



Full wwPDB EM Validation Report ⓘ

Jul 17, 2021 – 05:09 am BST

PDB ID : 7OGM
EMDB ID : EMD-12884
Title : A cooperative PNPase-Hfq-RNA carrier complex facilitates bacterial riboregulation. PNPase-3'ETS(leuZ)-Hfq
Authors : Dendooven, T.; Sinha, D.; Roesoleva, A.; Cameron, T.A.; De Lay, N.; Luisi, B.F.; Bandyra, K.
Deposited on : 2021-05-06
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

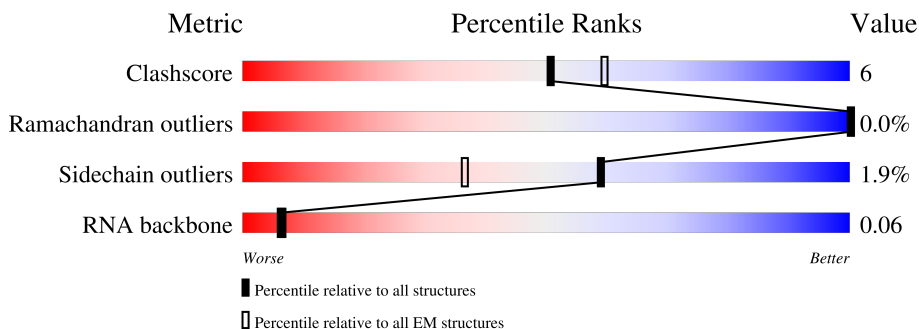
EMDB validation analysis : 0.0.0.dev84
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.22

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 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.



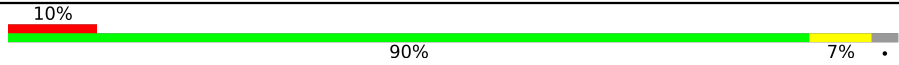
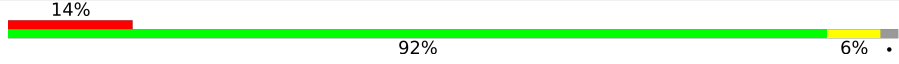

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	102	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 57%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: grey;"></div> </div>
1	E	102	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 56%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: grey;"></div> </div>
1	F	102	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 56%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: grey;"></div> </div>
1	I	102	<div style="display: flex; align-items: center;"> <div style="width: 23%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: grey;"></div> </div>
1	J	102	<div style="display: flex; align-items: center;"> <div style="width: 22%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 57%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: grey;"></div> </div>
1	K	102	<div style="display: flex; align-items: center;"> <div style="width: 17%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 51%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: grey;"></div> </div>
2	L	711	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	N	711	 <p>10% 90% 7%</p>
2	O	711	 <p>14% 92% 6%</p>
3	P	49	 <p>8% 12% 55% 33%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17683 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 RNA-binding protein Hfq.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	K	62	389	254	64	71	0	0
1	J	63	404	266	65	73	0	0
1	I	63	406	267	66	73	0	0
1	D	67	438	289	69	80	0	0
1	E	61	413	276	65	72	0	0
1	F	61	390	257	63	70	0	0

- Molecule 2 is a protein called Polyribonucleotide nucleotidyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	693	4777	3021	847	890	19	0	0
2	N	689	4841	3046	860	915	20	0	0
2	O	695	4672	2931	845	878	18	0	0

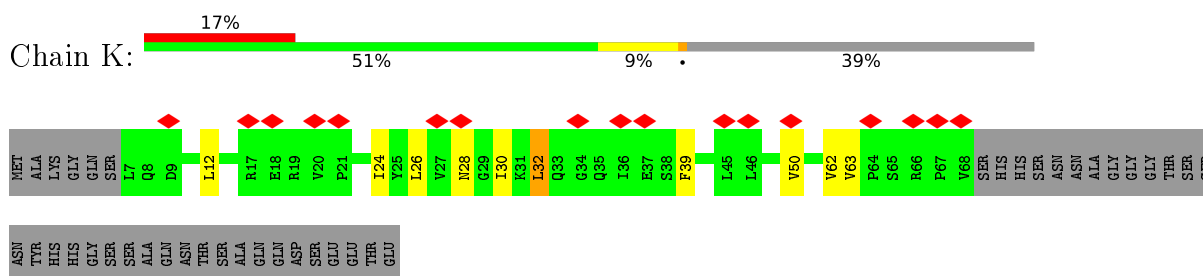
- Molecule 3 is a RNA chain called 3'ETS(LeuZ).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	P	49	953	422	162	320	49	0	0

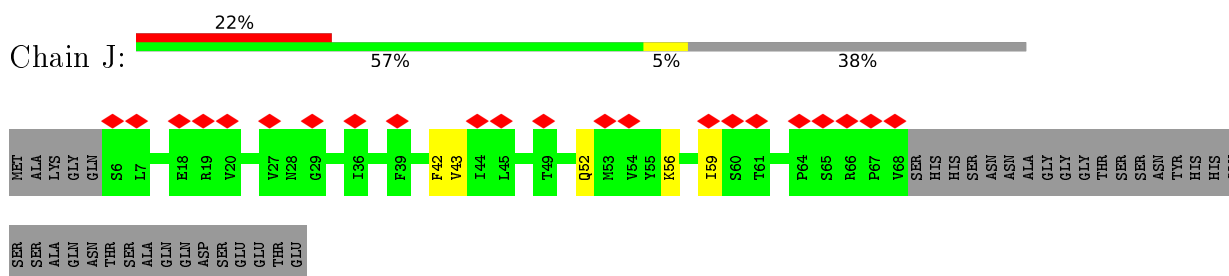
3 Residue-property plots

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

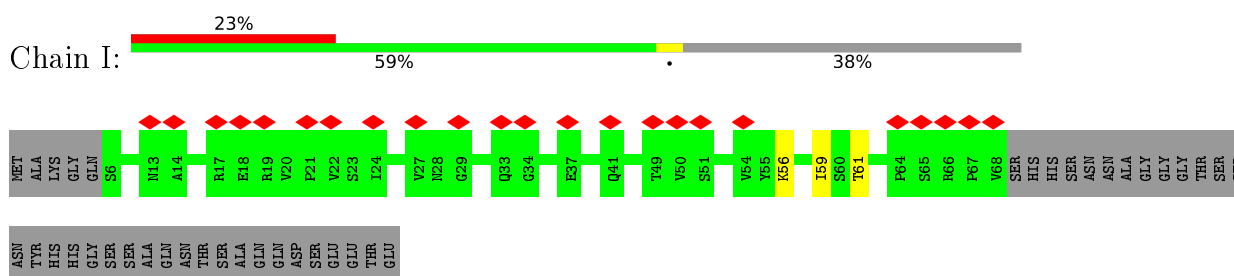
- Molecule 1: RNA-binding protein Hfq



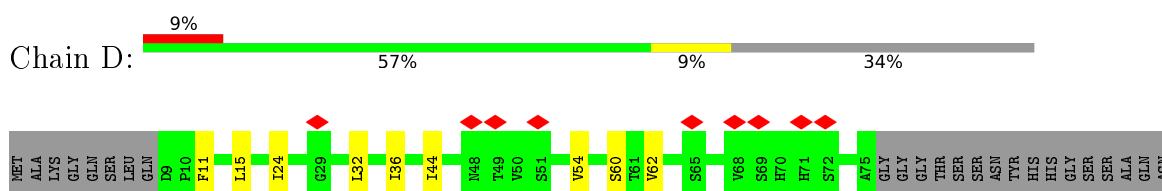
- Molecule 1: RNA-binding protein Hfq



- Molecule 1: RNA-binding protein Hfq



- Molecule 1: RNA-binding protein Hfq



THR
SER
ALA
GLY
GLN
ASP
SER
GLU
GLU
THR
GLU

- Molecule 1: RNA-binding protein Hfq



MET ALA LYS GLY GLN SER LEU Q8 I30 I36 S51 H57 A58 T61 S85 R66 P67 V68 SER R66 HIS R66 SER SER ASN ASN HIS ALA GLY GLY THR SER SER ASN TYR HIS HIS TYR SER SER ALA GLN ASP SER SER GLU THR GLU

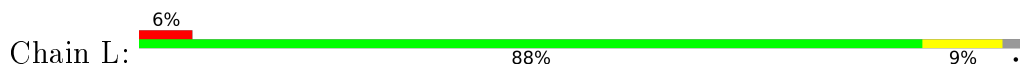
- Molecule 1: RNA-binding protein Hfq



MET ALA LYS GLY GLN SER LEU Q8 L26 V27 N28 Q35 I36 E37 V54 I59 S60 P64 S66 R66 P67 V68 SER SER HIS HIS SER SER ASN ASN ALA GLY GLY THR SER SER ASN TYR HIS HIS GLY SER SER ALA GLN ASP SER SER GLU THR GLU THR

