



wwPDB EM Validation Summary Report ⓘ

Aug 13, 2025 – 05:10 pm BST

PDB ID : 9I5T / pdb_00009i5t
EMDB ID : EMD-52635
Title : 50S subunit of P. gingivalis ribosome with Lefamulin
Authors : Hiregange, D.G.; Bashan, A.; Yonath, A.
Deposited on : 2025-01-28
Resolution : 2.60 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.dev126
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
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) : 2.45.1

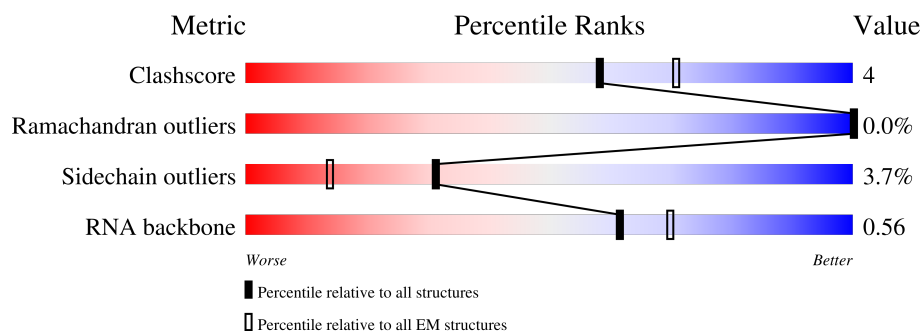
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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.















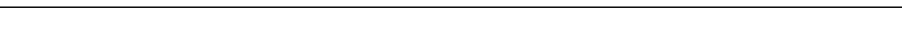

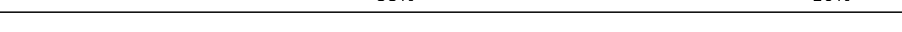

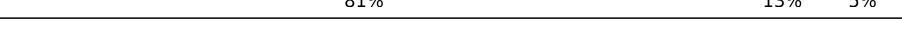








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 ≥ 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	0	79	89% 9% .
2	1	64	84% 14% .
3	11	186	74% 13% . 11%
4	12	85	58% . 39%
5	2	58	76% 21% .
6	4	61	80% 13% 7%
7	6	50	84% 12% .

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Mol	Chain	Length	Quality of chain
8	7	65	 77% 22% .
9	8	38	 82% 16% .
10	A	2882	 61% 23% . 12%
11	B	109	 52% 35% 6% 6%
12	D	274	 82% 17% .
13	E	205	 90% 10%
14	F	209	 93% 5% .
15	M	151	 91% 7% ..
16	O	148	 85% 12% ..
17	P	144	 83% 16% .
18	Q	160	 67% 10% 23%
19	R	114	 82% 13% . .
20	S	121	 82% 11% . 7%
21	T	115	 88% 10% .
22	U	105	 80% 18% ..
23	V	134	 81% 13% 5%
24	W	97	 82% 11% . 5%
25	X	106	 70% 22% 8%
26	Y	192	 78% 12% . 8%
27	Z	85	 84% 7% 9%
28	h	179	 25% . . 71%
29	15	49	 45% 24% . 29%
30	13	183	 73% 23% . .
31	N	121	 88% 12%
32	5	62	 73% 27%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 82341 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			600	387	117	93	3		

- Molecule 2 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	63	Total	C	N	O	S	0	0
			466	292	93	78	3		

- Molecule 3 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	11	166	Total	C	N	O	S	0	0
			1033	645	188	198	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	12	52	Total	C	N	O	0	0
			267	159	52	56		

- Molecule 5 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	56	Total	C	N	O	S	0	0
			434	275	89	68	2		

- Molecule 6 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	57	Total	C	N	O	S	0	0
			436	272	91	72	1		

- Molecule 7 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	48	Total	C	N	O	S	0	0
			382	230	89	61	2		

- Molecule 8 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	64	Total	C	N	O	S	0	0
			508	325	98	84	1		

- Molecule 9 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	38	Total	C	N	O	S	0	0
			297	185	63	47	2		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2529	Total	C	N	O	P	0	0
			54304	24248	10018	17509	2529		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	102	Total	C	N	O	P	0	0
			2187	975	400	710	102		

- Molecule 12 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	272	Total	C	N	O	S	0	0
			2036	1270	396	362	8		

- Molecule 13 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	204	Total	C	N	O	S	0	0
			1497	955	273	262	7		

- Molecule 14 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	208	Total	C	N	O	S	0	0
			1520	966	282	271	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	149	Total	C	N	O	S	0	0
			1136	726	212	193	5		

- Molecule 16 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	146	Total	C	N	O	S	0	0
			1021	641	195	184	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	142	Total	C	N	O	S	0	0
			1095	704	206	182	3		

- Molecule 18 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	123	Total	C	N	O	S	0	0
			968	618	183	161	6		

- Molecule 19 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	110	Total	C	N	O	S	0	0
			751	467	149	135			

- Molecule 20 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	113	Total	C	N	O	S	0	0
			854	548	161	145			

- Molecule 21 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	113	Total	C	N	O	S	0	0
			916	580	188	145	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	104	Total	C	N	O	S	0	0
			782	503	145	131	3		

- Molecule 23 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	127	Total	C	N	O	S	0	0
			1013	627	204	177	5		

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	92	Total	C	N	O	S	0	0
			682	439	119	120	4		

- Molecule 25 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	97	Total	C	N	O	S	0	0
			693	434	136	121	2		

- Molecule 26 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	176	Total	C	N	O	S	0	0
			1166	757	206	203			

- Molecule 27 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	77	Total	C	N	O	S	0	0
			574	354	113	106	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	h	52	Total	C	N	O	S	0	0
			349	226	61	61	1		

- Molecule 29 is a protein called DUF4295 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	15	35	Total	C	N	O	S	0	0
			256	164	41	49	2		

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	13	177	Total	C	N	O	S	0	0
			1309	828	240	237	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	N	121	Total	C	N	O	S	0	0
			875	547	168	156	4		

- Molecule 32 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	45	Total	C	N	O	S	0	0
			346	216	65	63	2		

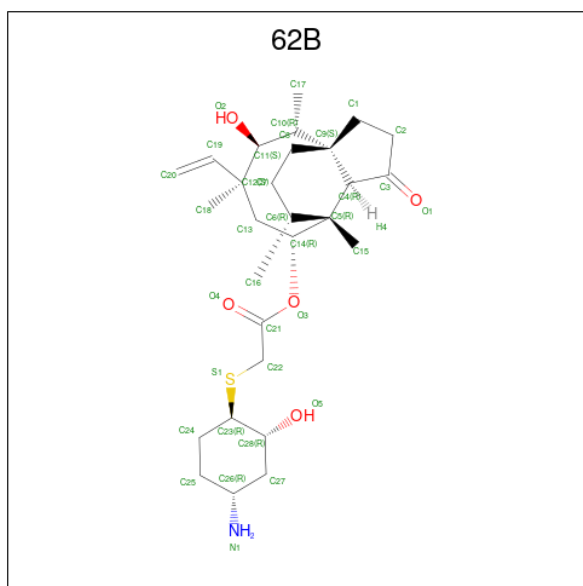
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	4	1	Total	Mg	0
			1	1	
33	A	134	Total	Mg	0
			134	134	
33	B	1	Total	Mg	0
			1	1	
33	F	1	Total	Mg	0
			1	1	
33	V	2	Total	Mg	0
			2	2	

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	4	1	Total	Zn	0
			1	1	

- Molecule 35 is Lefamulin (CCD ID: 62B) (formula: $C_{28}H_{45}NO_5S$).



Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	S	0
			35	28	1	5	1	

- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
36	A	18	Total	K	0
			18	18	

- Molecule 37 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
37	A	13	Total	Na	0
			13	13	
37	B	2	Total	Na	0
			2	2	


- Molecule 38 is water.

Mol	Chain	Residues	Atoms		AltConf
38	0	1	Total 1	O 1	0
38	4	6	Total 6	O 6	0
38	6	12	Total 12	O 12	0
38	7	1	Total 1	O 1	0
38	A	1225	Total 1225	O 1225	0
38	B	4	Total 4	O 4	0
38	D	26	Total 26	O 26	0
38	E	16	Total 16	O 16	0
38	F	19	Total 19	O 19	0
38	O	16	Total 16	O 16	0
38	Q	8	Total 8	O 8	0
38	S	1	Total 1	O 1	0
38	T	15	Total 15	O 15	0
38	U	8	Total 8	O 8	0
38	V	15	Total 15	O 15	0
38	W	2	Total 2	O 2	0
38	Z	5	Total 5	O 5	0

3 Residue-property plots [i](#)


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

- Molecule 1: Large ribosomal subunit protein bL28

Chain 0: 



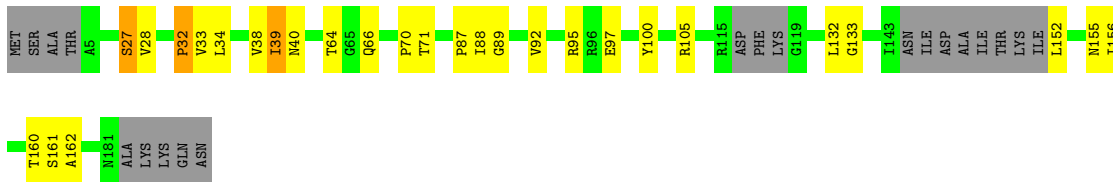
- Molecule 2: Large ribosomal subunit protein uL29

Chain 1: 



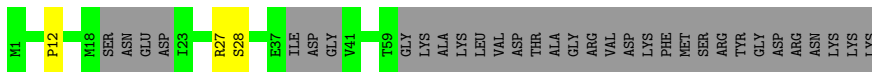
- Molecule 3: Large ribosomal subunit protein uL5

Chain 11: 



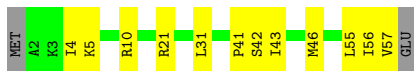
- Molecule 4: Large ribosomal subunit protein bL31B

Chain 12: 



