



## Full wwPDB EM Validation Report ⓘ

May 31, 2025 – 02:07 PM EDT

PDB ID : 9D9W / pdb\_00009d9w  
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 Full wwPDB EM Validation 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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.43.1

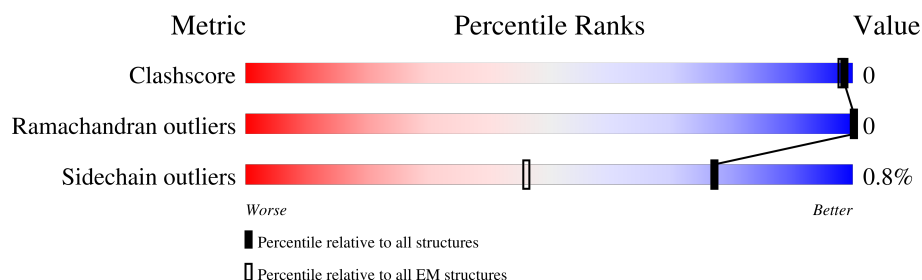
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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	<div> <div>8%</div> <div>97%</div> <div>..</div> </div>
1	Ab	397	<div> <div>11%</div> <div>98%</div> <div>.</div> </div>
1	Ac	397	<div> <div>6%</div> <div>98%</div> <div>.</div> </div>
1	Ad	397	<div> <div>8%</div> <div>98%</div> <div>.</div> </div>
1	Ae	397	<div> <div>.</div> <div>97%</div> <div>.</div> </div>
1	Af	397	<div> <div>5%</div> <div>98%</div> <div>.</div> </div>
1	Ba	397	<div> <div>7%</div> <div>97%</div> <div>..</div> </div>
1	Bb	397	<div> <div>10%</div> <div>97%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	Bc	397	6% 98% .
1	Bd	397	11% 98% .
1	Be	397	. 98% .
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	. 98% .
1	Cf	397	6% 98% .
1	Da	397	8% 96% ..
1	Db	397	11% 97% .
1	Dc	397	6% 99% .
1	Dd	397	6% 97% .
1	De	397	6% 98% .
1	Df	397	7% 99% .
1	Ea	397	7% 98% ..
1	Eb	397	10% 98% .
1	Ec	397	7% 99% .
1	Ed	397	8% 97% .
1	Ee	397	. 97% ..
1	Ef	397	7% 98% .
2	Fa	488	6% 89% 8%
2	Fb	488	6% 89% 8%
2	Fc	488	5% 90% 8%

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Mol	Chain	Length	Quality of chain
2	Fd	488	 6% 90% 8%
2	Fe	488	 90% 8%
2	Ff	488	 5% 90% 8%
2	Fg	488	 90% 8%
2	Fh	488	 5% 89% 8%
2	Fi	488	 7% 89% 8%
2	Fj	488	 6% 90% 8%
2	Fk	488	 5% 91% 8%
2	Fl	488	 5% 89% 8%

## 2 Entry composition

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

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

- Molecule 2 is a protein called Portal protein.

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

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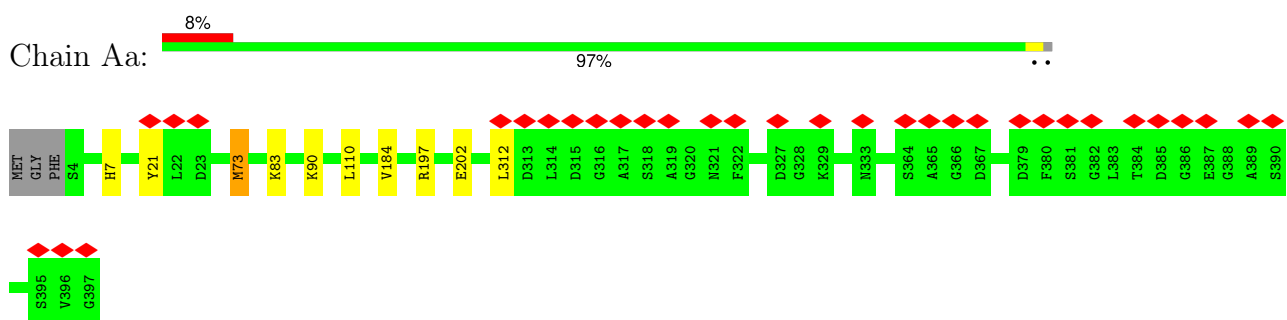
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Mol	Chain	Residues	Atoms						AltConf	Trace
2	Fg	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fh	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fi	450	Total 6951	C 2219	H 3425	N 603	O 690	S 14	0	0
2	Fj	450	Total 6951	C 2219	H 3425	N 603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

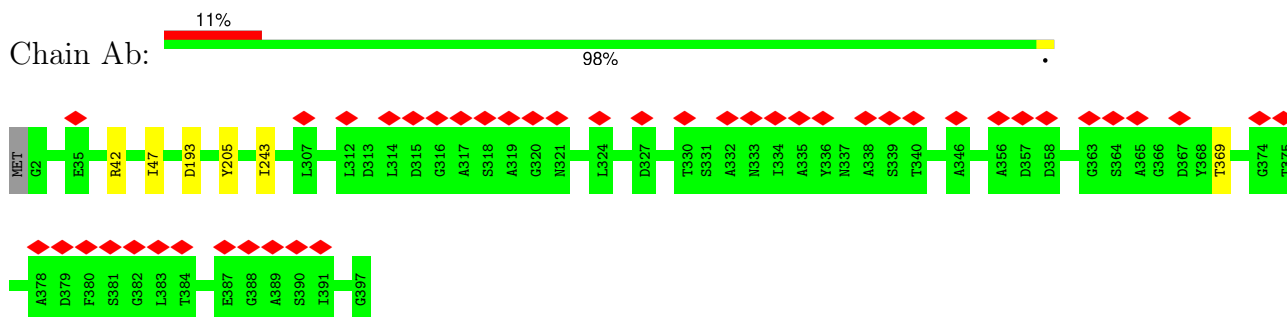
### 3 Residue-property plots [i](#)

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.

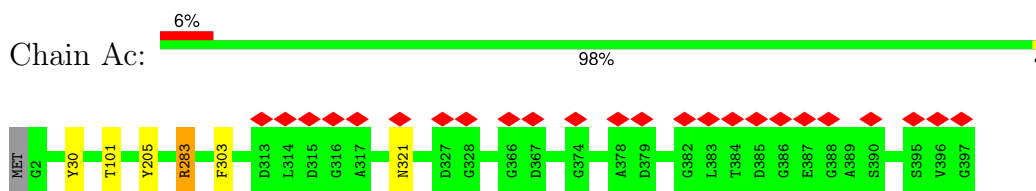
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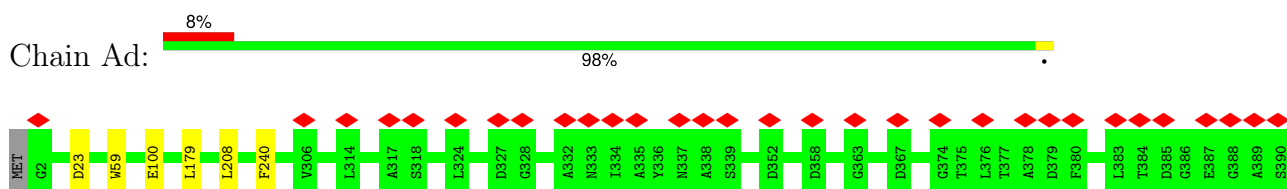
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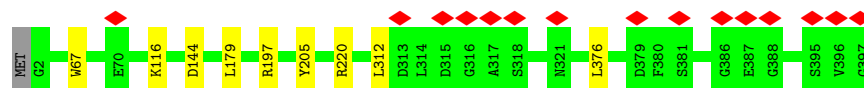
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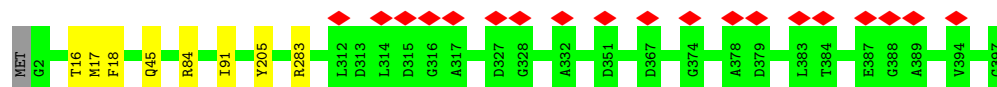
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Chain Ae: 97%



- Molecule 1: Major capsid protein

Chain Af: 98%



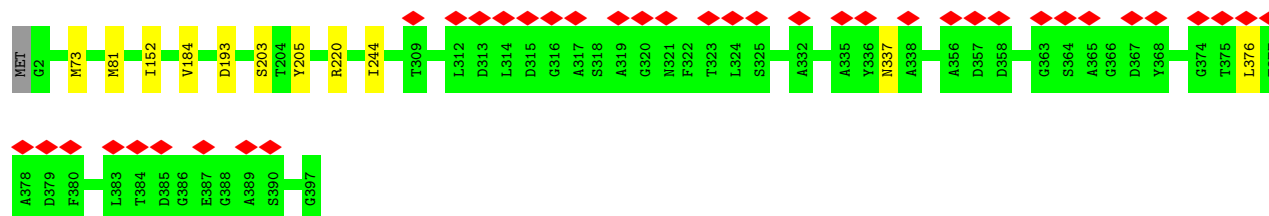
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Chain Ba: 97%



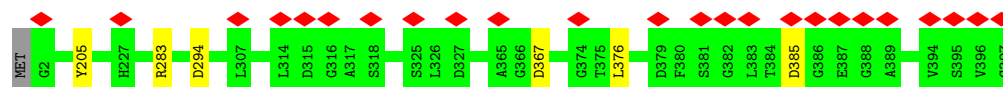
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Chain Bb: 97%



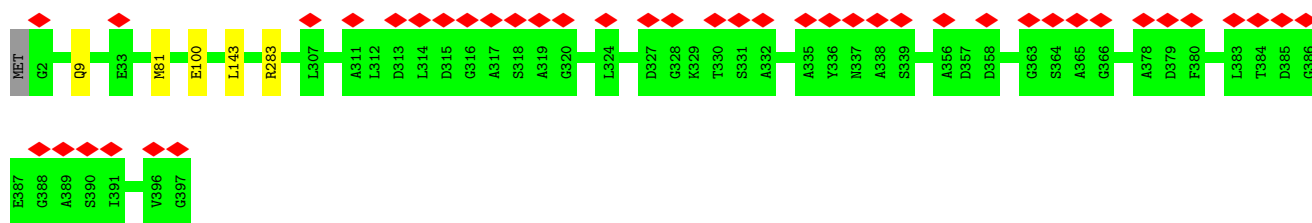
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Chain Bc: 98%

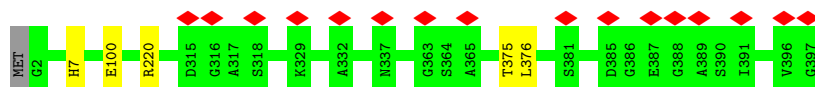


- Molecule 1: Major capsid protein

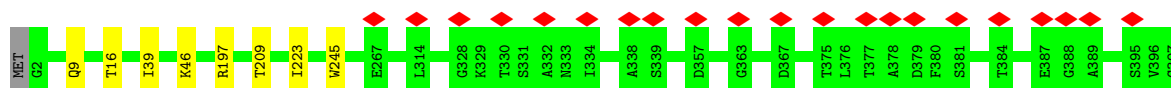
Chain Bd: 98%



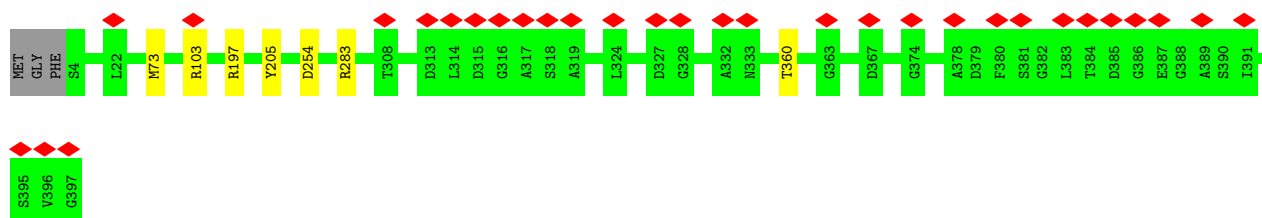
- Molecule 1: Major capsid protein



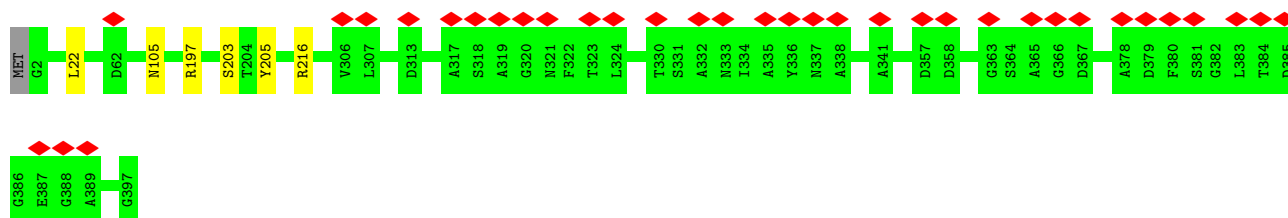
- Molecule 1: Major capsid protein



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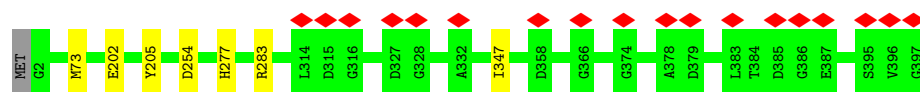