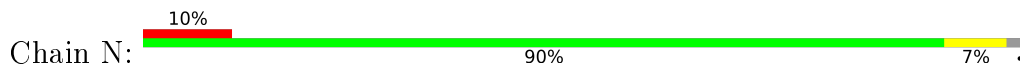
GLU

- Molecule 2: Polyribonucleotide nucleotidyltransferase



M1 L2 I5 V6 F9 Q10 Y11 V16 M22 Q26 V33 G318 R319 F103 P104 F107 E410 G133 I143 P144 P148 I157 N164 Q167 D168 K174 L216 M220 A226 W231 N239 L242 V246 L254 V270 I273 L282 A283 E284 D285 Q286 T287 L288 L293 I296 D317 G318 R319 R325 G326 L327 V329 R330 L334 R335 P336 T344 R345 G346 Q349 A350 L351 H379 G394 S395 I431 I481 R499 V536 E550 R554 K559 I560 N561 V568 I569 G570 K571 G572 V575 I576 T585 I589 E590 E591 D592 T594 V595 A617 E618 I619 E620 V621 G622 R623 T630 R631 I632 V633 D634 V639 G642 G643 G644 A655 D656 K657 R658 V659 T663 L666 Q667 M668 G669 Q670 E671 V672 P673 L677 E678 V679 D680 R681 T693 G694 G695 P696 G697 G698 G699 G700 G701 G702 G703 G704 G705 G706 G707 G708 G709 G710 G711 G712 G713 G714 G715 G716 G717 G718 G719 G720 G721 G722 G723 G724 G725 G726 G727 G728 G729 G730 G731 G732 G733 G734 G735 G736 G737 G738 G739 G740 G741 G742 G743 G744 G745 G746 G747 G748 G749 G750 G751 G752 G753 G754 G755 G756 G757 G758 G759 G760 G761 G762 G763 G764 G765 G766 G767 G768 G769 G770 G771 G772 G773 G774 G775 G776 G777 G778 G779 G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 G792 G793 G794 G795 G796 G797 G798 G799 G800 G801 G802 G803 G804 G805 G806 G807 G808 G809 G810 G811 G812 G813 G814 G815 G816 G817 G818 G819 G820 G821 G822 G823 G824 G825 G826 G827 G828 G829 G830 G831 G832 G833 G834 G835 G836 G837 G838 G839 G840 G841 G842 G843 G844 G845 G846 G847 G848 G849 G850 G851 G852 G853 G854 G855 G856 G857 G858 G859 G860 G861 G862 G863 G864 G865 G866 G867 G868 G869 G870 G871 G872 G873 G874 G875 G876 G877 G878 G879 G880 G881 G882 G883 G884 G885 G886 G887 G888 G889 G890 G891 G892 G893 G894 G895 G896 G897 G898 G899 G900 G901 G902 G903 G904 G905 G906 G907 G908 G909 G910 G911 G912 G913 G914 G915 G916 G917 G918 G919 G920 G921 G922 G923 G924 G925 G926 G927 G928 G929 G930 G931 G932 G933 G934 G935 G936 G937 G938 G939 G940 G941 G942 G943 G944 G945 G946 G947 G948 G949 G950 G951 G952 G953 G954 G955 G956 G957 G958 G959 G960 G961 G962 G963 G964 G965 G966 G967 G968 G969 G970 G971 G972 G973 G974 G975 G976 G977 G978 G979 G980 G981 G982 G983 G984 G985 G986 G987 G988 G989 G990 G991 G992 G993 G994 G995 G996 G997 G998 G999

- Molecule 2: Polyribonucleotide nucleotidyltransferase



M1 L2 N3 P4 R7 I8 F9 V16 M22 M23 V40 D55 F56 F78 R79 R80 V118 S119 V120 A130 N218 E221 K228 P229 R230 V238 A241 L254 L282 A283 E284 D285 E286 T287 L288 D289 L293 E301 E313 P314 R315 I316 D317 G318 R319 E320 M323 D328 V329 R330 T344 Q349 D361 A362 Q363 R372 V387 V428 E433 G467 L478 I481 E485 L488 I555 D563 R571 G584 E588 I589 E590 D591 D592 G593 K596 I615 T616 A617 E618 E619 I619 I620 E621 E622 E623 E624 E625 E626 E627 E628 E629 E630 E631 E632 E633 E634 E635 E636 E637 E638 E639 E640 E641 E642 E643 E644 E645 E646 E647 E648 E649 E650 E651 E652 E653 E654 E655 E656 E657 E658 E659 E660 E661 E662 E663 E664 E665 E666 E667 E668 E669 E670 E671 E672 E673 E674 E675 E676 E677 E678 E679 E680 E681 E682 E683 E684 E685 E686 E687 E688 E689 E690 E691 E692 E693 E694 E695 E696 E697 E698 E699 E700 E701 E702 E703 E704 E705 E706 E707 E708 E709 E710 E711 E712 E713 E714 E715 E716 E717 E718 E719 E720 E721 E722 E723 E724 E725 E726 E727 E728 E729 E730 E731 E732 E733 E734 E735 E736 E737 E738 E739 E740 E741 E742 E743 E744 E745 E746 E747 E748 E749 E750 E751 E752 E753 E754 E755 E756 E757 E758 E759 E760 E761 E762 E763 E764 E765 E766 E767 E768 E769 E770 E771 E772 E773 E774 E775 E776 E777 E778 E779 E780 E781 E782 E783 E784 E785 E786 E787 E788 E789 E790 E791 E792 E793 E794 E795 E796 E797 E798 E799 E800 E801 E802 E803 E804 E805 E806 E807 E808 E809 E810 E811 E812 E813 E814 E815 E816 E817 E818 E819 E820 E821 E822 E823 E824 E825 E826 E827 E828 E829 E830 E831 E832 E833 E834 E835 E836 E837 E838 E839 E840 E841 E842 E843 E844 E845 E846 E847 E848 E849 E850 E851 E852 E853 E854 E855 E856 E857 E858 E859 E860 E861 E862 E863 E864 E865 E866 E867 E868 E869 E870 E871 E872 E873 E874 E875 E876 E877 E878 E879 E880 E881 E882 E883 E884 E885 E886 E887 E888 E889 E890 E891 E892 E893 E894 E895 E896 E897 E898 E899 E900 E901 E902 E903 E904 E905 E906 E907 E908 E909 E910 E911 E912 E913 E914 E915 E916 E917 E918 E919 E920 E921 E922 E923 E924 E925 E926 E927 E928 E929 E930 E931 E932 E933 E934 E935 E936 E937 E938 E939 E940 E941 E942 E943 E944 E945 E946 E947 E948 E949 E950 E951 E952 E953 E954 E955 E956 E957 E958 E959 E960 E961 E962 E963 E964 E965 E966 E967 E968 E969 E970 E971 E972 E973 E974 E975 E976 E977 E978 E979 E980 E981 E982 E983 E984 E985 E986 E987 E988 E989 E990 E991 E992 E993 E994 E995 E996 E997 E998 E999

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133607	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.6	Depositor
Minimum defocus (nm)	-1	Depositor
Maximum defocus (nm)	-2.6	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.176	Depositor
Minimum map value	-1.698	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.41	Depositor
Map size (\AA)	319.50003, 319.50003, 319.50003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.065, 1.065, 1.065	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	D	0.81	0/446	0.86	0/619
1	E	0.84	0/422	0.90	0/585
1	F	0.81	0/396	0.85	0/552
1	I	0.82	0/412	0.85	0/573
1	J	0.82	0/411	0.83	0/572
1	K	0.84	0/393	0.83	0/547
2	L	0.74	0/4844	0.85	0/6629
2	N	0.72	0/4913	0.83	0/6704
2	O	0.76	0/4739	0.85	0/6487
3	P	0.33	0/1063	0.81	1/1651 (0.1%)
All	All	0.74	0/18039	0.84	1/24919 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1	A	OP1-P-OP2	-7.65	108.12	119.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	D	438	0	394	12	0
1	E	413	0	379	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	390	0	355	5	0
1	I	406	0	375	2	0
1	J	404	0	360	3	0
1	K	389	0	355	8	0
2	L	4777	0	4567	67	0
2	N	4841	0	4617	59	0
2	O	4672	0	4268	47	0
3	P	953	0	484	20	0
All	All	17683	0	16154	199	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 6.

