



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:04 AM UTC

PDB ID : 6LQH / pdb_00006lqh
EMDB ID : EMD-0945
Title : High resolution architecture of curli complex
Authors : Zhang, M.; Shi, H.; Huang, Y.
Deposited on : 2020-01-13
Resolution : 2.94 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

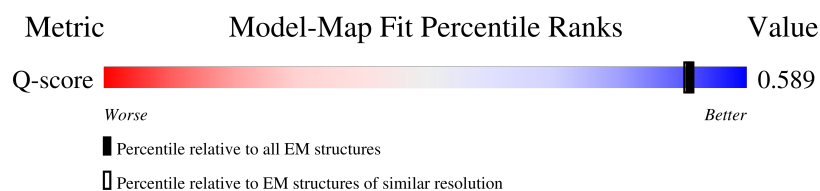
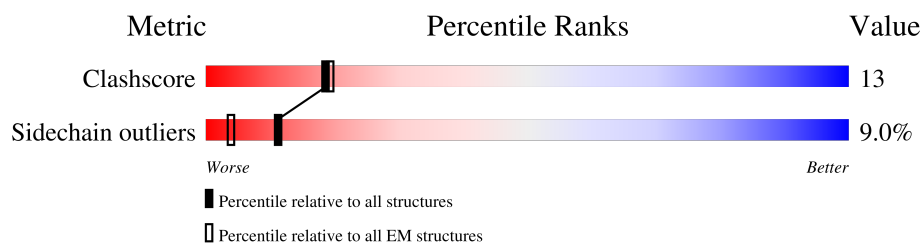
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13068 (2.44 - 3.44)

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

Mol	Chain	Length	Quality of chain
1	A	285	51% 18% • 28%
1	B	285	50% 20% • 28%
1	C	285	50% 20% • 28%
1	D	285	51% 19% • 28%
1	E	285	51% 19% • 28%

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Mol	Chain	Length	Quality of chain
1	F	285	
1	G	285	
1	H	285	
1	I	285	
2	a	144	
2	b	144	
2	c	144	
2	d	144	
2	e	144	
2	f	144	
2	g	144	
2	h	144	
2	i	144	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16623 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 1589	C 1008	N 270	O 306	S 5	0	0
1	B	206	Total 1589	C 1008	N 270	O 306	S 5	0	0
1	C	206	Total 1589	C 1008	N 270	O 306	S 5	0	0
1	D	206	Total 1589	C 1008	N 270	O 306	S 5	0	0
1	E	206	Total 1589	C 1008	N 270	O 306	S 5	0	0
1	F	206	Total 1589	C 1008	N 270	O 306	S 5	0	0
1	G	206	Total 1589	C 1008	N 270	O 306	S 5	0	0
1	H	206	Total 1589	C 1008	N 270	O 306	S 5	0	0
1	I	206	Total 1589	C 1008	N 270	O 306	S 5	0	0

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	34	Total	C	N	O	S	0	0
			258	159	47	51	1		
2	b	34	Total	C	N	O	S	0	0
			258	159	47	51	1		
2	c	34	Total	C	N	O	S	0	0
			258	159	47	51	1		
2	d	34	Total	C	N	O	S	0	0
			258	159	47	51	1		
2	e	34	Total	C	N	O	S	0	0
			258	159	47	51	1		
2	f	34	Total	C	N	O	S	0	0
			258	159	47	51	1		
2	g	34	Total	C	N	O	S	0	0
			258	159	47	51	1		
2	h	34	Total	C	N	O	S	0	0
			258	159	47	51	1		
2	i	34	Total	C	N	O	S	0	0
			258	159	47	51	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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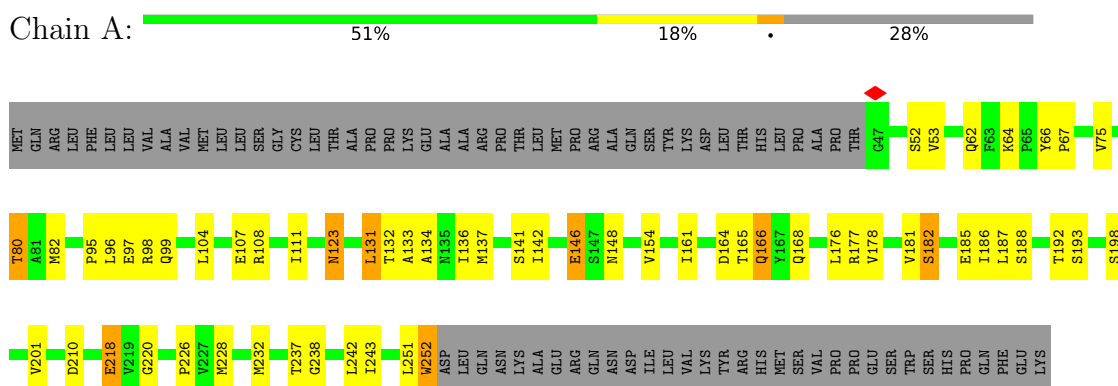
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Chain	Residue	Modelled	Actual	Comment	Reference
h	140	HIS	-	expression tag	UNP P0AE98
h	141	HIS	-	expression tag	UNP P0AE98
h	142	HIS	-	expression tag	UNP P0AE98
h	143	HIS	-	expression tag	UNP P0AE98
h	144	HIS	-	expression tag	UNP P0AE98
i	139	HIS	-	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

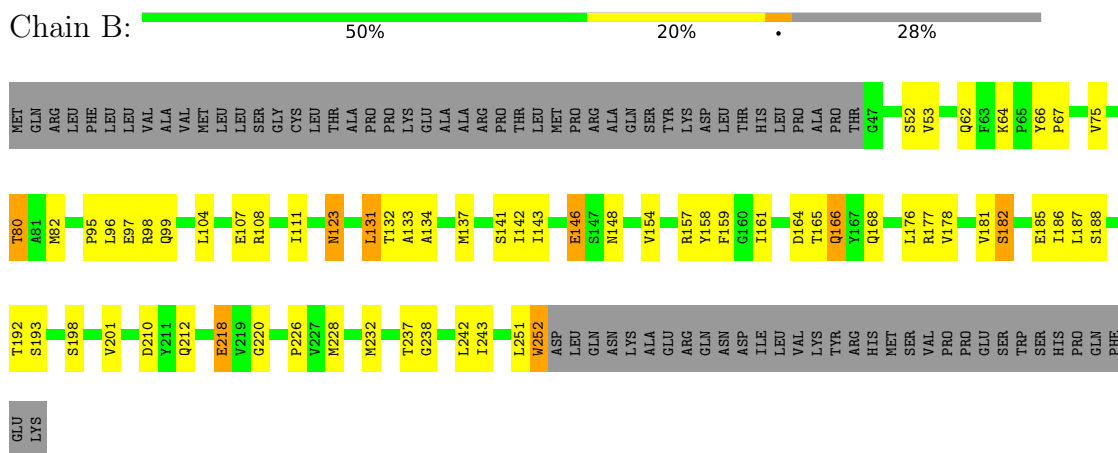
3 Residue-property plots

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.

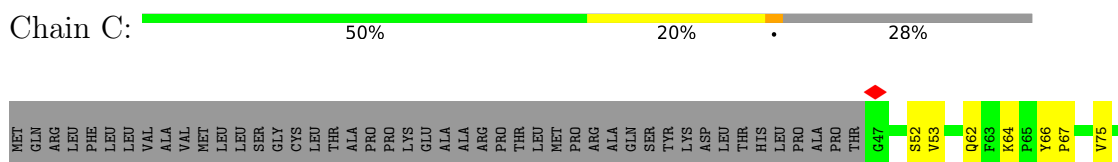
- Molecule 1: Curli production assembly/transport component CsgG

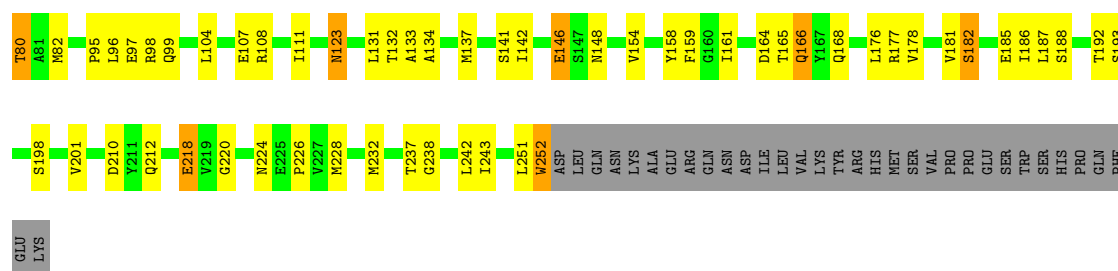


- Molecule 1: Curli production assembly/transport component CsgG



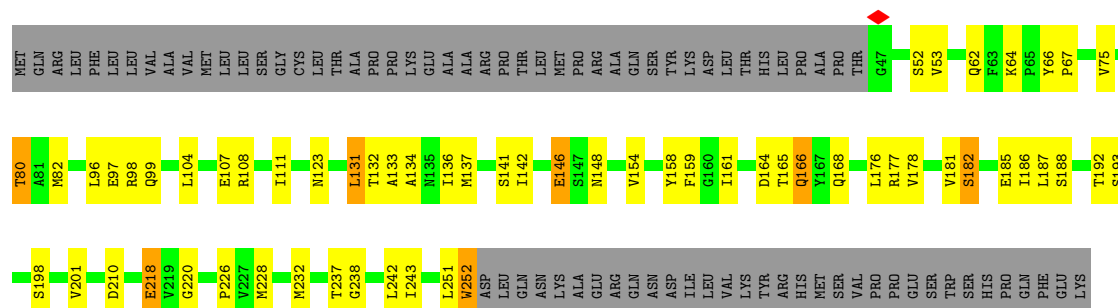
- Molecule 1: Curli production assembly/transport component CsgG





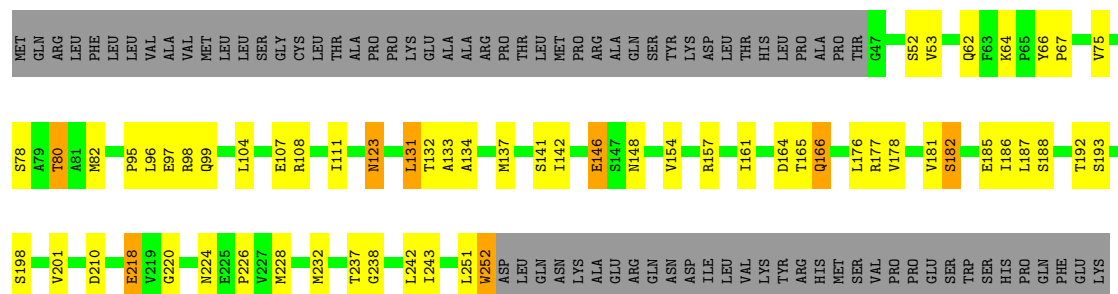
- Molecule 1: Curli production assembly/transport component CsgG

Chain D: 51% 19% 28%



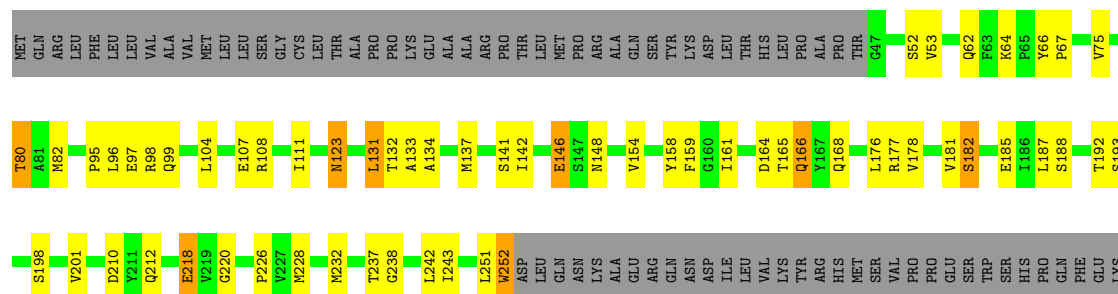
- Molecule 1: Curli production assembly/transport component CsgG

Chain E: 51% 19% 28%



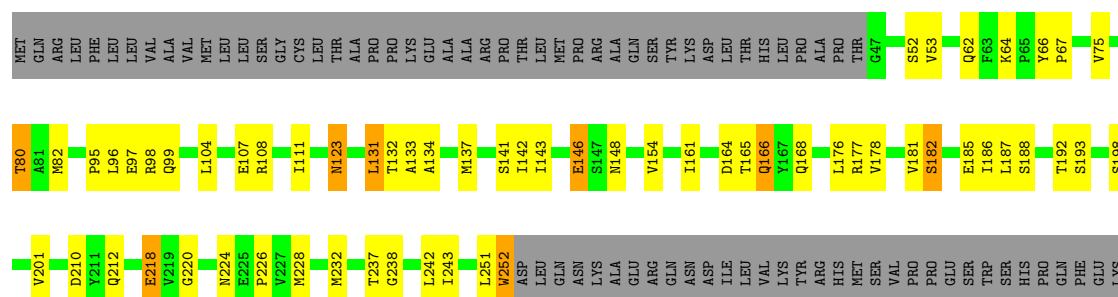
- Molecule 1: Curli production assembly/transport component CsgG