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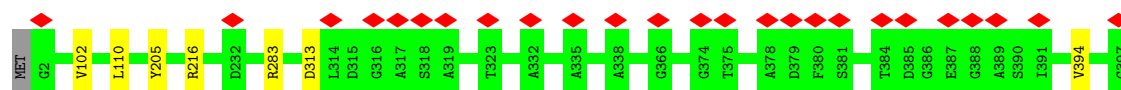


- Molecule 1: Major capsid protein

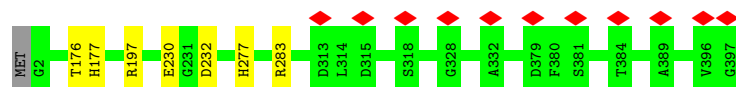




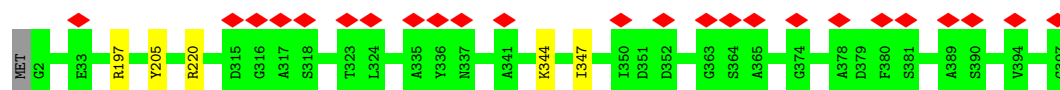
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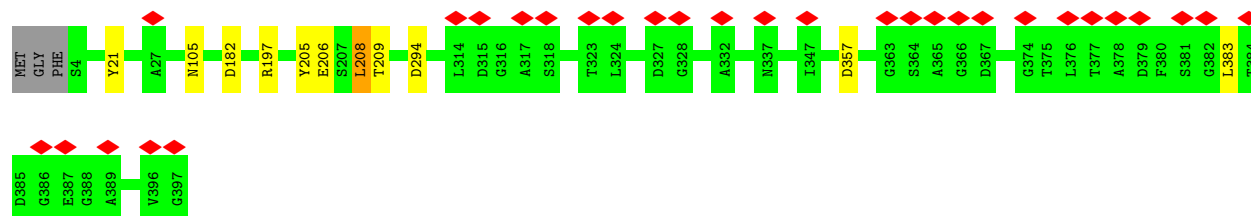
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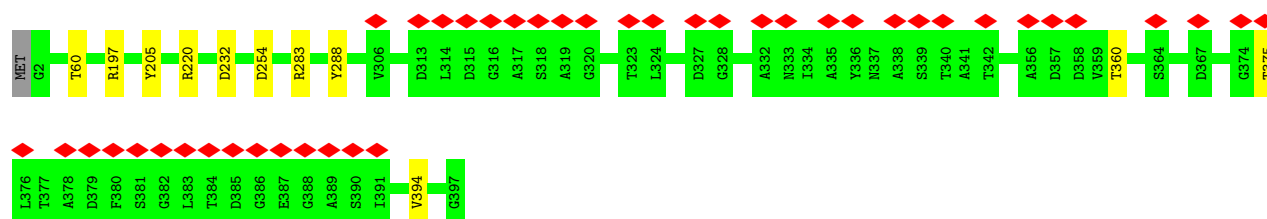
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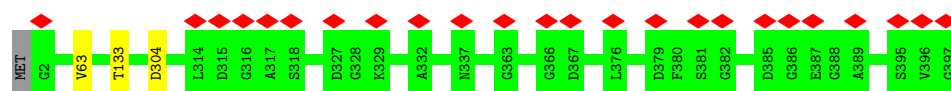
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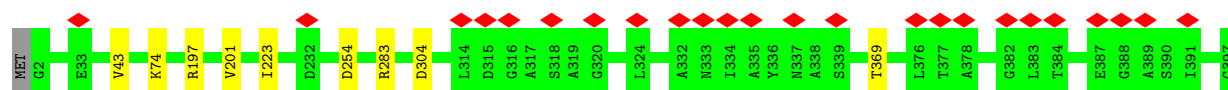
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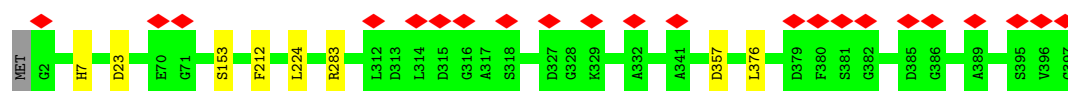
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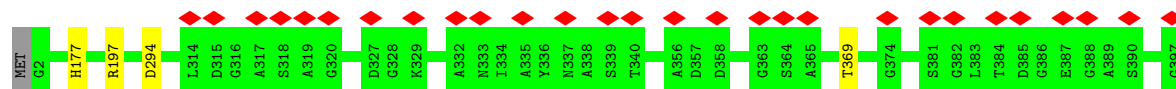
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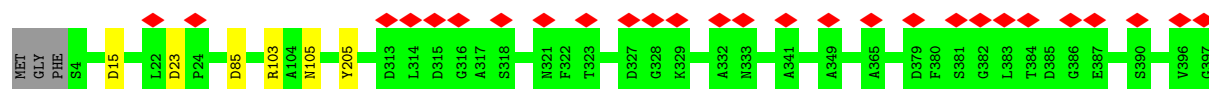
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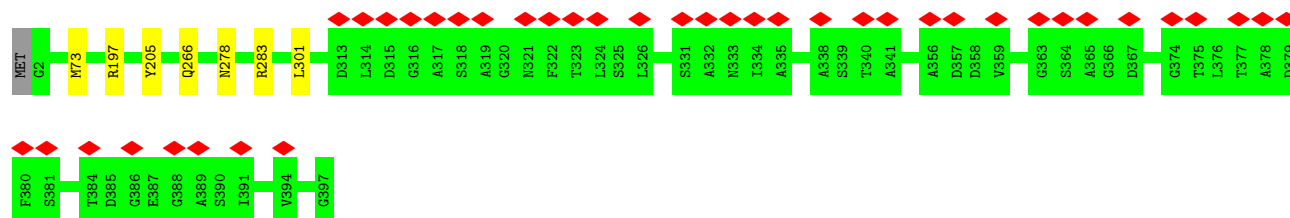
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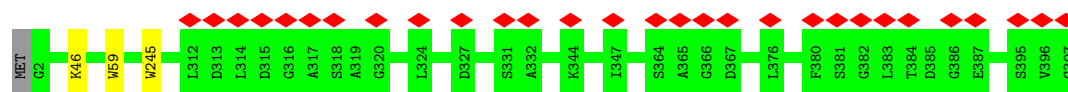


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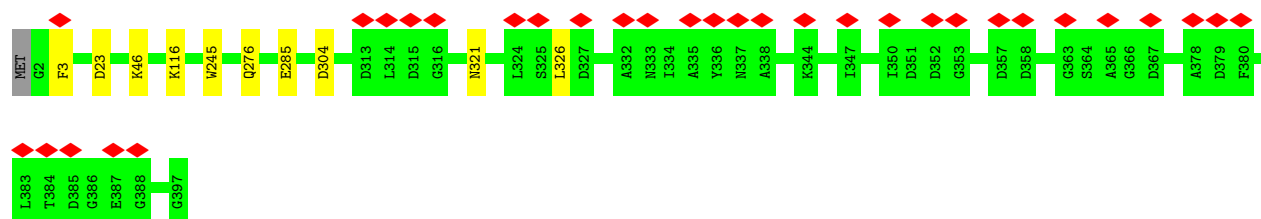


- Molecule 1: Major capsid protein

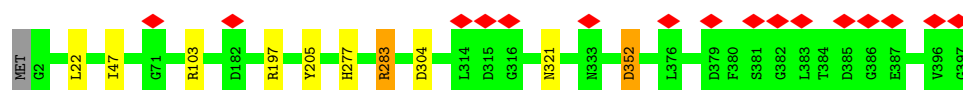




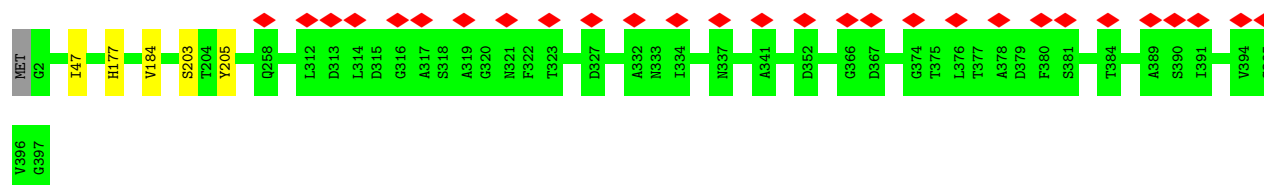
- Molecule 1: Major capsid protein



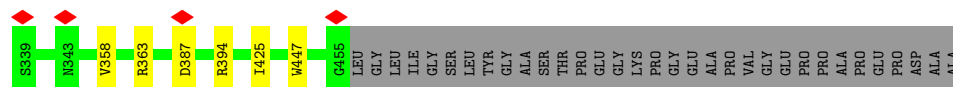
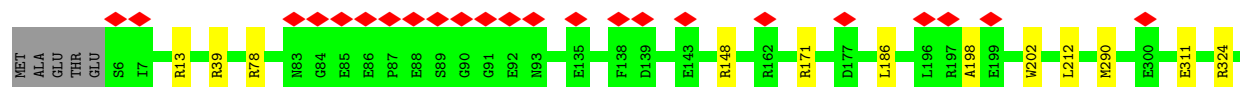
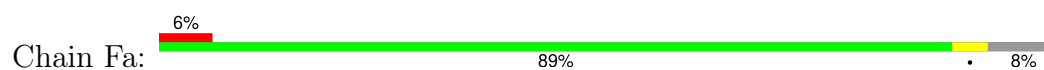
- Molecule 1: Major capsid protein