All (199) 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)
2:N:555:ILE:HG21	2:N:596:LYS:CE	1.58	1.31
2:N:555:ILE:HG21	2:N:596:LYS:HE2	1.26	1.14
2:N:555:ILE:CG2	2:N:596:LYS:CE	2.25	1.14
2:L:569:ILE:HA	2:L:576:ILE:CD1	1.82	1.09
2:N:555:ILE:CG2	2:N:596:LYS:HE3	1.81	1.08
2:L:325:ARG:HD2	2:L:346:GLY:HA3	1.38	1.05
2:N:555:ILE:CG2	2:N:596:LYS:HE2	1.88	0.99
2:N:555:ILE:HG21	2:N:596:LYS:HE3	1.39	0.99
2:N:316:ILE:HD12	2:N:485:GLU:HG3	1.50	0.92
2:O:2:LEU:H	2:O:2:LEU:HD13	1.33	0.92
2:O:2:LEU:H	2:O:2:LEU:CD1	1.83	0.90
2:L:5:ILE:O	2:L:6:VAL:HG23	1.72	0.90
2:L:569:ILE:HA	2:L:576:ILE:CG1	2.04	0.87
2:L:569:ILE:HA	2:L:576:ILE:HG13	1.58	0.85
2:N:625:TYR:CE2	2:N:626:THR:O	2.31	0.84
1:D:24:ILE:HD11	1:D:32:LEU:HD12	1.58	0.83
2:L:2:LEU:HD11	2:L:22:MET:O	1.79	0.83
2:L:5:ILE:HD13	2:L:226:ALA:HB2	1.63	0.80
2:L:569:ILE:HA	2:L:576:ILE:HD12	1.62	0.80
2:L:568:VAL:O	2:L:576:ILE:HG13	1.82	0.78
2:L:5:ILE:O	2:L:6:VAL:CG2	2.32	0.78
2:N:555:ILE:HG22	2:N:596:LYS:HE3	1.67	0.77
1:D:24:ILE:HG22	1:D:62:VAL:HG22	1.65	0.77
2:N:9:PHE:CD1	2:N:218:ASN:ND2	2.49	0.76
2:L:5:ILE:CD1	2:L:226:ALA:HB2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:589:ILE:HG21	2:N:596:LYS:HD3	1.68	0.73
3:P:11:A:OP2	3:P:11:A:H4'	1.87	0.73
2:O:2:LEU:CD1	2:O:2:LEU:N	2.49	0.73
2:O:2:LEU:HD23	2:O:22:MET:HG3	1.70	0.72
2:L:589:ILE:HG22	2:L:595:VAL:HG22	1.72	0.71
2:L:568:VAL:O	2:L:576:ILE:CG1	2.39	0.71
1:D:24:ILE:HD11	1:D:32:LEU:HB2	1.73	0.70
2:N:2:LEU:HD13	2:N:22:MET:HB2	1.74	0.70
3:P:7:G:H5'	3:P:7:G:N3	2.05	0.70
2:N:330:ARG:CZ	2:O:2:LEU:HD21	2.21	0.70
2:N:7:ARG:CZ	2:N:221:GLU:HG2	2.22	0.69
2:N:55:ASP:OD1	2:N:56:PHE:N	2.27	0.68
2:N:330:ARG:NE	2:O:2:LEU:HD11	2.09	0.67
2:O:258:TYR:OH	2:O:301:GLU:HG3	1.94	0.67
1:K:26:LEU:HB2	1:K:30:ILE:HB	1.77	0.67
2:O:159:ASP:O	2:O:160:GLN:NE2	2.28	0.67
1:K:50:VAL:HG11	1:F:64:PRO:O	1.93	0.67
2:O:334:LEU:HD11	2:O:351:LEU:HD11	1.77	0.65
1:D:24:ILE:HD11	1:D:32:LEU:CD1	2.27	0.65
2:N:330:ARG:NH1	2:O:2:LEU:HD21	2.12	0.65
3:P:40:A:H8	3:P:40:A:O5'	1.81	0.64
2:N:330:ARG:CZ	2:O:2:LEU:HD11	2.27	0.64
2:L:570:GLY:HA3	2:L:575:VAL:HG13	1.80	0.63
2:L:344:THR:HB	2:L:349:GLN:HG2	1.80	0.62
2:O:2:LEU:HD13	2:O:2:LEU:O	2.00	0.62
2:O:347:GLU:OE2	2:O:435:ASN:ND2	2.33	0.62
2:L:148:PRO:HG2	2:L:216:ILE:HG23	1.80	0.62
2:L:242:LEU:HD22	2:L:296:ILE:HD13	1.83	0.61
2:L:550:GLU:HA	2:L:554:ARG:HH21	1.66	0.61
2:L:559:LYS:HA	2:L:594:THR:CG2	2.31	0.60
2:N:9:PHE:CD2	2:N:16:VAL:HB	2.36	0.60
2:L:351:LEU:HD23	2:L:351:LEU:O	2.00	0.60
2:L:2:LEU:HD21	2:L:22:MET:HG3	1.84	0.60
2:L:327:LEU:HD22	2:L:536:VAL:HG21	1.83	0.60
1:D:24:ILE:CD1	1:D:32:LEU:HD12	2.29	0.59
1:E:57:HIS:HB3	3:P:47:U:H1'	1.84	0.59
2:O:2:LEU:HD23	2:O:22:MET:CG	2.32	0.59
2:L:569:ILE:CA	2:L:576:ILE:CD1	2.70	0.59
2:L:317:ASP:OD1	2:L:318:GLY:N	2.37	0.58
2:L:569:ILE:CA	2:L:576:ILE:HG13	2.33	0.56
2:O:651:ILE:HA	2:O:662:VAL:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:334:LEU:CD1	2:O:351:LEU:HD11	2.35	0.56
2:O:405:ARG:HG3	2:O:409:ARG:NH1	2.22	0.55
3:P:7:G:OP1	3:P:7:G:N2	2.37	0.55
3:P:17:A:N3	3:P:17:A:H2'	2.22	0.55
1:I:61:THR:HG22	1:D:54:VAL:HG22	1.89	0.55
2:L:569:ILE:HG12	2:L:576:ILE:CD1	2.37	0.55
2:L:569:ILE:CG1	2:L:589:ILE:HD11	2.37	0.55
2:N:330:ARG:NH2	2:O:2:LEU:CD1	2.69	0.55
2:O:306:ARG:HA	2:O:488:LEU:HD21	1.89	0.55
2:N:363:GLN:HB2	2:O:79:ARG:HG3	1.89	0.55
2:L:5:ILE:C	2:L:6:VAL:HG23	2.27	0.54
1:D:24:ILE:CD1	1:D:32:LEU:HB2	2.37	0.54
2:L:9:PHE:CE1	2:L:16:VAL:HB	2.43	0.54
1:I:56:LYS:HA	1:I:59:ILE:HD12	1.89	0.54
2:L:569:ILE:HG23	2:L:576:ILE:HD12	1.90	0.54
2:O:157:ILE:HD12	2:O:157:ILE:O	2.08	0.54
2:N:2:LEU:C	2:N:2:LEU:HD12	2.28	0.54
1:F:26:LEU:HD22	1:F:26:LEU:N	2.23	0.54
2:N:589:ILE:CG2	2:N:596:LYS:HD3	2.38	0.53
2:O:2:LEU:C	2:O:2:LEU:HD22	2.29	0.53
2:N:7:ARG:NE	2:N:221:GLU:HG2	2.24	0.53
2:L:104:PRO:HG2	2:L:107:PHE:HB2	1.89	0.53
3:P:7:G:N3	3:P:7:G:H2'	2.23	0.53
2:N:320:GLU:HB3	2:N:323:MET:HB2	1.91	0.52
2:O:380:TYR:OH	2:O:438:SER:OG	2.27	0.52
2:N:387:VAL:O	2:N:387:VAL:HG12	2.08	0.52
2:N:330:ARG:NH2	2:O:2:LEU:HD11	2.25	0.52
2:N:625:TYR:CD2	2:N:626:THR:O	2.63	0.52
2:L:254:LEU:HD12	2:L:273:ILE:HD11	1.92	0.51
2:O:258:TYR:OH	2:O:301:GLU:CG	2.58	0.51
1:K:24:ILE:HD13	1:K:62:VAL:HG13	1.92	0.51
2:N:344:THR:HG22	2:N:349:GLN:HG3	1.92	0.51
1:K:50:VAL:HG12	1:F:64:PRO:HD2	1.91	0.51
2:N:254:LEU:HD21	2:N:301:GLU:HG3	1.91	0.51
2:L:559:LYS:HA	2:L:594:THR:HG22	1.92	0.51
2:L:569:ILE:HA	2:L:576:ILE:HD11	1.81	0.51
2:N:9:PHE:CE2	2:N:16:VAL:HG11	2.45	0.51
1:K:50:VAL:CG1	1:F:64:PRO:HG2	2.41	0.50
2:N:649:VAL:HG22	2:N:685:ILE:HB	1.92	0.50
2:L:589:ILE:HD12	2:L:589:ILE:O	2.11	0.50
3:P:6:A:H4'	3:P:6:A:OP1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:5:ILE:HG22	2:L:6:VAL:N	2.27	0.49
3:P:9:A:H5''	3:P:9:A:H8	1.76	0.49
2:L:1:MET:HG3	2:L:2:LEU:N	2.28	0.49
2:L:143:ILE:HG23	2:L:144:PRO:HD2	1.95	0.49
2:O:6:VAL:HG11	2:O:8:LYS:HE3	1.96	0.48
2:N:467:GLY:HA3	2:N:481:ILE:CD1	2.43	0.48
2:O:2:LEU:CD2	2:O:22:MET:SD	3.01	0.48
3:P:13:A:H2'	3:P:13:A:N3	2.29	0.48
2:L:242:LEU:HD22	2:L:296:ILE:CD1	2.43	0.48
1:J:42:PHE:HB3	3:P:49:U:H2'	1.96	0.47
1:K:12:LEU:HD21	1:K:39:PHE:CB	2.44	0.47
2:L:319:ARG:CZ	2:L:325:ARG:HG3	2.44	0.47
1:D:24:ILE:HG22	1:D:62:VAL:CG2	2.39	0.47
2:N:9:PHE:CE1	2:N:218:ASN:CB	2.97	0.47
2:O:2:LEU:HD21	2:O:22:MET:SD	2.54	0.47
2:O:258:TYR:OH	2:O:301:GLU:OE2	2.33	0.47
3:P:21:U:H1'	3:P:22:A:H5'	1.96	0.47
2:L:143:ILE:CD1	2:L:231:TRP:CH2	2.98	0.46
2:N:555:ILE:HG23	2:N:596:LYS:HE2	1.85	0.46
3:P:39:A:H3'	3:P:40:A:C8	2.50	0.46
1:K:24:ILE:HB	1:K:32:LEU:HG	1.97	0.46
2:L:351:LEU:CD1	2:N:23:MET:HE1	2.45	0.46
2:O:6:VAL:HG13	2:O:17:THR:HG23	1.98	0.46
3:P:39:A:O5'	3:P:39:A:C8	2.68	0.46
2:L:246:VAL:HG21	2:L:293:LEU:HD11	1.97	0.46
2:N:315:ARG:NH2	2:N:319:ARG:HH22	2.14	0.46
2:N:625:TYR:CG	2:N:626:THR:N	2.85	0.45
3:P:16:C:O2	3:P:16:C:O4'	2.31	0.45
2:L:431:ILE:HD12	2:L:431:ILE:N	2.32	0.45
2:N:313:GLU:N	2:N:314:PRO:HD2	2.31	0.45
2:N:478:LEU:HD23	2:N:478:LEU:H	1.81	0.45
2:L:589:ILE:HG22	2:L:595:VAL:CG2	2.45	0.45
1:E:61:THR:HB	1:F:54:VAL:HG12	1.99	0.45
2:N:478:LEU:HD23	2:N:478:LEU:N	2.31	0.45
2:L:336:ARG:HG2	2:N:120:VAL:O	2.17	0.44
2:N:328:ASP:OD2	2:O:2:LEU:HD11	2.16	0.44
2:L:589:ILE:HG22	2:L:595:VAL:HG13	1.99	0.44
2:N:2:LEU:HD13	2:N:22:MET:CB	2.43	0.44
2:N:485:GLU:HG2	2:N:488:LEU:HD12	1.98	0.44
2:O:405:ARG:HG3	2:O:409:ARG:CZ	2.47	0.44
2:L:569:ILE:HG12	2:L:589:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:428:VAL:HG11	2:O:68:TYR:CD2	2.52	0.44
3:P:37:A:OP2	3:P:37:A:C8	2.71	0.44
2:L:157:ILE:H	2:L:157:ILE:HG13	1.69	0.44
2:N:317:ASP:OD2	2:N:319:ARG:NE	2.44	0.44
1:J:56:LYS:HA	1:J:59:ILE:HD12	2.00	0.44
2:L:287:THR:HG22	2:L:293:LEU:HD22	2.00	0.44
2:L:569:ILE:CA	2:L:576:ILE:HD11	2.44	0.43
2:L:569:ILE:CG1	2:L:576:ILE:HD11	2.48	0.43
2:O:2:LEU:N	2:O:2:LEU:HD12	2.33	0.43
2:L:102:LEU:HD12	2:L:102:LEU:HA	1.80	0.43
2:N:40:VAL:HG21	2:N:130:ALA:HA	2.00	0.43
3:P:32:A:H8	3:P:33:A:H2'	1.83	0.43
2:L:569:ILE:HG12	2:L:576:ILE:HD11	2.00	0.43
2:N:330:ARG:HE	2:O:2:LEU:HD11	1.84	0.43
2:L:327:LEU:CD2	2:L:536:VAL:HG11	2.48	0.43
2:L:630:THR:H	2:L:669:GLY:H	1.66	0.43
2:N:330:ARG:NH2	2:O:2:LEU:HD13	2.34	0.43
2:N:228:LYS:O	2:N:230:ARG:NH2	2.51	0.43
1:D:11:PHE:CZ	1:D:15:LEU:HD11	2.54	0.43
2:O:106:GLY:O	2:O:233:TRP:HZ2	2.01	0.43
1:D:36:ILE:HG22	1:D:44:ILE:HG21	2.00	0.42
2:L:334:LEU:HD21	2:N:118:VAL:HB	2.01	0.42
2:L:254:LEU:HD11	2:L:270:VAL:HG13	2.00	0.42
2:L:242:LEU:HD21	2:L:293:LEU:CD1	2.50	0.42
1:K:63:VAL:HG12	1:J:52:GLN:HA	2.02	0.41
2:L:143:ILE:HD11	2:L:231:TRP:CH2	2.55	0.41
2:O:35:MET:O	2:O:36:ASP:C	2.56	0.41
2:O:509:ILE:N	2:O:509:ILE:HD12	2.35	0.41
2:L:33:VAL:HG21	2:L:133:GLY:HA2	2.01	0.41
2:O:2:LEU:O	2:O:2:LEU:HD22	2.20	0.41
3:P:39:A:H2'	3:P:39:A:N3	2.34	0.41
2:L:11:TYR:CE2	2:L:164:ASN:ND2	2.86	0.41
2:L:379:HIS:ND1	2:N:80:ARG:HD3	2.36	0.41
2:N:330:ARG:CZ	2:O:2:LEU:CD2	2.94	0.41
2:O:2:LEU:H	2:O:2:LEU:HD12	1.75	0.41
1:E:30:ILE:HD12	1:E:30:ILE:HA	1.99	0.41
2:L:329:VAL:HG12	2:L:330:ARG:N	2.36	0.41
2:N:328:ASP:OD2	2:O:2:LEU:CD1	2.68	0.41
3:P:17:A:N3	3:P:17:A:C2'	2.84	0.41
1:D:60:SER:HA	1:E:58:ALA:HB2	2.03	0.41
2:L:589:ILE:CG2	2:L:595:VAL:HG22	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:361:ASP:CB	2:O:73:ILE:HD11	2.51	0.41
2:N:372:ARG:HE	2:N:372:ARG:HB3	1.48	0.41
2:N:9:PHE:CE1	2:N:218:ASN:HB3	2.56	0.40
3:P:29:A:O2'	3:P:30:A:O3'	2.38	0.40
2:L:26:GLN:HE21	2:O:433:GLU:HB2	1.86	0.40
2:N:349:GLN:HB3	2:N:433:GLU:HG2	2.02	0.40
2:O:491:MET:HG3	2:O:509:ILE:HG13	2.02	0.40
2:L:568:VAL:O	2:L:576:ILE:HG12	2.17	0.40
1:D:60:SER:HA	1:E:58:ALA:CB	2.52	0.40
2:O:9:PHE:HE1	2:O:18:LEU:HD23	1.85	0.40

