



## wwPDB EM Validation Summary Report ⓘ

Sep 30, 2024 – 12:53 PM EDT

PDB ID : 9D9W  
EMDB ID : EMD-46681  
Title : Mycobacteriophage Bxb1 C1 Capsid and Portal - Composite map and model  
Authors : Freeman, K.G.  
Deposited on : 2024-08-21  
Resolution : 3.50 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

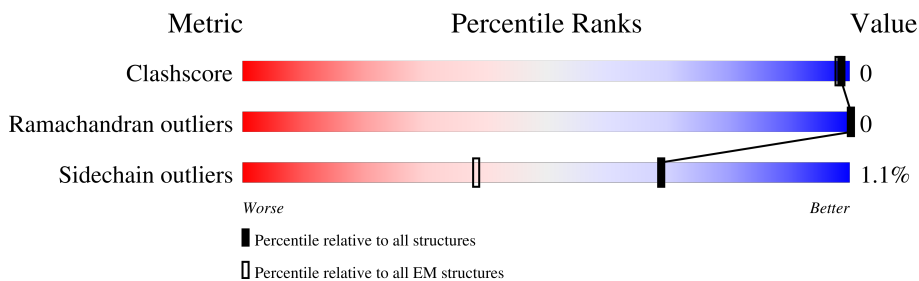
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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.



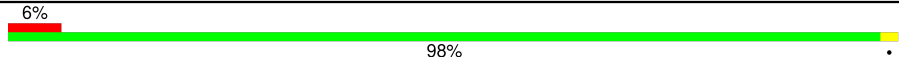
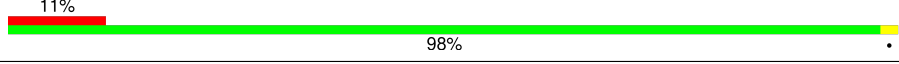
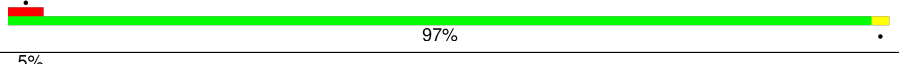
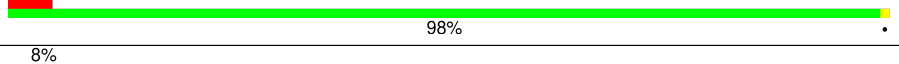
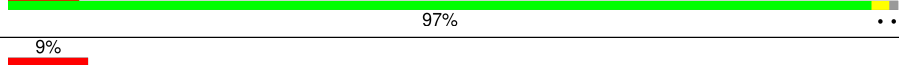
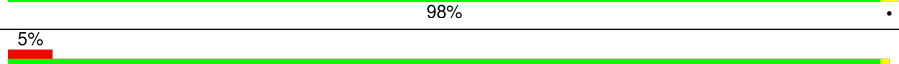
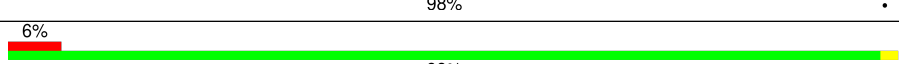
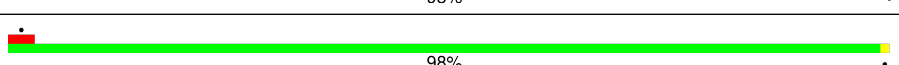
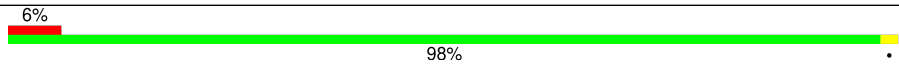
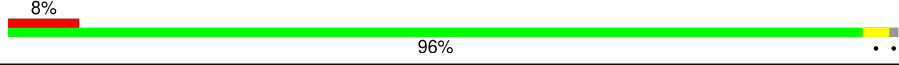
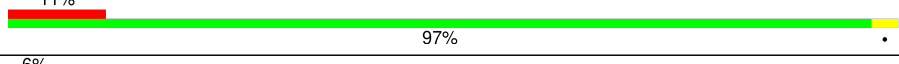
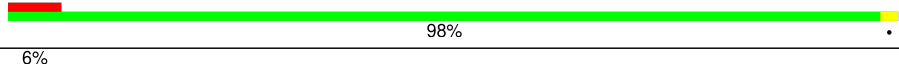
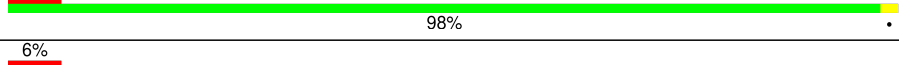
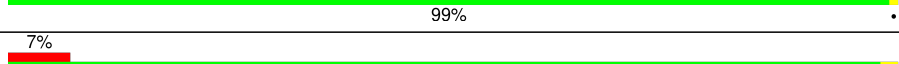
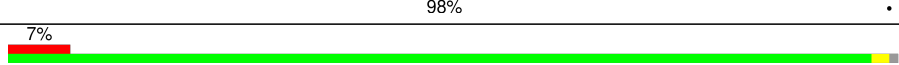
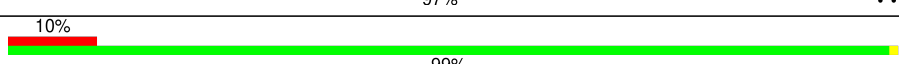
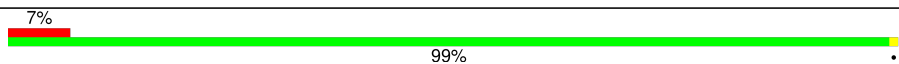
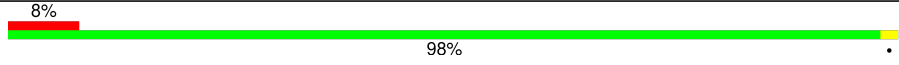
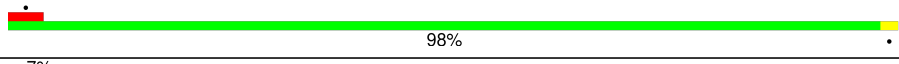
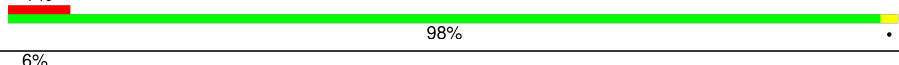





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	Aa	397	8% 97% . .
1	Ab	397	11% 98% .
1	Ac	397	6% 98% .
1	Ad	397	8% 98% .
1	Ae	397	. 97% .
1	Af	397	5% 98% .
1	Ba	397	7% 97% . .
1	Bb	397	10% 96% .

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Mol	Chain	Length	Quality of chain
1	Bc	397	 6% 98%
1	Bd	397	 11% 98%
1	Be	397	 1% 97%
1	Bf	397	 5% 98%
1	Ca	397	 8% 97%
1	Cb	397	 9% 98%
1	Cc	397	 5% 98%
1	Cd	397	 6% 98%
1	Ce	397	 1% 98%
1	Cf	397	 6% 98%
1	Da	397	 8% 96%
1	Db	397	 11% 97%
1	Dc	397	 6% 98%
1	Dd	397	 6% 98%
1	De	397	 6% 99%
1	Df	397	 7% 98%
1	Ea	397	 7% 97%
1	Eb	397	 10% 99%
1	Ec	397	 7% 99%
1	Ed	397	 8% 98%
1	Ee	397	 1% 98%
1	Ef	397	 7% 98%
2	Fa	488	 6% 88% 8%
2	Fb	488	 6% 87% 5% 8%
2	Fc	488	 5% 88% 8%

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Mol	Chain	Length	Quality of chain
2	Fd	488	
2	Fe	488	
2	Ff	488	
2	Fg	488	
2	Fh	488	
2	Fi	488	
2	Fj	488	
2	Fk	488	
2	Fl	488	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 257618 atoms, of which 127151 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 Major capsid protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	Aa	394	5785	1838	2859	488	594	6	0	0
1	Ab	396	5812	1849	2871	490	596	6	0	0
1	Ac	396	5811	1849	2870	490	596	6	0	0
1	Ad	396	5811	1849	2870	490	596	6	0	0
1	Ae	396	5811	1849	2870	490	596	6	0	0
1	Af	396	5811	1849	2870	490	596	6	0	0
1	Ba	394	5784	1838	2858	488	594	6	0	0
1	Bb	396	5811	1849	2870	490	596	6	0	0
1	Bc	396	5811	1849	2870	490	596	6	0	0
1	Bd	396	5812	1849	2871	490	596	6	0	0
1	Be	396	5811	1849	2870	490	596	6	0	0
1	Bf	396	5812	1849	2871	490	596	6	0	0
1	Ca	394	5784	1838	2858	488	594	6	0	0
1	Cb	396	5811	1849	2870	490	596	6	0	0
1	Cc	396	5811	1849	2870	490	596	6	0	0
1	Cd	396	5812	1849	2871	490	596	6	0	0
1	Ce	396	5811	1849	2870	490	596	6	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	Cf	396	Total 5811	C 1849	H 2870	N 490	O 596	S 6	0	0
1	Da	394	Total 5785	C 1838	H 2859	N 488	O 594	S 6	0	0
1	Db	396	Total 5811	C 1849	H 2870	N 490	O 596	S 6	0	0
1	Dc	396	Total 5812	C 1849	H 2871	N 490	O 596	S 6	0	0
1	Dd	396	Total 5812	C 1849	H 2871	N 490	O 596	S 6	0	0
1	De	396	Total 5811	C 1849	H 2870	N 490	O 596	S 6	0	0
1	Df	396	Total 5811	C 1849	H 2870	N 490	O 596	S 6	0	0
1	Ea	394	Total 5784	C 1838	H 2858	N 488	O 594	S 6	0	0
1	Eb	396	Total 5811	C 1849	H 2870	N 490	O 596	S 6	0	0
1	Ec	396	Total 5811	C 1849	H 2870	N 490	O 596	S 6	0	0
1	Ed	396	Total 5811	C 1849	H 2870	N 490	O 596	S 6	0	0
1	Ee	396	Total 5812	C 1849	H 2871	N 490	O 596	S 6	0	0
1	Ef	396	Total 5812	C 1849	H 2871	N 490	O 596	S 6	0	0

- Molecule 2 is a protein called Portal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	Fa	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fb	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fc	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fd	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fe	450	Total 6952	C 2219	H 3426	N 603	O 690	S 14	0	0
2	Ff	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0

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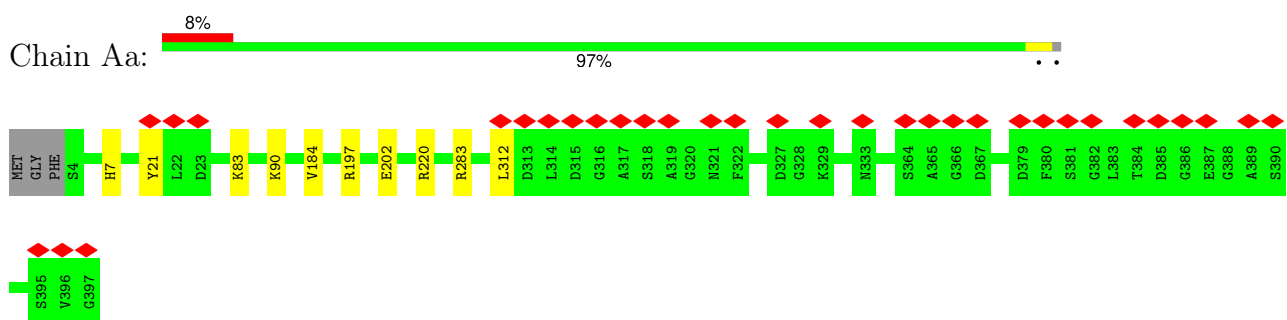
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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	Fg	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fh	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fi	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fj	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fk	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fl	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0