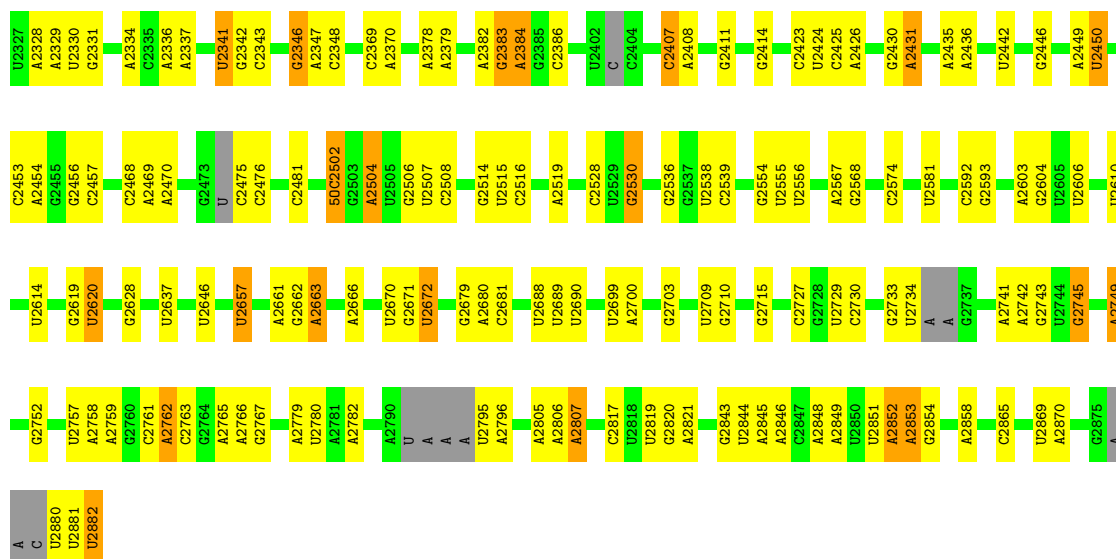
- Molecule 5: Large ribosomal subunit protein uL30

Chain 2: 



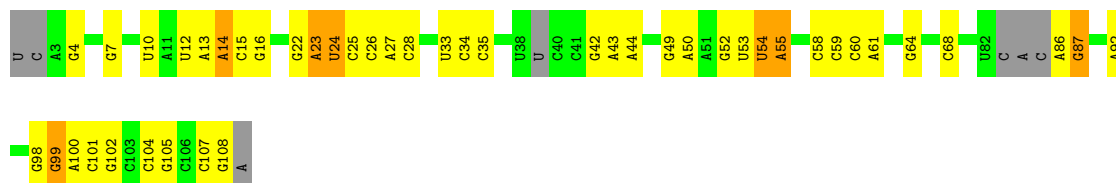
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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 0572 | 0573 | 0574 | 0575 | 0576 | 0577 | 0578 | 0579 | 0580 | 0581 | 0582 | 0583 | 0584 | 0585 | 0586 | 0587 | 0588 | 0589 | 0590 | 0591 | 0592 | 0593 | 0594 | 0595 | 0596 | 0597 | 0598 | 0599 | 0600 | 0601 | 0602 | 0603 | 0604 | 0605 | 0606 | 0607 | 0608 | 0609 | 0610 | 0611 | 0612 | 0613 | 0614 | 0615 | 0616 | 0617 | 0618 | 0619 | 0620 | 0621 | 0622 | 0623 | 0624 | 0625 | 0626 | 0627 | 0628 | 0629 | 0630 | 0631 | 0632 | 0633 | 0634 | 0635 | 0636 | 0637 | 0638 | 0639 | 0640 | 0641 | 0642 | 0643 | 0644 | 0645 | 0646 | 0647 | 0648 | 0649 | 0650 | 0651 | 0652 | 0653 | 0654 | 0655 | 0656 | 0657 | 0658 | 0659 | 0660 | 0661 | 0662 | 0663 | 0664 | 0665 | 0666 | 0667 | 0668 | 0669 | 0670 | 0671 | 0672 | 0673 | 0674 | 0675 | 0676 | 0677 | 0678 | 0679 | 0680 | 0681 | 0682 | 0683 | 0684 | 0685 | 0686 | 0687 | 0688 | 0689 | 0690 | 0691 | 0692 | 0693 | 0694 | 0695 | 0696 | 0697 | 0698 | 0699 | 0700 | 0701 | 0702 | 0703 | 0704 | 0705 | 0706 | 0707 | 0708 | 0709 | 0710 | 0711 | 0712 | 0713 | 0714 | 0715 | 0716 | 0717 | 0718 | 0719 | 0720 | 0721 | 0722 | 0723 | 0724 | 0725 | 0726 | 0727 | 0728 | 0729 | 0730 | 0731 | 0732 | 0733 | 0734 | 0735 | 0736 | 0737 | 0738 | 0739 | 0740 | 0741 | 0742 | 0743 | 0744 | 0745 | 0746 | 0747 | 0748 | 0749 | 0750 | 0751 | 0752 | 0753 | 0754 | 0755 | 0756 | 0757 | 0758 | 0759 | 0760 | 0761 | 0762 | 0763 | 0764 | 0765 | 0766 | 0767 | 0768 | 0769 | 0770 | 0771 | 0772 | 0773 | 0774 | 0775 | 0776 | 0777 | 0778 | 0779 | 0780 | 0781 | 0782 | 0783 | 0784 | 0785 | 0786 | 0787 | 0788 | 0789 | 0790 | 0791 | 0792 | 0793 | 0794 | 0795 | 0796 | 0797 | 0798 | 0799 | 0800 | 0801 | 0802 | 0803 | 0804 | 0805 | 0806 | 0807 | 0808 | 0809 | 0810 | 0811 | 0812 | 0813 | 0814 | 0815 | 0816 | 0817 | 0818 | 0819 | 0820 | 0821 | 0822 | 0823 | 0824 | 0825 | 0826 | 0827 | 0828 | 0829 | 0830 | 0831 | 0832 | 0833 | 0834 | 0835 | 0836 | 0837 | 0838 | 0839 | 0840 | 0841 | 0842 | 0843 | 0844 | 0845 | 0846 | 0847 | 0848 | 0849 | 0850 | 0851 | 0852 | 0853 | 0854 | 0855 | 0856 | 0857 | 0858 | 0859 | 0860 | 0861 | 0862 | 0863 | 0864 | 0865 | 0866 | 0867 | 0868 | 0869 | 0870 | 0871 | 0872 | 0873 | 0874 | 0875 | 0876 | 0877 | 0878 | 0879 | 0880 | 0881 | 0882 | 0883 | 0884 | 0885 | 0886 | 0887 | 0888 | 0889 | 0890 | 0891 | 0892 | 0893 | 0894 | 0895 | 0896 | 0897 | 0898 | 0899 | 0900 | 0901 | 0902 | 0903 | 0904 | 0905 | 0906 | 0907 | 0908 | 0909 | 0910 | 0911 | 0912 | 0913 | 0914 | 0915 | 0916 | 0917 | 0918 | 0919 | 0920 | 0921 | 0922 | 0923 | 0924 | 0925 | 0926 | 0927 | 0928 | 0929 | 0930 | 0931 | 0932 | 0933 | 0934 | 0935 | 0936 | 0937 | 0938 | 0939 | 0940 | 0941 | 0942 | 0943 | 0944 | 0945 | 0946 | 0947 | 0948 | 0949 | 0950 | 0951 | 0952 | 0953 | 0954 | 0955 | 0956 | 0957 | 0958 | 0959 | 0960 | 0961 | 0962 | 0963 | 0964 | 0965 | 0966 | 0967 | 0968 | 0969 | 0970 | 0971 | 0972 | 0973 | 0974 | 0975 | 0976 | 0977 | 0978 | 0979 | 0980 | 0981 | 0982 | 0983 | 0984 | 0985 | 0986 | 0987 | 0988 | 0989 | 0990 | 0991 | 0992 | 0993 | 0994 | 0995 | 0996 | 0997 | 0998 | 0999 | 1000 | 1001 | 1002 | 1003 | 1004 | 1005 | 1006 | 1007 | 1008 | 1009 | 1010 | 1011 | 1012 | 1013 | 1014 | 1015 | 1016 | 1017 | 1018 | 1019 | 1020 | 1021 | 1022 | 1023 | 1024 | 1025 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|





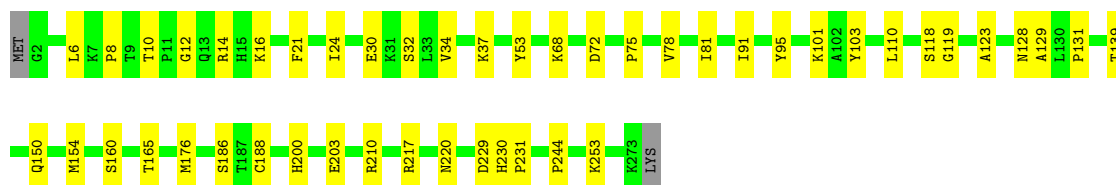
• Molecule 11: 5S rRNA

Chain B: 52% 35% 6% 6%



• Molecule 12: Large ribosomal subunit protein uL2

Chain D: 82% 17%



• Molecule 13: Large ribosomal subunit protein uL3

Chain E: 90% 10%



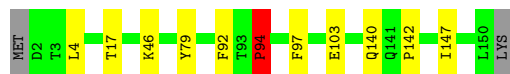
• Molecule 14: Large ribosomal subunit protein uL4

Chain F: 93% 5%




- Molecule 15: Large ribosomal subunit protein uL13

Chain M:  91% 7% ..




- Molecule 16: Large ribosomal subunit protein uL15

Chain O:  85% 12% ..



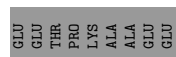
- Molecule 17: Large ribosomal subunit protein uL16

Chain P:  83% 16% .




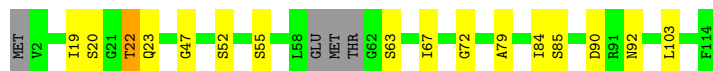
- Molecule 18: Large ribosomal subunit protein bL17

Chain Q:  67% 10% 23%




- Molecule 19: Large ribosomal subunit protein uL18

Chain R:  82% 13% . .



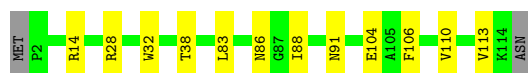
- Molecule 20: Large ribosomal subunit protein bL19

Chain S:  82% 11% 7%



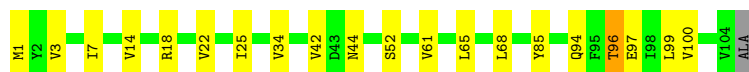
- Molecule 21: Large ribosomal subunit protein bL20

Chain T:  88% 10% .



- Molecule 22: Large ribosomal subunit protein bL21

Chain U: 80% 18% ..



