



## Full wwPDB EM Validation Report ⓘ

Jun 24, 2025 – 09:23 PM JST

PDB ID : 6LQJ / pdb\_00006lqj  
EMDB ID : EMD-0947  
Title : Low resolution architecture of curli complex  
Authors : Zhang, M.; Shi, H.; Huang, Y.  
Deposited on : 2020-01-13  
Resolution : 3.24 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) : 2.44

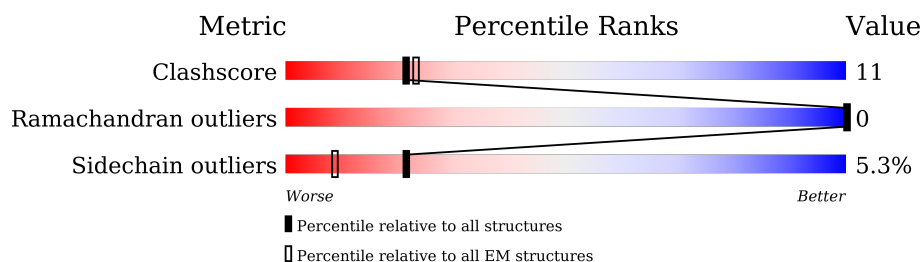
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.24 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	A	285	47% 25% • 28%
1	B	285	47% 25% • 28%
1	C	285	48% 24% • 28%
1	D	285	48% 24% • 28%
1	E	285	47% 25% 28%
1	F	285	46% 25% • 28%
1	G	285	48% 24% • 28%
1	H	285	45% 26% • 28%

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Mol	Chain	Length	Quality of chain
1	I	285	<div><div></div><div>46%25%28%</div></div>
2	a	144	<div><div></div><div>22%6%72%</div></div>
2	b	144	<div><div></div><div>22%6%72%</div></div>
2	c	144	<div><div></div><div>19%8%72%</div></div>
2	d	144	<div><div></div><div>20%7%72%</div></div>
2	e	144	<div><div></div><div>23%.72%</div></div>
2	f	144	<div><div></div><div>20%7%72%</div></div>
2	g	144	<div><div></div><div>19%8%72%</div></div>
2	h	144	<div><div></div><div>23%.72%</div></div>
2	i	144	<div><div></div><div>19%8%72%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17100 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Curli production assembly/transport component CsgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	206	Total	C	N	O	S	0	0
			1589	1008	270	306	5		
1	B	206	Total	C	N	O	S	0	0
			1589	1008	270	306	5		
1	C	206	Total	C	N	O	S	0	0
			1589	1008	270	306	5		
1	D	206	Total	C	N	O	S	0	0
			1589	1008	270	306	5		
1	E	206	Total	C	N	O	S	0	0
			1589	1008	270	306	5		
1	F	206	Total	C	N	O	S	0	0
			1589	1008	270	306	5		
1	G	206	Total	C	N	O	S	0	0
			1589	1008	270	306	5		
1	H	206	Total	C	N	O	S	0	0
			1589	1008	270	306	5		
1	I	206	Total	C	N	O	S	0	0
			1589	1008	270	306	5		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	TRP	-	expression tag	UNP P0AEA2
A	279	SER	-	expression tag	UNP P0AEA2
A	280	HIS	-	expression tag	UNP P0AEA2
A	281	PRO	-	expression tag	UNP P0AEA2
A	282	GLN	-	expression tag	UNP P0AEA2
A	283	PHE	-	expression tag	UNP P0AEA2
A	284	GLU	-	expression tag	UNP P0AEA2
A	285	LYS	-	expression tag	UNP P0AEA2
B	278	TRP	-	expression tag	UNP P0AEA2
B	279	SER	-	expression tag	UNP P0AEA2
B	280	HIS	-	expression tag	UNP P0AEA2
B	281	PRO	-	expression tag	UNP P0AEA2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	282	GLN	-	expression tag	UNP P0AEA2
B	283	PHE	-	expression tag	UNP P0AEA2
B	284	GLU	-	expression tag	UNP P0AEA2
B	285	LYS	-	expression tag	UNP P0AEA2
C	278	TRP	-	expression tag	UNP P0AEA2
C	279	SER	-	expression tag	UNP P0AEA2
C	280	HIS	-	expression tag	UNP P0AEA2
C	281	PRO	-	expression tag	UNP P0AEA2
C	282	GLN	-	expression tag	UNP P0AEA2
C	283	PHE	-	expression tag	UNP P0AEA2
C	284	GLU	-	expression tag	UNP P0AEA2
C	285	LYS	-	expression tag	UNP P0AEA2
D	278	TRP	-	expression tag	UNP P0AEA2
D	279	SER	-	expression tag	UNP P0AEA2
D	280	HIS	-	expression tag	UNP P0AEA2
D	281	PRO	-	expression tag	UNP P0AEA2
D	282	GLN	-	expression tag	UNP P0AEA2
D	283	PHE	-	expression tag	UNP P0AEA2
D	284	GLU	-	expression tag	UNP P0AEA2
D	285	LYS	-	expression tag	UNP P0AEA2
E	278	TRP	-	expression tag	UNP P0AEA2
E	279	SER	-	expression tag	UNP P0AEA2
E	280	HIS	-	expression tag	UNP P0AEA2
E	281	PRO	-	expression tag	UNP P0AEA2
E	282	GLN	-	expression tag	UNP P0AEA2
E	283	PHE	-	expression tag	UNP P0AEA2
E	284	GLU	-	expression tag	UNP P0AEA2
E	285	LYS	-	expression tag	UNP P0AEA2
F	278	TRP	-	expression tag	UNP P0AEA2
F	279	SER	-	expression tag	UNP P0AEA2
F	280	HIS	-	expression tag	UNP P0AEA2
F	281	PRO	-	expression tag	UNP P0AEA2
F	282	GLN	-	expression tag	UNP P0AEA2
F	283	PHE	-	expression tag	UNP P0AEA2
F	284	GLU	-	expression tag	UNP P0AEA2
F	285	LYS	-	expression tag	UNP P0AEA2
G	278	TRP	-	expression tag	UNP P0AEA2
G	279	SER	-	expression tag	UNP P0AEA2
G	280	HIS	-	expression tag	UNP P0AEA2
G	281	PRO	-	expression tag	UNP P0AEA2
G	282	GLN	-	expression tag	UNP P0AEA2
G	283	PHE	-	expression tag	UNP P0AEA2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	284	GLU	-	expression tag	UNP P0AEA2
G	285	LYS	-	expression tag	UNP P0AEA2
H	278	TRP	-	expression tag	UNP P0AEA2
H	279	SER	-	expression tag	UNP P0AEA2
H	280	HIS	-	expression tag	UNP P0AEA2
H	281	PRO	-	expression tag	UNP P0AEA2
H	282	GLN	-	expression tag	UNP P0AEA2
H	283	PHE	-	expression tag	UNP P0AEA2
H	284	GLU	-	expression tag	UNP P0AEA2
H	285	LYS	-	expression tag	UNP P0AEA2
I	278	TRP	-	expression tag	UNP P0AEA2
I	279	SER	-	expression tag	UNP P0AEA2
I	280	HIS	-	expression tag	UNP P0AEA2
I	281	PRO	-	expression tag	UNP P0AEA2
I	282	GLN	-	expression tag	UNP P0AEA2
I	283	PHE	-	expression tag	UNP P0AEA2
I	284	GLU	-	expression tag	UNP P0AEA2
I	285	LYS	-	expression tag	UNP P0AEA2

- Molecule 2 is a protein called Curli production assembly/transport component CsgF.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	40	Total	C	N	O	S	0	0
			311	191	55	64	1		
2	b	40	Total	C	N	O	S	0	0
			311	191	55	64	1		
2	c	40	Total	C	N	O	S	0	0
			311	191	55	64	1		
2	d	40	Total	C	N	O	S	0	0
			311	191	55	64	1		
2	e	40	Total	C	N	O	S	0	0
			311	191	55	64	1		
2	f	40	Total	C	N	O	S	0	0
			311	191	55	64	1		
2	g	40	Total	C	N	O	S	0	0
			311	191	55	64	1		
2	h	40	Total	C	N	O	S	0	0
			311	191	55	64	1		
2	i	40	Total	C	N	O	S	0	0
			311	191	55	64	1		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	139	HIS	-	expression tag	UNP P0AE98
a	140	HIS	-	expression tag	UNP P0AE98
a	141	HIS	-	expression tag	UNP P0AE98
a	142	HIS	-	expression tag	UNP P0AE98
a	143	HIS	-	expression tag	UNP P0AE98
a	144	HIS	-	expression tag	UNP P0AE98
b	139	HIS	-	expression tag	UNP P0AE98
b	140	HIS	-	expression tag	UNP P0AE98
b	141	HIS	-	expression tag	UNP P0AE98
b	142	HIS	-	expression tag	UNP P0AE98
b	143	HIS	-	expression tag	UNP P0AE98
b	144	HIS	-	expression tag	UNP P0AE98
c	139	HIS	-	expression tag	UNP P0AE98
c	140	HIS	-	expression tag	UNP P0AE98
c	141	HIS	-	expression tag	UNP P0AE98
c	142	HIS	-	expression tag	UNP P0AE98
c	143	HIS	-	expression tag	UNP P0AE98
c	144	HIS	-	expression tag	UNP P0AE98
d	139	HIS	-	expression tag	UNP P0AE98
d	140	HIS	-	expression tag	UNP P0AE98
d	141	HIS	-	expression tag	UNP P0AE98
d	142	HIS	-	expression tag	UNP P0AE98
d	143	HIS	-	expression tag	UNP P0AE98
d	144	HIS	-	expression tag	UNP P0AE98
e	139	HIS	-	expression tag	UNP P0AE98
e	140	HIS	-	expression tag	UNP P0AE98
e	141	HIS	-	expression tag	UNP P0AE98
e	142	HIS	-	expression tag	UNP P0AE98
e	143	HIS	-	expression tag	UNP P0AE98
e	144	HIS	-	expression tag	UNP P0AE98
f	139	HIS	-	expression tag	UNP P0AE98
f	140	HIS	-	expression tag	UNP P0AE98
f	141	HIS	-	expression tag	UNP P0AE98
f	142	HIS	-	expression tag	UNP P0AE98
f	143	HIS	-	expression tag	UNP P0AE98
f	144	HIS	-	expression tag	UNP P0AE98
g	139	HIS	-	expression tag	UNP P0AE98
g	140	HIS	-	expression tag	UNP P0AE98
g	141	HIS	-	expression tag	UNP P0AE98
g	142	HIS	-	expression tag	UNP P0AE98
g	143	HIS	-	expression tag	UNP P0AE98
g	144	HIS	-	expression tag	UNP P0AE98
h	139	HIS	-	expression tag	UNP P0AE98

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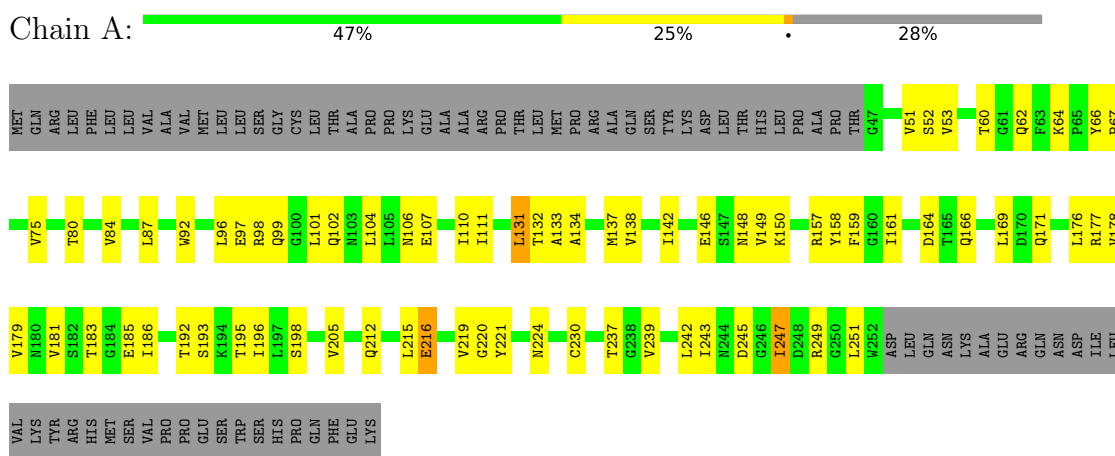
Chain	Residue	Modelled	Actual	Comment	Reference
h	140	HIS	-	expression tag	UNP P0AE98
h	141	HIS	-	expression tag	UNP P0AE98
h	142	HIS	-	expression tag	UNP P0AE98
h	143	HIS	-	expression tag	UNP P0AE98
h	144	HIS	-	expression tag	UNP P0AE98
i	139	HIS	-	expression tag	UNP P0AE98
i	140	HIS	-	expression tag	UNP P0AE98
i	141	HIS	-	expression tag	UNP P0AE98
i	142	HIS	-	expression tag	UNP P0AE98
i	143	HIS	-	expression tag	UNP P0AE98
i	144	HIS	-	expression tag	UNP P0AE98