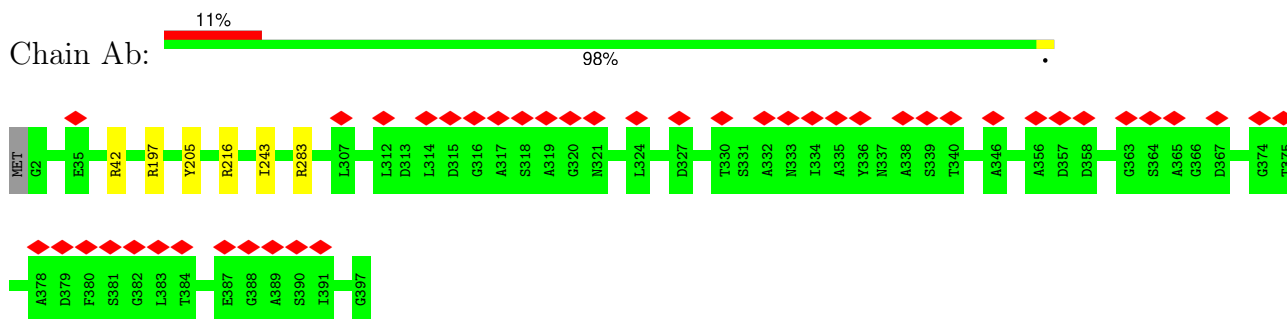
### 3 Residue-property plots [i](#)

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.

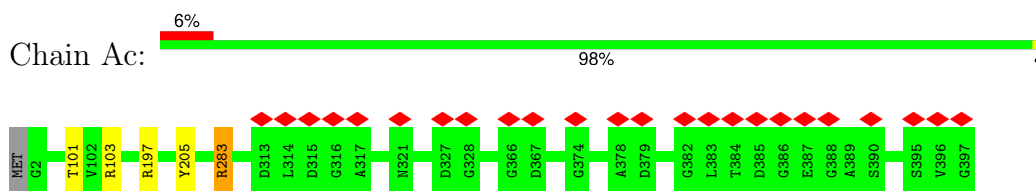
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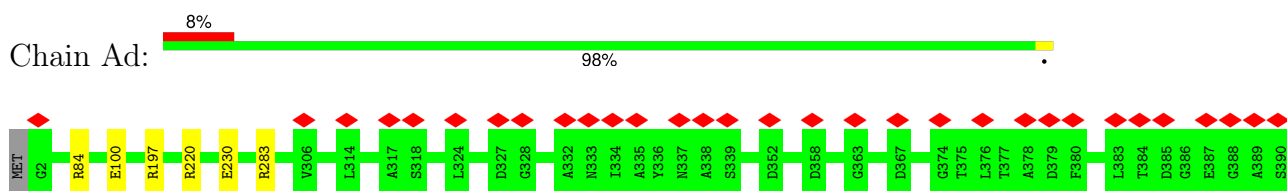
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- Molecule 1: Major capsid protein



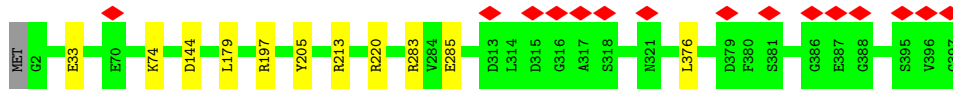
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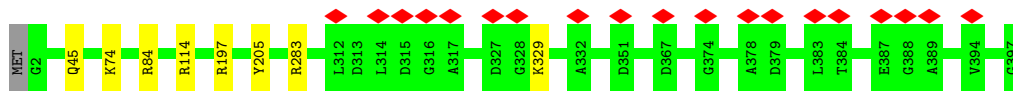




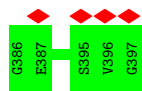
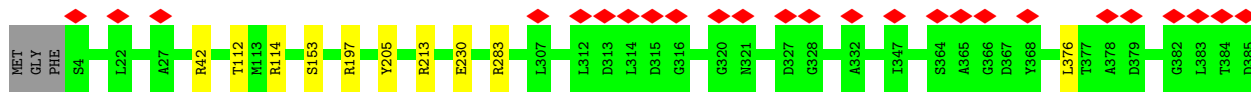
• Molecule 1: Major capsid protein



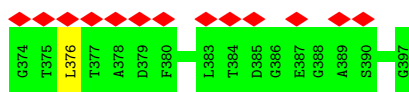
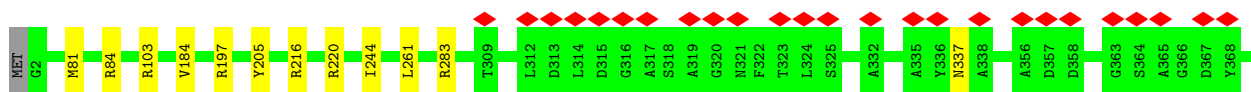
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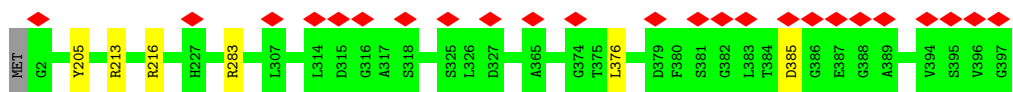
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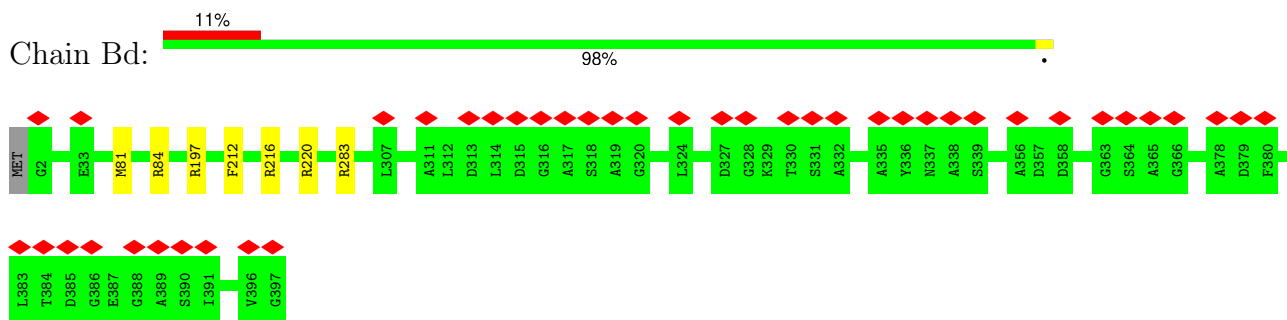
• Molecule 1: Major capsid protein



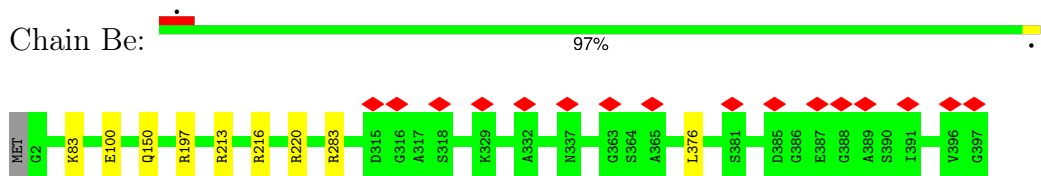
• Molecule 1: Major capsid protein



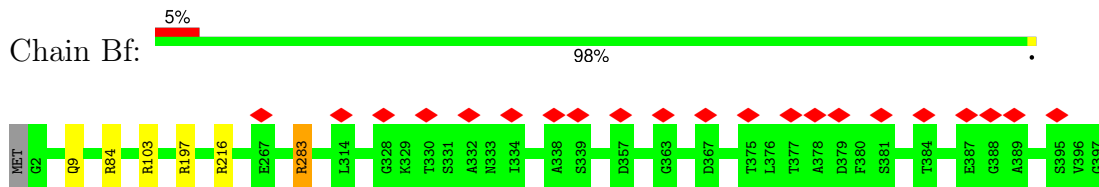
• Molecule 1: Major capsid protein



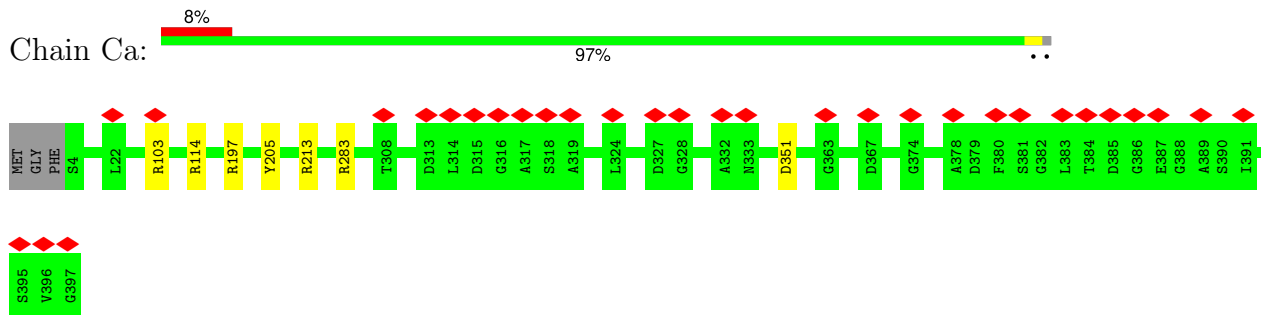
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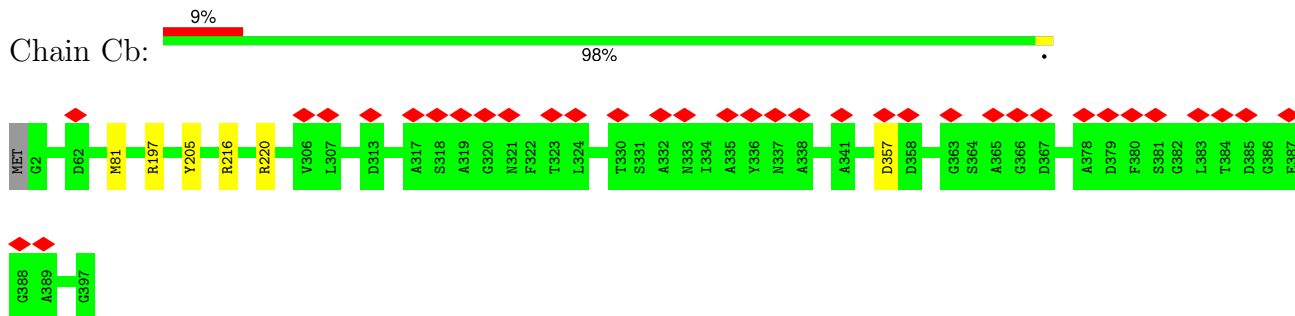
• Molecule 1: Major capsid protein