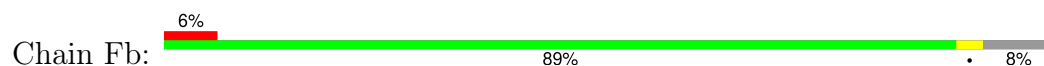
- Molecule 1: Major capsid protein

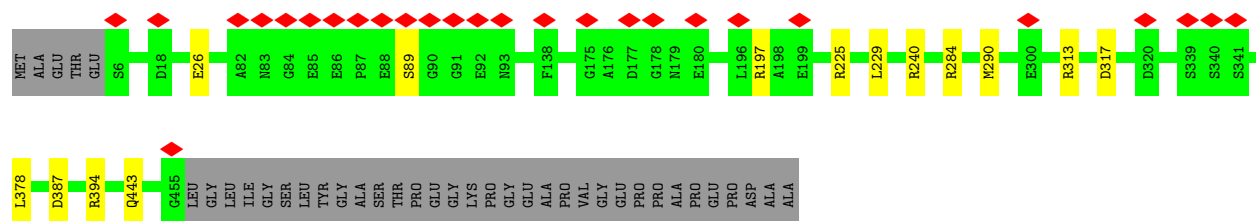


- Molecule 2: Portal protein

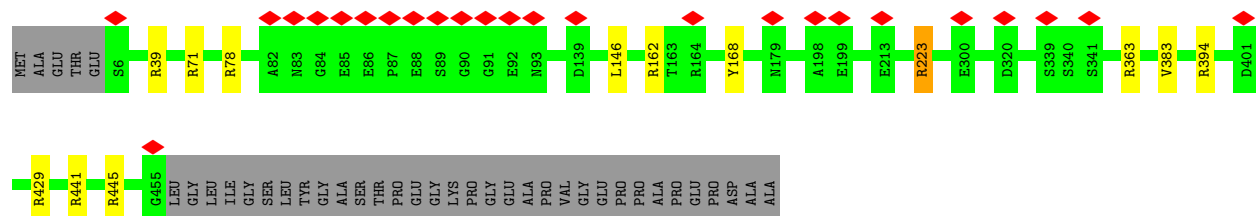
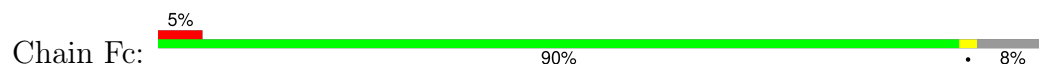


- Molecule 2: Portal protein

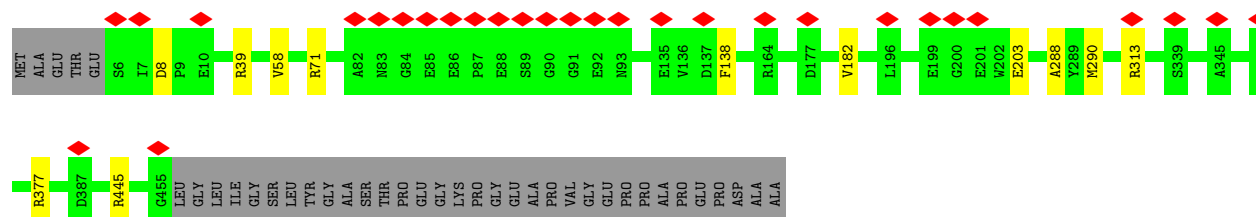




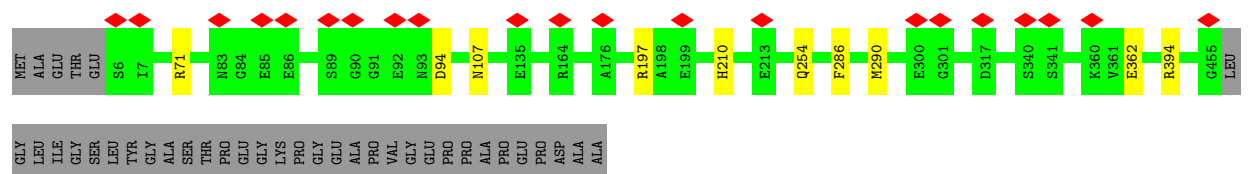
- Molecule 2: Portal protein



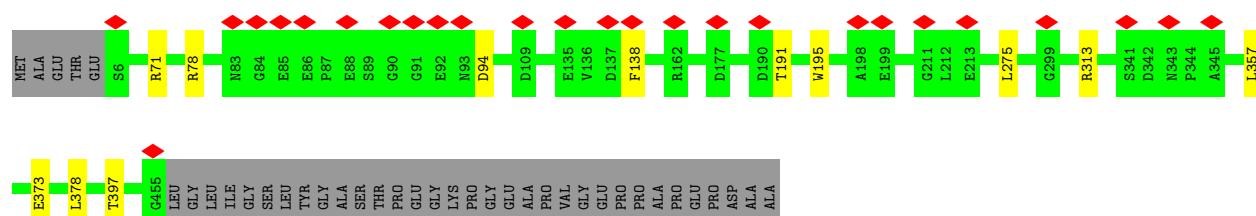
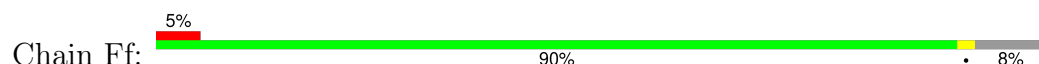
- Molecule 2: Portal protein



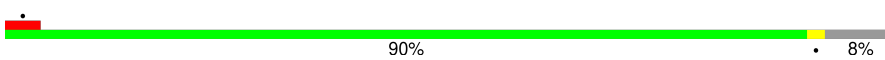
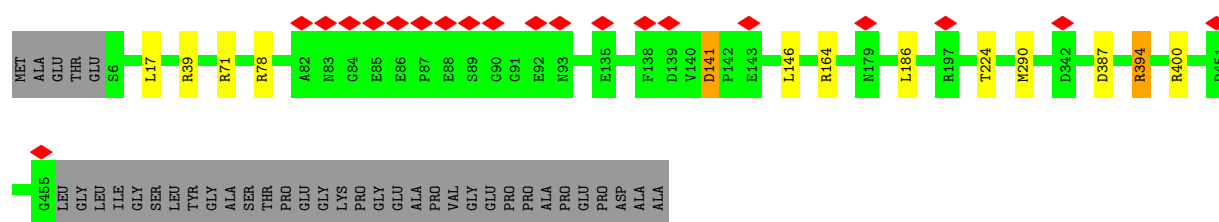
- Molecule 2: Portal protein



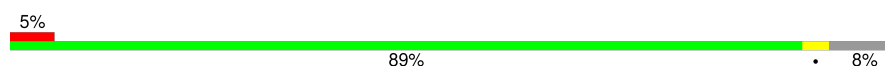
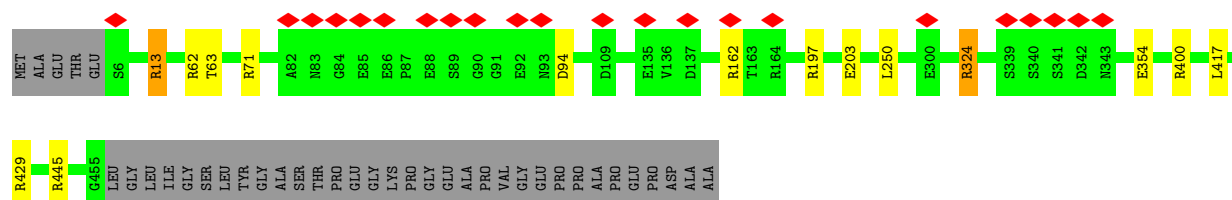
- Molecule 2: Portal protein




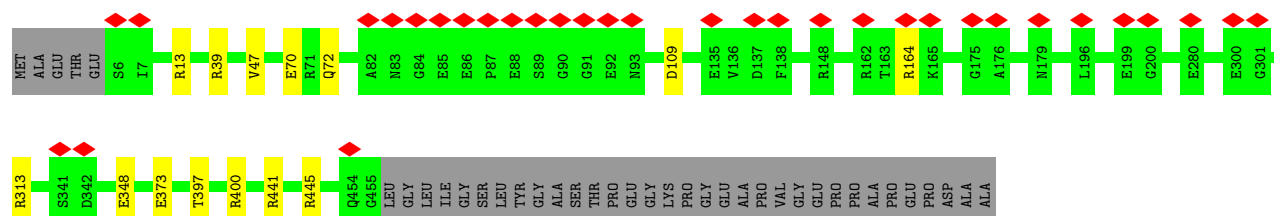
## • Molecule 2: Portal protein

Chain Fg:  90% 8%

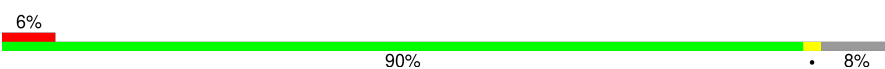
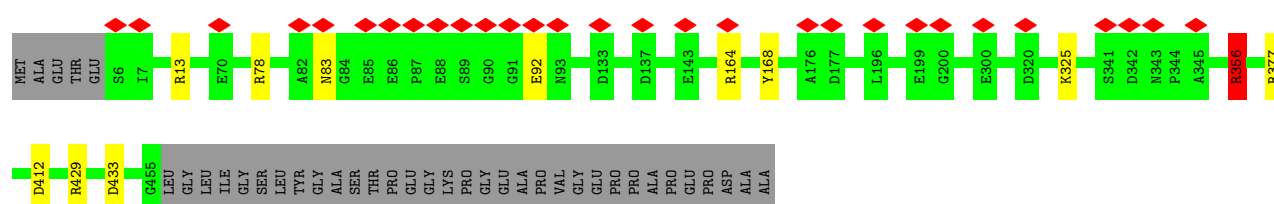
## • Molecule 2: Portal protein

Chain Fh:  89% 5% 8%

## • Molecule 2: Portal protein

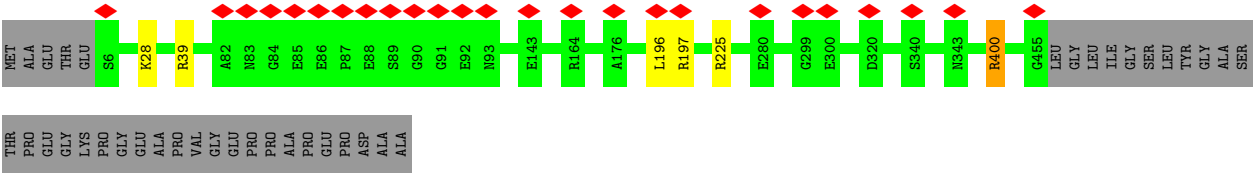
Chain Fi:  89% 7% 8%

## • Molecule 2: Portal protein

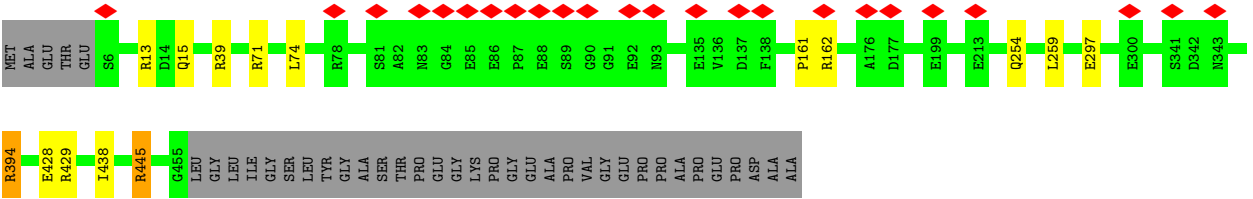
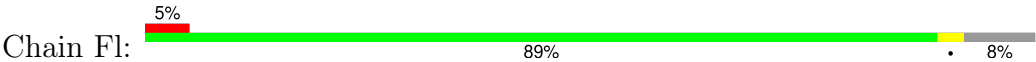
Chain Fj:  90% 6% 8%