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	D	65/102 (64%)	62 (95%)	3 (5%)	0	100	100
1	E	59/102 (58%)	58 (98%)	1 (2%)	0	100	100
1	F	59/102 (58%)	57 (97%)	2 (3%)	0	100	100
1	I	61/102 (60%)	59 (97%)	2 (3%)	0	100	100
1	J	61/102 (60%)	60 (98%)	1 (2%)	0	100	100
1	K	60/102 (59%)	60 (100%)	0	0	100	100
2	L	691/711 (97%)	657 (95%)	34 (5%)	0	100	100
2	N	687/711 (97%)	666 (97%)	20 (3%)	1 (0%)	51	83
2	O	693/711 (98%)	668 (96%)	25 (4%)	0	100	100
All	All	2436/2745 (89%)	2347 (96%)	88 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	4	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	39/89 (44%)	39 (100%)	0	100	100
1	E	38/89 (43%)	38 (100%)	0	100	100
1	F	34/89 (38%)	33 (97%)	1 (3%)	42	66
1	I	37/89 (42%)	37 (100%)	0	100	100
1	J	35/89 (39%)	34 (97%)	1 (3%)	42	66
1	K	34/89 (38%)	32 (94%)	2 (6%)	19	51
2	L	438/575 (76%)	426 (97%)	12 (3%)	44	68
2	N	454/575 (79%)	450 (99%)	4 (1%)	78	88
2	O	397/575 (69%)	389 (98%)	8 (2%)	55	74
All	All	1506/2259 (67%)	1478 (98%)	28 (2%)	59	76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	28	ASN
1	K	32	LEU
1	J	43	VAL
1	F	27	VAL
2	L	110	GLU
2	L	157	ILE
2	L	167	GLN
2	L	168	ASP
2	L	174	LYS
2	L	220	ASN
2	L	287	THR
2	L	344	THR
2	L	481	ILE
2	L	499	ARG

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Mol	Chain	Res	Type
2	L	585	THR
2	L	633	VAL
2	N	363	GLN
2	N	372	ARG
2	N	478	LEU
2	N	621	VAL
2	O	2	LEU
2	O	7	ARG
2	O	33	VAL
2	O	76	SER
2	O	120	VAL
2	O	121	ASN
2	O	316	ILE
2	O	321	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	28	ASN
2	L	26	GLN
2	L	146	ASN
2	L	218	ASN
2	L	532	HIS
2	N	109	ASN
2	N	291	ASN
2	O	10	GLN
2	O	26	GLN
2	O	64	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	47/49 (95%)	39 (82%)	5 (10%)

All (39) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	3	A
3	P	4	U
3	P	5	A

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Mol	Chain	Res	Type
3	P	6	A
3	P	7	G
3	P	8	A
3	P	9	A
3	P	10	U
3	P	11	A
3	P	12	A
3	P	13	A
3	P	14	A
3	P	15	U
3	P	16	C
3	P	17	A
3	P	18	A
3	P	19	U
3	P	20	U
3	P	21	U
3	P	22	A
3	P	23	A
3	P	24	A
3	P	25	A
3	P	26	A
3	P	27	A
3	P	28	A
3	P	29	A
3	P	30	A
3	P	31	A
3	P	32	A
3	P	34	A
3	P	37	A
3	P	39	A
3	P	40	A
3	P	43	U
3	P	46	U
3	P	47	U
3	P	48	U
3	P	50	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	P	2	G
3	P	9	A

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Mol	Chain	Res	Type
3	P	10	U
3	P	29	A
3	P	31	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	40:A	O3'	42:U	P	9.61

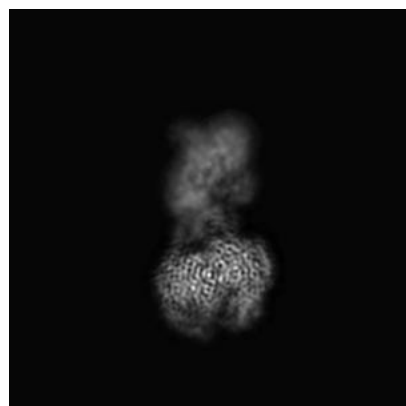
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12884. These allow visual inspection of the internal detail of the map and identification of artifacts.

