



## wwPDB EM Validation Summary Report ⓘ

Jan 1, 2025 – 11:57 PM EST

PDB ID : 9E6Q  
EMDB ID : EMD-47578  
Title : Cryo-EM structure of the Pyrobaculum calidifontis 50S ribosomal subunit in complex with Dri  
Authors : Nissley, A.J.; Cate, J.H.D.  
Deposited on : 2024-10-30  
Resolution : 1.95 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](mailto: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>.

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

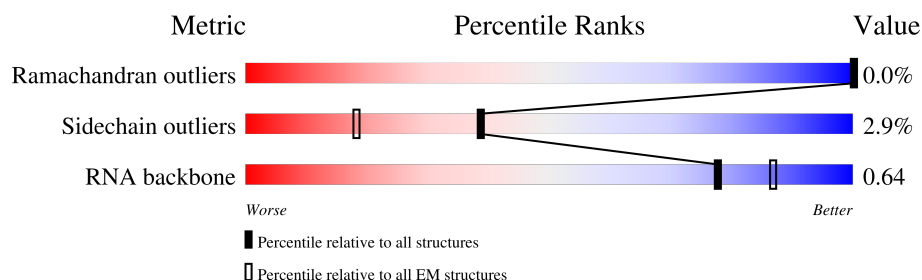
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

# 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 1.95 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	1	3024	
2	2	129	
3	3	655	
4	AA	244	
5	AB	338	
6	AC	285	
7	AD	178	
8	AE	196	

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Mol	Chain	Length	Quality of chain
9	AF	149	
10	AG	186	
11	AH	157	
12	AI	144	
13	AJ	103	
13	AK	103	
14	AL	156	
15	AM	189	
16	AN	178	
17	AO	205	
18	AP	122	
19	AQ	147	
20	AR	78	
21	AS	99	
22	AT	184	
23	AU	81	
24	AV	128	
25	AW	62	
26	AX	79	
27	AY	179	
28	AZ	101	
29	Aa	91	
30	Ab	153	
31	Ac	84	
32	Ad	52	

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Mol	Chain	Length	Quality of chain
33	Ae	67	<div><div></div><div>9%</div><div>99%</div><div></div></div>
34	Af	51	<div><div></div><div></div><div>96%</div><div></div></div>
35	Ag	53	<div><div></div><div>23%</div><div>92%</div><div>6%</div></div>
36	Ah	91	<div><div></div><div></div><div>98%</div><div></div></div>
37	Ai	102	<div><div></div><div>23%</div><div>94%</div><div></div></div>
38	Aj	184	<div><div></div><div>12%</div><div>96%</div><div></div></div>
39	Ak	93	<div><div></div><div>9%</div><div>92%</div><div></div></div>

## 2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 114588 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2842	Total	C	N	O	P	0	0
			61237	27268	11426	19701	2842		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	129	Total	C	N	O	P	0	0
			2769	1231	512	897	129		

- Molecule 3 is a protein called Putative signal-transduction protein with CBS domains.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	290	Total	C	N	O	S	0	0
			2272	1470	400	399	3		

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AA	239	Total	C	N	O	S	0	0
			1803	1136	354	308	5		

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AB	336	Total	C	N	O	S	0	0
			2611	1681	476	450	4		

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AC	278	Total	C	N	O	S	0	0
			2178	1406	395	371	6		

- Molecule 7 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AD	178	Total	C	N	O	S	0	0
			1412	894	273	238	7		

- Molecule 8 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AE	195	Total	C	N	O	S	0	0
			1520	990	254	272	4		

- Molecule 9 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AF	145	Total	C	N	O	S	0	0
			1095	705	187	202	1		

- Molecule 10 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AG	183	Total	C	N	O	S	0	0
			1510	979	278	246	7		

- Molecule 11 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AH	155	Total	C	N	O	S	0	0
			1244	785	249	209	1		

- Molecule 12 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AI	138	Total	C	N	O	S	0	0
			1068	682	202	181	3		

- Molecule 13 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AJ	101	Total	C	N	O	S	0	0
			788	500	143	144	1		
13	AK	90	Total	C	N	O	S	0	0
			700	441	130	128	1		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AL	152	Total	C	N	O	S	0	0
			1198	761	232	202	3		

- Molecule 15 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AM	184	Total	C	N	O	S	0	0
			1558	992	315	245	6		

- Molecule 16 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AN	169	Total	C	N	O	S	0	0
			1336	847	254	227	8		

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AO	200	Total	C	N	O	S	0	0
			1615	1027	309	278	1		

- Molecule 18 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AP	121	Total	C	N	O	S	0	0
			920	583	181	155	1		

- Molecule 19 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AQ	146	Total	C	N	O	S	0	0
			1214	759	244	208	3		

- Molecule 20 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AR	76	Total	C	N	O	S	0	0
			603	382	109	109	3		

- Molecule 21 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AS	98	Total	C	N	O	S	0	0
			788	503	150	134	1		

- Molecule 22 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AT	183	Total	C	N	O	S	0	0
			1496	978	268	247	3		

- Molecule 23 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AU	81	Total	C	N	O	S	0	0
			651	417	115	117	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AV	121	Total	C	N	O	S	0	0
			976	619	194	161	2		

- Molecule 25 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AW	56	Total	C	N	O	S	0	0
			449	287	86	70	6		

- Molecule 26 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AX	67	Total	C	N	O	S	0	0
			554	343	117	92	2		

- Molecule 27 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AY	172	Total	C	N	O	S	0	0
			1374	888	245	235	6		

- Molecule 28 is a protein called Large ribosomal subunit protein eL30.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	AZ	98	Total	C	N	O	S	0	0
			742	481	128	132	1		

- Molecule 29 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Aa	88	Total	C	N	O		0	0
			726	460	146	120			

- Molecule 30 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ab	140	Total	C	N	O	S	0	0
			1183	757	239	186	1		

- Molecule 31 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ac	83	Total	C	N	O	S	0	0
			649	407	138	102	2		

- Molecule 32 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ad	52	Total	C	N	O	S	0	0
			429	265	93	65	6		

- Molecule 33 is a protein called LSU ribosomal protein L38E.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ae	66	Total	C	N	O		0	0
			552	363	93	96			

- Molecule 34 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Af	50	Total	C	N	O		0	0
			415	260	96	59			

- Molecule 35 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ag	50	Total	C	N	O	S	0	0
			417	259	88	66	4		

- Molecule 36 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ah	91	Total	C	N	O	S	0	0
			739	467	142	123	7		

- Molecule 37 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ai	99	Total	C	N	O	S	0	0
			769	489	148	127	5		

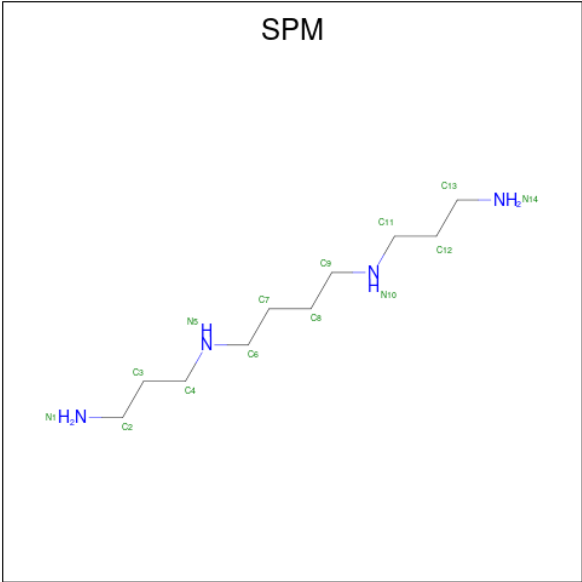
- Molecule 38 is a protein called DJ-1/PfpI domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Aj	183	Total	C	N	O	S	0	0
			1469	954	248	265	2		

- Molecule 39 is a protein called PaREP1 domain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ak	90	Total	C	N	O	S	0	0
			743	478	127	136	2		

- Molecule 40 is SPERMINE (three-letter code: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	AL	1	Total	C	N	0
			14	10	4	
40	AM	1	Total	C	N	0
			14	10	4	

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
41	1	168	Total	Mg	0
			168	168	
41	AA	1	Total	Mg	0
			1	1	
41	AL	2	Total	Mg	0
			2	2	
41	AN	1	Total	Mg	0
			1	1	
41	AT	1	Total	Mg	0
			1	1	

- Molecule 42 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
42	AW	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
42	Ad	1	Total 1	Zn 1	0
42	Ag	1	Total 1	Zn 1	0
42	Ah	1	Total 1	Zn 1	0
42	Ai	1	Total 1	Zn 1	0

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		AltConf
43	1	6534	Total 6534	O 6534	0
43	2	147	Total 147	O 147	0
43	3	58	Total 58	O 58	0
43	AA	83	Total 83	O 83	0
43	AB	85	Total 85	O 85	0
43	AC	83	Total 83	O 83	0
43	AD	16	Total 16	O 16	0
43	AE	22	Total 22	O 22	0
43	AF	19	Total 19	O 19	0
43	AG	50	Total 50	O 50	0
43	AH	49	Total 49	O 49	0
43	AI	30	Total 30	O 30	0
43	AJ	13	Total 13	O 13	0
43	AK	15	Total 15	O 15	0
43	AL	49	Total 49	O 49	0

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Mol	Chain	Residues	Atoms		AltConf
43	AM	66	Total 66	O 66	0
43	AN	51	Total 51	O 51	0
43	AO	32	Total 32	O 32	0
43	AP	28	Total 28	O 28	0
43	AQ	45	Total 45	O 45	0
43	AR	13	Total 13	O 13	0
43	AS	37	Total 37	O 37	0
43	AT	46	Total 46	O 46	0
43	AU	22	Total 22	O 22	0
43	AV	30	Total 30	O 30	0
43	AW	13	Total 13	O 13	0
43	AX	32	Total 32	O 32	0
43	AY	38	Total 38	O 38	0
43	AZ	18	Total 18	O 18	0
43	Aa	22	Total 22	O 22	0
43	Ab	42	Total 42	O 42	0
43	Ac	21	Total 21	O 21	0
43	Ad	26	Total 26	O 26	0
43	Ae	17	Total 17	O 17	0
43	Af	18	Total 18	O 18	0
43	Ag	11	Total 11	O 11	0

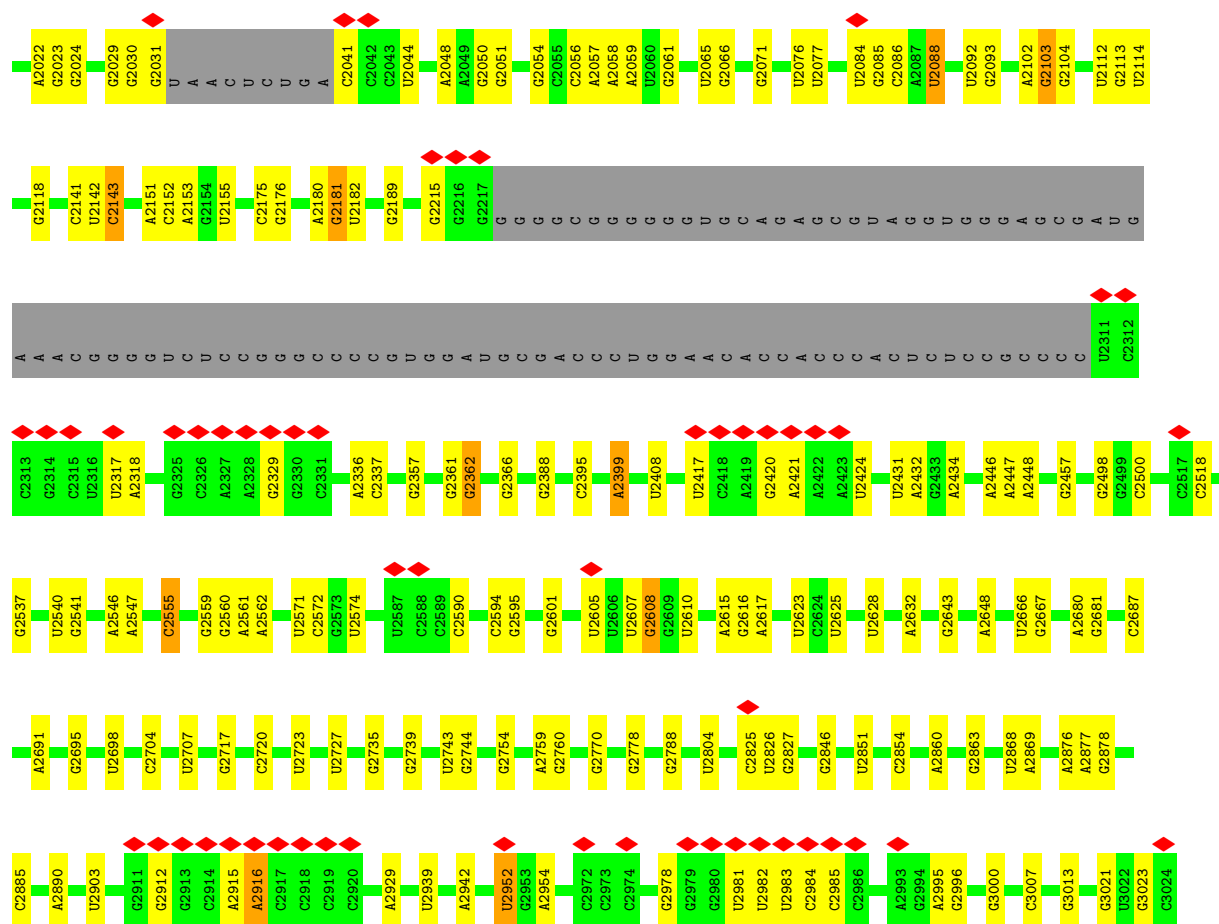
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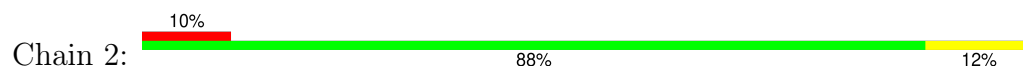
Mol	Chain	Residues	Atoms		AltConf
43	Ah	26	Total 26	O 26	0
43	Ai	34	Total 34	O 34	0
43	Aj	41	Total 41	O 41	0
43	Ak	12	Total 12	O 12	0