## • Molecule 2: Portal protein

Chain Fk:  91% 5% 8%



● 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 (Å)	865.62006, 865.62006, 865.62006	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2366, 1.2366, 1.2366	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.70	0/2982	1.23	1/4070 (0.0%)
1	Ab	0.71	0/2998	1.23	2/4091 (0.0%)
1	Ac	0.70	0/2998	1.19	3/4091 (0.1%)
1	Ad	0.70	0/2998	1.22	3/4091 (0.1%)
1	Ae	0.70	0/2998	1.22	2/4091 (0.0%)
1	Af	0.70	0/2998	1.21	3/4091 (0.1%)
1	Ba	0.71	0/2982	1.25	4/4070 (0.1%)
1	Bb	0.72	0/2998	1.25	5/4091 (0.1%)
1	Bc	0.70	0/2998	1.21	3/4091 (0.1%)
1	Bd	0.71	0/2998	1.22	2/4091 (0.0%)
1	Be	0.69	0/2998	1.20	3/4091 (0.1%)
1	Bf	0.70	0/2998	1.19	3/4091 (0.1%)
1	Ca	0.71	0/2982	1.24	5/4070 (0.1%)
1	Cb	0.72	0/2998	1.23	4/4091 (0.1%)
1	Cc	0.69	0/2998	1.20	6/4091 (0.1%)
1	Cd	0.70	0/2998	1.23	3/4091 (0.1%)
1	Ce	0.69	0/2998	1.22	4/4091 (0.1%)
1	Cf	0.69	0/2998	1.22	2/4091 (0.0%)
1	Da	0.71	0/2982	1.24	4/4070 (0.1%)
1	Db	0.71	0/2998	1.24	6/4091 (0.1%)
1	Dc	0.70	0/2998	1.19	0/4091
1	Dd	0.70	0/2998	1.23	4/4091 (0.1%)
1	De	0.69	0/2998	1.22	4/4091 (0.1%)
1	Df	0.69	0/2998	1.19	2/4091 (0.0%)
1	Ea	0.72	0/2982	1.23	4/4070 (0.1%)
1	Eb	0.70	0/2998	1.22	2/4091 (0.0%)
1	Ec	0.70	0/2998	1.21	0/4091
1	Ed	0.71	0/2998	1.23	5/4091 (0.1%)
1	Ee	0.69	0/2998	1.22	5/4091 (0.1%)
1	Ef	0.70	0/2998	1.23	2/4091 (0.0%)
2	Fa	0.71	0/3606	1.23	9/4901 (0.2%)
2	Fb	0.71	0/3606	1.22	10/4901 (0.2%)
2	Fc	0.72	0/3606	1.22	7/4901 (0.1%)
2	Fd	0.72	0/3606	1.23	10/4901 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	Fe	0.72	0/3606	1.20	6/4901 (0.1%)
2	Ff	0.72	0/3606	1.23	5/4901 (0.1%)
2	Fg	0.71	0/3606	1.21	8/4901 (0.2%)
2	Fh	0.72	0/3606	1.22	8/4901 (0.2%)
2	Fi	0.72	0/3606	1.21	6/4901 (0.1%)
2	Fj	0.72	0/3606	1.22	5/4901 (0.1%)
2	Fk	0.71	0/3606	1.19	4/4901 (0.1%)
2	Fl	0.72	0/3606	1.24	10/4901 (0.2%)
All	All	0.71	0/133132	1.22	184/181437 (0.1%)

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.

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bb	244	ILE	CA-CB-CG1	7.53	123.20	110.40
2	Fa	290	MET	N-CA-C	7.00	118.56	111.07
2	Fa	13	ARG	NE-CZ-NH2	6.68	125.22	119.20
1	Ed	304	ASP	CA-CB-CG	6.50	119.10	112.60
2	Fg	141	ASP	CA-CB-CG	6.46	119.06	112.60
1	Dd	304	ASP	CA-CB-CG	6.44	119.04	112.60
1	Be	220	ARG	NE-CZ-NH2	6.43	124.99	119.20
1	Ee	352	ASP	CA-CB-CG	6.32	118.92	112.60
2	Fb	89	SER	CA-C-N	6.32	126.10	120.10
2	Fb	89	SER	C-N-CA	6.32	126.10	120.10
1	Ab	193	ASP	CA-CB-CG	6.31	118.91	112.60
2	Fd	445	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	Bc	367	ASP	CA-CB-CG	6.29	118.89	112.60
2	Fi	39	ARG	NE-CZ-NH2	6.21	124.79	119.20
2	Ff	78	ARG	NE-CZ-NH2	6.15	124.74	119.20
2	Fg	394	ARG	NE-CZ-NH2	6.10	124.69	119.20
2	Fd	203	GLU	N-CA-C	6.09	118.41	110.43
1	Cc	283	ARG	NE-CZ-NH2	6.06	124.66	119.20
1	Ba	15	ASP	CA-CB-CG	6.04	118.64	112.60
2	Fl	161	PRO	CA-C-N	6.02	128.35	120.28
2	Fl	161	PRO	C-N-CA	6.02	128.35	120.28
2	Fe	290	MET	N-CA-C	6.01	117.83	111.28
1	Db	394	VAL	N-CA-C	6.00	116.78	110.72
1	Da	105	ASN	CB-CA-C	5.96	115.43	111.20
2	Fh	94	ASP	CA-CB-CG	5.95	118.55	112.60
2	Fg	400	ARG	NE-CZ-NH2	5.90	124.51	119.20
2	Fi	13	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	Dd	283	ARG	NE-CZ-NH2	5.88	124.50	119.20
2	Ff	94	ASP	CA-CB-CG	5.88	118.48	112.60
2	Fe	94	ASP	CA-CB-CG	5.88	118.48	112.60
2	Fd	138	PHE	CA-CB-CG	5.87	119.67	113.80
2	Fa	324	ARG	NE-CZ-NH2	5.86	124.48	119.20
1	Bc	294	ASP	CA-CB-CG	5.85	118.45	112.60
2	Fb	313	ARG	NE-CZ-NH2	5.83	124.45	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Dd	254	ASP	CA-CB-CG	5.83	118.43	112.60
2	Fh	445	ARG	NE-CZ-NH2	5.80	124.42	119.20
2	Fl	297	GLU	N-CA-C	5.79	118.99	110.59
2	Fd	288	ALA	N-CA-C	5.79	120.16	113.38
1	Ef	203	SER	N-CA-C	5.79	119.81	112.87
1	De	23	ASP	CA-CB-CG	5.78	118.38	112.60
2	Fd	71	ARG	NE-CZ-NH2	5.77	124.40	119.20
1	Bd	283	ARG	NE-CZ-NH2	5.77	124.39	119.20
2	Fa	78	ARG	NE-CZ-NH2	5.77	124.39	119.20
2	Fl	71	ARG	NE-CZ-NH2	5.76	124.39	119.20
2	Fk	400	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	Ea	105	ASN	CB-CA-C	5.75	115.28	111.20
2	Fg	39	ARG	NE-CZ-NH2	5.72	124.34	119.20
2	Fl	394	ARG	NE-CZ-NH2	5.71	124.34	119.20
2	Fa	387	ASP	CA-CB-CG	5.70	118.30	112.60
1	Cc	73	MET	CA-C-N	5.69	129.33	120.68
1	Cc	73	MET	C-N-CA	5.69	129.33	120.68
1	Da	182	ASP	CA-CB-CG	5.69	118.29	112.60
2	Fj	433	ASP	CA-CB-CG	-5.68	106.92	112.60
2	Fh	71	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	Da	357	ASP	CA-CB-CG	5.65	118.25	112.60
2	Fc	71	ARG	NE-CZ-NH2	5.64	124.28	119.20
2	Fe	394	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	Ce	232	ASP	CA-CB-CG	5.63	118.23	112.60
1	Ee	321	ASN	CA-CB-CG	5.62	118.22	112.60
2	Fa	171	ARG	NE-CZ-NH2	5.62	124.26	119.20
2	Fc	445	ARG	NE-CZ-NH2	5.58	124.22	119.20
2	Fd	290	MET	N-CA-C	5.58	117.36	111.28
2	Fb	225	ARG	NE-CZ-NH2	5.55	124.19	119.20
2	Fc	223	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	De	283	ARG	NE-CZ-NH2	5.53	124.18	119.20
2	Fa	39	ARG	NE-CZ-NH2	5.53	124.18	119.20
2	Fc	78	ARG	NE-CZ-NH2	5.53	124.17	119.20
2	Fd	39	ARG	NE-CZ-NH2	5.53	124.17	119.20
2	Fg	290	MET	N-CA-C	5.52	117.30	111.28
1	Db	254	ASP	CA-CB-CG	5.51	118.11	112.60
2	Fd	313	ARG	NE-CZ-NH2	5.50	124.15	119.20
2	Fj	164	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	Ce	283	ARG	NE-CZ-NH2	5.49	124.14	119.20
2	Fb	387	ASP	CA-CB-CG	5.47	118.07	112.60
1	Ed	3	PHE	CA-CB-CG	5.46	119.26	113.80
2	Fb	394	ARG	NE-CZ-NH2	5.46	124.11	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ea	85	ASP	CA-CB-CG	5.45	118.05	112.60
2	Fl	445	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	Af	283	ARG	NE-CZ-NH2	5.45	124.10	119.20
2	Fe	107	ASN	CA-CB-CG	5.43	118.03	112.60
1	Af	16	THR	CA-C-N	5.42	128.29	120.38
1	Af	16	THR	C-N-CA	5.42	128.29	120.38
1	Ac	321	ASN	CA-CB-CG	5.41	118.01	112.60
2	Fd	377	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	De	357	ASP	CA-CB-CG	5.40	118.00	112.60
1	Db	232	ASP	CA-CB-CG	5.39	117.99	112.60
1	Ee	304	ASP	CA-CB-CG	5.39	117.99	112.60
2	Fl	429	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	Ed	23	ASP	CA-CB-CG	5.37	117.97	112.60
1	Eb	283	ARG	NE-CZ-NH2	5.37	124.03	119.20
2	Fc	39	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	Db	220	ARG	NE-CZ-NH2	5.37	124.03	119.20
2	Fb	443	GLN	OE1-CD-NE2	-5.37	117.23	122.60
1	Ca	283	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	Fk	39	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	Fe	210	HIS	CB-CG-CD2	-5.35	124.24	131.20
1	Db	197	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	Cd	394	VAL	N-CA-C	5.34	116.82	111.00
1	Be	7	HIS	CB-CG-CD2	-5.33	124.27	131.20
2	Fe	71	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	Cb	197	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	Cd	283	ARG	NE-CZ-NH2	5.32	123.98	119.20
2	Fh	162	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	Fa	394	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	Fj	412	ASP	CA-CB-CG	5.30	117.90	112.60
1	Bc	283	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	Df	197	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	Fj	78	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	Ee	283	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	Fd	8	ASP	CA-CB-CG	5.28	117.88	112.60
1	Bf	16	THR	CA-C-N	5.27	127.61	120.38
1	Bf	16	THR	C-N-CA	5.27	127.61	120.38
1	Cf	220	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	Da	197	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	Bb	193	ASP	CA-CB-CG	5.27	117.87	112.60
1	Bf	197	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	Ea	103	ARG	NE-CZ-NH2	5.25	123.93	119.20
2	Fj	356	ARG	NE-CZ-NH2	5.24	123.92	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Db	283	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	Bb	73	MET	CA-C-N	5.23	128.62	120.68
1	Bb	73	MET	C-N-CA	5.23	128.62	120.68
1	Ca	73	MET	CA-C-N	5.23	128.60	120.60
1	Ca	73	MET	C-N-CA	5.23	128.60	120.60
1	Cc	202	GLU	N-CA-C	5.23	116.93	109.14
2	Fc	429	ARG	NE-CZ-NH2	5.23	123.90	119.20
1	Cb	203	SER	N-CA-C	5.22	118.75	112.38
1	Cb	105	ASN	CB-CA-C	5.22	114.90	111.20
1	Ed	276	GLN	OE1-CD-NE2	-5.22	117.38	122.60
2	Fl	13	ARG	NE-CZ-NH2	5.22	123.89	119.20
1	Ac	283	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	Ae	220	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	Eb	197	ARG	NE-CZ-NH2	5.20	123.88	119.20
2	Fh	429	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	Ce	277	HIS	CB-CG-CD2	-5.18	124.47	131.20
2	Fa	148	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	Bb	203	SER	N-CA-C	5.17	119.08	112.87
2	Fi	400	ARG	NE-CZ-NH2	5.17	123.85	119.20
2	Fl	39	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	Ba	327	ASP	CA-CB-CG	5.15	117.75	112.60
1	Ed	321	ASN	CA-CB-CG	5.14	117.74	112.60
1	Ca	197	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	Ce	197	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	Fh	62	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	Fi	72	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	Ea	15	ASP	CA-CB-CG	5.12	117.72	112.60
2	Fb	317	ASP	CA-CB-CG	5.12	117.72	112.60
1	Ad	23	ASP	CA-CB-CG	5.12	117.72	112.60
1	Ac	303	PHE	CA-CB-CG	5.11	118.91	113.80
2	Fk	196	LEU	N-CA-C	5.10	119.78	113.50
1	Ba	42	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	De	7	HIS	CB-CG-CD2	-5.09	124.58	131.20
2	Fb	197	ARG	NE-CZ-NH2	5.08	123.78	119.20
2	Fk	197	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	Ba	367	ASP	CA-CB-CG	5.07	117.67	112.60
1	Bd	9	GLN	OE1-CD-NE2	-5.07	117.53	122.60
2	Ff	138	PHE	CA-CB-CG	5.07	118.87	113.80
2	Fg	387	ASP	CA-CB-CG	5.07	117.67	112.60
1	Be	220	ARG	CB-CA-C	5.07	115.45	109.47
2	Fb	284	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	Aa	197	ARG	NE-CZ-NH2	5.07	123.76	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Df	177	HIS	CB-CG-CD2	-5.06	124.62	131.20
2	Ff	71	ARG	NE-CZ-NH2	5.06	123.75	119.20
2	Fi	441	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	Ae	197	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	Ca	254	ASP	CA-CB-CG	5.05	117.65	112.60
1	Dd	197	ARG	NE-CZ-NH2	5.05	123.74	119.20
2	Fh	324	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	Cf	197	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	Cc	277	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	Ee	197	ARG	NE-CZ-NH2	5.04	123.74	119.20
2	Fc	441	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	Ab	42	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	Cc	254	ASP	CA-CB-CG	5.03	117.63	112.60
1	Ef	177	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	Cb	216	ARG	NE-CZ-NH2	5.03	123.73	119.20
2	Fg	164	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	Ad	208	LEU	CA-C-N	5.02	127.84	120.71
1	Ad	208	LEU	C-N-CA	5.02	127.84	120.71
1	Cd	216	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	Fi	164	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	Ff	313	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	Fg	71	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	Fh	400	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	Fl	162	ARG	NE-CZ-NH2	5.01	123.71	119.20