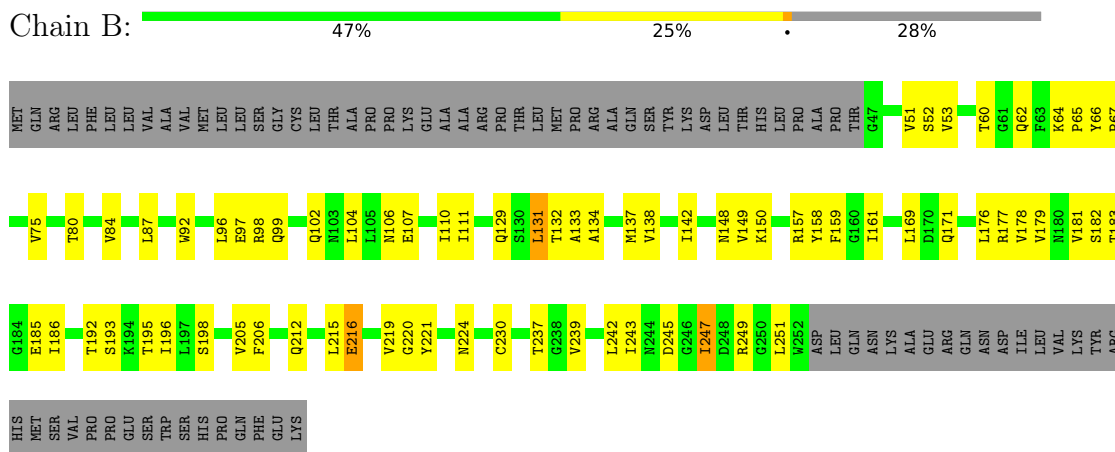
### 3 Residue-property plots

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

#### • Molecule 1: Curli production assembly/transport component CsgG

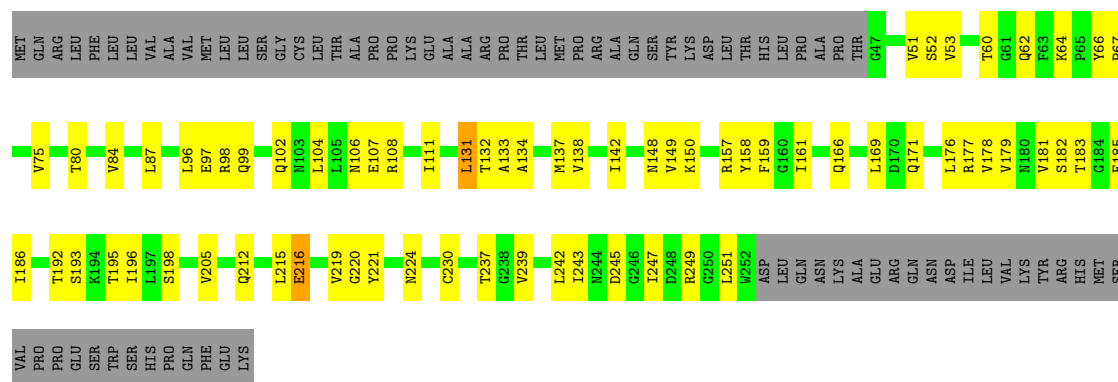


#### • Molecule 1: Curli production assembly/transport component CsgG



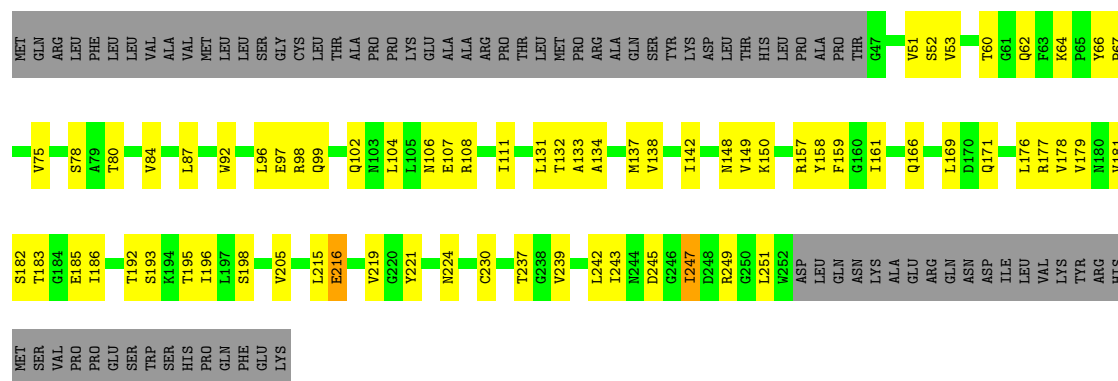
#### • Molecule 1: Curli production assembly/transport component CsgG





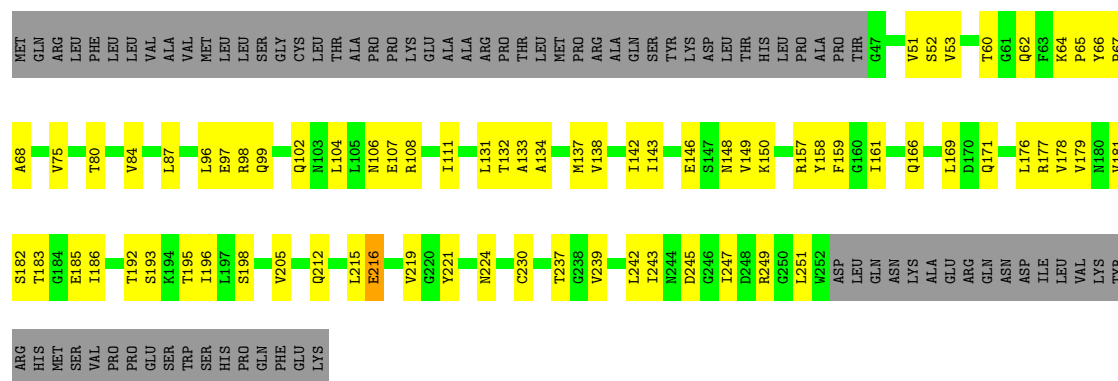
• Molecule 1: Curli production assembly/transport component CsgG

Chain D: 48% 24% 28%



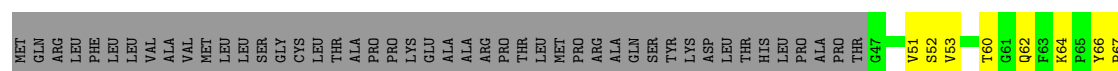
• Molecule 1: Curli production assembly/transport component CsgG

Chain E: 47% 25% 28%



• Molecule 1: Curli production assembly/transport component CsgG

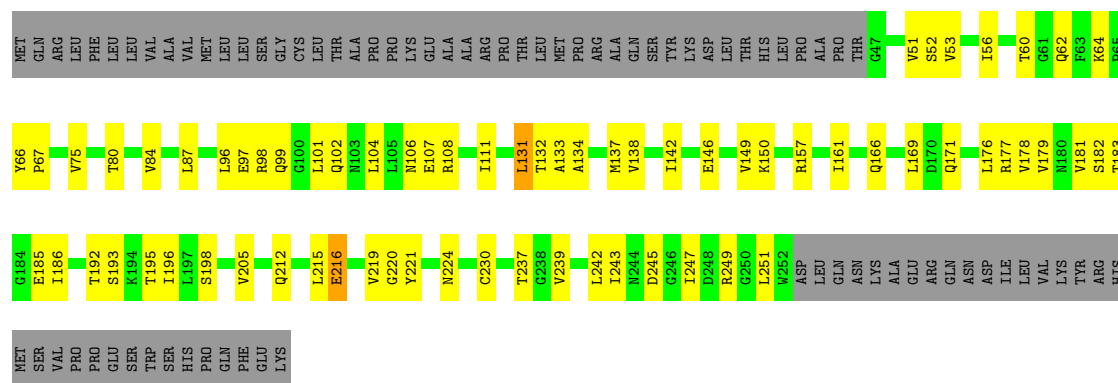
Chain F: 46% 25% 28%





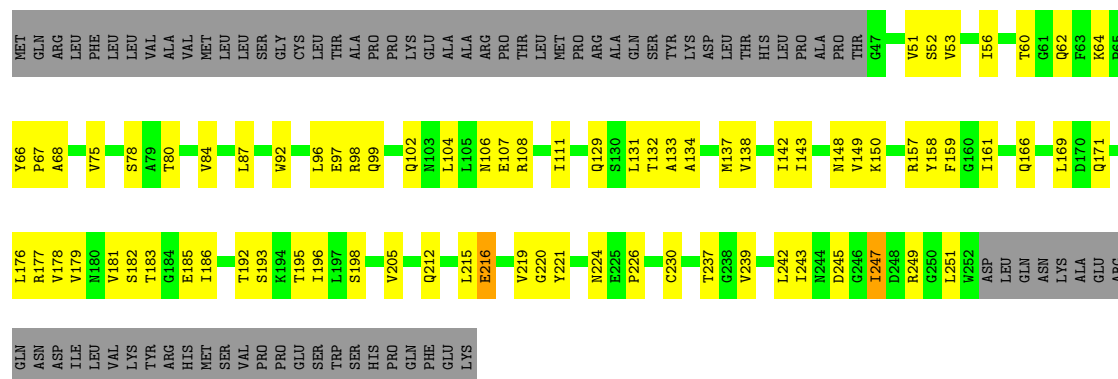
- Molecule 1: Curli production assembly/transport component CsgG

Chain G: 48% 24% 28%



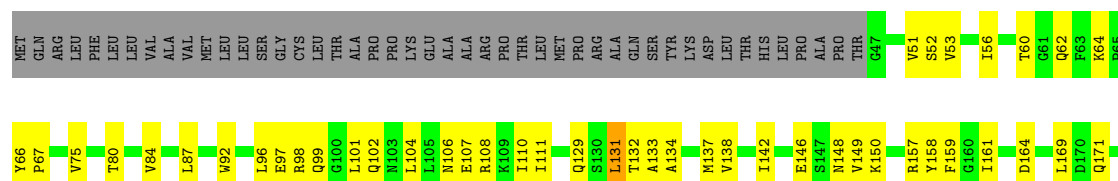
- Molecule 1: Curli production assembly/transport component CsgG

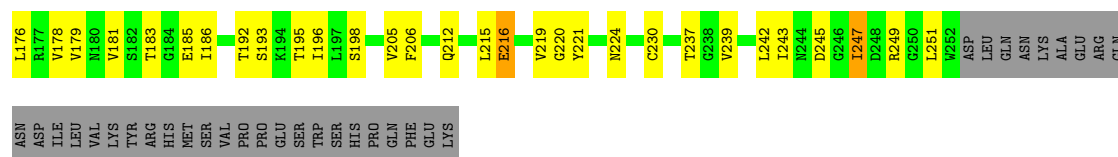
Chain H: 45% 26% 28%



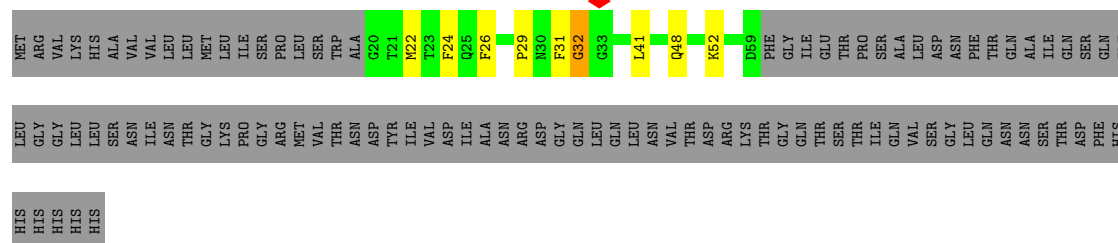
- Molecule 1: Curli production assembly/transport component CsgG

Chain I: 46% 25% 28%

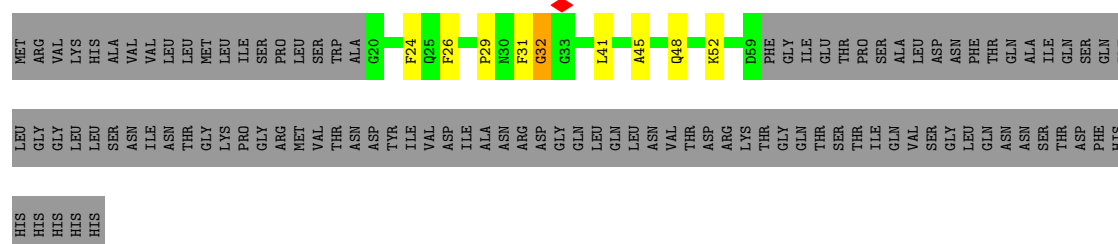




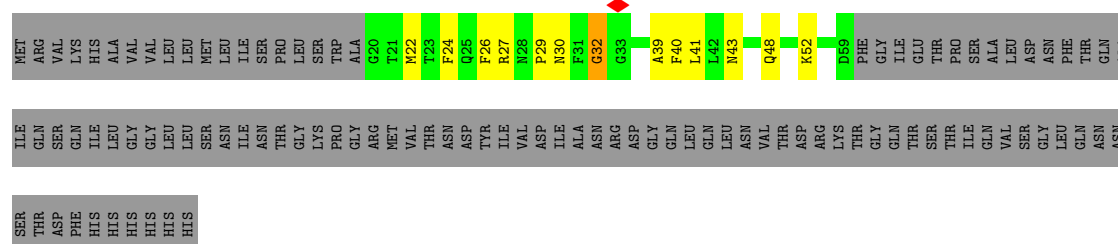
• Molecule 2: Curli production assembly/transport component CsgF



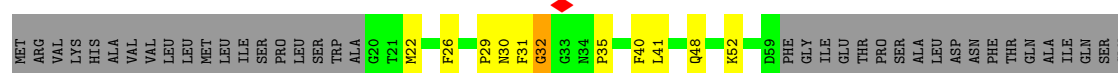
• Molecule 2: Curli production assembly/transport component CsgF