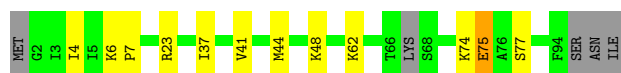
- Molecule 23: Large ribosomal subunit protein uL22

Chain V: 81% 13% 5%



- Molecule 24: Large ribosomal subunit protein uL23

Chain W: 82% 11% 5%



- Molecule 25: Large ribosomal subunit protein uL24

Chain X: 70% 22% 8%



- Molecule 26: Large ribosomal subunit protein bL25

Chain Y: 78% 12% 8%

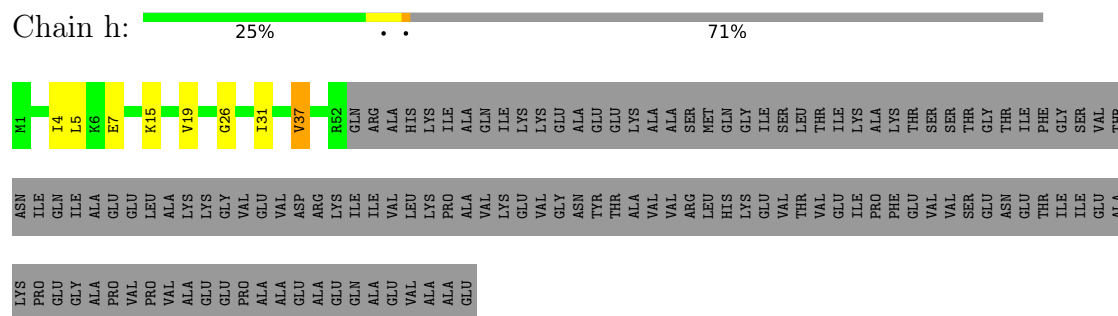


- Molecule 27: Large ribosomal subunit protein bL27

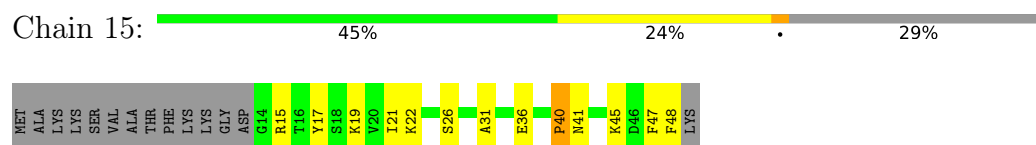
Chain Z: 84% 7% 9%



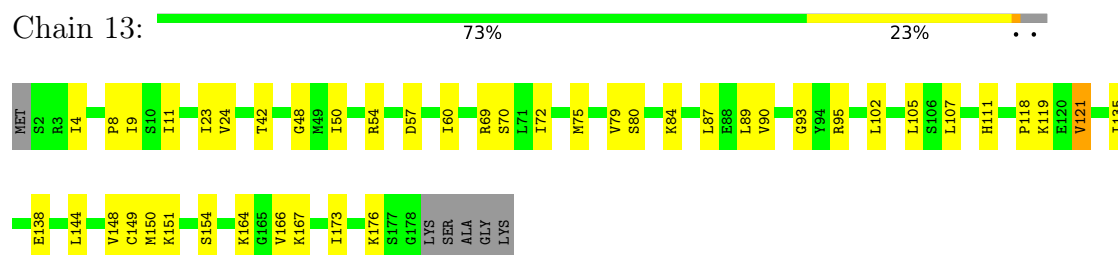
- Molecule 28: Large ribosomal subunit protein bL9



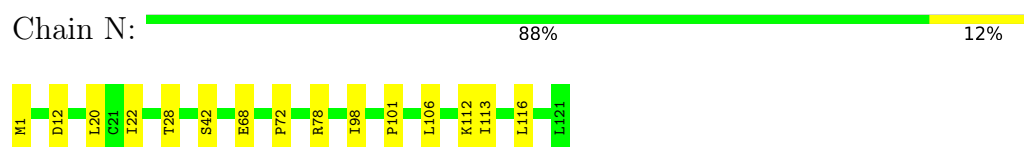
- Molecule 29: DUF4295 domain-containing protein



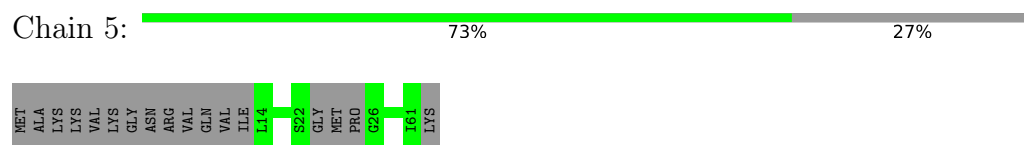
- Molecule 30: Large ribosomal subunit protein uL6



- Molecule 31: Large ribosomal subunit protein uL14



- Molecule 32: Large ribosomal subunit protein bL33



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	223396	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.294	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.005	Depositor
Map size (\AA)	370.48, 370.48, 370.48	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.842, 0.842, 0.842	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, ZN, 5MC, 62B, K, MG, PSU, OMU, 2MG, 2MA, 6MA, MA6, 5MU, OMG, NA, 5OC

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	0	0.17	0/609	0.31	0/815
2	1	0.14	0/470	0.28	0/633
3	11	0.70	4/1042 (0.4%)	1.13	9/1425 (0.6%)
4	12	0.11	0/265	0.39	0/366
5	2	0.23	0/437	0.55	1/587 (0.2%)
6	4	0.18	0/447	0.34	0/604
7	6	0.17	0/385	0.34	0/508
8	7	0.18	0/515	0.41	0/683
9	8	0.20	0/299	0.43	0/395
10	A	0.23	0/60371	0.36	0/94092
11	B	0.17	0/2445	0.30	0/3807
12	D	0.20	0/2075	0.45	2/2788 (0.1%)
13	E	0.18	0/1525	0.40	0/2050
14	F	0.16	0/1543	0.30	0/2097
15	M	0.40	1/1161 (0.1%)	0.70	5/1571 (0.3%)
16	O	0.17	0/1032	0.39	0/1387
17	P	0.17	0/1118	0.35	0/1503
18	Q	0.19	0/985	0.37	0/1321
19	R	0.12	0/755	0.30	0/1015
20	S	0.16	0/869	0.33	0/1170
21	T	0.17	0/933	0.32	0/1248
22	U	0.16	0/792	0.37	0/1068
23	V	0.20	0/1026	0.46	2/1370 (0.1%)
24	W	0.16	0/690	0.33	0/924
25	X	0.16	0/698	0.40	0/937
26	Y	0.46	2/1184 (0.2%)	0.95	7/1622 (0.4%)
27	Z	0.16	0/581	0.35	0/777
28	h	0.18	0/351	0.45	0/477
29	15	0.25	0/260	0.78	2/349 (0.6%)
30	13	0.23	1/1327 (0.1%)	0.53	4/1792 (0.2%)
31	N	0.22	0/882	0.49	3/1190 (0.3%)
32	5	0.14	0/348	0.33	0/468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.24	8/87420 (0.0%)	0.40	35/131039 (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
13	E	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	11	32	PRO	CG-CD	-11.94	1.10	1.50
3	11	87	PRO	CG-CD	-11.39	1.12	1.50
3	11	70	PRO	CG-CD	-11.27	1.12	1.50
15	M	142	PRO	CG-CD	-11.14	1.12	1.50
26	Y	139	PRO	CG-CD	-10.69	1.14	1.50

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	11	32	PRO	N-CD-CG	-18.81	74.98	103.20
26	Y	139	PRO	CB-CG-CD	18.29	164.63	106.10
26	Y	139	PRO	N-CD-CG	-17.78	76.53	103.20
3	11	87	PRO	N-CD-CG	-16.76	78.06	103.20
15	M	142	PRO	N-CD-CG	-16.06	79.11	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	E	151	TYR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	600	0	632	4	0
2	1	466	0	475	5	0
3	11	1033	0	801	16	0
4	12	267	0	126	2	0
5	2	434	0	482	6	0
6	4	436	0	419	5	0
7	6	382	0	409	4	0
8	7	508	0	557	9	0
9	8	297	0	315	6	0
10	A	54304	0	27363	346	0
11	B	2187	0	1105	22	0
12	D	2036	0	2092	22	0
13	E	1497	0	1527	11	0
14	F	1520	0	1504	5	0
15	M	1136	0	1133	8	0
16	O	1021	0	1035	11	0
17	P	1095	0	1124	13	0
18	Q	968	0	1003	10	0
19	R	751	0	711	6	0
20	S	854	0	831	10	0
21	T	916	0	969	7	0
22	U	782	0	804	12	0
23	V	1013	0	1058	10	0
24	W	682	0	685	8	0
25	X	693	0	701	11	0
26	Y	1166	0	1057	10	0
27	Z	574	0	578	3	0
28	h	349	0	344	4	0
29	15	256	0	243	9	0
30	13	1309	0	1300	24	0
31	N	875	0	906	10	0
32	5	346	0	338	0	0
33	4	1	0	0	0	0
33	A	134	0	0	0	0
33	B	1	0	0	0	0
33	F	1	0	0	0	0
33	V	2	0	0	0	0
34	4	1	0	0	0	0
35	A	35	0	0	0	0
36	A	18	0	0	0	0
37	A	13	0	0	0	0
37	B	2	0	0	0	0
38	0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	4	6	0	0	0	0
38	6	12	0	0	1	0
38	7	1	0	0	0	0
38	A	1225	0	0	6	0
38	B	4	0	0	0	0
38	D	26	0	0	0	0
38	E	16	0	0	0	0
38	F	19	0	0	0	0
38	O	16	0	0	0	0
38	Q	8	0	0	1	0
38	S	1	0	0	0	0
38	T	15	0	0	0	0
38	U	8	0	0	0	0
38	V	15	0	0	0	0
38	W	2	0	0	0	0
38	Z	5	0	0	0	0
All	All	82341	0	52627	582	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 582 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1521:G:OP2	12:D:101:LYS:NZ	2.16	0.75
10:A:2671:G:C4	10:A:2672:H2U:H51	2.22	0.74
10:A:2820:G:OP2	13:E:56:LYS:NZ	2.21	0.73
10:A:1862:A:H2'	10:A:1863:A:C8	2.24	0.72
7:6:45:SER:OG	10:A:114:A:OP1	2.08	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	75/79 (95%)	75 (100%)	0	0	100	100
2	1	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
3	11	160/186 (86%)	145 (91%)	15 (9%)	0	100	100
4	12	46/85 (54%)	34 (74%)	12 (26%)	0	100	100
5	2	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
6	4	55/61 (90%)	52 (94%)	3 (6%)	0	100	100
7	6	46/50 (92%)	46 (100%)	0	0	100	100
8	7	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
9	8	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
12	D	270/274 (98%)	264 (98%)	6 (2%)	0	100	100
13	E	202/205 (98%)	190 (94%)	11 (5%)	1 (0%)	25	47
14	F	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
15	M	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
16	O	142/148 (96%)	137 (96%)	5 (4%)	0	100	100
17	P	140/144 (97%)	135 (96%)	5 (4%)	0	100	100
18	Q	121/160 (76%)	119 (98%)	2 (2%)	0	100	100
19	R	106/114 (93%)	102 (96%)	4 (4%)	0	100	100
20	S	111/121 (92%)	109 (98%)	2 (2%)	0	100	100
21	T	111/115 (96%)	111 (100%)	0	0	100	100
22	U	102/105 (97%)	89 (87%)	13 (13%)	0	100	100
23	V	125/134 (93%)	123 (98%)	2 (2%)	0	100	100
24	W	88/97 (91%)	86 (98%)	2 (2%)	0	100	100
25	X	91/106 (86%)	89 (98%)	2 (2%)	0	100	100
26	Y	172/192 (90%)	158 (92%)	14 (8%)	0	100	100
27	Z	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
28	h	50/179 (28%)	44 (88%)	6 (12%)	0	100	100
29	15	33/49 (67%)	30 (91%)	3 (9%)	0	100	100
30	13	175/183 (96%)	170 (97%)	5 (3%)	0	100	100
31	N	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
32	5	41/62 (66%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3222/3640 (88%)	3081 (96%)	140 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	E	152	PRO