There are no chirality outliers.

All (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
1	Af	205	TYR	Sidechain
1	Af	84	ARG	Sidechain
1	Ba	205	TYR	Sidechain
1	Bb	205	TYR	Sidechain
1	Bb	220	ARG	Sidechain
1	Bc	205	TYR	Sidechain
1	Ca	103	ARG	Sidechain
1	Ca	205	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	Cb	205	TYR	Sidechain
1	Cc	205	TYR	Sidechain
1	Cd	205	TYR	Sidechain
1	Cf	205	TYR	Sidechain
1	Da	205	TYR	Sidechain
1	Da	21	TYR	Sidechain
1	Db	205	TYR	Sidechain
1	Db	288	TYR	Sidechain
1	Ea	205	TYR	Sidechain
1	Eb	205	TYR	Sidechain
1	Ee	205	TYR	Sidechain
1	Ef	205	TYR	Sidechain
2	Fb	240	ARG	Sidechain
2	Fc	223	ARG	Sidechain
2	Fc	363	ARG	Sidechain
2	Fc	394	ARG	Sidechain
2	Fe	197	ARG	Sidechain
2	Fg	394	ARG	Sidechain
2	Fg	78	ARG	Sidechain
2	Fh	13	ARG	Sidechain
2	Fh	324	ARG	Sidechain
2	Fi	313	ARG	Sidechain
2	Fi	445	ARG	Sidechain
2	Fj	13	ARG	Sidechain
2	Fj	377	ARG	Sidechain
2	Fj	429	ARG	Sidechain
2	Fk	225	ARG	Sidechain
2	Fk	400	ARG	Sidechain
2	Fl	394	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	2926	2859	2857	2	0
1	Ab	2941	2871	2869	1	0
1	Ac	2941	2870	2869	1	0
1	Ad	2941	2870	2869	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ae	2941	2870	2869	3	0
1	Af	2941	2870	2869	2	0
1	Ba	2926	2858	2857	0	0
1	Bb	2941	2870	2869	0	0
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	2	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	1	0
1	Ce	2941	2870	2869	0	0
1	Cf	2941	2870	2869	1	0
1	Da	2926	2859	2857	1	0
1	Db	2941	2870	2869	0	0
1	Dc	2941	2871	2869	0	0
1	Dd	2941	2871	2869	2	0
1	De	2941	2870	2869	1	0
1	Df	2941	2870	2869	0	0
1	Ea	2926	2858	2857	0	0
1	Eb	2941	2870	2869	2	0
1	Ec	2941	2870	2869	2	0
1	Ed	2941	2870	2869	2	0
1	Ee	2941	2871	2869	0	0
1	Ef	2941	2871	2869	0	0
2	Fa	3526	3425	3424	3	0
2	Fb	3526	3425	3424	2	0
2	Fc	3526	3425	3424	1	0
2	Fd	3526	3425	3424	0	0
2	Fe	3526	3426	3424	0	0
2	Ff	3526	3425	3424	1	0
2	Fg	3526	3425	3424	0	0
2	Fh	3526	3425	3424	0	0
2	Fi	3526	3425	3424	1	0
2	Fj	3526	3425	3424	1	0
2	Fk	3526	3425	3424	0	0
2	Fl	3526	3425	3424	3	0
All	All	130467	127151	127098	30	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.

All (30) 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)
1:Bf:46:LYS:HE2	1:Bf:245:TRP:CH2	2.45	0.50
2:Fa:198:ALA:HB1	2:Fa:202:TRP:CZ3	2.47	0.50
1:Dd:74:LYS:HE3	1:Eb:278:ASN:HD21	1.76	0.50
1:Bf:39:ILE:HD11	1:Bf:223:ILE:CG2	2.43	0.49
1:Ad:59:TRP:CG	1:Ae:116:LYS:HE2	2.47	0.48
1:Aa:73:MET:HA	1:Aa:73:MET:HE2	1.98	0.46
1:Ed:46:LYS:HE2	1:Ed:245:TRP:CH2	2.50	0.46
1:Ec:59:TRP:CG	1:Ed:116:LYS:HE3	2.51	0.46
2:Fl:438:ILE:H	2:Fl:438:ILE:HD12	1.83	0.44
1:Af:17:MET:HE3	1:Af:18:PHE:CZ	2.53	0.44
1:Da:208:LEU:HD23	1:Da:209:THR:H	1.83	0.43
1:Dd:43:VAL:HG12	1:Dd:223:ILE:HD13	2.01	0.43
1:Ad:59:TRP:CD2	1:Ae:116:LYS:HE2	2.53	0.43
2:Fc:162:ARG:HD2	2:Fc:162:ARG:H	1.84	0.43
1:Eb:266:GLN:H	1:Eb:266:GLN:CD	2.28	0.42
2:Fa:212:LEU:HD12	2:Fa:212:LEU:H	1.85	0.42
2:Fb:229:LEU:HD23	2:Fb:229:LEU:H	1.85	0.42
2:Fi:373:GLU:HG3	2:Fi:397:THR:HG23	2.01	0.42
1:Cd:102:VAL:HG23	1:Cd:110:LEU:CD1	2.50	0.42
1:Ec:46:LYS:HE2	1:Ec:245:TRP:CH2	2.56	0.41
2:Ff:373:GLU:HG3	2:Ff:397:THR:HG23	2.02	0.41
1:De:212:PHE:HA	1:De:224:LEU:HD11	2.02	0.41
2:Fj:356:ARG:HG3	2:Fj:356:ARG:HH21	1.86	0.41
1:Ab:47:ILE:HD12	1:Ac:30:TYR:CE1	2.56	0.41
2:Fa:447:TRP:CE2	2:Fl:428:GLU:HG2	2.56	0.41
2:Fb:290:MET:HE3	2:Fl:259:LEU:HD12	2.03	0.41
1:Aa:110:LEU:HD13	1:Aa:110:LEU:C	2.47	0.40
1:Ad:179:LEU:HD13	1:Ad:240:PHE:CZ	2.56	0.40
1:Ae:67:TRP:CE2	1:Af:91:ILE:HD11	2.57	0.40
1:Cf:344:LYS:HA	1:Cf:347:ILE:HG22	2.03	0.40

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	307 (98%)	7 (2%)	47	70
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%)	314 (100%)	1 (0%)	91	96
1	Ae	315/316 (100%)	311 (99%)	4 (1%)	65	81
1	Af	315/316 (100%)	314 (100%)	1 (0%)	91	96
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bd	315/316 (100%)	312 (99%)	3 (1%)	73	84
1	Be	315/316 (100%)	312 (99%)	3 (1%)	73	84
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%)	314 (100%)	1 (0%)	91	96
1	Cc	315/316 (100%)	314 (100%)	1 (0%)	91	96
1	Cd	315/316 (100%)	314 (100%)	1 (0%)	91	96
1	Ce	315/316 (100%)	312 (99%)	3 (1%)	73	84
1	Cf	315/316 (100%)	315 (100%)	0	100	100
1	Da	314/316 (99%)	310 (99%)	4 (1%)	65	81
1	Db	315/316 (100%)	312 (99%)	3 (1%)	73	84
1	Dc	315/316 (100%)	312 (99%)	3 (1%)	73	84
1	Dd	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	De	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	Df	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	Ea	314/316 (99%)	313 (100%)	1 (0%)	91	96
1	Eb	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	Ec	315/316 (100%)	315 (100%)	0	100	100
1	Ed	315/316 (100%)	313 (99%)	2 (1%)	84	91
1	Ee	315/316 (100%)	309 (98%)	6 (2%)	52	73
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%)	362 (100%)	2 (0%)	86	93
2	Fc	364/390 (93%)	361 (99%)	3 (1%)	79	88
2	Fd	364/390 (93%)	362 (100%)	2 (0%)	86	93
2	Fe	364/390 (93%)	361 (99%)	3 (1%)	79	88
2	Ff	364/390 (93%)	359 (99%)	5 (1%)	62	79
2	Fg	364/390 (93%)	359 (99%)	5 (1%)	62	79
2	Fh	364/390 (93%)	357 (98%)	7 (2%)	52	73
2	Fi	364/390 (93%)	360 (99%)	4 (1%)	70	83
2	Fj	364/390 (93%)	359 (99%)	5 (1%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Fk	364/390 (93%)	363 (100%)	1 (0%)	91	96
2	F1	364/390 (93%)	360 (99%)	4 (1%)	70	83
All	All	13813/14160 (98%)	13696 (99%)	117 (1%)	77	88

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	7	HIS
1	Aa	73	MET
1	Aa	83	LYS
1	Aa	90	LYS
1	Aa	184	VAL
1	Aa	202	GLU
1	Aa	312	LEU
1	Ab	243	ILE
1	Ab	369	THR
1	Ac	101	THR
1	Ad	100	GLU
1	Ae	144	ASP
1	Ae	179	LEU
1	Ae	312	LEU
1	Ae	376	LEU
1	Af	45	GLN
1	Ba	112	THR
1	Ba	153	SER
1	Ba	312	LEU
1	Ba	376	LEU
1	Bb	81	MET
1	Bb	152	ILE
1	Bb	184	VAL
1	Bb	337	ASN
1	Bb	376	LEU
1	Bc	376	LEU
1	Bc	385	ASP
1	Bd	81	MET
1	Bd	100	GLU
1	Bd	143	LEU
1	Be	100	GLU
1	Be	375	THR
1	Be	376	LEU
1	Bf	9	GLN

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Mol	Chain	Res	Type
1	Bf	209	THR
1	Ca	360	THR
1	Cb	22	LEU
1	Cc	347	ILE
1	Cd	313	ASP
1	Ce	176	THR
1	Ce	177	HIS
1	Ce	230	GLU
1	Da	206	GLU
1	Da	208	LEU
1	Da	294	ASP
1	Da	383	LEU
1	Db	60	THR
1	Db	360	THR
1	Db	375	THR
1	Dc	63	VAL
1	Dc	133	THR
1	Dc	304	ASP
1	Dd	201	VAL
1	Dd	369	THR
1	De	153	SER
1	De	376	LEU
1	Df	294	ASP
1	Df	369	THR
1	Ea	23	ASP
1	Eb	73	MET
1	Eb	301	LEU
1	Ed	285	GLU
1	Ed	326	LEU
1	Ee	22	LEU
1	Ee	47	ILE
1	Ee	103	ARG
1	Ee	277	HIS
1	Ee	283	ARG
1	Ee	352	ASP
1	Ef	47	ILE
1	Ef	184	VAL
2	Fa	186	LEU
2	Fa	311	GLU
2	Fa	358	VAL
2	Fa	363	ARG
2	Fa	425	ILE