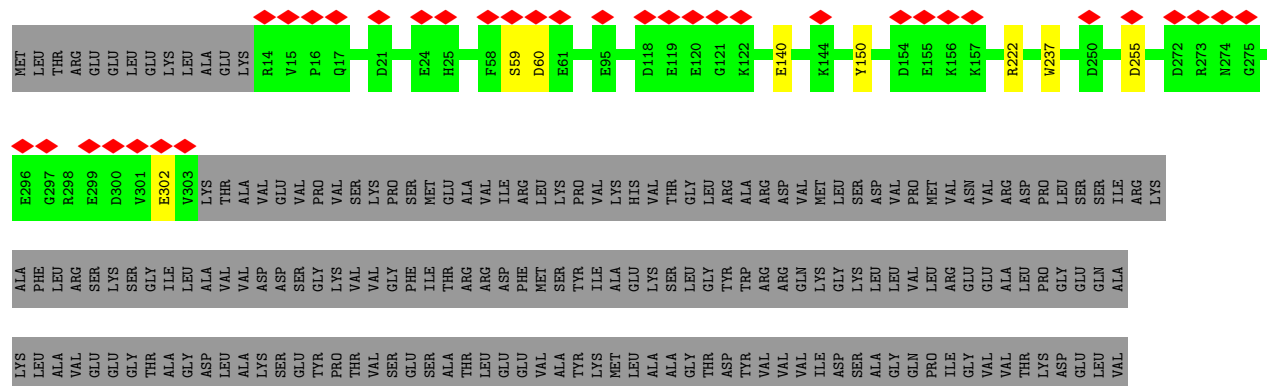




### • Molecule 2: 5S rRNA



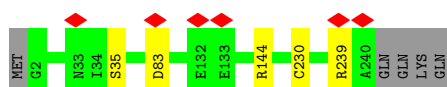
### • Molecule 3: Putative signal-transduction protein with CBS domains



LYS	ASP	ASP	ASP
LEU	LEU	VAL	VAL
TYR	ALA	LYS	LYS
	LEU	VAL	GLU
	ARG	PRO	ARG
	GLU	VAL	GLY
	ARG	ASP	ARG
	GLY	LYS	SER
	SER	LEU	VAL
	THR	THR	VAL
	VAL	GLN	VAL
	LYS	GLY	GLY
	VAL	VAL	GLU
	GLU	ARG	LEU
	LEU	PRO	MET
	THR	VAL	THR
	PRO	TYR	ALA
	ASP	PHE	ASP
	VAL	THR	THR
	ALA	LYS	LYS
	ALA	GLY	LEU
	VAL	ARG	ARG
	ASN	VAL	LYS
	PRO	GLY	ASN
	PHE	VAL	ALA
	LYS	THR	VAL
	SER	THR	GLY
	GLY	LEU	ASP
	MET	ILE	GLY
	SER	VAL	VAL
	THR	ASP	VAL
	THR	LYS	GLU
	GLY	ALA	GLY
	VAL	LEU	GLY
	VAL	PRO	ASN
	VAL	VAL	ILE
	VAL	ASP	HIS
	VAL	VAL	VAL
	VAL	GLN	GLY
	VAL	GLU	VAL
	VAL	GLU	VAL
	VAL	GLU	THR
	VAL	GLU	VAL
	VAL	GLU	ASP

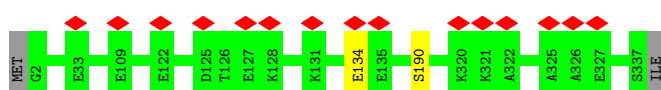
- Molecule 4: Large ribosomal subunit protein uL2

Chain AA:  96%



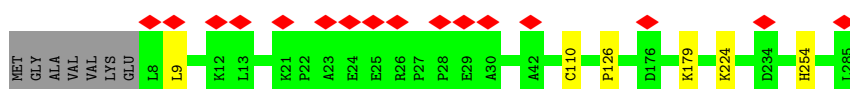
- Molecule 5: Large ribosomal subunit protein uL3

Chain AB:  99%

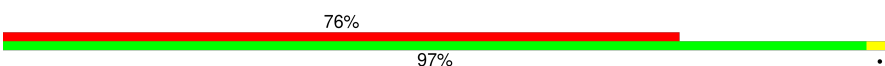


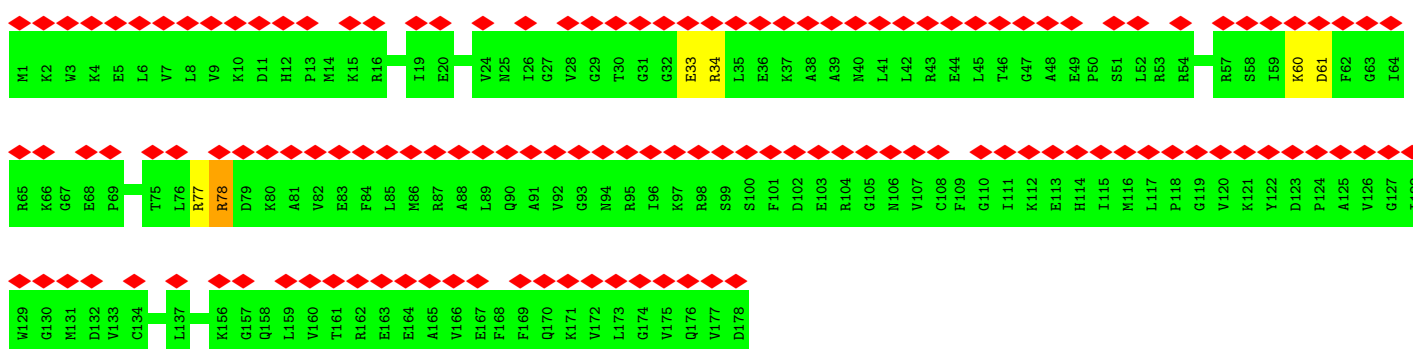
- Molecule 6: Large ribosomal subunit protein uL4

Chain AC:  6% 95%



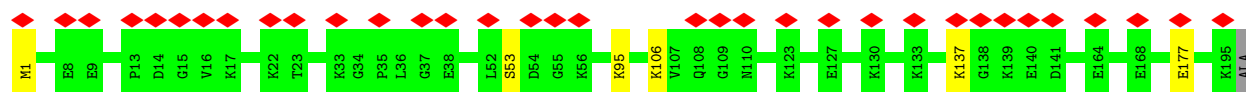
- Molecule 7: Large ribosomal subunit protein uL5

Chain AD:  76% 97%

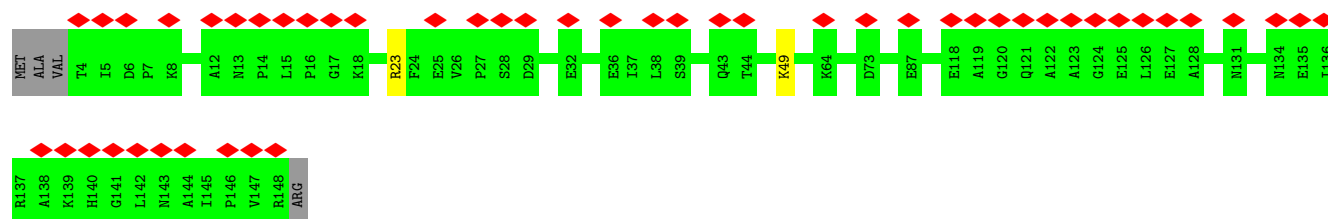


- Molecule 8: Large ribosomal subunit protein uL6

Chain AE:  17% 96%



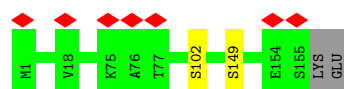
- Molecule 9: Large ribosomal subunit protein eL8



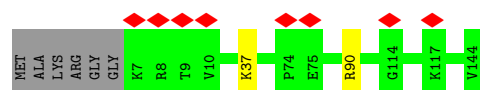
- Molecule 10: Large ribosomal subunit protein uL13



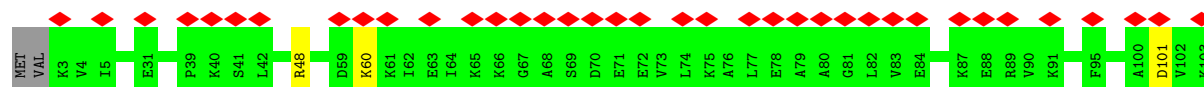
- Molecule 11: Large ribosomal subunit protein eL13



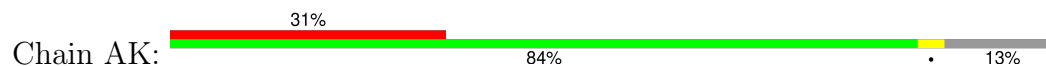
- Molecule 12: Large ribosomal subunit protein uL14

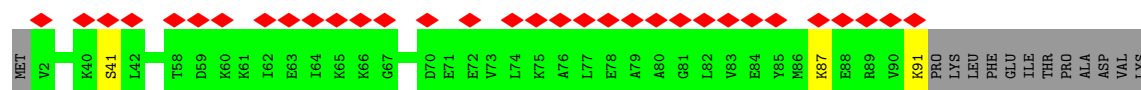


- Molecule 13: eL14

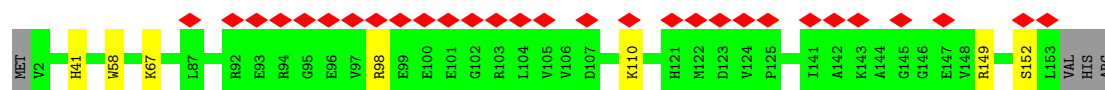


- Molecule 13: eL14

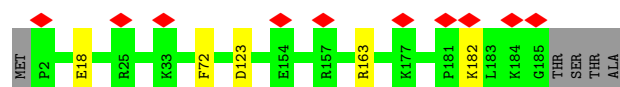




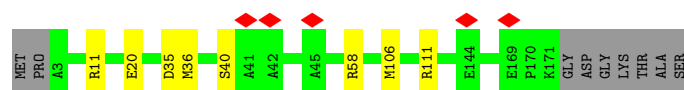
- Molecule 14: Large ribosomal subunit protein uL15



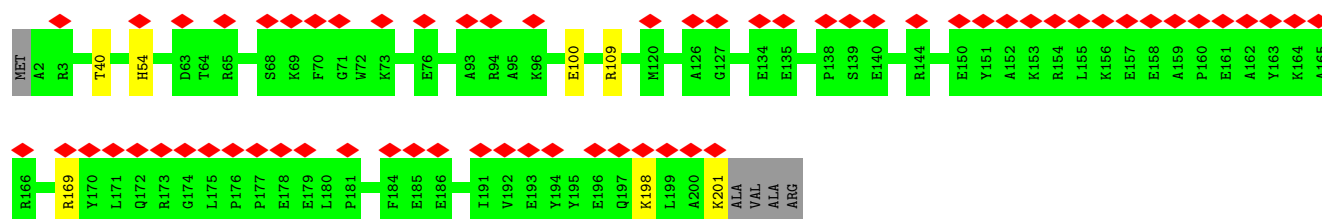
- Molecule 15: 50S ribosomal protein L15e



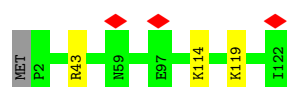
- Molecule 16: Large ribosomal subunit protein uL16



- Molecule 17: Large ribosomal subunit protein uL18

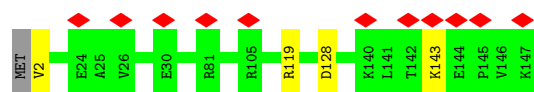


- Molecule 18: Large ribosomal subunit protein eL18

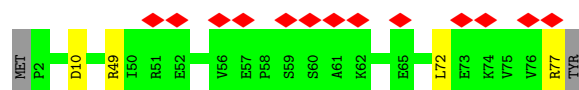


- Molecule 19: Large ribosomal subunit protein eL19

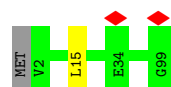




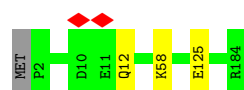
- Molecule 20: Large ribosomal subunit protein eL20



- Molecule 21: Large ribosomal subunit protein eL21



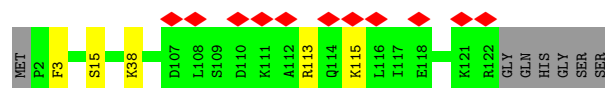
- Molecule 22: Large ribosomal subunit protein uL22



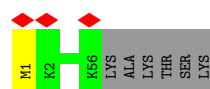
- Molecule 23: Large ribosomal subunit protein uL23