Chain F: 51% 19% 28%



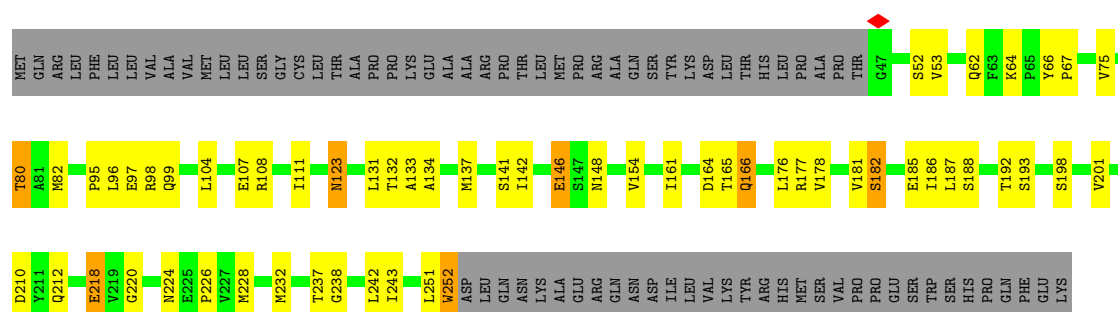
- Molecule 1: Curli production assembly/transport component CsgG

Chain G:  51% 19% 28%



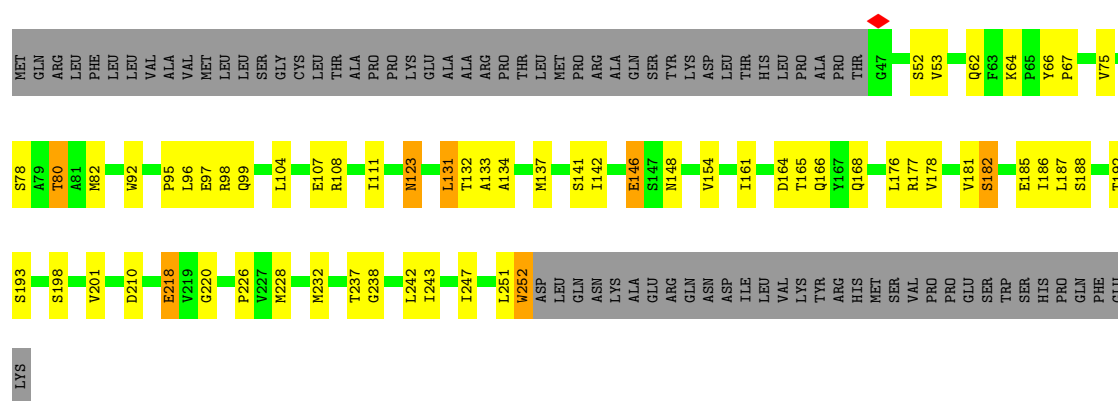
• Molecule 1: Curli production assembly/transport component CsgG

Chain H:  51% 19% 28%



• Molecule 1: Curli production assembly/transport component CsgG

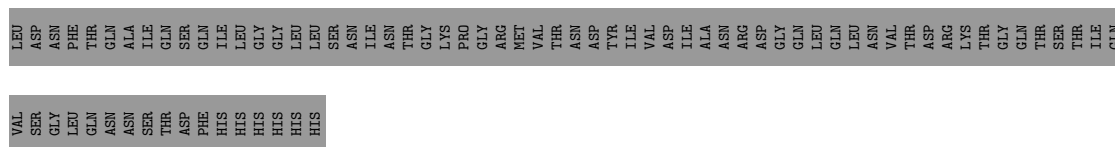
Chain I:  51% 19% 28%



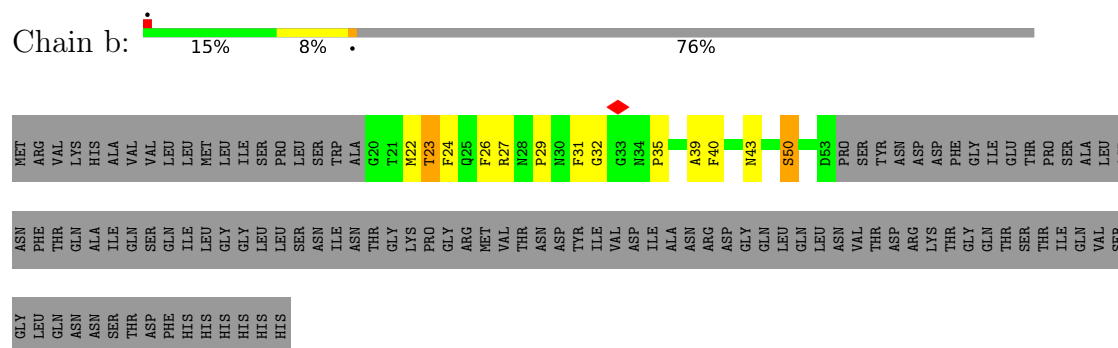
• Molecule 2: Curli production assembly/transport component CsgF

Chain a:  14% 8% 76%

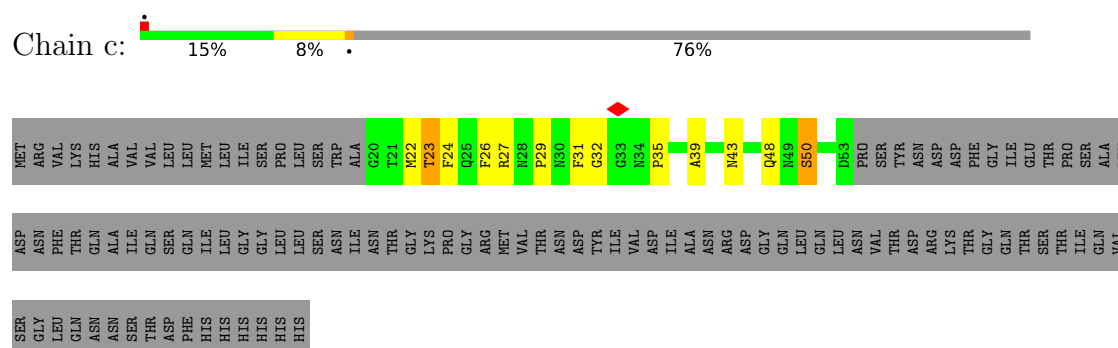




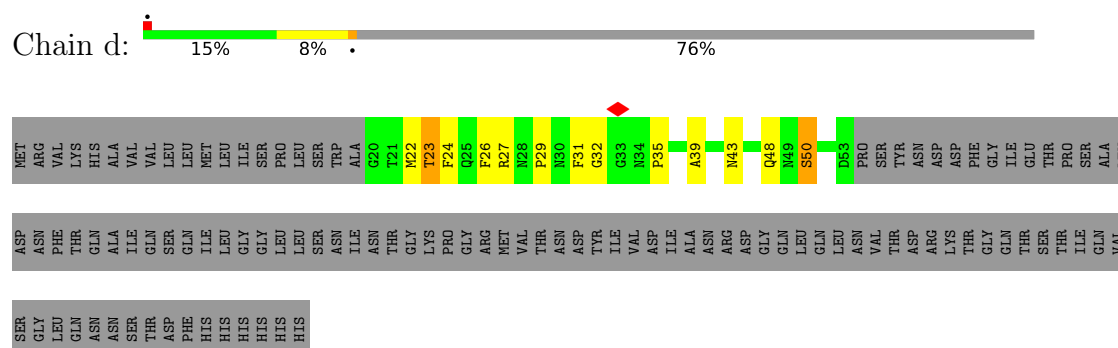
• Molecule 2: Curli production assembly/transport component CsgF



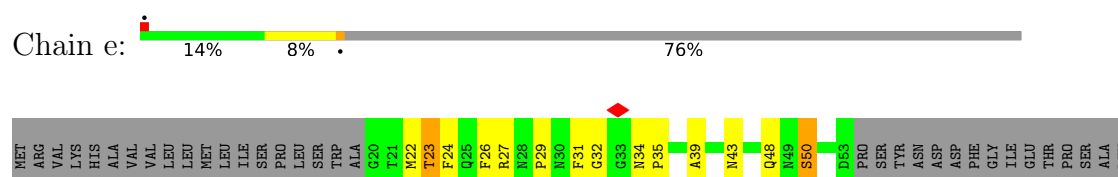
• Molecule 2: Curli production assembly/transport component CsgF

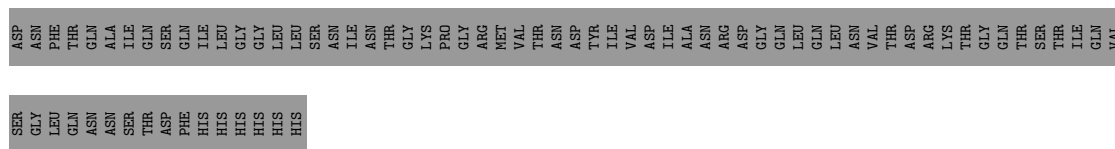


• Molecule 2: Curli production assembly/transport component CsgF

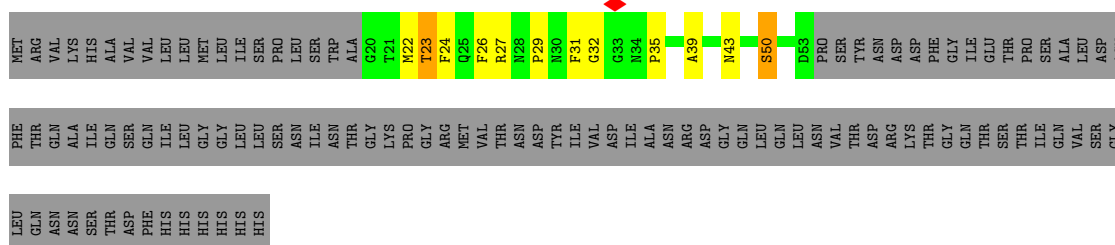


• Molecule 2: Curli production assembly/transport component CsgF

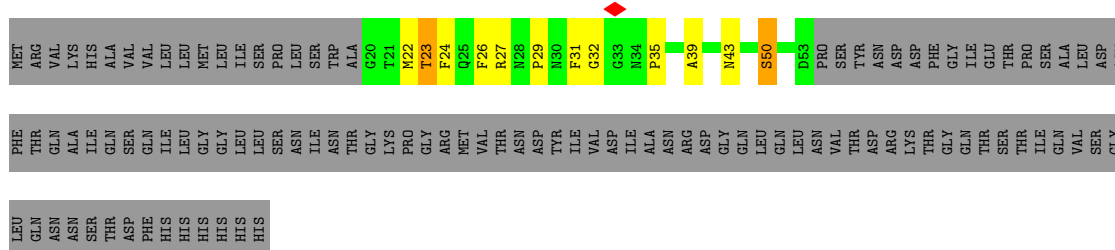




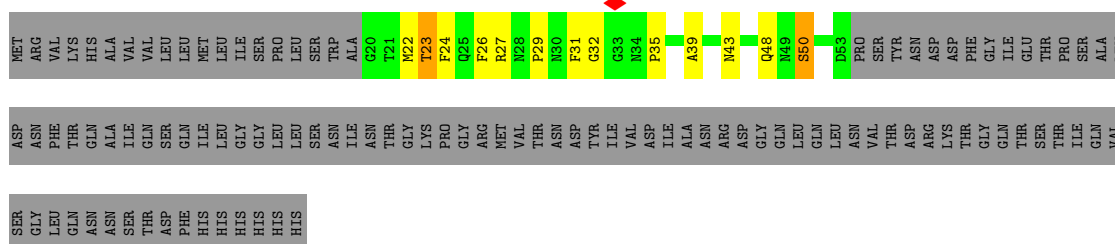
- Molecule 2: Curli production assembly/transport component CsgF



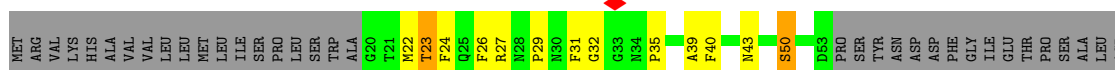
- Molecule 2: Curli production assembly/transport component CsgF



- Molecule 2: Curli production assembly/transport component CsgF



- Molecule 2: Curli production assembly/transport component CsgF



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

GLY
LEU
GLN
ASN
SER
THR
ASP
PHE
HIS
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HIS
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D9	Depositor
Number of particles used	101241	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	0.140	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/1614	0.48	0/2190
1	B	0.39	0/1614	0.48	0/2190
1	C	0.39	0/1614	0.48	0/2190
1	D	0.39	0/1614	0.48	0/2190
1	E	0.39	0/1614	0.48	0/2190
1	F	0.39	0/1614	0.48	0/2190
1	G	0.39	0/1614	0.48	0/2190
1	H	0.39	0/1614	0.48	0/2190
1	I	0.39	0/1614	0.48	0/2190
2	a	0.23	0/264	0.52	0/357
2	b	0.23	0/264	0.52	0/357
2	c	0.23	0/264	0.52	0/357
2	d	0.23	0/264	0.52	0/357
2	e	0.23	0/264	0.52	0/357
2	f	0.23	0/264	0.52	0/357
2	g	0.23	0/264	0.52	0/357
2	h	0.23	0/264	0.52	0/357
2	i	0.23	0/264	0.52	0/357
All	All	0.37	0/16902	0.48	0/22923

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1589	0	1596	52	0
1	B	1589	0	1596	52	0
1	C	1589	0	1596	51	0
1	D	1589	0	1596	50	0
1	E	1589	0	1596	51	0
1	F	1589	0	1596	49	0
1	G	1589	0	1596	53	0
1	H	1589	0	1596	51	0
1	I	1589	0	1596	49	0
2	a	258	0	225	18	0
2	b	258	0	225	18	0
2	c	258	0	225	19	0
2	d	258	0	225	14	0
2	e	258	0	225	20	0
2	f	258	0	225	17	0
2	g	258	0	225	18	0
2	h	258	0	225	20	0
2	i	258	0	225	18	0
All	All	16623	0	16389	430	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 13.