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Mol	Chain	Res	Type
2	Fb	26	GLU
2	Fb	378	LEU
2	Fc	146	LEU
2	Fc	168	TYR
2	Fc	383	VAL
2	Fd	58	VAL
2	Fd	182	VAL
2	Fe	254	GLN
2	Fe	286	PHE
2	Fe	362	GLU
2	Ff	191	THR
2	Ff	195	TRP
2	Ff	275	LEU
2	Ff	357	LEU
2	Ff	378	LEU
2	Fg	17	LEU
2	Fg	141	ASP
2	Fg	146	LEU
2	Fg	186	LEU
2	Fg	224	THR
2	Fh	13	ARG
2	Fh	63	THR
2	Fh	197	ARG
2	Fh	203	GLU
2	Fh	250	LEU
2	Fh	354	GLU
2	Fh	417	LEU
2	Fi	47	VAL
2	Fi	70	GLU
2	Fi	109	ASP
2	Fi	348	GLU
2	Fj	83	ASN
2	Fj	92	GLU
2	Fj	168	TYR
2	Fj	325	LYS
2	Fj	356	ARG
2	Fk	28	LYS
2	Fl	15	GLN
2	Fl	74	LEU
2	Fl	254	GLN
2	Fl	445	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180)

such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	26	GLN
1	Aa	105	ASN
1	Aa	266	GLN
1	Aa	296	ASN
1	Ab	105	ASN
1	Ab	108	ASN
1	Ab	140	GLN
1	Ab	145	GLN
1	Ac	66	GLN
1	Ac	105	ASN
1	Ac	108	ASN
1	Ac	131	HIS
1	Ac	145	GLN
1	Ad	105	ASN
1	Ad	108	ASN
1	Ad	127	ASN
1	Ad	134	ASN
1	Ad	227	HIS
1	Ad	296	ASN
1	Ad	321	ASN
1	Ad	333	ASN
1	Ae	66	GLN
1	Ae	266	GLN
1	Af	12	GLN
1	Ba	140	GLN
1	Ba	321	ASN
1	Bb	9	GLN
1	Bb	12	GLN
1	Bb	145	GLN
1	Bb	177	HIS
1	Bb	293	ASN
1	Bb	337	ASN
1	Bc	105	ASN
1	Bc	108	ASN
1	Bc	127	ASN
1	Bd	12	GLN
1	Bd	145	GLN
1	Bd	147	ASN
1	Be	105	ASN
1	Be	108	ASN
1	Be	140	GLN
1	Be	145	GLN

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Mol	Chain	Res	Type
1	Be	321	ASN
1	Be	333	ASN
1	Bf	12	GLN
1	Bf	58	HIS
1	Bf	145	GLN
1	Bf	242	GLN
1	Bf	293	ASN
1	Bf	333	ASN
1	Ca	87	HIS
1	Ca	127	ASN
1	Ca	140	GLN
1	Ca	147	ASN
1	Ca	177	HIS
1	Ca	195	ASN
1	Ca	278	ASN
1	Cb	105	ASN
1	Cb	321	ASN
1	Cb	333	ASN
1	Cc	227	HIS
1	Cc	293	ASN
1	Cd	321	ASN
1	Cd	333	ASN
1	Ce	145	GLN
1	Ce	158	GLN
1	Ce	266	GLN
1	Ce	277	HIS
1	Cf	58	HIS
1	Cf	127	ASN
1	Cf	145	GLN
1	Cf	195	ASN
1	Cf	266	GLN
1	Cf	293	ASN
1	Cf	296	ASN
1	Cf	333	ASN
1	Da	127	ASN
1	Da	131	HIS
1	Da	276	GLN
1	Da	293	ASN
1	Db	12	GLN
1	Db	45	GLN
1	Db	105	ASN
1	Db	108	ASN

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Mol	Chain	Res	Type
1	Db	195	ASN
1	Db	227	HIS
1	Db	293	ASN
1	Dc	12	GLN
1	Dc	127	ASN
1	Dc	131	HIS
1	Dc	321	ASN
1	Dd	9	GLN
1	Dd	12	GLN
1	Dd	105	ASN
1	Dd	108	ASN
1	Dd	147	ASN
1	Dd	150	GLN
1	Dd	242	GLN
1	Dd	266	GLN
1	Dd	293	ASN
1	Dd	296	ASN
1	De	87	HIS
1	De	105	ASN
1	De	108	ASN
1	De	145	GLN
1	De	147	ASN
1	De	266	GLN
1	Df	7	HIS
1	Df	158	GLN
1	Df	258	GLN
1	Ea	87	HIS
1	Ea	177	HIS
1	Ea	277	HIS
1	Ea	293	ASN
1	Eb	7	HIS
1	Eb	12	GLN
1	Eb	145	GLN
1	Eb	195	ASN
1	Eb	242	GLN
1	Eb	258	GLN
1	Eb	293	ASN
1	Eb	333	ASN
1	Ec	105	ASN
1	Ec	108	ASN
1	Ec	134	ASN
1	Ec	147	ASN

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Mol	Chain	Res	Type
1	Ec	195	ASN
1	Ec	293	ASN
1	Ed	7	HIS
1	Ed	195	ASN
1	Ed	333	ASN
1	Ee	9	GLN
1	Ee	140	GLN
1	Ee	177	HIS
1	Ef	247	GLN
1	Ef	270	ASN
1	Ef	293	ASN
1	Ef	321	ASN
1	Ef	333	ASN
2	Fa	72	GLN
2	Fa	252	ASN
2	Fa	306	GLN
2	Fa	335	GLN
2	Fb	72	GLN
2	Fb	254	GLN
2	Fc	72	GLN
2	Fc	252	ASN
2	Fc	254	GLN
2	Fc	452	GLN
2	Fd	72	GLN
2	Fd	107	ASN
2	Fd	454	GLN
2	Fe	104	GLN
2	Fe	107	ASN
2	Fe	446	GLN
2	Ff	252	ASN
2	Ff	420	ASN
2	Fg	72	GLN
2	Fg	179	ASN
2	Fg	374	GLN
2	Fg	443	GLN
2	Fh	24	GLN
2	Fh	254	GLN
2	Fh	452	GLN
2	Fi	72	GLN
2	Fi	343	ASN
2	Fi	420	ASN
2	Fi	446	GLN

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Mol	Chain	Res	Type
2	Fi	450	GLN
2	Fi	454	GLN
2	Fj	72	GLN
2	Fj	365	ASN
2	Fk	57	HIS
2	Fk	72	GLN
2	Fk	179	ASN
2	Fk	306	GLN
2	Fk	365	ASN
2	Fk	420	ASN
2	Fk	454	GLN
2	Fl	343	ASN

### 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.

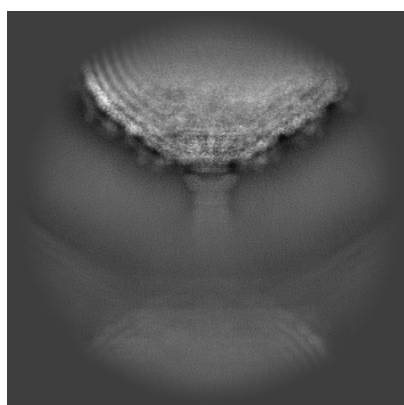
## 6 Map visualisation [i](#)

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.

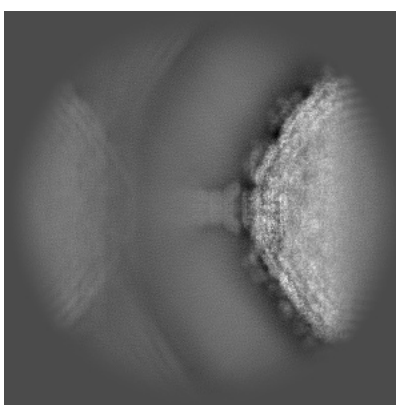
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

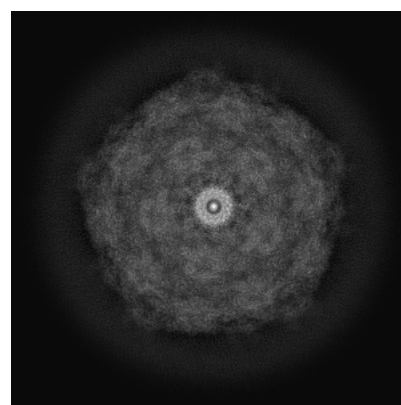
#### 6.1.1 Primary map



X



Y

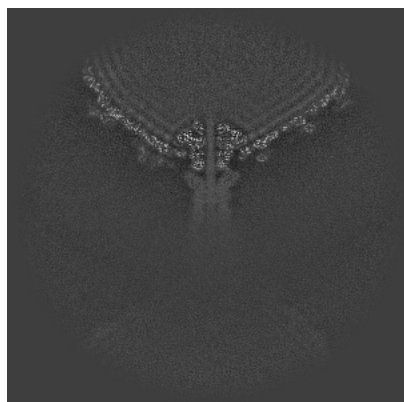


Z

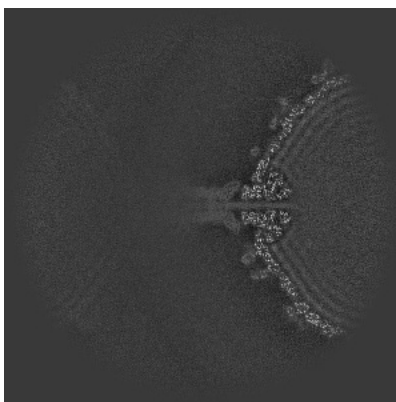
The images above show the map projected in three orthogonal directions.

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

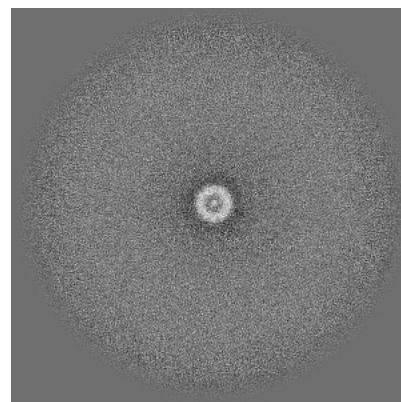
#### 6.2.1 Primary map



X Index: 350



Y Index: 350



Z Index: 350

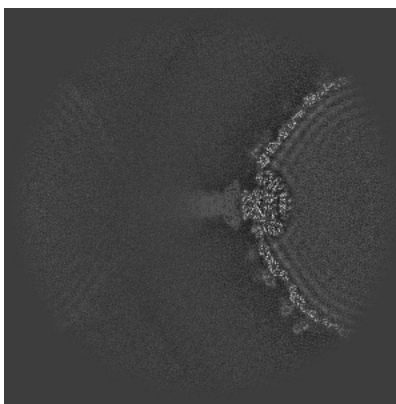
The images above show central slices of the map in three orthogonal directions.