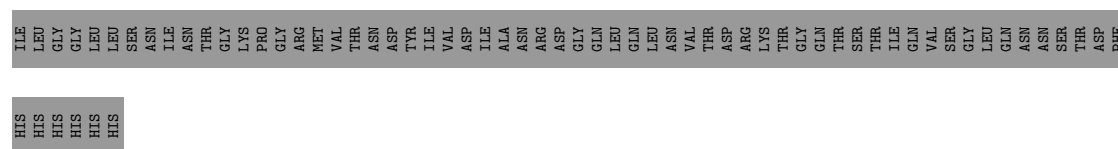


• Molecule 2: Curli production assembly/transport component CsgF

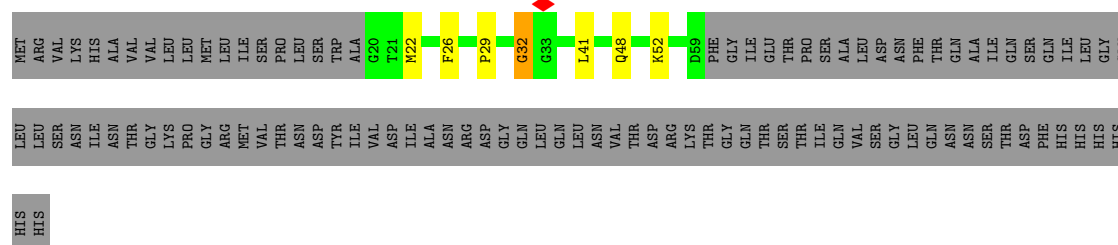


• Molecule 2: Curli production assembly/transport component CsgF





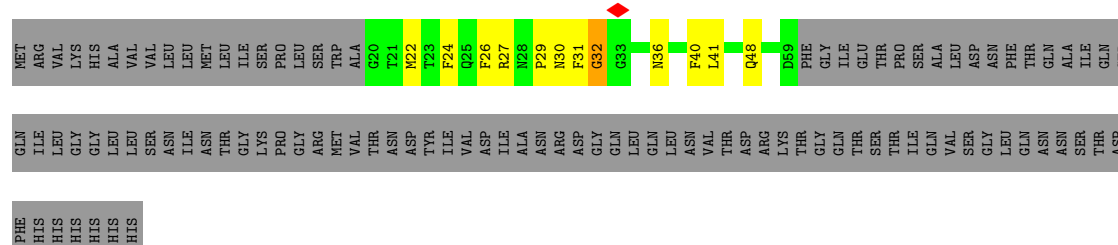
- Molecule 2: Curli production assembly/transport component CsgF



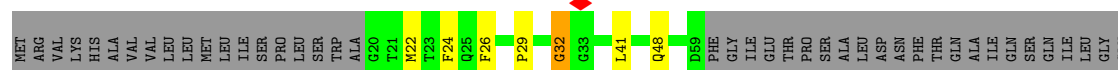
- Molecule 2: Curli production assembly/transport component CsgF



- Molecule 2: Curli production assembly/transport component CsgF



- Molecule 2: Curli production assembly/transport component CsgF



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

● Molecule 2: Curli production assembly/transport component CsgF



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

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C9	Depositor
Number of particles used	96558	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	A	0.32	0/1614	0.45	0/2190
1	B	0.31	0/1614	0.45	0/2190
1	C	0.31	0/1614	0.45	0/2190
1	D	0.31	0/1614	0.45	0/2190
1	E	0.31	0/1614	0.45	0/2190
1	F	0.31	0/1614	0.45	0/2190
1	G	0.32	0/1614	0.45	0/2190
1	H	0.31	0/1614	0.45	0/2190
1	I	0.31	0/1614	0.45	0/2190
2	a	0.34	0/319	0.44	0/432
2	b	0.34	0/319	0.44	0/432
2	c	0.34	0/319	0.44	0/432
2	d	0.34	0/319	0.44	0/432
2	e	0.34	0/319	0.44	0/432
2	f	0.34	0/319	0.44	0/432
2	g	0.34	0/319	0.44	0/432
2	h	0.34	0/319	0.44	0/432
2	i	0.34	0/319	0.44	0/432
All	All	0.32	0/17397	0.45	0/23598

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
2	a	0	1
2	b	0	1
2	c	0	1
2	d	0	1
2	e	0	1
2	f	0	1
2	g	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	h	0	1
2	i	0	1
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	a	32	GLY	Peptide
2	b	32	GLY	Peptide
2	c	32	GLY	Peptide
2	d	32	GLY	Peptide
2	e	32	GLY	Peptide
2	f	32	GLY	Peptide
2	g	32	GLY	Peptide
2	h	32	GLY	Peptide
2	i	32	GLY	Peptide

## 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	A	1589	0	1596	49	0
1	B	1589	0	1596	50	0
1	C	1589	0	1596	47	0
1	D	1589	0	1596	46	0
1	E	1589	0	1596	49	0
1	F	1589	0	1596	51	0
1	G	1589	0	1596	48	0
1	H	1589	0	1596	52	0
1	I	1589	0	1596	53	0
2	a	311	0	271	10	0
2	b	311	0	271	7	0
2	c	311	0	271	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	311	0	271	10	0
2	e	311	0	271	5	0
2	f	311	0	271	9	0
2	g	311	0	271	12	0
2	h	311	0	271	5	0
2	i	311	0	271	13	0
All	All	17100	0	16803	389	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 11.