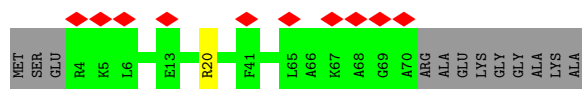
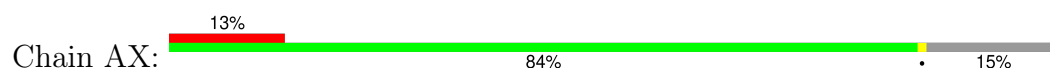
- Molecule 24: Large ribosomal subunit protein uL24



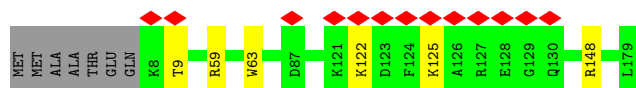
- Molecule 25: Large ribosomal subunit protein eL24



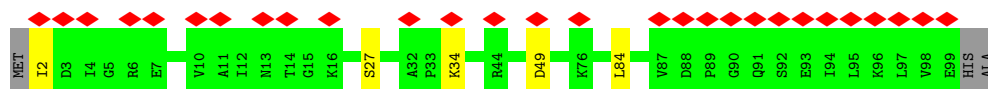
- Molecule 26: Large ribosomal subunit protein uL29



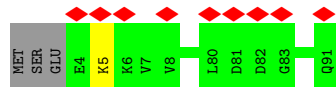
- Molecule 27: Large ribosomal subunit protein uL30



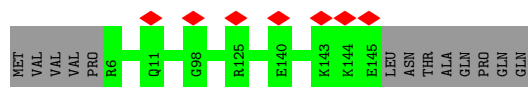
- Molecule 28: Large ribosomal subunit protein eL30



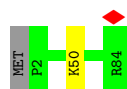
- Molecule 29: Large ribosomal subunit protein eL31



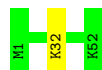
- Molecule 30: Large ribosomal subunit protein eL32



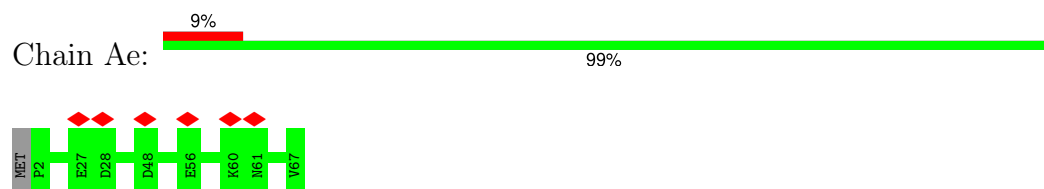
- Molecule 31: Large ribosomal subunit protein eL34



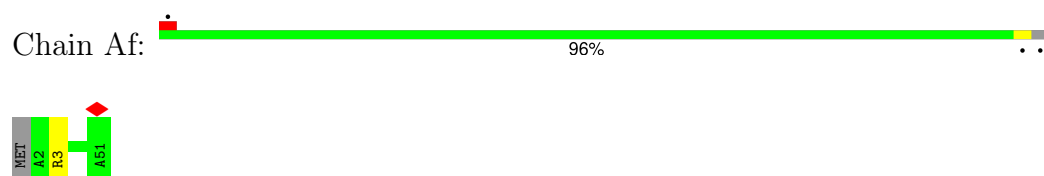
- Molecule 32: Large ribosomal subunit protein eL37



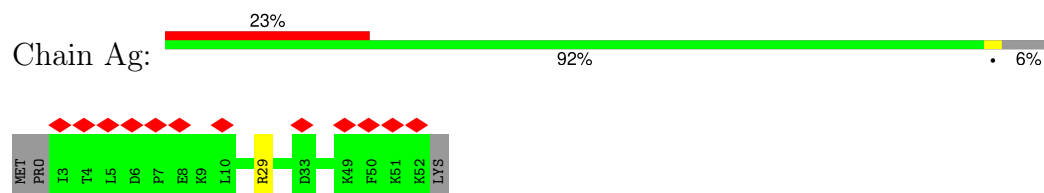
- Molecule 33: LSU ribosomal protein L38E



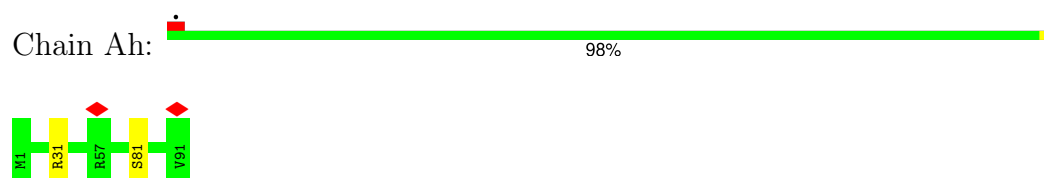
- Molecule 34: Large ribosomal subunit protein eL39



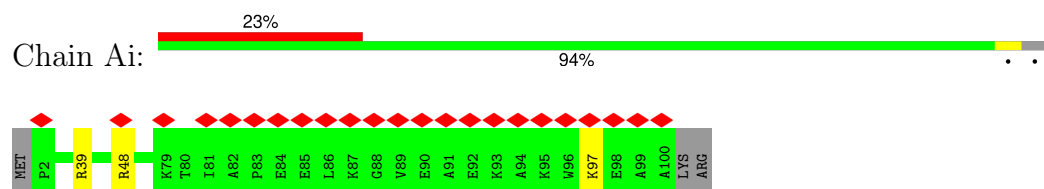
- Molecule 35: Large ribosomal subunit protein eL40



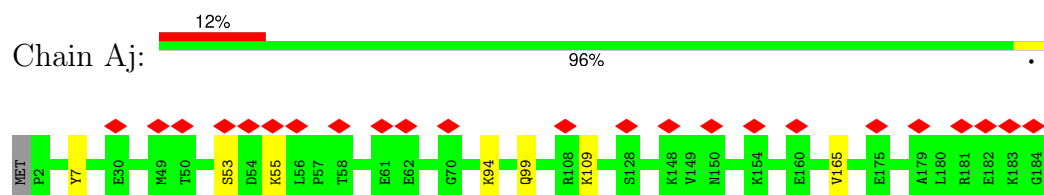
- Molecule 36: eL42



- Molecule 37: Large ribosomal subunit protein eL43



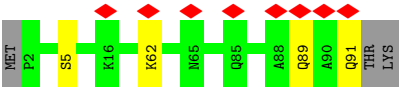
- Molecule 38: DJ-1/PfpI domain-containing protein



- Molecule 39: PaREP1 domain containing protein







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.352	Depositor
Minimum map value	-0.518	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.152	Depositor
Map size (Å)	504.2144, 504.2144, 504.2144	wwPDB
Map dimensions	608, 608, 608	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8293, 0.8293, 0.8293	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8T, MG, 5MC, UR3, OMC, ZN, A2M, OMU, SPM, OMG, 4AC, PSU, G7M

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	1	0.87	0/66967	0.86	41/104542 (0.0%)
2	2	0.70	0/3096	0.84	1/4830 (0.0%)
3	3	0.37	0/2323	0.53	0/3153
4	AA	0.42	0/1847	0.61	0/2489
5	AB	0.41	0/2678	0.57	0/3643
6	AC	0.38	0/2234	0.54	0/3024
7	AD	0.33	0/1431	0.58	0/1913
8	AE	0.38	0/1548	0.53	0/2087
9	AF	0.33	0/1114	0.49	0/1513
10	AG	0.38	0/1542	0.54	0/2076
11	AH	0.35	0/1265	0.57	0/1692
12	AI	0.39	0/1093	0.59	0/1487
13	AJ	0.33	0/795	0.54	0/1068
13	AK	0.36	0/704	0.57	0/944
14	AL	0.37	0/1225	0.58	0/1639
15	AM	0.40	0/1594	0.60	0/2138
16	AN	0.38	0/1365	0.57	0/1841
17	AO	0.34	0/1647	0.57	0/2212
18	AP	0.34	0/933	0.55	0/1263
19	AQ	0.34	0/1233	0.57	0/1645
20	AR	0.38	0/610	0.55	0/817
21	AS	0.43	0/805	0.60	0/1081
22	AT	0.37	0/1536	0.51	0/2075
23	AU	0.35	0/655	0.53	0/877
24	AV	0.35	0/990	0.58	0/1325
25	AW	0.40	0/460	0.56	0/613
26	AX	0.31	0/557	0.58	0/738
27	AY	0.38	0/1407	0.55	0/1905
28	AZ	0.31	0/754	0.52	0/1021
29	Aa	0.37	0/735	0.58	0/986
30	Ab	0.37	0/1209	0.59	0/1621
31	Ac	0.41	0/663	0.62	0/889

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Ad	0.43	0/442	0.60	0/587
33	Ae	0.39	0/562	0.46	0/753
34	Af	0.34	0/423	0.62	0/566
35	Ag	0.34	0/424	0.58	0/564
36	Ah	0.40	0/753	0.54	0/1001
37	Ai	0.37	0/788	0.58	0/1057
38	Aj	0.36	0/1497	0.53	0/2029
39	Ak	0.34	0/754	0.45	0/1005
All	All	0.72	0/112658	0.77	42/166709 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	AD	0	2

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2030	G	P-O3'-C3'	-11.54	105.85	119.70
1	1	2041	C	P-O3'-C3'	-10.63	106.94	119.70
1	1	1677	G	P-O3'-C3'	-10.20	107.46	119.70
1	1	2903	U	P-O3'-C3'	-9.81	107.93	119.70
1	1	1678	G	P-O3'-C3'	-8.99	108.91	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	AD	77	ARG	Sidechain
7	AD	78	ARG	Sidechain

## 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 ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	288/655 (44%)	282 (98%)	6 (2%)	0	100	100
4	AA	237/244 (97%)	229 (97%)	8 (3%)	0	100	100
5	AB	334/338 (99%)	327 (98%)	7 (2%)	0	100	100
6	AC	276/285 (97%)	267 (97%)	9 (3%)	0	100	100
7	AD	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
8	AE	193/196 (98%)	190 (98%)	3 (2%)	0	100	100
9	AF	143/149 (96%)	141 (99%)	2 (1%)	0	100	100
10	AG	181/186 (97%)	180 (99%)	1 (1%)	0	100	100
11	AH	153/157 (98%)	152 (99%)	1 (1%)	0	100	100
12	AI	136/144 (94%)	134 (98%)	2 (2%)	0	100	100
13	AJ	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
13	AK	88/103 (85%)	84 (96%)	3 (3%)	1 (1%)	12	4
14	AL	150/156 (96%)	144 (96%)	6 (4%)	0	100	100
15	AM	182/189 (96%)	179 (98%)	3 (2%)	0	100	100
16	AN	167/178 (94%)	165 (99%)	2 (1%)	0	100	100
17	AO	198/205 (97%)	197 (100%)	1 (0%)	0	100	100
18	AP	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
19	AQ	144/147 (98%)	144 (100%)	0	0	100	100
20	AR	74/78 (95%)	73 (99%)	1 (1%)	0	100	100
21	AS	96/99 (97%)	91 (95%)	5 (5%)	0	100	100
22	AT	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
23	AU	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
24	AV	119/128 (93%)	117 (98%)	1 (1%)	1 (1%)	16	8
25	AW	54/62 (87%)	54 (100%)	0	0	100	100
26	AX	65/79 (82%)	65 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	AY	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
28	AZ	96/101 (95%)	92 (96%)	4 (4%)	0	100	100
29	Aa	86/91 (94%)	85 (99%)	1 (1%)	0	100	100
30	Ab	138/153 (90%)	137 (99%)	1 (1%)	0	100	100
31	Ac	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
32	Ad	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
33	Ae	64/67 (96%)	64 (100%)	0	0	100	100
34	Af	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
35	Ag	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
36	Ah	89/91 (98%)	89 (100%)	0	0	100	100
37	Ai	97/102 (95%)	91 (94%)	6 (6%)	0	100	100
38	Aj	181/184 (98%)	172 (95%)	9 (5%)	0	100	100
39	Ak	88/93 (95%)	88 (100%)	0	0	100	100
All	All	5168/5747 (90%)	5051 (98%)	115 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	AK	41	SER
24	AV	3	PHE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	243/552 (44%)	235 (97%)	8 (3%)	33	23
4	AA	181/186 (97%)	176 (97%)	5 (3%)	38	29
5	AB	280/282 (99%)	278 (99%)	2 (1%)	81	81
6	AC	226/231 (98%)	220 (97%)	6 (3%)	40	31
7	AD	149/149 (100%)	144 (97%)	5 (3%)	32	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AE	165/165 (100%)	159 (96%)	6 (4%)	30	20
9	AF	115/118 (98%)	113 (98%)	2 (2%)	56	52
10	AG	163/165 (99%)	157 (96%)	6 (4%)	29	19
11	AH	133/135 (98%)	131 (98%)	2 (2%)	60	57
12	AI	115/118 (98%)	113 (98%)	2 (2%)	56	52
13	AJ	87/89 (98%)	84 (97%)	3 (3%)	32	22
13	AK	77/89 (86%)	75 (97%)	2 (3%)	41	33
14	AL	121/125 (97%)	114 (94%)	7 (6%)	17	7
15	AM	161/165 (98%)	156 (97%)	5 (3%)	35	25
16	AN	134/140 (96%)	126 (94%)	8 (6%)	16	6
17	AO	166/169 (98%)	159 (96%)	7 (4%)	25	15
18	AP	99/100 (99%)	96 (97%)	3 (3%)	36	27
19	AQ	127/128 (99%)	123 (97%)	4 (3%)	35	25
20	AR	69/71 (97%)	65 (94%)	4 (6%)	17	7
21	AS	84/85 (99%)	83 (99%)	1 (1%)	67	65
22	AT	157/158 (99%)	154 (98%)	3 (2%)	52	47
23	AU	71/71 (100%)	70 (99%)	1 (1%)	62	59
24	AV	107/112 (96%)	103 (96%)	4 (4%)	29	19
25	AW	48/53 (91%)	47 (98%)	1 (2%)	48	43
26	AX	58/65 (89%)	57 (98%)	1 (2%)	56	52
27	AY	147/152 (97%)	141 (96%)	6 (4%)	26	15
28	AZ	77/79 (98%)	72 (94%)	5 (6%)	14	5
29	Aa	78/81 (96%)	77 (99%)	1 (1%)	65	62
30	Ab	125/137 (91%)	125 (100%)	0	100	100
31	Ac	67/68 (98%)	66 (98%)	1 (2%)	60	57
32	Ad	44/44 (100%)	43 (98%)	1 (2%)	45	39
33	Ae	60/61 (98%)	60 (100%)	0	100	100
34	Af	42/43 (98%)	41 (98%)	1 (2%)	44	37
35	Ag	46/49 (94%)	45 (98%)	1 (2%)	47	41
36	Ah	82/82 (100%)	80 (98%)	2 (2%)	44	37
37	Ai	77/80 (96%)	74 (96%)	3 (4%)	27	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Aj	161/162 (99%)	154 (96%)	7 (4%)	25	14
39	Ak	79/82 (96%)	75 (95%)	4 (5%)	20	9
All	All	4421/4841 (91%)	4291 (97%)	130 (3%)	39	28