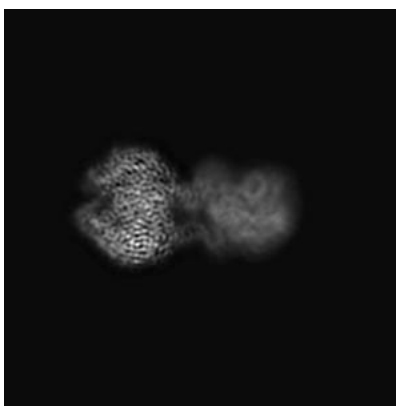
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

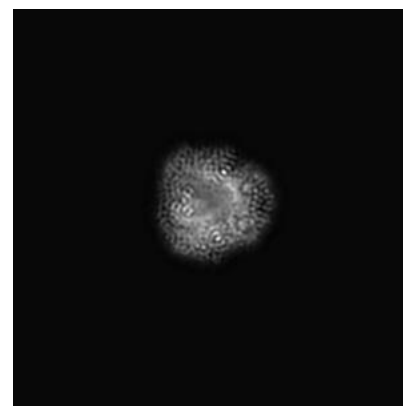
6.1.1 Primary map



X

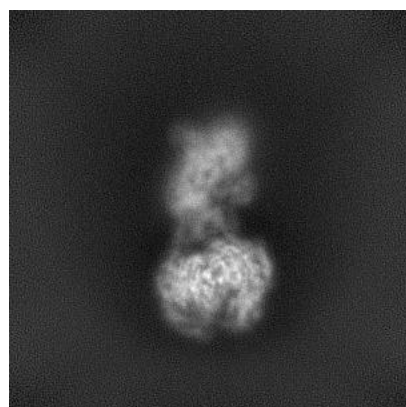


Y

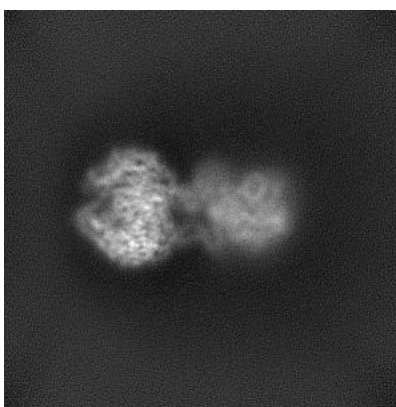


Z

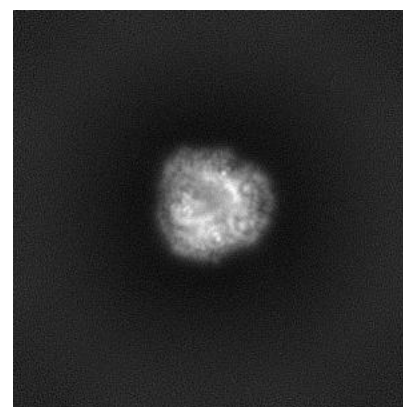
6.1.2 Raw map



X



Y

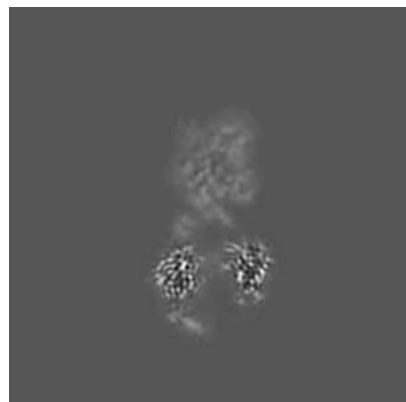


Z

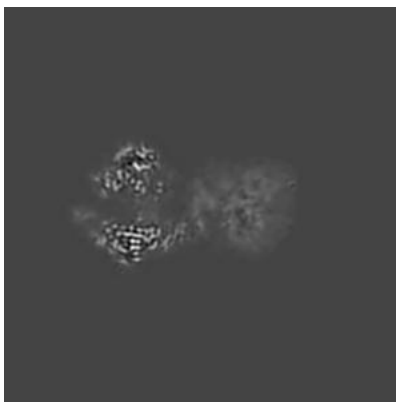
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

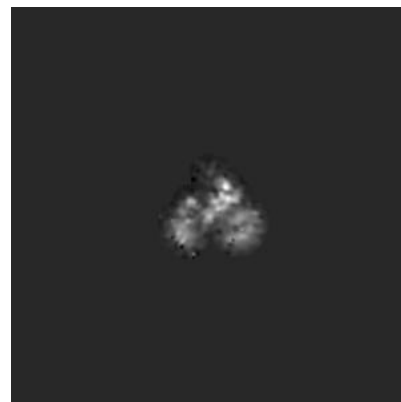
6.2.1 Primary map



X Index: 150

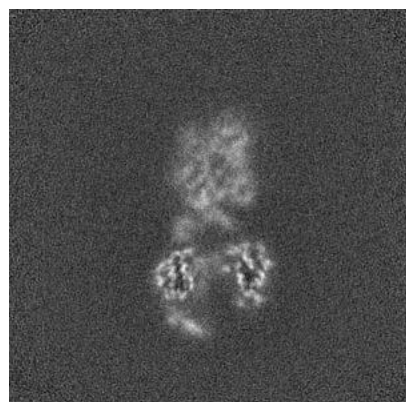


Y Index: 150

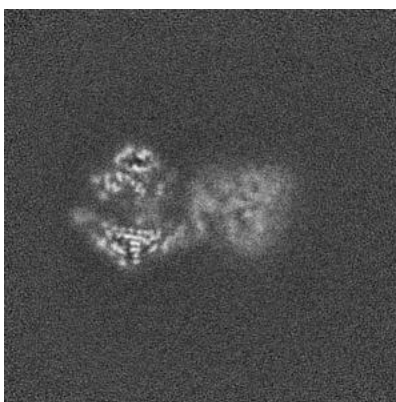


Z Index: 150

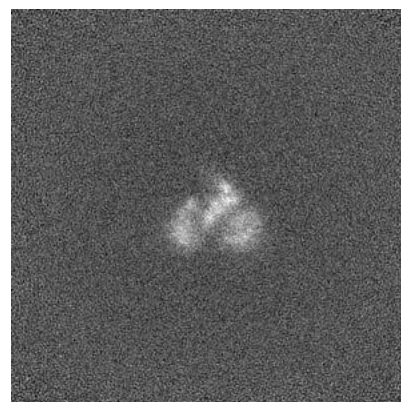
6.2.2 Raw map



X Index: 150



Y Index: 150

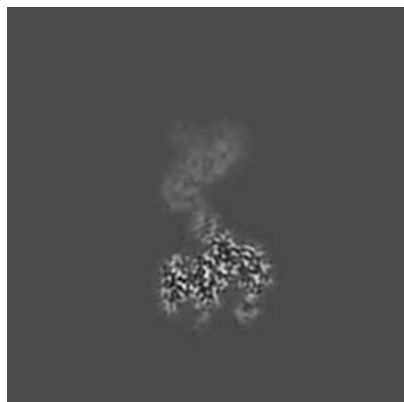


Z Index: 150

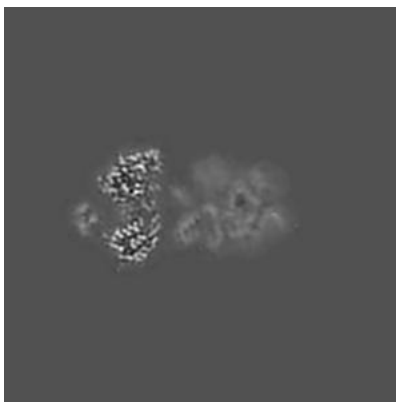
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