All (389) 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:B:133:ALA:HB1	1:E:111:ILE:HG12	1.55	0.87
1:E:133:ALA:HB1	1:H:111:ILE:HG12	1.59	0.84
1:A:133:ALA:HB1	1:B:111:ILE:HG12	1.59	0.84
1:B:62:GLN:HE22	1:E:64:LYS:HD2	1.42	0.83
1:C:111:ILE:HG12	1:D:133:ALA:HB1	1.61	0.82
1:C:133:ALA:HB1	1:G:111:ILE:HG12	1.61	0.82
1:D:111:ILE:HG12	1:F:133:ALA:HB1	1.61	0.81
1:F:111:ILE:HG12	1:H:133:ALA:HB1	1.60	0.81
1:C:62:GLN:HE22	1:G:64:LYS:HD2	1.52	0.74
1:C:137:MET:HE1	1:G:104:LEU:HA	1.71	0.72
1:A:102:GLN:O	1:A:106:ASN:ND2	2.23	0.72
1:I:102:GLN:O	1:I:106:ASN:ND2	2.23	0.72
1:H:102:GLN:O	1:H:106:ASN:ND2	2.23	0.71
1:E:102:GLN:O	1:E:106:ASN:ND2	2.23	0.71
1:D:102:GLN:O	1:D:106:ASN:ND2	2.23	0.71
1:G:102:GLN:O	1:G:106:ASN:ND2	2.23	0.71
1:C:102:GLN:O	1:C:106:ASN:ND2	2.23	0.71
1:F:102:GLN:O	1:F:106:ASN:ND2	2.23	0.71
1:B:102:GLN:O	1:B:106:ASN:ND2	2.23	0.71
1:D:64:LYS:HD2	1:F:62:GLN:HE22	1.56	0.71
1:D:104:LEU:HA	1:F:137:MET:HE1	1.73	0.70
1:E:75:VAL:HG11	1:E:142:ILE:HG21	1.74	0.70
1:E:137:MET:HE1	1:H:104:LEU:HA	1.73	0.70
1:F:64:LYS:HD2	1:H:62:GLN:HE22	1.56	0.70
1:H:75:VAL:HG11	1:H:142:ILE:HG21	1.74	0.70
1:B:75:VAL:HG11	1:B:142:ILE:HG21	1.73	0.69
1:C:64:LYS:HD2	1:D:62:GLN:HE22	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:GLN:HE22	1:H:64:LYS:HD2	1.56	0.69
2:a:26:PHE:HB2	2:a:32:GLY:HA3	1.75	0.69
1:A:75:VAL:HG11	1:A:142:ILE:HG21	1.74	0.69
1:F:75:VAL:HG11	1:F:142:ILE:HG21	1.74	0.69
2:i:26:PHE:HB2	2:i:32:GLY:HA3	1.75	0.69
1:C:75:VAL:HG11	1:C:142:ILE:HG21	1.74	0.69
2:b:26:PHE:HB2	2:b:32:GLY:HA3	1.74	0.69
2:e:26:PHE:HB2	2:e:32:GLY:HA3	1.74	0.69
2:g:26:PHE:HB2	2:g:32:GLY:HA3	1.74	0.69
1:A:221:TYR:OH	1:I:150:LYS:NZ	2.26	0.69
1:C:104:LEU:HA	1:D:137:MET:HE1	1.75	0.69
1:G:75:VAL:HG11	1:G:142:ILE:HG21	1.73	0.68
1:A:111:ILE:HG12	1:I:133:ALA:HB1	1.75	0.68
1:D:75:VAL:HG11	1:D:142:ILE:HG21	1.74	0.68
1:F:104:LEU:HA	1:H:137:MET:HE1	1.76	0.68
2:h:26:PHE:HB2	2:h:32:GLY:HA3	1.75	0.68
2:c:26:PHE:HB2	2:c:32:GLY:HA3	1.74	0.68
1:D:52:SER:HB2	1:D:98:ARG:HG3	1.76	0.68
1:G:52:SER:HB2	1:G:98:ARG:HG3	1.76	0.68
1:I:52:SER:HB2	1:I:98:ARG:HG3	1.76	0.68
1:I:75:VAL:HG11	1:I:142:ILE:HG21	1.73	0.68
1:C:52:SER:HB2	1:C:98:ARG:HG3	1.76	0.68
2:f:26:PHE:HB2	2:f:32:GLY:HA3	1.75	0.68
1:A:52:SER:HB2	1:A:98:ARG:HG3	1.76	0.67
2:d:26:PHE:HB2	2:d:32:GLY:HA3	1.74	0.67
1:B:52:SER:HB2	1:B:98:ARG:HG3	1.76	0.67
1:B:137:MET:HE1	1:E:104:LEU:HA	1.77	0.67
1:F:52:SER:HB2	1:F:98:ARG:HG3	1.76	0.67
1:H:52:SER:HB2	1:H:98:ARG:HG3	1.76	0.67
1:A:64:LYS:HD2	1:I:62:GLN:HE22	1.59	0.66
1:B:157:ARG:HB3	1:E:216:GLU:HG2	1.76	0.66
1:E:52:SER:HB2	1:E:98:ARG:HG3	1.76	0.66
1:B:186:ILE:HD12	1:E:84:VAL:HG11	1.78	0.66
1:B:148:ASN:O	1:E:224:ASN:ND2	2.30	0.64
1:A:62:GLN:HE22	1:B:64:LYS:HD2	1.62	0.64
1:B:150:LYS:NZ	1:E:221:TYR:OH	2.27	0.63
1:G:133:ALA:HB1	1:I:111:ILE:HG12	1.81	0.61
1:A:138:VAL:HG22	1:A:178:VAL:HG22	1.83	0.61
1:D:138:VAL:HG22	1:D:178:VAL:HG22	1.83	0.61
1:E:138:VAL:HG22	1:E:178:VAL:HG22	1.83	0.61
1:F:138:VAL:HG22	1:F:178:VAL:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:VAL:HG22	1:B:178:VAL:HG22	1.83	0.61
1:F:221:TYR:OH	1:H:150:LYS:NZ	2.31	0.60
1:C:138:VAL:HG22	1:C:178:VAL:HG22	1.83	0.60
1:G:138:VAL:HG22	1:G:178:VAL:HG22	1.83	0.60
1:H:138:VAL:HG22	1:H:178:VAL:HG22	1.83	0.60
1:C:182:SER:O	1:G:108:ARG:NH1	2.34	0.60
1:I:138:VAL:HG22	1:I:178:VAL:HG22	1.83	0.60
1:F:84:VAL:HG11	1:H:186:ILE:HD12	1.84	0.60
1:A:216:GLU:HG2	1:I:157:ARG:HB3	1.84	0.59
1:E:177:ARG:NH1	1:H:97:GLU:OE1	2.35	0.59
1:H:166:GLN:HB3	2:h:22:MET:HE1	1.86	0.57
1:I:212:GLN:HB3	2:g:48:GLN:HA	1.86	0.57
1:C:221:TYR:OH	1:D:150:LYS:NZ	2.36	0.57
1:C:84:VAL:HG11	1:D:186:ILE:HD12	1.86	0.57
1:D:108:ARG:NH1	1:F:182:SER:O	2.37	0.57
1:E:157:ARG:HB3	1:H:216:GLU:HG2	1.86	0.57
1:D:84:VAL:HG11	1:F:186:ILE:HD12	1.87	0.56
1:A:186:ILE:HD12	1:B:84:VAL:HG11	1.87	0.56
1:A:137:MET:HE1	1:B:104:LEU:HA	1.86	0.56
1:B:212:GLN:HB3	2:a:48:GLN:HA	1.87	0.56
1:C:186:ILE:HD12	1:G:84:VAL:HG11	1.88	0.56
1:F:216:GLU:HG2	1:H:157:ARG:HB3	1.88	0.56
1:A:53:VAL:HG12	1:A:80:THR:HG23	1.89	0.55
1:B:53:VAL:HG12	1:B:80:THR:HG23	1.89	0.55
1:E:53:VAL:HG12	1:E:80:THR:HG23	1.88	0.55
1:F:53:VAL:HG12	1:F:80:THR:HG23	1.88	0.55
1:I:220:GLY:HA3	2:i:24:PHE:CE1	2.41	0.55
1:G:166:GLN:HB3	2:g:22:MET:HE1	1.87	0.55
1:H:53:VAL:HG12	1:H:80:THR:HG23	1.88	0.55
1:D:53:VAL:HG12	1:D:80:THR:HG23	1.89	0.55
1:H:137:MET:HE3	1:H:181:VAL:HG22	1.89	0.55
1:C:108:ARG:NH1	1:D:182:SER:O	2.40	0.55
1:E:137:MET:HE3	1:E:181:VAL:HG22	1.89	0.55
1:F:137:MET:HE3	1:F:181:VAL:HG22	1.89	0.55
1:I:53:VAL:HG12	1:I:80:THR:HG23	1.89	0.55
1:C:157:ARG:HB3	1:G:216:GLU:HG2	1.88	0.55
1:D:137:MET:HE3	1:D:181:VAL:HG22	1.89	0.54
1:I:159:PHE:HA	2:i:48:GLN:OE1	2.08	0.54
1:A:84:VAL:HG11	1:I:186:ILE:HD12	1.88	0.54
1:C:53:VAL:HG12	1:C:80:THR:HG23	1.89	0.54
1:G:53:VAL:HG12	1:G:80:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:MET:HE3	1:B:181:VAL:HG22	1.89	0.54
1:C:137:MET:HE3	1:C:181:VAL:HG22	1.89	0.54
1:B:220:GLY:HA3	2:b:24:PHE:CE1	2.42	0.53
1:G:62:GLN:HE22	1:I:64:LYS:HD2	1.74	0.53
1:A:137:MET:HE3	1:A:181:VAL:HG22	1.89	0.53
1:I:137:MET:HE3	1:I:181:VAL:HG22	1.89	0.53
1:G:137:MET:HE3	1:G:181:VAL:HG22	1.89	0.53
1:A:177:ARG:NH1	1:B:97:GLU:OE1	2.42	0.53
1:I:224:ASN:OD1	2:i:22:MET:N	2.22	0.53
1:C:150:LYS:NZ	1:G:221:TYR:OH	2.37	0.52
1:C:216:GLU:HG2	1:D:157:ARG:HB3	1.91	0.52
1:A:224:ASN:ND2	1:I:148:ASN:O	2.41	0.52
1:F:98:ARG:NH2	1:F:132:THR:O	2.43	0.52
1:D:98:ARG:NH2	1:D:132:THR:O	2.43	0.51
1:E:148:ASN:O	1:H:224:ASN:ND2	2.39	0.51
1:F:166:GLN:HB3	2:f:22:MET:HE1	1.92	0.51
1:E:186:ILE:HD12	1:H:84:VAL:HG11	1.92	0.51
1:A:98:ARG:NH2	1:A:132:THR:O	2.43	0.51
1:A:212:GLN:HB3	2:i:48:GLN:HA	1.92	0.51
1:C:224:ASN:ND2	1:D:148:ASN:O	2.43	0.51
1:E:98:ARG:NH2	1:E:132:THR:O	2.43	0.51
1:E:143:ILE:O	1:H:78:SER:OG	2.27	0.51
1:F:224:ASN:ND2	1:H:148:ASN:O	2.42	0.51
1:C:166:GLN:HB3	2:c:22:MET:HE1	1.91	0.51
1:I:98:ARG:NH2	1:I:132:THR:O	2.43	0.51
1:B:98:ARG:NH2	1:B:132:THR:O	2.43	0.51
1:D:216:GLU:HG2	1:F:157:ARG:HB3	1.92	0.51
1:F:108:ARG:NH1	1:H:182:SER:O	2.44	0.51
1:A:101:LEU:HD21	1:B:110:ILE:HD11	1.94	0.50
1:G:98:ARG:NH2	1:G:132:THR:O	2.43	0.50
1:H:98:ARG:NH2	1:H:132:THR:O	2.43	0.50
1:C:148:ASN:O	1:G:224:ASN:ND2	2.42	0.50
1:C:97:GLU:OE1	1:D:177:ARG:NH1	2.45	0.50
1:H:158:TYR:CG	1:H:159:PHE:N	2.80	0.50
1:D:221:TYR:OH	1:F:150:LYS:NZ	2.37	0.50
1:C:96:LEU:HD12	1:C:134:ALA:HB2	1.94	0.49
1:A:176:LEU:HB3	1:A:242:LEU:HD11	1.94	0.49
1:C:98:ARG:NH2	1:C:132:THR:O	2.43	0.49
1:E:158:TYR:CG	1:E:159:PHE:N	2.80	0.49
1:I:96:LEU:HD12	1:I:134:ALA:HB2	1.95	0.49
1:C:169:LEU:HD22	1:C:195:THR:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:LEU:HD12	1:D:134:ALA:HB2	1.95	0.49
1:F:169:LEU:HD22	1:F:195:THR:HB	1.94	0.49
1:G:96:LEU:HD12	1:G:134:ALA:HB2	1.94	0.49
1:D:97:GLU:OE1	1:F:177:ARG:NH1	2.44	0.49
1:F:96:LEU:HD12	1:F:134:ALA:HB2	1.95	0.49
1:G:176:LEU:HB3	1:G:242:LEU:HD11	1.94	0.49
1:I:176:LEU:HB3	1:I:242:LEU:HD11	1.94	0.49
1:A:220:GLY:HA3	2:a:24:PHE:CE1	2.48	0.49
1:F:158:TYR:CG	1:F:159:PHE:N	2.80	0.49
1:H:96:LEU:HD12	1:H:134:ALA:HB2	1.94	0.49
1:A:150:LYS:NZ	1:B:221:TYR:OH	2.41	0.49
1:B:96:LEU:HD12	1:B:134:ALA:HB2	1.94	0.49
1:G:177:ARG:NH1	1:I:97:GLU:OE1	2.46	0.49
1:A:96:LEU:HD12	1:A:134:ALA:HB2	1.95	0.49
1:B:176:LEU:HB3	1:B:242:LEU:HD11	1.94	0.49
1:B:245:ASP:OD2	1:B:249:ARG:NH2	2.42	0.49
1:C:176:LEU:HB3	1:C:242:LEU:HD11	1.94	0.49
1:A:169:LEU:HD22	1:A:195:THR:HB	1.94	0.48
1:F:97:GLU:OE1	1:H:177:ARG:NH1	2.46	0.48
1:G:137:MET:HE1	1:I:104:LEU:HA	1.93	0.48
2:g:40:PHE:HE2	2:i:30:ASN:ND2	2.11	0.48
1:B:169:LEU:HD22	1:B:195:THR:HB	1.94	0.48
1:E:96:LEU:HD12	1:E:134:ALA:HB2	1.94	0.48
1:G:212:GLN:HB3	2:c:48:GLN:HA	1.95	0.48
1:H:56:ILE:H	1:H:80:THR:HG1	1.59	0.48
1:B:158:TYR:CG	1:B:159:PHE:N	2.80	0.48
1:F:176:LEU:HB3	1:F:242:LEU:HD11	1.94	0.48
1:A:148:ASN:O	1:B:224:ASN:ND2	2.43	0.48
1:C:177:ARG:NH1	1:G:97:GLU:OE1	2.45	0.48
1:D:169:LEU:HD22	1:D:195:THR:HB	1.94	0.48
1:D:224:ASN:ND2	1:F:148:ASN:O	2.44	0.48
1:H:245:ASP:OD2	1:H:249:ARG:NH2	2.42	0.48
1:A:66:TYR:CG	1:A:67:PRO:HA	2.49	0.48
1:E:66:TYR:CG	1:E:67:PRO:HA	2.49	0.48
1:E:169:LEU:HD22	1:E:195:THR:HB	1.94	0.48
1:E:176:LEU:HB3	1:E:242:LEU:HD11	1.94	0.48
1:H:176:LEU:HB3	1:H:242:LEU:HD11	1.94	0.48
1:G:169:LEU:HD22	1:G:195:THR:HB	1.94	0.48
1:F:66:TYR:CG	1:F:67:PRO:HA	2.49	0.48
1:H:169:LEU:HD22	1:H:195:THR:HB	1.94	0.48
2:d:31:PHE:HA	2:f:27:ARG:HE	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASP:OD2	1:A:249:ARG:NH2	2.42	0.48
1:D:176:LEU:HB3	1:D:242:LEU:HD11	1.94	0.48
1:E:245:ASP:OD2	1:E:249:ARG:NH2	2.42	0.48
1:H:212:GLN:HB3	2:e:48:GLN:HA	1.96	0.48
1:I:169:LEU:HD22	1:I:195:THR:HB	1.94	0.48
1:E:182:SER:O	1:H:108:ARG:NH1	2.47	0.48
1:F:245:ASP:OD2	1:F:249:ARG:NH2	2.42	0.48
1:H:66:TYR:CG	1:H:67:PRO:HA	2.49	0.48
1:G:66:TYR:CG	1:G:67:PRO:HA	2.49	0.47
1:D:66:TYR:CG	1:D:67:PRO:HA	2.49	0.47
1:I:66:TYR:CG	1:I:67:PRO:HA	2.49	0.47
2:c:27:ARG:HE	2:g:31:PHE:HA	1.79	0.47
1:B:66:TYR:CG	1:B:67:PRO:HA	2.49	0.47
1:C:66:TYR:CG	1:C:67:PRO:HA	2.49	0.47
1:D:245:ASP:OD2	1:D:249:ARG:NH2	2.42	0.47
1:B:182:SER:O	1:E:108:ARG:NH1	2.48	0.47
1:C:212:GLN:HB3	2:d:48:GLN:HA	1.97	0.47
1:D:158:TYR:CG	1:D:159:PHE:N	2.80	0.47
1:F:220:GLY:HA3	2:f:24:PHE:CE1	2.49	0.47
1:B:206:PHE:HD2	2:b:45:ALA:HB2	1.80	0.46
1:I:56:ILE:H	1:I:80:THR:HG1	1.61	0.46
1:I:245:ASP:OD2	1:I:249:ARG:NH2	2.42	0.46
2:d:30:ASN:ND2	2:f:40:PHE:HE2	2.13	0.46
1:C:131:LEU:HD12	1:C:131:LEU:HA	1.76	0.46
1:C:220:GLY:HA3	2:c:24:PHE:CE1	2.51	0.46
1:A:51:VAL:HG11	1:A:87:LEU:HD13	1.98	0.46
1:C:181:VAL:HA	1:G:104:LEU:HD11	1.97	0.46
1:G:220:GLY:HA3	2:g:24:PHE:CE1	2.50	0.46
1:C:245:ASP:OD2	1:C:249:ARG:NH2	2.42	0.46
1:A:183:THR:HG22	1:B:129:GLN:OE1	2.16	0.45
1:G:149:VAL:HG22	1:G:169:LEU:O	2.16	0.45
1:D:51:VAL:HG11	1:D:87:LEU:HD13	1.98	0.45
1:D:149:VAL:HG22	1:D:169:LEU:O	2.16	0.45
1:E:212:GLN:HB3	2:b:48:GLN:HA	1.98	0.45
1:A:157:ARG:HB3	1:B:216:GLU:HG2	1.98	0.45
1:D:166:GLN:HB3	2:d:22:MET:HE1	1.98	0.45
1:E:178:VAL:HG23	1:E:242:LEU:HD13	1.99	0.45
1:A:149:VAL:HG22	1:A:169:LEU:O	2.16	0.45
1:A:178:VAL:HG23	1:A:242:LEU:HD13	1.99	0.45
1:B:178:VAL:HG23	1:B:242:LEU:HD13	1.99	0.45
1:H:178:VAL:HG23	1:H:242:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:VAL:HG22	1:C:169:LEU:O	2.16	0.45
1:I:149:VAL:HG22	1:I:169:LEU:O	2.16	0.45
2:e:52:LYS:HE2	2:e:52:LYS:HB2	1.80	0.45
1:B:149:VAL:HG22	1:B:169:LEU:O	2.16	0.45
1:F:51:VAL:HG11	1:F:87:LEU:HD13	1.98	0.45
1:G:51:VAL:HG11	1:G:87:LEU:HD13	1.98	0.45
1:G:245:ASP:OD2	1:G:249:ARG:NH2	2.42	0.45
1:B:51:VAL:HG11	1:B:87:LEU:HD13	1.98	0.45
1:E:65:PRO:HB3	1:H:68:ALA:HA	1.99	0.45
1:E:149:VAL:HG22	1:E:169:LEU:O	2.16	0.45
1:G:56:ILE:H	1:G:80:THR:HG1	1.61	0.45
1:H:51:VAL:HG11	1:H:87:LEU:HD13	1.98	0.45
1:D:171:GLN:NE2	1:D:193:SER:OG	2.50	0.45
1:G:182:SER:O	1:I:108:ARG:NH1	2.50	0.45
1:I:178:VAL:HG23	1:I:242:LEU:HD13	1.99	0.45
1:C:51:VAL:HG11	1:C:87:LEU:HD13	1.98	0.44
1:E:51:VAL:HG11	1:E:87:LEU:HD13	1.98	0.44
1:F:149:VAL:HG22	1:F:169:LEU:O	2.16	0.44
1:H:220:GLY:HA3	2:h:24:PHE:CE1	2.52	0.44
2:a:52:LYS:HE2	2:a:52:LYS:HB2	1.81	0.44
1:A:110:ILE:HD11	1:I:101:LEU:HD21	1.99	0.44
1:A:166:GLN:HB3	2:a:22:MET:HE1	2.00	0.44
1:B:171:GLN:NE2	1:B:193:SER:OG	2.50	0.44
1:H:149:VAL:HG22	1:H:169:LEU:O	2.16	0.44
2:g:40:PHE:HE2	2:i:30:ASN:HD21	1.65	0.44
1:C:171:GLN:NE2	1:C:193:SER:OG	2.50	0.44
1:F:178:VAL:HG23	1:F:242:LEU:HD13	1.99	0.44
1:G:150:LYS:NZ	1:I:221:TYR:OH	2.44	0.44
2:c:40:PHE:HE2	2:g:30:ASN:ND2	2.15	0.44
2:g:27:ARG:HE	2:i:31:PHE:HA	1.83	0.44
1:A:171:GLN:NE2	1:A:193:SER:OG	2.50	0.44
1:D:104:LEU:HD11	1:F:181:VAL:HA	1.99	0.44
1:E:171:GLN:NE2	1:E:193:SER:OG	2.50	0.44
1:A:107:GLU:O	1:A:111:ILE:HG13	2.18	0.44
1:G:178:VAL:HG23	1:G:242:LEU:HD13	1.99	0.44
1:A:104:LEU:HA	1:I:137:MET:HE1	1.99	0.44
1:F:171:GLN:NE2	1:F:193:SER:OG	2.50	0.44
2:c:52:LYS:HE2	2:c:52:LYS:HB2	1.80	0.44
1:I:164:ASP:HB3	2:a:31:PHE:CB	2.48	0.44
2:d:35:PRO:HG2	2:f:36:ASN:HB2	1.99	0.44
1:I:51:VAL:HG11	1:I:87:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:36:ASN:HB2	2:i:35:PRO:HG2	2.00	0.44
1:D:178:VAL:HG23	1:D:242:LEU:HD13	1.99	0.43
1:G:183:THR:OG1	1:G:185:GLU:HG2	2.18	0.43
1:G:186:ILE:HD12	1:I:84:VAL:HG11	1.99	0.43
1:C:178:VAL:HG23	1:C:242:LEU:HD13	1.99	0.43
1:C:183:THR:OG1	1:C:185:GLU:HG2	2.18	0.43
1:I:171:GLN:NE2	1:I:193:SER:OG	2.50	0.43
1:B:107:GLU:O	1:B:111:ILE:HG13	2.18	0.43
1:B:177:ARG:NH1	1:E:97:GLU:OE1	2.51	0.43
1:E:183:THR:HG22	1:H:129:GLN:OE1	2.17	0.43
1:C:107:GLU:O	1:C:111:ILE:HG13	2.18	0.43
1:F:131:LEU:HD12	1:F:131:LEU:HA	1.76	0.43
1:I:183:THR:OG1	1:I:185:GLU:HG2	2.18	0.43
2:d:52:LYS:HB2	2:d:52:LYS:HE2	1.81	0.43
1:B:183:THR:OG1	1:B:185:GLU:HG2	2.18	0.43
1:D:107:GLU:O	1:D:111:ILE:HG13	2.18	0.43
1:I:107:GLU:O	1:I:111:ILE:HG13	2.18	0.43
1:F:196:ILE:HG12	1:F:230:CYS:SG	2.59	0.43
1:H:171:GLN:NE2	1:H:193:SER:OG	2.50	0.43
1:I:196:ILE:HG12	1:I:230:CYS:SG	2.59	0.43
1:D:78:SER:OG	1:F:143:ILE:O	2.36	0.43
1:F:107:GLU:O	1:F:111:ILE:HG13	2.18	0.43
1:H:196:ILE:HG12	1:H:230:CYS:SG	2.59	0.43
1:H:239:VAL:O	1:H:243:ILE:HG13	2.19	0.43
2:f:44:SER:O	2:f:48:GLN:NE2	2.33	0.43
1:A:196:ILE:HG12	1:A:230:CYS:SG	2.59	0.43
1:B:181:VAL:HA	1:E:104:LEU:HD11	2.00	0.43
1:D:183:THR:OG1	1:D:185:GLU:HG2	2.19	0.43
1:G:107:GLU:O	1:G:111:ILE:HG13	2.18	0.43
1:G:171:GLN:NE2	1:G:193:SER:OG	2.50	0.43
1:A:158:TYR:CG	1:A:159:PHE:N	2.80	0.42
1:C:158:TYR:CG	1:C:159:PHE:N	2.80	0.42
1:D:196:ILE:HG12	1:D:230:CYS:SG	2.59	0.42
1:G:157:ARG:HB3	1:I:216:GLU:HG2	2.01	0.42
1:H:107:GLU:O	1:H:111:ILE:HG13	2.18	0.42
1:H:161:ILE:HG13	1:H:205:VAL:HG13	2.01	0.42
2:c:40:PHE:HE2	2:g:30:ASN:HD21	1.67	0.42
1:B:196:ILE:HG12	1:B:230:CYS:SG	2.59	0.42
1:E:196:ILE:HG12	1:E:230:CYS:SG	2.59	0.42
1:E:239:VAL:O	1:E:243:ILE:HG13	2.19	0.42
1:F:183:THR:OG1	1:F:185:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:VAL:O	1:F:243:ILE:HG13	2.19	0.42
1:H:183:THR:OG1	1:H:185:GLU:HG2	2.19	0.42
1:B:131:LEU:HA	1:B:131:LEU:HD12	1.76	0.42
1:B:161:ILE:HG13	1:B:205:VAL:HG13	2.01	0.42
1:E:183:THR:OG1	1:E:185:GLU:HG2	2.18	0.42
1:G:183:THR:HG22	1:I:129:GLN:OE1	2.19	0.42
1:G:239:VAL:O	1:G:243:ILE:HG13	2.19	0.42
1:I:239:VAL:O	1:I:243:ILE:HG13	2.19	0.42
1:B:239:VAL:O	1:B:243:ILE:HG13	2.19	0.42
1:C:239:VAL:O	1:C:243:ILE:HG13	2.19	0.42
1:E:107:GLU:O	1:E:111:ILE:HG13	2.18	0.42
1:E:150:LYS:NZ	1:H:221:TYR:OH	2.45	0.42
1:E:161:ILE:HG13	1:E:205:VAL:HG13	2.01	0.42
1:G:101:LEU:HD21	1:I:110:ILE:HD11	2.02	0.42
1:G:196:ILE:HG12	1:G:230:CYS:SG	2.59	0.42
1:B:97:GLU:C	1:B:99:GLN:H	2.28	0.42
1:C:104:LEU:HD11	1:D:181:VAL:HA	2.01	0.42
1:C:196:ILE:HG12	1:C:230:CYS:SG	2.59	0.42
1:F:97:GLU:C	1:F:99:GLN:H	2.28	0.42
1:G:131:LEU:HD12	1:G:131:LEU:HA	1.77	0.42
1:F:161:ILE:HG13	1:F:205:VAL:HG13	2.01	0.42
1:G:97:GLU:C	1:G:99:GLN:H	2.28	0.42
2:b:52:LYS:HE2	2:b:52:LYS:HB2	1.80	0.42
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.77	0.42
1:A:183:THR:OG1	1:A:185:GLU:HG2	2.19	0.42
1:I:164:ASP:CB	2:a:31:PHE:HB2	2.50	0.42
1:A:239:VAL:O	1:A:243:ILE:HG13	2.19	0.42
1:C:97:GLU:C	1:C:99:GLN:H	2.28	0.42
1:D:97:GLU:C	1:D:99:GLN:H	2.28	0.42
1:G:161:ILE:HG13	1:G:205:VAL:HG13	2.01	0.42
1:H:97:GLU:C	1:H:99:GLN:H	2.28	0.42
1:C:161:ILE:HG13	1:C:205:VAL:HG13	2.01	0.42
1:F:168:GLN:HG3	2:f:22:MET:HE3	2.02	0.42
1:I:206:PHE:HD2	2:i:45:ALA:HB2	1.85	0.42
1:A:131:LEU:HB3	1:B:110:ILE:HG23	2.02	0.41
1:I:161:ILE:HG13	1:I:205:VAL:HG13	2.01	0.41
2:b:29:PRO:HD2	2:b:41:LEU:HD12	2.02	0.41
1:A:97:GLU:C	1:A:99:GLN:H	2.28	0.41
1:A:164:ASP:HB3	2:b:31:PHE:CB	2.50	0.41
1:E:97:GLU:C	1:E:99:GLN:H	2.28	0.41
2:h:29:PRO:HD2	2:h:41:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HG13	1:A:205:VAL:HG13	2.01	0.41
1:D:239:VAL:O	1:D:243:ILE:HG13	2.19	0.41
1:E:166:GLN:HB3	2:e:22:MET:HE1	2.01	0.41
2:e:29:PRO:HD2	2:e:41:LEU:HD12	2.02	0.41
1:D:161:ILE:HG13	1:D:205:VAL:HG13	2.01	0.41
1:F:104:LEU:HD11	1:H:181:VAL:HA	2.02	0.41
2:f:29:PRO:HD2	2:f:41:LEU:HD12	2.02	0.41
1:I:158:TYR:CG	1:I:159:PHE:N	2.80	0.41
2:c:29:PRO:HD2	2:c:41:LEU:HD12	2.02	0.41
2:g:29:PRO:HD2	2:g:41:LEU:HD12	2.02	0.41
1:B:65:PRO:HB3	1:E:68:ALA:HA	2.02	0.41
1:E:146:GLU:HG2	1:H:226:PRO:HA	2.01	0.41
1:I:97:GLU:C	1:I:99:GLN:H	2.28	0.41
1:A:92:TRP:CH2	1:A:247:ILE:HD11	2.56	0.41
1:F:78:SER:OG	1:H:143:ILE:O	2.36	0.41
1:B:92:TRP:CH2	1:B:247:ILE:HD11	2.56	0.41
1:F:212:GLN:HB3	2:h:48:GLN:HA	2.03	0.41
1:I:164:ASP:HB3	2:a:31:PHE:HB2	2.03	0.41
2:a:29:PRO:HD2	2:a:41:LEU:HD12	2.02	0.41
2:i:29:PRO:HD2	2:i:41:LEU:HD12	2.02	0.41
1:F:92:TRP:CH2	1:F:247:ILE:HD11	2.56	0.41
1:I:92:TRP:CH2	1:I:247:ILE:HD11	2.56	0.41
2:a:29:PRO:HG2	2:i:40:PHE:CE2	2.56	0.41
2:i:52:LYS:HE2	2:i:52:LYS:HB2	1.80	0.41
2:d:29:PRO:HD2	2:d:41:LEU:HD12	2.02	0.40
1:A:146:GLU:HG2	1:A:149:VAL:HG12	2.04	0.40
1:D:92:TRP:CH2	1:D:247:ILE:HD11	2.56	0.40
1:I:131:LEU:HD12	1:I:131:LEU:HA	1.76	0.40
1:I:146:GLU:HG2	1:I:149:VAL:HG12	2.04	0.40
2:c:30:ASN:ND2	2:d:40:PHE:HE2	2.18	0.40
1:G:146:GLU:HG2	1:G:149:VAL:HG12	2.04	0.40
2:c:39:ALA:O	2:c:43:ASN:ND2	2.55	0.40
1:H:92:TRP:CH2	1:H:247:ILE:HD11	2.56	0.40
2:d:31:PHE:O	2:d:31:PHE:CD1	2.75	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	A	204/285 (72%)	188 (92%)	16 (8%)	0	100	100
1	B	204/285 (72%)	188 (92%)	16 (8%)	0	100	100
1	C	204/285 (72%)	188 (92%)	16 (8%)	0	100	100
1	D	204/285 (72%)	188 (92%)	16 (8%)	0	100	100
1	E	204/285 (72%)	188 (92%)	16 (8%)	0	100	100
1	F	204/285 (72%)	188 (92%)	16 (8%)	0	100	100
1	G	204/285 (72%)	188 (92%)	16 (8%)	0	100	100
1	H	204/285 (72%)	188 (92%)	16 (8%)	0	100	100
1	I	204/285 (72%)	188 (92%)	16 (8%)	0	100	100
2	a	38/144 (26%)	32 (84%)	6 (16%)	0	100	100
2	b	38/144 (26%)	32 (84%)	6 (16%)	0	100	100
2	c	38/144 (26%)	32 (84%)	6 (16%)	0	100	100
2	d	38/144 (26%)	32 (84%)	6 (16%)	0	100	100
2	e	38/144 (26%)	32 (84%)	6 (16%)	0	100	100
2	f	38/144 (26%)	32 (84%)	6 (16%)	0	100	100
2	g	38/144 (26%)	32 (84%)	6 (16%)	0	100	100
2	h	38/144 (26%)	32 (84%)	6 (16%)	0	100	100
2	i	38/144 (26%)	32 (84%)	6 (16%)	0	100	100
All	All	2178/3861 (56%)	1980 (91%)	198 (9%)	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	A	173/244 (71%)	162 (94%)	11 (6%)	14	43
1	B	173/244 (71%)	162 (94%)	11 (6%)	14	43
1	C	173/244 (71%)	162 (94%)	11 (6%)	14	43
1	D	173/244 (71%)	162 (94%)	11 (6%)	14	43
1	E	173/244 (71%)	162 (94%)	11 (6%)	14	43
1	F	173/244 (71%)	162 (94%)	11 (6%)	14	43
1	G	173/244 (71%)	162 (94%)	11 (6%)	14	43
1	H	173/244 (71%)	162 (94%)	11 (6%)	14	43
1	I	173/244 (71%)	162 (94%)	11 (6%)	14	43
2	a	33/124 (27%)	33 (100%)	0	100	100
2	b	33/124 (27%)	33 (100%)	0	100	100
2	c	33/124 (27%)	33 (100%)	0	100	100
2	d	33/124 (27%)	33 (100%)	0	100	100
2	e	33/124 (27%)	33 (100%)	0	100	100
2	f	33/124 (27%)	33 (100%)	0	100	100
2	g	33/124 (27%)	33 (100%)	0	100	100
2	h	33/124 (27%)	33 (100%)	0	100	100
2	i	33/124 (27%)	33 (100%)	0	100	100
All	All	1854/3312 (56%)	1755 (95%)	99 (5%)	21	49

