210	 0.4770
z	 0.0470	 0.4800