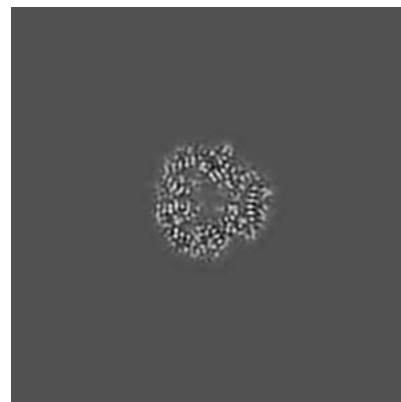
6.3.1 Primary map



X Index: 128

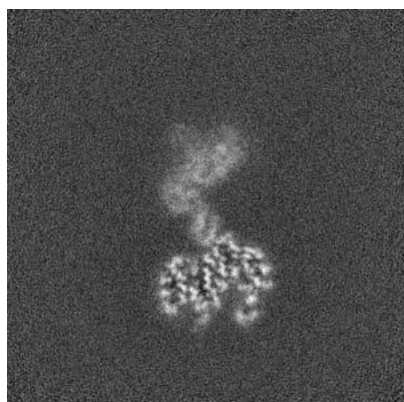


Y Index: 141

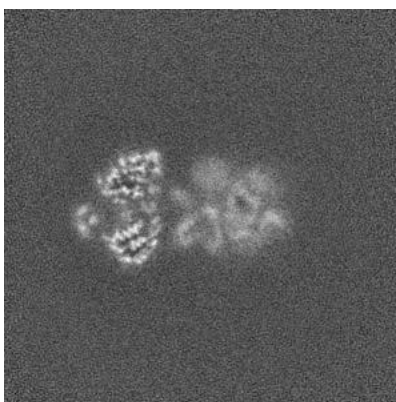


Z Index: 100

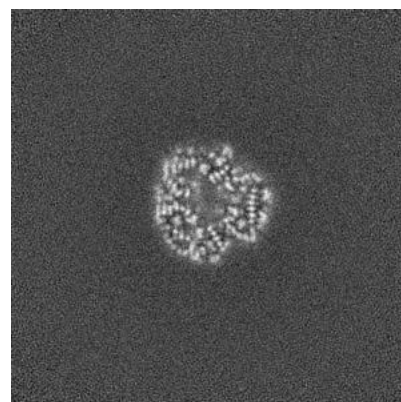
6.3.2 Raw map



X Index: 128



Y Index: 141

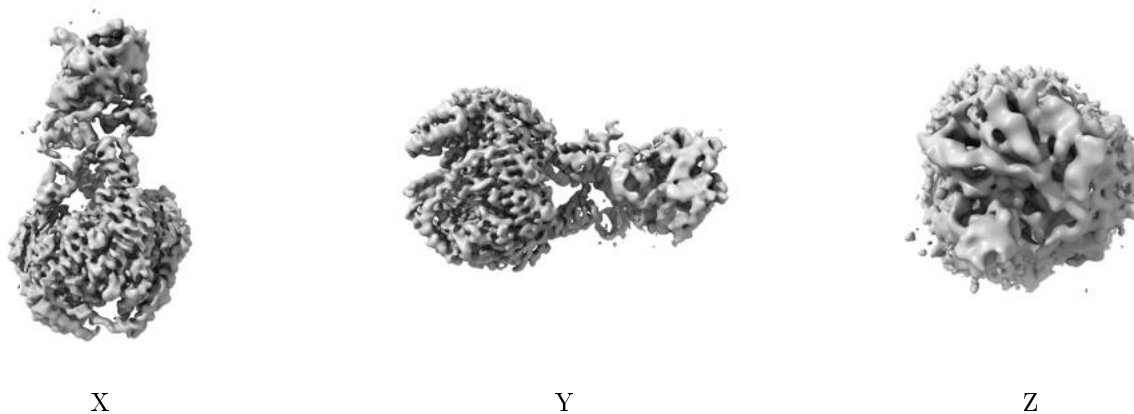


Z Index: 99

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

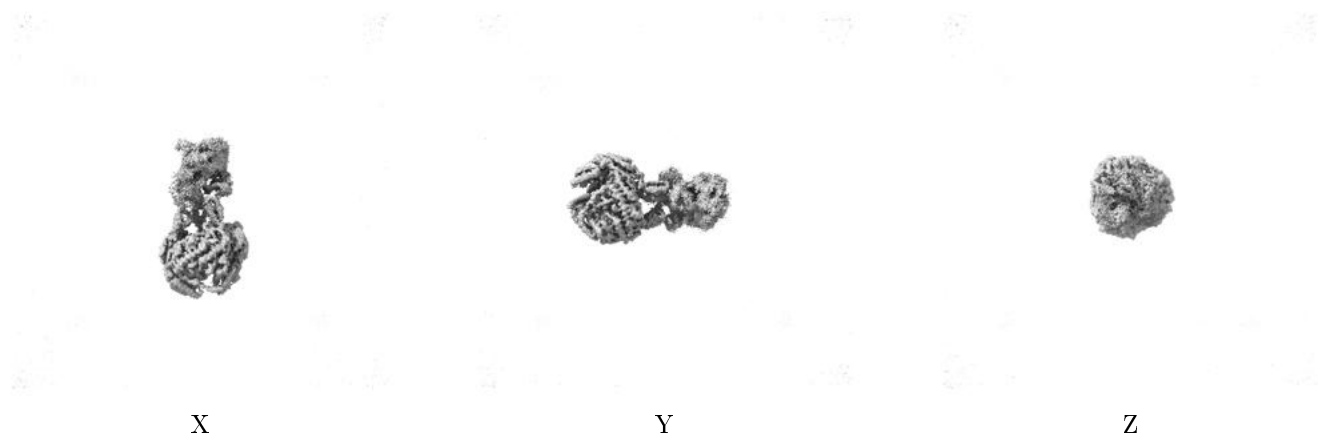
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.41. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

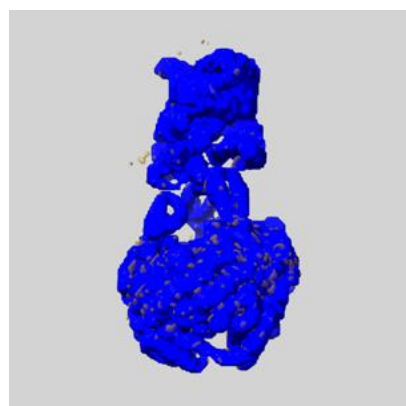
6.5 Mask visualisation [i](#)

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

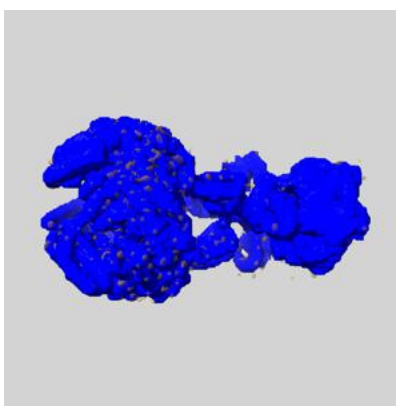
A mask typically either:

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

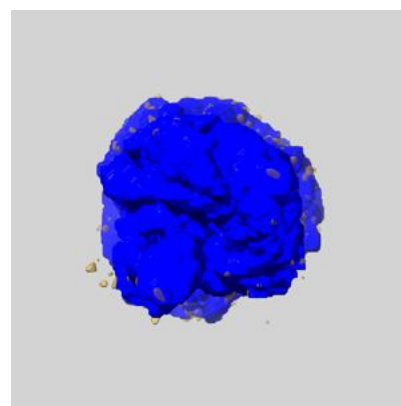
6.5.1 emd_12884_msk_1.map [i](#)