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

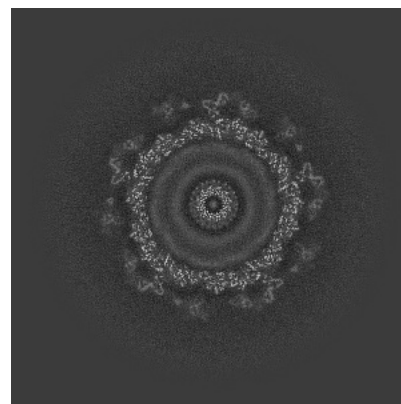
### 6.3.1 Primary map



X Index: 373



Y Index: 333

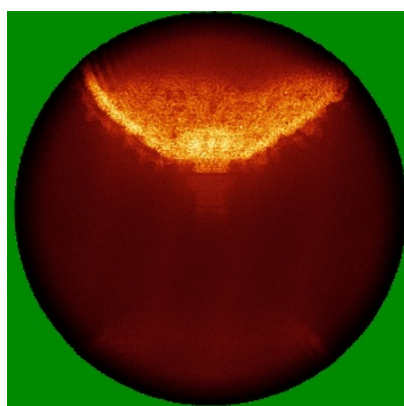


Z Index: 491

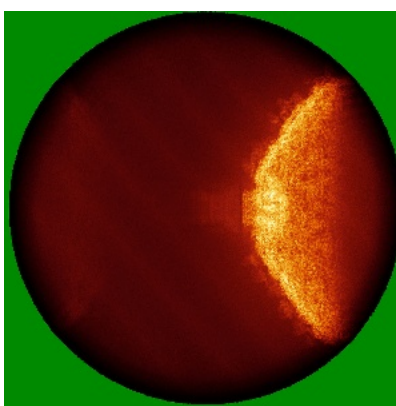
The images above show the largest variance slices of the map in three orthogonal directions.

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

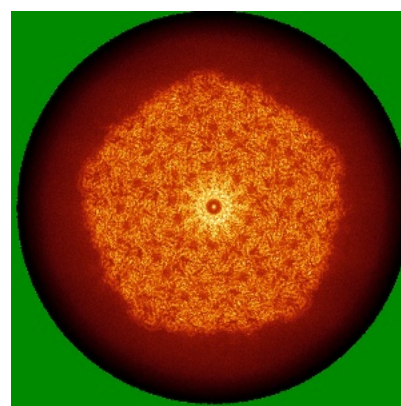
### 6.4.1 Primary map



X



Y

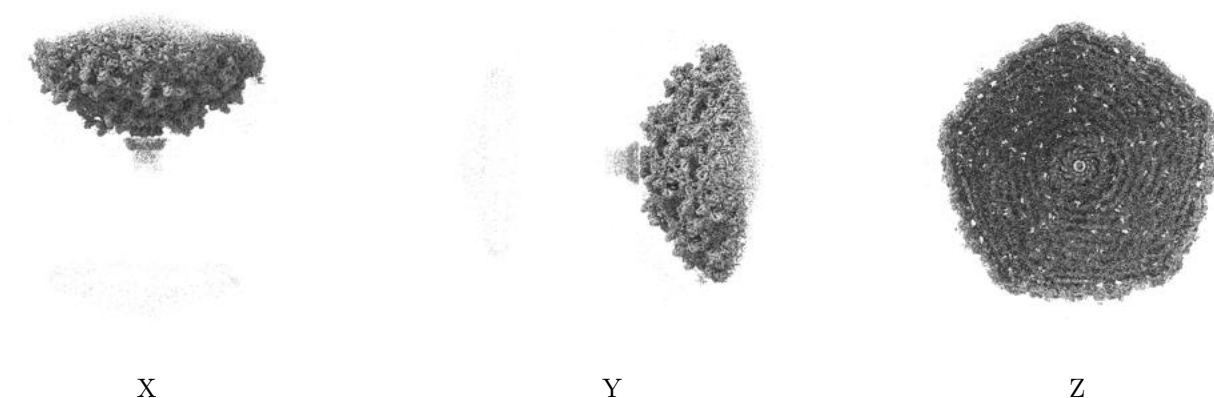


Z

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.

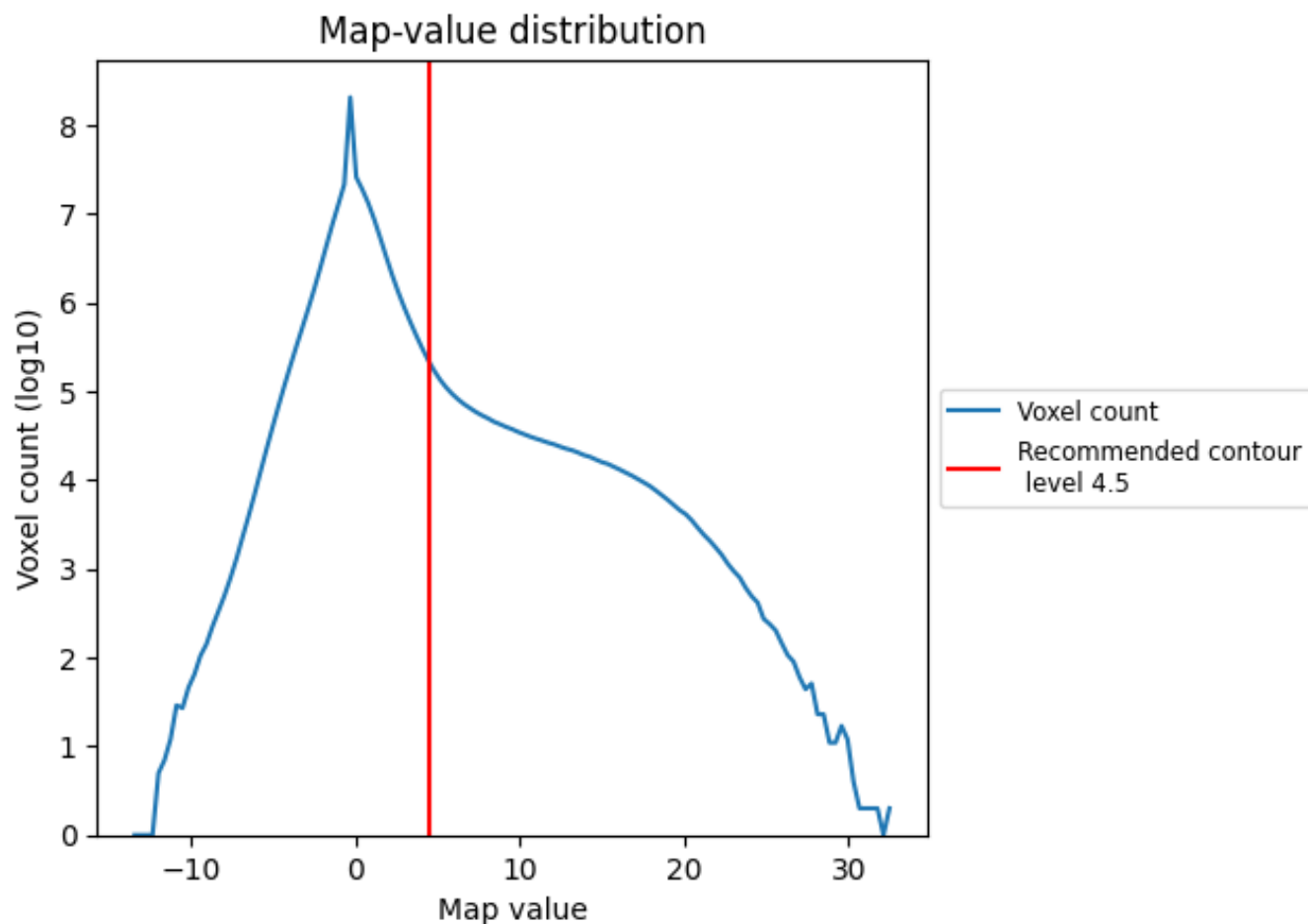
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

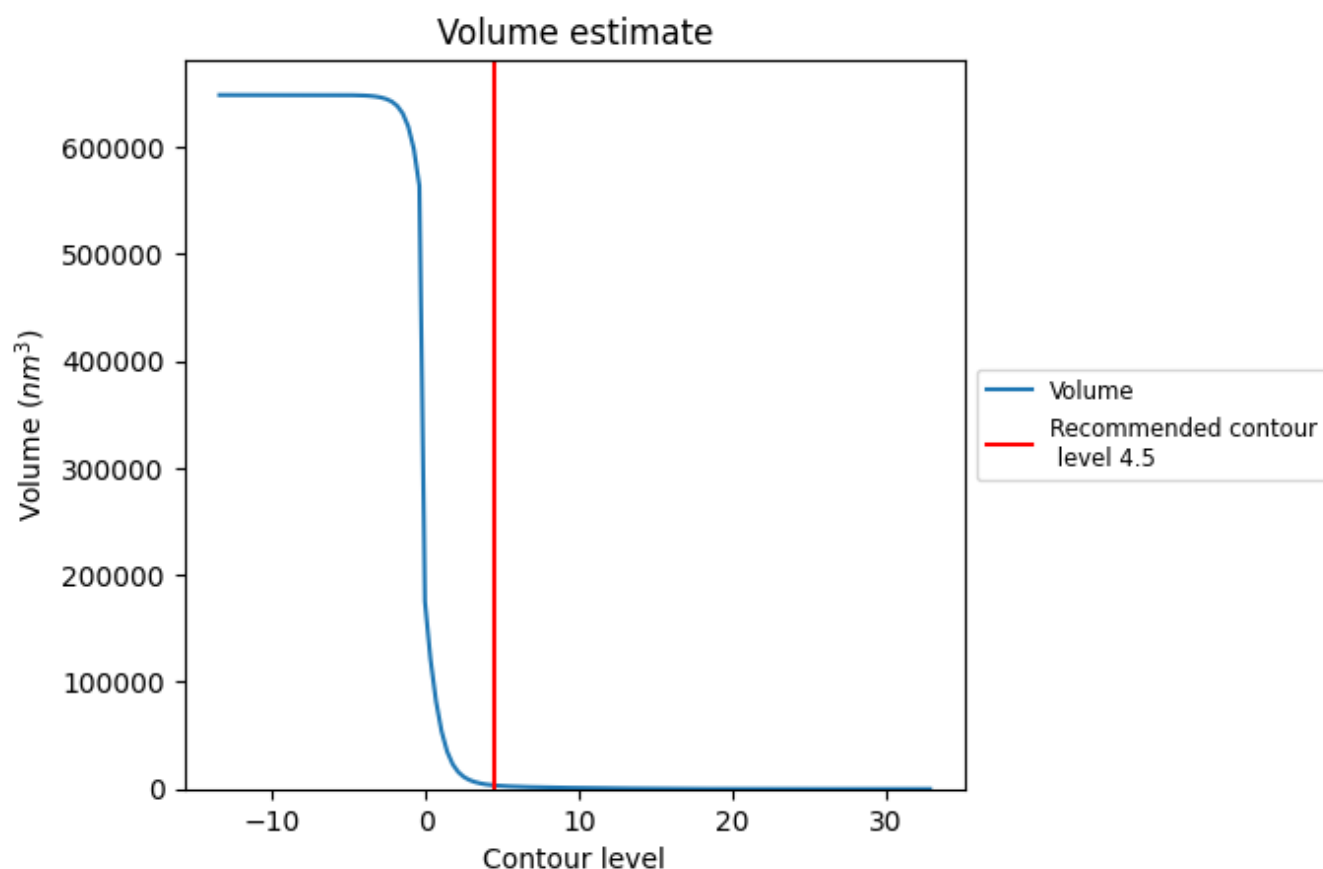
This section contains the results of statistical analysis of the map.