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	
1	0	59/66 (89%)	59 (100%)	0	100	100
2	1	43/56 (77%)	42 (98%)	1 (2%)	45	71
3	11	66/161 (41%)	62 (94%)	4 (6%)	15	34
4	12	5/77 (6%)	5 (100%)	0	100	100
5	2	47/53 (89%)	45 (96%)	2 (4%)	25	49
6	4	39/50 (78%)	39 (100%)	0	100	100
7	6	37/40 (92%)	36 (97%)	1 (3%)	40	66
8	7	55/58 (95%)	55 (100%)	0	100	100
9	8	29/35 (83%)	28 (97%)	1 (3%)	32	58
12	D	208/218 (95%)	199 (96%)	9 (4%)	25	49
13	E	152/163 (93%)	146 (96%)	6 (4%)	27	53
14	F	147/177 (83%)	140 (95%)	7 (5%)	21	44
15	M	113/128 (88%)	110 (97%)	3 (3%)	40	66
16	O	97/117 (83%)	94 (97%)	3 (3%)	35	62
17	P	107/118 (91%)	104 (97%)	3 (3%)	38	65
18	Q	96/129 (74%)	95 (99%)	1 (1%)	73	88
19	R	59/90 (66%)	53 (90%)	6 (10%)	6	12
20	S	79/107 (74%)	77 (98%)	2 (2%)	42	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	T	90/93 (97%)	89 (99%)	1 (1%)	70	86
22	U	80/92 (87%)	77 (96%)	3 (4%)	28	54
23	V	105/113 (93%)	105 (100%)	0	100	100
24	W	66/85 (78%)	62 (94%)	4 (6%)	15	34
25	X	67/89 (75%)	62 (92%)	5 (8%)	11	24
26	Y	91/159 (57%)	82 (90%)	9 (10%)	6	13
27	Z	59/69 (86%)	57 (97%)	2 (3%)	32	58
28	h	30/146 (20%)	29 (97%)	1 (3%)	33	59
29	15	26/42 (62%)	25 (96%)	1 (4%)	28	54
30	13	133/159 (84%)	125 (94%)	8 (6%)	16	35
31	N	88/100 (88%)	86 (98%)	2 (2%)	45	71
32	5	35/58 (60%)	35 (100%)	0	100	100
All	All	2308/3048 (76%)	2223 (96%)	85 (4%)	31	55

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	X	7	LYS
27	Z	9	SER
25	X	23	SER
26	Y	82	PRO
30	13	23	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	16	HIS
21	T	7	HIS
29	15	35	GLN
20	S	17	HIS
22	U	78	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2492/2882 (86%)	322 (12%)	21 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	B	99/109 (90%)	21 (21%)	1 (1%)
All	All	2591/2991 (86%)	343 (13%)	22 (0%)

5 of 343 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	23	A
10	A	52	A
10	A	60	A
10	A	63	A
10	A	64	G

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	1530	A
10	A	2431	A
10	A	2407	C
10	A	2475	C
10	A	1482	U

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

18 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
10	OMU	A	2450	10	19,22,23	3.01	8 (42%)	26,31,34	1.82	6 (23%)
10	5MU	A	1949	10	19,22,23	0.50	0	28,32,35	0.51	0
10	PSU	A	2606	10	18,21,22	1.09	1 (5%)	22,30,33	1.80	3 (13%)
10	5MC	A	1935	10	18,22,23	0.53	0	26,32,35	0.57	0
10	H2U	A	2620	10	18,21,22	0.64	0	21,30,33	1.02	1 (4%)
10	H2U	A	876	10	18,21,22	0.56	0	21,30,33	0.90	2 (9%)
10	H2U	A	781	10	18,21,22	0.50	0	21,30,33	1.24	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	6MA	A	2067	10,33	18,24,25	0.70	0	15,34,37	0.75	1 (6%)
10	2MG	A	2446	10	18,26,27	1.23	2 (11%)	16,38,41	0.96	2 (12%)
10	OMG	A	2252	10	18,26,27	1.19	2 (11%)	19,38,41	0.83	1 (5%)
10	PSU	A	2581	10	18,21,22	1.08	1 (5%)	22,30,33	1.79	4 (18%)
10	5OC	A	2502	10,36	18,21,22	4.28	13 (72%)	25,30,33	1.44	2 (8%)
10	6MA	A	2069	10	18,24,25	0.73	0	15,34,37	0.74	1 (6%)
10	2MA	A	2504	10,36	19,25,26	3.57	6 (31%)	21,37,40	2.42	3 (14%)
10	H2U	A	2672	10	18,21,22	0.53	0	21,30,33	0.97	2 (9%)
10	MA6	A	2068	10	18,26,27	1.00	2 (11%)	19,38,41	4.17	2 (10%)
10	5MC	A	1972	10	18,22,23	0.63	0	26,32,35	0.56	0
10	OMG	A	2554	10	18,26,27	1.18	2 (11%)	19,38,41	0.88	1 (5%)

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
10	OMU	A	2450	10	-	0/9/27/28	0/2/2/2
10	5MU	A	1949	10	-	0/7/25/26	0/2/2/2
10	PSU	A	2606	10	-	0/7/25/26	0/2/2/2
10	5MC	A	1935	10	-	0/7/25/26	0/2/2/2
10	H2U	A	2620	10	-	0/7/38/39	0/2/2/2
10	H2U	A	876	10	-	0/7/38/39	0/2/2/2
10	H2U	A	781	10	-	0/7/38/39	0/2/2/2
10	6MA	A	2067	10,33	-	1/5/23/24	0/3/3/3
10	2MG	A	2446	10	-	2/5/27/28	0/3/3/3
10	OMG	A	2252	10	-	1/5/27/28	0/3/3/3
10	PSU	A	2581	10	-	0/7/25/26	0/2/2/2
10	5OC	A	2502	10,36	-	5/7/21/22	0/2/2/2
10	6MA	A	2069	10	-	0/5/23/24	0/3/3/3
10	2MA	A	2504	10,36	-	3/3/25/26	0/3/3/3
10	H2U	A	2672	10	-	0/7/38/39	0/2/2/2
10	MA6	A	2068	10	-	0/7/29/30	0/3/3/3
10	5MC	A	1972	10	-	1/7/25/26	0/2/2/2
10	OMG	A	2554	10	-	0/5/27/28	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2504	2MA	C4-N3	9.27	1.50	1.35
10	A	2502	5OC	C2'-C3'	-8.26	1.31	1.52
10	A	2504	2MA	C2-N3	7.82	1.47	1.34
10	A	2450	OMU	C2-N1	7.05	1.49	1.38
10	A	2450	OMU	C2-N3	6.58	1.49	1.38

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2068	MA6	N1-C6-N6	-16.99	99.17	117.06
10	A	2504	2MA	C2-N3-C4	7.23	121.40	115.52
10	A	2504	2MA	C1'-N9-C4	-6.79	114.71	126.64
10	A	2068	MA6	N3-C2-N1	-5.68	119.80	128.68
10	A	2450	OMU	C4-N3-C2	-5.42	119.44	126.58

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2067	6MA	N1-C6-N6-C1
10	A	2502	5OC	C3'-C4'-C5'-O5'
10	A	2502	5OC	O4'-C4'-C5'-O5'
10	A	2446	2MG	C3'-C4'-C5'-O5'
10	A	2504	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2450	OMU	2	0
10	A	2620	H2U	1	0
10	A	876	H2U	2	0
10	A	2067	6MA	1	0
10	A	2502	5OC	2	0
10	A	2672	H2U	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 174 ligands modelled in this entry, 173 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
35	62B	A	2901	-	37,38,38	0.52	0	55,60,60	1.37	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	62B	A	2901	-	-	0/12/86/86	0/4/4/4

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	2901	62B	C18-C12-C13	-4.47	102.27	105.60
35	A	2901	62B	C15-C5-C14	-3.60	105.41	108.95
35	A	2901	62B	O1-C3-C2	-3.51	120.47	125.56
35	A	2901	62B	C28-C23-S1	-2.89	106.04	111.10
35	A	2901	62B	C12-C11-C10	2.61	117.14	114.58

There are no chirality outliers.

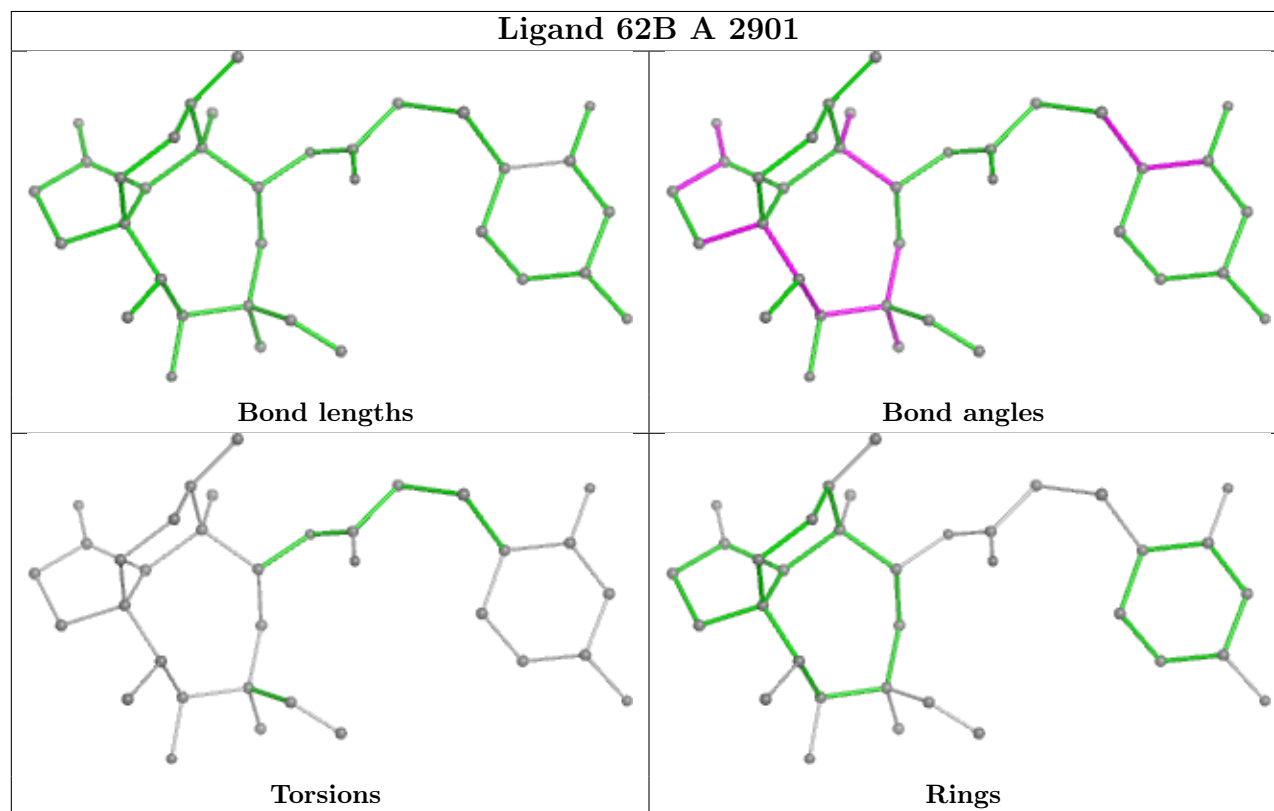
There are no torsion outliers.