X



Y

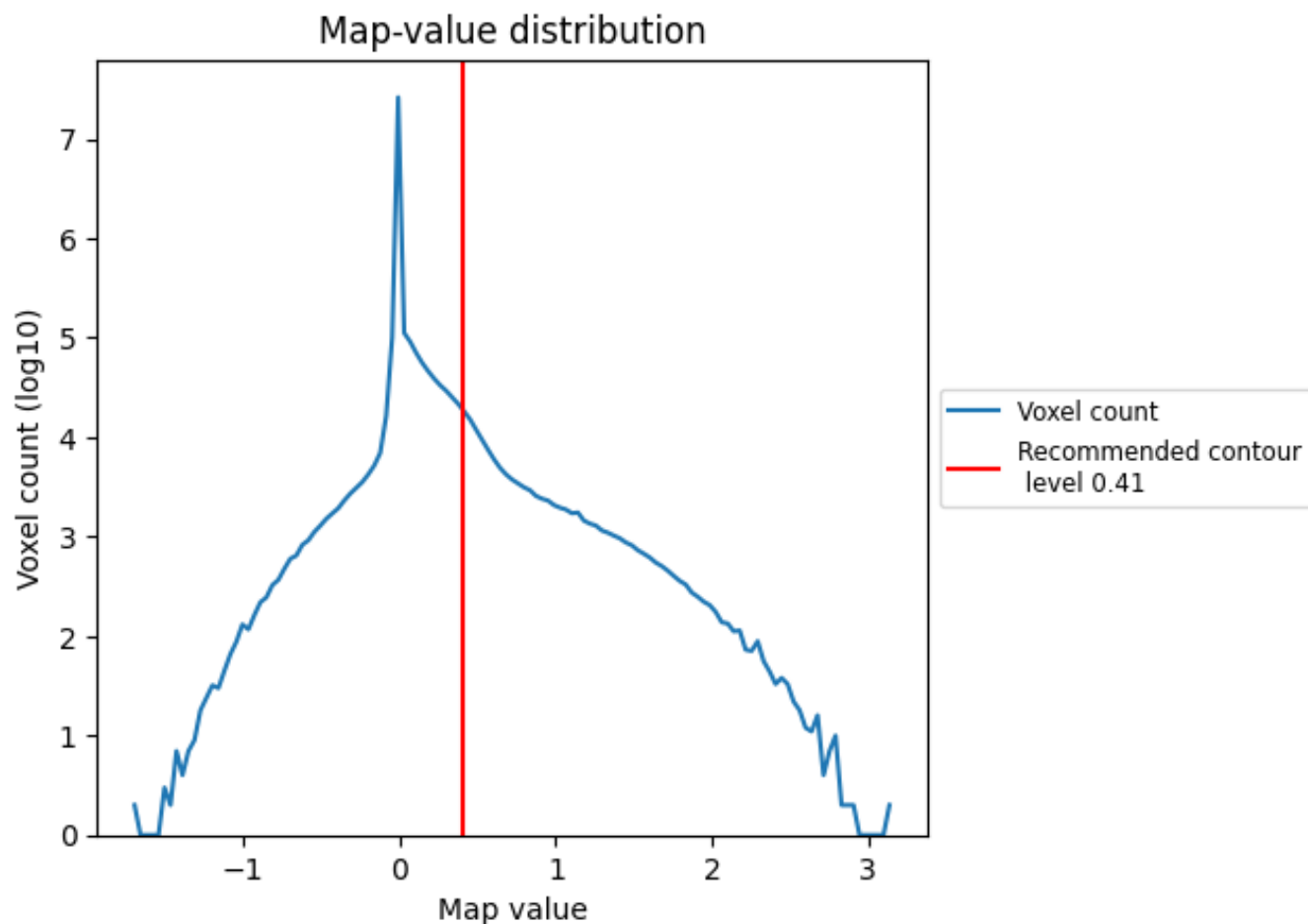


Z

7 Map analysis [i](#)

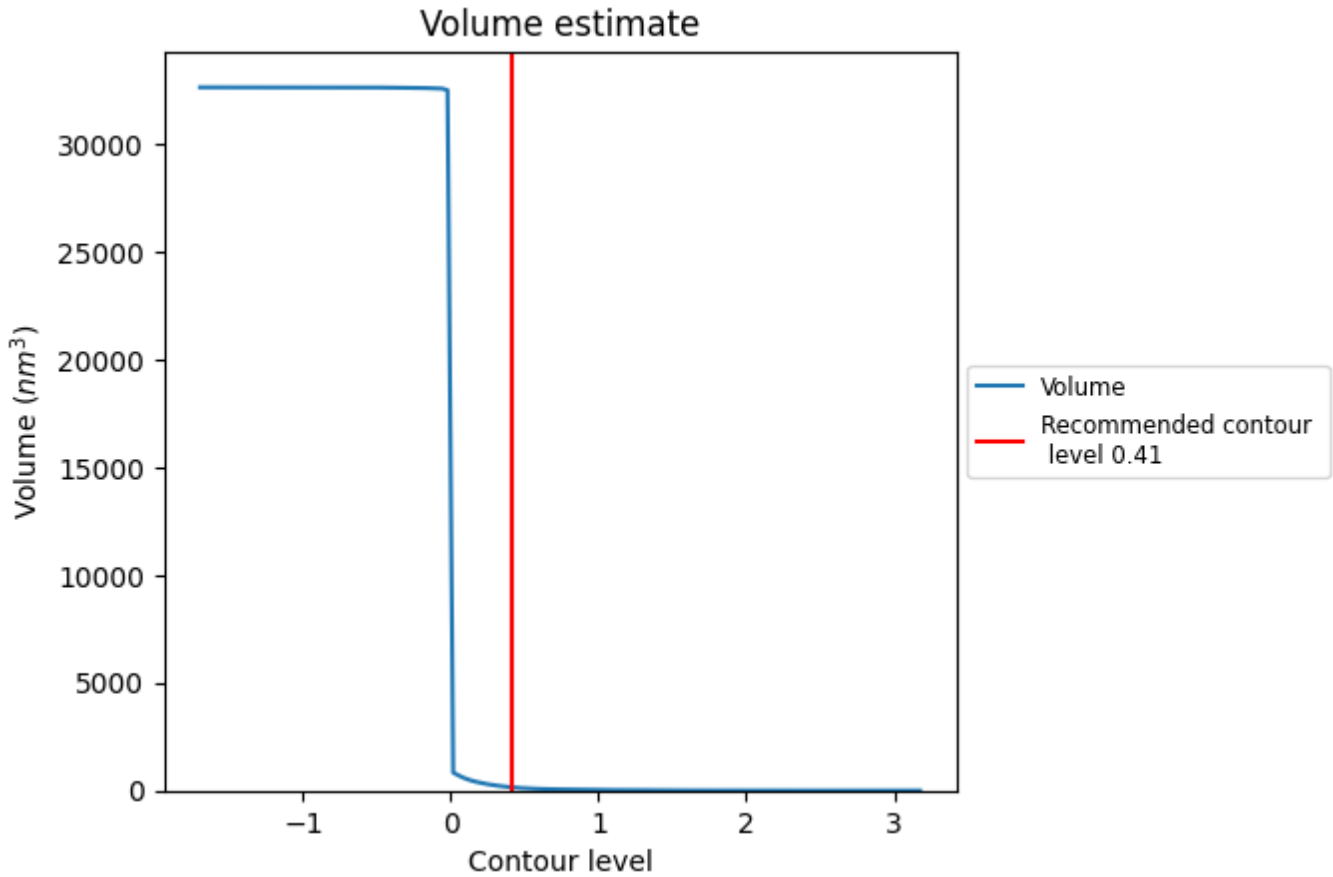
This section contains the results of statistical analysis of the map.

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.

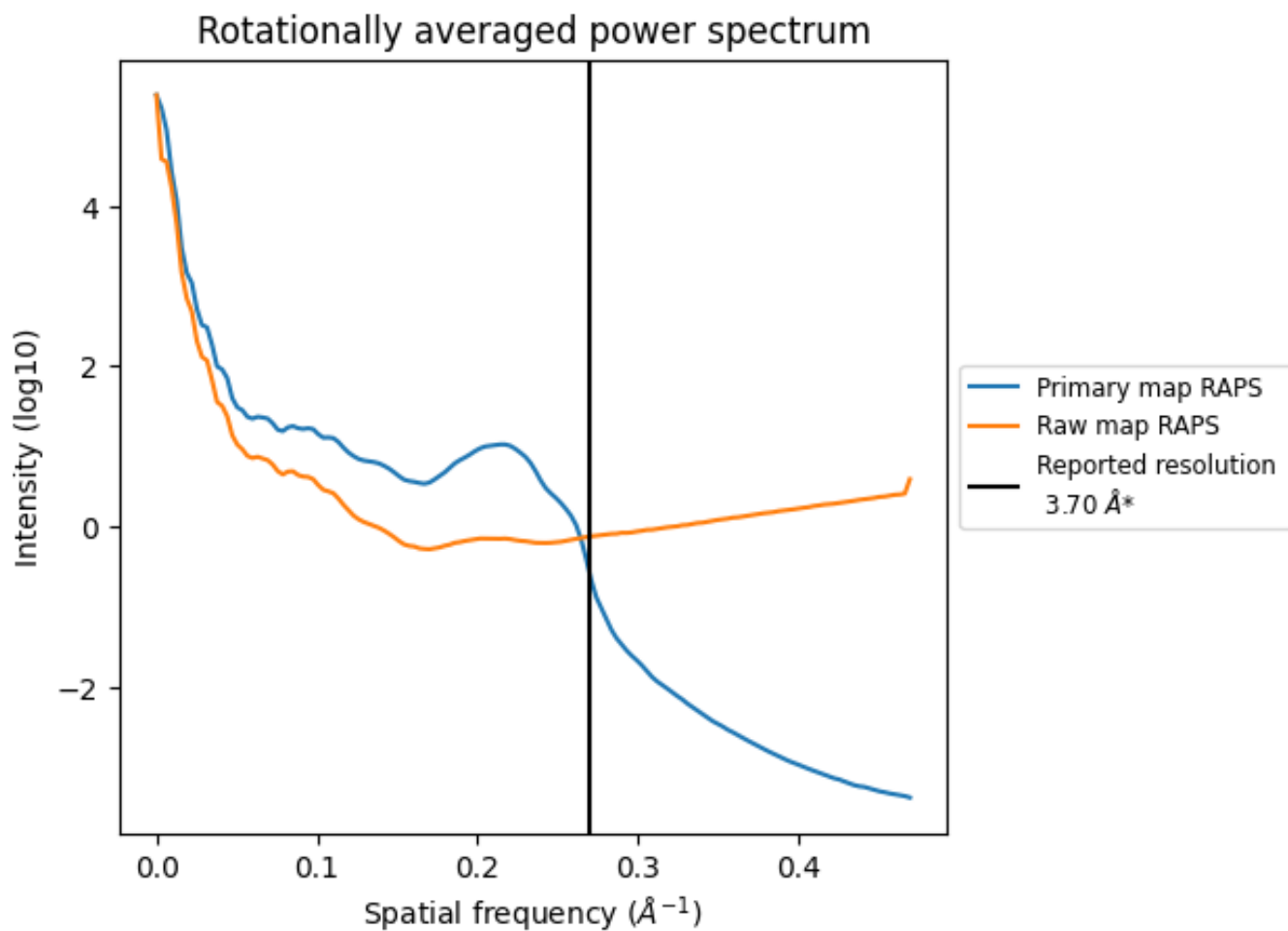
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 138 kDa.