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	Ah	81	SER
38	Aj	7	TYR
13	AK	91	LYS
13	AK	87	LYS
38	Aj	55	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2834/3024 (93%)	342 (12%)	32 (1%)
2	2	128/129 (99%)	13 (10%)	1 (0%)
All	All	2962/3153 (93%)	355 (11%)	33 (1%)

5 of 355 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	A
1	1	27	C
1	1	43	G
1	1	63	A
1	1	66	A

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	2615	A
1	1	2868	U
2	2	7	A
1	1	902	OMG
1	1	882	A



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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	1	1987	1	18,21,22	0.92	1 (5%)	21,30,33	0.72	0
1	OMG	1	2071	1	19,26,27	0.96	1 (5%)	21,38,41	1.09	2 (9%)
1	PSU	1	2571	1	18,21,22	0.93	1 (5%)	21,30,33	0.68	0
1	PSU	1	2625	1	18,21,22	0.92	1 (5%)	21,30,33	0.78	0
1	OMC	1	493	1	19,22,23	0.82	1 (5%)	25,31,34	0.79	0
1	OMU	1	2574	1	19,22,23	1.34	3 (15%)	25,31,34	1.81	4 (16%)
1	OMC	1	2116	1	19,22,23	0.79	0	25,31,34	0.74	0
1	OMU	1	2623	1	19,22,23	1.34	4 (21%)	25,31,34	1.94	4 (16%)
1	OMG	1	2066	1	19,26,27	0.93	1 (5%)	21,38,41	1.07	2 (9%)
1	A2M	1	2059	1,41	18,25,26	0.69	0	20,36,39	0.92	1 (5%)
1	OMU	1	2666	1	19,22,23	1.29	3 (15%)	25,31,34	1.99	5 (20%)
1	OMG	1	2366	1	19,26,27	0.93	1 (5%)	21,38,41	1.08	2 (9%)
1	OMG	1	2667	1	19,26,27	0.92	1 (5%)	21,38,41	1.08	2 (9%)
1	OMC	1	2624	1	19,22,23	0.29	0	25,31,34	0.31	0
1	A2M	1	2691	1,41	18,25,26	0.67	0	20,36,39	0.76	1 (5%)
1	OMG	1	2608	1	19,26,27	1.06	3 (15%)	21,38,41	0.72	1 (4%)
1	OMG	1	902	1,41	19,26,27	0.93	1 (5%)	21,38,41	1.19	2 (9%)
1	PSU	1	1911	1	18,21,22	0.93	1 (5%)	21,30,33	0.77	0
1	OMC	1	2143	1	19,22,23	0.29	0	25,31,34	0.38	0
1	OMG	1	1949	1	19,26,27	0.96	1 (5%)	21,38,41	1.11	2 (9%)
1	OMC	1	872	1	19,22,23	0.79	0	25,31,34	0.80	0
1	OMU	1	908	1,41	19,22,23	1.35	4 (21%)	25,31,34	2.02	8 (32%)
1	OMC	1	2720	1	19,22,23	0.78	0	25,31,34	0.94	1 (4%)
1	B8T	1	79	1	19,22,23	0.43	0	25,31,34	0.35	0
1	OMC	1	2555	1	19,22,23	0.79	0	25,31,34	0.88	1 (4%)
1	G7M	1	3023	1	20,26,27	2.37	3 (15%)	16,39,42	0.38	0
1	OMU	1	875	1	19,22,23	1.28	3 (15%)	25,31,34	1.87	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4AC	1	2016	1	21,24,25	0.37	0	28,34,37	0.40	0
1	PSU	1	2610	1	18,21,22	0.91	1 (5%)	21,30,33	0.83	1 (4%)
1	OMG	1	2388	1	19,26,27	0.91	1 (5%)	21,38,41	1.20	2 (9%)
1	OMU	1	2851	1	19,22,23	1.33	3 (15%)	25,31,34	1.81	4 (16%)
1	OMU	1	2408	1	19,22,23	1.31	4 (21%)	25,31,34	1.91	5 (20%)
1	OMC	1	2018	1	19,22,23	0.80	1 (5%)	25,31,34	0.81	0
1	OMC	1	673	1	19,22,23	0.80	0	25,31,34	0.87	0
1	UR3	1	2698	1	19,22,23	0.94	1 (5%)	26,32,35	1.77	4 (15%)
1	OMC	1	2704	1	19,22,23	0.82	1 (5%)	25,31,34	0.85	0
1	OMG	1	1947	1	19,26,27	0.90	1 (5%)	21,38,41	1.21	2 (9%)
1	OMU	1	2088	1	19,22,23	1.37	3 (15%)	25,31,34	1.84	5 (20%)
1	OMG	1	2537	1	19,26,27	0.92	1 (5%)	21,38,41	1.08	2 (9%)
1	OMU	1	2155	1	19,22,23	1.39	3 (15%)	25,31,34	2.03	5 (20%)
1	PSU	1	2044	1	18,21,22	0.88	1 (5%)	21,30,33	0.68	0
1	OMG	1	2017	1	19,26,27	0.87	1 (5%)	21,38,41	1.11	3 (14%)
1	5MC	1	38	1	19,22,23	1.42	3 (15%)	26,32,35	1.31	3 (11%)
1	OMC	1	2538	1	19,22,23	0.78	0	25,31,34	0.75	0
1	OMU	1	2077	1	19,22,23	1.34	3 (15%)	25,31,34	1.86	4 (16%)
1	OMG	1	1957	1	19,26,27	0.95	1 (5%)	21,38,41	1.07	2 (9%)
1	OMC	1	1976	1	19,22,23	0.82	1 (5%)	25,31,34	0.98	1 (4%)
1	A2M	1	2011	1	18,25,26	0.67	0	20,36,39	0.73	1 (5%)
1	5MC	1	2056	1,41	19,22,23	1.41	3 (15%)	26,32,35	1.13	3 (11%)
1	OMG	1	2104	1	19,26,27	0.96	1 (5%)	21,38,41	1.22	2 (9%)
1	PSU	1	2607	1	18,21,22	0.95	1 (5%)	21,30,33	0.72	0
1	OMC	1	492	1	19,22,23	0.80	1 (5%)	25,31,34	0.88	1 (4%)
1	OMG	1	2176	1,41	19,26,27	0.89	1 (5%)	21,38,41	1.12	3 (14%)
1	OMC	1	2884	1	19,22,23	0.80	0	25,31,34	0.77	0
1	OMU	1	2707	1	19,22,23	1.36	4 (21%)	25,31,34	1.84	5 (20%)
1	OMC	1	1816	1	19,22,23	0.76	0	25,31,34	0.77	0
1	OMG	1	2362	1	19,26,27	0.98	1 (5%)	21,38,41	1.10	2 (9%)
1	OMC	1	2115	1	19,22,23	0.81	0	25,31,34	0.76	0
1	OMG	1	2103	1	19,26,27	0.89	1 (5%)	21,38,41	1.14	2 (9%)
1	OMG	1	2601	1,41	19,26,27	0.91	1 (5%)	21,38,41	1.09	3 (14%)
1	OMC	1	2885	1	19,22,23	0.80	0	25,31,34	0.78	1 (4%)
1	A2M	1	1990	1	18,25,26	0.69	0	20,36,39	0.83	1 (5%)
1	OMU	1	2628	1	19,22,23	1.36	3 (15%)	25,31,34	1.89	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMG	1	1971	1	19,26,27	0.93	1 (5%)	21,38,41	0.99	2 (9%)
1	B8T	1	2937	1	19,22,23	0.42	0	25,31,34	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	1987	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2071	1	-	0/5/27/28	0/3/3/3
1	PSU	1	2571	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2625	1	-	0/7/25/26	0/2/2/2
1	OMC	1	493	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2574	1	-	0/9/27/28	0/2/2/2
1	OMC	1	2116	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2623	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2066	1	-	0/5/27/28	0/3/3/3
1	A2M	1	2059	1,41	-	1/5/27/28	0/3/3/3
1	OMU	1	2666	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2366	1	-	0/5/27/28	0/3/3/3
1	OMG	1	2667	1	-	0/5/27/28	0/3/3/3
1	OMC	1	2624	1	-	0/9/27/28	0/2/2/2
1	A2M	1	2691	1,41	-	0/5/27/28	0/3/3/3
1	OMG	1	2608	1	-	2/5/27/28	0/3/3/3
1	OMG	1	902	1,41	-	0/5/27/28	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2143	1	-	2/9/27/28	0/2/2/2
1	OMG	1	1949	1	-	0/5/27/28	0/3/3/3
1	OMC	1	872	1	-	0/9/27/28	0/2/2/2
1	OMU	1	908	1,41	-	5/9/27/28	0/2/2/2
1	OMC	1	2720	1	-	0/9/27/28	0/2/2/2
1	B8T	1	79	1	-	0/7/27/28	0/2/2/2
1	OMC	1	2555	1	-	1/9/27/28	0/2/2/2
1	G7M	1	3023	1	-	0/3/25/26	0/3/3/3
1	OMU	1	875	1	-	0/9/27/28	0/2/2/2
1	4AC	1	2016	1	-	0/11/29/30	0/2/2/2
1	PSU	1	2610	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2388	1	-	1/5/27/28	0/3/3/3
1	OMU	1	2851	1	-	1/9/27/28	0/2/2/2
1	OMU	1	2408	1	-	0/9/27/28	0/2/2/2
1	OMC	1	2018	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	1	673	1	-	0/9/27/28	0/2/2/2
1	UR3	1	2698	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2704	1	-	0/9/27/28	0/2/2/2
1	OMG	1	1947	1	-	2/5/27/28	0/3/3/3
1	OMU	1	2088	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2537	1	-	1/5/27/28	0/3/3/3
1	OMU	1	2155	1	-	3/9/27/28	0/2/2/2
1	PSU	1	2044	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2017	1	-	0/5/27/28	0/3/3/3
1	5MC	1	38	1	-	1/7/25/26	0/2/2/2
1	OMC	1	2538	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2077	1	-	0/9/27/28	0/2/2/2
1	OMG	1	1957	1	-	0/5/27/28	0/3/3/3
1	OMC	1	1976	1	-	0/9/27/28	0/2/2/2
1	A2M	1	2011	1	-	0/5/27/28	0/3/3/3
1	5MC	1	2056	1,41	-	0/7/25/26	0/2/2/2
1	OMG	1	2104	1	-	0/5/27/28	0/3/3/3
1	PSU	1	2607	1	-	0/7/25/26	0/2/2/2
1	OMC	1	492	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2176	1,41	-	0/5/27/28	0/3/3/3
1	OMC	1	2884	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2707	1	-	0/9/27/28	0/2/2/2
1	OMC	1	1816	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2362	1	-	0/5/27/28	0/3/3/3
1	OMC	1	2115	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2103	1	-	0/5/27/28	0/3/3/3
1	OMG	1	2601	1,41	-	1/5/27/28	0/3/3/3
1	OMC	1	2885	1	-	0/9/27/28	0/2/2/2
1	A2M	1	1990	1	-	1/5/27/28	0/3/3/3
1	OMU	1	2628	1	-	0/9/27/28	0/2/2/2
1	OMG	1	1971	1	-	1/5/27/28	0/3/3/3
1	B8T	1	2937	1	-	2/7/27/28	0/2/2/2

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	3023	G7M	C8-N9	7.30	1.46	1.33
1	1	3023	G7M	C8-N7	7.02	1.45	1.33
1	1	2056	5MC	C5-C4	4.75	1.47	1.44
1	1	38	5MC	C5-C4	4.75	1.47	1.44
1	1	2571	PSU	C6-C5	3.61	1.39	1.35