All (430) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:29:PRO:HB3	2:a:35:PRO:HA	1.63	0.80
2:f:29:PRO:HB3	2:f:35:PRO:HA	1.63	0.80
2:i:29:PRO:HB3	2:i:35:PRO:HA	1.63	0.80
2:d:29:PRO:HB3	2:d:35:PRO:HA	1.63	0.80
2:h:29:PRO:HB3	2:h:35:PRO:HA	1.63	0.80
2:b:29:PRO:HB3	2:b:35:PRO:HA	1.63	0.80
2:e:29:PRO:HB3	2:e:35:PRO:HA	1.63	0.80
1:E:164:ASP:HB3	2:h:31:PHE:HB2	1.63	0.79
2:c:29:PRO:HB3	2:c:35:PRO:HA	1.63	0.79
2:g:29:PRO:HB3	2:g:35:PRO:HA	1.63	0.79
1:F:111:ILE:HG12	1:H:133:ALA:HB1	1.66	0.78
1:B:133:ALA:HB1	1:E:111:ILE:HG12	1.65	0.78
1:D:111:ILE:HG12	1:F:133:ALA:HB1	1.67	0.76
1:C:133:ALA:HB1	1:G:111:ILE:HG12	1.66	0.76
1:C:111:ILE:HG12	1:D:133:ALA:HB1	1.67	0.76
1:A:111:ILE:HG12	1:I:133:ALA:HB1	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:ASP:HB3	2:i:31:PHE:HB2	1.69	0.74
1:A:133:ALA:HB1	1:B:111:ILE:HG12	1.68	0.74
1:E:133:ALA:HB1	1:H:111:ILE:HG12	1.70	0.74
1:H:220:GLY:HA3	2:h:24:PHE:CE1	2.24	0.73
2:c:27:ARG:HE	2:g:31:PHE:HA	1.54	0.72
1:G:133:ALA:HB1	1:I:111:ILE:HG12	1.69	0.72
1:B:164:ASP:HB3	2:e:31:PHE:HB2	1.71	0.71
1:H:164:ASP:HB3	2:f:31:PHE:HB2	1.74	0.69
1:C:146:GLU:HG2	1:G:226:PRO:HA	1.74	0.69
1:A:146:GLU:HG2	1:B:226:PRO:HA	1.75	0.68
1:D:164:ASP:HB3	2:c:31:PHE:HB2	1.75	0.68
1:A:164:ASP:HB3	2:b:31:PHE:HB2	1.76	0.67
1:G:146:GLU:HG2	1:I:226:PRO:HA	1.77	0.67
1:B:146:GLU:HG2	1:E:226:PRO:HA	1.77	0.66
1:A:226:PRO:HA	1:I:146:GLU:HG2	1.77	0.66
1:C:148:ASN:ND2	2:g:23:THR:OG1	2.28	0.66
1:B:148:ASN:ND2	2:e:23:THR:OG1	2.28	0.66
1:C:226:PRO:HA	1:D:146:GLU:HG2	1.76	0.66
1:E:146:GLU:HG2	1:H:226:PRO:HA	1.77	0.66
1:C:220:GLY:HA3	2:c:24:PHE:CE1	2.31	0.66
1:A:98:ARG:NH2	1:A:132:THR:O	2.30	0.65
1:B:98:ARG:NH2	1:B:132:THR:O	2.30	0.65
1:E:98:ARG:NH2	1:E:132:THR:O	2.30	0.65
1:G:98:ARG:NH2	1:G:132:THR:O	2.30	0.65
1:I:98:ARG:NH2	1:I:132:THR:O	2.30	0.65
2:c:31:PHE:HA	2:d:27:ARG:HE	1.61	0.65
1:D:98:ARG:NH2	1:D:132:THR:O	2.30	0.65
1:F:98:ARG:NH2	1:F:132:THR:O	2.30	0.65
1:F:226:PRO:HA	1:H:146:GLU:HG2	1.77	0.65
1:H:98:ARG:NH2	1:H:132:THR:O	2.30	0.65
1:E:148:ASN:ND2	2:h:23:THR:OG1	2.29	0.65
1:D:226:PRO:HA	1:F:146:GLU:HG2	1.77	0.65
1:G:148:ASN:ND2	2:i:23:THR:OG1	2.30	0.64
2:d:31:PHE:HA	2:f:27:ARG:HE	1.62	0.64
1:C:98:ARG:NH2	1:C:132:THR:O	2.30	0.64
1:I:164:ASP:HB3	2:a:31:PHE:HB2	1.81	0.63
1:E:220:GLY:HA3	2:e:24:PHE:CE1	2.33	0.63
1:I:148:ASN:ND2	2:a:23:THR:OG1	2.33	0.61
1:D:148:ASN:ND2	2:c:23:THR:OG1	2.33	0.61
1:H:224:ASN:OD1	2:h:22:MET:N	2.28	0.61
1:G:220:GLY:HA3	2:g:24:PHE:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ASP:HB3	2:g:31:PHE:HB2	1.83	0.60
1:H:148:ASN:ND2	2:f:23:THR:OG1	2.34	0.60
2:f:39:ALA:O	2:f:43:ASN:ND2	2.35	0.60
2:b:39:ALA:O	2:b:43:ASN:ND2	2.35	0.60
2:g:39:ALA:O	2:g:43:ASN:ND2	2.35	0.60
2:e:39:ALA:O	2:e:43:ASN:ND2	2.35	0.60
2:i:39:ALA:O	2:i:43:ASN:ND2	2.35	0.60
2:d:39:ALA:O	2:d:43:ASN:ND2	2.35	0.60
2:c:39:ALA:O	2:c:43:ASN:ND2	2.35	0.59
1:A:97:GLU:OE2	1:I:177:ARG:NH1	2.35	0.59
1:E:187:LEU:HD13	1:E:251:LEU:HD21	1.84	0.59
2:a:39:ALA:O	2:a:43:ASN:ND2	2.35	0.59
2:h:39:ALA:O	2:h:43:ASN:ND2	2.35	0.59
1:B:187:LEU:HD13	1:B:251:LEU:HD21	1.84	0.59
1:A:187:LEU:HD13	1:A:251:LEU:HD21	1.84	0.59
1:D:97:GLU:OE2	1:F:177:ARG:NH1	2.36	0.59
1:H:218:GLU:HG2	2:h:26:PHE:CD1	2.37	0.59
1:I:220:GLY:HA3	2:i:24:PHE:CE1	2.38	0.59
1:G:187:LEU:HD13	1:G:251:LEU:HD21	1.84	0.59
1:A:148:ASN:ND2	2:b:23:THR:OG1	2.36	0.58
1:C:187:LEU:HD13	1:C:251:LEU:HD21	1.84	0.58
1:I:187:LEU:HD13	1:I:251:LEU:HD21	1.84	0.58
2:a:31:PHE:HA	2:i:27:ARG:HE	1.67	0.58
2:g:26:PHE:HB2	2:g:32:GLY:HA3	1.86	0.58
2:e:26:PHE:HB2	2:e:32:GLY:HA3	1.86	0.58
1:A:220:GLY:HA3	2:a:24:PHE:CE1	2.39	0.58
1:F:187:LEU:HD13	1:F:251:LEU:HD21	1.84	0.58
1:F:220:GLY:HA3	2:f:24:PHE:CE1	2.39	0.58
1:H:187:LEU:HD13	1:H:251:LEU:HD21	1.84	0.58
2:a:26:PHE:HB2	2:a:32:GLY:HA3	1.86	0.58
1:I:123:ASN:OD1	1:I:123:ASN:N	2.36	0.58
2:h:26:PHE:HB2	2:h:32:GLY:HA3	1.86	0.58
1:E:243:ILE:HA	1:E:252:TRP:HE1	1.69	0.58
1:G:243:ILE:HA	1:G:252:TRP:HE1	1.69	0.58
2:i:26:PHE:HB2	2:i:32:GLY:HA3	1.86	0.58
1:D:187:LEU:HD13	1:D:251:LEU:HD21	1.84	0.58
1:I:243:ILE:HA	1:I:252:TRP:HE1	1.69	0.58
2:b:26:PHE:HB2	2:b:32:GLY:HA3	1.86	0.58
2:f:26:PHE:HB2	2:f:32:GLY:HA3	1.86	0.58
1:B:137:MET:HE1	1:E:104:LEU:HA	1.85	0.57
1:C:97:GLU:OE2	1:D:177:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:ASN:OD1	2:g:22:MET:N	2.33	0.57
2:d:26:PHE:HB2	2:d:32:GLY:HA3	1.86	0.57
1:F:243:ILE:HA	1:F:252:TRP:HE1	1.69	0.57
2:c:26:PHE:HB2	2:c:32:GLY:HA3	1.86	0.57
1:A:104:LEU:HA	1:I:137:MET:HE1	1.86	0.57
2:a:27:ARG:HE	2:b:31:PHE:HA	1.68	0.57
1:H:166:GLN:HB3	2:h:22:MET:HE1	1.84	0.57
1:A:177:ARG:NH1	1:B:97:GLU:OE2	2.36	0.57
1:G:177:ARG:NH1	1:I:97:GLU:OE2	2.37	0.57
1:A:243:ILE:HA	1:A:252:TRP:HE1	1.69	0.57
1:B:177:ARG:NH1	1:E:97:GLU:OE2	2.36	0.57
1:C:177:ARG:NH1	1:G:97:GLU:OE2	2.37	0.57
1:E:123:ASN:OD1	1:E:123:ASN:N	2.36	0.57
1:D:243:ILE:HA	1:D:252:TRP:HE1	1.69	0.57
1:H:218:GLU:HG2	2:h:26:PHE:HD1	1.67	0.57
1:C:243:ILE:HA	1:C:252:TRP:HE1	1.69	0.57
1:B:243:ILE:HA	1:B:252:TRP:HE1	1.69	0.56
1:C:218:GLU:HG2	2:c:26:PHE:CD1	2.41	0.56
1:H:243:ILE:HA	1:H:252:TRP:HE1	1.69	0.56
1:E:177:ARG:NH1	1:H:97:GLU:OE2	2.38	0.56
1:C:218:GLU:HG2	2:c:26:PHE:HD1	1.71	0.56
1:G:123:ASN:OD1	1:G:123:ASN:N	2.36	0.56
1:G:137:MET:HE1	1:I:104:LEU:HA	1.89	0.55
2:f:31:PHE:HA	2:h:27:ARG:HE	1.70	0.55
1:B:53:VAL:HG12	1:B:80:THR:HG23	1.88	0.55
1:D:104:LEU:HA	1:F:137:MET:HE1	1.88	0.55
1:F:97:GLU:OE2	1:H:177:ARG:NH1	2.38	0.55
1:B:182:SER:O	1:E:108:ARG:NH1	2.40	0.55
1:F:104:LEU:HA	1:H:137:MET:HE1	1.88	0.55
1:I:53:VAL:HG12	1:I:80:THR:HG23	1.88	0.55
1:A:53:VAL:HG12	1:A:80:THR:HG23	1.88	0.55
1:G:164:ASP:CB	2:i:31:PHE:HB2	2.36	0.55
1:E:53:VAL:HG12	1:E:80:THR:HG23	1.88	0.55
1:B:123:ASN:OD1	1:B:123:ASN:N	2.36	0.55
1:C:137:MET:HE1	1:G:104:LEU:HA	1.89	0.54
2:b:27:ARG:HE	2:e:31:PHE:HA	1.72	0.54
1:F:123:ASN:OD1	1:F:123:ASN:N	2.36	0.54
1:G:53:VAL:HG12	1:G:80:THR:HG23	1.88	0.54
1:C:104:LEU:HA	1:D:137:MET:HE1	1.90	0.54
1:D:168:GLN:HG3	2:d:22:MET:HE3	1.89	0.54
1:D:53:VAL:HG12	1:D:80:THR:HG23	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:VAL:HG12	1:F:80:THR:HG23	1.88	0.53
1:H:53:VAL:HG12	1:H:80:THR:HG23	1.88	0.53
1:C:53:VAL:HG12	1:C:80:THR:HG23	1.88	0.53
1:B:220:GLY:HA3	2:b:24:PHE:CE1	2.44	0.53
1:A:137:MET:HE1	1:B:104:LEU:HA	1.90	0.52
1:E:164:ASP:CB	2:h:31:PHE:HB2	2.35	0.52
1:D:108:ARG:NH1	1:F:182:SER:O	2.41	0.52
1:F:218:GLU:HG2	2:f:26:PHE:CD1	2.44	0.52
2:g:27:ARG:HE	2:i:31:PHE:HA	1.73	0.52
1:B:146:GLU:HA	1:B:146:GLU:OE1	2.10	0.52
1:D:146:GLU:HA	1:D:146:GLU:OE1	2.10	0.52
1:I:218:GLU:HG2	2:i:26:PHE:HD1	1.74	0.52
1:A:146:GLU:OE1	1:A:146:GLU:HA	2.10	0.52
1:C:123:ASN:OD1	1:C:123:ASN:N	2.36	0.52
1:E:218:GLU:HG2	2:e:26:PHE:HD1	1.73	0.52
1:I:218:GLU:HG2	2:i:26:PHE:CD1	2.44	0.52
1:A:165:THR:HG23	1:A:201:VAL:HG22	1.92	0.52
1:E:218:GLU:HG2	2:e:26:PHE:CD1	2.44	0.52
1:G:165:THR:HG23	1:G:201:VAL:HG22	1.92	0.52
1:G:182:SER:O	1:I:108:ARG:NH1	2.42	0.52
1:C:146:GLU:OE1	1:C:146:GLU:HA	2.10	0.52
1:B:165:THR:HG23	1:B:201:VAL:HG22	1.92	0.52
1:B:218:GLU:HG2	2:b:26:PHE:CD1	2.44	0.52
2:a:50:SER:O	2:a:50:SER:OG	2.27	0.52
2:d:50:SER:O	2:d:50:SER:OG	2.27	0.52
1:C:165:THR:HG23	1:C:201:VAL:HG22	1.92	0.51
1:E:146:GLU:OE1	1:E:146:GLU:HA	2.10	0.51
1:F:146:GLU:OE1	1:F:146:GLU:HA	2.10	0.51
1:I:165:THR:HG23	1:I:201:VAL:HG22	1.92	0.51
1:D:165:THR:HG23	1:D:201:VAL:HG22	1.92	0.51
1:F:218:GLU:HG2	2:f:26:PHE:HD1	1.75	0.51
1:F:164:ASP:HB3	2:d:31:PHE:HB2	1.93	0.51
2:i:50:SER:O	2:i:50:SER:OG	2.27	0.51
1:E:165:THR:HG23	1:E:201:VAL:HG22	1.92	0.51
1:D:218:GLU:HG2	2:d:26:PHE:CD1	2.46	0.51
1:F:165:THR:HG23	1:F:201:VAL:HG22	1.92	0.51
1:G:146:GLU:HA	1:G:146:GLU:OE1	2.10	0.51
1:H:165:THR:HG23	1:H:201:VAL:HG22	1.92	0.51
1:I:146:GLU:HA	1:I:146:GLU:OE1	2.10	0.51
1:D:220:GLY:HA3	2:d:24:PHE:CE1	2.46	0.51
1:G:164:ASP:HB3	2:i:31:PHE:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:50:SER:O	2:g:50:SER:OG	2.27	0.51
1:E:137:MET:HE1	1:H:104:LEU:HA	1.92	0.50
2:b:50:SER:O	2:b:50:SER:OG	2.27	0.50
1:H:123:ASN:OD1	1:H:123:ASN:N	2.36	0.50
1:H:146:GLU:OE1	1:H:146:GLU:HA	2.10	0.50
1:H:176:LEU:HB3	1:H:242:LEU:HD11	1.94	0.50
1:A:176:LEU:HB3	1:A:242:LEU:HD11	1.94	0.50
1:E:157:ARG:HB2	2:h:31:PHE:HE2	1.76	0.50
2:e:50:SER:O	2:e:50:SER:OG	2.27	0.50
1:E:176:LEU:HB3	1:E:242:LEU:HD11	1.94	0.50
1:I:176:LEU:HB3	1:I:242:LEU:HD11	1.94	0.50
1:F:176:LEU:HB3	1:F:242:LEU:HD11	1.94	0.50
1:F:108:ARG:NH1	1:H:182:SER:O	2.44	0.50
1:D:176:LEU:HB3	1:D:242:LEU:HD11	1.94	0.50
1:B:176:LEU:HB3	1:B:242:LEU:HD11	1.94	0.50
1:G:176:LEU:HB3	1:G:242:LEU:HD11	1.94	0.50
1:H:164:ASP:CB	2:f:31:PHE:HB2	2.42	0.50
1:C:176:LEU:HB3	1:C:242:LEU:HD11	1.94	0.49
1:G:166:GLN:HB3	2:g:22:MET:HE1	1.93	0.49
1:A:108:ARG:NH1	1:I:182:SER:O	2.42	0.49
1:C:108:ARG:NH1	1:D:182:SER:O	2.44	0.49
2:c:50:SER:O	2:c:50:SER:OG	2.27	0.49
1:A:218:GLU:HG2	2:a:26:PHE:CD1	2.47	0.49
1:B:161:ILE:H	1:B:161:ILE:HD12	1.78	0.49
1:F:161:ILE:HD12	1:F:161:ILE:H	1.78	0.49
1:I:168:GLN:HG3	2:i:22:MET:HE3	1.95	0.49
1:C:166:GLN:HB3	2:c:22:MET:HE1	1.93	0.49
1:E:166:GLN:HB3	2:e:22:MET:HE1	1.94	0.49
2:h:50:SER:O	2:h:50:SER:OG	2.27	0.49
1:D:161:ILE:H	1:D:161:ILE:HD12	1.78	0.49
1:A:218:GLU:HG2	2:a:26:PHE:HD1	1.77	0.48
1:D:66:TYR:CG	1:D:67:PRO:HA	2.48	0.48
1:G:161:ILE:H	1:G:161:ILE:HD12	1.78	0.48
1:A:66:TYR:CG	1:A:67:PRO:HA	2.49	0.48
1:A:161:ILE:HD12	1:A:161:ILE:H	1.78	0.48
1:E:107:GLU:O	1:E:111:ILE:HG13	2.13	0.48
1:E:161:ILE:HD12	1:E:161:ILE:H	1.78	0.48
1:G:66:TYR:CG	1:G:67:PRO:HA	2.48	0.48
1:B:107:GLU:O	1:B:111:ILE:HG13	2.13	0.48
1:F:66:TYR:CG	1:F:67:PRO:HA	2.49	0.48
1:G:218:GLU:HG2	2:g:26:PHE:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ASN:OD1	2:c:22:MET:N	2.39	0.48
1:F:148:ASN:ND2	2:d:23:THR:OG1	2.47	0.48
1:H:66:TYR:CG	1:H:67:PRO:HA	2.49	0.48
2:f:50:SER:O	2:f:50:SER:OG	2.27	0.48