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

7.3 Rotationally averaged power spectrum i

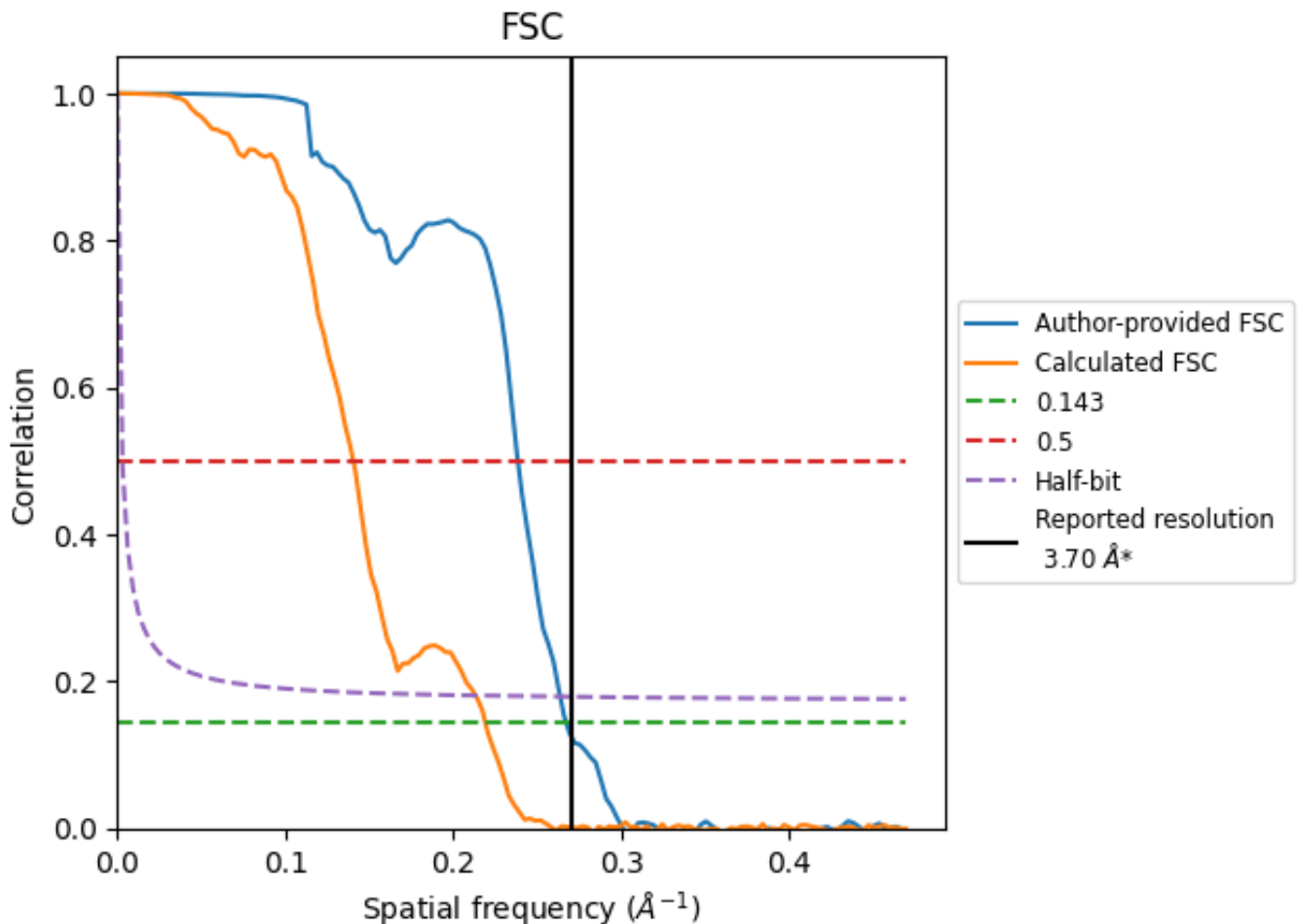


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

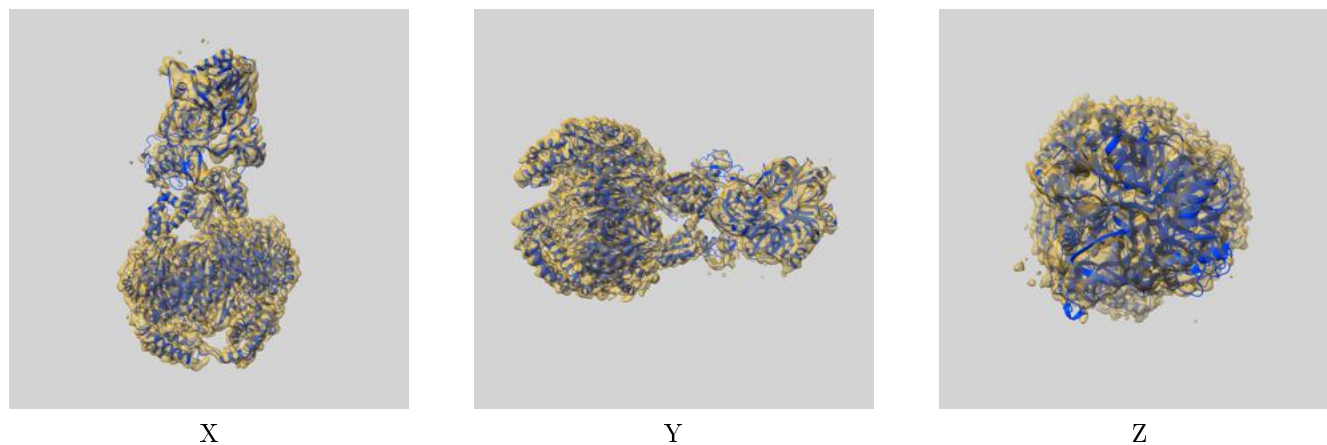
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.19	3.79
Calculated*	4.56	7.12	4.69

*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 4.56 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

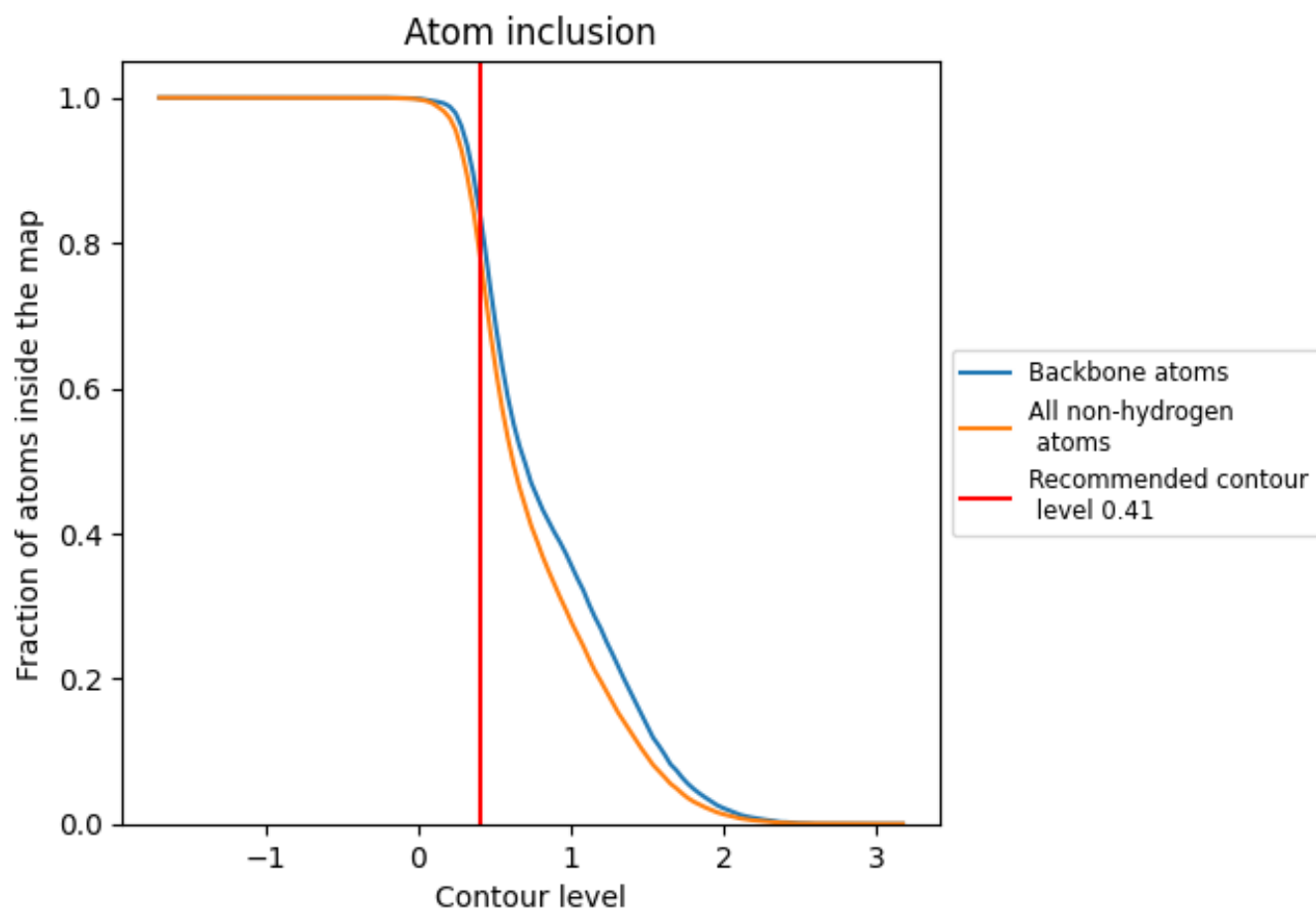
This section contains information regarding the fit between EMDB map EMD-12884 and PDB model 7OGM. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.41 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 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.