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	131	LEU
1	A	179	VAL
1	A	192	THR
1	A	198	SER
1	A	215	LEU
1	A	216	GLU
1	A	219	VAL
1	A	237	THR
1	A	247	ILE
1	A	251	LEU

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Mol	Chain	Res	Type
1	B	60	THR
1	B	131	LEU
1	B	179	VAL
1	B	192	THR
1	B	198	SER
1	B	215	LEU
1	B	216	GLU
1	B	219	VAL
1	B	237	THR
1	B	247	ILE
1	B	251	LEU
1	C	60	THR
1	C	131	LEU
1	C	179	VAL
1	C	192	THR
1	C	198	SER
1	C	215	LEU
1	C	216	GLU
1	C	219	VAL
1	C	237	THR
1	C	247	ILE
1	C	251	LEU
1	D	60	THR
1	D	131	LEU
1	D	179	VAL
1	D	192	THR
1	D	198	SER
1	D	215	LEU
1	D	216	GLU
1	D	219	VAL
1	D	237	THR
1	D	247	ILE
1	D	251	LEU
1	E	60	THR
1	E	131	LEU
1	E	179	VAL
1	E	192	THR
1	E	198	SER
1	E	215	LEU
1	E	216	GLU
1	E	219	VAL
1	E	237	THR

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Mol	Chain	Res	Type
1	E	247	ILE
1	E	251	LEU
1	F	60	THR
1	F	131	LEU
1	F	179	VAL
1	F	192	THR
1	F	198	SER
1	F	215	LEU
1	F	216	GLU
1	F	219	VAL
1	F	237	THR
1	F	247	ILE
1	F	251	LEU
1	G	60	THR
1	G	131	LEU
1	G	179	VAL
1	G	192	THR
1	G	198	SER
1	G	215	LEU
1	G	216	GLU
1	G	219	VAL
1	G	237	THR
1	G	247	ILE
1	G	251	LEU
1	H	60	THR
1	H	131	LEU
1	H	179	VAL
1	H	192	THR
1	H	198	SER
1	H	215	LEU
1	H	216	GLU
1	H	219	VAL
1	H	237	THR
1	H	247	ILE
1	H	251	LEU
1	I	60	THR
1	I	131	LEU
1	I	179	VAL
1	I	192	THR
1	I	198	SER
1	I	215	LEU
1	I	216	GLU

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Mol	Chain	Res	Type
1	I	219	VAL
1	I	237	THR
1	I	247	ILE
1	I	251	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	77	GLN
1	A	106	ASN
1	A	171	GLN
1	A	244	ASN
1	B	62	GLN
1	B	77	GLN
1	B	106	ASN
1	B	171	GLN
1	B	244	ASN
1	C	62	GLN
1	C	77	GLN
1	C	106	ASN
1	C	171	GLN
1	C	180	ASN
1	C	244	ASN
1	D	62	GLN
1	D	77	GLN
1	D	106	ASN
1	D	148	ASN
1	D	171	GLN
1	D	180	ASN
1	D	244	ASN
1	E	62	GLN
1	E	77	GLN
1	E	106	ASN
1	E	148	ASN
1	E	171	GLN
1	E	244	ASN
1	F	62	GLN
1	F	77	GLN
1	F	106	ASN
1	F	148	ASN
1	F	171	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	F	180	ASN
1	F	244	ASN
1	G	62	GLN
1	G	77	GLN
1	G	106	ASN
1	G	171	GLN
1	G	244	ASN
1	H	62	GLN
1	H	77	GLN
1	H	106	ASN
1	H	148	ASN
1	H	171	GLN
1	H	180	ASN
1	H	244	ASN
1	I	62	GLN
1	I	77	GLN
1	I	106	ASN
1	I	171	GLN
1	I	244	ASN
2	a	30	ASN
2	a	46	GLN
2	b	30	ASN
2	c	30	ASN
2	c	46	GLN
2	d	30	ASN
2	d	46	GLN
2	e	30	ASN
2	e	46	GLN
2	f	30	ASN
2	g	30	ASN
2	g	46	GLN
2	h	30	ASN
2	h	46	GLN
2	i	30	ASN
2	i	46	GLN

### 5.3.3 RNA ⓘ

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.