1:E:66:TYR:CG	1:E:67:PRO:HA	2.48	0.48
1:B:168:GLN:HG3	2:b:22:MET:HE3	1.96	0.48
1:I:66:TYR:CG	1:I:67:PRO:HA	2.48	0.48
1:I:161:ILE:H	1:I:161:ILE:HD12	1.78	0.48
1:B:66:TYR:CG	1:B:67:PRO:HA	2.49	0.47
1:F:107:GLU:O	1:F:111:ILE:HG13	2.14	0.47
2:b:40:PHE:CE2	2:e:29:PRO:HG2	2.49	0.47
1:C:182:SER:O	1:G:108:ARG:NH1	2.46	0.47
1:E:182:SER:O	1:H:108:ARG:NH1	2.45	0.47
1:G:148:ASN:ND2	2:i:23:THR:HG1	2.11	0.47
1:H:161:ILE:HD12	1:H:161:ILE:H	1.78	0.47
1:I:107:GLU:O	1:I:111:ILE:HG13	2.14	0.47
1:C:161:ILE:HD12	1:C:161:ILE:H	1.78	0.47
1:D:107:GLU:O	1:D:111:ILE:HG13	2.14	0.47
1:A:107:GLU:O	1:A:111:ILE:HG13	2.14	0.47
1:A:164:ASP:CB	2:b:31:PHE:HB2	2.44	0.47
1:C:107:GLU:O	1:C:111:ILE:HG13	2.14	0.47
1:G:166:GLN:HG3	2:i:26:PHE:CE2	2.49	0.47
1:H:107:GLU:O	1:H:111:ILE:HG13	2.14	0.47
1:H:212:GLN:HB3	2:e:48:GLN:HA	1.95	0.47
1:C:66:TYR:CG	1:C:67:PRO:HA	2.49	0.47
1:E:224:ASN:OD1	2:e:22:MET:N	2.39	0.47
1:D:218:GLU:HG2	2:d:26:PHE:HD1	1.80	0.47
1:F:96:LEU:HD12	1:F:134:ALA:HB2	1.97	0.47
1:G:218:GLU:HG2	2:g:26:PHE:CD1	2.50	0.47
1:D:96:LEU:HD12	1:D:134:ALA:HB2	1.97	0.47
1:D:164:ASP:CB	2:c:31:PHE:HB2	2.43	0.47
1:G:107:GLU:O	1:G:111:ILE:HG13	2.14	0.47
1:H:96:LEU:HD12	1:H:134:ALA:HB2	1.97	0.47
1:E:164:ASP:HB3	2:h:31:PHE:CB	2.39	0.47
1:E:131:LEU:HD12	1:E:131:LEU:HA	1.68	0.46
2:e:27:ARG:HE	2:h:31:PHE:HA	1.79	0.46
1:C:168:GLN:HG3	2:c:22:MET:HE3	1.97	0.46
1:E:96:LEU:HD12	1:E:134:ALA:HB2	1.97	0.46
1:C:96:LEU:HD12	1:C:134:ALA:HB2	1.97	0.46
1:G:166:GLN:HG3	2:i:26:PHE:HE2	1.79	0.46
1:H:224:ASN:CG	2:h:22:MET:H	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:HG2	2:b:26:PHE:HD1	1.78	0.46
1:H:137:MET:HE3	1:H:181:VAL:HG22	1.98	0.46
1:A:75:VAL:HG11	1:A:142:ILE:HG21	1.98	0.46
1:A:137:MET:HE3	1:A:181:VAL:HG22	1.98	0.46
1:B:137:MET:HE3	1:B:181:VAL:HG22	1.98	0.46
1:G:137:MET:HE3	1:G:181:VAL:HG22	1.98	0.46
1:I:137:MET:HE3	1:I:181:VAL:HG22	1.98	0.46
1:A:96:LEU:HD12	1:A:134:ALA:HB2	1.97	0.46
1:C:166:GLN:HG3	2:g:26:PHE:CE2	2.51	0.46
1:E:137:MET:HE3	1:E:181:VAL:HG22	1.98	0.46
1:F:137:MET:HE3	1:F:181:VAL:HG22	1.98	0.46
1:H:164:ASP:HB3	2:f:31:PHE:CB	2.45	0.46
1:B:164:ASP:CB	2:e:31:PHE:HB2	2.41	0.45
1:C:146:GLU:HB2	1:G:228:MET:HE2	1.98	0.45
1:D:137:MET:HE3	1:D:181:VAL:HG22	1.98	0.45
1:E:157:ARG:HB2	2:h:31:PHE:CE2	2.51	0.45
1:G:96:LEU:HD12	1:G:134:ALA:HB2	1.97	0.45
1:B:75:VAL:HG11	1:B:142:ILE:HG21	1.98	0.45
1:B:96:LEU:HD12	1:B:134:ALA:HB2	1.97	0.45
1:F:212:GLN:HB3	2:h:48:GLN:HA	1.97	0.45
1:A:166:GLN:HB3	2:a:22:MET:HE1	1.97	0.45
1:C:137:MET:HE3	1:C:181:VAL:HG22	1.98	0.45
1:H:192:THR:HG21	1:H:237:THR:HB	1.99	0.45
1:A:146:GLU:HB2	1:B:228:MET:HE2	1.99	0.45
1:G:251:LEU:HB3	1:G:252:TRP:CE3	2.52	0.45
1:I:75:VAL:HG11	1:I:142:ILE:HG21	1.98	0.45
1:D:131:LEU:HD12	1:D:131:LEU:HA	1.68	0.45
1:E:192:THR:HG21	1:E:237:THR:HB	1.99	0.45
1:I:96:LEU:HD12	1:I:134:ALA:HB2	1.97	0.45
1:B:62:GLN:HE22	1:E:64:LYS:HD2	1.82	0.45
1:B:192:THR:HG21	1:B:237:THR:HB	1.99	0.45
1:B:251:LEU:HB3	1:B:252:TRP:CE3	2.52	0.45
1:C:251:LEU:HB3	1:C:252:TRP:CE3	2.52	0.45
1:G:212:GLN:HB3	2:c:48:GLN:HA	1.99	0.45
1:G:238:GLY:O	1:G:242:LEU:HG	2.17	0.45
1:E:251:LEU:HB3	1:E:252:TRP:CE3	2.52	0.45
1:F:168:GLN:HG3	2:f:22:MET:HE3	1.97	0.45
1:F:192:THR:HG21	1:F:237:THR:HB	1.99	0.45
1:A:238:GLY:O	1:A:242:LEU:HG	2.17	0.45
1:B:181:VAL:HA	1:E:104:LEU:HD11	1.99	0.45
1:I:251:LEU:HB3	1:I:252:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:THR:HG21	1:A:237:THR:HB	1.99	0.45
1:F:75:VAL:HG11	1:F:142:ILE:HG21	1.98	0.45
1:A:251:LEU:HB3	1:A:252:TRP:CE3	2.52	0.45
1:E:75:VAL:HG11	1:E:142:ILE:HG21	1.98	0.45
1:F:64:LYS:HD2	1:H:62:GLN:HE22	1.82	0.45
1:C:212:GLN:HB3	2:d:48:GLN:HA	1.98	0.44
1:D:192:THR:HG21	1:D:237:THR:HB	1.99	0.44
1:H:251:LEU:HB3	1:H:252:TRP:CE3	2.52	0.44
1:F:238:GLY:O	1:F:242:LEU:HG	2.17	0.44
1:G:75:VAL:HG11	1:G:142:ILE:HG21	1.98	0.44
1:H:75:VAL:HG11	1:H:142:ILE:HG21	1.98	0.44
1:D:166:GLN:HB3	2:d:22:MET:HE1	2.00	0.44
1:D:238:GLY:O	1:D:242:LEU:HG	2.17	0.44
1:F:158:TYR:CG	1:F:159:PHE:N	2.85	0.44
1:D:228:MET:HE2	1:F:146:GLU:HB2	1.99	0.44
1:D:251:LEU:HB3	1:D:252:TRP:CE3	2.52	0.44
1:A:228:MET:HE2	1:I:146:GLU:HB2	1.99	0.44
1:C:238:GLY:O	1:C:242:LEU:HG	2.17	0.44
1:F:251:LEU:HB3	1:F:252:TRP:CE3	2.52	0.44
1:B:238:GLY:O	1:B:242:LEU:HG	2.17	0.44
1:D:75:VAL:HG11	1:D:142:ILE:HG21	1.98	0.44
1:I:192:THR:HG21	1:I:237:THR:HB	1.99	0.44
1:A:182:SER:O	1:B:108:ARG:NH1	2.45	0.44
1:B:157:ARG:HB2	2:e:31:PHE:HE2	1.83	0.44
1:E:146:GLU:HB2	1:H:228:MET:HE2	2.00	0.44
1:E:238:GLY:O	1:E:242:LEU:HG	2.17	0.44
1:F:166:GLN:HB3	2:f:22:MET:HE1	2.00	0.44
1:G:62:GLN:HE22	1:I:64:LYS:HD2	1.82	0.43
1:G:131:LEU:HA	1:G:131:LEU:HD12	1.68	0.43
1:G:192:THR:HG21	1:G:237:THR:HB	1.99	0.43
1:A:178:VAL:HG23	1:A:242:LEU:HD13	2.01	0.43
1:C:192:THR:HG21	1:C:237:THR:HB	1.99	0.43
1:C:228:MET:HE2	1:D:146:GLU:HB2	2.00	0.43
1:I:178:VAL:HG23	1:I:242:LEU:HD13	2.01	0.43
1:I:238:GLY:O	1:I:242:LEU:HG	2.17	0.43
1:B:178:VAL:HG23	1:B:242:LEU:HD13	2.01	0.43
1:C:64:LYS:HD2	1:D:62:GLN:HE22	1.84	0.43
1:C:75:VAL:HG11	1:C:142:ILE:HG21	1.98	0.43
1:C:186:ILE:HD12	1:G:95:PRO:HB2	2.00	0.43
1:G:178:VAL:HG23	1:G:242:LEU:HD13	2.01	0.43
1:I:148:ASN:ND2	2:a:23:THR:HG1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASN:ND2	2:e:23:THR:HG1	2.15	0.43
1:C:178:VAL:HG23	1:C:242:LEU:HD13	2.01	0.43
1:H:238:GLY:O	1:H:242:LEU:HG	2.17	0.43
1:D:64:LYS:HD2	1:F:62:GLN:HE22	1.84	0.43
1:D:158:TYR:CG	1:D:159:PHE:N	2.85	0.43
1:F:228:MET:HE2	1:H:146:GLU:HB2	2.01	0.43
1:G:97:GLU:C	1:G:99:GLN:H	2.27	0.43
1:D:97:GLU:C	1:D:99:GLN:H	2.27	0.43
1:G:143:ILE:O	1:I:78:SER:OG	2.36	0.43
1:A:164:ASP:HB3	2:b:31:PHE:CB	2.47	0.43
1:C:62:GLN:HE22	1:G:64:LYS:HD2	1.84	0.43
1:F:97:GLU:C	1:F:99:GLN:H	2.27	0.43
1:H:97:GLU:C	1:H:99:GLN:H	2.27	0.43
1:B:146:GLU:HB2	1:E:228:MET:HE2	2.01	0.43
1:D:166:GLN:HG3	2:c:26:PHE:CE2	2.54	0.43
1:B:158:TYR:CG	1:B:159:PHE:N	2.85	0.42
1:E:178:VAL:HG23	1:E:242:LEU:HD13	2.01	0.42
1:E:62:GLN:HE22	1:H:64:LYS:HD2	1.84	0.42
1:G:146:GLU:HB2	1:I:228:MET:HE2	2.01	0.42
1:B:131:LEU:HD12	1:B:131:LEU:HA	1.68	0.42
1:C:97:GLU:C	1:C:99:GLN:H	2.27	0.42
1:D:178:VAL:HG23	1:D:242:LEU:HD13	2.01	0.42
1:E:97:GLU:C	1:E:99:GLN:H	2.27	0.42
1:H:166:GLN:HG3	2:f:26:PHE:HE2	1.84	0.42
1:H:178:VAL:HG23	1:H:242:LEU:HD13	2.01	0.42
1:A:168:GLN:HG3	2:a:22:MET:HE3	2.01	0.42
1:C:148:ASN:ND2	2:g:23:THR:HG1	2.15	0.42
1:F:178:VAL:HG23	1:F:242:LEU:HD13	2.01	0.42
1:I:164:ASP:CB	2:a:31:PHE:HB2	2.49	0.42
1:A:62:GLN:HE22	1:B:64:LYS:HD2	1.84	0.42
1:H:218:GLU:OE1	2:h:27:ARG:HG2	2.19	0.42
1:I:97:GLU:C	1:I:99:GLN:H	2.27	0.42
2:e:34:ASN:HA	2:e:35:PRO:HD3	1.93	0.42
1:F:95:PRO:HB2	1:H:186:ILE:HD12	2.01	0.42
1:A:97:GLU:C	1:A:99:GLN:H	2.27	0.42
1:B:97:GLU:C	1:B:99:GLN:H	2.27	0.42
1:C:166:GLN:HG3	2:g:26:PHE:HE2	1.84	0.42
1:A:95:PRO:HB2	1:I:186:ILE:HD12	2.02	0.42
1:A:104:LEU:HD11	1:I:181:VAL:HA	2.02	0.42
1:A:64:LYS:HD2	1:I:62:GLN:HE22	1.84	0.42
1:D:166:GLN:HG3	2:c:26:PHE:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HD12	1:B:95:PRO:HB2	2.02	0.41
1:D:164:ASP:HB3	2:c:31:PHE:CB	2.47	0.41
1:A:123:ASN:OD1	1:A:123:ASN:N	2.36	0.41
1:B:82:MET:HB3	1:B:232:MET:SD	2.61	0.41
1:E:82:MET:HB3	1:E:232:MET:SD	2.61	0.41
1:I:82:MET:HB3	1:I:232:MET:SD	2.61	0.41
1:A:82:MET:HB3	1:A:232:MET:SD	2.61	0.41
1:B:186:ILE:HD12	1:E:95:PRO:HB2	2.02	0.41
1:C:95:PRO:HB2	1:D:186:ILE:HD12	2.02	0.41
1:D:97:GLU:O	1:D:99:GLN:N	2.54	0.41
1:G:82:MET:HB3	1:G:232:MET:SD	2.61	0.41
1:H:166:GLN:HG3	2:f:26:PHE:CE2	2.54	0.41
1:C:82:MET:HB3	1:C:232:MET:SD	2.61	0.41
1:F:104:LEU:HD11	1:H:181:VAL:HA	2.03	0.41
1:I:97:GLU:O	1:I:99:GLN:N	2.54	0.41
1:A:97:GLU:O	1:A:99:GLN:N	2.54	0.41
1:B:143:ILE:O	1:E:78:SER:OG	2.36	0.41
1:B:166:GLN:HG3	2:e:26:PHE:CE2	2.55	0.41
1:C:97:GLU:O	1:C:99:GLN:N	2.54	0.41
1:F:97:GLU:O	1:F:99:GLN:N	2.54	0.41
1:G:168:GLN:HG3	2:g:22:MET:HE3	2.03	0.41
1:D:82:MET:HB3	1:D:232:MET:SD	2.61	0.41
1:E:186:ILE:HD12	1:H:95:PRO:HB2	2.03	0.40
1:F:82:MET:HB3	1:F:232:MET:SD	2.61	0.40
1:G:97:GLU:O	1:G:99:GLN:N	2.54	0.40
2:a:29:PRO:HG2	2:i:40:PHE:CE2	2.56	0.40
2:a:40:PHE:CE2	2:b:29:PRO:HG2	2.56	0.40
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.68	0.40
1:A:166:GLN:HG3	2:b:26:PHE:HE2	1.87	0.40
1:E:97:GLU:O	1:E:99:GLN:N	2.54	0.40
1:B:97:GLU:O	1:B:99:GLN:N	2.54	0.40
1:B:212:GLN:HB3	2:a:48:GLN:HA	2.02	0.40
1:D:104:LEU:HD11	1:F:181:VAL:HA	2.03	0.40
1:F:131:LEU:HA	1:F:131:LEU:HD12	1.68	0.40
1:H:82:MET:HB3	1:H:232:MET:SD	2.61	0.40
1:C:158:TYR:CG	1:C:159:PHE:N	2.85	0.40
1:C:164:ASP:CB	2:g:31:PHE:HB2	2.48	0.40
1:F:243:ILE:HA	1:F:252:TRP:NE1	2.36	0.40
1:G:186:ILE:HD12	1:I:95:PRO:HB2	2.04	0.40
1:I:92:TRP:CZ2	1:I:247:ILE:HD11	2.57	0.40
1:A:136:ILE:HD13	1:A:252:TRP:CH2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLN:HG3	2:b:26:PHE:CE2	2.56	0.40
1:A:243:ILE:HA	1:A:252:TRP:NE1	2.36	0.40
1:D:136:ILE:HD13	1:D:252:TRP:CH2	2.57	0.40
1:I:131:LEU:HD12	1:I:131:LEU:HA	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	173/244 (71%)	157 (91%)	16 (9%)	8	22
1	B	173/244 (71%)	157 (91%)	16 (9%)	8	22
1	C	173/244 (71%)	157 (91%)	16 (9%)	8	22
1	D	173/244 (71%)	157 (91%)	16 (9%)	8	22
1	E	173/244 (71%)	157 (91%)	16 (9%)	8	22
1	F	173/244 (71%)	157 (91%)	16 (9%)	8	22
1	G	173/244 (71%)	157 (91%)	16 (9%)	8	22
1	H	173/244 (71%)	157 (91%)	16 (9%)	8	22
1	I	173/244 (71%)	157 (91%)	16 (9%)	8	22
2	a	26/124 (21%)	24 (92%)	2 (8%)	12	28
2	b	26/124 (21%)	24 (92%)	2 (8%)	12	28
2	c	26/124 (21%)	24 (92%)	2 (8%)	12	28
2	d	26/124 (21%)	24 (92%)	2 (8%)	12	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	e	26/124 (21%)	24 (92%)	2 (8%)	12	28
2	f	26/124 (21%)	24 (92%)	2 (8%)	12	28
2	g	26/124 (21%)	24 (92%)	2 (8%)	12	28
2	h	26/124 (21%)	24 (92%)	2 (8%)	12	28
2	i	26/124 (21%)	24 (92%)	2 (8%)	12	28
All	All	1791/3312 (54%)	1629 (91%)	162 (9%)	11	23