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](#)

There are no chain breaks in this entry.

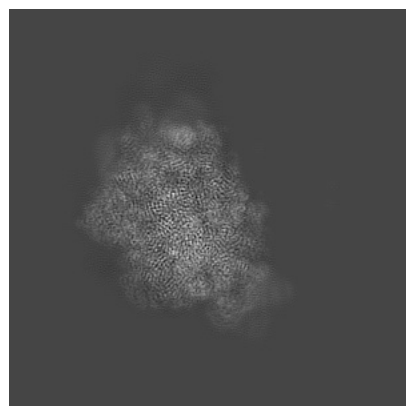
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52635. These allow visual inspection of the internal detail of the map and identification of artifacts.

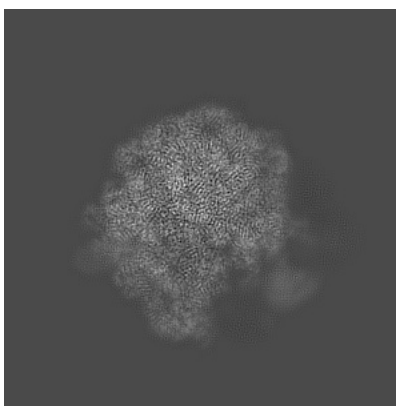
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

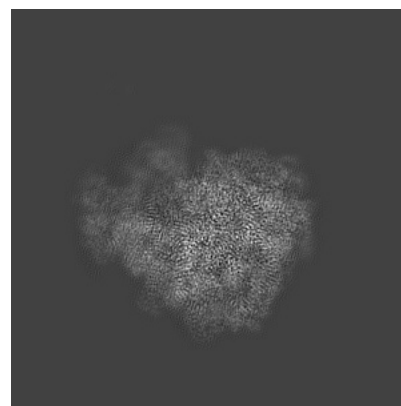
6.1.1 Primary map



X

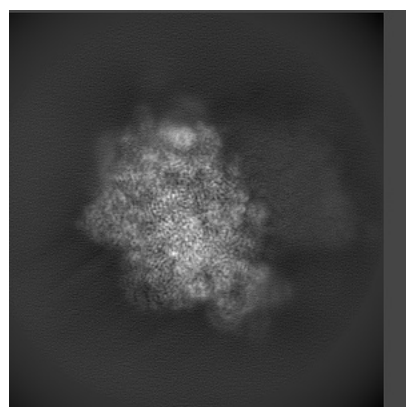


Y

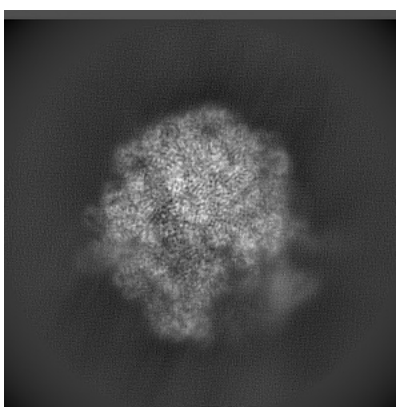


Z

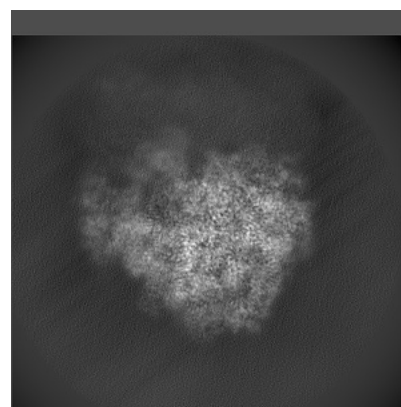
6.1.2 Raw map



X



Y

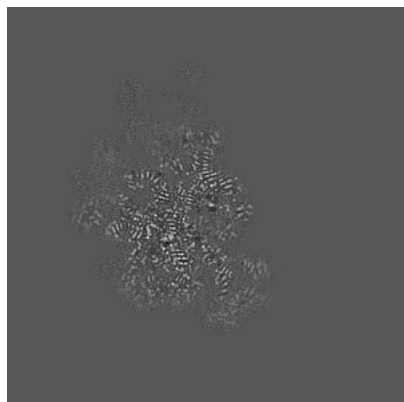


Z

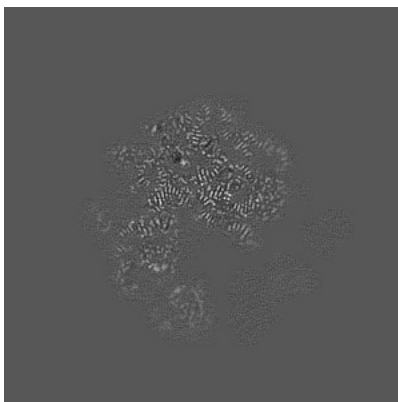
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

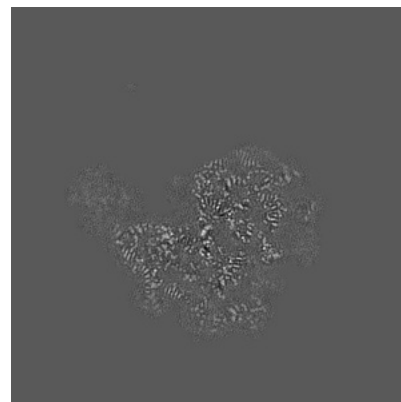
6.2.1 Primary map



X Index: 220

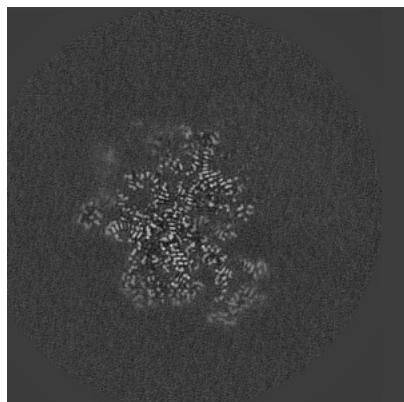


Y Index: 220

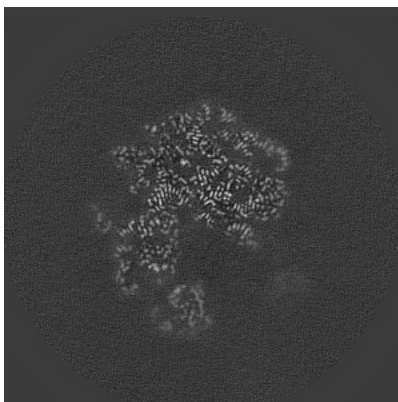


Z Index: 220

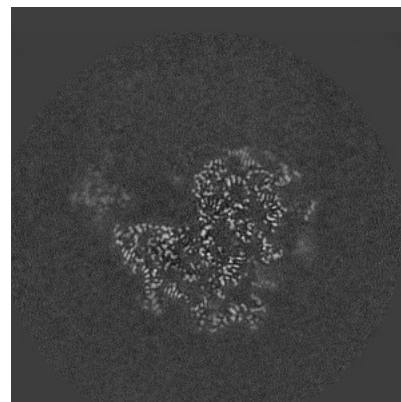
6.2.2 Raw map



X Index: 220



Y Index: 220

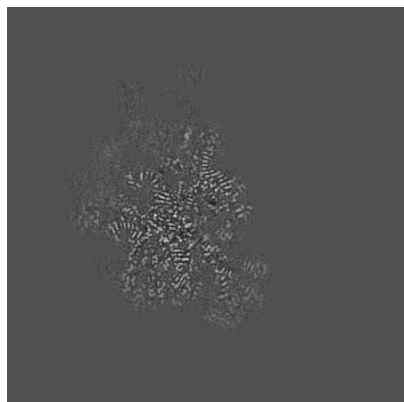


Z Index: 220

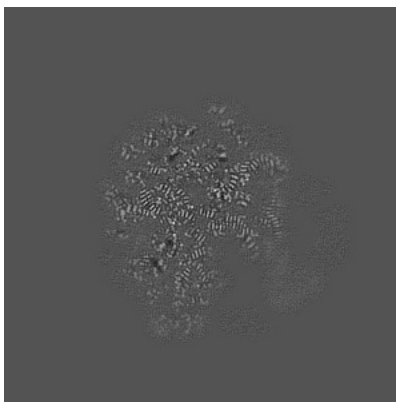
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

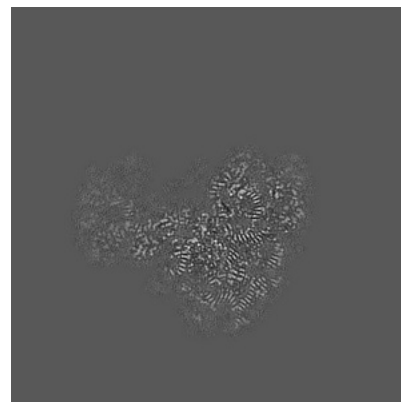
6.3.1 Primary map



X Index: 219

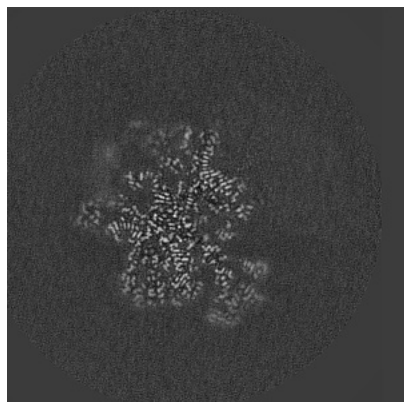


Y Index: 194

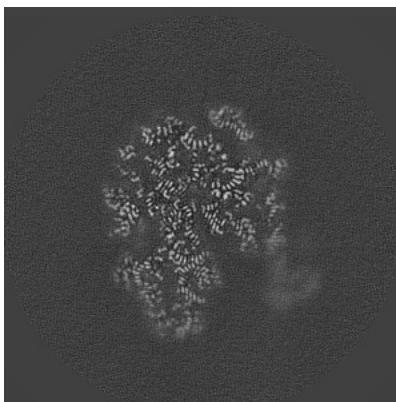


Z Index: 192

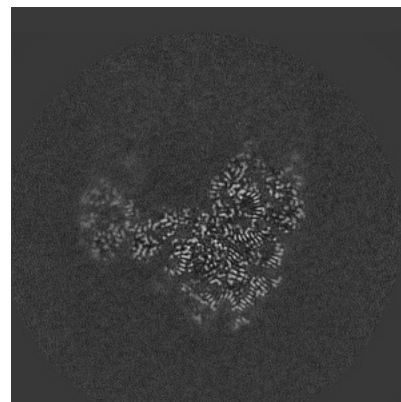
6.3.2 Raw map



X Index: 219



Y Index: 199

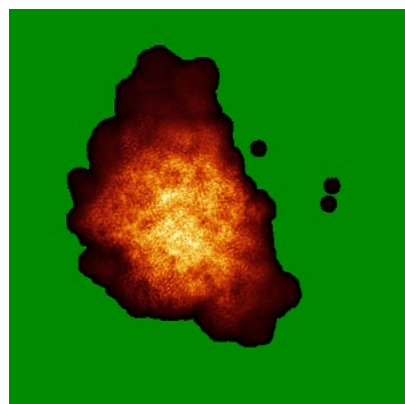


Z Index: 192

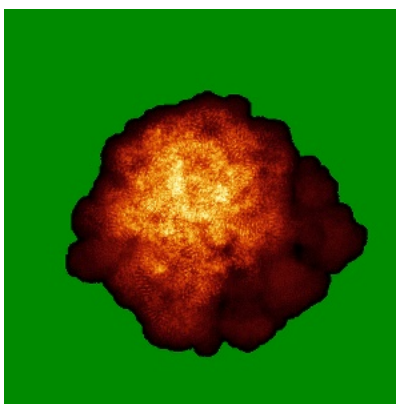
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