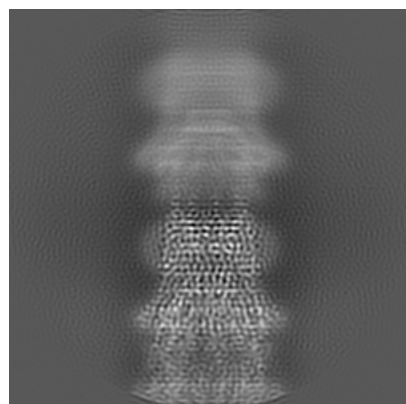
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0947. These allow visual inspection of the internal detail of the map and identification of artifacts.

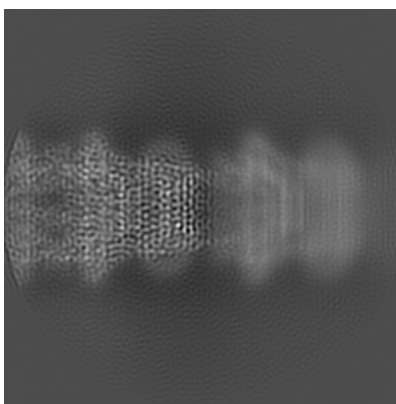
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

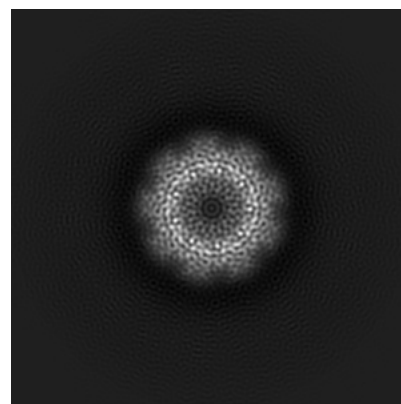
#### 6.1.1 Primary map



X

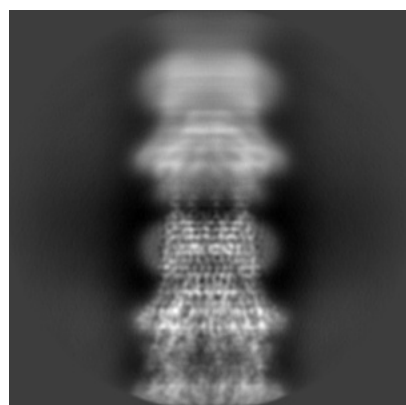


Y

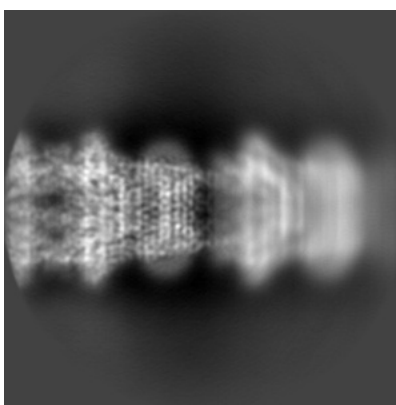


Z

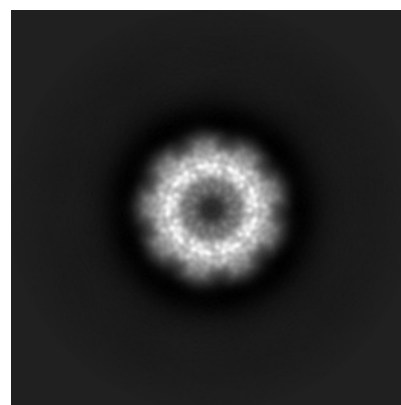
#### 6.1.2 Raw map



X



Y

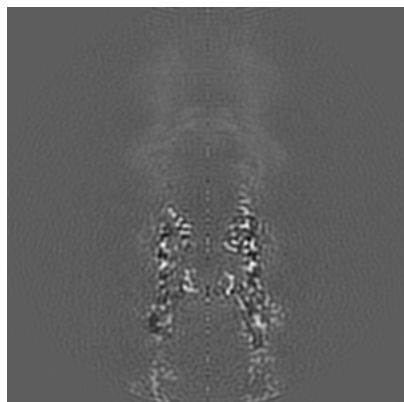


Z

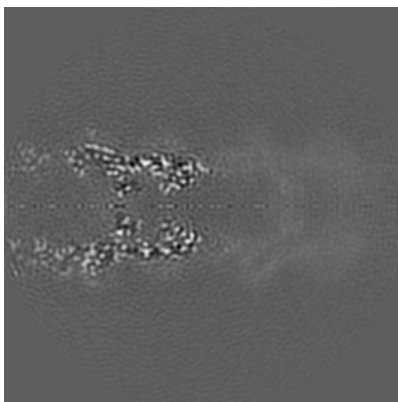
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

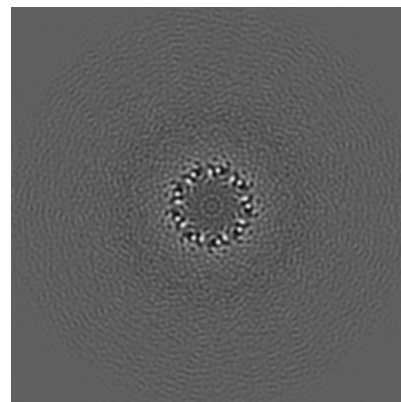
### 6.2.1 Primary map



X Index: 128

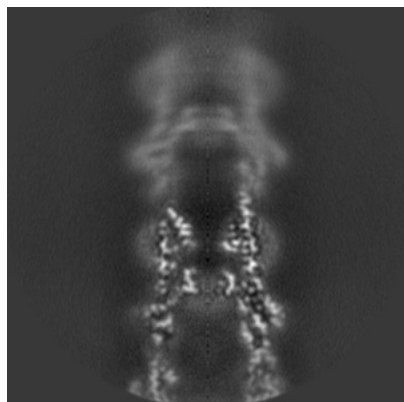


Y Index: 128

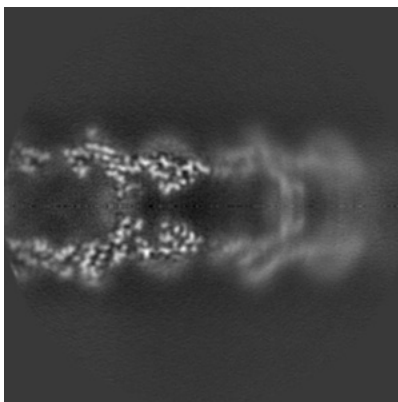


Z Index: 128

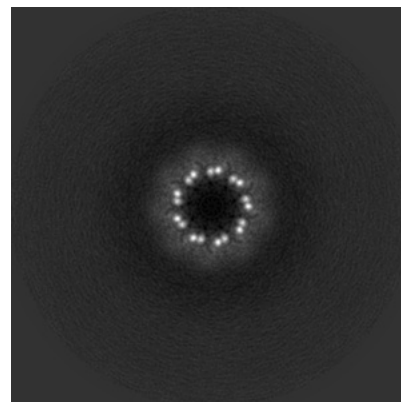
### 6.2.2 Raw map



X Index: 128



Y Index: 128

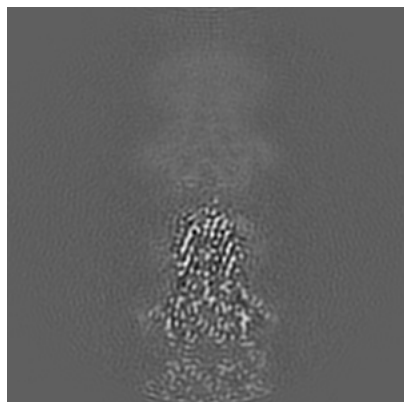


Z Index: 128

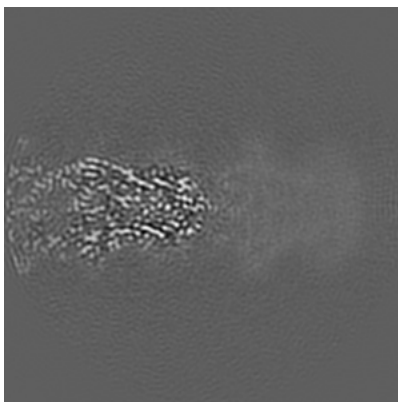
The images above show central slices of the map in three orthogonal directions.

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

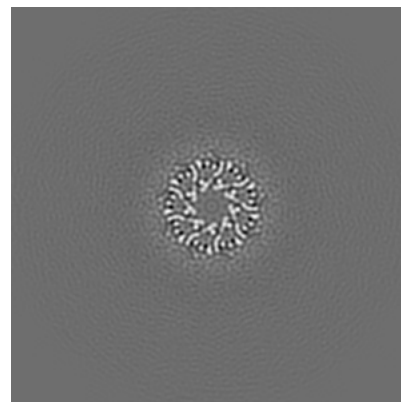
### 6.3.1 Primary map



X Index: 153

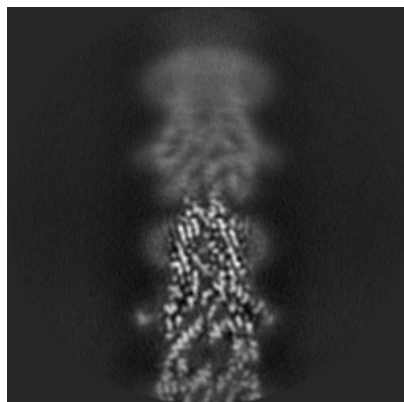


Y Index: 152

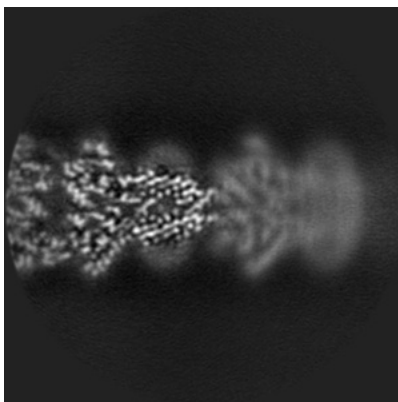


Z Index: 111

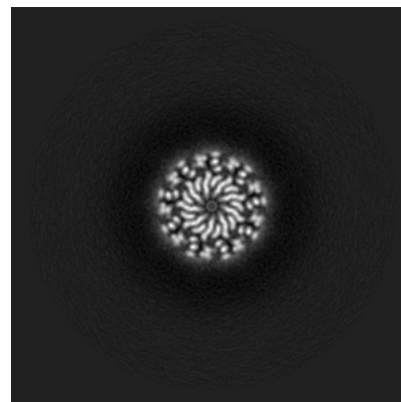
### 6.3.2 Raw map



X Index: 105



Y Index: 105

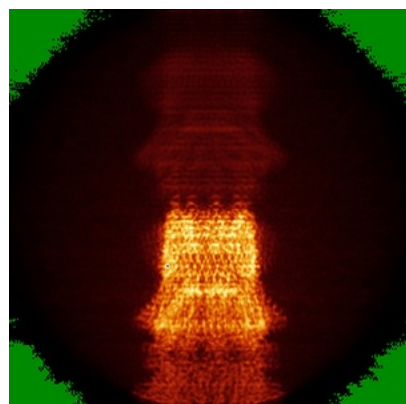


Z Index: 75

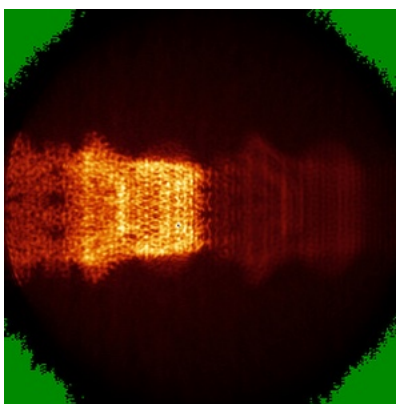
The images above show the largest variance slices of the map in three orthogonal directions.