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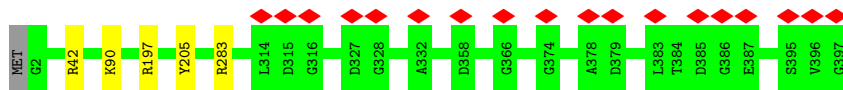


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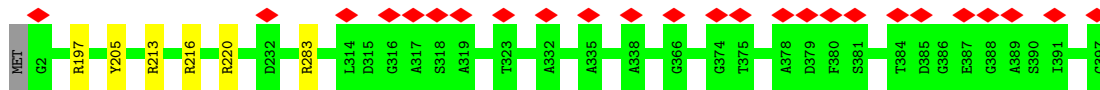


• Molecule 1: Major capsid protein

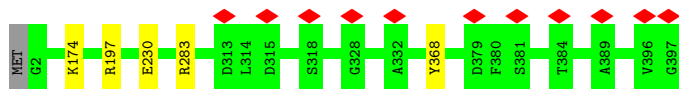




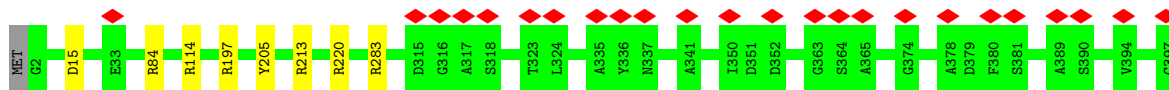
• Molecule 1: Major capsid protein



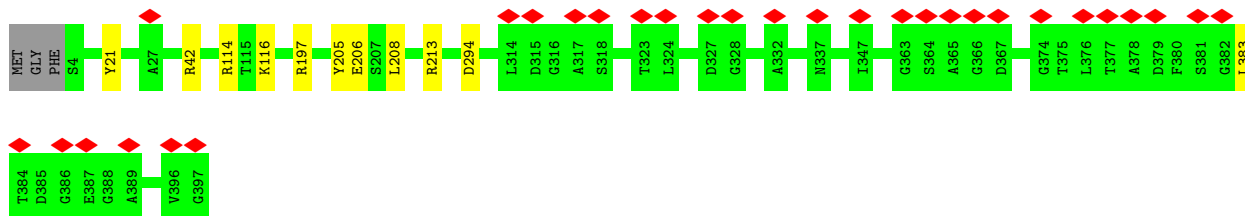
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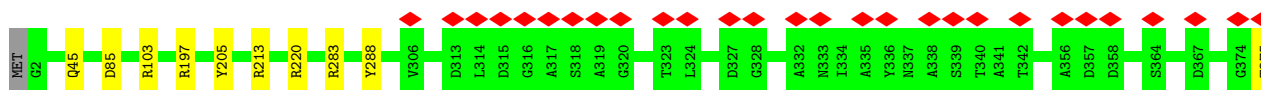
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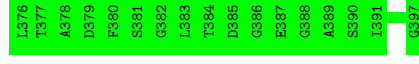
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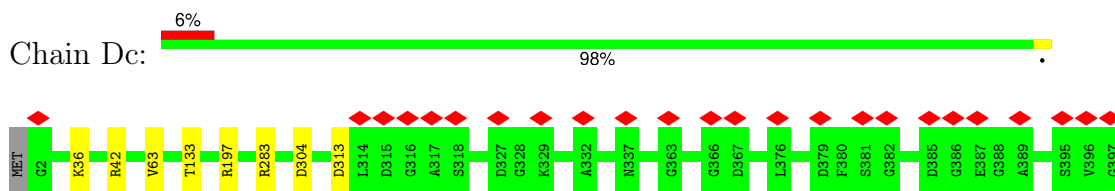


• Molecule 1: Major capsid protein

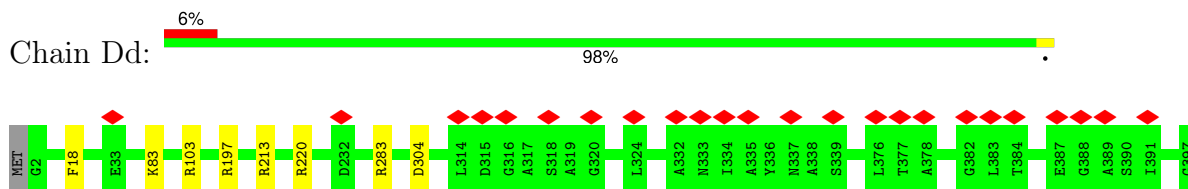


• Molecule 1: Major capsid protein

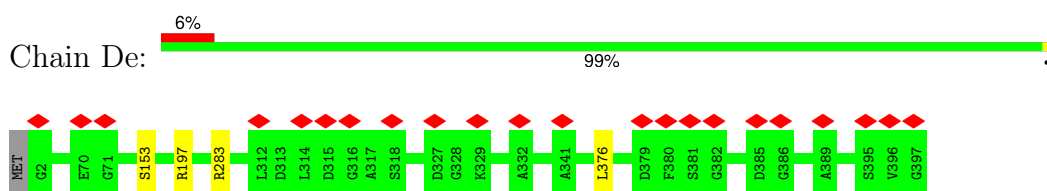




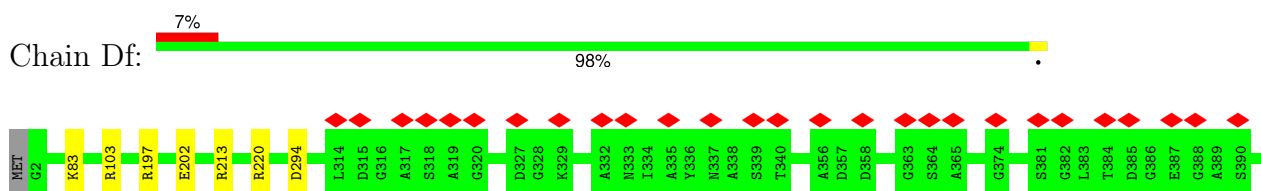
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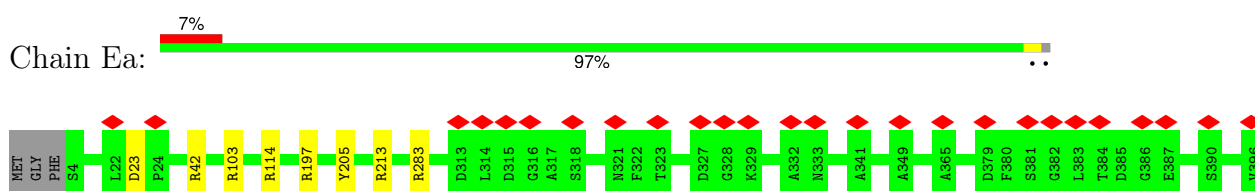
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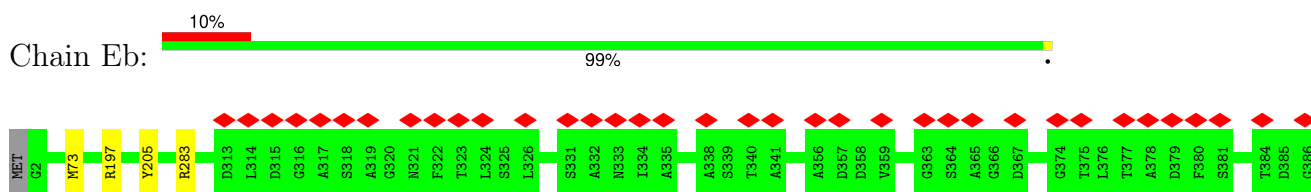
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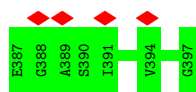


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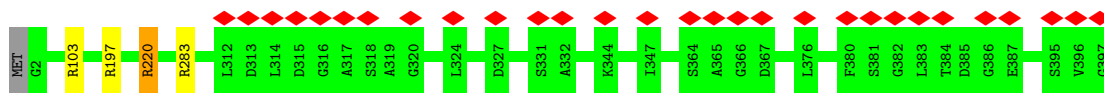


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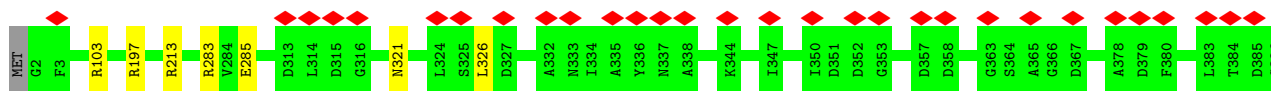




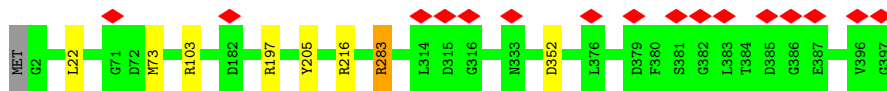
• Molecule 1: Major capsid protein



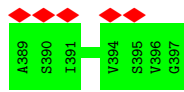
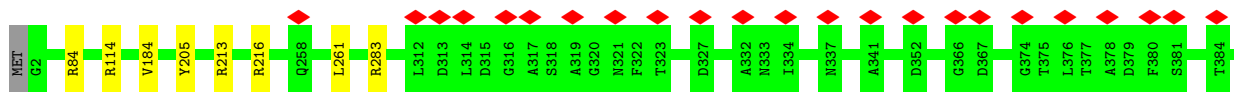
• Molecule 1: Major capsid protein



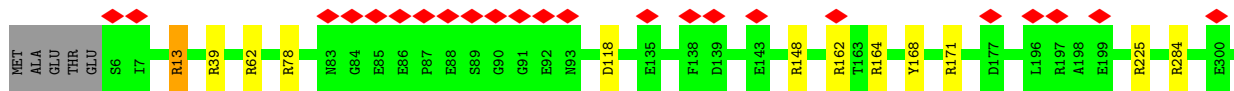
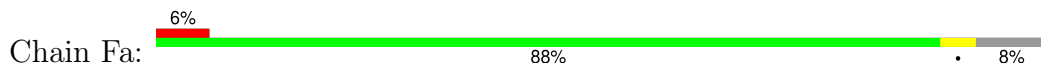
• Molecule 1: Major capsid protein

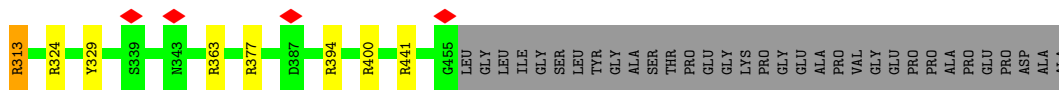


• Molecule 1: Major capsid protein

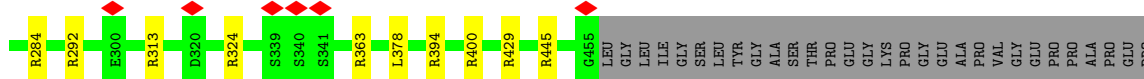
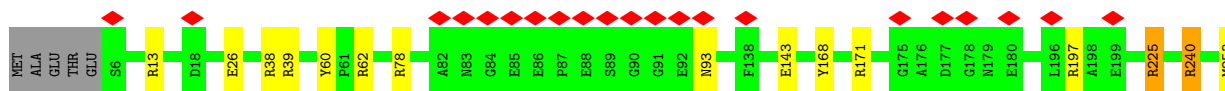
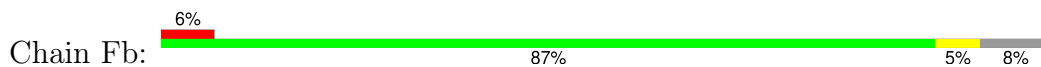