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	80	THR
1	A	123	ASN
1	A	131	LEU
1	A	141	SER
1	A	146	GLU
1	A	154	VAL
1	A	166	GLN
1	A	182	SER
1	A	185	GLU
1	A	188	SER
1	A	193	SER
1	A	198	SER
1	A	210	ASP
1	A	218	GLU
1	A	252	TRP
1	B	52	SER
1	B	80	THR
1	B	123	ASN
1	B	131	LEU
1	B	141	SER
1	B	146	GLU
1	B	154	VAL
1	B	166	GLN
1	B	182	SER
1	B	185	GLU
1	B	188	SER
1	B	193	SER
1	B	198	SER
1	B	210	ASP

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Mol	Chain	Res	Type
1	B	218	GLU
1	B	252	TRP
1	C	52	SER
1	C	80	THR
1	C	123	ASN
1	C	131	LEU
1	C	141	SER
1	C	146	GLU
1	C	154	VAL
1	C	166	GLN
1	C	182	SER
1	C	185	GLU
1	C	188	SER
1	C	193	SER
1	C	198	SER
1	C	210	ASP
1	C	218	GLU
1	C	252	TRP
1	D	52	SER
1	D	80	THR
1	D	123	ASN
1	D	131	LEU
1	D	141	SER
1	D	146	GLU
1	D	154	VAL
1	D	166	GLN
1	D	182	SER
1	D	185	GLU
1	D	188	SER
1	D	193	SER
1	D	198	SER
1	D	210	ASP
1	D	218	GLU
1	D	252	TRP
1	E	52	SER
1	E	80	THR
1	E	123	ASN
1	E	131	LEU
1	E	141	SER
1	E	146	GLU
1	E	154	VAL
1	E	166	GLN

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Mol	Chain	Res	Type
1	E	182	SER
1	E	185	GLU
1	E	188	SER
1	E	193	SER
1	E	198	SER
1	E	210	ASP
1	E	218	GLU
1	E	252	TRP
1	F	52	SER
1	F	80	THR
1	F	123	ASN
1	F	131	LEU
1	F	141	SER
1	F	146	GLU
1	F	154	VAL
1	F	166	GLN
1	F	182	SER
1	F	185	GLU
1	F	188	SER
1	F	193	SER
1	F	198	SER
1	F	210	ASP
1	F	218	GLU
1	F	252	TRP
1	G	52	SER
1	G	80	THR
1	G	123	ASN
1	G	131	LEU
1	G	141	SER
1	G	146	GLU
1	G	154	VAL
1	G	166	GLN
1	G	182	SER
1	G	185	GLU
1	G	188	SER
1	G	193	SER
1	G	198	SER
1	G	210	ASP
1	G	218	GLU
1	G	252	TRP
1	H	52	SER
1	H	80	THR

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Mol	Chain	Res	Type
1	H	123	ASN
1	H	131	LEU
1	H	141	SER
1	H	146	GLU
1	H	154	VAL
1	H	166	GLN
1	H	182	SER
1	H	185	GLU
1	H	188	SER
1	H	193	SER
1	H	198	SER
1	H	210	ASP
1	H	218	GLU
1	H	252	TRP
1	I	52	SER
1	I	80	THR
1	I	123	ASN
1	I	131	LEU
1	I	141	SER
1	I	146	GLU
1	I	154	VAL
1	I	166	GLN
1	I	182	SER
1	I	185	GLU
1	I	188	SER
1	I	193	SER
1	I	198	SER
1	I	210	ASP
1	I	218	GLU
1	I	252	TRP
2	a	23	THR
2	a	50	SER
2	b	23	THR
2	b	50	SER
2	c	23	THR
2	c	50	SER
2	d	23	THR
2	d	50	SER
2	e	23	THR
2	e	50	SER
2	f	23	THR
2	f	50	SER

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Mol	Chain	Res	Type
2	g	23	THR
2	g	50	SER
2	h	23	THR
2	h	50	SER
2	i	23	THR
2	i	50	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	B	62	GLN
1	C	62	GLN
1	D	62	GLN
1	E	62	GLN
1	E	148	ASN
1	F	62	GLN
1	G	62	GLN
1	H	62	GLN
1	H	148	ASN
1	I	62	GLN
2	a	43	ASN
2	a	49	ASN
2	b	37	ASN
2	b	43	ASN
2	b	49	ASN
2	c	43	ASN
2	c	49	ASN
2	d	43	ASN
2	d	49	ASN
2	e	43	ASN
2	e	49	ASN
2	f	37	ASN
2	f	43	ASN
2	f	49	ASN
2	g	43	ASN
2	g	49	ASN
2	h	43	ASN
2	h	49	ASN
2	i	43	ASN
2	i	49	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.