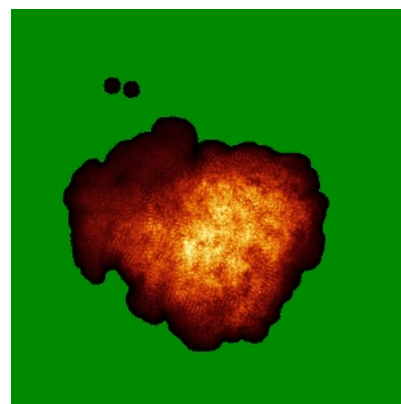
6.4.1 Primary map



X

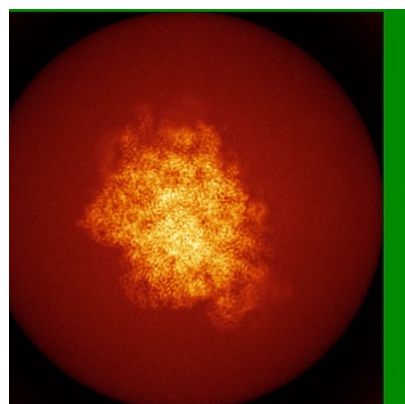


Y

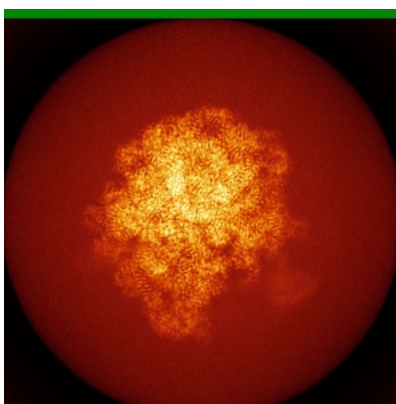


Z

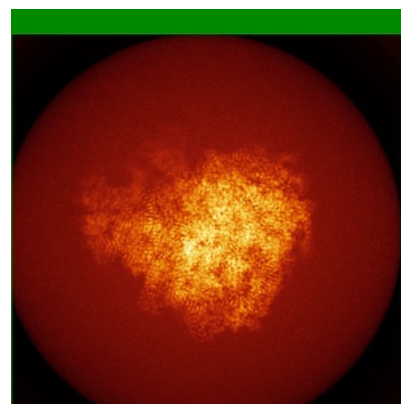
6.4.2 Raw map



X



Y

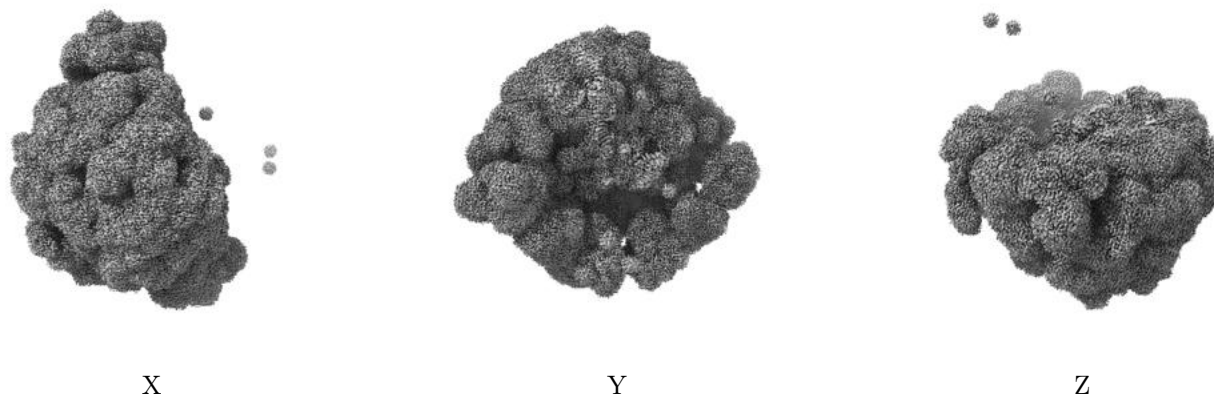


Z

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.

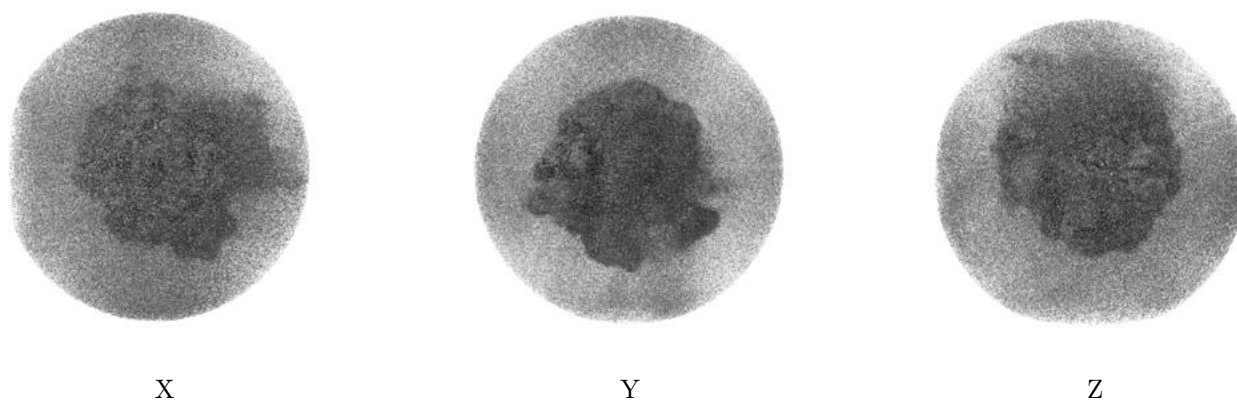
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

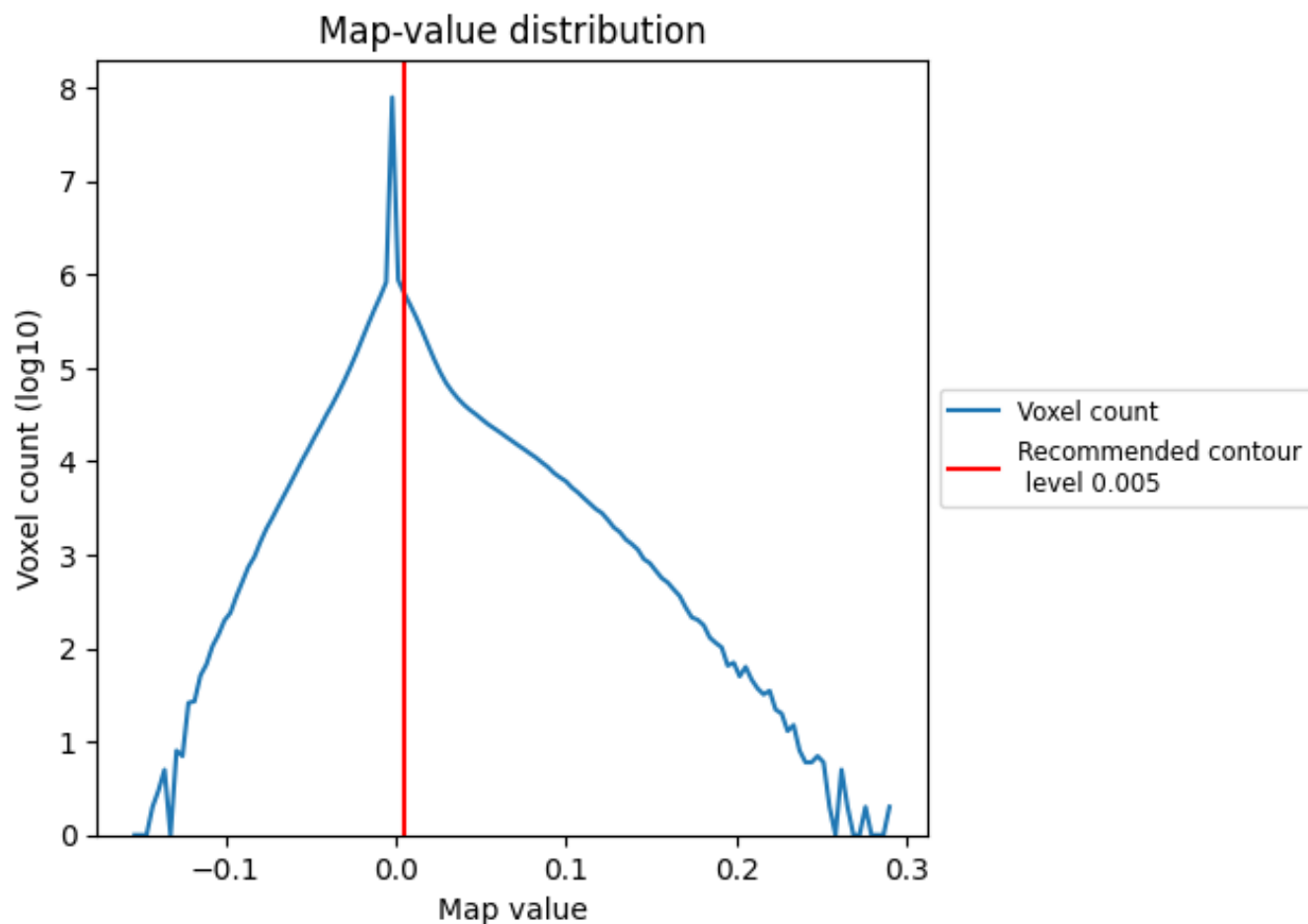
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