• Molecule 2: Portal protein

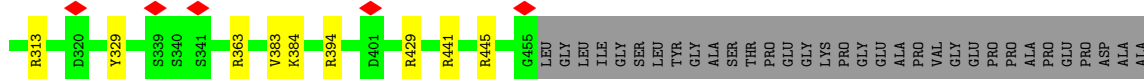
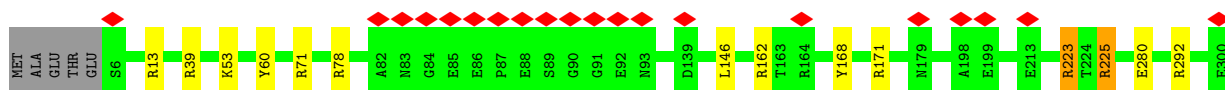
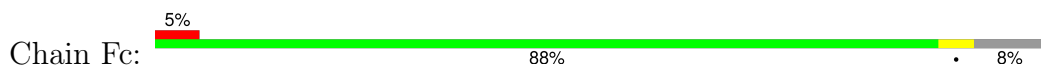




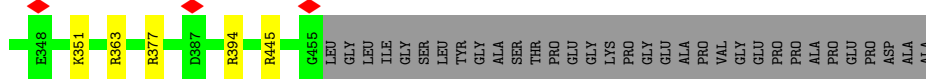
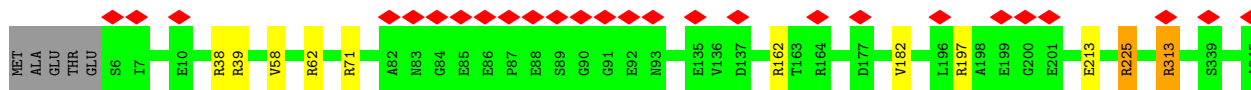
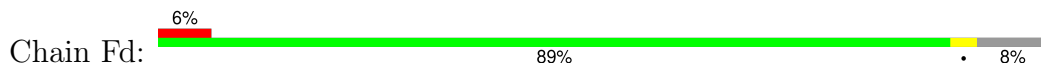
• Molecule 2: Portal protein



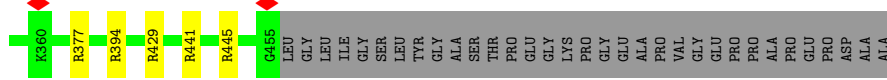
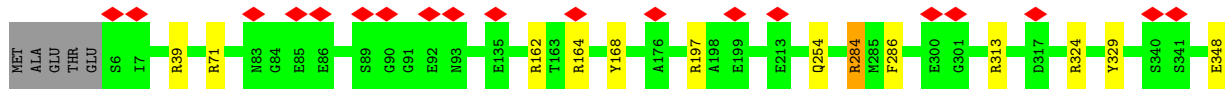
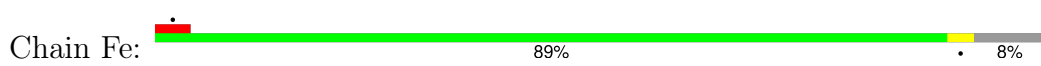
• Molecule 2: Portal protein



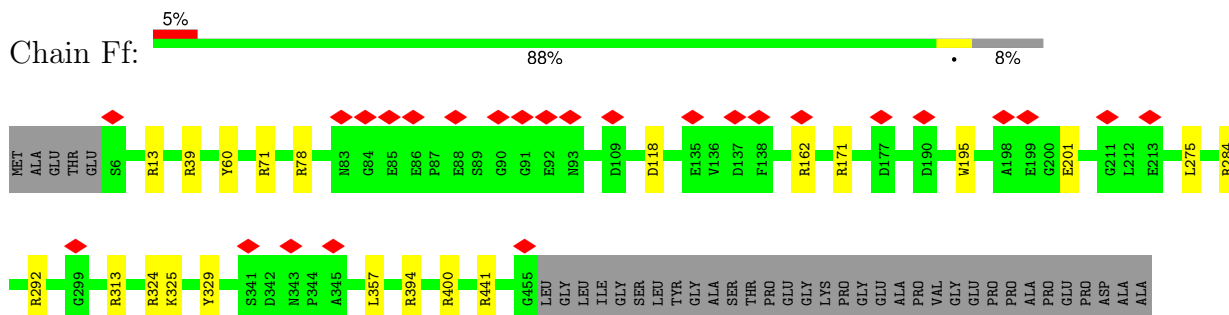
• Molecule 2: Portal protein



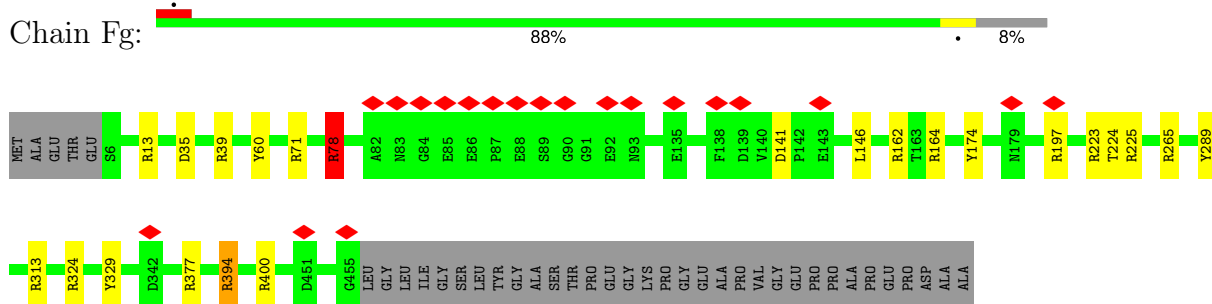
• Molecule 2: Portal protein



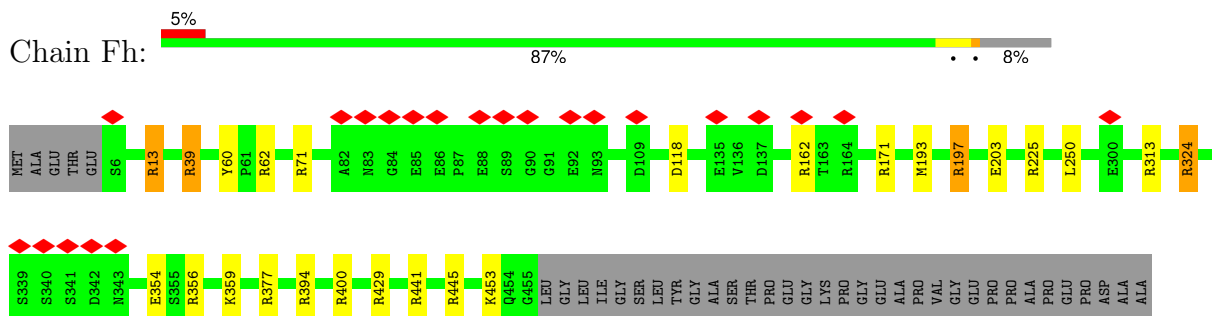
• Molecule 2: Portal protein



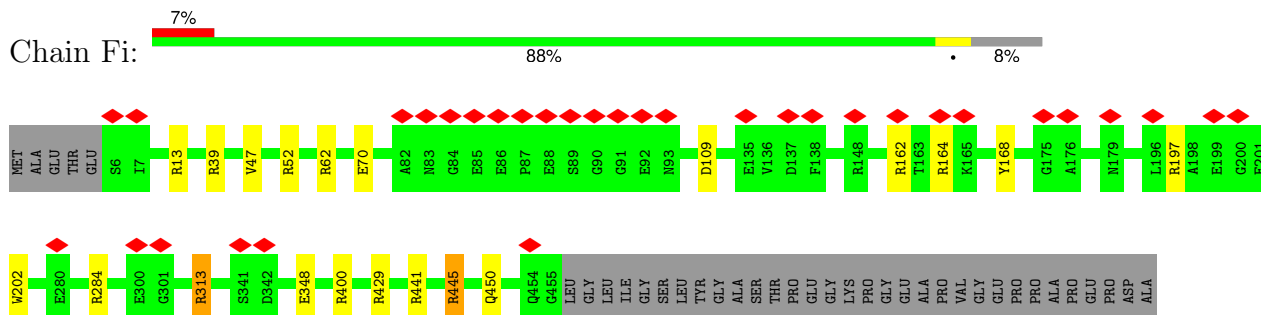
• Molecule 2: Portal protein



• Molecule 2: Portal protein

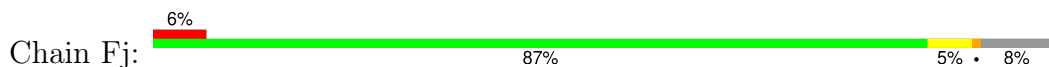


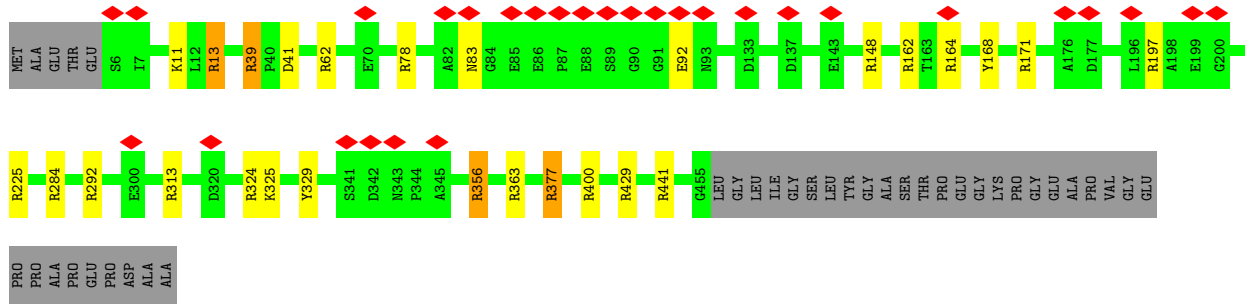
• Molecule 2: Portal protein



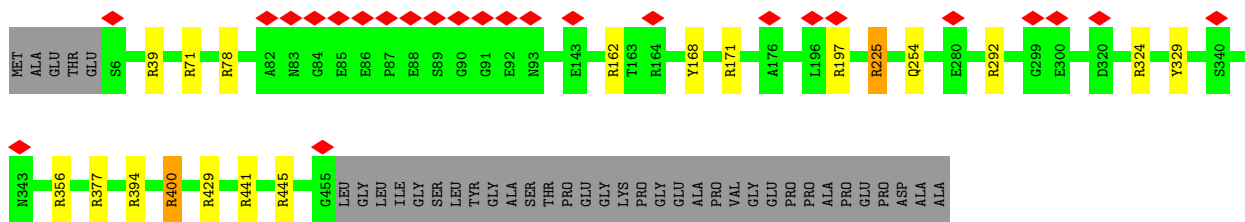
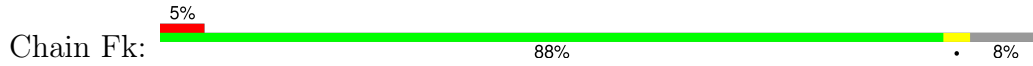
ALA