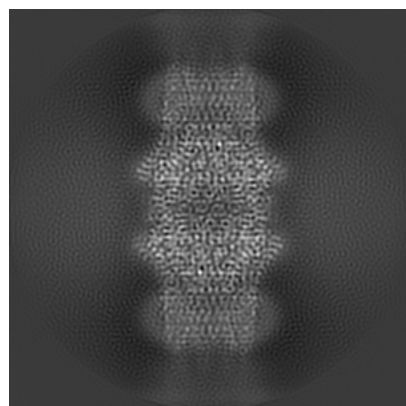
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0945. These allow visual inspection of the internal detail of the map and identification of artifacts.

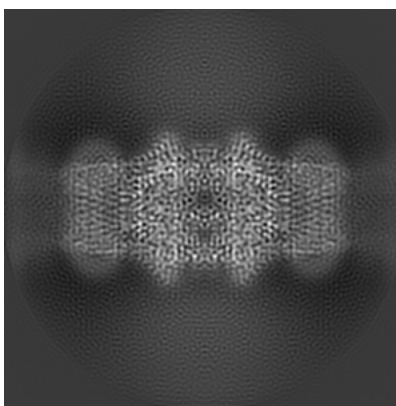
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

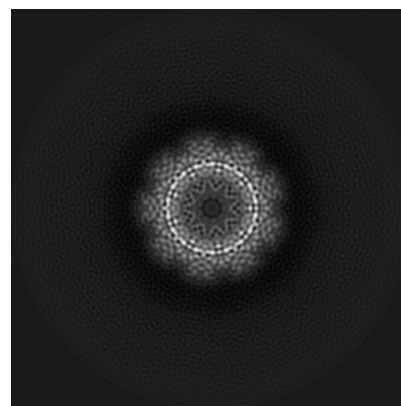
6.1.1 Primary map



X

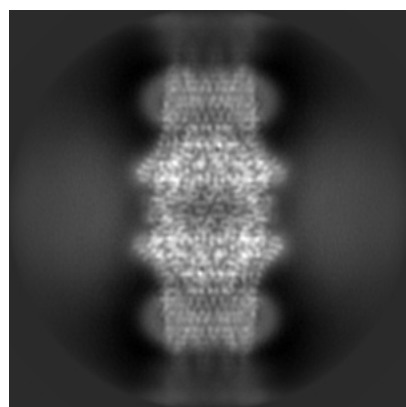


Y

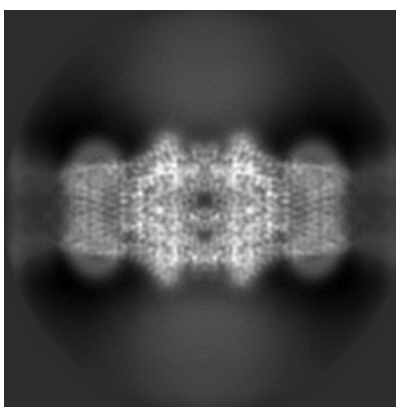


Z

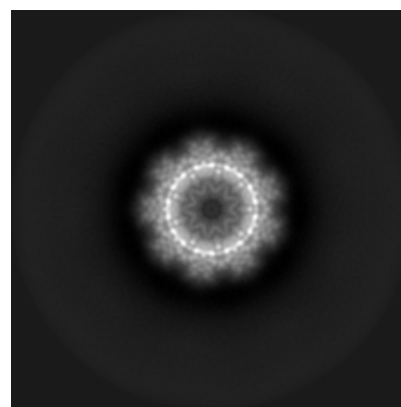
6.1.2 Raw map



X



Y

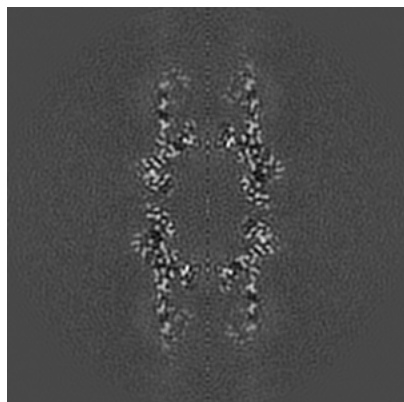


Z

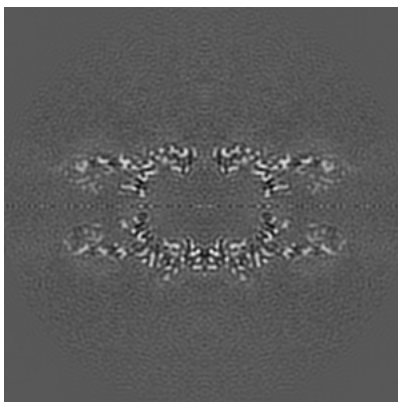
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

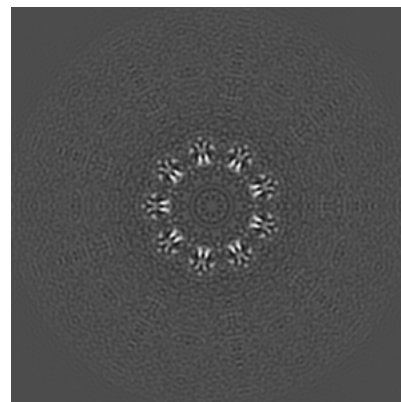
6.2.1 Primary map



X Index: 128

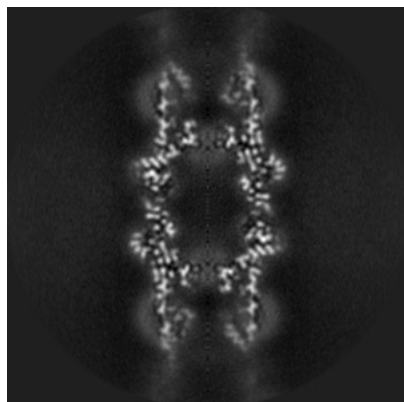


Y Index: 128

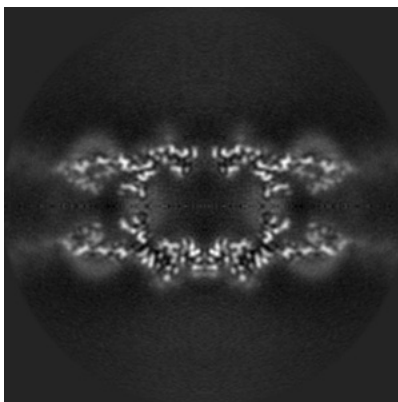


Z Index: 128

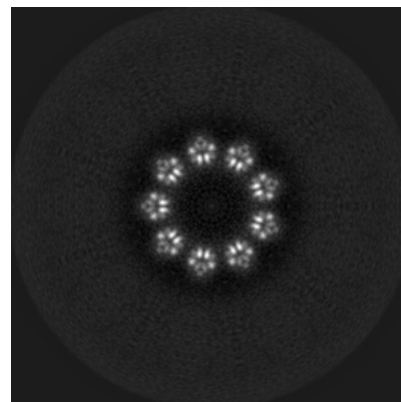
6.2.2 Raw map



X Index: 128



Y Index: 128

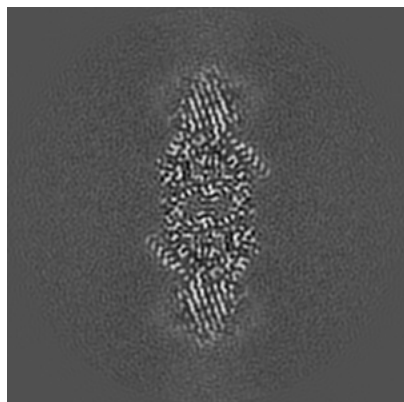


Z Index: 128

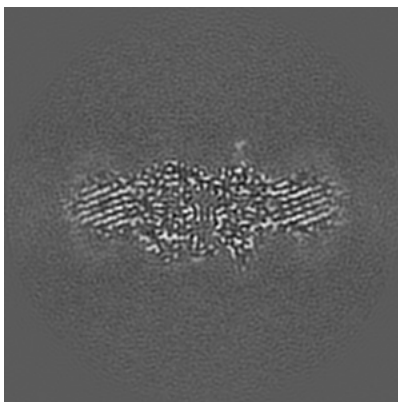
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

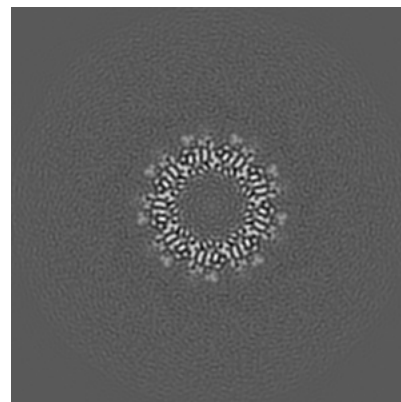
6.3.1 Primary map



X Index: 101

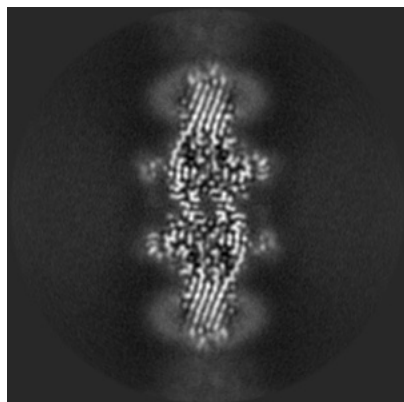


Y Index: 101

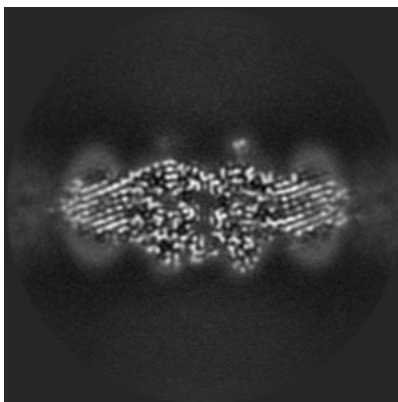


Z Index: 109

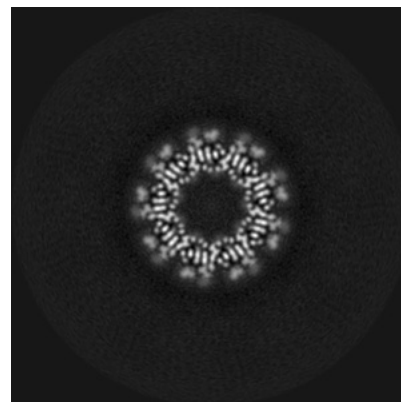
6.3.2 Raw map



X Index: 156



Y Index: 102

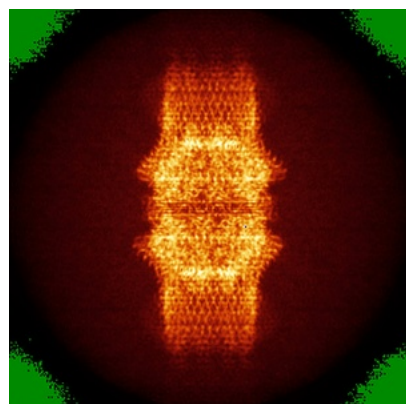


Z Index: 147

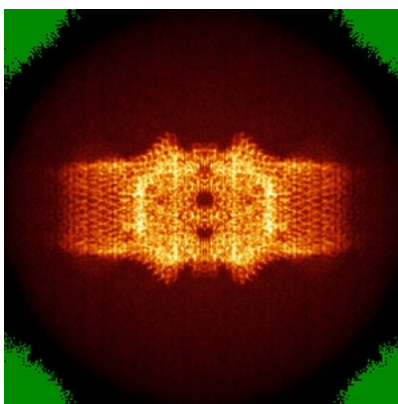
The images above show the largest variance slices of the map in three orthogonal directions.