### 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.

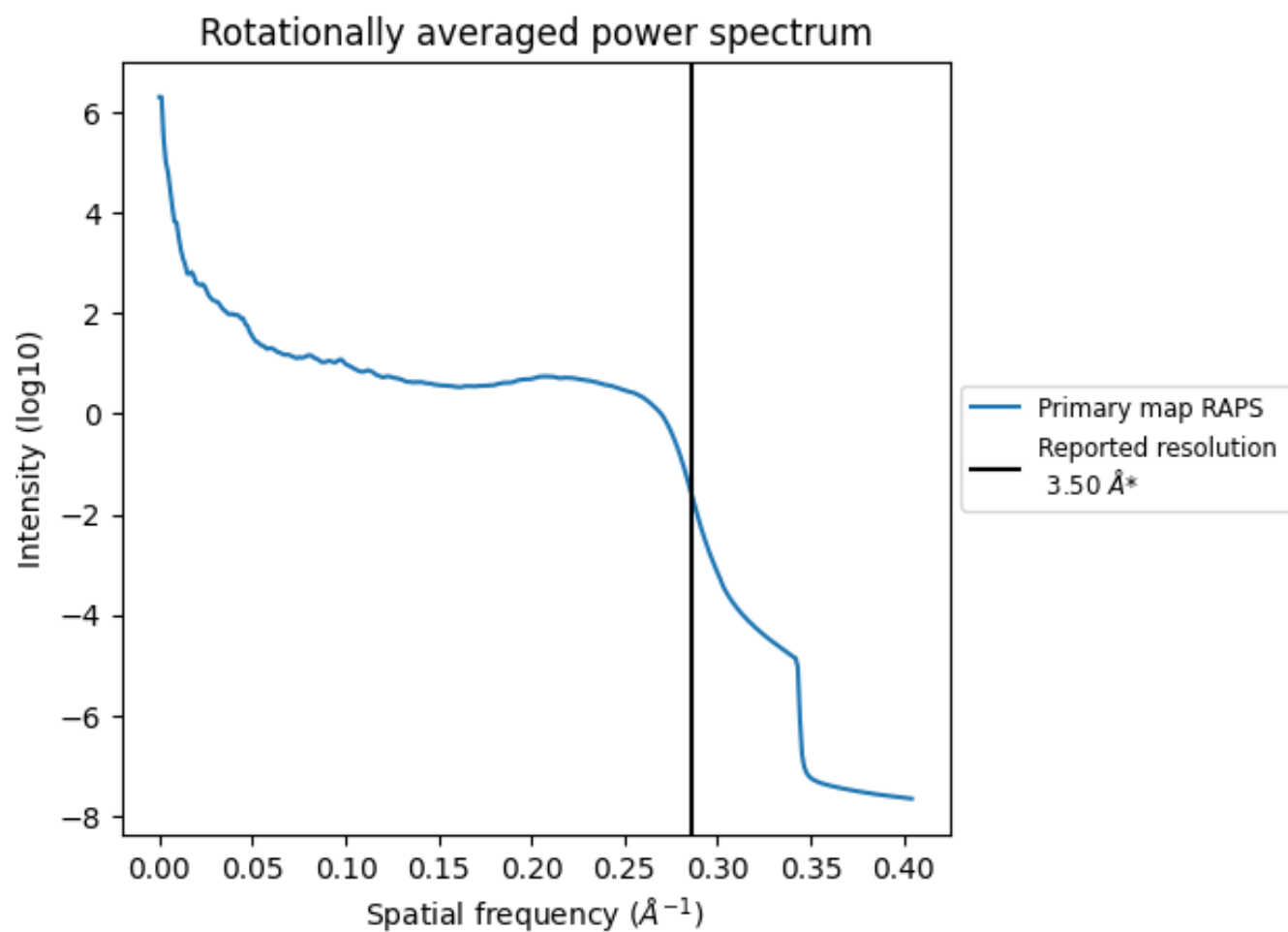
## 7.2 Volume estimate [i](#)



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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

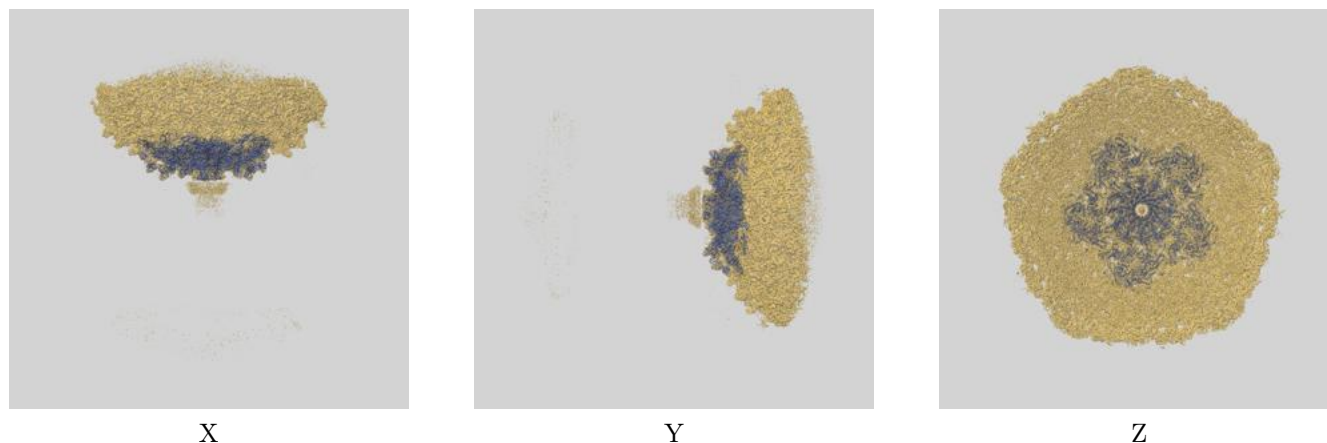
## 8 Fourier-Shell correlation ⓘ

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

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

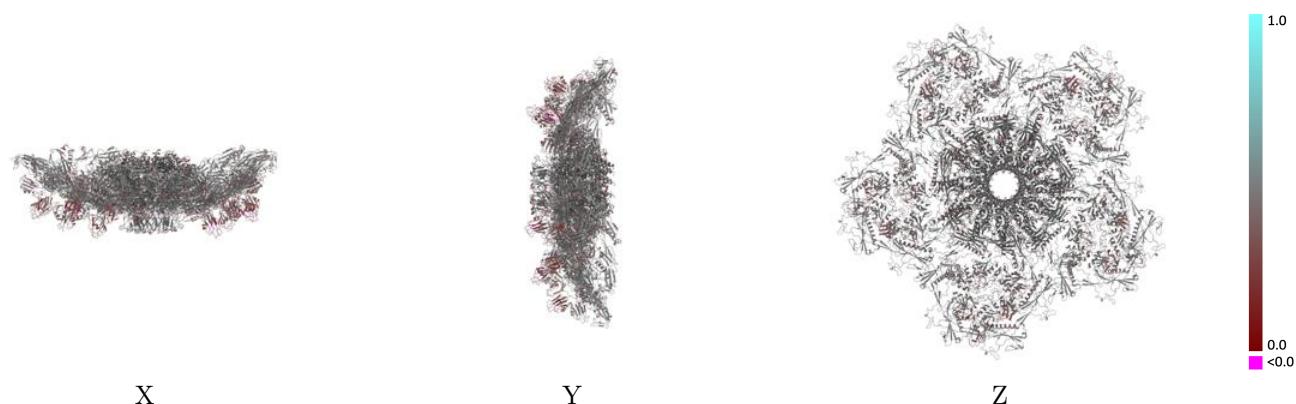
This section contains information regarding the fit between EMDB map EMD-46681 and PDB model 9D9W. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

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



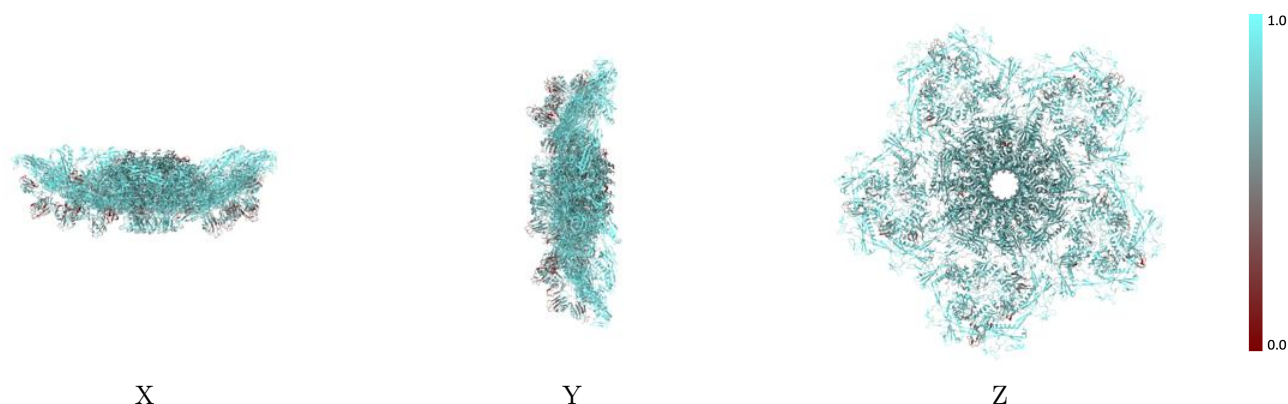
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



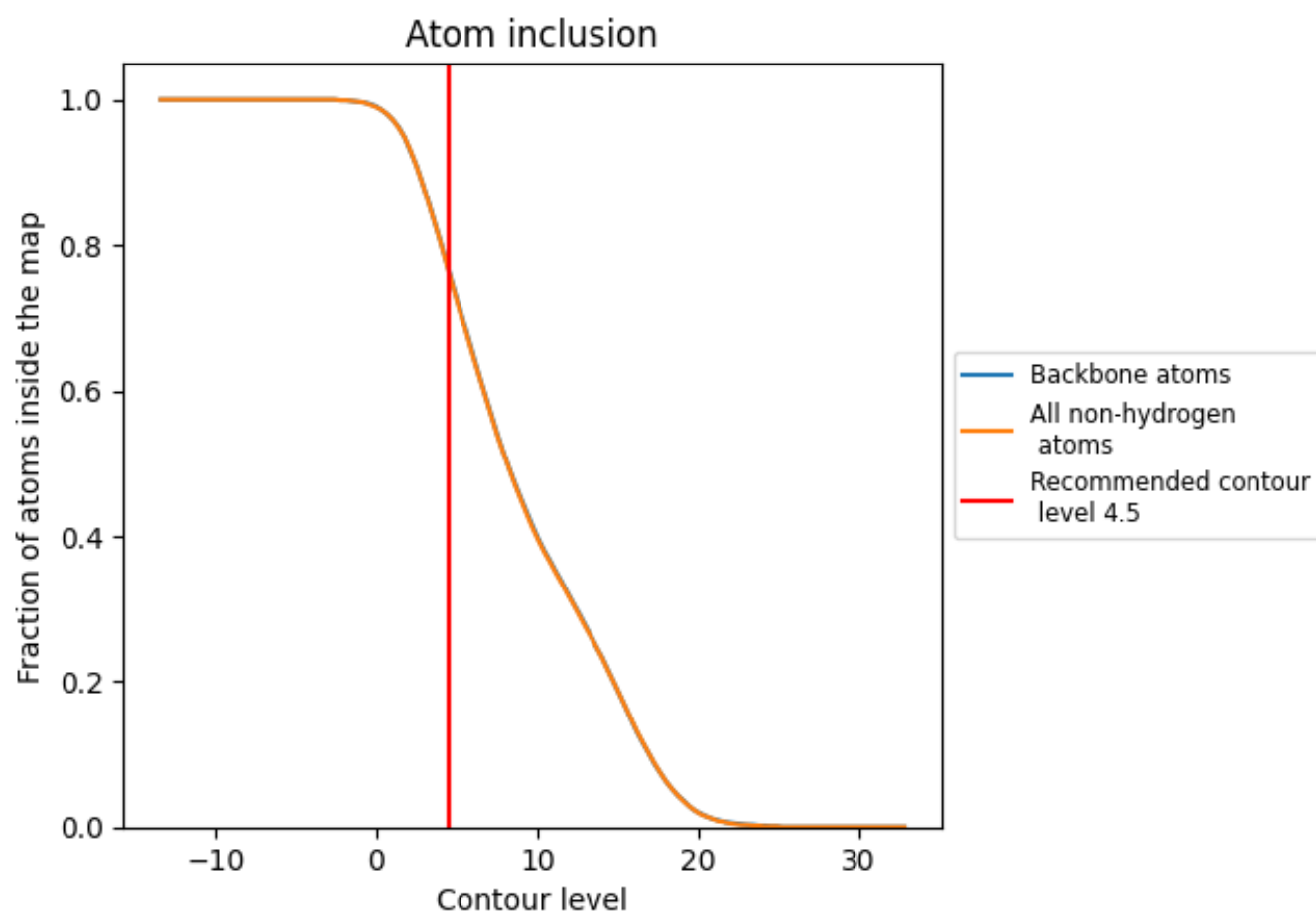
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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