• Molecule 2: Portal protein

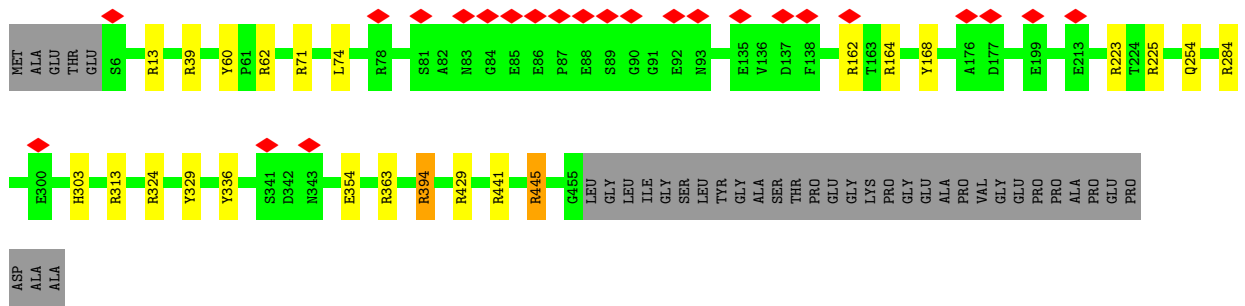
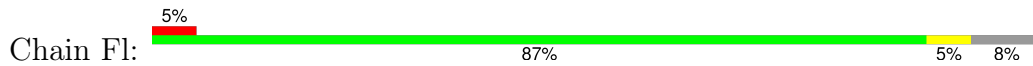




• Molecule 2: Portal protein



• Molecule 2: Portal protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33132	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	32.850	Depositor
Minimum map value	-13.408	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.022	Depositor
Recommended contour level	4.5	Depositor
Map size ( $\text{\AA}$ )	865.62006, 865.62006, 865.62006	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.2366, 1.2366, 1.2366	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	Aa	0.58	0/2982	0.93	3/4070 (0.1%)
1	Ab	0.59	0/2998	0.93	3/4091 (0.1%)
1	Ac	0.58	0/2998	0.92	3/4091 (0.1%)
1	Ad	0.59	0/2998	0.92	3/4091 (0.1%)
1	Ae	0.58	0/2998	0.94	5/4091 (0.1%)
1	Af	0.58	0/2998	0.92	3/4091 (0.1%)
1	Ba	0.59	0/2982	0.95	5/4070 (0.1%)
1	Bb	0.59	0/2998	0.94	6/4091 (0.1%)
1	Bc	0.58	0/2998	0.92	3/4091 (0.1%)
1	Bd	0.59	0/2998	0.92	5/4091 (0.1%)
1	Be	0.58	0/2998	0.92	5/4091 (0.1%)
1	Bf	0.58	0/2998	0.91	5/4091 (0.1%)
1	Ca	0.58	0/2982	0.94	4/4070 (0.1%)
1	Cb	0.59	0/2998	0.92	3/4091 (0.1%)
1	Cc	0.58	0/2998	0.91	3/4091 (0.1%)
1	Cd	0.59	0/2998	0.94	6/4091 (0.1%)
1	Ce	0.58	0/2998	0.93	3/4091 (0.1%)
1	Cf	0.58	0/2998	0.93	6/4091 (0.1%)
1	Da	0.58	0/2982	0.94	4/4070 (0.1%)
1	Db	0.59	0/2998	0.94	6/4091 (0.1%)
1	Dc	0.58	0/2998	0.91	4/4091 (0.1%)
1	Dd	0.59	0/2998	0.95	5/4091 (0.1%)
1	De	0.58	0/2998	0.92	2/4091 (0.0%)
1	Df	0.58	0/2998	0.91	4/4091 (0.1%)
1	Ea	0.59	0/2982	0.93	6/4070 (0.1%)
1	Eb	0.58	0/2998	0.92	2/4091 (0.0%)
1	Ec	0.58	0/2998	0.91	4/4091 (0.1%)
1	Ed	0.59	0/2998	0.94	4/4091 (0.1%)
1	Ee	0.58	0/2998	0.93	3/4091 (0.1%)
1	Ef	0.58	0/2998	0.93	5/4091 (0.1%)
2	Fa	0.65	0/3606	1.03	19/4901 (0.4%)
2	Fb	0.64	0/3606	1.03	20/4901 (0.4%)
2	Fc	0.64	0/3606	1.04	14/4901 (0.3%)
2	Fd	0.65	0/3606	1.01	12/4901 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	Fe	0.64	0/3606	1.00	13/4901 (0.3%)
2	Ff	0.65	0/3606	1.03	16/4901 (0.3%)
2	Fg	0.64	0/3606	1.03	18/4901 (0.4%)
2	Fh	0.64	0/3606	1.02	17/4901 (0.3%)
2	Fi	0.64	0/3606	1.01	15/4901 (0.3%)
2	Fj	0.65	0/3606	1.02	22/4901 (0.4%)
2	Fk	0.64	0/3606	1.01	18/4901 (0.4%)
2	Fl	0.65	0/3606	1.04	21/4901 (0.4%)
All	All	0.60	0/133132	0.96	328/181437 (0.2%)

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
1	Aa	0	1
1	Ab	0	1
1	Ac	0	2
1	Ae	0	1
1	Af	0	2
1	Ba	0	1
1	Bb	0	2
1	Bc	0	1
1	Ca	0	2
1	Cb	0	1
1	Cc	0	1
1	Cd	0	1
1	Cf	0	1
1	Da	0	2
1	Db	0	2
1	Ea	0	1
1	Eb	0	1
1	Ee	0	1
1	Ef	0	1
2	Fb	0	1
2	Fc	0	3
2	Fe	0	1
2	Fg	0	2
2	Fh	0	2
2	Fi	0	2
2	Fj	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	Fk	0	2
2	Fl	0	1
All	All	0	42

There are no bond length outliers.

The worst 5 of 328 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Fa	13	ARG	NE-CZ-NH2	9.83	125.22	120.30
1	Be	220	ARG	NE-CZ-NH2	9.37	124.99	120.30
2	Fd	445	ARG	NE-CZ-NH2	9.14	124.87	120.30
2	Fi	39	ARG	NE-CZ-NH2	8.98	124.79	120.30
2	Ff	78	ARG	NE-CZ-NH2	8.88	124.74	120.30

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Aa	21	TYR	Sidechain
1	Ab	205	TYR	Sidechain
1	Ac	205	TYR	Sidechain
1	Ac	283	ARG	Sidechain
1	Ae	205	TYR	Sidechain

## 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	Aa	2926	2859	2857	0	0
1	Ab	2941	2871	2869	0	0
1	Ac	2941	2870	2869	0	0
1	Ad	2941	2870	2869	0	0
1	Ae	2941	2870	2869	0	0
1	Af	2941	2870	2869	0	0
1	Ba	2926	2858	2857	0	0
1	Bb	2941	2870	2869	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Bc	2941	2870	2869	0	0
1	Bd	2941	2871	2869	0	0
1	Be	2941	2870	2869	0	0
1	Bf	2941	2871	2869	0	0
1	Ca	2926	2858	2857	0	0
1	Cb	2941	2870	2869	0	0
1	Cc	2941	2870	2869	0	0
1	Cd	2941	2871	2869	0	0
1	Ce	2941	2870	2869	0	0
1	Cf	2941	2870	2869	0	0
1	Da	2926	2859	2857	0	0
1	Db	2941	2870	2869	0	0
1	Dc	2941	2871	2869	0	0
1	Dd	2941	2871	2869	0	0
1	De	2941	2870	2869	0	0
1	Df	2941	2870	2869	0	0
1	Ea	2926	2858	2857	0	0
1	Eb	2941	2870	2869	0	0
1	Ec	2941	2870	2869	0	0
1	Ed	2941	2870	2869	0	0
1	Ee	2941	2871	2869	0	0
1	Ef	2941	2871	2869	0	0
2	Fa	3526	3425	3424	0	0
2	Fb	3526	3425	3424	0	0
2	Fc	3526	3425	3424	0	0
2	Fd	3526	3425	3424	0	0
2	Fe	3526	3426	3424	0	0
2	Ff	3526	3425	3424	0	0
2	Fg	3526	3425	3424	0	0
2	Fh	3526	3425	3424	0	0
2	Fi	3526	3425	3424	0	0
2	Fj	3526	3425	3424	0	0
2	Fk	3526	3425	3424	0	0
2	Fl	3526	3425	3424	0	0
All	All	130467	127151	127098	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	392/397 (99%)	364 (93%)	28 (7%)	0	100	100
1	Ab	394/397 (99%)	374 (95%)	20 (5%)	0	100	100
1	Ac	394/397 (99%)	377 (96%)	17 (4%)	0	100	100
1	Ad	394/397 (99%)	374 (95%)	20 (5%)	0	100	100
1	Ae	394/397 (99%)	379 (96%)	15 (4%)	0	100	100
1	Af	394/397 (99%)	376 (95%)	18 (5%)	0	100	100
1	Ba	392/397 (99%)	369 (94%)	23 (6%)	0	100	100
1	Bb	394/397 (99%)	377 (96%)	17 (4%)	0	100	100
1	Bc	394/397 (99%)	380 (96%)	14 (4%)	0	100	100
1	Bd	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
1	Be	394/397 (99%)	375 (95%)	19 (5%)	0	100	100
1	Bf	394/397 (99%)	376 (95%)	18 (5%)	0	100	100
1	Ca	392/397 (99%)	372 (95%)	20 (5%)	0	100	100
1	Cb	394/397 (99%)	376 (95%)	18 (5%)	0	100	100
1	Cc	394/397 (99%)	381 (97%)	13 (3%)	0	100	100
1	Cd	394/397 (99%)	378 (96%)	16 (4%)	0	100	100
1	Ce	394/397 (99%)	377 (96%)	17 (4%)	0	100	100
1	Cf	394/397 (99%)	376 (95%)	18 (5%)	0	100	100
1	Da	392/397 (99%)	371 (95%)	21 (5%)	0	100	100
1	Db	394/397 (99%)	376 (95%)	18 (5%)	0	100	100
1	Dc	394/397 (99%)	382 (97%)	12 (3%)	0	100	100
1	Dd	394/397 (99%)	375 (95%)	19 (5%)	0	100	100
1	De	394/397 (99%)	376 (95%)	18 (5%)	0	100	100
1	Df	394/397 (99%)	379 (96%)	15 (4%)	0	100	100
1	Ea	392/397 (99%)	375 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Eb	394/397 (99%)	380 (96%)	14 (4%)	0	100	100
1	Ec	394/397 (99%)	380 (96%)	14 (4%)	0	100	100
1	Ed	394/397 (99%)	374 (95%)	20 (5%)	0	100	100
1	Ee	394/397 (99%)	376 (95%)	18 (5%)	0	100	100
1	Ef	394/397 (99%)	375 (95%)	19 (5%)	0	100	100
2	Fa	448/488 (92%)	430 (96%)	18 (4%)	0	100	100
2	Fb	448/488 (92%)	430 (96%)	18 (4%)	0	100	100
2	Fc	448/488 (92%)	427 (95%)	21 (5%)	0	100	100
2	Fd	448/488 (92%)	433 (97%)	15 (3%)	0	100	100
2	Fe	448/488 (92%)	426 (95%)	22 (5%)	0	100	100
2	Ff	448/488 (92%)	429 (96%)	19 (4%)	0	100	100
2	Fg	448/488 (92%)	428 (96%)	20 (4%)	0	100	100
2	Fh	448/488 (92%)	432 (96%)	16 (4%)	0	100	100
2	Fi	448/488 (92%)	436 (97%)	12 (3%)	0	100	100
2	Fj	448/488 (92%)	435 (97%)	13 (3%)	0	100	100
2	Fk	448/488 (92%)	429 (96%)	19 (4%)	0	100	100
2	Fl	448/488 (92%)	432 (96%)	16 (4%)	0	100	100
All	All	17186/17766 (97%)	16450 (96%)	736 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	Aa	314/316 (99%)	308 (98%)	6 (2%)	52	73
1	Ab	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	Ac	315/316 (100%)	314 (100%)	1 (0%)	91	96
1	Ad	315/316 (100%)	312 (99%)	3 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ae	315/316 (100%)	309 (98%)	6 (2%)	52	73
1	Af	315/316 (100%)	312 (99%)	3 (1%)	73	84
1	Ba	314/316 (99%)	310 (99%)	4 (1%)	65	81
1	Bb	315/316 (100%)	310 (98%)	5 (2%)	58	76
1	Bc	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	Bd	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	Be	315/316 (100%)	311 (99%)	4 (1%)	65	81
1	Bf	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	Ca	314/316 (99%)	313 (100%)	1 (0%)	91	96
1	Cb	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	Cc	315/316 (100%)	314 (100%)	1 (0%)	91	96
1	Cd	315/316 (100%)	315 (100%)	0	100	100
1	Ce	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	Cf	315/316 (100%)	314 (100%)	1 (0%)	91	96
1	Da	314/316 (99%)	309 (98%)	5 (2%)	58	76
1	Db	315/316 (100%)	312 (99%)	3 (1%)	73	84
1	Dc	315/316 (100%)	310 (98%)	5 (2%)	58	76
1	Dd	315/316 (100%)	312 (99%)	3 (1%)	73	84
1	De	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	Df	315/316 (100%)	312 (99%)	3 (1%)	73	84
1	Ea	314/316 (99%)	313 (100%)	1 (0%)	91	96
1	Eb	315/316 (100%)	314 (100%)	1 (0%)	91	96
1	Ec	315/316 (100%)	314 (100%)	1 (0%)	91	96
1	Ed	315/316 (100%)	312 (99%)	3 (1%)	73	84
1	Ee	315/316 (100%)	310 (98%)	5 (2%)	58	76
1	Ef	315/316 (100%)	313 (99%)	2 (1%)	84	91
2	Fa	364/390 (93%)	359 (99%)	5 (1%)	62	79
2	Fb	364/390 (93%)	357 (98%)	7 (2%)	52	73
2	Fc	364/390 (93%)	356 (98%)	8 (2%)	47	70
2	Fd	364/390 (93%)	358 (98%)	6 (2%)	58	76
2	Fe	364/390 (93%)	359 (99%)	5 (1%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Ff	364/390 (93%)	358 (98%)	6 (2%)	58	76
2	Fg	364/390 (93%)	358 (98%)	6 (2%)	58	76
2	Fh	364/390 (93%)	354 (97%)	10 (3%)	40	65
2	Fi	364/390 (93%)	357 (98%)	7 (2%)	52	73
2	Fj	364/390 (93%)	356 (98%)	8 (2%)	47	70
2	Fk	364/390 (93%)	362 (100%)	2 (0%)	86	93
2	Fl	364/390 (93%)	358 (98%)	6 (2%)	58	76
All	All	13813/14160 (98%)	13656 (99%)	157 (1%)	69	83