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

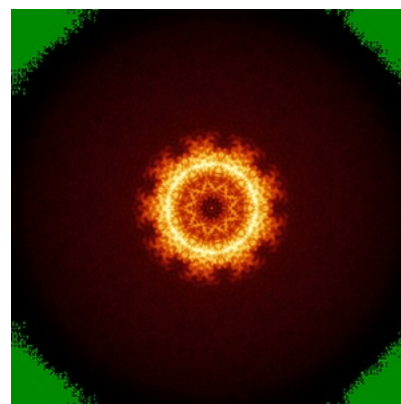
6.4.1 Primary map



X

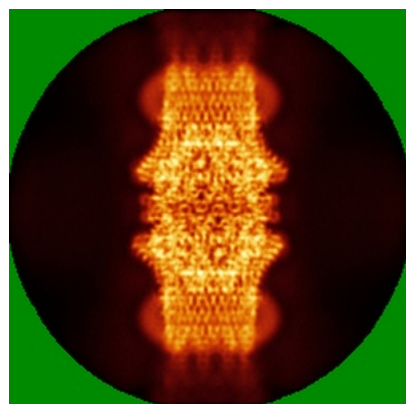


Y

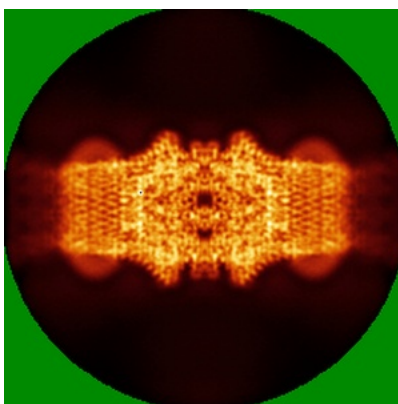


Z

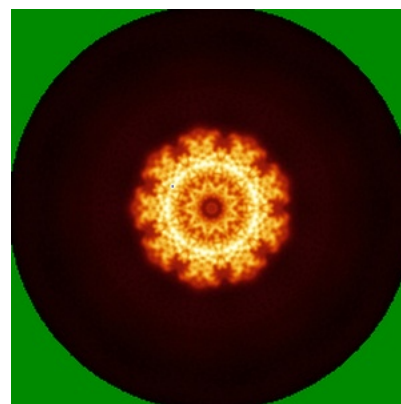
6.4.2 Raw map



X



Y

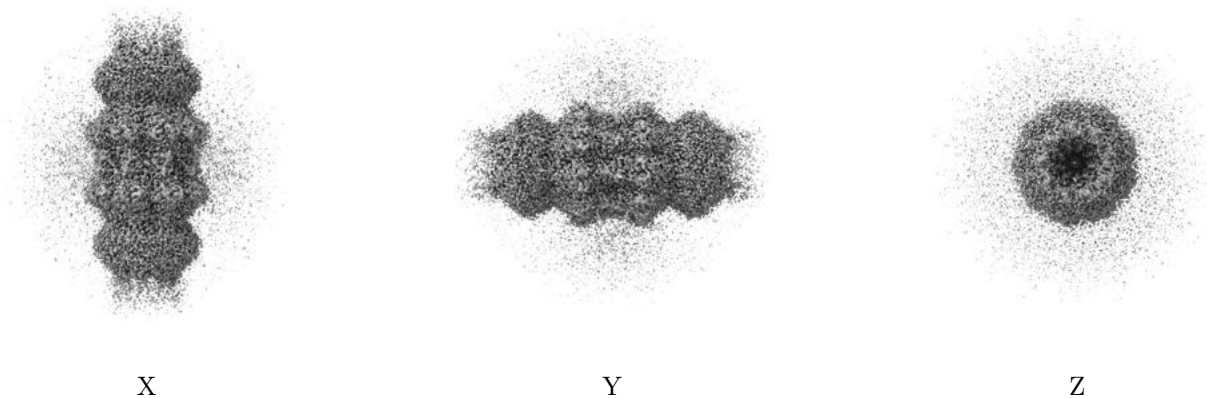


Z

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.

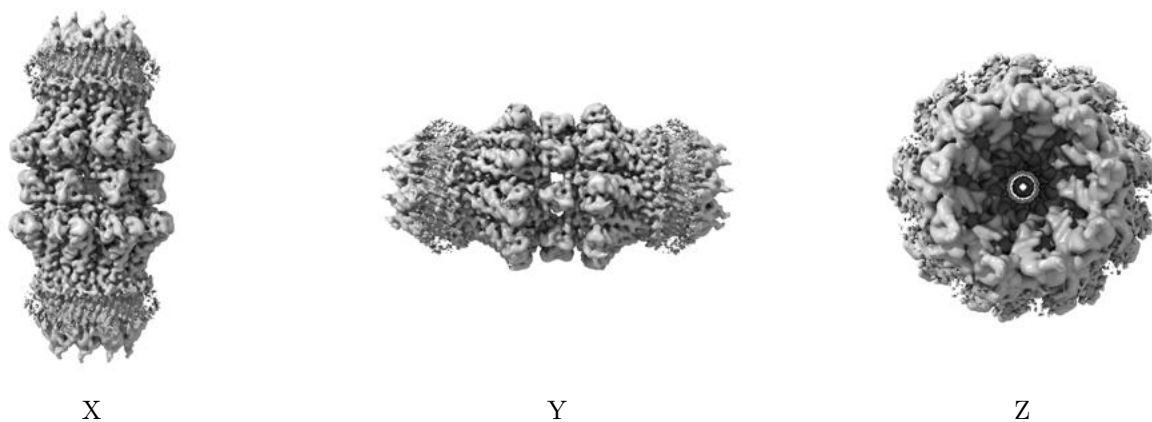
6.5 Orthogonal surface views [i](#)

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.

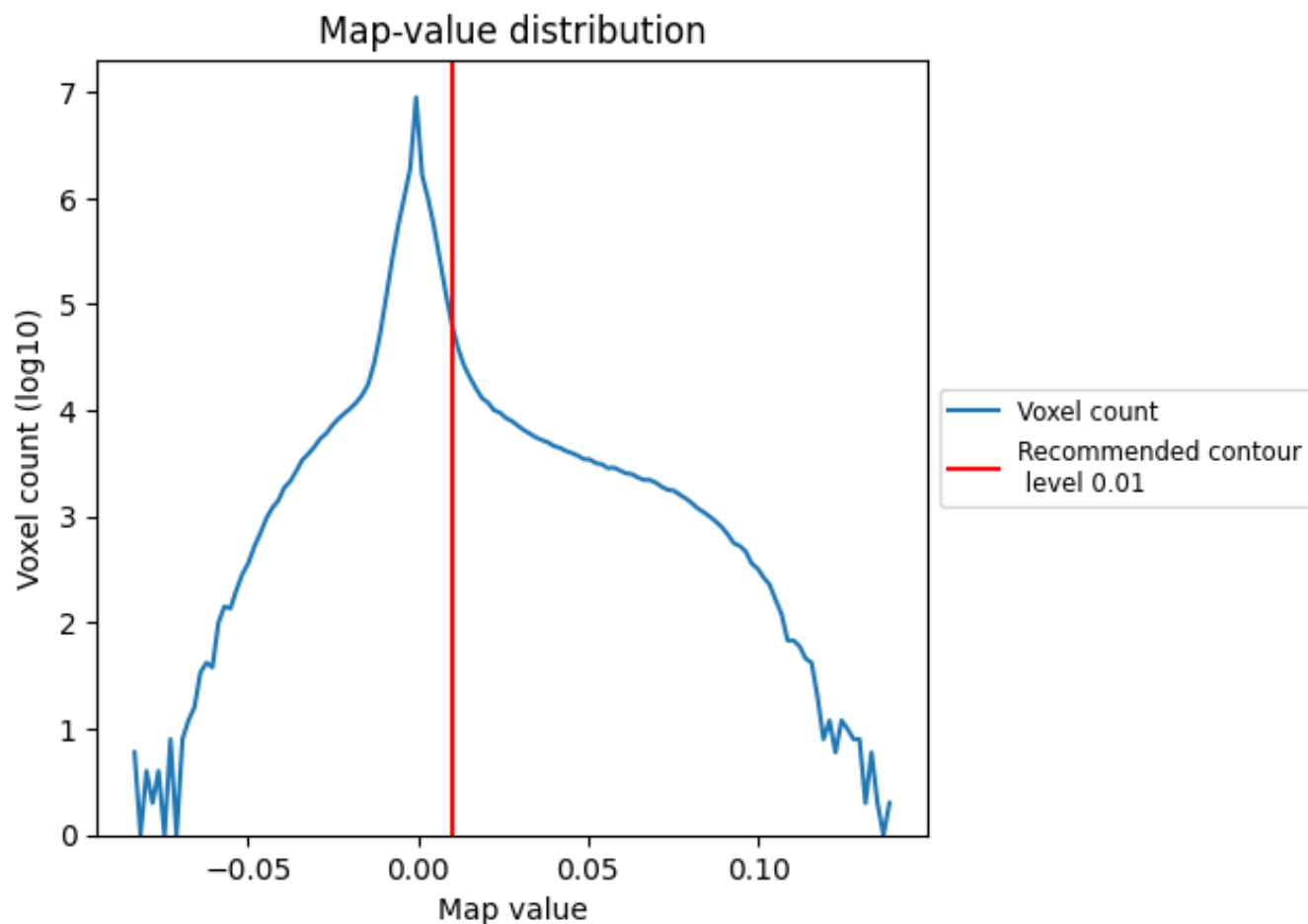
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

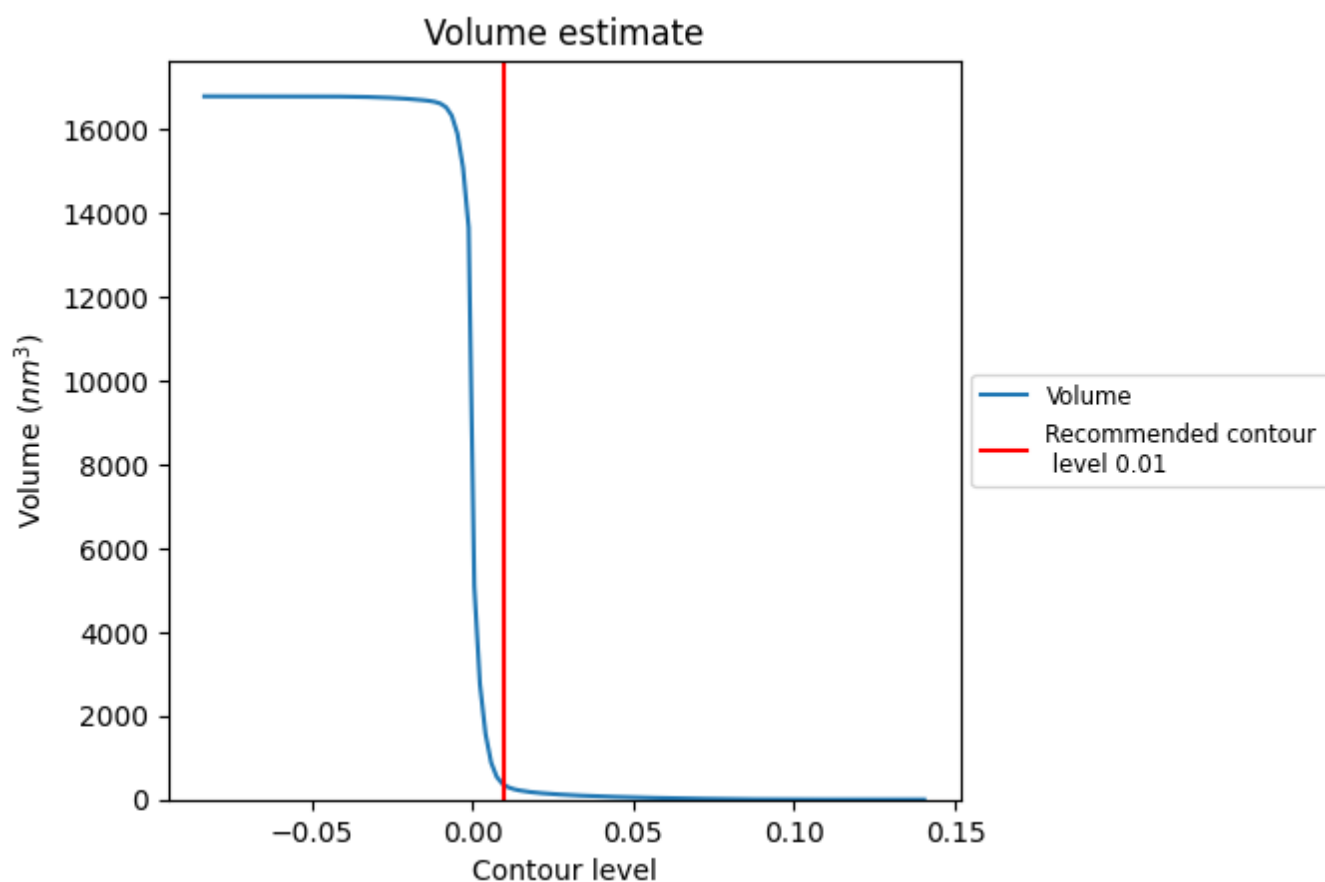
This section contains the results of statistical analysis of the map.

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.