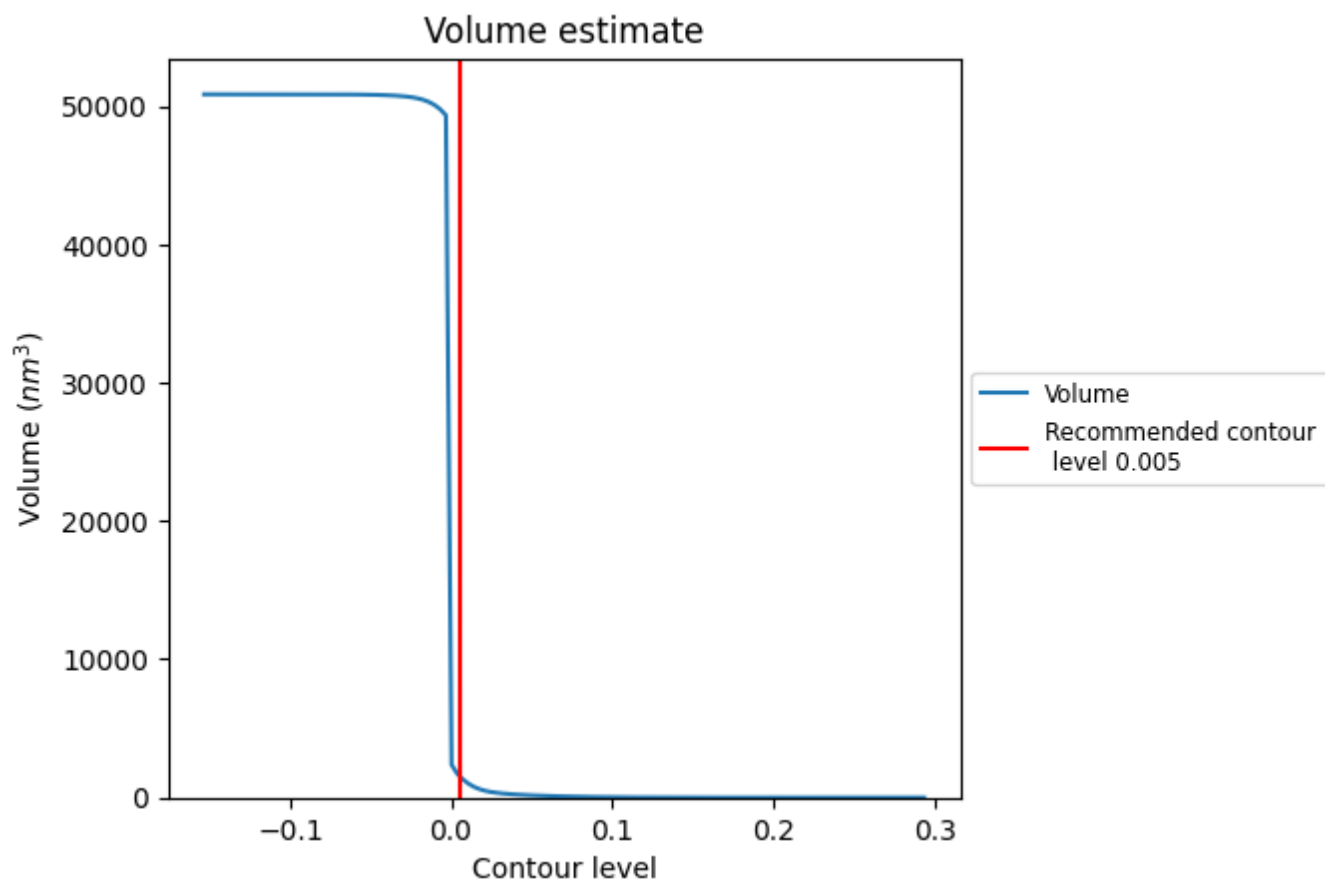
This section contains the results of statistical analysis of the map.

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.

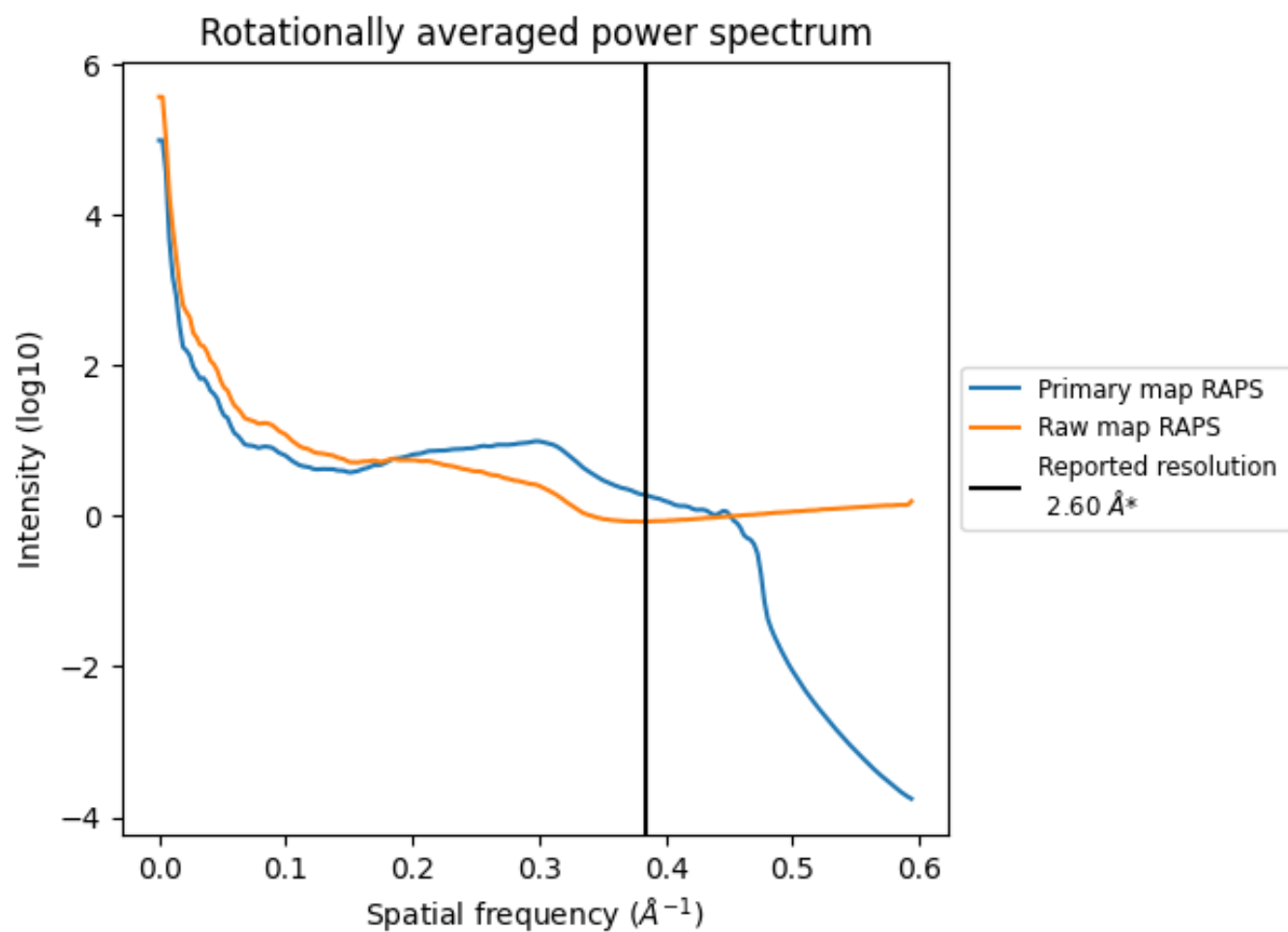
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1587 nm³; this corresponds to an approximate mass of 1434 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 ⓘ