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Ff	275	LEU
2	Fj	41	ASP
2	Fg	78	ARG
2	Fh	250	LEU
2	Fk	254	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ba	266	GLN
1	Bb	337	ASN
1	Ca	12	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 oligosaccharides 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](#)

There are no chain breaks in this entry.

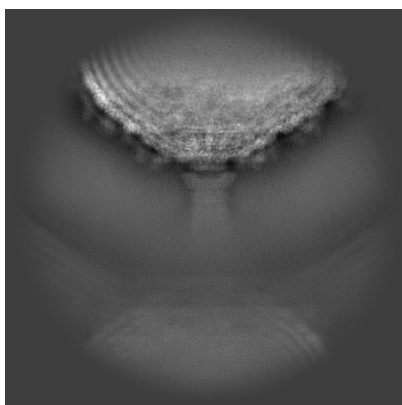
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46681. These allow visual inspection of the internal detail of the map and identification of artifacts.

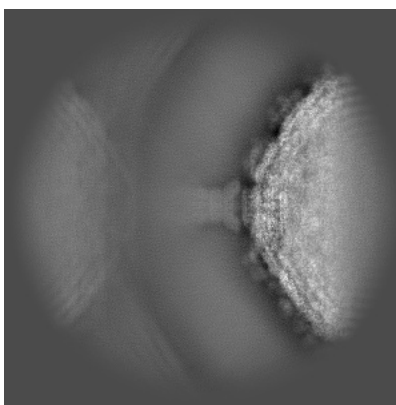
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

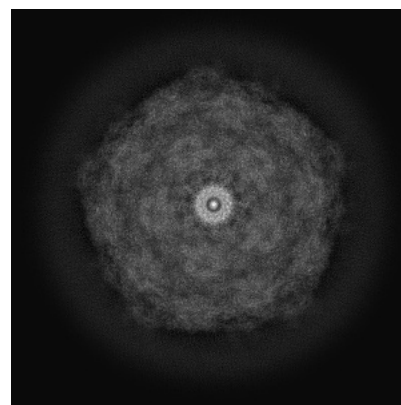
#### 6.1.1 Primary map



X



Y



Z

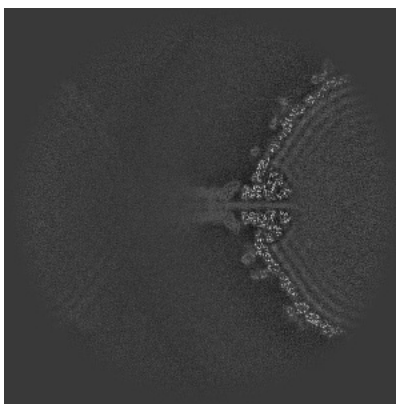
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

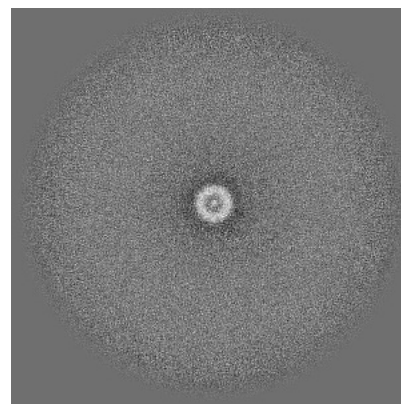
#### 6.2.1 Primary map



X Index: 350



Y Index: 350



Z Index: 350

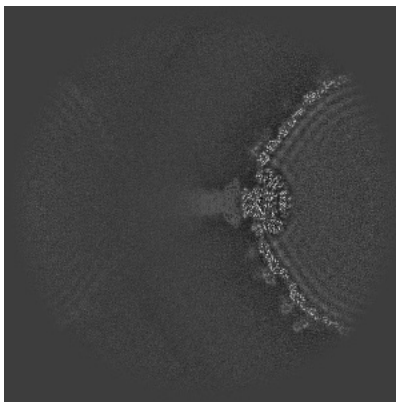
The images above show central slices of the map in three orthogonal directions.

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

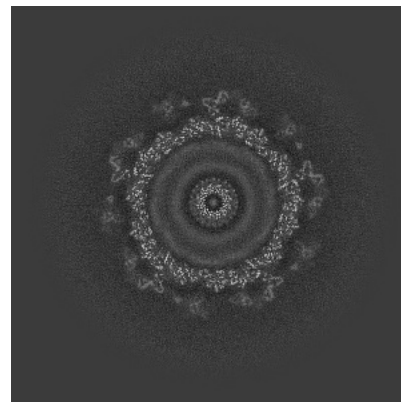
### 6.3.1 Primary map



X Index: 373



Y Index: 333

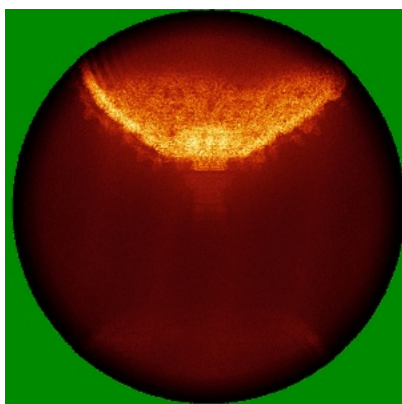


Z Index: 491

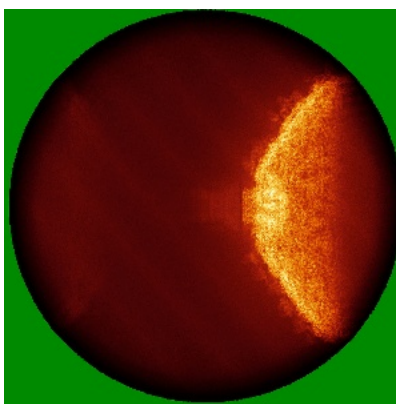
The images above show the largest variance slices of the map in three orthogonal directions.

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

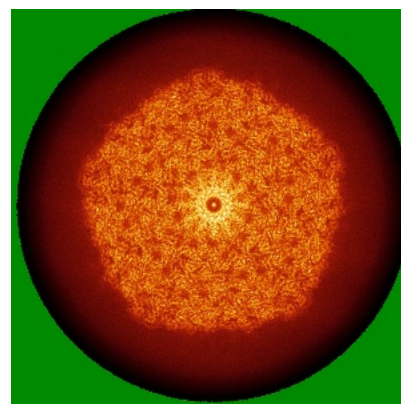
### 6.4.1 Primary map



X



Y

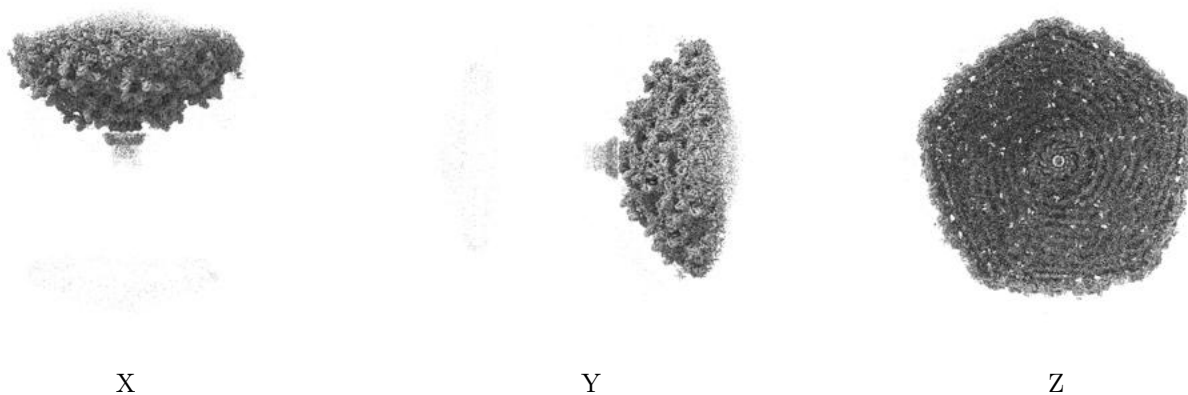


Z

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 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