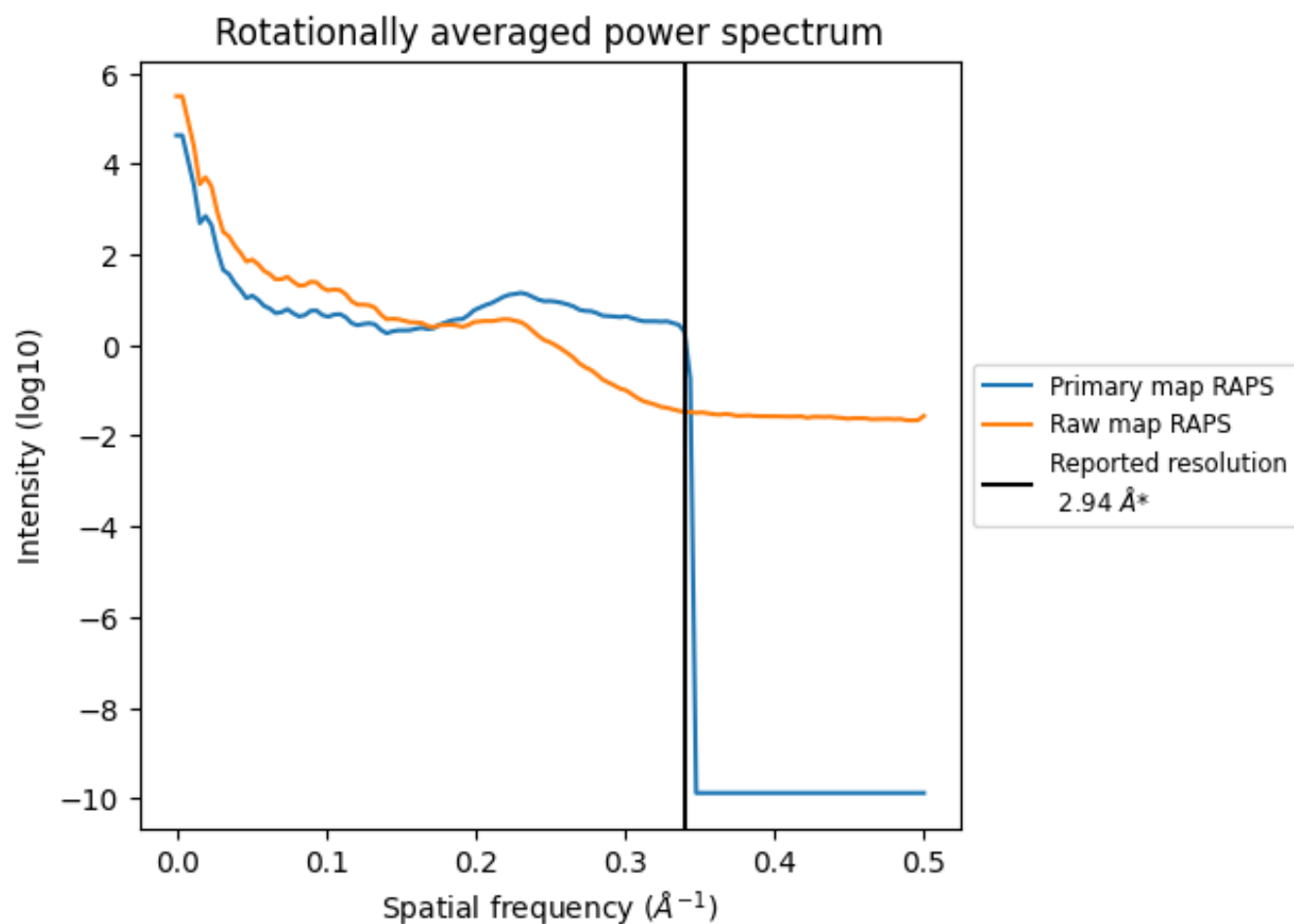
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 345 nm³; this corresponds to an approximate mass of 312 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 ⓘ

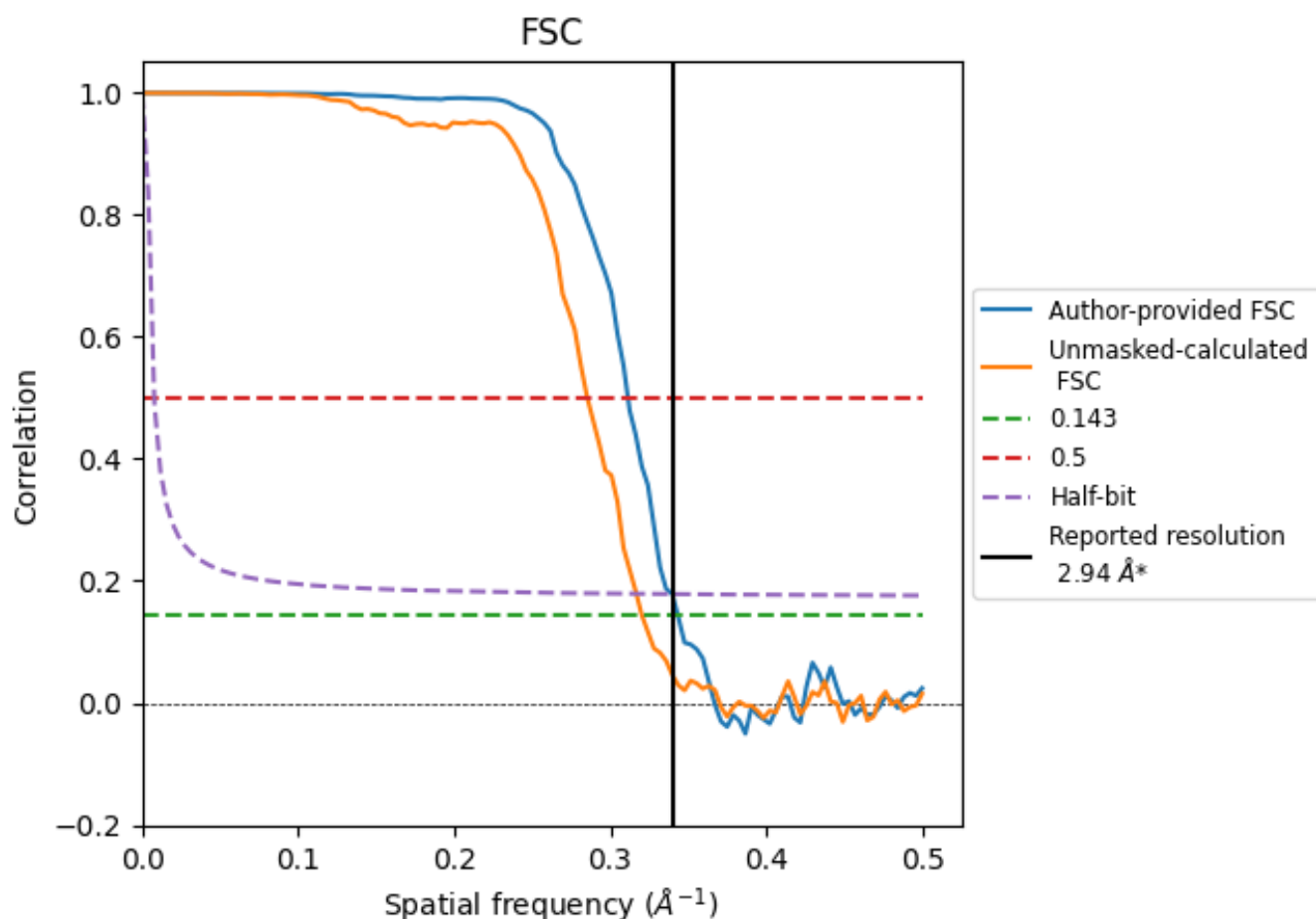


*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.340 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.91	3.21	2.94
Unmasked-calculated*	3.12	3.51	3.16

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

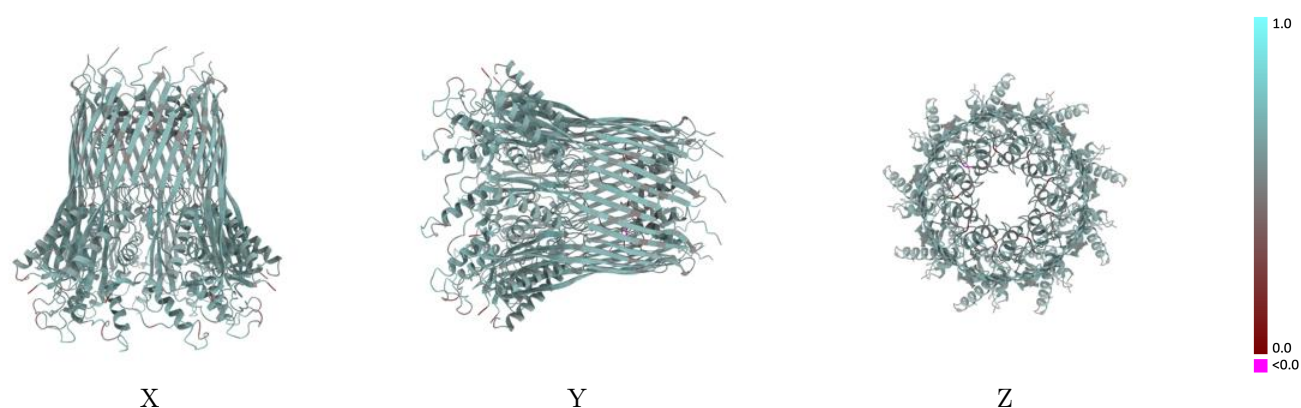
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0945 and PDB model 6LQH. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

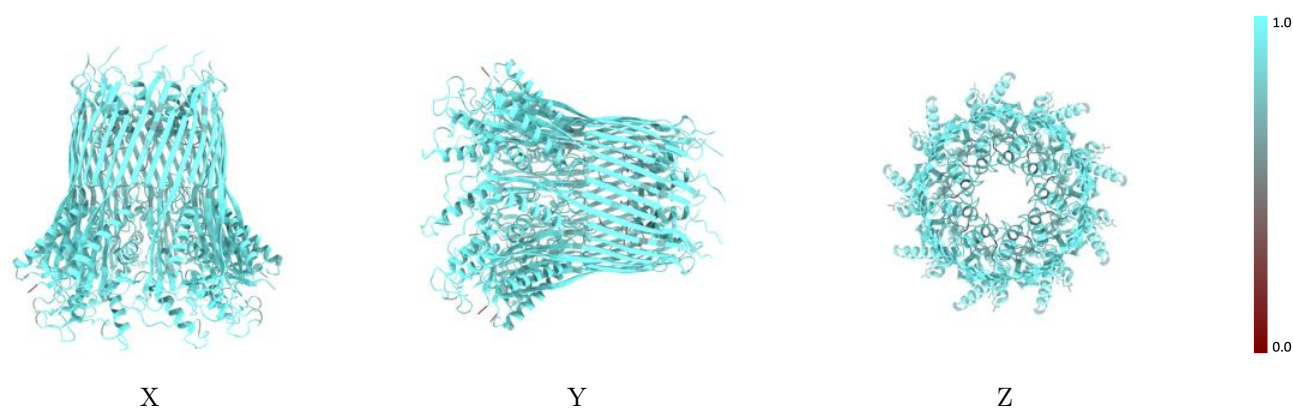
This section was not generated.

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



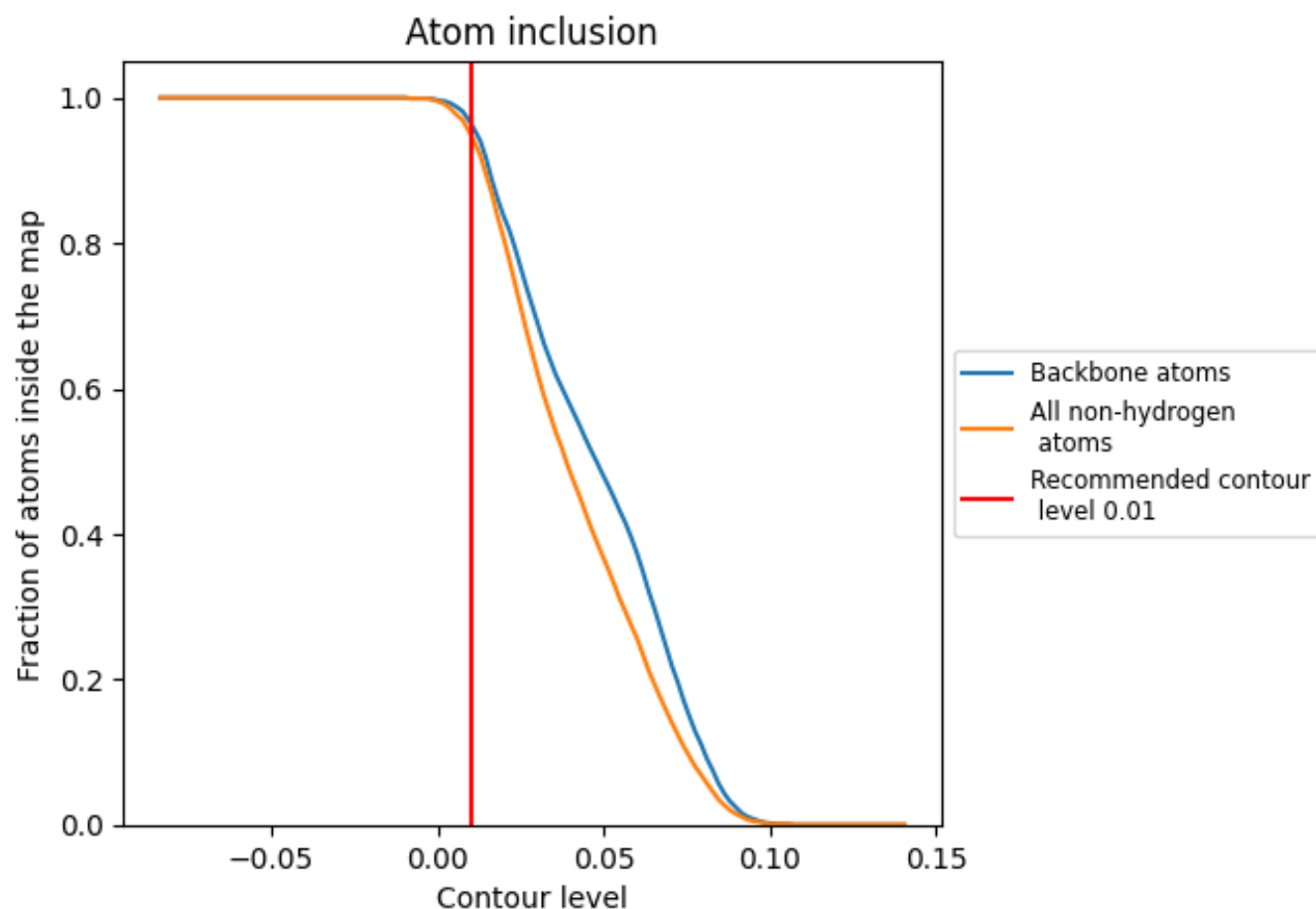
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 96% of all backbone atoms, 95% 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	0.9490	0.5890
A	0.9550	0.5950
B	0.9600	0.5950
C	0.9550	0.5940
D	0.9550	0.5920
E	0.9600	0.5960
F	0.9550	0.5940
G	0.9600	0.5930
H	0.9620	0.5940
I	0.9570	0.5940
a	0.9060	0.5530
b	0.8860	0.5480
c	0.8980	0.5570
d	0.8900	0.5520
e	0.8980	0.5550
f	0.9060	0.5600
g	0.9020	0.5580
h	0.8980	0.5590
i	0.8980	0.5550

1.0

0.0

<0.0