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2698	UR3	C4-N3-C2	-6.86	119.06	124.58
1	1	2666	OMU	C4-N3-C2	-5.44	119.85	126.61
1	1	2155	OMU	C4-N3-C2	-5.41	119.90	126.61
1	1	2408	OMU	C4-N3-C2	-5.18	120.18	126.61
1	1	2623	OMU	C4-N3-C2	-5.17	120.19	126.61

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1947	OMG	O4'-C4'-C5'-O5'
1	1	1990	A2M	C1'-C2'-O2'-CM'
1	1	2155	OMU	C1'-C2'-O2'-CM2
1	1	2608	OMG	O4'-C4'-C5'-O5'
1	1	1947	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 224 ligands modelled in this entry, 178 are monoatomic - leaving 46 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	$\# Z  > 2$
40	SPM	1	3120	-	13,13,13	0.17	0	12,12,12	0.23	0
40	SPM	1	3110	-	13,13,13	0.14	0	12,12,12	0.16	0
40	SPM	1	3138	-	13,13,13	0.16	0	12,12,12	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	SPM	AL	201	-	13,13,13	0.16	0	12,12,12	0.20	0
40	SPM	1	3143	-	13,13,13	0.19	0	12,12,12	0.44	0
40	SPM	1	3127	-	13,13,13	0.16	0	12,12,12	0.22	0
40	SPM	1	3102	-	13,13,13	0.17	0	12,12,12	0.43	0
40	SPM	1	3131	-	13,13,13	0.15	0	12,12,12	0.25	0
40	SPM	1	3137	-	13,13,13	0.17	0	12,12,12	0.27	0
40	SPM	1	3144	-	13,13,13	0.19	0	12,12,12	0.24	0
40	SPM	AM	201	-	13,13,13	0.18	0	12,12,12	0.28	0
40	SPM	1	3116	-	13,13,13	0.21	0	12,12,12	0.29	0
40	SPM	1	3124	-	13,13,13	0.16	0	12,12,12	0.34	0
40	SPM	1	3133	-	13,13,13	0.16	0	12,12,12	0.29	0
40	SPM	1	3142	-	13,13,13	0.17	0	12,12,12	0.37	0
40	SPM	1	3111	-	13,13,13	0.14	0	12,12,12	0.19	0
40	SPM	1	3109	-	13,13,13	0.17	0	12,12,12	0.26	0
40	SPM	1	3134	-	13,13,13	0.17	0	12,12,12	0.29	0
40	SPM	1	3139	-	13,13,13	0.18	0	12,12,12	0.14	0
40	SPM	1	3119	-	13,13,13	0.20	0	12,12,12	0.21	0
40	SPM	1	3135	-	13,13,13	0.15	0	12,12,12	0.33	0
40	SPM	1	3105	-	13,13,13	0.17	0	12,12,12	0.18	0
40	SPM	1	3104	-	13,13,13	0.16	0	12,12,12	0.40	0
40	SPM	1	3114	-	13,13,13	0.20	0	12,12,12	0.31	0
40	SPM	1	3122	-	13,13,13	0.17	0	12,12,12	0.20	0
40	SPM	1	3129	-	13,13,13	0.18	0	12,12,12	0.31	0
40	SPM	1	3125	-	13,13,13	0.14	0	12,12,12	0.28	0
40	SPM	1	3123	-	13,13,13	0.18	0	12,12,12	0.33	0
40	SPM	1	3113	-	13,13,13	0.16	0	12,12,12	0.21	0
40	SPM	1	3121	-	13,13,13	0.24	0	12,12,12	0.24	0
40	SPM	1	3108	-	13,13,13	0.18	0	12,12,12	0.35	0
40	SPM	1	3106	-	13,13,13	0.20	0	12,12,12	0.24	0
40	SPM	1	3112	-	13,13,13	0.19	0	12,12,12	0.40	0
40	SPM	1	3132	-	13,13,13	0.17	0	12,12,12	0.19	0
40	SPM	1	3115	-	13,13,13	0.18	0	12,12,12	0.26	0
40	SPM	1	3126	-	13,13,13	0.14	0	12,12,12	0.42	0
40	SPM	1	3117	-	13,13,13	0.20	0	12,12,12	0.32	0
40	SPM	1	3140	-	13,13,13	0.15	0	12,12,12	0.26	0
40	SPM	1	3103	-	13,13,13	0.16	0	12,12,12	0.34	0
40	SPM	1	3130	-	13,13,13	0.15	0	12,12,12	0.22	0
40	SPM	1	3136	-	13,13,13	0.18	0	12,12,12	0.37	0
40	SPM	1	3118	-	13,13,13	0.16	0	12,12,12	0.26	0
40	SPM	1	3141	-	13,13,13	0.16	0	12,12,12	0.17	0
40	SPM	1	3107	-	13,13,13	0.16	0	12,12,12	0.18	0
40	SPM	1	3128	-	13,13,13	0.19	0	12,12,12	0.32	0
40	SPM	1	3101	-	13,13,13	0.18	0	12,12,12	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	SPM	1	3120	-	-	1/11/11/11	-
40	SPM	1	3110	-	-	4/11/11/11	-
40	SPM	1	3138	-	-	8/11/11/11	-
40	SPM	AL	201	-	-	3/11/11/11	-
40	SPM	1	3143	-	-	4/11/11/11	-
40	SPM	1	3127	-	-	0/11/11/11	-
40	SPM	1	3102	-	-	1/11/11/11	-
40	SPM	1	3131	-	-	1/11/11/11	-
40	SPM	1	3137	-	-	2/11/11/11	-
40	SPM	1	3144	-	-	2/11/11/11	-
40	SPM	AM	201	-	-	0/11/11/11	-
40	SPM	1	3116	-	-	3/11/11/11	-
40	SPM	1	3124	-	-	0/11/11/11	-
40	SPM	1	3133	-	-	2/11/11/11	-
40	SPM	1	3142	-	-	1/11/11/11	-
40	SPM	1	3111	-	-	8/11/11/11	-
40	SPM	1	3109	-	-	1/11/11/11	-
40	SPM	1	3134	-	-	1/11/11/11	-
40	SPM	1	3139	-	-	2/11/11/11	-
40	SPM	1	3119	-	-	2/11/11/11	-
40	SPM	1	3135	-	-	1/11/11/11	-
40	SPM	1	3105	-	-	1/11/11/11	-
40	SPM	1	3104	-	-	2/11/11/11	-
40	SPM	1	3114	-	-	3/11/11/11	-
40	SPM	1	3122	-	-	9/11/11/11	-
40	SPM	1	3129	-	-	2/11/11/11	-
40	SPM	1	3125	-	-	1/11/11/11	-
40	SPM	1	3123	-	-	3/11/11/11	-
40	SPM	1	3113	-	-	9/11/11/11	-
40	SPM	1	3121	-	-	1/11/11/11	-
40	SPM	1	3108	-	-	4/11/11/11	-
40	SPM	1	3106	-	-	7/11/11/11	-
40	SPM	1	3112	-	-	1/11/11/11	-
40	SPM	1	3132	-	-	9/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	SPM	1	3115	-	-	1/11/11/11	-
40	SPM	1	3126	-	-	1/11/11/11	-
40	SPM	1	3117	-	-	1/11/11/11	-
40	SPM	1	3140	-	-	1/11/11/11	-
40	SPM	1	3103	-	-	0/11/11/11	-
40	SPM	1	3130	-	-	0/11/11/11	-
40	SPM	1	3136	-	-	0/11/11/11	-
40	SPM	1	3118	-	-	0/11/11/11	-
40	SPM	1	3141	-	-	7/11/11/11	-
40	SPM	1	3107	-	-	3/11/11/11	-
40	SPM	1	3128	-	-	1/11/11/11	-
40	SPM	1	3101	-	-	4/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 118 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	1	3106	SPM	C12-C11-N10-C9
40	1	3113	SPM	C12-C11-N10-C9
40	1	3122	SPM	C12-C11-N10-C9
40	1	3138	SPM	C3-C4-N5-C6
40	1	3134	SPM	N5-C6-C7-C8

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.



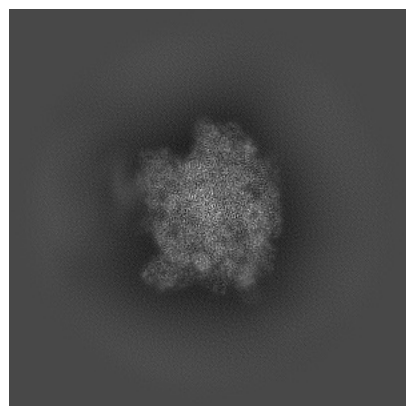
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47578. These allow visual inspection of the internal detail of the map and identification of artifacts.

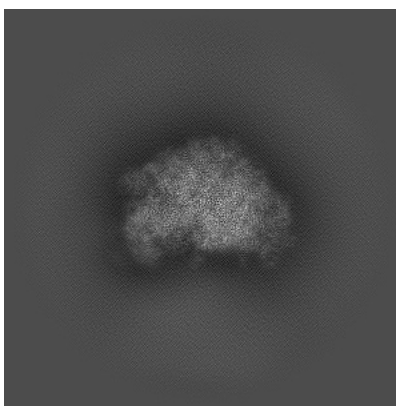
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

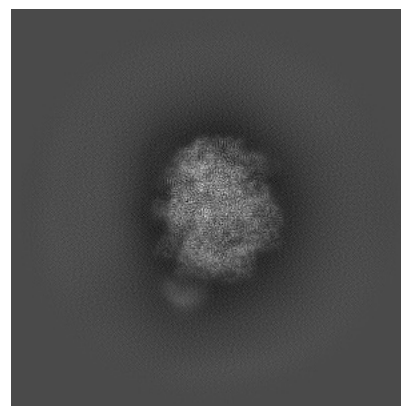
#### 6.1.1 Primary map



X

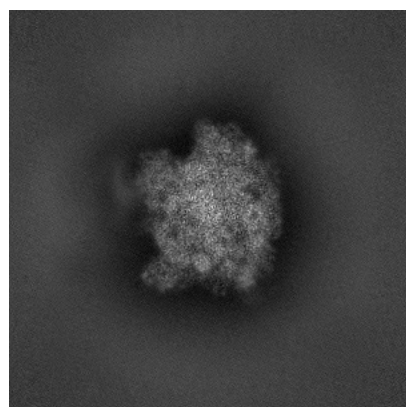


Y

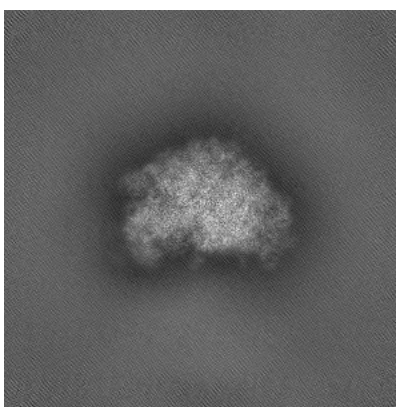


Z

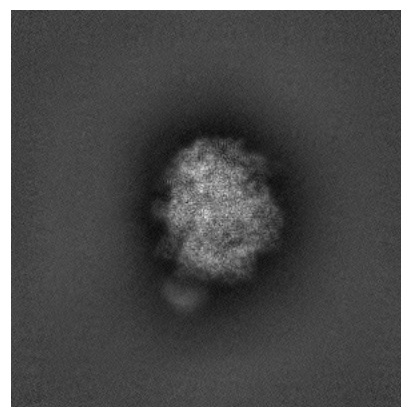
#### 6.1.2 Raw map



X



Y

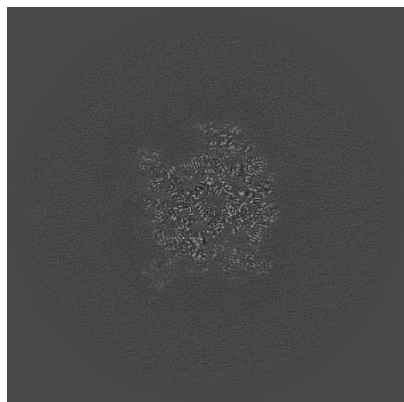


Z

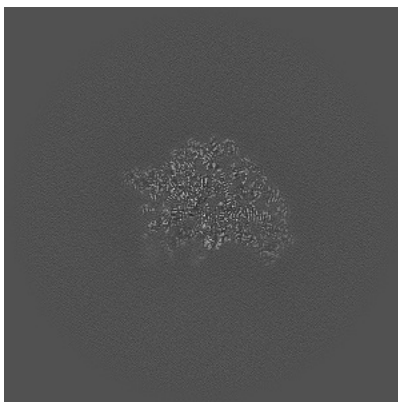
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