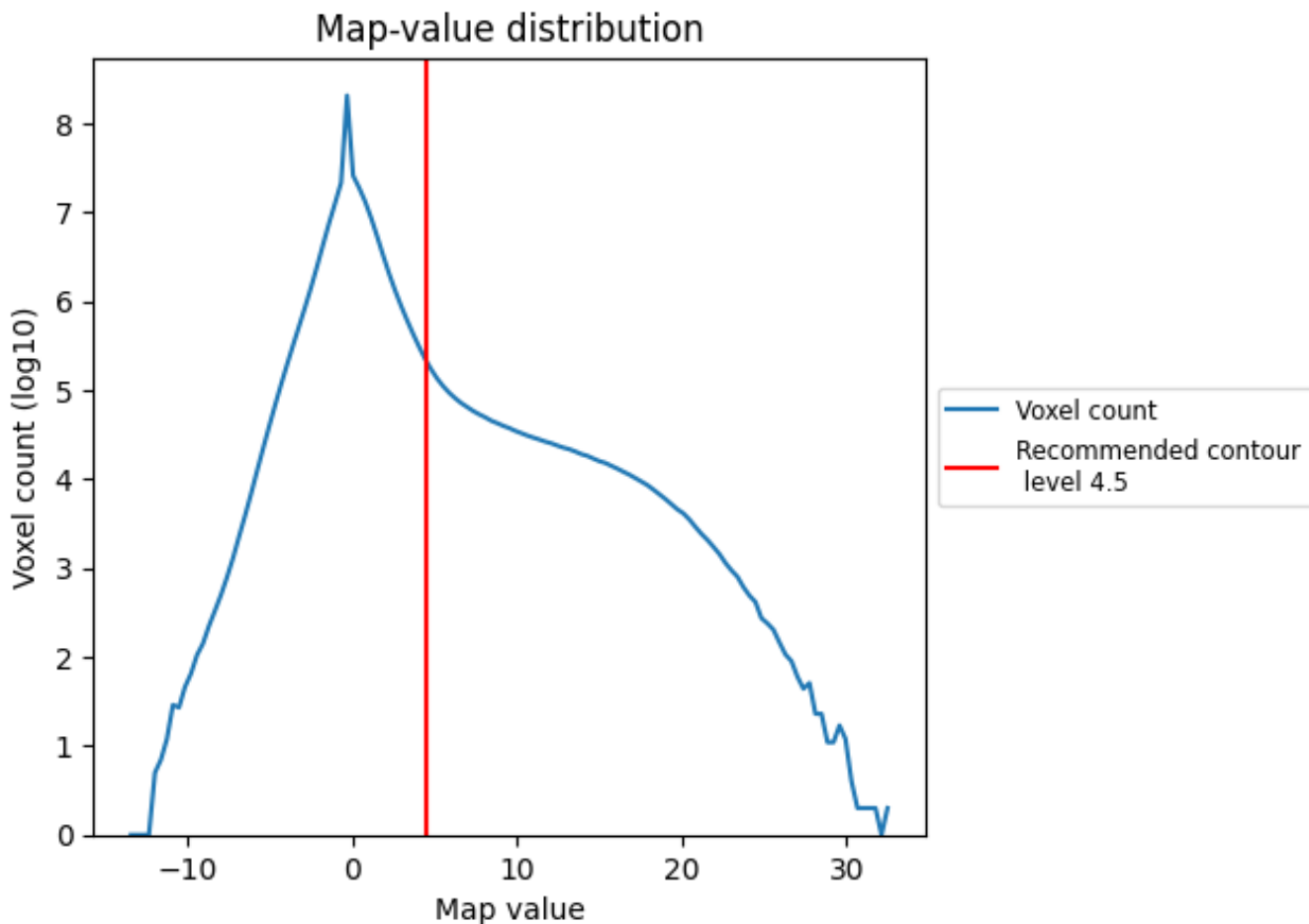
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

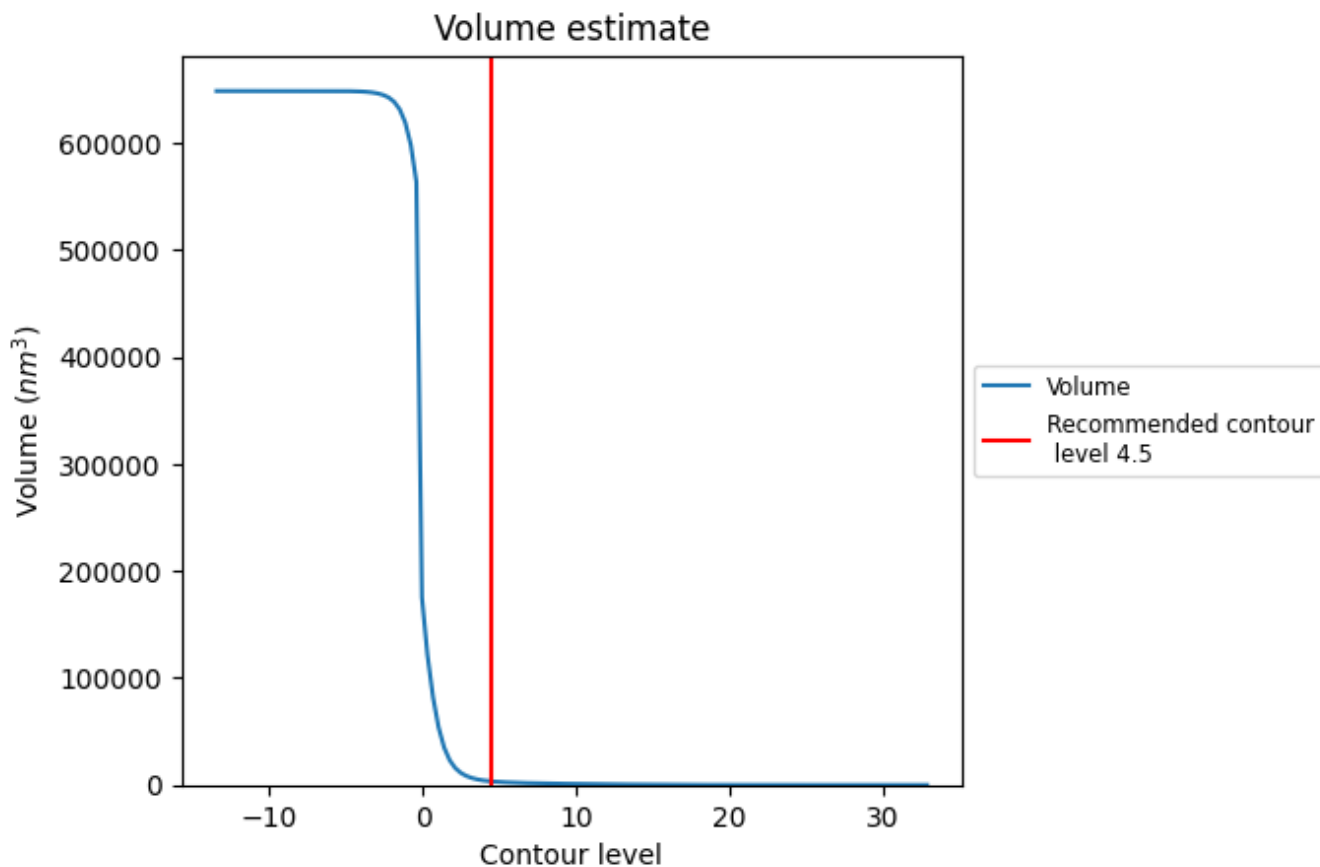
This section contains the results of statistical analysis of the map.

### 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.

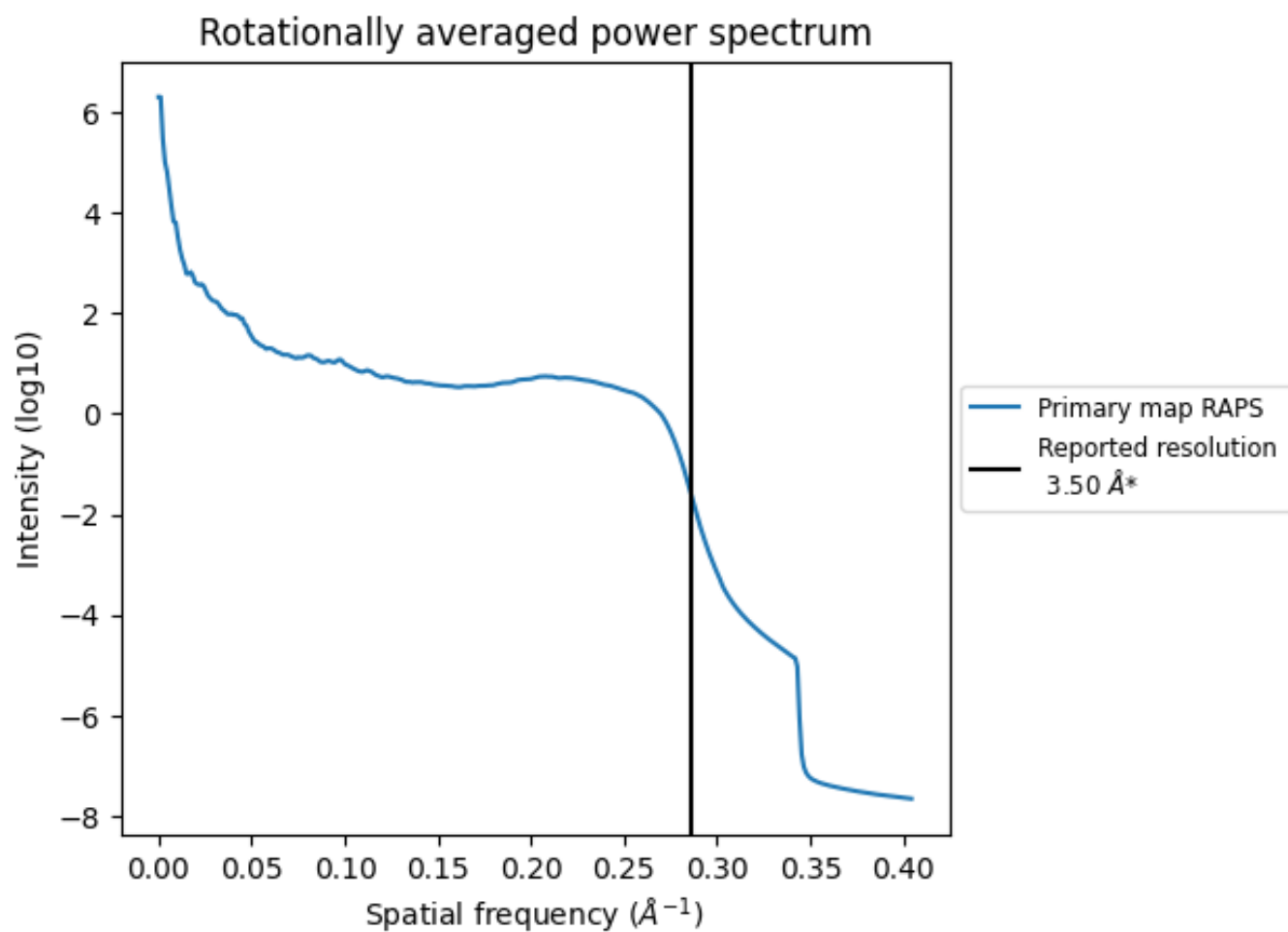
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3345  $\text{nm}^3$ ; this corresponds to an approximate mass of 3022 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 0.286 Å<sup>-1</sup>