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

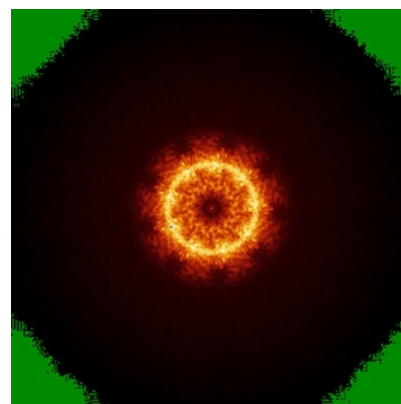
### 6.4.1 Primary map



X

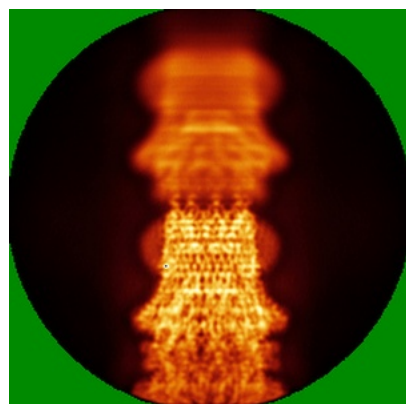


Y

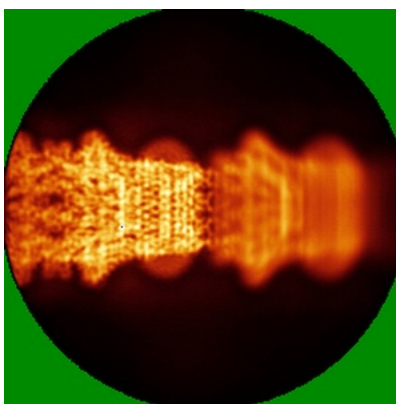


Z

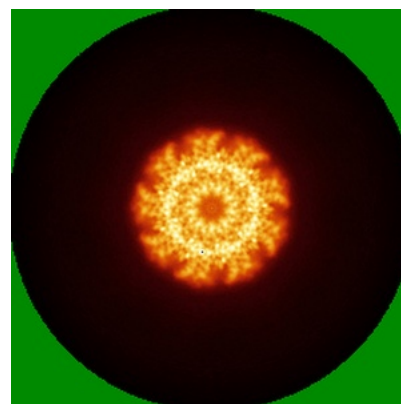
### 6.4.2 Raw map



X



Y

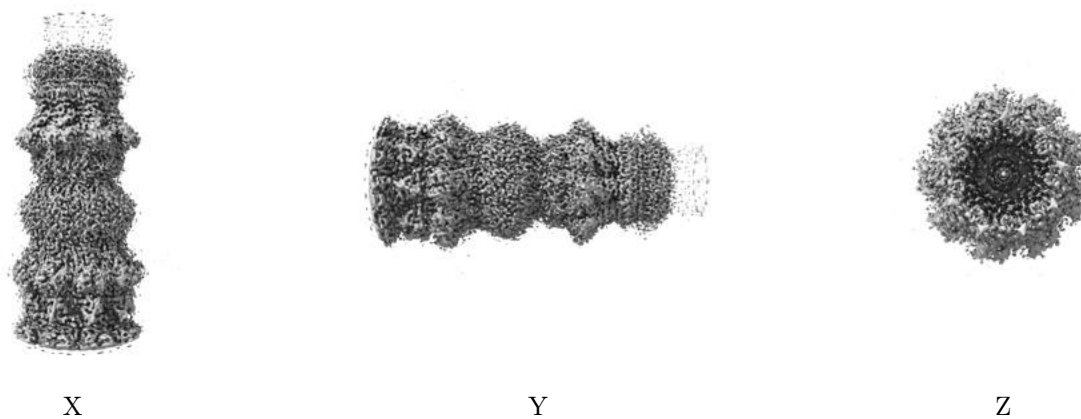


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

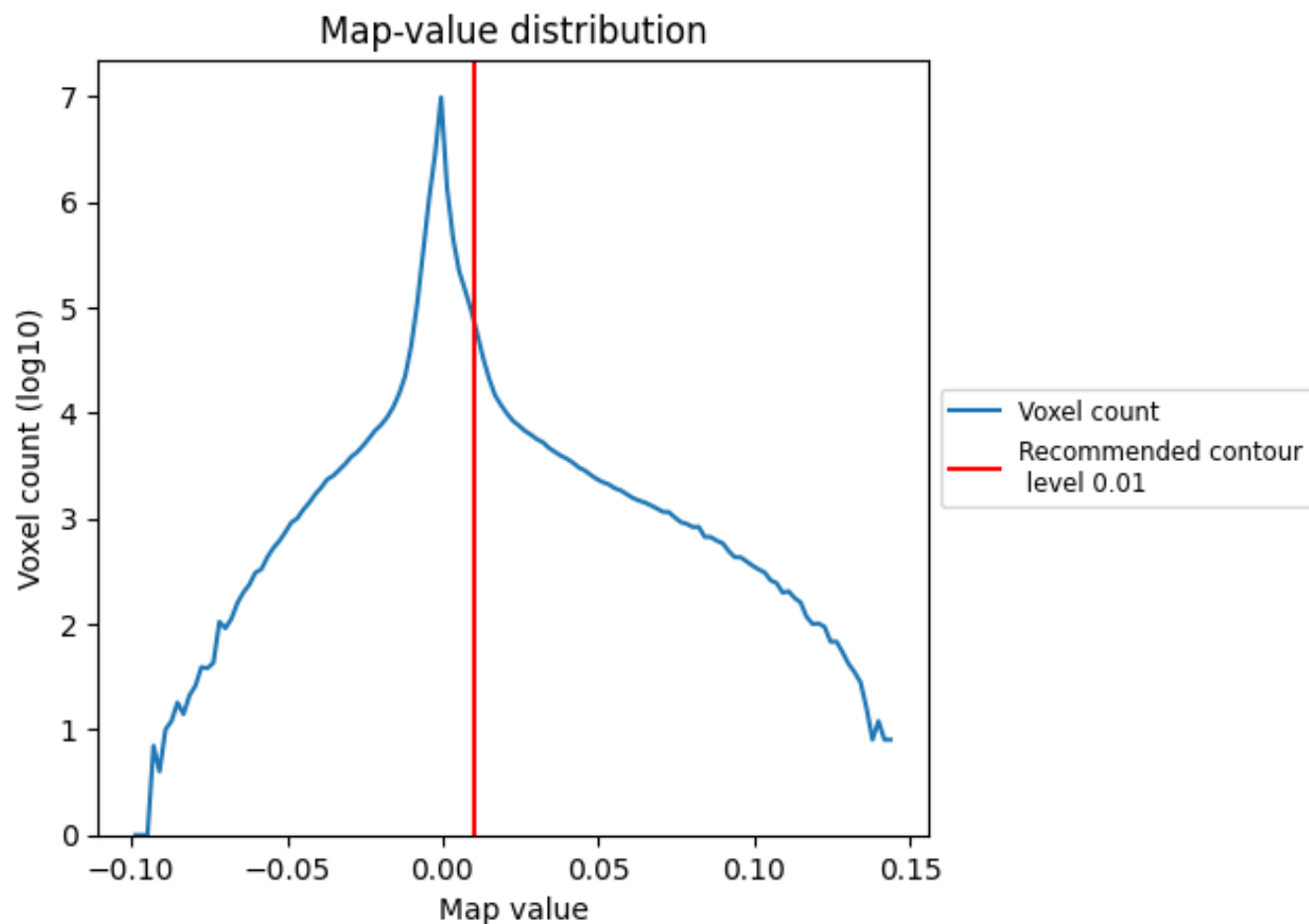
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

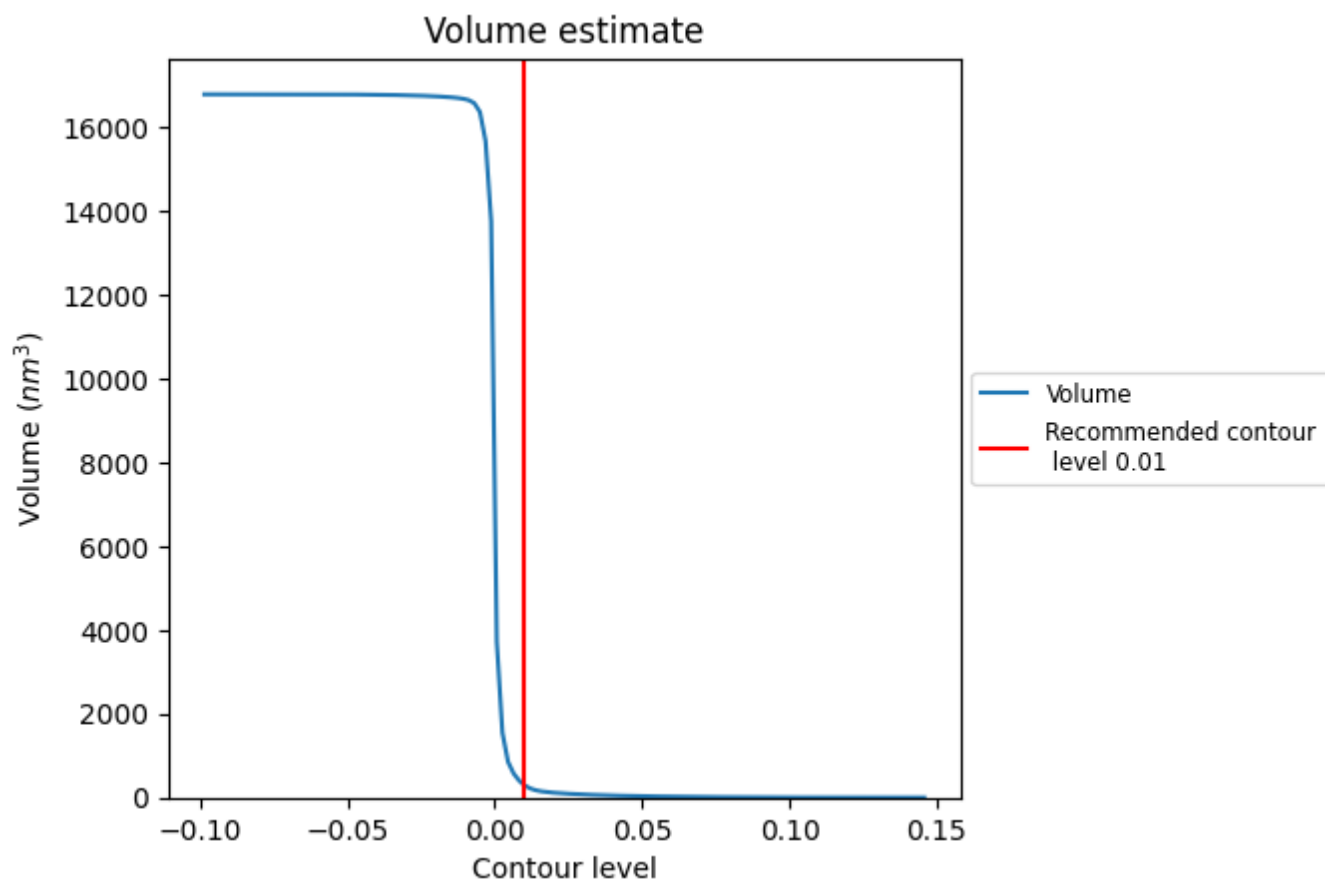
### 7.1 Map-value distribution [i](#)



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



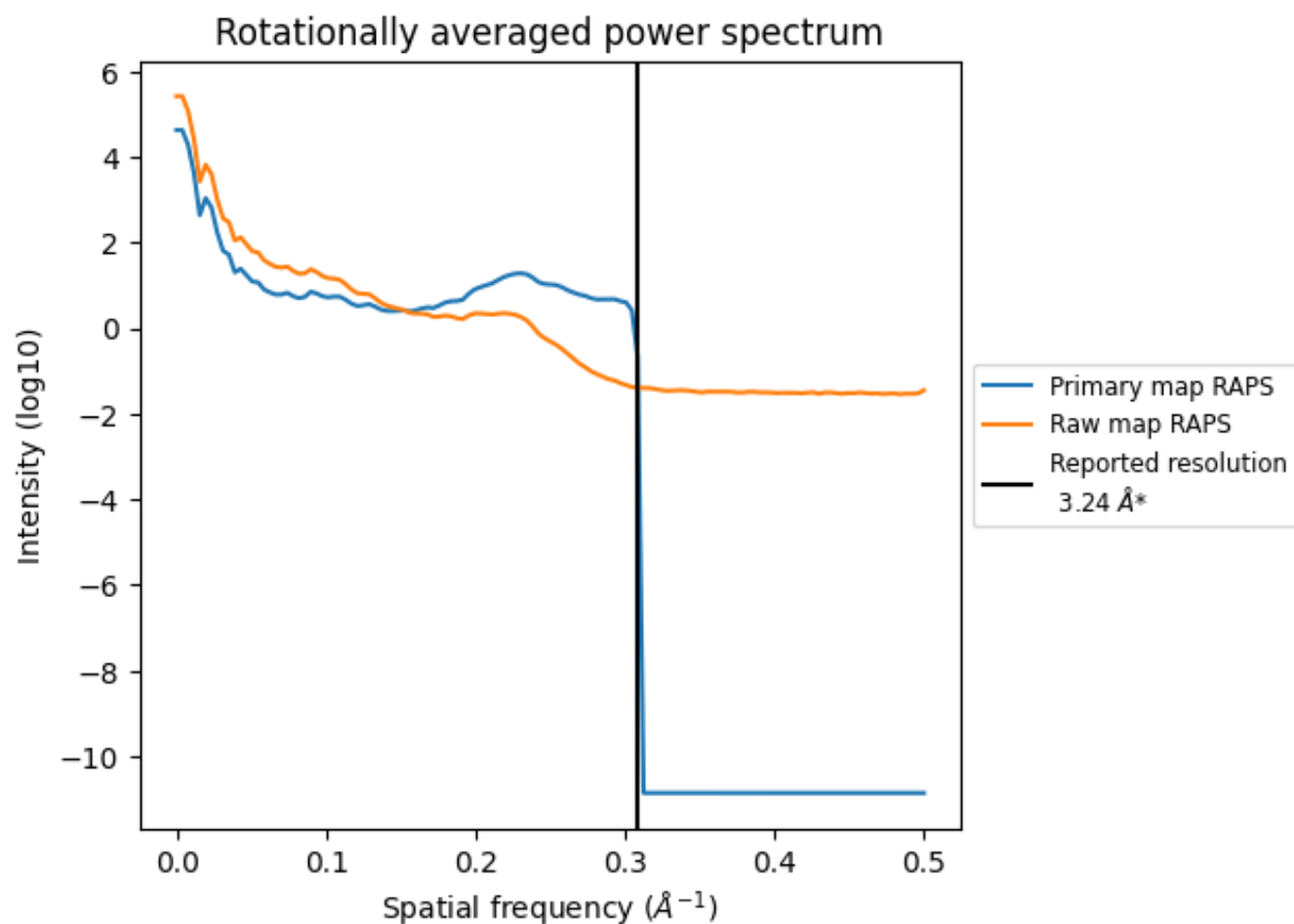
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300 nm<sup>3</sup>; this corresponds to an approximate mass of 271 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 ⓘ