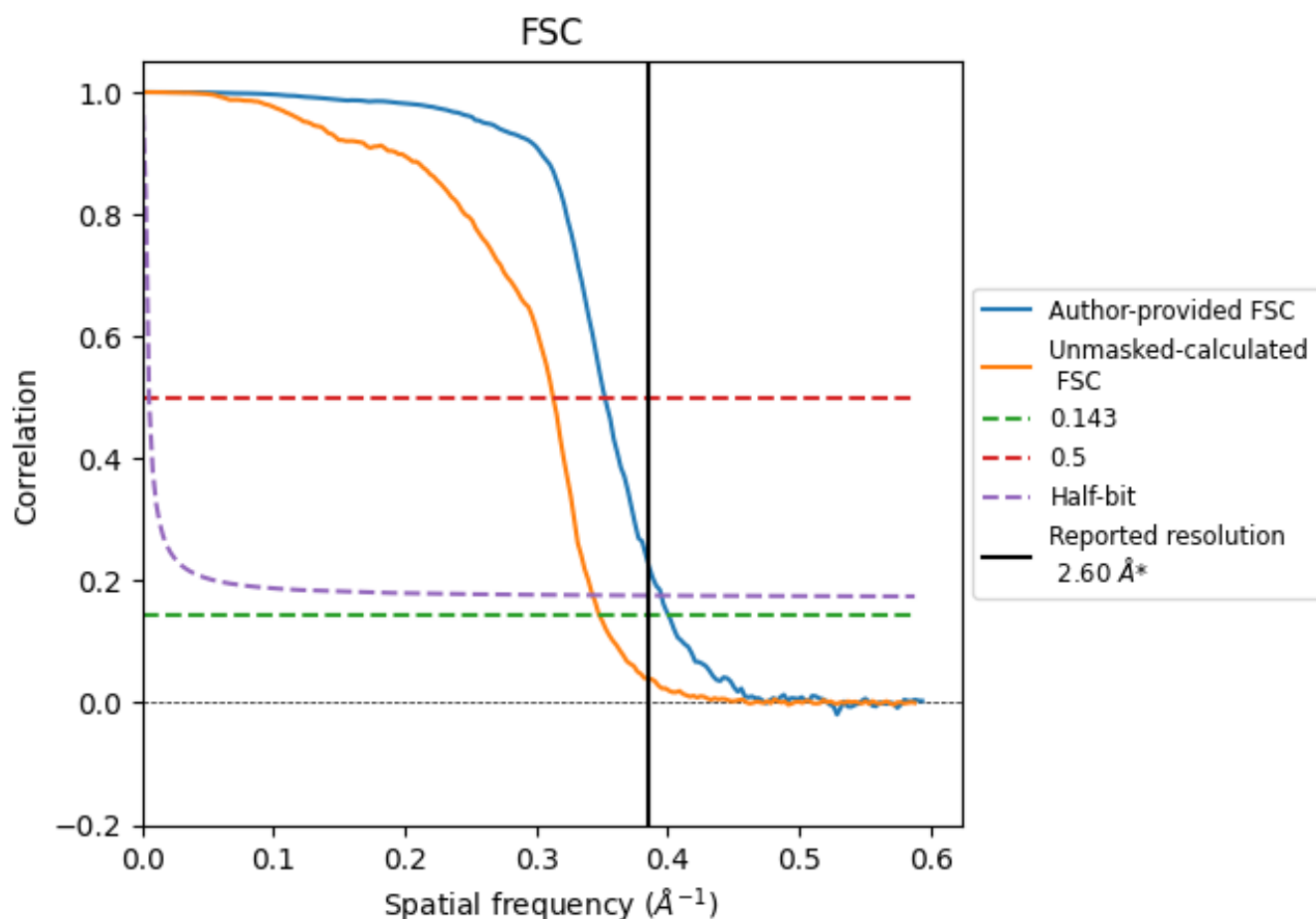


*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

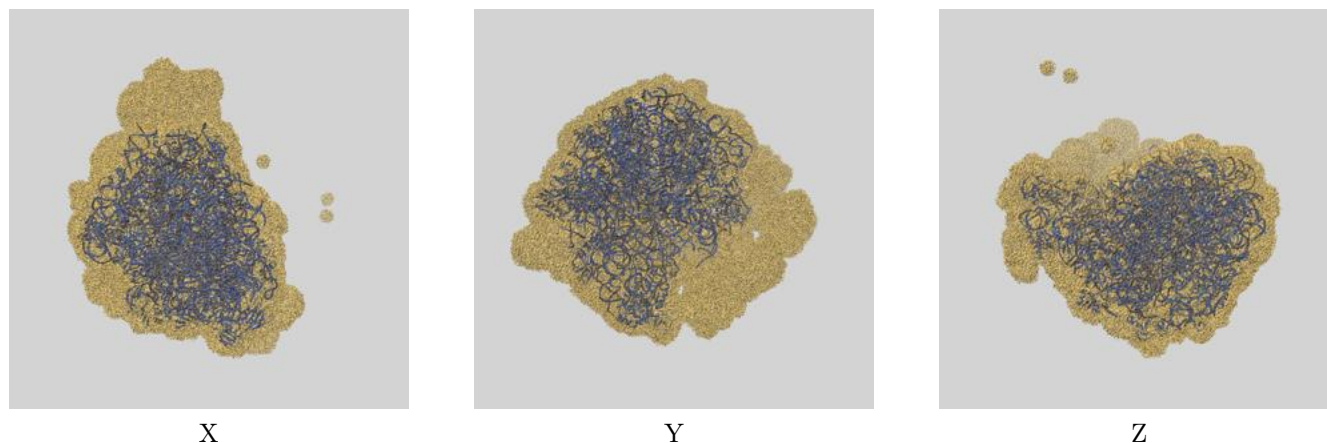
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.50	2.84	2.53
Unmasked-calculated*	2.87	3.20	2.92

*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 2.87 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

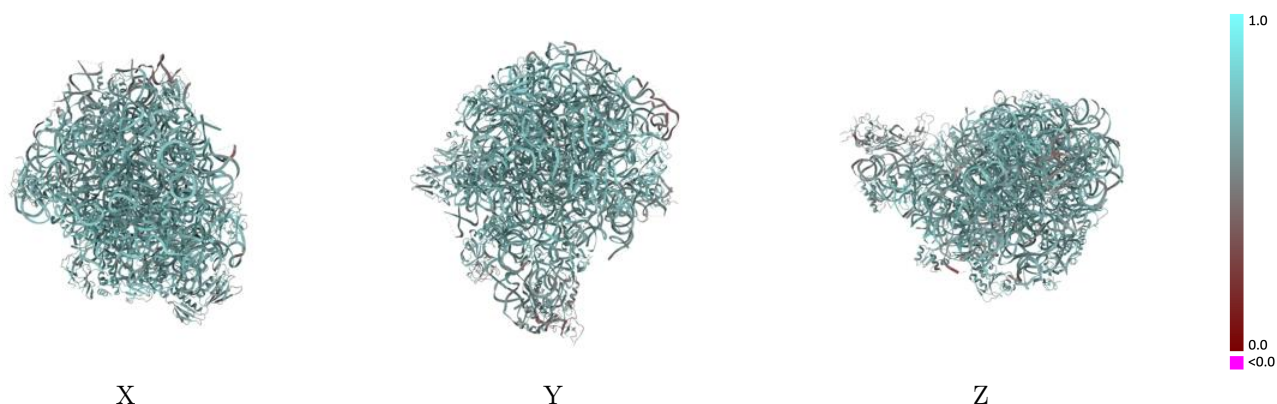
This section contains information regarding the fit between EMDB map EMD-52635 and PDB model 9I5T. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



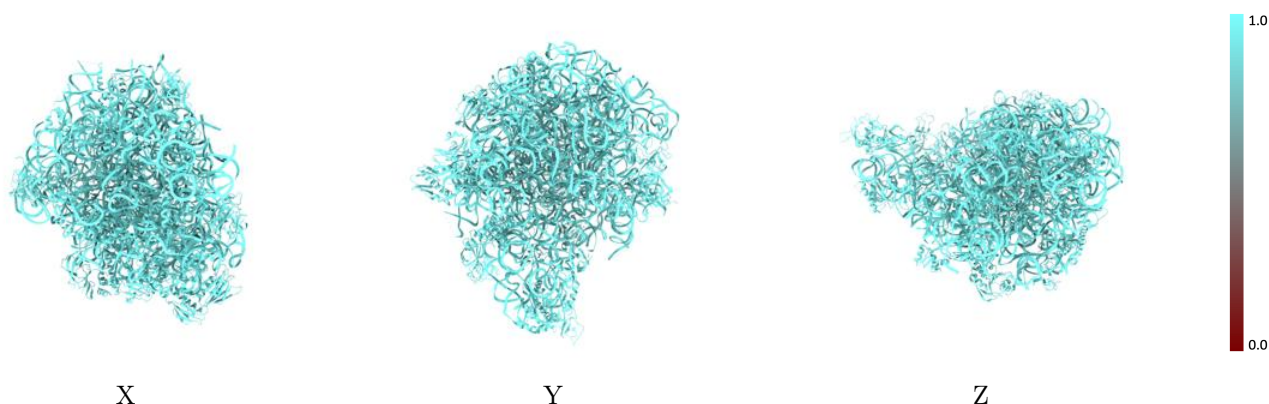
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



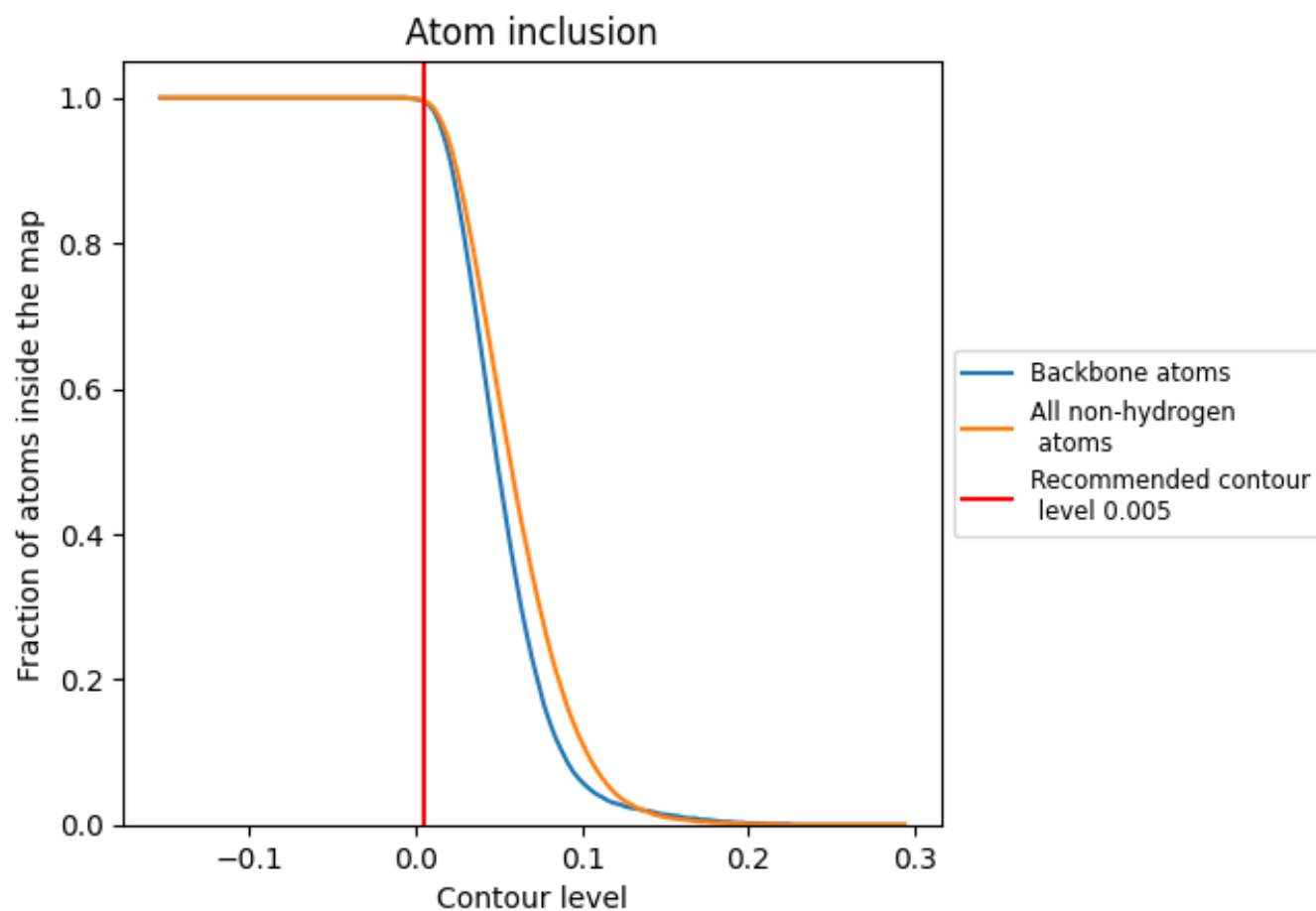
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).



































































9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9960	 0.6710
0	 0.9980	 0.6930
1	 0.9980	 0.6520
11	 0.9900	 0.5420
12	 0.9850	 0.4620
13	 0.9910	 0.5970
15	 0.9920	 0.5930
2	 0.9980	 0.6910
4	 1.0000	 0.7030
5	 0.9940	 0.6780
6	 1.0000	 0.7370
7	 0.9960	 0.7060
8	 0.9930	 0.6790
A	 0.9960	 0.6760
B	 0.9950	 0.5950
D	 0.9990	 0.7050
E	 0.9970	 0.6960
F	 0.9990	 0.6840
M	 0.9940	 0.6890
N	 0.9980	 0.6860
O	 0.9950	 0.6660
P	 0.9970	 0.6840
Q	 0.9990	 0.7150
R	 0.9990	 0.6260
S	 0.9950	 0.6770
T	 0.9980	 0.7210
U	 0.9920	 0.6620
V	 1.0000	 0.7040
W	 0.9930	 0.6600
X	 0.9970	 0.6540
Y	 0.9900	 0.5960
Z	 0.9980	 0.7090
h	 0.9910	 0.6090