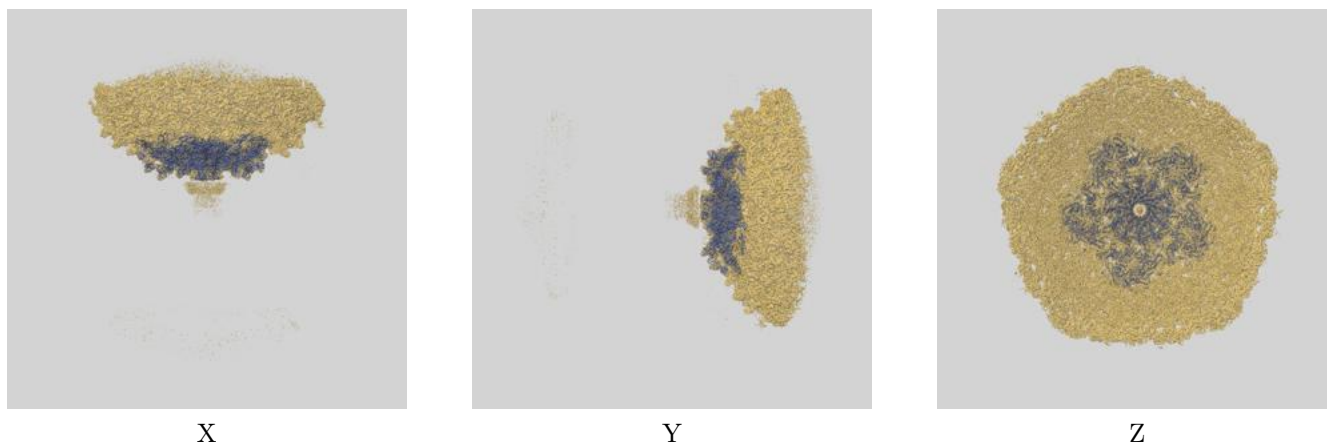
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

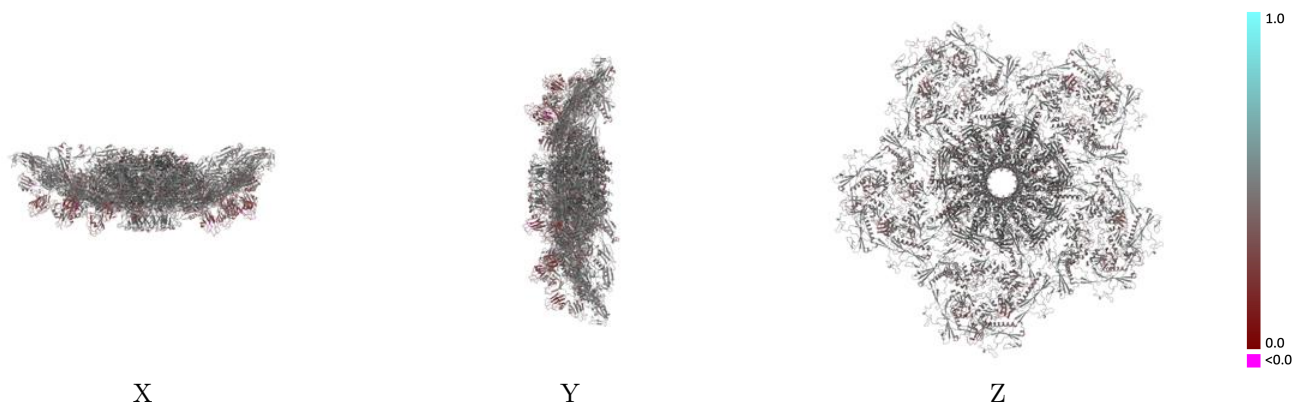
This section contains information regarding the fit between EMDB map EMD-46681 and PDB model 9D9W. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



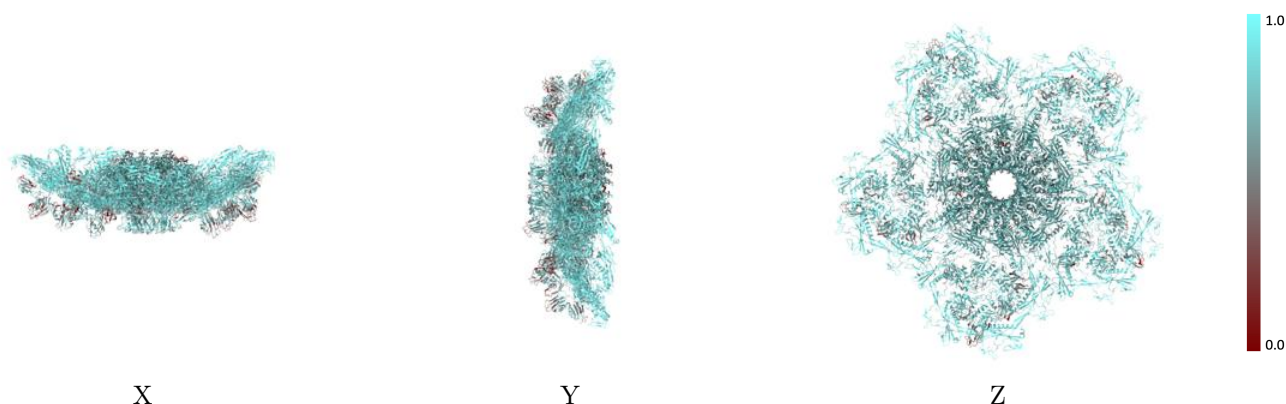
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



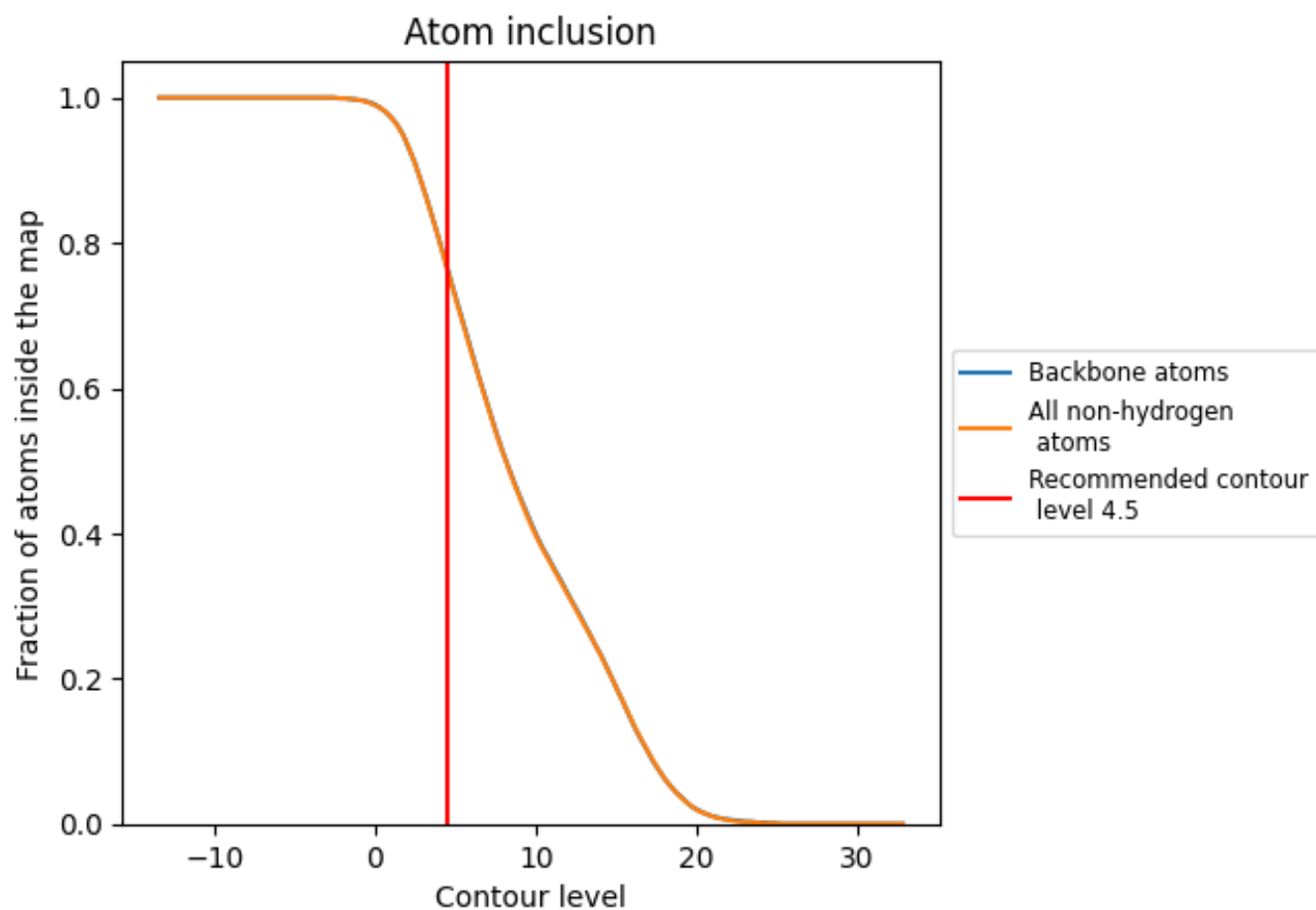
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7630	 0.4420
Aa	 0.7600	 0.4360
Ab	 0.7640	 0.4330
Ac	 0.7810	 0.4460
Ad	 0.7680	 0.4280
Ae	 0.7980	 0.4520
Af	 0.7950	 0.4370
Ba	 0.7630	 0.4360
Bb	 0.7680	 0.4270
Bc	 0.7760	 0.4460
Bd	 0.7640	 0.4260
Be	 0.7960	 0.4480
Bf	 0.7990	 0.4370
Ca	 0.7640	 0.4390
Cb	 0.7720	 0.4310
Cc	 0.7850	 0.4430
Cd	 0.7740	 0.4280
Ce	 0.7900	 0.4460
Cf	 0.7840	 0.4240
Da	 0.7720	 0.4360
Db	 0.7650	 0.4300
Dc	 0.7770	 0.4430
Dd	 0.7900	 0.4340
De	 0.7980	 0.4470
Df	 0.7820	 0.4250
Ea	 0.7720	 0.4410
Eb	 0.7670	 0.4210
Ec	 0.7680	 0.4400
Ed	 0.7790	 0.4250
Ee	 0.7950	 0.4490
Ef	 0.7830	 0.4300
Fa	 0.7550	 0.4510
Fb	 0.7590	 0.4550
Fc	 0.7750	 0.4620
Fd	 0.7620	 0.4590



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Chain	Atom inclusion	Q-score
Fe	 0.7710	 0.4620
Ff	 0.7570	 0.4480
Fg	 0.7510	 0.4500
Fh	 0.7510	 0.4520
Fi	 0.7390	 0.4470
Fj	 0.7620	 0.4540
Fk	 0.7660	 0.4590
Fl	 0.7590	 0.4530