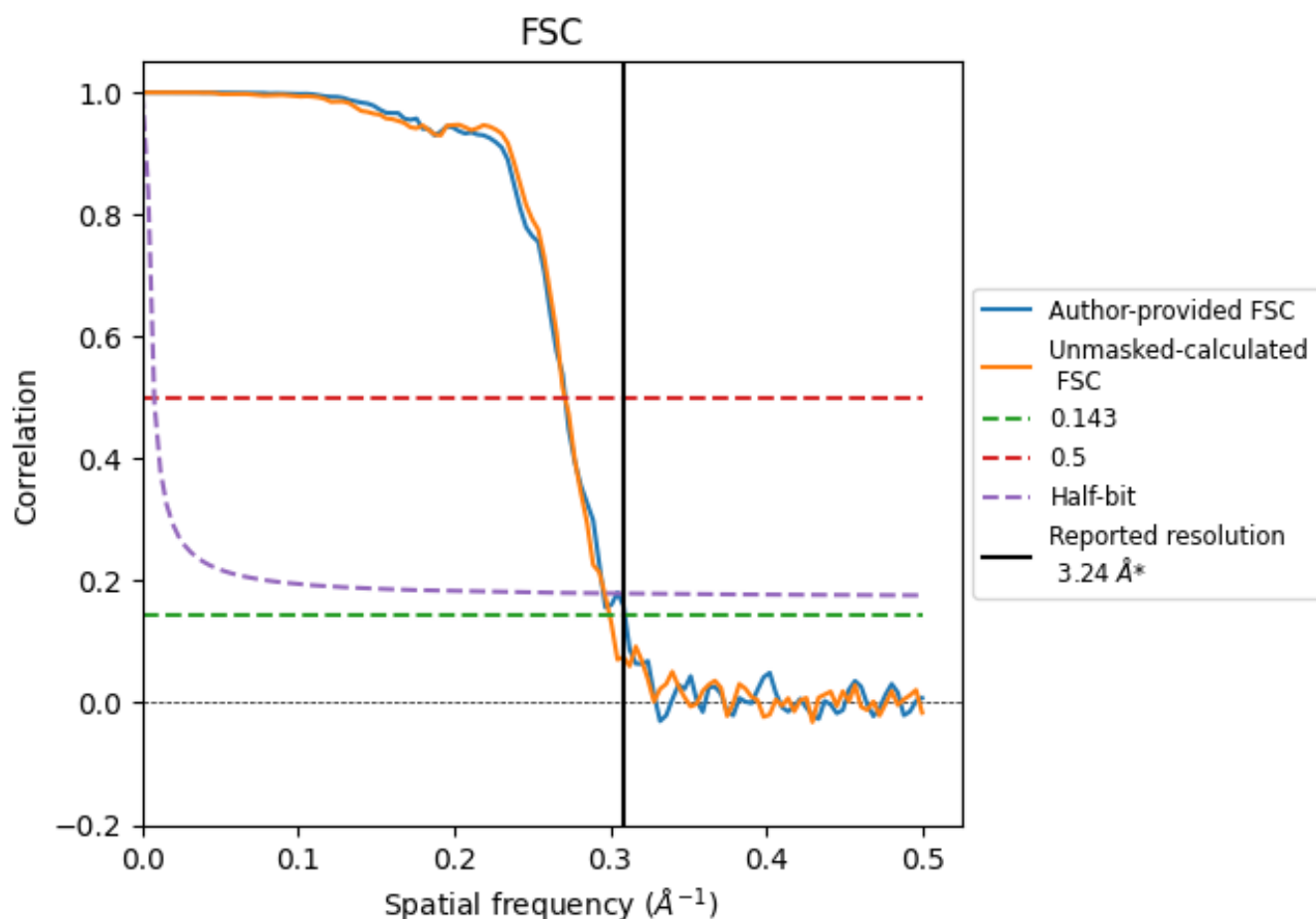


\*Reported resolution corresponds to spatial frequency of 0.309 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.309  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

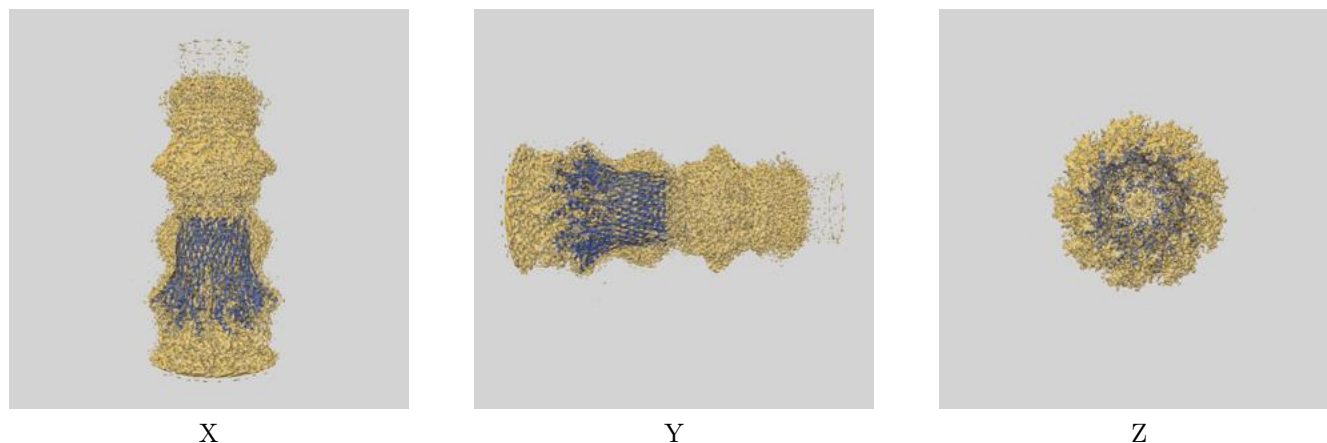
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	3.23	3.69	3.38
Unmasked-calculated*	3.34	3.69	3.37

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

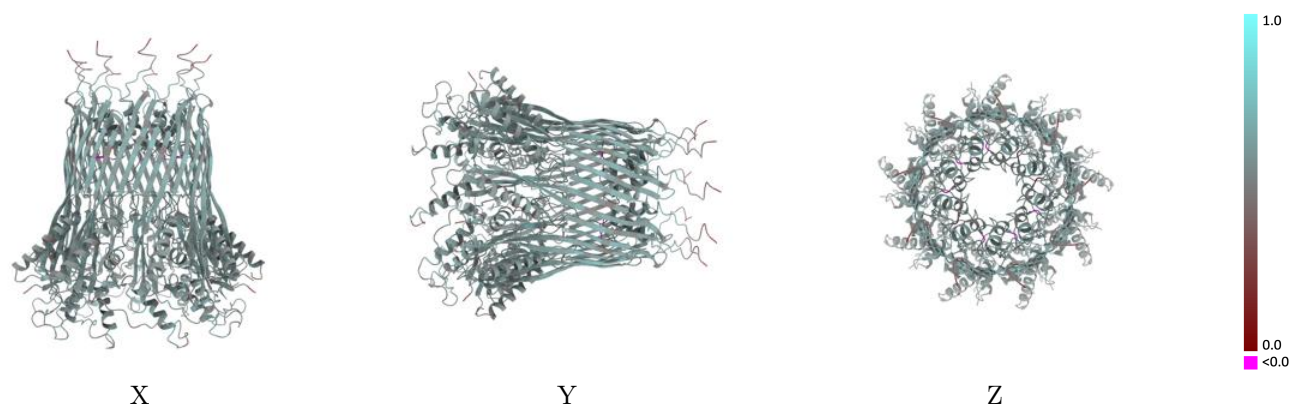
This section contains information regarding the fit between EMDB map EMD-0947 and PDB model 6LQJ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



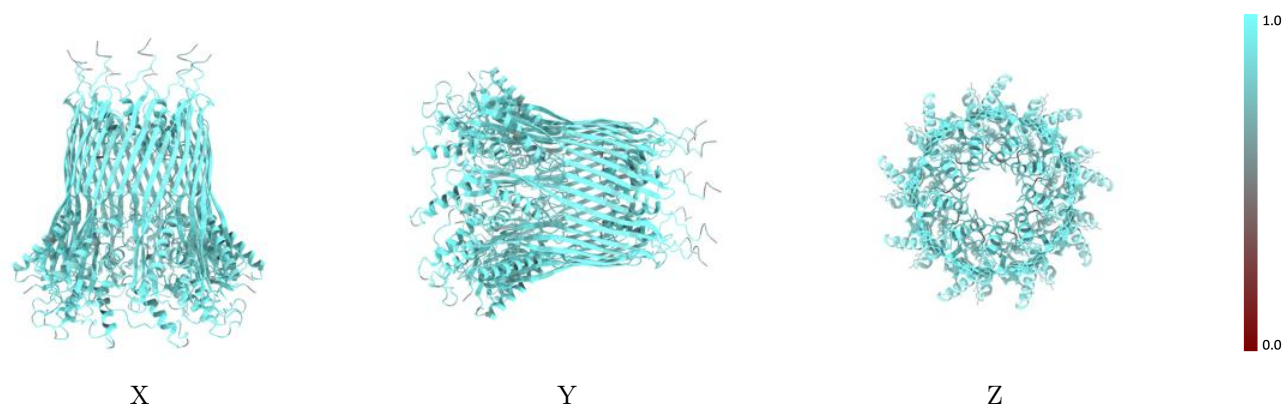
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



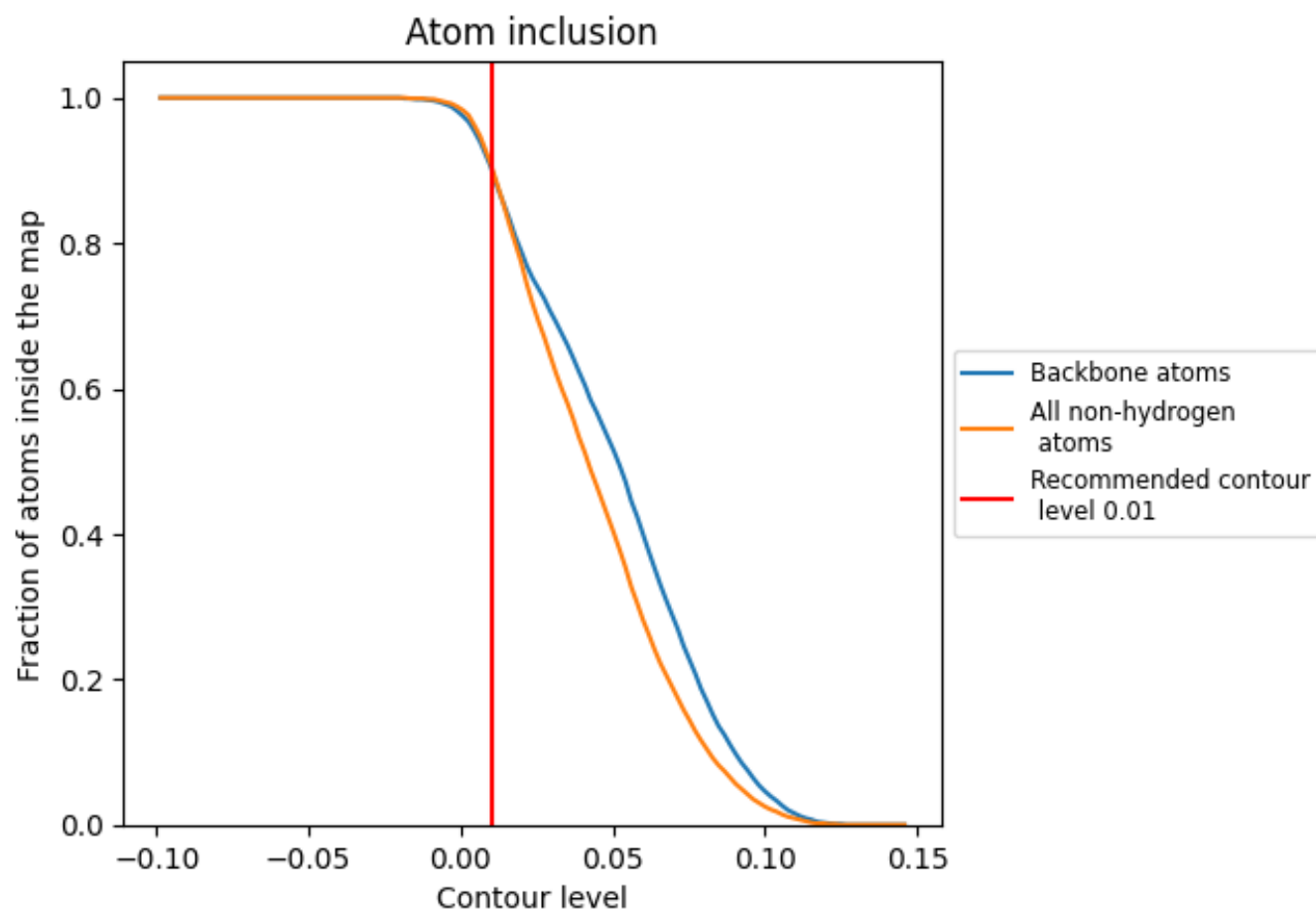
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9080	 0.5450
A	 0.9100	 0.5480
B	 0.9120	 0.5500
C	 0.9110	 0.5520
D	 0.9140	 0.5500
E	 0.9050	 0.5500
F	 0.9160	 0.5490
G	 0.9130	 0.5510
H	 0.9110	 0.5500
I	 0.9120	 0.5490
a	 0.8860	 0.5230
b	 0.8860	 0.5220
c	 0.8890	 0.5170
d	 0.8830	 0.5230
e	 0.8860	 0.5240
f	 0.8920	 0.5240
g	 0.8960	 0.5200
h	 0.8920	 0.5240
i	 0.8920	 0.5200