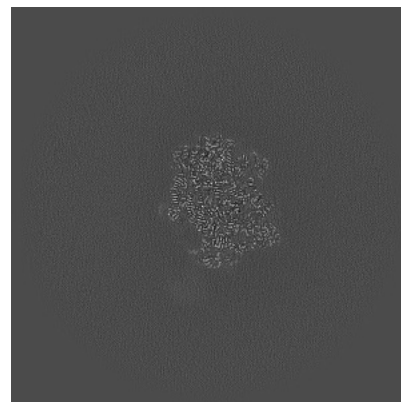
### 6.2.1 Primary map



X Index: 304

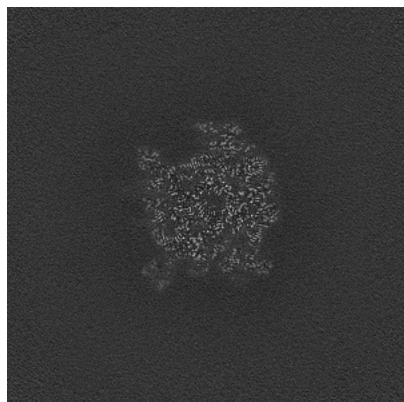


Y Index: 304

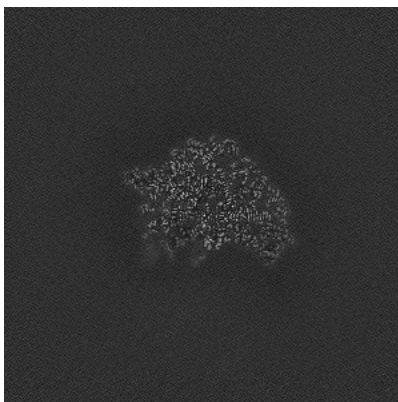


Z Index: 304

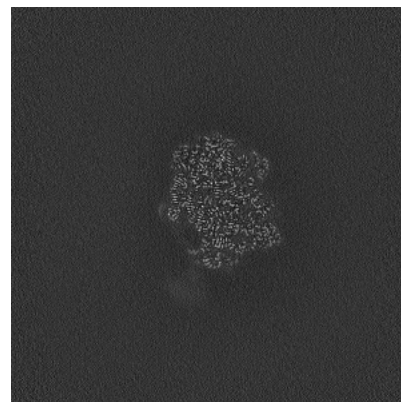
### 6.2.2 Raw map



X Index: 304



Y Index: 304

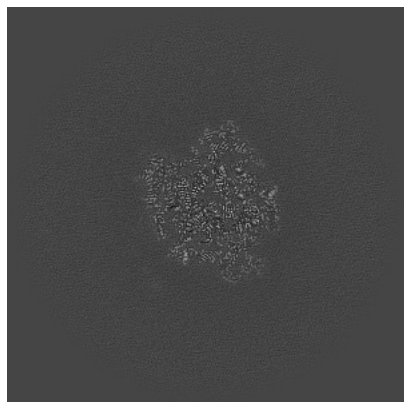


Z Index: 304

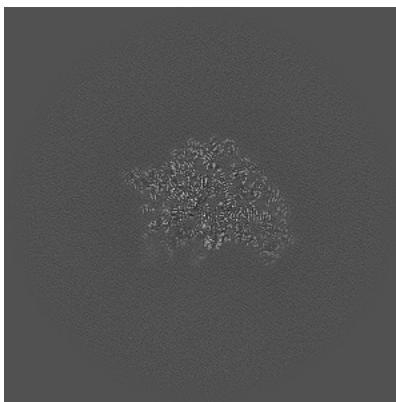
The images above show central slices of the map in three orthogonal directions.

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

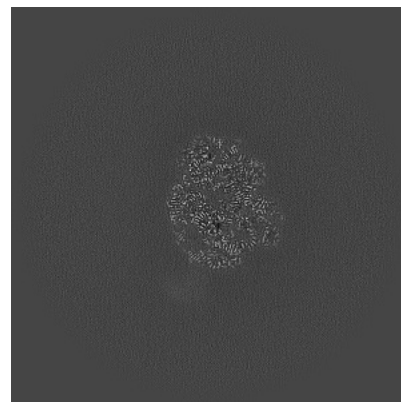
### 6.3.1 Primary map



X Index: 316

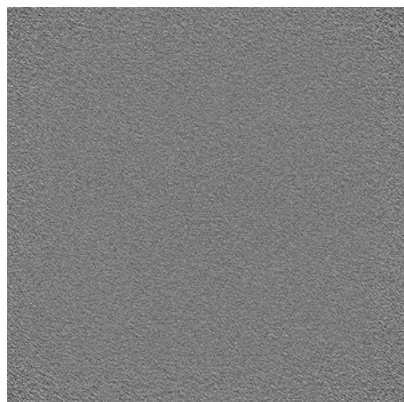


Y Index: 304

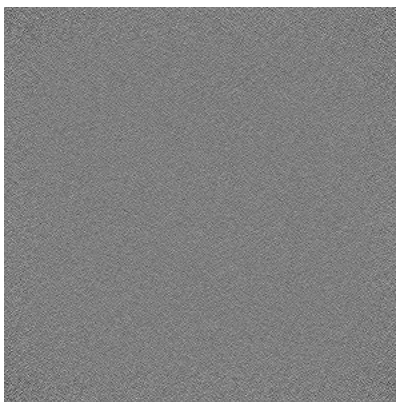


Z Index: 311

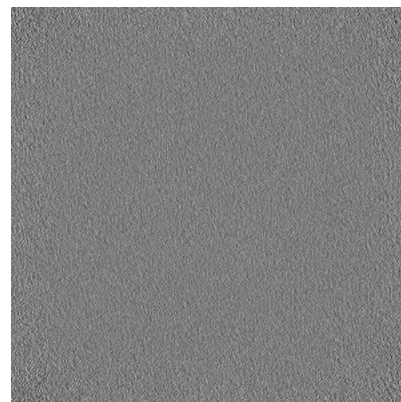
### 6.3.2 Raw map



X Index: 0



Y Index: 0



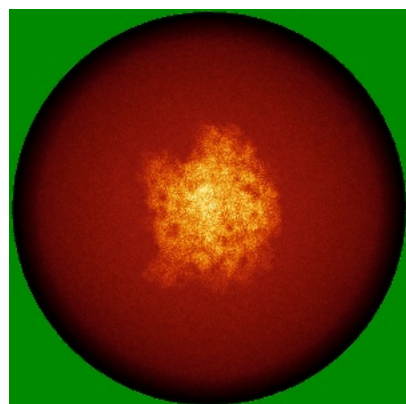
Z Index: 0

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

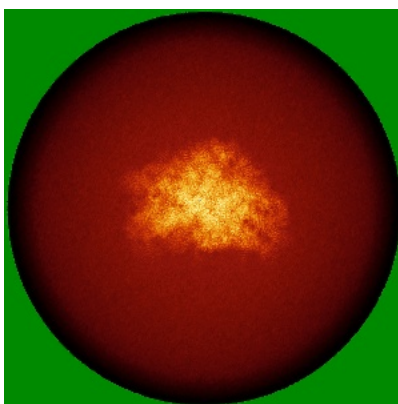


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

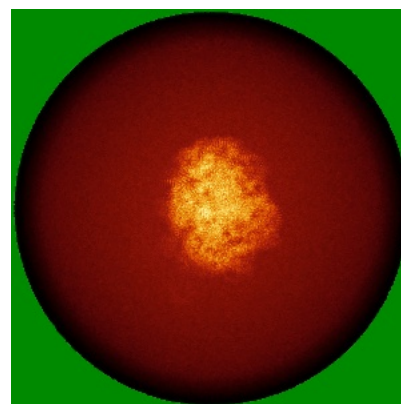
### 6.4.1 Primary map



X

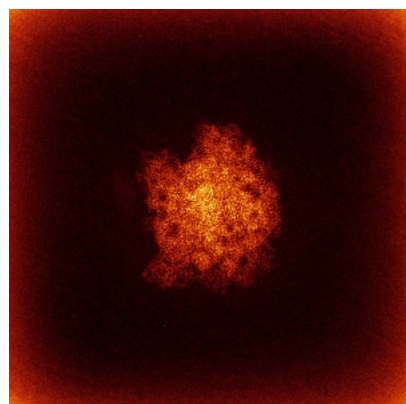


Y

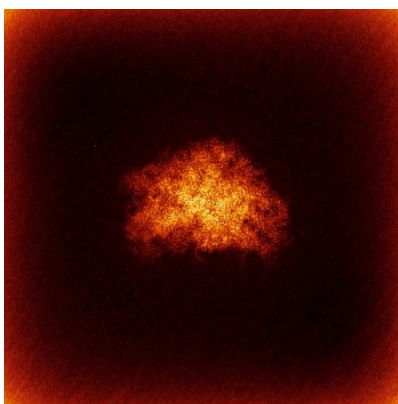


Z

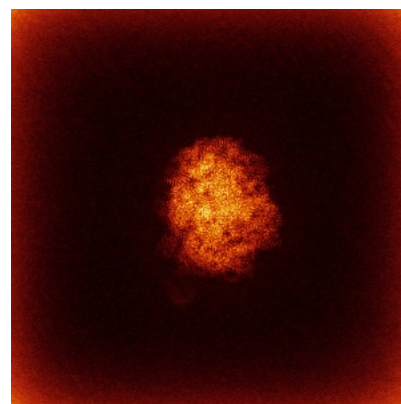
### 6.4.2 Raw map



X



Y

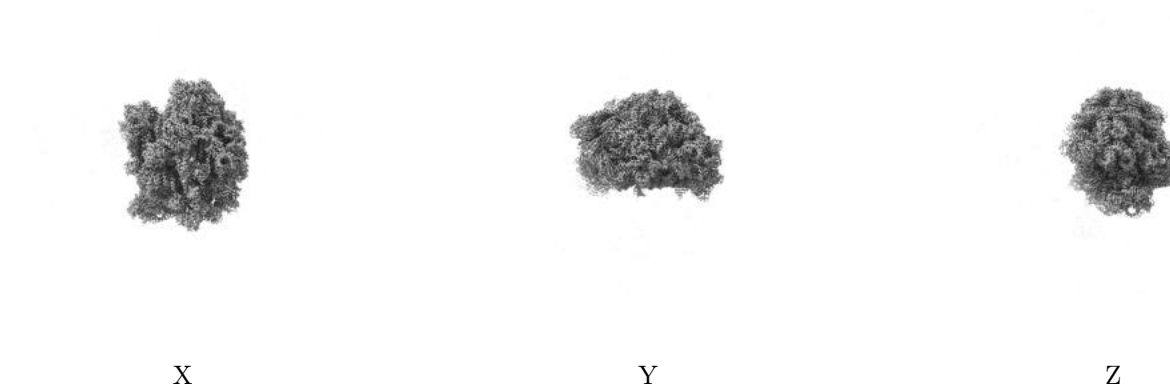


Z

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.

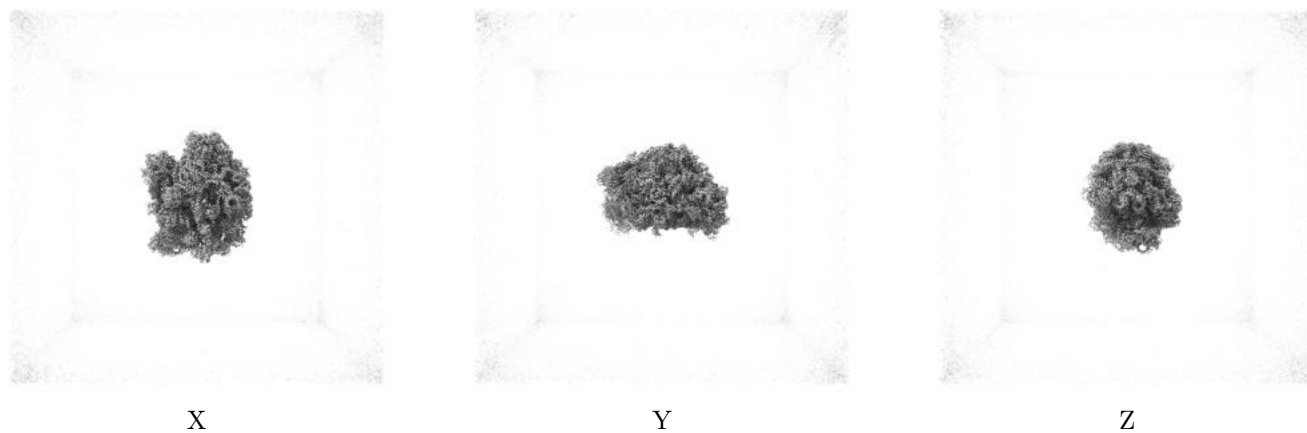
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.152. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

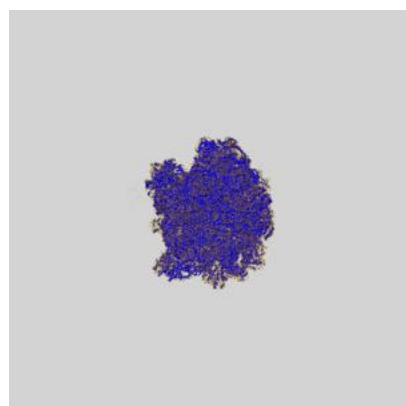
## 6.6 Mask visualisation [i](#)

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

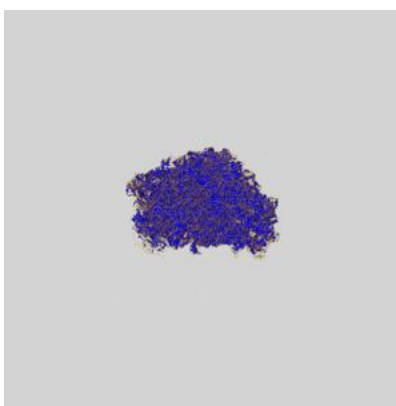
A mask typically either:

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

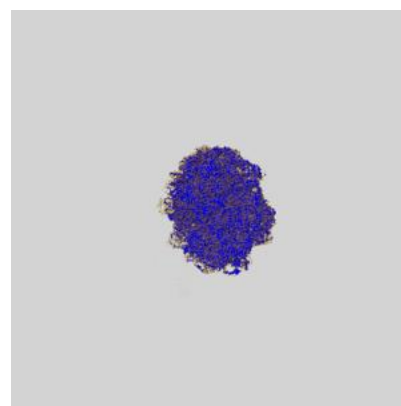
### 6.6.1 emd\_47578\_msk\_1.map [i](#)



X



Y

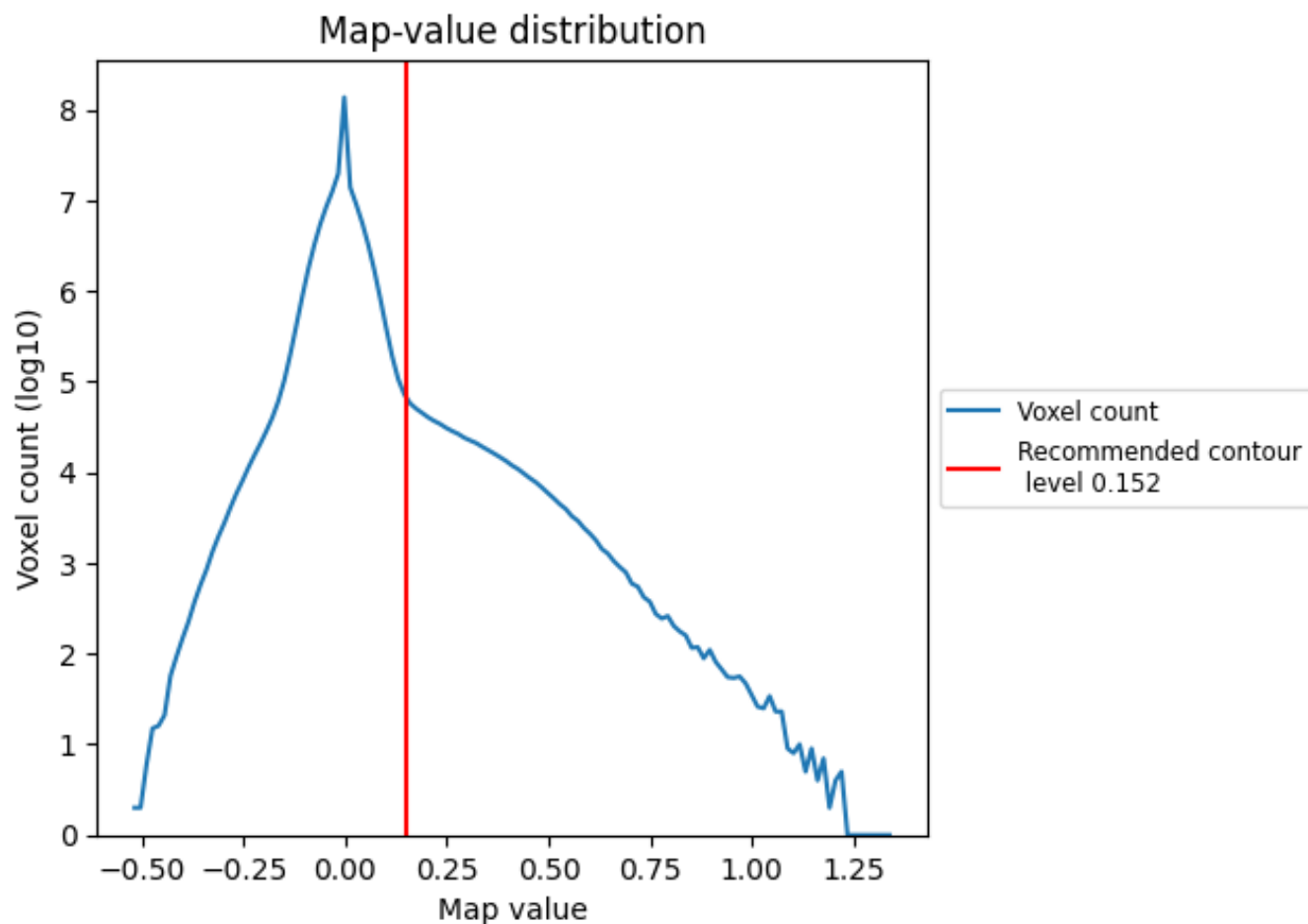


Z

## 7 Map analysis [i](#)

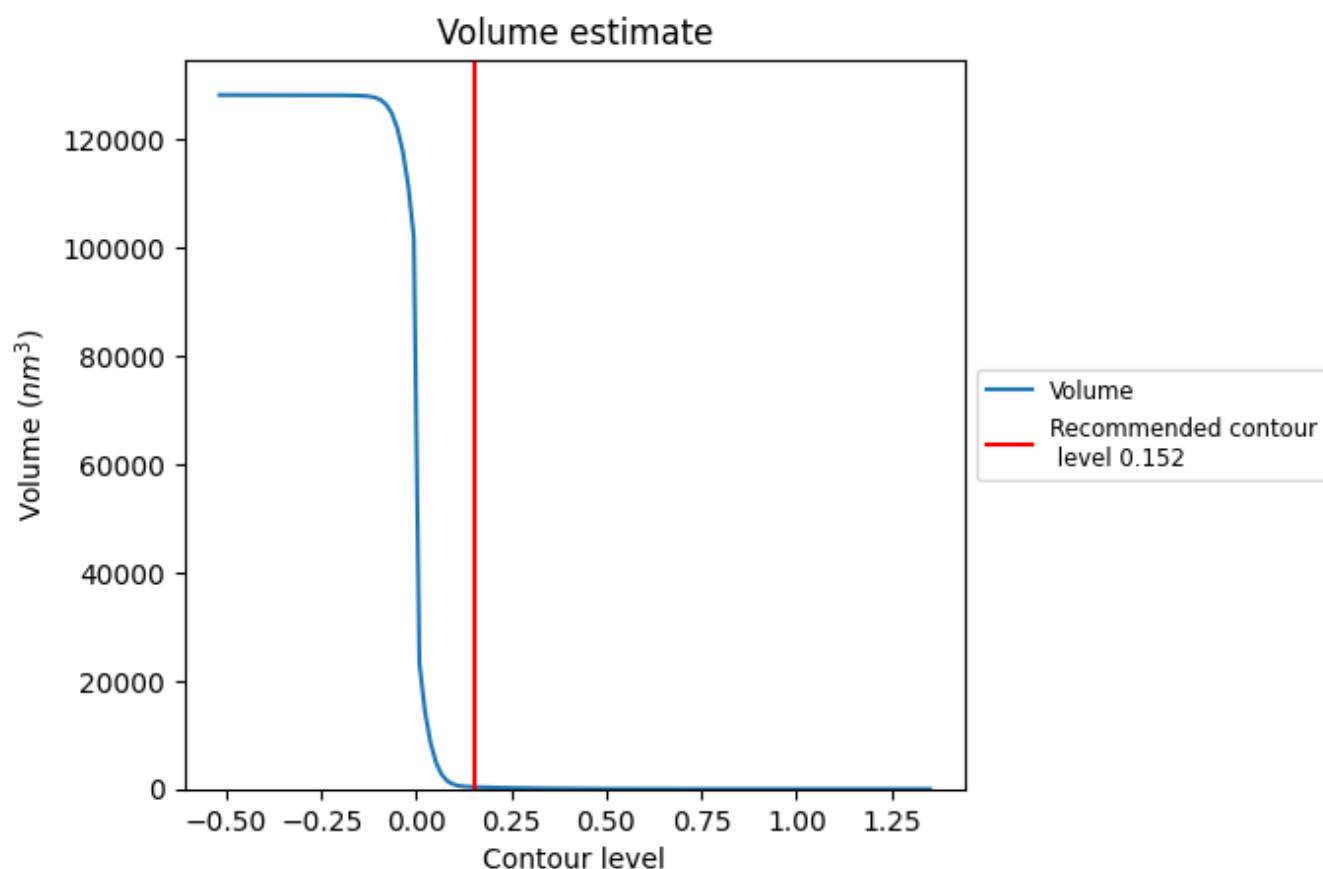
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

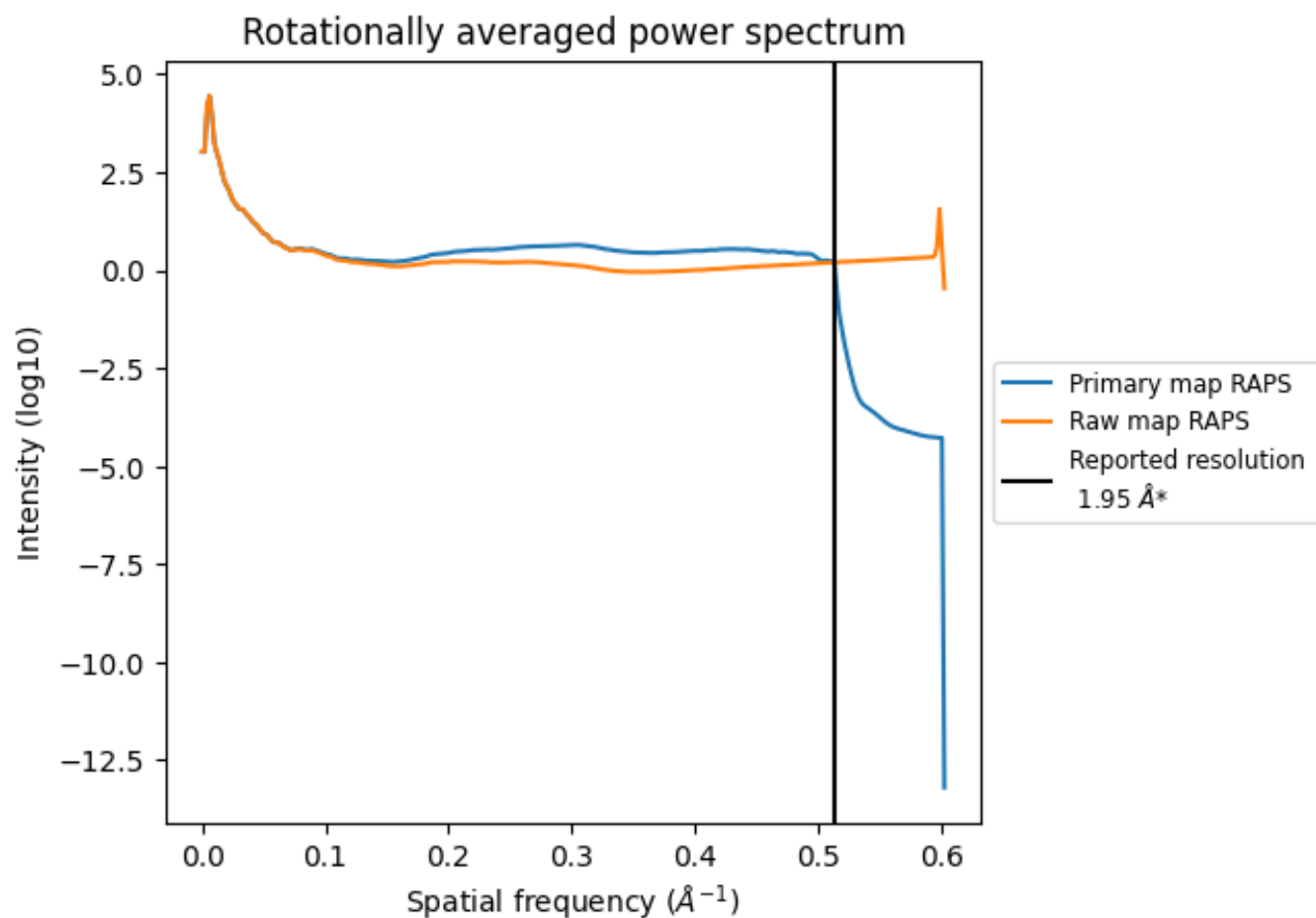


The volume at the recommended contour level is 360  $\text{nm}^3$ ; this corresponds to an approximate mass of 325 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

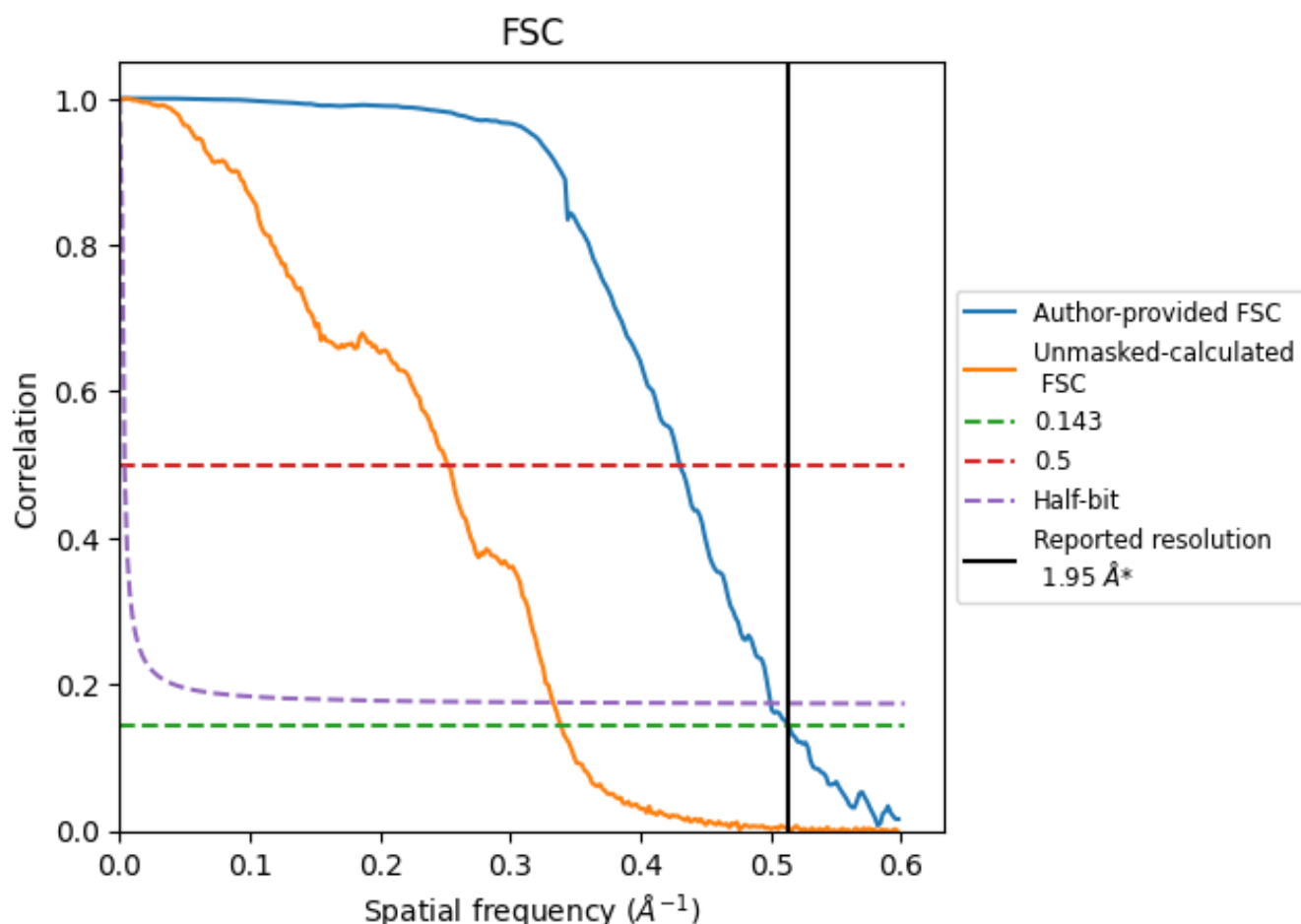


\*Reported resolution corresponds to spatial frequency of  $0.513 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.513 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

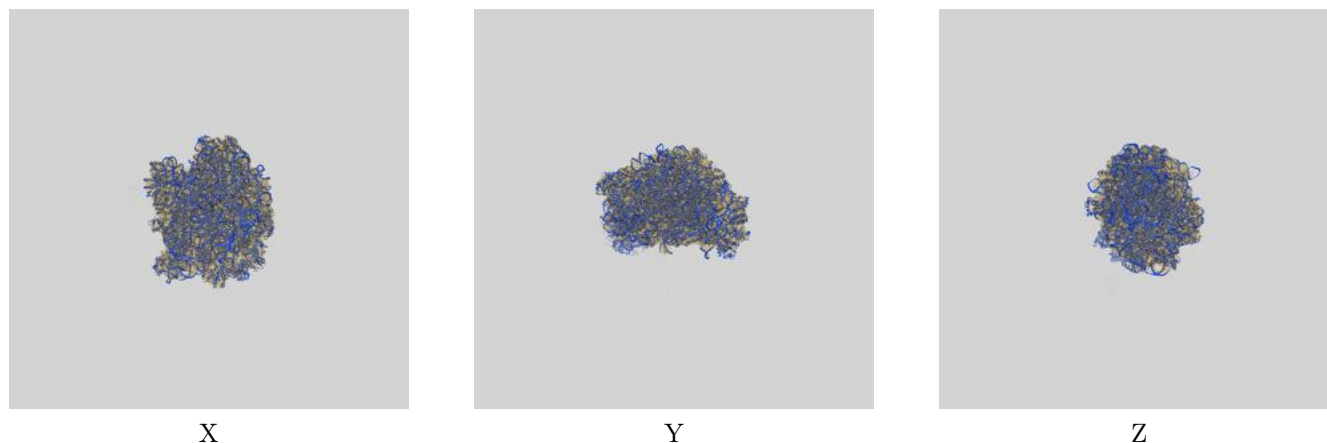
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.95	-	-
Author-provided FSC curve	1.95	2.32	2.00
Unmasked-calculated*	2.95	3.97	3.00

\*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 2.95 differs from the reported value 1.95 by more than 10 %

## 9 Map-model fit [i](#)

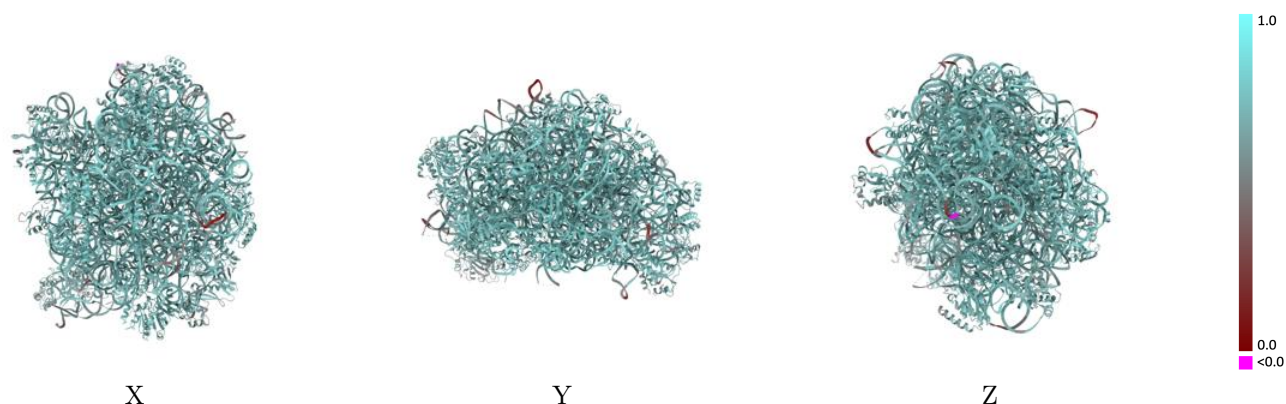
This section contains information regarding the fit between EMDB map EMD-47578 and PDB model 9E6Q. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

### 9.1 Map-model overlay [i](#)



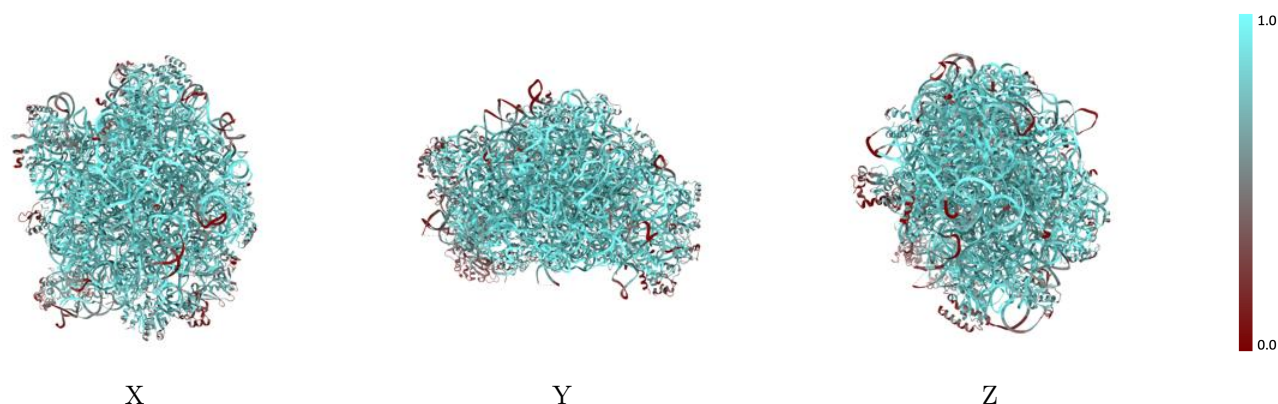
The images above show the 3D surface view of the map at the recommended contour level 0.152 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



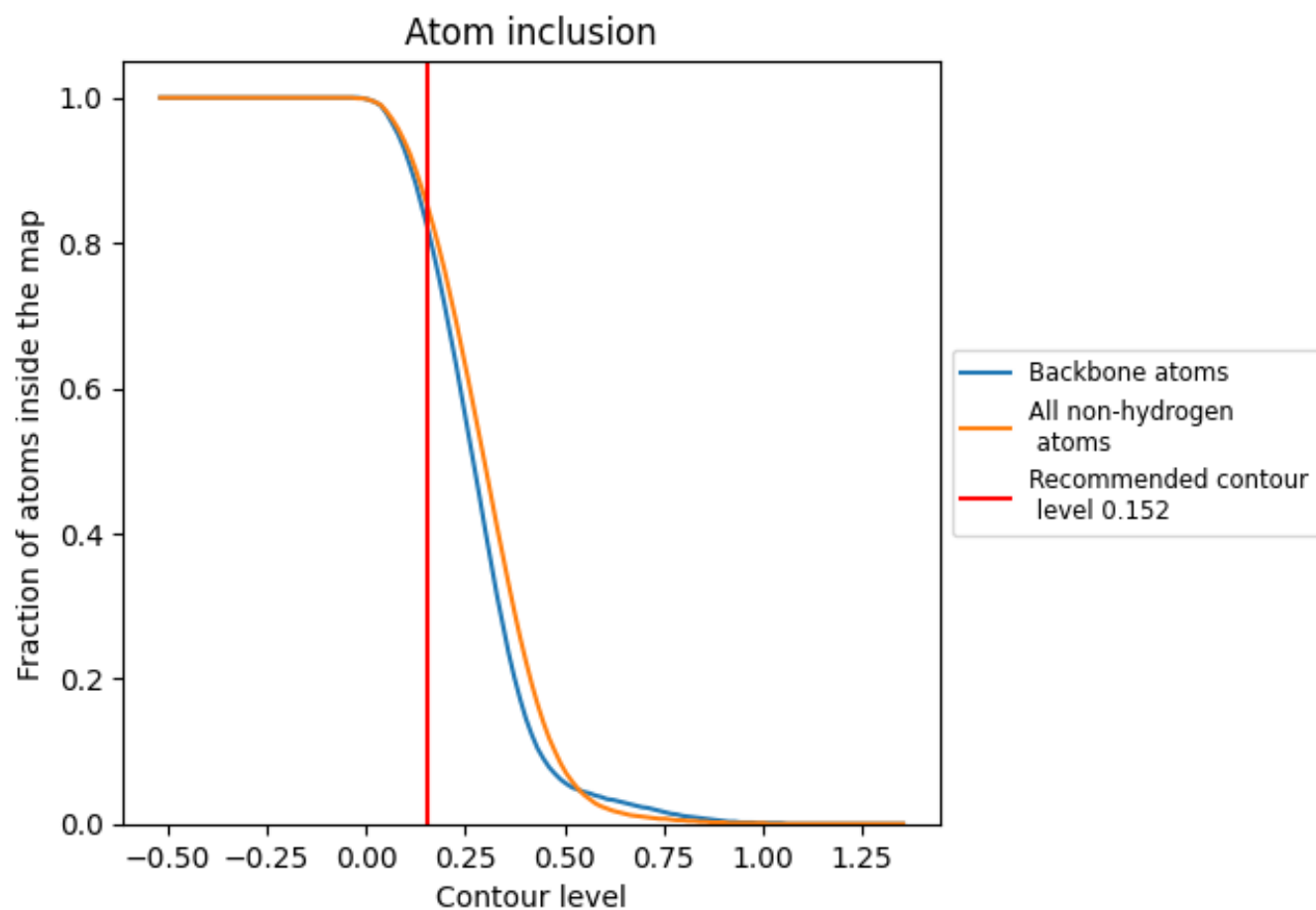
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.152).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 86% 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 (0.152) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.7260
1	 0.9130	 0.7290
2	 0.7540	 0.6710
3	 0.7710	 0.7220
AA	 0.9030	 0.7590
AB	 0.8970	 0.7600
AC	 0.8650	 0.7470
AD	 0.2720	 0.5760
AE	 0.6660	 0.6980
AF	 0.6050	 0.6730
AG	 0.8300	 0.7460
AH	 0.8600	 0.7470
AI	 0.8620	 0.7510
AJ	 0.5470	 0.6460
AK	 0.6000	 0.6720
AL	 0.7260	 0.7070
AM	 0.8720	 0.7510
AN	 0.8770	 0.7540
AO	 0.5930	 0.6730
AP	 0.8620	 0.7470
AQ	 0.8160	 0.7380
AR	 0.6980	 0.7080
AS	 0.9020	 0.7540
AT	 0.8960	 0.7620
AU	 0.8540	 0.7510
AV	 0.8030	 0.7280
AW	 0.8430	 0.7430
AX	 0.7160	 0.7100
AY	 0.8510	 0.7400
AZ	 0.5860	 0.6720
Aa	 0.8210	 0.7410
Ab	 0.8490	 0.7490
Ac	 0.9060	 0.7420
Ad	 0.9830	 0.7900
Ae	 0.7940	 0.7310



*Continued on next page...*

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Chain	Atom inclusion	Q-score
Af	 0.9240	 0.7650
Ag	 0.6930	 0.6920
Ah	 0.8760	 0.7430
Ai	 0.7120	 0.7150
Aj	 0.7260	 0.7120
Ak	 0.7250	 0.7020